Supporting Information

Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes

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Table 1S: Geometry of the **C'C'**, **A'C'**, **A'A'**, **B'C'**, **A'B'**, **B'B'**, **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** Dimers in the Gas Phase, in DMF and CCl_4 Solvents and in **1.2$_4$.1** Capsules, at Various Levels of Theory.

Table 2S: Encapsulated Dimer % Distribution of the **C'C'**, **A'C'**, **A'A'**, **B'C'**, **A'B'**, and **B'B'** Species at Various Levels of Theory.

Table 3S: Encapsulated Dimer % Distribution of the **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** Species at Various Levels of Theory.

Table 4S-7S: Absolute Energies and BSSE Corrections of the Calculated Structures at Various Levels of Theory.

Table 8S: Cartesian Coordinates of the Calculated Species at Various Levels of Theory.

Figure 1S. Dimerization energies of the **C'C'**, **A'C'**, **A'A'**, **B'C'**, **A'B'**, and **B'B'** dimers at various levels of theory.

Figure 2S. Dimerization energies of the **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** dimers at various levels of theory.

Figure 3S: Structures of the encapsulated dimers in the capsule **1.2$_4$.1a**. The atoms of the capsule are designed with stick bonds for clarity. (H atoms = white spheres, C = grey spheres, O = red spheres and N = blue spheres).

Complete Reference 36

Table 1S: Geometry of the **C'C'**, **A'C'**, **A'A'**, **B'C'**, **A'B'**, **B'B'**, **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** Dimers in the Gas Phase, in DMF and CCl_4 Solvents and in **1.2$_4$.1** Capsules, at Various Levels of Theory.

Method	**R_{1-2}**	**R_{2-3}**	**R_{3-4}**	**R_{4-5}**	**R_{5-6}**	**R_{6-7}**	**R_{7-8}**	**R_{8-1}**	**φ_{812}**	**φ_{234}**	**φ_{456}**	**φ_{678}**	**d_1**[a]	**d_2**[b]
							A'A'							
M06-2X/6-31G(d,p)	1.231	1.846	1.026	1.343	1.231	1.846	1.026	1.343	123.1	176.3	123.1	176.3	0.0	
M06-2X/6-311+G(d,p)	1.226	1.866	1.024	1.345	1.226	1.866	1.024	1.345	122.6	172.6	122.6	172.6	0.0	
M06-2X/6-311+G(d,p)[c]	1.226	1.879	1.024	1.345	1.226	1.879	1.024	1.345	122.7	172.6	122.7	172.6	0.0	
M06-L/6-311+G(d,p)	1.232	1.839	1.027	1.348	1.232	1.839	1.027	1.348	122.7	174.9	122.7	174.9	0.0	
MP2/6-31G(d,p)	1.242	1.878	1.022	1.349	1.242	1.878	1.022	1.349	123.2	176.8	123.2	176.8	0.0	
MP2/6-31G(d,p)[c]	1.239	1.949	1.019	1.352	1.239	1.949	1.019	1.352	123.0	176.1	123.0	176.1	0.0	
MP2/6-311+G(d,p)	1.235	1.880	1.024	1.356	1.235	1.880	1.024	1.356	122.7	174.9	122.7	174.9	0.0	
M06-2X/6-31G(d,p)[d]	1.237	1.881	1.024	1.340	1.237	1.881	1.024	1.340	122.7	177.0	122.7	177.0	0.0	
M06-2X/6-311+G(d,p)[d]	1.234	1.900	1.022	1.341	1.234	1.900	1.022	1.341	122.1	173.8	122.1	173.8	0.0	
MP2/6-31G(d,p)[d]	1.247	1.907	1.020	1.345	1.247	1.907	1.020	1.345	122.8	177.4	122.8	177.4	0.0	
M06-2X/6-311+G(d,p)[e]	1.230	1.882	1.023	1.343	1.230	1.882	1.023	1.343	122.4	173.6	122.4	173.6	0.0	
MP2/6-31G(d,p)[e]	1.245	1.890	1.021	1.347	1.245	1.890	1.021	1.347	123.0	177.2	123.0	177.2	0.0	
							AA							
M06-2X/6-31G(d,p)/trans	1.233	1.858	1.025	1.346	1.233	1.858	1.025	1.346	122.9	176.1	122.9	176.1	0.0	0.0
M06-2X/6-311+G(d,p)/trans	1.228	1.867	1.023	1.346	1.228	1.867	1.023	1.346	122.5	173.5	122.5	173.5	0.0	0.0
M06-2X/6-311+G(d,p)/trans[c]	1.227	1.882	1.023	1.347	1.227	1.882	1.023	1.347	122.5	173.5	122.5	173.5	0.0	0.0
M06-2X/6-311+G(d,p)/cis	1.228	1.869	1.023	1.346	1.228	1.867	1.023	1.347	122.6	173.4	122.5	173.4	3.4	4.7
M06-L/6-311+G(d,p)/trans	1.235	1.839	1.026	1.350	1.235	1.839	1.026	1.350	122.1	175.8	122.1	175.8	0.0	0.0
MP2/6-31G(d,p)/trans	1.245	1.879	1.022	1.352	1.245	1.879	1.022	1.352	123.3	177.0	123.3	177.0	0.0	0.0
MP2/6-31G(d,p)/cis	1.245	1.878	1.022	1.352	1.245	1.878	1.022	1.352	123.3	177.0	123.3	177.0	0.0	0.7
MP2/6-31G(d,p)/trans[c]	1.242	1.951	1.019	1.356	1.242	1.951	1.019	1.356	123.0	176.6	123.0	176.6	0.0	0.0
M06-2X/6-31G(d,p)/trans[d]	1.238	1.881	1.023	1.342	1.238	1.881	1.023	1.342	122.5	177.1	122.5	177.1	0.0	0.0
M06-2X/6-31G(d,p)/cis[d]	1.238	1.883	1.023	1.342	1.238	1.878	1.024	1.342	122.5	176.5	122.4	177.0	8.2	9.2
M06-2X/6-311+G(d,p)/trans[d]	1.234	1.897	1.022	1.342	1.234	1.897	1.022	1.342	122.1	174.1	122.1	174.1	0.0	0
M06-2X/6-311+G(d,p)/cis[d]	1.234	1.898	1.022	1.342	1.234	1.895	1.022	1.342	122.1	174.0	122.0	174.1	6.5	7.5
MP2/6-31G(d,p)/cis[d]	1.249	1.903	1.021	1.347	1.249	1.903	1.021	1.347	122.9	177.4	122.9	177.4	0.0	0
M06-2X/6-311+G(d,p)/trans[e]	1.231	1.879	1.023	1.345	1.231	1.879	1.023	1.345	122.3	174.2	122.3	174.2	0.0	0
M06-2X/6-311+G(d,p)/cis[e]	1.230	1.880	1.023	1.345	1.230	1.880	1.023	1.345	122.4	174.1	122.3	174.0	2.5	3.3

MP2/6-31G(d,p)/trans[e]	1.247	1.887	1.022	1.350	1.247	1.887	1.022	1.350	123.1	177.3	123.1	177.3	0.0	0
MP2/6-31G(d,p)/cis[e]	1.247	1.889	1.022	1.350	1.247	1.889	1.022	1.350	123.1	177.3	123.1	177.3	0.4	1.2
oniom-M06-2X/6-31G(d,p)/trans[f]	1.236	1.877	1.025	1.342	1.234	1.875	1.025	1.342	122.9	176.1	123.2	176.7	3.1	6.8
oniom-M06-2X/6-31G(d,p)/cis[f]	1.236	1.878	1.024	1.338	1.236	1.836	1.026	1.341	123.2	177.1	123.2	178.0	15.0	17.5
oniom-M06-2X/6-31G(d,p)/trans[g]	1.238	1.872	1.023	1.338	1.237	1.850	1.026	1.338	122.7	176.5	122.9	180.0	11.2	7.9
oniom-MP2/6-31G(d,p)/trans[f]	1.249	1.903	1.022	1.348	1.247	1.908	1.022	1.347	123.1	176.7	123.4	176.9	3.2	5.7
oniom-MP2/6-31G(d,p)/cis[f]	1.250	1.897	1.021	1.343	1.249	1.866	1.022	1.345	123.5	176.8	123.4	178.3	18.8	22.4
M06-2X/6-31G(d,p)/trans[f]	1.235	1.902	1.026	1.338	1.238	1.904	1.025	1.346	122.7	176.7	123.8	177.7	13.5	22.7
							C'C'							
M06-2X/6-31G(d,p)	1.309	1.009	1.586	1.227	1.309	1.009	1.586	1.227	124.2	180.0	124.2	180.0	0.0	
M06-2X/6-311+G(d,p)	1.316	0.992	1.685	1.218	1.316	0.992	1.686	1.218	123.6	176.8	123.6	176.8	0.0	
M06-2X/6-311+G(d,p)[c]	1.317	0.991	1.701	1.218	1.317	0.991	1.701	1.218	123.6	176.9	123.6	176.9	0.0	
M06-L/6-311+G(d,p)	1.322	0.995	1.697	1.223	1.322	0.995	1.697	1.223	123.9	179.1	123.9	179.1	0.1	
MP2/6-31G(d,p)	1.329	0.995	1.699	1.234	1.329	0.995	1.699	1.234	124.4	179.2	124.4	179.2	0.0	
MP2/6-31G(d,p)[c]	1.335	0.989	1.781	1.231	1.335	0.989	1.781	1.231	124.1	179.5	124.1	179.5	0.0	
MP2/6-311+G(d,p)	1.327	0.991	1.704	1.227	1.327	0.991	1.704	1.227	123.9	179.8	123.9	179.8	0.2	
M06-2X/6-31G(d,p)[d]	1.311	1.010	1.584	1.229	1.311	1.010	1.583	1.229	123.5	178.1	123.5	178.2	0.0	
M06-2X/6-311+G(d,p)[d]	1.318	0.992	1.685	1.221	1.318	0.992	1.686	1.221	122.8	179.5	122.8	179.6	0.0	
MP2/6-31G(d,p)[d]	1.330	0.995	1.702	1.235	1.330	0.995	1.702	1.235	123.8	177.3	123.8	177.3	0.0	
M06-2X/6-311+G(d,p)[e]	1.317	0.993	1.683	1.220	1.317	0.993	1.683	1.220	123.2	178.0	123.2	178.0	0.0	
MP2/6-31G(d,p)[e]	1.329	0.995	1.699	1.235	1.329	0.995	1.699	1.235	124.1	178.3	124.1	178.4	0.0	
							CC							
M06-2X/6-31G(d,p)/cis	1.308	1.014	1.557	1.232	1.308	1.014	1.557	1.232	123.8	179.5	123.8	179.5	0.1	0.6
M06-2X/6-311+G(d,p)/trans	1.315	0.995	1.657	1.223	1.315	0.995	1.657	1.223	123.4	177.9	123.4	177.9	0.0	0
M06-2X/6-311+G(d,p)/trans[c]	1.316	0.993	1.674	1.222	1.316	0.993	1.674	1.222	123.4	177.9	123.4	177.9	0.0	0
M06-2X/6-311+G(d,p)/cis	1.315	0.995	1.657	1.223	1.315	0.995	1.656	1.223	123.4	177.9	123.4	177.9	0.2	0.2
M06-L/6-311+G(d,p)/trans	1.323	0.996	1.683	1.228	1.323	0.996	1.683	1.228	123.6	179.8	123.6	179.8	0.0	0
MP2/6-31G(d,p)/trans	1.328	0.997	1.676	1.239	1.328	0.997	1.676	1.239	124.0	178.5	124.0	178.5	0.0	0
MP2/6-31G(d,p)/trans[c]	1.334	0.991	1.757	1.235	1.334	0.991	1.757	1.235	123.7	178.7	123.7	178.7	0.0	0
MP2/6-31G(d,p)/cis	1.328	0.997	1.677	1.239	1.328	0.997	1.677	1.239	124.0	178.5	124.0	178.5	0.0	1
M06-2X/6-31G(d,p)/trans[d]	1.309	1.014	1.557	1.234	1.309	1.014	1.557	1.234	123.4	178.1	123.4	178.1	0.0	0
M06-2X/6-31G(d,p)/cis[d]	1.309	1.014	1.557	1.234	1.309	1.014	1.556	1.234	123.4	178.1	123.4	178.1	0.2	0.8
M06-2X/6-311+G(d,p)/trans[d]	1.316	0.995	1.659	1.225	1.316	0.995	1.659	1.225	122.8	179.9	122.8	179.9	0.0	0
M06-2X/6-311+G(d,p)/cis[d]	1.316	0.995	1.658	1.225	1.316	0.995	1.658	1.225	122.8	179.9	122.8	179.9	0.1	0.3

MP2/6-31G(d,p)/cis[d]	1.329	0.997	1.681	1.239	1.329	0.997	1.681	1.239	123.6	177.1	123.6	177.1	0.0	0
M06-2X/6-311+G(d,p)/trans[e]	1.315	0.995	1.657	1.224	1.315	0.995	1.657	1.224	123.1	178.8	123.1	178.8	0.0	0
M06-2X/6-311+G(d,p)/cis[e]	1.315	0.995	1.656	1.224	1.315	0.995	1.656	1.224	123.1	178.8	123.1	178.8	0.1	0.1
MP2/6-31G(d,p)/trans[e]	1.328	0.997	1.677	1.239	1.328	0.997	1.677	1.239	123.8	177.9	123.8	177.9	0.0	0
MP2/6-31G(d,p)/cis[e]	1.329	0.997	1.679	1.239	1.329	0.997	1.680	1.239	123.8	177.9	123.8	177.9	0.1	1.3
oniom-M06-2X/6-31G(d,p)/trans[f]	1.305	1.020	1.536	1.235	1.308	1.018	1.531	1.233	124.3	177.8	123.7	178.2	7.1	23.3
oniom-M06-2X/6-31G(d,p)/cis[f]	1.305	1.019	1.549	1.235	1.309	1.017	1.528	1.233	124.2	176.4	123.7	176.3	12.4	28.6
oniom-M06-2X/6-31G(d,p)/cis[g]	1.313	0.990	1.650	1.224	1.316	0.995	1.652	1.224	123.7	175.8	124.8	178.4	2.4	3.4
oniom-MP2/6-31G(d,p)/trans[f]	1.325	1.000	1.669	1.241	1.329	0.999	1.644	1.239	124.6	177.1	123.9	176.7	4.2	29.8
oniom-MP2/6-31G(d,p)/cis[f]	1.326	0.999	1.686	1.241	1.329	0.999	1.642	1.239	124.5	175.5	123.8	175.1	12.2	36.3
M06-2X/6-31G(d,p)/trans[f]	1.309	1.007	1.602	1.230	1.313	1.006	1.641	1.230	124.8	169.4	123.7	173.6	15.9	21
							B'B'							
M06-2X/6-31G(d,p)	1.392	1.842	0.974	1.347	1.392	1.842	0.974	1.347	118.0	178.6	118.0	178.6	0.9	
M06-2X/6-311+G(d,p)	1.392	1.848	0.972	1.347	1.393	1.848	0.972	1.347	117.6	179.1	117.6	179.1	3.4	
M06-2X/6-311+G(d,p)[c]	1.392	1.870	0.972	1.347	1.392	1.870	0.972	1.347	117.5	179.2	117.5	179.2	0.0	
M06-L/6-311+G(d,p)	1.395	1.844	0.974	1.348	1.395	1.844	0.974	1.348	117.4	179.2	117.4	179.2	0.0	
MP2/6-31G(d,p)	1.401	1.859	0.975	1.355	1.401	1.859	0.975	1.355	118.1	179.4	118.1	179.4	0.0	
MP2/6-31G(d,p)[c]	1.397	1.936	0.973	1.357	1.397	1.936	0.973	1.357	118.1	179.6	118.1	179.6	0.0	
MP2/6-311+G(d,p)	1.400	1.856	0.973	1.354	1.400	1.856	0.973	1.354	117.7	177.5	117.7	177.5	31.0	
MP2/aug-cc-pVDZ	1.411	1.840	0.979	1.366	1.411	1.840	0.979	1.366	117.6	179.7	117.6	179.7	0.0	
M06-2X/6-31G(d,p)[d]	1.387	1.825	0.976	1.354	1.387	1.825	0.976	1.354	117.7	178.4	117.6	178.4	7.0	
M06-2X/6-311+G(d,p)[d]	1.387	1.829	0.974	1.356	1.387	1.829	0.974	1.356	117.1	179.3	117.1	179.3	0.1	
MP2/6-31G(d,p)[d]	1.395	1.841	0.977	1.362	1.395	1.841	0.977	1.362	117.7	179.4	117.7	179.4	0.0	
M06-2X/6-311+G(d,p)[e]	1.390	1.840	0.973	1.351	1.390	1.840	0.973	1.351	117.3	179.1	117.3	179.2	0.1	
MP2/6-31G(d,p)[e]	1.398	1.851	0.976	1.358	1.398	1.851	0.976	1.358	117.9	179.5	117.9	179.5	0.0	
							BB							
M06-2X/6-31G(d,p)/trans	1.389	1.832	0.974	1.347	1.389	1.841	0.974	1.347	118.9	177.7	118.9	177.5	6.5	24.5
M06-2X/6-311+G(d,p)/trans	1.388	1.850	0.972	1.349	1.388	1.841	0.972	1.349	118.2	178.2	118.2	178.5	13.1	9.1
M06-2X/6-311+G(d,p)/trans[c]	1.387	1.866	0.971	1.349	1.387	1.867	0.971	1.349	118.2	178.8	118.2	178.5	0.8	1.9
M06-L/6-311+G(d,p)/trans	1.391	1.841	0.973	1.350	1.391	1.840	0.973	1.350	118.1	178.4	118.1	178.4	0.1	0
M06-L/6-311+G(d,p)/cis	1.391	1.842	0.973	1.350	1.391	1.842	0.973	1.350	118.0	177.3	118.0	177.3	24.1	25.3
MP2/6-31G(d,p)/trans	1.398	1.850	0.975	1.355	1.398	1.850	0.975	1.355	119.1	178.3	119.1	178.3	5.6	39
MP2/6-31G(d,p)/cis	1.398	1.850	0.975	1.355	1.398	1.850	0.975	1.355	119.1	178.3	119.1	178.3	5.8	39.1
MP2/6-31G(d,p)/trans[c]	1.394	1.926	0.973	1.357	1.394	1.926	0.973	1.357	119.1	179.6	119.1	179.6	6.0	38.3

M06-2X/6-31G(d,p)/trans[d]	1.384	1.833	0.976	1.353	1.384	1.815	0.976	1.353	118.3	176.8	118.4	176.8	22.1	12
M06-2X/6-31G(d,p)/cis[d]	1.384	1.823	0.976	1.353	1.384	1.823	0.976	1.353	118.5	177.7	118.5	177.7	6.2	25.8
M06-2X/6-311+G(d,p)/trans[d]	1.383	1.838	0.973	1.355	1.383	1.825	0.974	1.355	117.7	178.2	117.7	178.5	16.1	12.8
M06-2X/6-311+G(d,p)/cis[d]	1.383	1.831	0.974	1.355	1.383	1.831	0.974	1.355	117.8	178.7	117.8	178.8	2.2	19.6
MP2/6-31G(d,p)/cis[d]	1.392	1.835	0.977	1.361	1.392	1.836	0.977	1.361	118.6	177.9	118.5	177.9	19.5	30.6
M06-2X/6-311+G(d,p)/trans[e]	1.386	1.838	0.973	1.351	1.386	1.838	0.973	1.351	118.1	178.7	118.1	178.7	1.3	17.7
M06-2X/6-311+G(d,p)/cis[e]	1.386	1.838	0.973	1.351	1.386	1.838	0.973	1.351	118.1	178.7	118.1	178.7	1.3	17.7
MP2/6-31G(d,p)/trans[e]	1.395	1.844	0.976	1.357	1.395	1.844	0.976	1.358	118.8	178.5	118.8	178.9	4.4	3.5
MP2/6-31G(d,p)/cis[e]	1.395	1.844	0.976	1.357	1.395	1.844	0.976	1.357	118.9	178.6	118.9	178.6	6.2	40.8
oniom-M06-2X/6-31G(d,p)/trans[f]	1.382	1.868	0.975	1.349	1.380	1.766	0.977	1.349	118.9	175.7	118.9	178.5	9.8	41.6
oniom-M06-2X/6-31G(d,p)/cis[f]	1.382	1.833	0.975	1.349	1.380	1.806	0.976	1.348	119.4	179.8	119.2	173.9	4.9	25.9
oniom-M06-2X/6-31G(d,p)/cis[g]	1.383	1.867	0.976	1.355	1.378	1.814	0.975	1.351	118.6	172.1	117.7	165.0	36.3	23.9
oniom-MP2/6-31G(d,p)/trans[f]	1.391	1.877	0.976	1.357	1.389	1.786	0.978	1.357	119.0	177.2	118.9	178.1	6.1	47.5
oniom-MP2/6-31G(d,p)/cis[f]	1.390	1.853	0.976	1.357	1.388	1.817	0.977	1.356	119.3	179.7	119.2	174.0	5.5	32.5
M06-2X/6-31G(d,p)/trans[f]	1.371	1.781	0.979	1.354	1.381	1.799	0.978	1.358	119.9	170.9	119.5	171.2	16.6	8.5
							A'B'							
M06-2X/6-31G(d,p)	1.346	1.018	1.921	1.397	1.340	0.981	1.765	1.228	122.8	168.2	119.2	177.5	0.7	
M06-2X/6-311+G(d,p)	1.348	1.017	1.951	1.398	1.341	0.978	1.775	1.224	122.3	166.9	118.8	179.0	0.1	
M06-2X/6-311+G(d,p)[c]	1.349	1.017	1.973	1.397	1.341	0.978	1.791	1.223	122.3	166.8	118.7	178.6	0.3	
M06-L/6-311+G(d,p)	1.351	1.019	1.928	1.400	1.342	0.981	1.781	1.228	122.3	167.8	118.4	177.3	0.1	
MP2/6-31G(d,p)	1.352	1.015	1.949	1.404	1.349	0.981	1.793	1.240	122.9	168.5	119.1	175.9	0.4	
MP2/6-31G(d,p)[c]	1.355	1.013	2.028	1.401	1.352	0.978	1.865	1.237	122.6	168.7	119.2	175.5	0.4	
MP2/6-311+G(d,p)	1.359	1.017	1.970	1.404	1.349	0.979	1.785	1.232	122.5	166.5	118.7	176.5	27.2	
M06-2X/6-31G(d,p)[d]	1.338	1.018	1.933	1.387	1.351	0.986	1.729	1.238	122.7	166.7	118.1	173.7	0.3	
M06-2X/6-311+G(d,p)[d]	1.339	1.017	1.964	1.387	1.354	0.982	1.744	1.236	122.0	165.7	117.5	174.9	0.4	
MP2/6-31G(d,p)[d]	1.344	1.015	1.961	1.394	1.360	0.984	1.767	1.248	122.7	167.4	118.1	172.6	1.5	
M06-2X/6-311+G(d,p)[e]	1.345	1.017	1.959	1.393	1.346	0.980	1.763	1.228	122.2	166.6	118.3	177.3	0.1	
MP2/6-31G(d,p)[e]	1.348	1.015	1.955	1.400	1.354	0.982	1.780	1.244	122.9	168.1	118.7	174.6	0.0	
							AB							
M06-2X/6-31G(d,p)/trans	1.349	1.018	1.926	1.392	1.342	0.982	1.759	1.231	122.6	169.3	120.0	177.5	3.2	7.1
M06-2X/6-311+G(d,p)/trans	1.350	1.017	1.956	1.391	1.343	0.979	1.768	1.226	122.2	168.2	119.3	177.8	7.8	24.3
M06-2X/6-311+G(d,p)/trans[c]	1.350	1.016	1.976	1.390	1.343	0.978	1.782	1.225	122.2	168.1	119.3	178.4	5.0	23.6
M06-L/6-311+G(d,p)/trans	1.355	1.018	1.931	1.394	1.344	0.981	1.771	1.232	121.9	169.5	119.1	177.0	7.6	20.7
M06-L/6-311+G(d,p)/cis	1.354	1.018	1.927	1.394	1.344	0.981	1.774	1.232	121.9	169.4	119.1	177.5	1.2	13.5

MP2/6-31G(d,p)/trans	1.355	1.016	1.952	1.400	1.350	0.982	1.781	1.243	123.0	169.2	120.1	176.6	4.4	10.0
MP2/6-31G(d,p)/cis	1.355	1.016	1.952	1.400	1.350	0.982	1.781	1.243	123.0	169.2	120.1	176.6	4.3	9.7
MP2/6-31G(d,p)/cis[c]	1.359	1.014	2.030	1.397	1.353	0.979	1.854	1.240	122.7	169.7	120.1	176.2	6.7	10.7
M06-2X/6-31G(d,p)/trans[d]	1.341	1.018	1.941	1.383	1.351	0.985	1.726	1.239	122.5	167.2	118.7	174.5	11.9	21.6
M06-2X/6-31G(d,p)/cis[d]	1.341	1.018	1.938	1.383	1.351	0.985	1.728	1.239	122.5	167.6	118.7	174.4	2.7	13.9
M06-2X/6-311+G(d,p)/trans[d]	1.341	1.017	1.968	1.382	1.353	0.982	1.740	1.236	122.0	166.7	118.1	175.0	4.6	25.5
M06-2X/6-311+G(d,p)/cis[d]	1.341	1.017	1.968	1.382	1.353	0.982	1.740	1.236	122.0	166.6	118.1	175.2	0.5	17.5
MP2/6-31G(d,p)/cis[d]	1.346	1.015	1.961	1.391	1.359	0.985	1.756	1.250	122.9	167.8	119.0	173.3	4.5	5
M06-2X/6-311+G(d,p)/trans[e]	1.347	1.017	1.962	1.388	1.347	0.980	1.756	1.230	122.1	167.8	118.8	176.9	5.5	24.6
M06-2X/6-311+G(d,p)/cis[e]	1.347	1.017	1.962	1.388	1.346	0.980	1.756	1.230	122.1	167.7	118.9	177.4	0.8	17.5
MP2/6-31G(d,p)/cis[e]	1.351	1.015	1.957	1.397	1.353	0.983	1.771	1.246	122.9	168.8	119.7	175.1	1.0	7.1
oniom-M06-2X/6-31G(d,p)/trans[f]	1.340	1.019	1.904	1.381	1.344	0.984	1.739	1.237	122.5	171.1	120.1	174.8	8.2	48.5
oniom-M06-2X/6-31G(d,p)/cis[f]	1.340	1.018	1.915	1.381	1.344	0.985	1.734	1.238	122.4	171.3	119.8	171.8	14.9	46.9
oniom-M06-2X/6-31G(d,p)/trans[g]	1.341	1.019	1.879	1.382	1.346	0.982	1.785	1.237	122.6	172.8	119.6	174.2	7.8	45
oniom-MP2/6-31G(d,p)/trans[f]	1.345	1.016	1.930	1.389	1.353	0.984	1.761	1.250	122.7	170.7	120.1	173.5	3.4	52.4
oniom-MP2/6-31G(d,p)/cis[f]	1.345	1.016	1.938	1.390	1.354	0.984	1.773	1.250	122.6	171.3	119.8	171.0	14.4	57.5
M06-2X/6-31G(d,p)/trans[f]	1.347	1.021	1.906	1.382	1.348	0.983	1.782	1.233	122.6	166.2	121.6	177.2	31.4	18.6
							A'C'							
M06-2X/6-31G(d,p)	1.338	1.024	1.843	1.221	1.314	1.009	1.593	1.236	122.8	166.4	124.6	174.1	0.0	
M06-2X/6-311+G(d,p)	1.342	1.021	1.887	1.215	1.318	0.998	1.648	1.230	122.5	163.1	123.9	177.0	0.1	
M06-2X/6-311+G(d,p)[c]	1.342	1.020	1.902	1.215	1.318	0.997	1.662	1.229	122.5	163.0	123.9	176.8	0.1	
M06-L/6-311+G(d,p)	1.345	1.023	1.865	1.221	1.324	0.999	1.677	1.234	122.4	165.7	124.3	175.4	0.2	
MP2/6-31G(d,p)	1.345	1.019	1.889	1.232	1.330	0.999	1.678	1.245	122.8	167.6	124.9	173.2	0.3	
MP2/6-31G(d,p)[c]	1.350	1.016	1.967	1.229	1.335	0.993	1.750	1.242	122.7	166.4	124.5	173.1	0.3	
MP2/6-311+G(d,p)	1.353	1.021	1.907	1.224	1.329	0.995	1.681	1.237	122.5	165.4	124.3	174.0	6.6	
M06-2X/6-31G(d,p)[d]	1.332	1.021	1.890	1.223	1.316	1.019	1.547	1.245	122.5	165.8	124.0	171.1	0.0	
M06-2X/6-311+G(d,p)[d]	1.335	1.018	1.950	1.217	1.320	1.005	1.606	1.240	122.0	163.0	123.1	172.9	0.1	
MP2/6-31G(d,p)[d]	1.340	1.016	1.939	1.232	1.332	1.004	1.648	1.252	122.5	167.2	124.3	170.3	0.3	
M06-2X/6-311+G(d,p)[e]	1.339	1.020	1.908	1.217	1.318	1.002	1.626	1.234	122.3	163.3	123.5	175.1	0.0	
MP2/6-31G(d,p)[e]	1.343	1.018	1.911	1.232	1.331	1.001	1.663	1.248	122.7	167.5	124.6	172.0	0.0	
							AC							
M06-2X/6-31G(d,p)/trans	1.340	1.024	1.841	1.225	1.314	1.010	1.582	1.239	122.5	166.9	124.3	173.8	0.4	19.9
M06-2X/6-31G(d,p)/cis	1.340	1.024	1.841	1.225	1.314	1.010	1.582	1.239	122.5	166.9	124.3	173.8	0.4	19.9
M06-2X/6-311+G(d,p)/trans	1.342	1.021	1.881	1.218	1.317	0.999	1.632	1.236	122.2	164.4	123.8	175.8	0.6	19.7

M06-2X/6-311+G(d,p)/cis	1.342	1.021	1.879	1.218	1.317	0.999	1.634	1.233	122.2	164.3	123.8	176.1	0.6	19.7
M06-2X/6-311+G(d,p)/trans[c]	1.343	1.021	1.895	1.218	1.317	0.998	1.647	1.232	122.2	164.4	123.8	175.8	2.7	23.4
M06-L/6-311+G(d,p)/trans	1.347	1.023	1.858	1.225	1.324	0.999	1.667	1.238	121.9	167.4	124.0	174.1	3.6	18.1
MP2/6-31G(d,p)/trans	1.348	1.020	1.884	1.235	1.330	1.000	1.666	1.248	122.9	167.9	124.5	172.7	0.7	29.5
MP2/6-31G(d,p)/cis	1.348	1.020	1.884	1.235	1.330	1.001	1.666	1.248	122.9	167.9	124.5	172.7	0.6	29.1
MP2/6-31G(d,p)/trans[c]	1.353	1.017	1.962	1.232	1.335	0.994	1.739	1.245	122.7	167.2	124.2	172.5	1.4	29.5
M06-2X/6-31G(d,p)/trans[d]	1.334	1.021	1.888	1.226	1.314	1.019	1.541	1.246	122.2	166.0	123.9	171.2	1.2	22.2
M06-2X/6-31G(d,p)/cis[d]	1.334	1.021	1.885	1.226	1.314	1.019	1.541	1.246	122.2	166.0	123.9	171.4	5.3	17.3
M06-2X/6-311+G(d,p)/trans[d]	1.336	1.019	1.930	1.220	1.318	1.006	1.594	1.241	121.9	163.9	123.2	172.7	1.7	24.1
M06-2X/6-311+G(d,p)/cis[d]	1.336	1.019	1.928	1.220	1.318	1.006	1.595	1.241	121.9	163.9	123.2	172.9	4.5	18.4
MP2/6-31G(d,p)/trans[d]	1.336	1.019	1.928	1.220	1.318	1.006	1.595	1.241	121.9	163.9	123.2	172.9	4.5	18.4
MP2/6-31G(d,p)/cis[d]	1.342	1.017	1.929	1.235	1.331	1.005	1.638	1.254	122.6	167.1	124.1	170.3	2.7	28.3
M06-2X/6-311+G(d,p)/trans[e]	1.340	1.020	1.900	1.219	1.317	1.002	1.614	1.236	122.1	164.4	123.5	174.4	2.2	23.7
M06-2X/6-311+G(d,p)/cis[e]	1.340	1.020	1.900	1.219	1.317	1.002	1.617	1.236	122.1	164.2	123.5	174.7	1.4	20.3
MP2/6-31G(d,p)/trans[e]	1.346	1.018	1.902	1.235	1.330	1.002	1.654	1.251	122.7	167.7	124.3	171.6	1.0	28.6
oniom-M06-2X/6-31G(d,p)/trans[f]	1.330	1.023	1.782	1.226	1.315	1.016	1.584	1.245	123.2	169.0	124.0	171.7	21.3	42.7
oniom-M06-2X/6-31G(d,p)/cis[f]	1.330	1.023	1.782	1.225	1.315	1.015	1.591	1.245	123.3	168.4	124.0	172.9	18.6	41.7
oniom-MP2/6-31G(d,p)/trans[f]	1.337	1.019	1.818	1.236	1.332	1.003	1.686	1.255	123.5	170.3	124.2	170.6	21.6	44.1
oniom-MP2/6-31G(d,p)/cis[f]	1.336	1.019	1.813	1.235	1.332	1.002	1.700	1.256	123.6	170.0	124.2	171.9	17.0	43.5
M06-2X/6-31G(d,p)/trans[f]	1.340	1.025	1.856	1.227	1.307	1.020	1.561	1.242	122.2	169.1	125.8	173.1	15.7	15.1
							B'C'							
M06-2X/6-31G(d,p)	1.341	0.977	1.811	1.217	1.324	0.988	1.729	1.400	118.3	175.2	123.7	179.5	0.9	
M06-2X/6-311+G(d,p)	1.342	0.974	1.825	1.212	1.326	0.984	1.756	1.401	118.0	174.1	123.2	179.8	0.3	
M06-2X/6-311+G(d,p)[c]	1.342	0.974	1.843	1.211	1.326	0.983	1.775	1.400	118.0	174.1	123.2	179.8	0.4	
M06-L/6-311+G(d,p)	1.342	0.977	1.816	1.217	1.332	0.986	1.765	1.403	117.7	176.1	123.6	179.7	0.2	
MP2/6-31G(d,p)	1.350	0.977	1.837	1.229	1.337	0.987	1.761	1.407	118.2	177.1	124.2	178.5	0.5	
MP2/6-31G(d,p)[c]	1.353	0.974	1.918	1.226	1.342	0.984	1.838	1.403	118.3	177.1	123.8	177.5	0.3	
MP2/6-311+G(d,p)	1.350	0.975	1.837	1.221	1.337	0.984	1.766	1.407	118.0	175.0	123.6	177.8	17.4	
M06-2X/6-31G(d,p)[d]	1.351	0.979	1.794	1.221	1.322	0.991	1.703	1.392	117.5	178.2	123.4	179.3	0.1	
M06-2X/6-311+G(d,p)[d]	1.354	0.976	1.810	1.217	1.324	0.987	1.733	1.392	117.0	177.3	122.7	179.8	0.1	
MP2/6-31G(d,p)[d]	1.360	0.978	1.826	1.232	1.335	0.989	1.741	1.399	117.5	179.8	123.8	178.4	0.2	
M06-2X/6-311+G(d,p)[e]	1.347	0.975	1.820	1.214	1.325	0.985	1.742	1.397	117.6	175.3	122.9	179.9	0.0	
MP2/6-31G(d,p)[e]	1.354	0.977	1.835	1.230	1.337	0.988	1.750	1.404	117.9	178.1	124.0	178.4	0.0	
							BC							

M06-2X/6-31G(d,p)/trans	1.342	0.978	1.795	1.221	1.324	0.987	1.729	1.396	119.2	174.3	123.4	179.3	4.5	11.6
M06-2X/6-31G(d,p)/cis	1.342	0.978	1.793	1.221	1.324	0.987	1.730	1.396	119.1	174.4	123.4	179.2	5.2	8.4
M06-2X/6-311+G(d,p)/trans	1.343	0.975	1.802	1.215	1.326	0.983	1.760	1.396	118.6	174.0	123.0	179.9	0.7	6.4
M06-2X/6-311+G(d,p)/cis	1.343	0.975	1.804	1.215	1.326	0.983	1.759	1.395	118.6	173.9	123.0	179.3	4.5	1.7
M06-2X/6-311+G(d,p)/trans[c]	1.344	0.974	1.818	1.215	1.326	0.982	1.780	1.395	118.6	174.0	123.0	179.7	0.7	5.8
M06-L/6-311+G(d,p)/trans	1.345	0.977	1.796	1.222	1.333	0.985	1.773	1.398	118.3	175.9	123.2	179.5	1.8	3.1
M06-L/6-311+G(d,p)/cis	1.345	0.977	1.796	1.222	1.333	0.985	1.772	1.398	118.3	175.8	123.2	179.1	1.3	3.0
MP2/6-31G(d,p)/trans	1.351	0.978	1.819	1.233	1.337	0.987	1.755	1.404	119.2	176.5	123.8	178.0	1.9	20.4
MP2/6-31G(d,p)/cis	1.351	0.978	1.819	1.233	1.337	0.987	1.755	1.404	119.2	176.5	123.8	178.0	1.9	20.2
MP2/6-31G(d,p)/trans[c]	1.353	0.976	1.897	1.230	1.342	0.984	1.831	1.400	119.2	176.5	123.5	177.2	2.9	19.3
MP2/6-31G(d,p)/cis[c]	1.353	0.976	1.897	1.230	1.342	0.984	1.831	1.400	119.2	176.5	123.5	177.2	2.9	19.1
M06-2X/6-31G(d,p)/trans[d]	1.350	0.979	1.779	1.224	1.321	0.991	1.706	1.389	118.3	177.3	123.3	179.3	4.7	10.1
M06-2X/6-31G(d,p)/cis[d]	1.350	0.979	1.777	1.224	1.321	0.991	1.707	1.389	118.2	177.4	123.3	179.2	4.7	7.2
M06-2X/6-311+G(d,p)/trans[d]	1.353	0.976	1.786	1.219	1.323	0.985	1.746	1.388	117.7	177.3	122.7	179.4	2.2	4.6
M06-2X/6-311+G(d,p)/cis[d]	1.353	0.976	1.788	1.219	1.323	0.985	1.744	1.388	117.6	177.2	122.7	179.7	2.4	2.1
MP2/6-31G(d,p)/trans[d]	1.359	0.979	1.809	1.235	1.335	0.990	1.737	1.396	118.3	178.8	123.6	178.1	1.0	23.5
M06-2X/6-311+G(d,p)/trans[e]	1.347	0.975	1.797	1.217	1.325	0.984	1.754	1.393	118.2	175.3	122.8	179.4	2.0	5.8
M06-2X/6-311+G(d,p)/cis[e]	1.347	0.975	1.799	1.217	1.325	0.984	1.751	1.392	118.2	175.3	122.8	179.4	2.6	2.4
MP2/6-31G(d,p)/trans[e]	1.354	0.979	1.815	1.234	1.337	0.988	1.748	1.401	118.8	177.6	123.7	177.9	0.5	22.7
MP2/6-31G(d,p)/cis[e]	1.354	0.979	1.816	1.234	1.337	0.988	1.748	1.401	118.8	177.5	123.7	177.9	1.0	22.3
oniom-M06-2X/6-31G(d,p)/trans[f]	1.344	0.980	1.781	1.223	1.321	0.993	1.673	1.387	119.4	175.7	123.5	176.5	4.3	22.3
oniom-M06-2X/6-31G(d,p)/cis[f]	1.344	0.979	1.774	1.223	1.321	0.993	1.683	1.386	119.3	173.8	123.6	177.0	10.4	19.5
oniom-M06-2X/6-31G(d,p)/trans[g]	1.347	0.979	1.808	1.225	1.318	0.992	1.680	1.384	118.9	175.7	123.7	175.6	5.9	15.1
oniom-MP2/6-31G(d,p)/trans[f]	1.353	0.980	1.813	1.235	1.335	0.991	1.710	1.394	119.3	177.0	123.8	175.6	5.6	25.3
oniom-MP2/6-31G(d,p)/cis[f]	1.353	0.979	1.792	1.235	1.334	0.991	1.733	1.393	119.2	175.3	123.9	176.7	9.1	19.8
M06-2X/6-31G(d,p)/trans[f]	1.358	0.981	1.796	1.222	1.320	0.992	1.682	1.383	119.7	168.2	124.3	169.0	28.0	13.3

[a] Dihedral angle between the (7,8,2) and (3,4,6) planes for the **A'A'**, **AA**, **B'B'**, and **BB** dimers, . between the (8,2,3) and (4,6,7) planes for the **C'C'**, **CC**, **A'B'**, **AB**, **A'C'**, **AC, B'C'**, and **BC** dimers, [b] Dihedral angle between the two phenyl groups. [c] BSSE. [d] In n,n-DiMethylFormamide solvent (ϵ = 37.219), PCM model. [e] In CCl_4 solvent (ϵ = 2.2280), PCM model. [f] In the capsule **a**. [g] In the capsule **b**.

Table 2S: Encapsulated Dimer % Distribution of the **C'C'**, **A'C'**, **A'A'**, **B'C'**, **A'B'**, and **B'B'** Species at Various Levels of Theory.

	A' + C'			**B' + C'**			**A' + B'**			**A' + B' + C'**					
	A'C'	**C'C'**	**A'A'**	**B'B'**	**B'C'**	**C'C'**	**B'B'**	**A'B'**	**A'A'**	**B'B'**	**A'C'**	**B'C'**	**C'C'**	**A'B'**	**A'A'**
M06-2X/6-31G(d,p)	51	27	23	50	30	20	53	29	18	27	21	17	11	15	9
M06-2X/6-311+G(d,p)	51	26	23	50	30	19	53	29	18	28	21	17	11	15	9
M06-L/6-311+G(d,p)	51	26	23	50	30	20	52	29	19	27	21	17	11	15	10
MP2/6-31G(d,p)	51	26	23	52	30	19	54	29	17	28	20	16	10	15	9
MP2/6-311+G(d,p)	50	26	24	51	30	19	53	29	18	28	20	17	10	15	10
M06-2X/6-31G(d,p)[a, b]	52	28	19	52	30	18	57	29	14	30	19	17	10	16	7
M06-2X/6-31G(d,p)[a, c]	53	27	20	53	30	17	57	29	13	31	20	17	10	16	7
M06-2X/6-311+G(d,p)[a, b]	53	28	19	52	30	18	57	29	13	30	19	18	10	16	7
M06-2X/6-311+G(d,p)[a, c]	53	27	20	53	30	17	58	29	13	31	19	18	10	15	7
MP2/6-31G(d,p)[a, b]	53	27	20	53	30	17	57	29	13	31	19	17	10	16	7
MP2/6-31G(d,p)[a, c]	53	27	20	55	29	16	58	29	13	32	19	17	9	16	7
M06-2X/6-311+G(d,p)[d, b]	52	27	21	51	30	19	55	29	16	29	20	17	10	15	8
MP2/6-31G(d,p)[d, b]	52	26	22	52	30	18	55	28	16	29	20	17	10	15	9
Expt[e]	53	36	11	61	21	18	75	12.5	12.5	34	23	18	15	6	4

[a] In n,n-DiMethylFormamide solvent (ϵ =37.219). [b] PCM model. [c] SCI-PCM model, single point calculation at the geometry of PCM model. [d] In CCl_4 solvent (ϵ = 2.2280). [e] Reference 16, % distribution of the corresponding **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** species in the **1.2$_4$.1** cage.

Table 3S: Encapsulated Dimer % Distribution of the **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** Species at Various Levels of Theory.

	A + C			**B + C**			**A + B**			**A + B + C**					
	AC	**CC**	**AA**	**BB**	**BC**	**CC**	**BB**	**AB**	**AA**	**BB**	**AC**	**BC**	**CC**	**AB**	**AA**
M06-2X/6-31G(d,p)	51	28	22	49	30	20	54	29	17	27	21	17	11	15	9
M06-2X/6-311+G(d,p)	51	27	22	49	31	20	53	29	17	27	21	17	11	15	9
M06-L/6-311+G(d,p)	51	27	22	48	31	21	52	30	18	26	21	17	11	15	9
MP2/6-31G(d,p)	51	27	22	50	30	19	54	29	17	28	20	17	11	15	9
M06-2X/6-31G(d,p)[a, b]	53	29	19	51	30	19	57	30	14	29	20	17	11	15	7
M06-2X/6-31G(d,p)[a, c]	52	29	19	50	30	20	56	30	14	29	20	17	11	15	7
M06-2X/6-311+G(d,p)[a, b]	52	29	19	51	30	19	57	30	13	29	20	18	11	16	7
MP2/6-31G(d,p)[a, b]	52	28	20	53	30	18	57	29	13	31	19	17	10	16	7
MP2/6-31G(d,p)[a, c]	53	27	20	52	30	17	57	29	14	30	20	17	10	16	7
M06-2X/6-311+G(d,p)[d, b]	51	28	21	50	30	20	55	29	16	28	20	17	11	15	8
MP2/6-31G(d,p)[d, b]	51	27	21	51	30	19	56	29	16	29	20	17	11	15	8
Oniom-M06-2X/6-31G(d,p)[e]	50	28	22	49	31	21	54	28	18	28	20	17	12	14	9
Oniom-M06-2X/6-31G(d,p)[f]							52	30	18						
Oniom-MP2/6-31G(d,p)[e]	49	28	23	51	30	19	54	28	18	29	20	17	11	15	9
M06-2X/6-31G(d,p)[e]	51	28	21	48	28	24	50	31	19	25	23	14	13	16	9
Expt[g]	53	36	11	61	21	18	75	12.5	12.5	34	23	18	15	6	4

[a] In n,n-DiMethylFormamide solvent (ϵ =37.219). [b] PCM model. [c] SCI-PCM model, single point calculation at the geometry of PCM model. [d] In CCl_4 solvent (ϵ = 2.2280). [e] In the capsule **a**. [f] In the capsule **b**. [g] Reference 16, % distribution of the **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** species in the **1.2$_4$.1** cage.

Table 4S: Absolute Energies and BSSE Corrections of the Calculated Structures at Various Levels of Theory in the Gas Phase.

Species	E	BSSE	E	BSSE	E	BSSE
	M06-2X/6-31G(d,p)		**M06-2X/6-311+G(d,p)**		**M06-L/6-311+G(d,p)**	
B'-syn	-216.4393443		-216.5119187		-216.5664565	
B'-anti	-216.4400109		-216.5128830		-216.5671755	
B'-ex-en	-216.4442644		-216.5169642		-216.5711390	
C'	-228.9910856		-229.0647238		-229.1290102	
A'	-209.1235471		-209.1892768		-209.2528872	
B'B'	-432.9093424	0.003737078773	-433.0521407	0.001307310996	-433.1593430	0.001021010893
C'C'	-458.0148152	0.005416193191	-458.1570870	0.001418995072	-458.2852111	0.001065355973
A'A'	-418.2753211	0.004987427566	-418.4022319	0.000897084490	-418.5294855	0.000621351986
B'C'	-445.46050697	0.004462076916	-445.6034007	0.001366133300	-445.7209724	0.001045756833
A'B'	-425.5909156	0.004344613613	-425.7257690	0.001058861169	-425.8428919	0.000814601751
A'C'	-438.1459712	0.005208385132	-438.2806816	0.001176044439	-438.4080019	0.000834631110
B-syn	-486.7003552		-486.8316633		-486.9622227	
B-anti	-486.6997252		-486.8307296		-486.9614511	
B-ex-en	-486.7041400		-486.8354606		-486.9661904	
C	-499.2534714		-499.384638		-499.5270706	
A	-479.3848540		-479.5079238		-479.6494361	
BB-cis	-973.4290501	0.00361799519	-973.6888832	0.001332711536	-973.9493714	0.001261758753
BB-trans	-973.4290141	0.003611715474	-973.6888835	0.001421654610	-973.9493244	0.001011313061
CC-cis	-998.5404601	0.005086104779	-998.7979805	0.001352219096	-999.0820997	
CC-trans	-998.5404518	0.00508319710	-998.7979683	0.001349805049	-999.0821136	0.000959202735
AA-cis	-958.7964359	0.004645243991	-959.0385713	0.000921169589	-959.3214125	
AA-trans	-958.7964013	0.00465167657	-959.0385210	0.000924512752	-959.3214053	0.000574906068
BC-cis	-985.9829854	0.00424088260	-986.2420742	0.001300798015	-986.5143185	0.000973943901
BC-trans	-985.9830163	0.004246809226	-986.2420841	0.001293105741	-986.5143407	0.000971579066
AB-cis	-966.1118931	0.00408966075	-966.3629166	0.001096773222	-966.6345390	0.000816809057
AB-trans	-966.1118868	0.004101045133	-966.3629110	0.001114529983	-966.6345841	0.000838609424
AC-cis	-978.6692001	0.004872175709	-978.9192070	0.001171821128	-979.2024598	
AC-trans	-978.6691886	0.00487401035	-978.9192112	0.001167958167	-979.2024704	0.000788779588

	MP2/6-31G(d,p)		**MP2/6-311+G(d,p)**	
B'-syn	-215.910904		-216.0250106	
B'-anti	-215.9108988		-216.0260219	
B'-ex-en	-215.9154005		-216.0300141	
C'	-228.4535885		-228.5679722	
A'	-208.6117729		-208.7092026	
B'B'	-431.8512996	0.00594175602	-432.0776894	0.004727527050
	-431.84563095[a]			
C'C'	-456.9370010	0.008551829199	-457.1604960	0.005025026175
A'A'	-417.2507088	0.007930741387	-417.4400949	0.003907583407
B'C'	-444.3930774	0.00708154019	-444.6181194	0.004729464086
	-444.3862820[a]			
A'B'	-424.5496492	0.006836604518	-424.7575547	0.004131774296
A'C'	-437.0946393	0.008228001625	-437.3010184	0.005025026175
B-syn	-485.4321197		-485.6362660	
B-anti	-485.4317602		-485.6364864	
B-ex-en	-485.4359257		-485.6404497	
C	-497.9761140			
A’	-478.1344046			
BB-cis	-970.8925597	0.005966542461		
BB-trans	-970.8925625	0.005968942317		
	-970.8868698[a]			
CC-cis	-995.9831294	0.008573038441		
CC-trans	-995.9831295	0.008580377876		
AA-cis	-956.2952742	0.007804205576		
AA-trans	-956.2952569	0.007805575557		
BC-cis	-983.4366975	0.007076472802		
	-983.4299014[a]			
BC-trans	-983.4366966	0.007076308258		
	-983.4299006[a]			

AB-cis	-963.5929865	0.006803052363
AB-trans	-963.5929858	0.006803267143
AC-cis	-976.1398436	0.008189854684
AC-trans	-976.1398418	0.008189728036
	-976.1319329[a]	

	M06-2X/6-311+G(d,p)		**MP2/6-311+G(d,p)**		**MP2/6-31G(d,p)**	
$HB(OH)_2$	-177.1900252		-176.8121929			
$HB(OH)_2$-anti	-177.1931257		-176.8159521			
$HB(OH)_2$-ex-en	-177.1958260		-176.8182369		-176.7180843	
HCOOH	-189.7491048		-189.3621442		-189.2604984	
$(HB(OH)_2)_2$	-354.4093384	0.001266918393	-353.6531201	0.004043445156	-353.4560056	0.005793683799
$(HCOOH)_2$	-379.5248399	0.001279134646	-378.7473632	0.004460464207	-378.5498795	0.008133311051
H_2O	-76.4208161		-76.2747201		-76.2197858	
$(H_2O)_2$	-152.8519694	0.001315582624	-152.5590632	0.002535533645	-152.4508025	0.003829946632
	LMP2/aug-cc-pvdz					
H_2O	-76.25991380					
$(H_2O)_2$	-152.526938026	-0.000195157				
	MP2/aug-cc-pvdz		**df-LMP2/ aug-cc-pvdz**			
B'-syn	-215.9794378					
B'-anti	-215.9802852					
B'-ex-en	-215.9834620		-215.97222770		-	
B'B'	-431.9850254	0.003698990602	-431.9585182	-0.00172		

[a] BSSE optimized geometry.

Table 5S: Absolute Energies of the Calculated Structures at Various Levels of Theory in n,n-DiMethylFormamide Solvent (ε=37.219).

Species	E[a]	E[b]	E[a]	E[b]	E[a]	E[b]
	M06-2X/6-31G(d,p)		M06-2X/6-311+G(d,p)		MP2/6-31G(d,p)	
B'-ex-en	-216.4508234	-216.4526181	-216.524194	-216.5247916	-215.921962	-215.9234791
C'	-228.9978276	-228.9993423	-229.0724031	-229.0728127	-228.4596795	-228.4608274
A'	-209.1340437	-209.1350029	-209.2011824	-209.2007721	-208.6213812	-208.622215
B'B'	-432.9199952	-432.9222452	-433.0634996	-433.0642653	-431.8617907	-431.8636467
C'C'	-458.0211834	-458.0212348	-458.1646525	-458.163792	-456.9426781	-456.9425261
A'A'	-418.2871647	-418.2875856	-418.4156916	-418.4143544	-417.2615262	-417.2618659
B'C'	-445.4699461	-445.4712594	-445.6138378	-445.6139271	-444.4019269	-444.4029234
A'B'	-425.6043195	-425.6056574	-425.7404197	-425.7399313	-424.5622714	-424.5632193
A'C'	-438.1559996	-438.1564624	-438.2920083	-438.2911274	-437.1036143	-437.1037938
B-ex-en	-486.7122305	-486.713696	-486.8443769	-486.8444583	-485.4434555	-485.4445367
C	-499.2608294	-499.2620952	-499.3928854	-499.392960	-497.9825546	-497.9834862
A’	-479.395666	-479.3963286	-479.5201079	-479.5194915	-478.1441122	-478.144517
BB-cis	-973.4422367		-973.7033119			
BB-trans	-973.4421474	-973.4427418	-973.7033339		-970.9047851	-970.9051749
CC-cis	-998.5476953		-998.8064901	-998.805041		
CC-trans	-998.5476888		-998.8064845		-995.9893286	-995.9885604
AA-cis	-958.8096653	-958.8091569	-959.053538		-956.3069623	-956.3064453
AA-trans	-958.8096238		-959.0534526		-956.3069274	
BC-cis	-985.9940275	-985.9941464	-986.2544261	-986.253264		
BC-trans	-985.9940566		-986.2544295	-986.253257	-983.4465665	
AB-cis	-966.1268401	-966.1267673	-966.3794492	-966.377901	-963.6065355	-963.6061425
AB-trans	-966.1267911		-966.3794604	-966.3779007		
AC-cis	-978.6803063	-978.6797457	-978.9316939	-978.9300992		
AC-trans	-978.6803179		-978.9317089	-978.9300989	-976.1494618	-976.1488984

[a] PCM model. [b] SCI-PCM model, single point calculations at the optimized geometry of the PCM model.

Table 6S: Absolute Energies of the Calculated Structures at Various Levels of Theory in CCl_4 Solvent (ε=2.2280).

Species	E[a]	E[a]
	M06-2X/6-311+G(d,p)	**MP2/6-31G(d,p)**
B'-ex-en	-216.5201855	-215.9183409
C'	-229.0682840	-228.4564364
A'	-209.1945478	-208.6160059
B'B'	-433.0571322	-431.8559450
C'C'	-458.1605094	-456.9395757
A'A'	-418.4081121	-417.2554866
B'C'	-445.6079494	-444.3969611
A'B'	-425.7318820	-424.5549344
A'C'	-438.2856757	-437.0986291
B-ex-en	-486.8392465	-485.439214
C	-499.3883130	-497.9790024
A’	-479.5131173	-478.1386043
BB-cis	-973.6948487	-970.897698
BB-trans	-973.6948439	-970.8976581
CC-cis	-998.8015733	-995.9857439
CC-trans	-998.8015675	-995.9857455
AA-cis	-959.0447769	-956.3002113
AA-trans	-959.0447320	-956.3001887
BC-cis	-986.2471220	-983.4407814
BC-trans	-986.2471323	-983.4407677
AB-cis	-966.3694801	-963.59841980
AB-trans	-966.3694778	
AC-cis	-978.9244034	
AC-trans	-978.9244181	-976.1438860

[a] PCM model. [b] SCI-PCM model, single point calculations at the optimized geometry of the PCM model.

Table 7S: Absolute Energies and BSSE Corrections of the Calculated Dimers in the Cage using the ONIOM Method[a] at Various Levels of Theory in the Gas Phase.

Species	**E**	**BSSE**	**E**	**BSSE**	**E**	**BSSE**
	M06-2X/6-31G(d,p)[b]		**MP2/6-31G(d,p)**[b]		**M06-2X/6-31G(d,p)**[c]	
BB-cis	-973.42817364	0.003594044885	-970.8915085	0.006011348356	-973.427442598	0.003949845308
BB-trans	-973.42758943	0.003614470822	-970.8911499	0.006058701161		
CC-cis	-998.53908594	0.005108305842	-995.9816575	0.008705816688	-998.525711330	0.0050430
CC-trans	-998.53941760	0.005141996298	-995.981931	0.008778483930		
AA-cis	-958.79536001	0.004633440868	-956.2935113	0.007875745931	-958.794313031	0.004571656860
AA-trans	-958.79572990	0.004621035459	-956.2942574	0.007699968908	-958.79486760	0.004595821532
BC-cis	-985.98167349	0.004297958350	-983.4352463	0.007216699157		
BC-trans	-985.98197832	0.004329252429	-983.4356968	0.007312093999	-985.981658010	0.004288180477
AB-cis	-966.11000051	0.004201776477	-963.5910095	0.007038811932		
AB-trans	-966.11022458	0.004167696784	-963.5913828	0.007018573437	-966.110430606	0.004085170010
AC-cis	-978.66700634	0.004950430541	-976.1377062	0.008410658971		
AC-trans	-978.66657551	0.004931638380	-976.1372635	0.008418729427		

[a] The systems were defined as two regions (layers) with the high layer that is the dimers calculated at the M06-2X/6-31G(d,p) or MP2/6-31G(d,p) levels of theory and the low layer, that is the capsule calculated at the PM6 level of theory. [b] Capsule **a**. [c] Capsule **b**.

Table 8S: Absolute Energies and BSSE Corrections of the Encapsulation Complexes (Capsule **a)** at the M06-2X/6-31G(d,p) Level of Theory in the Gas Phase.

A. DIMERS IN THE GAS PHASE

B'B': M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.683310	0.043848	0.030880
2	5	0	-2.116068	-0.068358	-0.009757
3	8	0	-1.315495	1.070239	-0.050024
4	8	0	-1.497388	-1.264950	0.006922
5	1	0	-0.526953	-1.207695	-0.007556
6	1	0	-1.813650	1.890082	-0.061233
7	1	0	-4.012597	0.425975	1.002723
8	1	0	-4.154846	-0.927290	-0.118289
9	1	0	-4.067596	0.734076	-0.725603
10	6	0	3.683617	-0.044242	0.019331
11	5	0	2.115920	0.068914	0.008273
12	8	0	1.315548	-1.069994	-0.030543
13	8	0	1.497013	1.265309	0.025480
14	1	0	0.526770	1.208096	0.000853
15	1	0	1.813864	-1.889773	-0.040417
16	1	0	4.047217	-0.449799	-0.930456
17	1	0	4.037656	-0.717797	0.805292
18	1	0	4.151614	0.928874	0.166168

B'C': M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.616926	-0.089717	0.007622
2	5	0	2.054862	0.082345	-0.006045
3	8	0	1.222060	-1.043915	-0.004479
4	8	0	1.476255	1.292975	-0.009847
5	1	0	0.502096	1.275804	-0.007050
6	1	0	1.707470	-1.871785	-0.002402
7	1	0	4.120394	0.868301	-0.118666
8	1	0	3.960925	-0.764922	-0.781494
9	1	0	3.950200	-0.518936	0.958134
10	6	0	-3.505926	0.090827	0.003240
11	8	0	-1.309283	1.055074	0.004883
12	8	0	-1.515077	-1.167987	-0.003099
13	1	0	-0.532216	-1.125794	-0.003924
14	6	0	-2.005897	0.063795	0.002185
15	1	0	-3.876344	-0.451203	0.874405
16	1	0	-3.875537	-0.421627	-0.886129
17	1	0	-3.853546	1.119830	0.019410

A'B': M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.677271	-0.058536	0.010108
2	5	0	-2.101995	-0.077235	-0.007471
3	8	0	-1.389809	1.125447	-0.007659
4	8	0	-1.419323	-1.231252	-0.010648
5	1	0	-0.443976	-1.152863	-0.006984
6	1	0	-1.970330	1.888976	-0.005940
7	1	0	-4.046514	0.322513	0.968153
8	1	0	-4.087467	-1.058586	-0.128159
9	1	0	-4.089136	0.592037	-0.767329
10	6	0	3.555393	-0.206545	0.003965
11	8	0	1.327977	-1.041931	0.001877
12	6	0	2.052465	-0.055823	0.001929
13	7	0	1.560738	1.199606	0.000346
14	1	0	0.551198	1.326513	-0.002014
15	1	0	2.169161	1.998834	-0.000705
16	1	0	3.839694	-0.782999	0.884712
17	1	0	4.085958	0.745232	0.004421
18	1	0	3.841943	-0.783406	-0.875799

C'C': M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.423304	0.113868	0.000155
2	8	0	-1.215640	1.041772	0.001091
3	8	0	-1.457407	-1.178987	0.000717
4	1	0	-0.465520	-1.162492	-0.000362
5	6	0	-1.925151	0.051343	0.001116
6	1	0	-3.806025	-0.417277	0.872678
7	1	0	-3.802486	-0.394715	-0.887382
8	1	0	-3.748797	1.150189	0.011833
9	6	0	3.423283	-0.113964	0.001884
10	8	0	1.215619	-1.041695	-0.002304
11	8	0	1.457436	1.179057	-0.002014
12	1	0	0.465555	1.162540	-0.000598
13	6	0	1.925149	-0.051274	-0.002177
14	1	0	3.797579	0.365089	0.907956
15	1	0	3.811010	0.445186	-0.850485
16	1	0	3.748751	-1.149523	-0.039427

A'C': M06-2X/6-311+G(d,p):

Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z

1	6	0	3.487463	-0.004263	0.000416
2	8	0	1.361052	1.102972	0.000027
3	6	0	1.985882	0.060448	0.000382
4	8	0	1.425229	-1.131873	0.000518
5	1	0	0.430185	-1.055997	-0.000315
6	1	0	3.823633	-0.552636	-0.880808
7	1	0	3.823821	-0.556771	0.878925
8	1	0	3.900421	1.000597	0.002477
9	6	0	-3.465239	-0.246488	0.001578
10	8	0	-1.217822	-1.016279	-0.001922
11	6	0	-1.970201	-0.043256	-0.000542
12	7	0	-1.515623	1.219008	-0.000870
13	1	0	-0.506423	1.372827	-0.001486
14	1	0	-2.148457	1.999233	0.000917
15	1	0	-3.732297	-0.833512	-0.877605
16	1	0	-4.026484	0.687314	0.001121
17	1	0	-3.730141	-0.831320	0.882880

A'A': M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.567553	0.090998	-0.002713
2	8	0	-1.412552	1.101181	0.004244
3	6	0	-2.055685	0.057013	0.004715
4	7	0	-1.471722	-1.154758	0.003271
5	1	0	-2.024246	-1.993935	0.004206
6	1	0	-0.449891	-1.221571	-0.001061
7	1	0	-3.895038	0.552400	-0.935400
8	1	0	-3.900711	0.727046	0.817175
9	1	0	-4.021876	-0.895175	0.091121
10	6	0	3.567552	-0.090998	0.002749
11	8	0	1.412551	-1.101181	-0.004284
12	6	0	2.055685	-0.057013	-0.004721
13	7	0	1.471723	1.154758	-0.003273
14	1	0	0.449892	1.221572	0.001038
15	1	0	2.024248	1.993935	-0.004173
16	1	0	3.900732	-0.727069	-0.817113
17	1	0	3.895013	-0.552375	0.935457
18	1	0	4.021879	0.895171	-0.091099

B'B': M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.695203	0.043150	-0.003390
2	5	0	2.127375	-0.067265	0.007675
3	8	0	1.326895	1.071126	0.006285
4	8	0	1.508392	-1.264163	0.006508
5	1	0	0.538409	-1.206853	0.001142
6	1	0	1.826967	1.889804	0.009956
7	1	0	4.044722	0.440426	-0.961968
8	1	0	4.163086	-0.930244	0.142021
9	1	0	4.063805	0.721409	0.771637
10	6	0	-3.695199	-0.043170	0.003981
11	5	0	-2.127375	0.067276	-0.007649
12	8	0	-1.326892	-1.071115	-0.006434
13	8	0	-1.508402	1.264177	-0.007018
14	1	0	-0.538418	1.206887	-0.001808
15	1	0	-1.826965	-1.889795	-0.009539
16	1	0	-4.044470	-0.441528	0.962190
17	1	0	-4.063951	-0.720596	-0.771714
18	1	0	-4.163150	0.930355	-0.140326

B'C': M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.625913	-0.088629	0.006539
2	5	0	2.063634	0.081178	-0.005741
3	8	0	1.231584	-1.044543	-0.002695
4	8	0	1.484436	1.291803	-0.009598
5	1	0	0.510750	1.275547	-0.006500
6	1	0	1.720196	-1.870449	-0.001869
7	1	0	4.127836	0.870476	-0.117472
8	1	0	3.970445	-0.760892	-0.784871
9	1	0	3.960657	-0.520164	0.955480
10	6	0	-3.514946	0.090132	0.002971
11	8	0	-1.318633	1.055708	0.005280
12	8	0	-1.523665	-1.167365	-0.003933
13	1	0	-0.541545	-1.126055	-0.004321
14	6	0	-2.014862	0.064590	0.001975
15	1	0	-3.885030	-0.452465	0.873928
16	1	0	-3.884255	-0.422042	-0.886669
17	1	0	-3.863627	1.118767	0.019652

A'B': M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.686110	-0.061877	0.008275
2	5	0	-2.110893	-0.075991	-0.007127
3	8	0	-1.401013	1.127185	-0.005298
4	8	0	-1.425471	-1.228665	-0.009799
5	1	0	-0.450892	-1.147954	-0.005431
6	1	0	-1.984329	1.888523	-0.006204
7	1	0	-4.058010	0.321489	0.964361
8	1	0	-4.093052	-1.063601	-0.127207
9	1	0	-4.098869	0.584581	-0.772114
10	6	0	3.564087	-0.206766	0.003329
11	8	0	1.336730	-1.042543	0.002329

12	6	0	2.060977	-0.056737	0.001677
13	7	0	1.570049	1.199360	-0.000393
14	1	0	0.561279	1.328770	-0.001888
15	1	0	2.178467	1.998570	-0.001956
16	1	0	3.848837	-0.782465	0.884414
17	1	0	4.094389	0.745127	0.002969
18	1	0	3.850604	-0.784146	-0.876091

C'C': M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.430764	0.113042	-0.000134
2	8	0	-1.223392	1.042580	0.000211
3	8	0	-1.464394	-1.178208	-0.000109
4	1	0	-0.473698	-1.162579	0.000138
5	6	0	-1.932487	0.052576	-0.000048
6	1	0	-3.810950	-0.405719	0.880980
7	1	0	-3.811182	-0.408843	-0.879278
8	1	0	-3.757776	1.148935	-0.001788
9	6	0	3.430758	-0.113082	-0.000168
10	8	0	1.223362	-1.042560	0.000249
11	8	0	1.464431	1.178227	-0.000076
12	1	0	0.473743	1.162642	0.000123
13	6	0	1.932481	-0.052574	-0.000007
14	1	0	3.811001	0.405764	0.880874
15	1	0	3.811145	0.408700	-0.879385
16	1	0	3.757742	-1.148982	-0.001731

A'C': M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.494144	-0.006769	0.000130
2	8	0	1.369641	1.104691	-0.000159
3	6	0	1.992733	0.061618	0.000136
4	8	0	1.429913	-1.130115	-0.000168
5	1	0	0.436156	-1.053500	-0.000506
6	1	0	3.829155	-0.555984	-0.880993
7	1	0	3.829139	-0.559714	0.878895
8	1	0	3.909443	0.997121	0.002128
9	6	0	-3.471935	-0.245358	0.001308
10	8	0	-1.225284	-1.017784	-0.000751
11	6	0	-1.976417	-0.044437	-0.000093
12	7	0	-1.521712	1.218164	-0.000571
13	1	0	-0.513433	1.374334	-0.001139
14	1	0	-2.154301	1.998577	0.000288
15	1	0	-3.739473	-0.831724	-0.878173
16	1	0	-4.031951	0.689152	0.000901
17	1	0	-3.738065	-0.830063	0.882332

A'A': M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.573814	-0.090065	-0.002808
2	8	0	1.419597	-1.101950	0.004374
3	6	0	2.061896	-0.057644	0.004698
4	7	0	1.477343	1.154007	0.003378
5	1	0	2.028552	1.994025	0.004313
6	1	0	0.455900	1.220858	-0.001052
7	1	0	3.901522	-0.552457	-0.934921
8	1	0	3.907675	-0.724718	0.817882
9	1	0	4.027390	0.896550	0.089672
10	6	0	-3.573814	0.090065	0.002838
11	8	0	-1.419597	1.101950	-0.004404
12	6	0	-2.061896	0.057645	-0.004703
13	7	0	-1.477343	-1.154007	-0.003383
14	1	0	-0.455900	-1.220859	0.001031
15	1	0	-2.028552	-1.994025	-0.004295
16	1	0	-3.907695	0.724738	-0.817827
17	1	0	-3.901500	0.552432	0.934971
18	1	0	-4.027391	-0.896549	-0.089654

B'B': MP2/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.629656	0.045595	0.282973
2	5	0	-2.086368	-0.084250	-0.008700
3	8	0	-1.325965	1.028682	-0.386466
4	8	0	-1.448023	-1.273134	0.106303
5	1	0	-0.496715	-1.204843	-0.085972
6	1	0	-1.860409	1.826585	-0.416655
7	1	0	-3.797512	0.637086	1.190827
8	1	0	-4.092695	-0.931573	0.430306
9	1	0	-4.154187	0.557201	-0.531408
10	6	0	3.629640	-0.045895	0.282978
11	5	0	2.086361	0.084243	-0.008611
12	8	0	1.325764	-1.028482	-0.386557
13	8	0	1.448261	1.273268	0.106388
14	1	0	0.496990	1.205212	-0.086067
15	1	0	1.859946	-1.826567	-0.416611
16	1	0	4.154313	-0.554603	-0.533137
17	1	0	3.797849	-0.640334	1.188833
18	1	0	4.092259	0.930999	0.433373

B'C': MP2/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.606459	-0.096495	0.162820
2	5	0	2.052740	0.083067	-0.027670
3	8	0	1.228040	-1.034764	-0.249344
4	8	0	1.469882	1.299227	0.023369
5	1	0	0.500882	1.259973	-0.077598
6	1	0	1.734227	-1.851477	-0.234090
7	1	0	4.120423	0.866146	0.165097
8	1	0	4.044797	-0.721023	-0.623172
9	1	0	3.817916	-0.590907	1.118515
10	6	0	-3.504054	0.068595	0.096521
11	8	0	-1.323730	1.066450	-0.163381
12	8	0	-1.493451	-1.164582	0.120296
13	1	0	-0.518169	-1.104302	0.007718
14	6	0	-2.003248	0.065811	0.006400
15	1	0	-3.820568	-0.458348	0.998991
16	1	0	-3.914244	-0.467130	-0.763313
17	1	0	-3.869833	1.093626	0.104244

A'B': MP2/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.658598	-0.049979	0.172355
2	5	0	2.092021	-0.079668	-0.026795
3	8	0	1.394850	1.102479	-0.323126
4	8	0	1.397719	-1.230354	0.087429
5	1	0	0.432848	-1.135146	-0.048977
6	1	0	2.001067	1.846122	-0.367961
7	1	0	4.163650	0.403587	-0.688125
8	1	0	4.061742	-1.054034	0.314825
9	1	0	3.927231	0.549227	1.050524
10	6	0	-3.551590	-0.171709	0.057354
11	8	0	-1.341077	-1.042972	-0.228535
12	6	0	-2.044231	-0.054681	-0.011015
13	7	0	-1.518838	1.172649	0.243218
14	1	0	-0.522000	1.301865	0.085411
15	1	0	-2.118948	1.980543	0.245610
16	1	0	-3.892184	-0.781014	-0.780920
17	1	0	-4.056736	0.796323	0.040855
18	1	0	-3.813513	-0.692689	0.981905

C'C': MP2/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.439189	0.096575	-0.000172
2	8	0	-1.236011	1.066963	0.003716
3	8	0	-1.456302	-1.177499	0.000305
4	1	0	-0.466509	-1.134919	-0.001053
5	6	0	-1.936844	0.059577	0.002325
6	1	0	-3.816862	-0.444046	0.870630
7	1	0	-3.811259	-0.410587	-0.893458
8	1	0	-3.782749	1.129097	0.017209
9	6	0	3.439181	-0.096598	0.004359
10	8	0	1.236050	-1.066936	-0.003209
11	8	0	1.456276	1.177530	-0.005530
12	1	0	0.466476	1.134955	-0.001914
13	6	0	1.936854	-0.059530	-0.003492
14	1	0	3.805441	0.382039	0.915798
15	1	0	3.822430	0.471063	-0.846354
16	1	0	3.782914	-1.128212	-0.041231

A'C': MP2/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.501734	-0.015576	0.024373
2	8	0	-1.378614	1.124483	0.085975
3	6	0	-1.998136	0.070043	0.025410
4	8	0	-1.429455	-1.129074	-0.046247
5	1	0	-0.439305	-1.033472	-0.045051
6	1	0	-3.831912	-0.625504	0.868422
7	1	0	-3.835797	-0.508819	-0.891478
8	1	0	-3.929127	0.983334	0.090953
9	6	0	3.479868	-0.219663	0.115492
10	8	0	1.241163	-1.046792	-0.053795
11	6	0	1.984244	-0.057827	-0.035673
12	7	0	1.516181	1.205552	-0.156642
13	1	0	0.506900	1.344490	-0.093859
14	1	0	2.132159	1.985225	0.004929
15	1	0	3.704158	-0.401565	1.170435
16	1	0	4.032800	0.660539	-0.219124
17	1	0	3.796646	-1.093897	-0.453809

A'A': MP2/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.567059	-0.069053	-0.090155
2	8	0	1.427581	-1.128520	0.119453
3	6	0	2.059492	-0.069612	0.060718
4	7	0	1.462489	1.145528	0.135888
5	1	0	2.000301	1.972436	-0.066334
6	1	0	0.442672	1.196972	0.059571
7	1	0	3.811019	-0.254216	-1.140264
8	1	0	3.978819	-0.886490	0.502467
9	1	0	4.020896	0.875396	0.218121
10	6	0	-3.567054	0.069055	0.090202
11	8	0	-1.427575	1.128520	-0.119388
12	6	0	-2.059490	0.069613	-0.060705
13	7	0	-1.462501	-1.145531	-0.136016

14	1	0	-0.442687	-1.196985	-0.059655
15	1	0	-2.000306	-1.972430	0.066262
16	1	0	-3.978823	0.886516	-0.502380
17	1	0	-3.810987	0.254182	1.140324
18	1	0	-4.020903	-0.875380	-0.218099

AA-trans: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.679578	-1.239577	-0.073937
2	6	0	-4.293111	-1.268688	0.012454
3	6	0	-3.553954	-0.098642	-0.157077
4	6	0	-4.224159	1.099838	-0.395985
5	6	0	-5.608124	1.120271	-0.491777
6	6	0	-6.356580	-0.047959	-0.334533
7	1	0	-6.245490	-2.154879	0.067619
8	1	0	-3.798290	-2.205601	0.243457
9	1	0	-3.639812	2.005343	-0.506253
10	1	0	-6.120218	2.056372	-0.691237
11	6	0	-7.863045	-0.010998	-0.378886
12	6	0	-8.458815	0.272528	1.005340
13	1	0	-8.240806	-0.966134	-0.753430
14	1	0	-8.187789	0.759747	-1.083004
15	1	0	-9.549514	0.299247	0.965014
16	1	0	-8.159463	-0.499335	1.717856
17	1	0	-8.104691	1.232868	1.386714
18	8	0	-1.477569	0.991570	0.187771
19	6	0	5.608095	-1.120339	0.491654
20	6	0	4.224136	-1.099882	0.395798
21	6	0	3.553951	0.098641	0.157042
22	6	0	4.293121	1.268707	-0.012271
23	6	0	5.679585	1.239576	0.074191
24	6	0	6.356566	0.047912	0.334630
25	1	0	6.120173	-2.056474	0.690992
26	1	0	3.639775	-2.005398	0.505895
27	1	0	3.798314	2.205662	-0.243137
28	1	0	6.245509	2.154899	-0.067182
29	6	0	7.863029	0.010929	0.379048
30	6	0	8.458857	-0.272482	-1.005176
31	1	0	8.187730	-0.759884	1.083111
32	1	0	8.240786	0.966026	0.753694
33	1	0	9.549553	-0.299233	-0.964800
34	1	0	8.104727	-1.232779	-1.386657
35	1	0	8.159559	0.499455	-1.717634
36	8	0	1.477565	-0.991499	-0.188047
37	6	0	-2.056450	-0.059131	-0.073739
38	6	0	2.056450	0.059151	0.073656
39	7	0	1.398172	1.212886	0.293768
40	1	0	0.374954	1.207557	0.271551
41	1	0	1.877390	2.015178	0.663043
42	7	0	-1.398155	-1.212845	-0.293915
43	1	0	-1.877386	-2.015148	-0.663147
44	1	0	-0.374936	-1.207482	-0.271812

AC-cis: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.699944	1.206534	-0.014577
2	6	0	4.312388	1.262837	0.032410
3	6	0	3.556779	0.100627	-0.117335
4	6	0	4.211292	-1.116868	-0.296239
5	6	0	5.596621	-1.164897	-0.352489
6	6	0	6.361853	-0.004962	-0.215184
7	1	0	6.278543	2.116364	0.110106
8	1	0	3.829060	2.216036	0.216959
9	1	0	3.613307	-2.015125	-0.391527
10	1	0	6.096350	-2.116301	-0.505807
11	6	0	7.868016	-0.069388	-0.218572
12	6	0	8.422814	-0.323845	1.188118
13	1	0	8.272186	0.868252	-0.609444
14	1	0	8.196627	-0.865218	-0.892301
15	1	0	9.513557	-0.369933	1.177149
16	1	0	8.118869	0.472621	1.870940
17	1	0	8.042605	-1.267186	1.586535
18	8	0	1.452833	-0.945288	0.195662
19	6	0	-5.624487	1.205043	0.048272
20	6	0	-4.237425	1.176104	0.059724
21	6	0	-3.557882	-0.019764	-0.164335
22	6	0	-4.288021	-1.178240	-0.427899
23	6	0	-5.676785	-1.139960	-0.449841
24	6	0	-6.365087	0.048806	-0.206092
25	1	0	-6.144584	2.140130	0.230791
26	1	0	-3.658153	2.074146	0.237498
27	1	0	-3.780556	-2.109014	-0.656560
28	1	0	-6.235632	-2.043431	-0.672346
29	6	0	-7.871988	0.073846	-0.172288
30	6	0	-8.407103	-0.222156	1.233846
31	1	0	-8.265281	-0.662991	-0.877819
32	1	0	-8.227311	1.053605	-0.502219
33	1	0	-9.498422	-0.197915	1.251723
34	1	0	-8.079423	-1.208325	1.570417
35	1	0	-8.034715	0.514285	1.949454
36	8	0	-1.456958	1.061988	-0.347927
37	6	0	2.057007	0.088465	-0.076206
38	6	0	-2.058231	0.011665	-0.141434
39	7	0	-1.424142	-1.149546	0.108838
40	1	0	-0.402098	-1.150160	0.162365
41	1	0	-1.933833	-1.951285	0.436524
42	7	0	1.424806	1.246352	-0.345376
43	1	0	1.927527	2.030428	-0.722417
44	1	0	0.401505	1.256689	-0.355418

AC-trans: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.436332	-1.277125	0.413761
2	6	0	4.055954	-1.187065	0.299977
3	6	0	3.453216	0.060713	0.144798
4	6	0	4.240371	1.210258	0.104935
5	6	0	5.619351	1.110231	0.219024
6	6	0	6.236448	-0.133103	0.375421
7	1	0	5.903720	-2.248871	0.538866
8	1	0	3.437436	-2.075017	0.333554
9	1	0	3.754187	2.171326	-0.012563
10	1	0	6.229789	2.007310	0.191615
11	6	0	7.738173	-0.244378	0.443345
12	6	0	8.346890	-0.455575	-0.948532
13	1	0	8.013207	-1.078590	1.094247
14	1	0	8.151551	0.663102	0.891203
15	1	0	9.434528	-0.534007	-0.893013
16	1	0	7.958693	-1.370104	-1.402277
17	1	0	8.094513	0.377520	-1.608173
18	8	0	1.429329	1.280884	-0.103202
19	6	0	-5.398911	-1.131668	-0.619590
20	6	0	-4.021539	-0.981368	-0.562444
21	6	0	-3.464686	0.238513	-0.180342
22	6	0	-4.307121	1.293135	0.168835
23	6	0	-5.686169	1.131983	0.118787
24	6	0	-6.252000	-0.078445	-0.281734
25	1	0	-5.823638	-2.080871	-0.931011
26	1	0	-3.356207	-1.798306	-0.813776
27	1	0	-3.900373	2.237259	0.514704
28	1	0	-6.333341	1.956021	0.400978
29	6	0	-7.747222	-0.269643	-0.287250
30	6	0	-8.237240	-0.893010	1.025260
31	1	0	-8.028448	-0.911721	-1.126300
32	1	0	-8.237482	0.694738	-0.443425
33	1	0	-9.320548	-1.027136	1.014719
34	1	0	-7.772151	-1.868303	1.185451
35	1	0	-7.976771	-0.256684	1.873844
36	8	0	-1.284664	-0.674223	-0.063134
37	6	0	1.974901	0.199175	0.026703
38	6	0	-1.972944	0.345102	-0.143719
39	7	0	-1.431722	1.572213	-0.200592
40	1	0	-0.413429	1.647748	-0.189178
41	1	0	-1.994268	2.378021	-0.409758
42	8	0	1.327460	-0.946028	0.076728
43	1	0	0.341250	-0.800372	0.007881

AC-cis: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.455169	-1.305167	-0.182541
2	6	0	4.070384	-1.211755	-0.170559
3	6	0	3.460628	0.042015	-0.173597
4	6	0	4.244942	1.194153	-0.189022
5	6	0	5.628313	1.090784	-0.199823
6	6	0	6.252510	-0.158623	-0.196927
7	1	0	5.928706	-2.281825	-0.183911
8	1	0	3.454340	-2.102090	-0.162401
9	1	0	3.752673	2.159208	-0.195183
10	1	0	6.236767	1.989514	-0.213844
11	6	0	7.755108	-0.269527	-0.152061
12	6	0	8.267974	-0.342397	1.291497
13	1	0	8.200838	0.591309	-0.657295
14	1	0	8.070676	-1.161894	-0.699282
15	1	0	9.356186	-0.427188	1.317399
16	1	0	7.978767	0.552080	1.847666
17	1	0	7.842988	-1.206716	1.806555
18	8	0	1.427936	1.272199	-0.175157
19	6	0	-5.411261	-1.114518	-0.555705
20	6	0	-4.032531	-0.968217	-0.522639
21	6	0	-3.465067	0.240254	-0.120623
22	6	0	-4.297944	1.286792	0.273453
23	6	0	-5.677999	1.129884	0.246253
24	6	0	-6.254785	-0.068481	-0.174938
25	1	0	-5.844289	-2.054589	-0.883030
26	1	0	-3.374375	-1.779314	-0.809224
27	1	0	-3.882430	2.221007	0.635448
28	1	0	-6.317689	1.947795	0.561540
29	6	0	-7.750527	-0.254620	-0.158171
30	6	0	-8.222008	-0.889509	1.155532
31	1	0	-8.047275	-0.887027	-0.999173
32	1	0	-8.239708	0.713043	-0.296773
33	1	0	-9.305687	-1.021065	1.159972
34	1	0	-7.756922	-1.867337	1.299465
35	1	0	-7.947561	-0.261984	2.006283
36	8	0	-1.283814	-0.677308	-0.090377
37	6	0	1.978034	0.185234	-0.163376
38	6	0	-1.972571	0.344440	-0.117672
39	7	0	-1.431283	1.572522	-0.146023
40	1	0	-0.412940	1.646451	-0.162018
41	1	0	-1.997731	2.385042	-0.314223
42	8	0	1.332041	-0.961702	-0.140051
43	1	0	0.344118	-0.812053	-0.125622

CC-trans: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.506298	-1.203551	0.287271
2	6	0	4.121306	-1.243901	0.208524
3	6	0	3.395720	-0.053223	0.182177
4	6	0	4.062240	1.170086	0.234413
5	6	0	5.446382	1.199116	0.312309
6	6	0	6.186948	0.014594	0.340532

7	1	0	6.071313	-2.129762	0.311598
8	1	0	3.594515	-2.189081	0.170709
9	1	0	3.480647	2.083856	0.216847
10	1	0	5.964766	2.151482	0.356733
11	6	0	7.693424	0.051318	0.371721
12	6	0	8.282377	0.074964	-1.044032
13	1	0	8.068170	-0.822655	0.910962
14	1	0	8.024549	0.935484	0.922783
15	1	0	9.373272	0.101831	-1.012883
16	1	0	7.976196	-0.811824	-1.603381
17	1	0	7.932401	0.952548	-1.592032
18	8	0	1.261509	0.979569	0.086539
19	8	0	1.372173	-1.251586	0.050092
20	1	0	0.381898	-1.172030	-0.001624
21	6	0	-5.446392	-1.199132	-0.312215
22	6	0	-4.062243	-1.170080	-0.234467
23	6	0	-3.395733	0.053240	-0.182324
24	6	0	-4.121342	1.243906	-0.208596
25	6	0	-5.506342	1.203534	-0.287195
26	6	0	-6.186979	-0.014622	-0.340369
27	1	0	-5.964767	-2.151506	-0.356577
28	1	0	-3.480634	-2.083841	-0.216960
29	1	0	-3.594562	2.189095	-0.170855
30	1	0	-6.071374	2.129736	-0.311474
31	6	0	-7.693458	-0.051370	-0.371390
32	6	0	-8.282252	-0.075009	1.044430
33	1	0	-8.024631	-0.935547	-0.922405
34	1	0	-8.068278	0.822592	-0.910598
35	1	0	-9.373149	-0.101893	1.013405
36	1	0	-7.932199	-0.952581	1.592401
37	1	0	-7.976022	0.811791	1.603734
38	8	0	-1.261498	-0.979518	-0.086800
39	8	0	-1.372175	1.251628	-0.050399
40	1	0	-0.381897	1.172096	0.001337
41	6	0	1.913628	-0.054694	0.102220
42	6	0	-1.913629	0.054735	-0.102539

CC-cis: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.512597	1.211677	-0.169023
2	6	0	-4.125112	1.250648	-0.169375
3	6	0	-3.400415	0.059359	-0.174440
4	6	0	-4.069918	-1.163591	-0.180017
5	6	0	-5.456024	-1.191240	-0.179864
6	6	0	-6.196019	-0.005805	-0.174349
7	1	0	-6.077282	2.138333	-0.168139
8	1	0	-3.596021	2.195272	-0.168947
9	1	0	-3.488990	-2.077921	-0.187766
10	1	0	-5.977272	-2.143054	-0.187820
11	6	0	-7.701589	-0.043708	-0.117075
12	6	0	-8.203638	-0.108422	1.330810
13	1	0	-8.065146	-0.913259	-0.671074
14	1	0	-8.108735	0.843910	-0.608027
15	1	0	-9.294280	-0.140383	1.365543
16	1	0	-7.817272	-0.998421	1.832237
17	1	0	-7.866737	0.764697	1.893967
18	8	0	-1.265499	-0.976106	-0.181563
19	8	0	-1.371247	1.255580	-0.174489
20	1	0	-0.379604	1.174924	-0.176161
21	6	0	5.456421	1.194059	-0.174253
22	6	0	4.070228	1.166829	-0.174558
23	6	0	3.400358	-0.055867	-0.174799
24	6	0	4.124703	-1.247448	-0.175460
25	6	0	5.512123	-1.208904	-0.175049
26	6	0	6.195982	0.008416	-0.174508
27	1	0	5.977943	2.145733	-0.177469
28	1	0	3.489591	2.081373	-0.177981
29	1	0	3.595308	-2.191889	-0.179587
30	1	0	6.076534	-2.135741	-0.178698
31	6	0	7.701577	0.044690	-0.116961
32	6	0	8.204036	0.084380	1.331686
33	1	0	8.065567	0.923206	-0.656245
34	1	0	8.108117	-0.834755	-0.622978
35	1	0	9.294726	0.114134	1.366690
36	1	0	7.819022	0.966386	1.848072
37	1	0	7.865961	-0.797543	1.880208
38	8	0	1.265563	0.980025	-0.177758
39	8	0	1.371040	-1.251687	-0.179841
40	1	0	0.379396	-1.170914	-0.181181
41	6	0	-1.916157	0.059200	-0.177471
42	6	0	1.916094	-0.055370	-0.177868

BB-trans: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.762542	1.226310	0.260816
2	6	0	-4.382374	1.221295	0.094303
3	6	0	-3.650965	0.029629	0.104730
4	6	0	-4.360694	-1.163705	0.287181
5	6	0	-5.738573	-1.162807	0.455395
6	6	0	-6.460389	0.032701	0.444626
7	1	0	-6.306927	2.165447	0.250538
8	1	0	-3.885706	2.178551	-0.047182
9	1	0	-3.811877	-2.098938	0.299269
10	1	0	-6.266667	-2.100459	0.600637
11	6	0	-7.962790	0.024642	0.570141
12	6	0	-8.637941	-0.199417	-0.788540
13	1	0	-8.300188	0.973139	0.996336
14	1	0	-8.265921	-0.764416	1.263783
15	1	0	-9.725259	-0.210239	-0.689777
16	1	0	-8.363062	0.592604	-1.488622
17	1	0	-8.321812	-1.151137	-1.221278
18	5	0	-2.097693	-0.030029	-0.074871

19	8	0	-1.322331	1.113462	-0.208910
20	8	0	-1.477744	-1.227569	-0.102877
21	1	0	-0.514157	-1.175112	-0.217483
22	6	0	5.759056	-1.216716	-0.243969
23	6	0	4.369780	-1.188939	-0.250790
24	6	0	3.664470	0.018730	-0.241082
25	6	0	4.409665	1.203887	-0.217799
26	6	0	5.797959	1.180294	-0.213797
27	6	0	6.493188	-0.030361	-0.227282
28	1	0	6.283470	-2.167241	-0.252778
29	1	0	3.842678	-2.140260	-0.257540
30	1	0	3.881480	2.151003	-0.207219
31	1	0	6.355838	2.111806	-0.202363
32	6	0	7.999354	-0.056678	-0.164720
33	6	0	8.500811	-0.070007	1.284480
34	1	0	9.591827	-0.089096	1.322529
35	1	0	8.153169	0.816690	1.819188
36	1	0	8.122529	-0.947537	1.813543
37	5	0	2.102110	0.098298	-0.258035
38	8	0	1.308514	-1.027800	-0.427185
39	8	0	1.491761	1.291798	-0.110357
40	1	0	0.521794	1.249181	-0.151265
41	1	0	1.803279	-1.836946	-0.571886
42	1	0	-1.818915	1.932111	-0.147729
43	1	0	8.401222	0.817666	-0.683683
44	1	0	8.371442	-0.940430	-0.690024

BB-cis: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.769107	-1.245621	-0.032987
2	6	0	-4.381719	-1.216894	0.044564
3	6	0	-3.667411	-0.023913	-0.102723
4	6	0	-4.401971	1.147143	-0.325464
5	6	0	-5.787695	1.122056	-0.406932
6	6	0	-6.492015	-0.074903	-0.262478
7	1	0	-6.299373	-2.185576	0.084603
8	1	0	-3.864624	-2.155193	0.231694
9	1	0	-3.867649	2.083944	-0.439880
10	1	0	-6.336052	2.041691	-0.587843
11	6	0	-7.999259	-0.090548	-0.294535
12	6	0	-8.593017	0.191038	1.090976
13	1	0	-8.347401	-1.062829	-0.653219
14	1	0	-8.356566	0.659395	-1.005584
15	1	0	-9.684343	0.178408	1.060960
16	1	0	-8.259245	-0.559412	1.811114
17	1	0	-8.269899	1.168651	1.455597
18	5	0	-2.106488	0.054700	-0.031972
19	8	0	-1.313370	-1.081750	0.046713
20	8	0	-1.497018	1.257627	-0.051420
21	1	0	-0.527036	1.211969	-0.013896
22	6	0	5.769123	1.245578	-0.033092
23	6	0	4.381728	1.216867	0.044316
24	6	0	3.667421	0.023902	-0.103107
25	6	0	4.401986	-1.147159	-0.325797
26	6	0	5.787718	-1.122083	-0.407141
27	6	0	6.492038	0.074862	-0.262576
28	1	0	6.299392	2.185518	0.084614
29	1	0	3.864617	2.155148	0.231492
30	1	0	3.867666	-2.083954	-0.440276
31	1	0	6.336083	-2.041718	-0.588032
32	6	0	7.999285	0.090497	-0.294497
33	6	0	8.592918	-0.191045	1.091077
34	1	0	8.347465	1.062762	-0.653183
35	1	0	8.356651	-0.659473	-1.005488
36	1	0	9.684247	-0.178417	1.061159
37	1	0	8.259084	0.559429	1.811161
38	1	0	8.269765	-1.168644	1.455702
39	5	0	2.106490	-0.054660	-0.032544
40	8	0	1.313395	1.081860	0.045402
41	8	0	1.496989	-1.257580	-0.051480
42	1	0	0.527013	-1.211877	-0.013830
43	1	0	1.804544	1.904979	0.001271
44	1	0	-1.804473	-1.904922	0.003107

BC-trans: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.667339	1.209634	0.210883
2	6	0	4.279921	1.202030	0.121450
3	6	0	3.553249	0.008286	0.162447
4	6	0	4.274853	-1.185154	0.290746
5	6	0	5.659642	-1.181378	0.383290
6	6	0	6.376809	0.016510	0.345464
7	1	0	6.208245	2.150211	0.176611
8	1	0	3.774663	2.158819	0.008983
9	1	0	3.729200	-2.121866	0.321226
10	1	0	6.197617	-2.118732	0.489010
11	6	0	7.883910	0.010710	0.389111
12	6	0	8.484965	-0.228187	-1.001345
13	1	0	8.225152	-0.770211	1.074350
14	1	0	8.242431	0.964056	0.786253
15	1	0	9.576055	-0.235002	-0.961954
16	1	0	8.149234	-1.185952	-1.405182
17	1	0	8.169732	0.554358	-1.695098
18	5	0	1.992481	-0.058557	0.074543
19	8	0	1.211022	1.097611	0.089993
20	8	0	1.377697	-1.249546	-0.012459
21	1	0	0.404618	-1.201412	-0.047924
22	6	0	-5.560954	-1.208656	-0.338310
23	6	0	-4.177583	-1.159139	-0.266460
24	6	0	-3.530154	0.073103	-0.183245
25	6	0	-4.275122	1.251594	-0.173327
26	6	0	-5.660341	1.190773	-0.245413

27	6	0	-6.321376	-0.035988	-0.328873
28	1	0	-6.063745	-2.168008	-0.407444
29	1	0	-3.580807	-2.063276	-0.276703
30	1	0	-3.765156	2.204730	-0.111647
31	1	0	-6.240253	2.107996	-0.240550
32	6	0	-7.826984	-0.101114	-0.350777
33	6	0	-8.399544	-0.263347	1.062939
34	1	0	-8.145671	-0.940613	-0.974439
35	1	0	-8.225742	0.808596	-0.806895
36	1	0	-9.489803	-0.313793	1.039877
37	1	0	-8.022840	-1.177105	1.527688
38	1	0	-8.106937	0.578126	1.694768
39	8	0	-1.375099	-0.924637	-0.115731
40	8	0	-1.521531	1.302355	-0.035824
41	1	0	-0.542366	1.227606	0.009281
42	1	0	1.718988	1.903558	0.205871
43	6	0	-2.047251	0.087728	-0.109685

BC-cis: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.670038	1.206341	-0.169912
2	6	0	4.279803	1.197353	-0.156178
3	6	0	3.557969	0.000116	-0.165759
4	6	0	4.287088	-1.195528	-0.195687
5	6	0	5.674753	-1.190711	-0.208262
6	6	0	6.387227	0.010584	-0.195101
7	1	0	6.207010	2.149668	-0.166610
8	1	0	3.767747	2.157084	-0.148162
9	1	0	3.745076	-2.134643	-0.212178
10	1	0	6.219704	-2.129678	-0.233724
11	6	0	7.894520	0.007501	-0.157031
12	6	0	8.420509	-0.177205	1.271495
13	1	0	8.272951	0.946198	-0.570246
14	1	0	8.272298	-0.797805	-0.793128
15	1	0	9.512126	-0.183797	1.290493
16	1	0	8.069344	0.630696	1.917234
17	1	0	8.063770	-1.119564	1.693281
18	5	0	1.994753	-0.068693	-0.148768
19	8	0	1.215034	1.081836	-0.023780
20	8	0	1.375969	-1.256562	-0.250162
21	1	0	0.402725	-1.210323	-0.216786
22	6	0	-5.572228	-1.206383	-0.218488
23	6	0	-4.187006	-1.161240	-0.198759
24	6	0	-3.533061	0.069606	-0.155891
25	6	0	-4.273248	1.250895	-0.134024
26	6	0	-5.660373	1.194472	-0.154520
27	6	0	-6.327890	-0.030778	-0.196989
28	1	0	-6.080746	-2.164456	-0.255707
29	1	0	-3.593880	-2.067625	-0.218975
30	1	0	-3.757870	2.202597	-0.104047
31	1	0	-6.236730	2.113821	-0.141136
32	6	0	-7.833491	-0.091071	-0.163629
33	6	0	-8.354865	-0.243684	1.270724
34	1	0	-8.177047	-0.932997	-0.770654
35	1	0	-8.245710	0.817281	-0.610378
36	1	0	-9.445349	-0.291514	1.287491
37	1	0	-7.963825	-1.155699	1.727056
38	1	0	-8.037703	0.600632	1.886760
39	8	0	-1.379227	-0.933660	-0.162145
40	8	0	-1.517571	1.294174	-0.091980
41	1	0	-0.537677	1.217162	-0.075299
42	1	0	1.728233	1.886102	0.079384
43	6	0	-2.048387	0.080402	-0.138040

AB-trans: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.821321	1.100472	0.235063
2	6	0	4.441953	1.218759	0.107766
3	6	0	3.606774	0.097487	0.126614
4	6	0	4.212933	-1.155488	0.282362
5	6	0	5.589748	-1.278689	0.408794
6	6	0	6.415273	-0.152261	0.387231
7	1	0	6.445932	1.988495	0.221981
8	1	0	4.028490	2.219440	0.000745
9	1	0	3.582003	-2.037284	0.306671
10	1	0	6.036633	-2.260999	0.531891
11	6	0	7.913961	-0.294472	0.472036
12	6	0	8.533387	-0.555071	-0.906232
13	1	0	8.163736	-1.117769	1.146937
14	1	0	8.343505	0.614218	0.902323
15	1	0	9.618483	-0.656980	-0.837005
16	1	0	8.129271	-1.471861	-1.341345
17	1	0	8.307046	0.266074	-1.589992
18	5	0	2.044829	0.173520	-0.006544
19	8	0	1.392285	1.383365	-0.220903
20	8	0	1.323097	-0.954864	0.085858
21	1	0	0.353378	-0.853417	0.002109
22	6	0	-5.531100	-1.141364	-0.626767
23	6	0	-4.153011	-0.995558	-0.572351
24	6	0	-3.591399	0.215110	-0.168838
25	6	0	-4.429828	1.264745	0.204366
26	6	0	-5.809613	1.108256	0.156364
27	6	0	-6.380156	-0.092485	-0.266082
28	1	0	-5.959448	-2.083312	-0.954935
29	1	0	-3.490247	-1.808855	-0.842043
30	1	0	-4.018486	2.200466	0.567332
31	1	0	-6.453834	1.928280	0.456693
32	6	0	-7.876112	-0.278268	-0.271470
33	6	0	-8.367069	-0.914039	1.034642
34	1	0	-8.160842	-0.909916	-1.117228
35	1	0	-8.362970	0.689659	-0.416439
36	1	0	-9.450864	-1.044418	1.023785

37	1	0	-7.905041	-1.892492	1.184009
38	1	0	-8.103649	-0.287718	1.889774
39	8	0	-1.404834	-0.693880	-0.086925
40	1	0	1.994870	2.125971	-0.293410
41	6	0	-2.097616	0.315919	-0.140881
42	7	0	-1.561498	1.554704	-0.171811
43	1	0	-0.547991	1.632506	-0.202829
44	1	0	-2.124680	2.354101	-0.403567

AB-cis: M06-2X/6-311+G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.833628	1.083760	-0.146743
2	6	0	4.449423	1.207408	-0.113203
3	6	0	3.614065	0.086424	-0.148609
4	6	0	4.225256	-1.171775	-0.211811
5	6	0	5.607158	-1.300068	-0.247687
6	6	0	6.432524	-0.173946	-0.216870
7	1	0	6.458877	1.971122	-0.120264
8	1	0	4.032443	2.210421	-0.051046
9	1	0	3.594805	-2.053958	-0.236592
10	1	0	6.057984	-2.286521	-0.304330
11	6	0	7.933258	-0.318754	-0.200051
12	6	0	8.466005	-0.484124	1.228367
13	1	0	8.390994	0.559406	-0.663488
14	1	0	8.221666	-1.185422	-0.801218
15	1	0	9.552619	-0.591974	1.233218
16	1	0	8.202841	0.382793	1.838694
17	1	0	8.030463	-1.367754	1.700092
18	5	0	2.047058	0.170947	-0.126663
19	8	0	1.387158	1.393572	-0.199579
20	8	0	1.329021	-0.960417	-0.043989
21	1	0	0.356363	-0.853023	-0.043966
22	6	0	-5.531493	-1.138503	-0.562836
23	6	0	-4.153388	-0.991737	-0.510122
24	6	0	-3.592124	0.217692	-0.102511
25	6	0	-4.430838	1.264915	0.276895
26	6	0	-5.810531	1.107508	0.230407
27	6	0	-6.380796	-0.091793	-0.196640
28	1	0	-5.959548	-2.079376	-0.894464
29	1	0	-3.490406	-1.803197	-0.784786
30	1	0	-4.019633	2.199461	0.643048
31	1	0	-6.454999	1.925738	0.535105
32	6	0	-7.876686	-0.278096	-0.201337
33	6	0	-8.366839	-0.914880	1.104567
34	1	0	-8.161646	-0.909226	-1.047394
35	1	0	-8.363894	0.689801	-0.345414
36	1	0	-9.450604	-1.045567	1.094107
37	1	0	-7.904428	-1.893291	1.253032
38	1	0	-8.103239	-0.289056	1.960012
39	8	0	-1.403694	-0.688278	-0.032461
40	1	0	1.986584	2.135485	-0.300486
41	6	0	-2.098374	0.320595	-0.079538
42	7	0	-1.564609	1.560355	-0.108598
43	1	0	-0.551343	1.640374	-0.141800
44	1	0	-2.130292	2.359777	-0.333990

BB-trans: M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.783232	1.239883	-0.215740
2	6	0	4.394564	1.222315	-0.153349
3	6	0	3.678237	0.022154	-0.186723
4	6	0	4.411655	-1.167238	-0.281512
5	6	0	5.798009	-1.153727	-0.346282
6	6	0	6.504747	0.050503	-0.314752
7	1	0	6.315781	2.185403	-0.188630
8	1	0	3.878946	2.176441	-0.071408
9	1	0	3.874759	-2.109114	-0.307968
10	1	0	6.345704	-2.088151	-0.425135
11	6	0	8.012425	0.056185	-0.329030
12	6	0	8.588241	-0.162798	1.075301
13	1	0	8.371086	1.008026	-0.729592
14	1	0	8.372902	-0.729249	-0.999107
15	1	0	9.679880	-0.161245	1.057129
16	1	0	8.253554	0.624581	1.754302
17	1	0	8.252348	-1.118838	1.483128
18	5	0	2.116505	-0.048458	-0.123941
19	8	0	1.323550	1.089514	-0.132334
20	8	0	1.506824	-1.250279	-0.061892
21	1	0	0.537188	-1.203490	-0.031085
22	1	0	1.817118	1.908121	-0.213292
23	6	0	-5.779240	-1.219483	0.266200
24	6	0	-4.392954	-1.204683	0.170297
25	6	0	-3.675396	-0.004315	0.159568
26	6	0	-4.405883	1.187169	0.243827
27	6	0	-5.790902	1.176565	0.340866
28	6	0	-6.498158	-0.027101	0.354843
29	1	0	-6.312834	-2.164882	0.275374
30	1	0	-3.879494	-2.161005	0.101336
31	1	0	-3.868204	2.128909	0.237028
32	1	0	-6.336012	2.113090	0.410867
33	6	0	-8.005007	-0.036502	0.407499
34	6	0	-8.617858	0.016298	-0.996989
35	1	0	-9.708687	0.014421	-0.949279
36	1	0	-8.298098	0.918999	-1.522208
37	1	0	-8.298290	-0.844442	-1.588812
38	5	0	-2.115165	0.064335	0.064858
39	8	0	-1.323073	-1.074227	0.056192
40	8	0	-1.505605	1.265657	-0.007470
41	1	0	-0.536493	1.218273	-0.051374
42	1	0	-1.815806	-1.893211	0.138044
43	1	0	-8.353224	0.819137	0.992384
44	1	0	-8.346666	-0.937824	0.923599

BC-trans: M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.676854	1.208420	0.220654
2	6	0	4.289319	1.202719	0.133103
3	6	0	3.561573	0.009386	0.165624
4	6	0	4.282227	-1.185600	0.284762
5	6	0	5.667123	-1.183777	0.375409
6	6	0	6.385397	0.013673	0.345246
7	1	0	6.218561	2.148737	0.193072
8	1	0	3.785058	2.161058	0.029540
9	1	0	3.735716	-2.121951	0.309523
10	1	0	6.204392	-2.122363	0.473661
11	6	0	7.892540	0.006013	0.386816
12	6	0	8.491388	-0.225341	-1.005886
13	1	0	8.233776	-0.779380	1.066918
14	1	0	8.252675	0.956594	0.789094
15	1	0	9.582518	-0.233946	-0.968011
16	1	0	8.153755	-1.180210	-1.414967
17	1	0	8.176364	0.561789	-1.694515
18	5	0	2.000585	-0.055399	0.078734
19	8	0	1.220045	1.100154	0.092600
20	8	0	1.385722	-1.247006	-0.005796
21	1	0	0.413300	-1.199852	-0.043631
22	1	0	1.731088	1.905358	0.198686
23	6	0	-5.569054	-1.210024	-0.334279
24	6	0	-4.185628	-1.159714	-0.264195
25	6	0	-3.538534	0.073079	-0.186372
26	6	0	-4.284015	1.251303	-0.180003
27	6	0	-5.669266	1.189665	-0.250237
28	6	0	-6.329949	-0.037636	-0.328271
29	1	0	-6.071553	-2.169824	-0.399197
30	1	0	-3.588697	-2.063792	-0.271649
31	1	0	-3.774443	2.204887	-0.122380
32	1	0	-6.249509	2.106687	-0.248033
33	6	0	-7.835560	-0.103427	-0.348289
34	6	0	-8.406438	-0.262732	1.066438
35	1	0	-8.154595	-0.944450	-0.969724
36	1	0	-8.235223	0.805062	-0.806029
37	1	0	-9.496696	-0.313755	1.044698
38	1	0	-8.028790	-1.175250	1.532850
39	1	0	-8.113531	0.580295	1.696060
40	8	0	-1.382403	-0.922913	-0.116631
41	8	0	-1.530757	1.304134	-0.044120
42	1	0	-0.552407	1.230647	0.001466
43	6	0	-2.055566	0.088277	-0.113775

AB-trans: M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.834341	1.097431	0.221773
2	6	0	4.454329	1.218896	0.105914
3	6	0	3.616230	0.100077	0.137586
4	6	0	4.220451	-1.153995	0.291833
5	6	0	5.597993	-1.280367	0.407239
6	6	0	6.426192	-0.156254	0.374613
7	1	0	6.461259	1.983636	0.199116
8	1	0	4.043220	2.220265	-0.003738
9	1	0	3.587473	-2.034059	0.324172
10	1	0	6.043322	-2.263379	0.530282
11	6	0	7.925167	-0.301629	0.448052
12	6	0	8.533867	-0.560759	-0.935282
13	1	0	8.178289	-1.126707	1.119490
14	1	0	8.359642	0.605403	0.876906
15	1	0	9.619257	-0.664645	-0.874317
16	1	0	8.124960	-1.476063	-1.369039
17	1	0	8.303896	0.262011	-1.615870
18	5	0	2.053052	0.180970	0.022643
19	8	0	1.399935	1.395508	-0.155319
20	8	0	1.331167	-0.948825	0.099329
21	1	0	0.361268	-0.844766	0.029746
22	1	0	2.004159	2.137856	-0.214761
23	6	0	-5.535484	-1.150076	-0.620734
24	6	0	-4.157891	-1.001205	-0.562226
25	6	0	-3.600034	0.215595	-0.172139
26	6	0	-4.441944	1.268386	0.184036
27	6	0	-5.821250	1.108834	0.132289
28	6	0	-6.387937	-0.098302	-0.276741
29	1	0	-5.960832	-2.096957	-0.938407
30	1	0	-3.492846	-1.817035	-0.818402
31	1	0	-4.033745	2.209228	0.537121
32	1	0	-6.468022	1.931429	0.419787
33	6	0	-7.883489	-0.287322	-0.285112
34	6	0	-8.376814	-0.913647	1.024705
35	1	0	-8.164445	-0.926431	-1.126521
36	1	0	-8.372005	0.678323	-0.439273
37	1	0	-9.460335	-1.046075	1.012017
38	1	0	-7.913416	-1.890060	1.182888
39	1	0	-8.116729	-0.280163	1.875550
40	8	0	-1.411640	-0.687211	-0.059617
41	6	0	-2.106495	0.319337	-0.135784
42	7	0	-1.573274	1.558986	-0.185807
43	1	0	-0.560217	1.640682	-0.200624
44	1	0	-2.135579	2.353983	-0.433960

CC-trans: M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.513728	1.204026	-0.286279
2	6	0	4.128677	1.243820	-0.208475

3	6	0	3.403416	0.052889	-0.183526
4	6	0	4.070519	-1.170103	-0.236322
5	6	0	5.454725	-1.198565	-0.313426
6	6	0	6.194910	-0.013781	-0.340115
7	1	0	6.078368	2.130497	-0.309390
8	1	0	3.601720	2.188876	-0.170222
9	1	0	3.489540	-2.084302	-0.219755
10	1	0	5.973409	-2.150747	-0.358359
11	6	0	7.701410	-0.049937	-0.370271
12	6	0	8.289231	-0.077077	1.045925
13	1	0	8.076308	0.825545	-0.906932
14	1	0	8.033250	-0.932580	-0.923347
15	1	0	9.380152	-0.103704	1.015571
16	1	0	7.982447	0.808254	1.607253
17	1	0	7.938927	-0.956097	1.591400
18	8	0	1.268478	-0.979612	-0.088007
19	8	0	1.380318	1.251538	-0.052550
20	1	0	0.391691	1.173354	-0.000414
21	6	0	1.921179	0.053432	-0.104045
22	6	0	-5.454710	1.198547	0.313600
23	6	0	-4.070513	1.170104	0.236332
24	6	0	-3.403405	-0.052880	0.183415
25	6	0	-4.128650	-1.243820	0.208402
26	6	0	-5.513691	-1.204043	0.286369
27	6	0	-6.194880	0.013755	0.340329
28	1	0	-5.973400	2.150723	0.358626
29	1	0	-3.489545	2.084309	0.219730
30	1	0	-3.601686	-2.188869	0.170053
31	1	0	-6.078319	-2.130521	0.309511
32	6	0	-7.701377	0.049895	0.370655
33	6	0	-8.289357	0.077082	-1.045474
34	1	0	-8.033163	0.932513	0.923801
35	1	0	-8.076206	-0.825611	0.907326
36	1	0	-9.380275	0.103696	-1.014997
37	1	0	-7.939123	0.956126	-1.590955
38	1	0	-7.982627	-0.808225	-1.606869
39	8	0	-1.268483	0.979634	0.087622
40	8	0	-1.380311	-1.251506	0.052069
41	1	0	-0.391693	-1.173281	-0.000273
42	6	0	-1.921179	-0.053411	0.103768

AC-trans: M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.443184	-1.276589	0.414557
2	6	0	4.062620	-1.185773	0.304096
3	6	0	3.460317	0.062194	0.148375
4	6	0	4.248211	1.211103	0.104702
5	6	0	5.627370	1.110308	0.215782
6	6	0	6.244012	-0.133195	0.372608
7	1	0	5.910198	-2.248484	0.539909
8	1	0	3.443716	-2.073336	0.340519
9	1	0	3.762604	2.172411	-0.013228
10	1	0	6.238317	2.006948	0.185628
11	6	0	7.745808	-0.245463	0.437223
12	6	0	8.351187	-0.458133	-0.955882
13	1	0	8.021732	-1.079345	1.088164
14	1	0	8.160815	0.662067	0.883477
15	1	0	9.438884	-0.537340	-0.902761
16	1	0	7.961298	-1.372697	-1.408115
17	1	0	8.097954	0.374666	-1.615570
18	8	0	1.436044	1.282666	-0.097973
19	6	0	1.981878	0.201786	0.033449
20	8	0	1.334199	-0.943731	0.088206
21	1	0	0.349436	-0.799018	0.018814
22	6	0	-5.406256	-1.131686	-0.621829
23	6	0	-4.028796	-0.982117	-0.564149
24	6	0	-3.471324	0.237230	-0.181218
25	6	0	-4.313465	1.291882	0.168808
26	6	0	-5.692561	1.131478	0.118163
27	6	0	-6.258939	-0.078354	-0.283417
28	1	0	-5.831307	-2.080477	-0.934068
29	1	0	-3.364175	-1.799474	-0.816029
30	1	0	-3.906343	2.235402	0.515856
31	1	0	-6.339389	1.955595	0.400914
32	6	0	-7.754272	-0.268719	-0.289688
33	6	0	-8.245207	-0.893017	1.022029
34	1	0	-8.035512	-0.909842	-1.129467
35	1	0	-8.243917	0.696085	-0.445183
36	1	0	-9.328577	-1.026601	1.010860
37	1	0	-7.780680	-1.868682	1.181585
38	1	0	-7.984836	-0.257577	1.871311
39	8	0	-1.290558	-0.675097	-0.061296
40	6	0	-1.979328	0.343185	-0.143055
41	7	0	-1.438866	1.571080	-0.200929
42	1	0	-0.421320	1.648228	-0.188247
43	1	0	-2.000955	2.376499	-0.412683

AA-trans: M06-2X/6-311+G(d,p), BSSE-optimized:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.686711	-1.239377	-0.073135
2	6	0	-4.300285	-1.268058	0.013814
3	6	0	-3.561315	-0.097918	-0.156243
4	6	0	-4.231854	1.100250	-0.395838
5	6	0	-5.615824	1.120310	-0.491700
6	6	0	-6.364043	-0.048024	-0.334151
7	1	0	-6.252389	-2.154796	0.068587
8	1	0	-3.805351	-2.204690	0.245687
9	1	0	-3.647940	2.005985	-0.506669
10	1	0	-6.128126	2.056237	-0.691428
11	6	0	-7.870516	-0.011519	-0.378892
12	6	0	-8.466692	0.272165	1.005109
13	1	0	-8.247885	-0.966861	-0.753312

14	1	0	-8.195329	0.758898	-1.083338
15	1	0	-9.557386	0.298607	0.964496
16	1	0	-8.167359	-0.499460	1.717896
17	1	0	-8.112899	1.232660	1.386405
18	8	0	-1.484298	0.991546	0.190240
19	6	0	-2.063734	-0.058222	-0.072368
20	7	0	-1.405858	-1.212004	-0.294927
21	1	0	-1.884449	-2.013704	-0.666235
22	1	0	-0.383155	-1.207196	-0.273867
23	6	0	5.615612	-1.120420	0.491745
24	6	0	4.231666	-1.100202	0.395575
25	6	0	3.561302	0.098063	0.155973
26	6	0	4.300436	1.268147	-0.013775
27	6	0	5.686838	1.239308	0.073479
28	6	0	6.363989	0.047854	0.334505
29	1	0	6.127771	-2.056426	0.691471
30	1	0	3.647632	-2.005889	0.506156
31	1	0	3.805664	2.204861	-0.245661
32	1	0	6.252645	2.154685	-0.068005
33	6	0	7.870447	0.011180	0.379576
34	6	0	8.466894	-0.272523	-1.004306
35	1	0	8.195018	-0.759301	1.084064
36	1	0	8.247844	0.966465	0.754113
37	1	0	9.557576	-0.299101	-0.963453
38	1	0	8.113067	-1.232961	-1.385714
39	1	0	8.167812	0.499166	-1.717127
40	8	0	1.484286	-0.991238	-0.190969
41	6	0	2.063736	0.058501	0.071728
42	7	0	1.405867	1.212272	0.294371
43	1	0	0.383166	1.207495	0.273193
44	1	0	1.884427	2.013892	0.665887

BB-trans: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.778549	1.190664	-0.082403
2	6	0	-4.389119	1.155972	-0.192334
3	6	0	-3.658571	-0.000752	0.127228
4	6	0	-4.378833	-1.125099	0.564781
5	6	0	-5.766621	-1.089862	0.683081
6	6	0	-6.487014	0.070590	0.369141
7	1	0	-6.319732	2.095347	-0.338548
8	1	0	-3.878242	2.040045	-0.563114
9	1	0	-3.838648	-2.031356	0.809861
10	1	0	-6.301075	-1.966745	1.033268
11	6	0	-7.991446	0.085273	0.435696
12	6	0	-8.621502	-0.387723	-0.876241
13	1	0	-8.336808	1.095862	0.664603
14	1	0	-8.325883	-0.555646	1.254395
15	1	0	-9.709875	-0.374409	-0.819077
16	1	0	-8.313083	0.255116	-1.700046
17	1	0	-8.302283	-1.403373	-1.107500
18	5	0	-2.097249	-0.061184	0.021567
19	8	0	-1.325995	1.103952	0.052543
20	8	0	-1.475310	-1.259494	-0.093343
21	1	0	-0.503174	-1.181198	-0.110940
22	6	0	5.755048	-1.058129	-0.685931
23	6	0	4.361580	-1.022313	-0.657499
24	6	0	3.667777	0.117759	-0.218543
25	6	0	4.429168	1.228621	0.182296
26	6	0	5.821797	1.192138	0.162162
27	6	0	6.506035	0.050219	-0.276048
28	1	0	6.266893	-1.945837	-1.042158
29	1	0	3.815338	-1.891177	-1.013516
30	1	0	3.916862	2.125295	0.508906
31	1	0	6.389283	2.061996	0.475987
32	6	0	8.010412	-0.007708	-0.241274
33	6	0	8.527319	-0.508365	1.109272
34	1	0	9.616468	-0.546552	1.126001
35	1	0	8.194716	0.149164	1.911801
36	1	0	8.145771	-1.507746	1.316135
37	5	0	2.103615	0.180008	-0.173676
38	8	0	1.336583	-0.986952	-0.116462
39	8	0	1.475898	1.380761	-0.180166
40	1	0	0.506317	1.301410	-0.108697
41	1	0	1.886339	-1.771241	-0.014958
42	1	0	-1.861912	1.882398	0.238165
43	1	0	8.417866	0.985140	-0.443913
44	1	0	8.368744	-0.664460	-1.036997

BB-cis: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.753032	1.232432	0.220681
2	6	0	4.360819	1.171157	0.262917
3	6	0	3.667905	0.008337	-0.113323
4	6	0	4.428931	-1.094288	-0.536920
5	6	0	5.819900	-1.032334	-0.587574
6	6	0	6.502871	0.134138	-0.217361
7	1	0	6.264527	2.141232	0.519677
8	1	0	3.816526	2.038605	0.625318
9	1	0	3.917932	-2.004847	-0.824886
10	1	0	6.386613	-1.892580	-0.928173
11	6	0	8.008233	0.176592	-0.211091
12	6	0	8.583466	-0.310425	1.120750
13	1	0	8.345384	1.197328	-0.404465
14	1	0	8.393252	-0.442448	-1.024381
15	1	0	9.672895	-0.276872	1.116329
16	1	0	8.224168	0.310904	1.940431
17	1	0	8.272385	-1.335797	1.317640
18	5	0	2.104707	-0.081605	-0.084064
19	8	0	1.314329	1.070125	-0.129843
20	8	0	1.500322	-1.292756	-0.022028
21	1	0	0.527197	-1.231931	-0.050118

22	6	0	-5.752973	-1.232474	0.220518
23	6	0	-4.360761	-1.171143	0.262702
24	6	0	-3.667909	-0.008281	-0.113526
25	6	0	-4.428997	1.094326	-0.537054
26	6	0	-5.819965	1.032316	-0.587659
27	6	0	-6.502874	-0.134196	-0.217457
28	1	0	-6.264419	-2.141304	0.519503
29	1	0	-3.816419	-2.038584	0.625049
30	1	0	-3.918048	2.004918	-0.825009
31	1	0	-6.386725	1.892550	-0.928208
32	6	0	-8.008235	-0.176711	-0.211130
33	6	0	-8.583435	0.310227	1.120754
34	1	0	-8.345351	-1.197453	-0.404533
35	1	0	-8.393311	0.442347	-1.024379
36	1	0	-9.672863	0.276629	1.116374
37	1	0	-8.224079	-0.311121	1.940394
38	1	0	-8.272388	1.335604	1.317673
39	5	0	-2.104717	0.081715	-0.084298
40	8	0	-1.314300	-1.069990	-0.130129
41	8	0	-1.500361	1.292878	-0.022220
42	1	0	-0.527231	1.232059	-0.050113
43	1	0	-1.843882	-1.861303	-0.275073
44	1	0	1.843920	1.861423	-0.274828

BC-trans: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.660253	1.214419	0.002362
2	6	0	4.271455	1.167383	-0.110998
3	6	0	3.558594	-0.021125	0.119627
4	6	0	4.295459	-1.164758	0.471101
5	6	0	5.682559	-1.117689	0.592643
6	6	0	6.385388	0.073966	0.368322
7	1	0	6.187895	2.143758	-0.184341
8	1	0	3.747731	2.069218	-0.415508
9	1	0	3.768417	-2.094708	0.645848
10	1	0	6.230167	-2.010585	0.875457
11	6	0	7.889456	0.105858	0.436929
12	6	0	8.525898	-0.259584	-0.905933
13	1	0	8.233493	-0.588890	1.206229
14	1	0	8.219985	1.101722	0.740219
15	1	0	9.613966	-0.234584	-0.847074
16	1	0	8.221548	-1.259913	-1.211876
17	1	0	8.207818	0.437807	-1.680205
18	5	0	1.999038	-0.100217	0.009630
19	8	0	1.215864	1.058736	0.130668
20	8	0	1.389734	-1.288263	-0.193550
21	1	0	0.413715	-1.222578	-0.204151
22	6	0	-5.593649	-1.187580	-0.406812
23	6	0	-4.203445	-1.162783	-0.349266
24	6	0	-3.536869	0.056389	-0.182172
25	6	0	-4.267697	1.246372	-0.082859
26	6	0	-5.658672	1.204591	-0.142212
27	6	0	-6.342424	-0.006571	-0.311603
28	1	0	-6.107896	-2.132838	-0.541057
29	1	0	-3.621299	-2.071064	-0.429591
30	1	0	-3.747966	2.186179	0.040747
31	1	0	-6.224521	2.126909	-0.069886
32	6	0	-7.847557	-0.047343	-0.312941
33	6	0	-8.410351	-0.225644	1.099130
34	1	0	-8.188860	-0.866241	-0.949757
35	1	0	-8.236544	0.875221	-0.749041
36	1	0	-9.499728	-0.254189	1.088003
37	1	0	-8.047265	-1.153466	1.539903
38	1	0	-8.095081	0.595799	1.741654
39	8	0	-1.390262	-0.989631	-0.218454
40	8	0	-1.516874	1.260728	0.028163
41	1	0	-0.534226	1.167638	0.057208
42	1	0	1.745469	1.823207	0.381709
43	6	0	-2.053347	0.045786	-0.128192

BC-cis: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.674528	-1.086088	-0.480949
2	6	0	-4.281137	-1.056639	-0.519011
3	6	0	-3.565823	0.115096	-0.220249
4	6	0	-4.305491	1.263616	0.108687
5	6	0	-5.697613	1.234159	0.154753
6	6	0	-6.403530	0.060562	-0.143056
7	1	0	-6.204086	-1.999761	-0.729285
8	1	0	-3.753926	-1.958324	-0.817881
9	1	0	-3.776338	2.183337	0.325990
10	1	0	-6.248306	2.133219	0.410742
11	6	0	-7.904882	0.015935	-0.035190
12	6	0	-8.360849	-0.350188	1.378985
13	1	0	-8.300437	-0.711378	-0.747548
14	1	0	-8.318918	0.987557	-0.313226
15	1	0	-9.448181	-0.379503	1.448361
16	1	0	-7.972471	-1.327750	1.663052
17	1	0	-7.990675	0.378751	2.099137
18	5	0	-2.001848	0.174816	-0.250893
19	8	0	-1.241104	-0.997749	-0.118111
20	8	0	-1.367455	1.358365	-0.394703
21	1	0	-0.393088	1.278882	-0.358214
22	6	0	5.615829	1.162047	-0.261908
23	6	0	4.224284	1.155913	-0.274295
24	6	0	3.534134	-0.057093	-0.169741
25	6	0	4.243290	-1.259443	-0.062587
26	6	0	5.635921	-1.236301	-0.051559
27	6	0	6.343232	-0.031496	-0.157738
28	1	0	6.148594	2.102669	-0.347794
29	1	0	3.658938	2.074087	-0.361831
30	1	0	3.705653	-2.194294	0.012504

31	1	0	6.185208	-2.168089	0.026813
32	6	0	7.846948	-0.012343	-0.083143
33	6	0	8.340555	0.125194	1.359046
34	1	0	8.230525	0.816052	-0.682514
35	1	0	8.245092	-0.930087	-0.521146
36	1	0	9.429403	0.138324	1.402870
37	1	0	7.968115	1.047715	1.803130
38	1	0	7.982654	-0.706251	1.965354
39	8	0	1.406043	1.020231	-0.287991
40	8	0	1.490413	-1.236820	-0.089111
41	1	0	0.508867	-1.130287	-0.106920
42	1	0	-1.792866	-1.760254	0.086993
43	6	0	2.050045	-0.026416	-0.189512

AB-trans: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.816625	1.066862	-0.386817
2	6	0	-4.425962	1.166040	-0.358695
3	6	0	-3.611947	0.027738	-0.235052
4	6	0	-4.251044	-1.220800	-0.152015
5	6	0	-5.640548	-1.322434	-0.171823
6	6	0	-6.444601	-0.180945	-0.293546
7	1	0	-6.421880	1.960552	-0.497300
8	1	0	-3.976588	2.149349	-0.466885
9	1	0	-3.643941	-2.114446	-0.075106
10	1	0	-6.111672	-2.297736	-0.106855
11	6	0	-7.946287	-0.288058	-0.255571
12	6	0	-8.483603	-0.224595	1.175841
13	1	0	-8.256488	-1.225981	-0.721399
14	1	0	-8.384926	0.518404	-0.847424
15	1	0	-9.570617	-0.303604	1.194488
16	1	0	-8.070289	-1.036203	1.773751
17	1	0	-8.199775	0.715805	1.647335
18	5	0	-2.044775	0.112454	-0.196406
19	8	0	-1.409335	1.299592	0.187662
20	8	0	-1.311472	-0.972043	-0.525439
21	1	0	-0.340306	-0.854243	-0.441116
22	6	0	5.529207	-1.174908	0.608108
23	6	0	4.148490	-1.053965	0.480732
24	6	0	3.584344	0.176721	0.126492
25	6	0	4.418655	1.274921	-0.117485
26	6	0	5.800778	1.138763	0.004690
27	6	0	6.376223	-0.080640	0.382336
28	1	0	5.959412	-2.127732	0.896723
29	1	0	3.492772	-1.898611	0.646018
30	1	0	3.997995	2.218854	-0.442721
31	1	0	6.442255	1.990642	-0.192929
32	6	0	7.872102	-0.236894	0.457313
33	6	0	8.462049	-0.693531	-0.878948
34	1	0	8.123235	-0.960879	1.235415
35	1	0	8.323428	0.712791	0.752424
36	1	0	9.544304	-0.804053	-0.814248
37	1	0	8.036437	-1.651262	-1.176341
38	1	0	8.236994	0.029829	-1.661920
39	8	0	1.431902	-0.745513	-0.302715
40	1	0	-2.053672	1.947869	0.490961
41	6	0	2.098223	0.257815	0.005376
42	7	0	1.541109	1.471495	0.233374
43	1	0	0.527501	1.536640	0.235270
44	1	0	2.076457	2.182441	0.698592

AB-cis: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.818925	1.115377	-0.009039
2	6	0	4.428403	1.204604	0.046142
3	6	0	3.613987	0.071003	-0.112956
4	6	0	4.252829	-1.161185	-0.331539
5	6	0	5.641760	-1.252051	-0.395414
6	6	0	6.445897	-0.114267	-0.243312
7	1	0	6.425039	2.005887	0.120853
8	1	0	3.981258	2.173977	0.248436
9	1	0	3.646331	-2.051015	-0.447583
10	1	0	6.112352	-2.213006	-0.575764
11	6	0	7.947815	-0.225975	-0.247238
12	6	0	8.497742	-0.529255	1.148232
13	1	0	8.382358	0.705199	-0.617712
14	1	0	8.252582	-1.013818	-0.939661
15	1	0	9.584805	-0.609011	1.136333
16	1	0	8.218842	0.259205	1.846520
17	1	0	8.088732	-1.466942	1.522869
18	5	0	2.046520	0.145222	-0.065269
19	8	0	1.386197	1.351415	-0.329001
20	8	0	1.336630	-0.966356	0.222187
21	1	0	0.361834	-0.851188	0.196585
22	6	0	-5.551347	-1.149503	-0.576248
23	6	0	-4.166634	-1.025473	-0.509749
24	6	0	-3.591999	0.182277	-0.098102
25	6	0	-4.418853	1.253125	0.264180
26	6	0	-5.804621	1.113538	0.201866
27	6	0	-6.391786	-0.081422	-0.231736
28	1	0	-5.990414	-2.083496	-0.909605
29	1	0	-3.515549	-1.850529	-0.766822
30	1	0	-3.987386	2.175604	0.633788
31	1	0	-6.439910	1.943653	0.490934
32	6	0	-7.888678	-0.245389	-0.242777
33	6	0	-8.407995	-0.800100	1.085665
34	1	0	-8.174829	-0.915097	-1.056579
35	1	0	-8.359437	0.718619	-0.447133
36	1	0	-9.491523	-0.915472	1.067445
37	1	0	-7.962759	-1.772526	1.293009
38	1	0	-8.147635	-0.131593	1.905578
39	8	0	-1.415697	-0.748478	0.157087

40	1	0	2.010566	2.025216	-0.618087
41	6	0	-2.102120	0.267975	-0.045868
42	7	0	-1.563856	1.499631	-0.215252
43	1	0	-0.552007	1.573951	-0.263029
44	1	0	-2.125846	2.236518	-0.602090

CC-trans: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.519057	-1.205450	0.288405
2	6	0	4.128915	-1.239837	0.211911
3	6	0	3.410182	-0.038775	0.180110
4	6	0	4.087148	1.184870	0.234869
5	6	0	5.476585	1.201895	0.311233
6	6	0	6.213501	0.010210	0.346488
7	1	0	6.075651	-2.135692	0.317619
8	1	0	3.599680	-2.181767	0.174498
9	1	0	3.514546	2.102432	0.214577
10	1	0	5.999346	2.150833	0.358132
11	6	0	7.718791	0.036340	0.367124
12	6	0	8.303914	0.059319	-1.046966
13	1	0	8.090887	-0.838912	0.903844
14	1	0	8.060026	0.914430	0.919503
15	1	0	9.393255	0.078365	-1.021838
16	1	0	7.988839	-0.822200	-1.604304
17	1	0	7.957702	0.938970	-1.588564
18	8	0	1.280804	1.029504	0.080667
19	8	0	1.380515	-1.234823	0.057839
20	1	0	0.388897	-1.142132	0.006402
21	6	0	-5.476557	-1.201924	-0.311203
22	6	0	-4.087117	-1.184863	-0.234898
23	6	0	-3.410187	0.038802	-0.180168
24	6	0	-4.128951	1.239847	-0.211933
25	6	0	-5.519095	1.205422	-0.288370
26	6	0	-6.213507	-0.010257	-0.346427
27	1	0	-5.999293	-2.150874	-0.358083
28	1	0	-3.514487	-2.102408	-0.214631
29	1	0	-3.599738	2.181790	-0.174541
30	1	0	-6.075716	2.135649	-0.317560
31	6	0	-7.718797	-0.036430	-0.367000
32	6	0	-8.303860	-0.059429	1.047114
33	1	0	-8.060030	-0.914528	-0.919367
34	1	0	-8.090940	0.838812	-0.903703
35	1	0	-9.393202	-0.078505	1.022031
36	1	0	-7.957601	-0.939071	1.588696
37	1	0	-7.988786	0.822098	1.604442
38	8	0	-1.280770	-1.029399	-0.080768
39	8	0	-1.380566	1.234918	-0.057939
40	1	0	-0.388956	1.142201	-0.006496
41	6	0	1.928571	-0.026081	0.102310
42	6	0	-1.928584	0.026157	-0.102439

CC-cis: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.527805	1.202788	-0.177774
2	6	0	-4.135549	1.238110	-0.175341
3	6	0	-3.415406	0.037524	-0.167775
4	6	0	-4.093503	-1.186724	-0.171915
5	6	0	-5.485030	-1.204659	-0.174445
6	6	0	-6.223560	-0.013467	-0.184530
7	1	0	-6.085768	2.132607	-0.188126
8	1	0	-3.605711	2.180435	-0.177249
9	1	0	-3.520039	-2.103961	-0.171351
10	1	0	-6.008939	-2.154095	-0.182176
11	6	0	-7.727845	-0.040094	-0.125341
12	6	0	-8.237585	-0.051958	1.317737
13	1	0	-8.097182	-0.922616	-0.651997
14	1	0	-8.128272	0.830766	-0.648632
15	1	0	-9.326725	-0.071301	1.350204
16	1	0	-7.862901	-0.927253	1.847306
17	1	0	-7.894021	0.833978	1.850698
18	8	0	-1.282978	-1.029467	-0.168686
19	8	0	-1.382796	1.234963	-0.167665
20	1	0	-0.389900	1.142657	-0.167837
21	6	0	5.485100	1.205319	-0.173437
22	6	0	4.093562	1.187384	-0.170997
23	6	0	3.415461	-0.036855	-0.167991
24	6	0	4.135599	-1.237447	-0.176804
25	6	0	5.527842	-1.202130	-0.179114
26	6	0	6.223611	0.014140	-0.184651
27	1	0	6.009023	2.154748	-0.180335
28	1	0	3.520102	2.104622	-0.169524
29	1	0	3.605747	-2.179763	-0.179679
30	1	0	6.085805	-2.131941	-0.190523
31	6	0	7.727874	0.040529	-0.125126
32	6	0	8.237177	0.046898	1.318164
33	1	0	8.097357	0.925049	-0.648301
34	1	0	8.128457	-0.828343	-0.651600
35	1	0	9.326305	0.066210	1.351083
36	1	0	7.862206	0.920136	1.850913
37	1	0	7.893507	-0.841099	1.847616
38	8	0	1.283041	1.030155	-0.167728
39	8	0	1.382859	-1.234284	-0.168720
40	1	0	0.389965	-1.141997	-0.168767
41	6	0	-1.931723	0.025742	-0.168602
42	6	0	1.931777	-0.025059	-0.168615

AC-trans: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.470409	-1.248670	-0.462853
2	6	0	-4.080941	-1.163047	-0.413018
3	6	0	-3.472282	0.077837	-0.190627
4	6	0	-4.260606	1.222653	-0.029762
5	6	0	-5.647816	1.121494	-0.082098
6	6	0	-6.274367	-0.111920	-0.306084
7	1	0	-5.940674	-2.209838	-0.639929
8	1	0	-3.466801	-2.043251	-0.542183
9	1	0	-3.772377	2.173787	0.135444
10	1	0	-6.255900	2.011492	0.038305
11	6	0	-7.775898	-0.225393	-0.300186
12	6	0	-8.318869	-0.490122	1.105986
13	1	0	-8.082982	-1.032014	-0.969387
14	1	0	-8.212301	0.695022	-0.694181
15	1	0	-9.405802	-0.570650	1.100495
16	1	0	-7.907984	-1.417101	1.504600
17	1	0	-8.037935	0.317568	1.781087
18	8	0	-1.444655	1.312859	0.056128
19	6	0	5.410447	-1.124404	0.705876
20	6	0	4.029143	-1.002630	0.585758
21	6	0	3.471248	0.194229	0.122482
22	6	0	4.311227	1.255744	-0.236861
23	6	0	5.693542	1.118054	-0.120413
24	6	0	6.263586	-0.065361	0.364841
25	1	0	5.836403	-2.049249	1.079248
26	1	0	3.368905	-1.820825	0.841155
27	1	0	3.894440	2.168603	-0.645272
28	1	0	6.339421	1.940712	-0.407126
29	6	0	7.758952	-0.228333	0.434912
30	6	0	8.326786	-0.812182	-0.860800
31	1	0	8.014489	-0.879608	1.273452
32	1	0	8.222072	0.740217	0.635050
33	1	0	9.408824	-0.926631	-0.799838
34	1	0	7.889188	-1.789194	-1.062820
35	1	0	8.097341	-0.162148	-1.704456
36	8	0	1.309335	-0.745621	-0.195377
37	6	0	-1.992086	0.221798	-0.132147
38	6	0	1.986148	0.282084	0.014529
39	7	0	1.436252	1.505912	0.144270
40	1	0	0.419286	1.576445	0.125593
41	1	0	1.983783	2.267682	0.502247
42	8	0	-1.344210	-0.927643	-0.299025
43	1	0	-0.355744	-0.780143	-0.252389

CC-cis: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.470854	-1.321218	-0.097590
2	6	0	4.081591	-1.225107	-0.063944
3	6	0	3.473239	0.032556	-0.152952
4	6	0	4.261626	1.181082	-0.284303
5	6	0	5.648640	1.069296	-0.316537
6	6	0	6.274863	-0.181534	-0.231125
7	1	0	5.940867	-2.296552	-0.033043
8	1	0	3.467397	-2.109462	0.032459
9	1	0	3.773633	2.143845	-0.356892
10	1	0	6.256760	1.961055	-0.422905
11	6	0	7.776466	-0.290948	-0.204122
12	6	0	8.325785	-0.201370	1.221516
13	1	0	8.210638	0.503765	-0.814676
14	1	0	8.081004	-1.237774	-0.655297
15	1	0	9.412727	-0.281360	1.231210
16	1	0	8.047366	0.747897	1.678036
17	1	0	7.917185	-1.001324	1.838054
18	8	0	1.446057	1.291398	-0.210267
19	6	0	-5.453336	-1.064175	-0.662041
20	6	0	-4.066726	-0.957357	-0.605798
21	6	0	-3.475896	0.203787	-0.094908
22	6	0	-4.287504	1.243588	0.375846
23	6	0	-5.675068	1.120656	0.322270
24	6	0	-6.279046	-0.025575	-0.209012
25	1	0	-5.905536	-1.960435	-1.072427
26	1	0	-3.427268	-1.760284	-0.947829
27	1	0	-3.842763	2.125650	0.820812
28	1	0	-6.298546	1.925926	0.695024
29	6	0	-7.777341	-0.176214	-0.212184
30	6	0	-8.282858	-0.840933	1.070308
31	1	0	-8.080919	-0.769849	-1.077080
32	1	0	-8.242044	0.805648	-0.324532
33	1	0	-9.367513	-0.945794	1.058016
34	1	0	-7.843617	-1.831237	1.185297
35	1	0	-8.005085	-0.248744	1.941570
36	8	0	-1.308417	-0.765547	0.048743
37	6	0	1.993249	0.187390	-0.124897
38	6	0	-1.986533	0.277042	-0.058390
39	7	0	-1.433870	1.504027	-0.136228
40	1	0	-0.416734	1.568168	-0.165678
41	1	0	-1.992669	2.290262	-0.415182
42	8	0	1.345259	-0.967268	0.000291
43	1	0	0.356992	-0.812048	0.015708

AA-trans: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.669857	-1.245286	-0.025545
2	6	0	-4.279032	-1.252962	0.072605
3	6	0	-3.556465	-0.071040	-0.133243
4	6	0	-4.242485	1.113519	-0.423599
5	6	0	-5.630546	1.107424	-0.528088
6	6	0	-6.365575	-0.071579	-0.340251
7	1	0	-6.223609	-2.162791	0.141660
8	1	0	-3.764237	-2.165878	0.347047
9	1	0	-3.672922	2.023352	-0.559755
10	1	0	-6.154563	2.026189	-0.768491

11	6	0	-7.870683	-0.056845	-0.389192
12	6	0	-8.479513	0.278452	0.974217
13	1	0	-8.234086	-1.030936	-0.723603
14	1	0	-8.203211	0.674686	-1.128835
15	1	0	-9.568404	0.287083	0.928500
16	1	0	-8.172971	-0.455256	1.718984
17	1	0	-8.142387	1.257940	1.311659
18	8	0	-1.496883	1.034032	0.325189
19	6	0	5.630513	-1.107450	0.528095
20	6	0	4.242456	-1.113528	0.423542
21	6	0	3.556462	0.071047	0.133194
22	6	0	4.279050	1.252969	-0.072582
23	6	0	5.669870	1.245276	0.025632
24	6	0	6.365562	0.071552	0.340330
25	1	0	6.154510	-2.026228	0.768491
26	1	0	3.672878	-2.023360	0.559643
27	1	0	3.764275	2.165899	-0.347015
28	1	0	6.223638	2.162781	-0.141517
29	6	0	7.870668	0.056801	0.389338
30	6	0	8.479556	-0.278459	-0.974053
31	1	0	8.203155	-0.674755	1.128973
32	1	0	8.234065	1.030878	0.723796
33	1	0	9.568446	-0.287102	-0.928287
34	1	0	8.142436	-1.257933	-1.311541
35	1	0	8.173055	0.455275	-1.718811
36	8	0	1.496887	-1.033986	-0.325369
37	6	0	-2.065182	-0.013930	-0.033271
38	6	0	2.065183	0.013956	0.033154
39	7	0	1.400603	1.150458	0.338812
40	1	0	0.378452	1.142843	0.344961
41	1	0	1.881927	1.892106	0.815277
42	7	0	-1.400600	-1.150427	-0.338940
43	1	0	-1.881937	-1.892095	-0.815361
44	1	0	-0.378450	-1.142798	-0.345137

A'C':-cis: MP2/6-31G(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.675209	1.215991	0.100601
2	6	0	4.281394	1.240144	0.128764
3	6	0	3.556073	0.067996	-0.118988
4	6	0	4.241675	-1.123511	-0.380523
5	6	0	5.633189	-1.133808	-0.415053
6	6	0	6.371852	0.035362	-0.184724
7	1	0	6.230726	2.125985	0.299922
8	1	0	3.764354	2.157977	0.381724
9	1	0	3.668829	-2.025717	-0.549654
10	1	0	6.157664	-2.057785	-0.633477
11	6	0	7.877235	0.002563	-0.158085
12	6	0	8.412754	-0.346088	1.232453
13	1	0	8.268586	0.973622	-0.468958
14	1	0	8.237804	-0.729689	-0.883746
15	1	0	9.502389	-0.367747	1.241392
16	1	0	8.077938	0.388018	1.964547
17	1	0	8.047451	-1.322883	1.547643
18	8	0	1.463032	-1.013909	0.229925
19	6	0	-5.641186	1.210577	0.070566
20	6	0	-4.249562	1.201112	0.040162
21	6	0	-3.562299	0.008441	-0.211403
22	6	0	-4.286154	-1.162928	-0.467126
23	6	0	-5.680053	-1.139907	-0.442851
24	6	0	-6.378589	0.043393	-0.173330
25	1	0	-6.167169	2.137688	0.271275
26	1	0	-3.677707	2.104585	0.205829
27	1	0	-3.767738	-2.079468	-0.721924
28	1	0	-6.234442	-2.047033	-0.657661
29	6	0	-7.881660	0.048123	-0.082271
30	6	0	-8.364629	-0.238821	1.341196
31	1	0	-8.290543	-0.699117	-0.765784
32	1	0	-8.262976	1.017577	-0.410078
33	1	0	-9.453042	-0.232429	1.397312
34	1	0	-8.009644	-1.213425	1.674710
35	1	0	-7.981137	0.511165	2.032191
36	8	0	-1.469391	1.091895	-0.559487
37	6	0	2.061161	0.028628	-0.094459
38	6	0	-2.067392	0.048900	-0.236450
39	7	0	-1.432231	-1.096685	0.096571
40	1	0	-0.411666	-1.100990	0.154326
41	1	0	-1.945734	-1.835431	0.542997
42	7	0	1.426201	1.174325	-0.427469
43	1	0	1.939424	1.912059	-0.875894
44	1	0	0.405615	1.178661	-0.484794

B. DIMERS IN SOLVENT: n,n-DiMethylFormamide

A'A': M06-2X/6-311+G(d,p),_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.587764	-0.084223	-0.003189
2	8	0	1.431672	-1.108656	0.004944
3	6	0	2.079578	-0.058098	0.005374
4	7	0	1.486564	1.144442	0.004257
5	1	0	2.032404	1.990298	0.003917
6	1	0	0.466118	1.203476	-0.000963
7	1	0	3.918740	-0.529151	-0.943048
8	1	0	3.928740	-0.726075	0.809191
9	1	0	4.030856	0.904746	0.101699
10	6	0	-3.587764	0.084222	0.003217
11	8	0	-1.431672	1.108656	-0.004973
12	6	0	-2.079579	0.058099	-0.005379
13	7	0	-1.486564	-1.144442	-0.004259
14	1	0	-0.466118	-1.203476	0.000945
15	1	0	-2.032404	-1.990298	-0.003895

16	1	0	-3.928758	0.726082	-0.809150
17	1	0	-3.918720	0.529142	0.943088
18	1	0	-4.030857	-0.904746	-0.101670

A'B': M06-2X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.680648	-0.068401	0.007840
2	5	0	-2.108679	-0.067208	-0.007404
3	8	0	-1.391490	1.119797	-0.004334
4	8	0	-1.404016	-1.223396	-0.010831
5	1	0	-0.429555	-1.101848	-0.005535
6	1	0	-1.949677	1.902419	-0.003941
7	1	0	-4.046881	0.304055	0.970172
8	1	0	-4.092037	-1.066842	-0.142867
9	1	0	-4.089689	0.595419	-0.758896
10	6	0	3.550452	-0.214541	0.003724
11	8	0	1.313521	-1.041101	0.003246
12	6	0	2.053016	-0.051101	0.001622
13	7	0	1.568232	1.196849	-0.001754
14	1	0	0.560869	1.337084	-0.002790
15	1	0	2.181299	1.995096	-0.003295
16	1	0	3.833289	-0.789708	0.886119
17	1	0	4.081648	0.735657	0.003467
18	1	0	3.835467	-0.791374	-0.876897

A'C':: M06-2X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.497838	-0.046506	0.000436
2	8	0	1.402078	1.126253	-0.000542
3	6	0	2.001805	0.066950	-0.000504
4	8	0	1.394108	-1.105014	-0.000148
5	1	0	0.395538	-0.992544	-0.000448
6	1	0	3.817171	-0.603921	-0.881428
7	1	0	3.816185	-0.607831	0.880158
8	1	0	3.947984	0.942248	0.002794
9	6	0	-3.469820	-0.259682	0.001623
10	8	0	-1.210589	-1.012664	-0.000808
11	6	0	-1.981693	-0.041061	-0.000025
12	7	0	-1.535380	1.216678	-0.000503
13	1	0	-0.530998	1.383465	-0.001293
14	1	0	-2.173027	1.995585	0.000346
15	1	0	-3.733120	-0.846464	-0.879137
16	1	0	-4.034270	0.670964	0.001481
17	1	0	-3.731363	-0.845061	0.883849

B'B':: M06-2X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.678002	0.047964	0.003444
2	5	0	-2.112816	-0.065038	-0.006590
3	8	0	-1.303844	1.061798	-0.005993
4	8	0	-1.491974	-1.270443	-0.005359
5	1	0	-0.519959	-1.205279	-0.000863
6	1	0	-1.792237	1.890122	-0.009179
7	1	0	-4.019719	0.470857	0.953583
8	1	0	-4.157863	-0.922581	-0.124782
9	1	0	-4.034818	0.718547	-0.783169
10	6	0	3.677998	-0.047992	-0.001989
11	5	0	2.112800	0.065043	0.006527
12	8	0	1.303826	-1.061800	0.004337
13	8	0	1.491997	1.270468	0.005490
14	1	0	0.519989	1.205350	0.000262
15	1	0	1.792279	-1.890090	0.007814
16	1	0	4.020696	-0.471395	-0.951538
17	1	0	4.033949	-0.718170	0.785369
18	1	0	4.157747	0.922599	0.126296

B'C':: M06-2X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.616592	-0.085606	0.000528
2	5	0	2.056859	0.075716	-0.000105
3	8	0	1.220213	-1.036653	0.000084
4	8	0	1.462269	1.291782	-0.000829
5	1	0	0.487884	1.241054	-0.001082
6	1	0	1.688534	-1.876831	0.000658
7	1	0	4.128463	0.876683	-0.000058
8	1	0	3.946758	-0.651076	-0.876094
9	1	0	3.946142	-0.649658	0.878297
10	6	0	-3.502800	0.076655	0.000379
11	8	0	-1.313040	1.063389	0.000521
12	8	0	-1.497042	-1.158961	-0.000746
13	1	0	-0.511502	-1.112797	-0.000655
14	6	0	-2.005530	0.063001	0.000063
15	1	0	-3.866834	-0.453859	0.881392
16	1	0	-3.867245	-0.453346	-0.880766
17	1	0	-3.865261	1.100489	0.000775

C'C':: M06-2X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.432156	0.094569	0.000478
2	8	0	-1.233541	1.053682	0.000887

3	8	0	-1.441956	-1.166506	0.000259
4	1	0	-0.450305	-1.129690	-0.000901
5	6	0	-1.936969	0.055486	0.001279
6	1	0	-3.805702	-0.439778	0.875078
7	1	0	-3.803121	-0.420418	-0.886894
8	1	0	-3.778260	1.123966	0.010549
9	6	0	3.432082	-0.094705	0.002177
10	8	0	1.233457	-1.053573	-0.002234
11	8	0	1.442101	1.166614	-0.002374
12	1	0	0.450499	1.129557	-0.001038
13	6	0	1.936958	-0.055416	-0.001795
14	1	0	3.798455	0.392169	0.907362
15	1	0	3.810413	0.466343	-0.853218
16	1	0	3.778042	-1.123488	-0.036077

AA-trans: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.693421	-1.237984	-0.068474
2	6	0	-4.305929	-1.264287	0.007347
3	6	0	-3.571443	-0.091063	-0.171632
4	6	0	-4.247245	1.104675	-0.416428
5	6	0	-5.632636	1.121599	-0.502748
6	6	0	-6.376557	-0.048673	-0.330834
7	1	0	-6.254584	-2.154647	0.081122
8	1	0	-3.809745	-2.201641	0.232478
9	1	0	-3.673925	2.014621	-0.546176
10	1	0	-6.147826	2.054648	-0.707286
11	6	0	-7.882972	-0.016825	-0.366252
12	6	0	-8.468811	0.265663	1.022693
13	1	0	-8.259113	-0.974334	-0.735040
14	1	0	-8.214037	0.754134	-1.066566
15	1	0	-9.559539	0.287401	0.986829
16	1	0	-8.163620	-0.506438	1.732744
17	1	0	-8.118021	1.229385	1.399203
18	8	0	-1.489454	0.996398	0.185549
19	6	0	-2.075982	-0.053130	-0.092835
20	7	0	-1.415282	-1.196388	-0.333965
21	1	0	-1.890436	-2.012959	-0.680961
22	1	0	-0.394306	-1.192846	-0.295094
23	6	0	5.632460	-1.121755	0.502617
24	6	0	4.247090	-1.104692	0.416037
25	6	0	3.571430	0.091165	0.171422
26	6	0	4.306047	1.264375	-0.007106
27	6	0	5.693524	1.237937	0.068976
28	6	0	6.376512	0.048501	0.331151
29	1	0	6.147533	-2.054902	0.707004
30	1	0	3.673666	-2.014623	0.545429
31	1	0	3.809991	2.201834	-0.232082
32	1	0	6.254791	2.154594	-0.080263
33	6	0	7.882917	0.016508	0.366842
34	6	0	8.468982	-0.265842	-1.022035
35	1	0	8.213780	-0.754583	1.067106
36	1	0	8.259083	0.973929	0.735834
37	1	0	9.559701	-0.287706	-0.985971
38	1	0	8.118155	-1.229471	-1.398749
39	1	0	8.164008	0.506396	-1.732030
40	8	0	1.489442	-0.996099	-0.186333
41	6	0	2.075981	0.053350	0.092326
42	7	0	1.415297	1.196599	0.333545
43	1	0	0.394329	1.193111	0.294497
44	1	0	1.890427	2.013083	0.680778

AA-cis: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.719432	1.200460	-0.053580
2	6	0	4.331952	1.260663	0.000768
3	6	0	3.574221	0.094496	-0.118140
4	6	0	4.227116	-1.127622	-0.281303
5	6	0	5.612683	-1.179278	-0.345702
6	6	0	6.379868	-0.016600	-0.233703
7	1	0	6.298783	2.112507	0.047227
8	1	0	3.854230	2.220655	0.161998
9	1	0	3.635229	-2.031082	-0.364494
10	1	0	6.109439	-2.133924	-0.486548
11	6	0	7.885521	-0.082306	-0.245504
12	6	0	8.445932	-0.304037	1.164923
13	1	0	8.287453	0.846643	-0.657562
14	1	0	8.208706	-0.895859	-0.899764
15	1	0	9.536291	-0.351518	1.146281
16	1	0	8.148762	0.510959	1.828870
17	1	0	8.068484	-1.238867	1.585860
18	8	0	1.465187	-0.933469	0.256215
19	6	0	2.077196	0.090381	-0.060636
20	7	0	1.442784	1.233548	-0.364417
21	1	0	1.938403	2.024774	-0.740108
22	1	0	0.421452	1.249906	-0.342108
23	6	0	-5.651798	1.201486	0.071437
24	6	0	-4.264446	1.178379	0.107413
25	6	0	-3.573374	-0.008477	-0.137547
26	6	0	-4.292283	-1.165971	-0.440369
27	6	0	-5.681034	-1.132898	-0.486784
28	6	0	-6.381030	0.047198	-0.227533
29	1	0	-6.179822	2.128195	0.271913
30	1	0	-3.701379	2.077242	0.328000
31	1	0	-3.779255	-2.092050	-0.674311
32	1	0	-6.230305	-2.034617	-0.737209
33	6	0	-7.888041	0.064958	-0.222135
34	6	0	-8.445267	-0.248483	1.171887
35	1	0	-8.263954	-0.668219	-0.940141
36	1	0	-8.241381	1.047261	-0.545512
37	1	0	-9.536588	-0.229286	1.167186
38	1	0	-8.120381	-1.237737	1.502501

39	1	0	-8.091830	0.484574	1.900765
40	8	0	-1.467818	1.082084	-0.278496
41	6	0	-2.076513	0.024903	-0.091420
42	7	0	-1.439821	-1.130132	0.157737
43	1	0	-0.419334	-1.127888	0.209498
44	1	0	-1.943503	-1.958006	0.430225

AB-trans: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.828736	1.093813	0.226519
2	6	0	4.449288	1.219860	0.099580
3	6	0	3.608436	0.100883	0.129206
4	6	0	4.210518	-1.154678	0.291374
5	6	0	5.587876	-1.285192	0.417506
6	6	0	6.418553	-0.161364	0.388212
7	1	0	6.456987	1.978896	0.204617
8	1	0	4.039712	2.219455	-0.018620
9	1	0	3.582407	-2.038680	0.321285
10	1	0	6.030061	-2.268941	0.544967
11	6	0	7.916456	-0.308707	0.475105
12	6	0	8.534732	-0.575453	-0.902788
13	1	0	8.162603	-1.132300	1.150484
14	1	0	8.348128	0.600774	0.900502
15	1	0	9.619163	-0.678811	-0.829622
16	1	0	8.131136	-1.494779	-1.333609
17	1	0	8.313050	0.245519	-1.588577
18	5	0	2.048260	0.196370	0.000959
19	8	0	1.386639	1.395607	-0.184011
20	8	0	1.308613	-0.934284	0.074222
21	1	0	0.340881	-0.790806	-0.007374
22	1	0	1.956715	2.166983	-0.239562
23	6	0	-5.528327	-1.144727	-0.643738
24	6	0	-4.149935	-0.990293	-0.598409
25	6	0	-3.591333	0.218274	-0.180586
26	6	0	-4.433094	1.259547	0.212983
27	6	0	-5.812349	1.093780	0.175147
28	6	0	-6.380286	-0.105343	-0.259772
29	1	0	-5.953181	-2.083535	-0.984613
30	1	0	-3.492269	-1.798326	-0.894964
31	1	0	-4.026829	2.196343	0.577843
32	1	0	-6.457820	1.906847	0.490666
33	6	0	-7.875115	-0.297333	-0.258075
34	6	0	-8.355377	-0.930252	1.053633
35	1	0	-8.160277	-0.935407	-1.098354
36	1	0	-8.365729	0.668453	-0.401583
37	1	0	-9.438728	-1.063192	1.046510
38	1	0	-7.890758	-1.907885	1.201917
39	1	0	-8.091833	-0.297959	1.904562
40	8	0	-1.393442	-0.674704	-0.089275
41	6	0	-2.100727	0.336210	-0.159658
42	7	0	-1.574490	1.567935	-0.219716
43	1	0	-0.562535	1.664682	-0.217204
44	1	0	-2.143540	2.378166	-0.400963

AB-cis: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.840246	1.076048	-0.140187
2	6	0	4.456009	1.208074	-0.109971
3	6	0	3.615371	0.088932	-0.147711
4	6	0	4.222596	-1.172522	-0.212991
5	6	0	5.604985	-1.308752	-0.246008
6	6	0	6.435359	-0.185091	-0.211027
7	1	0	6.468659	1.960908	-0.111653
8	1	0	4.042549	2.211429	-0.052714
9	1	0	3.595086	-2.056992	-0.242819
10	1	0	6.050919	-2.297233	-0.303696
11	6	0	7.935348	-0.335522	-0.193223
12	6	0	8.465016	-0.497478	1.236997
13	1	0	8.395812	0.540555	-0.656910
14	1	0	8.220738	-1.206558	-0.788918
15	1	0	9.551161	-0.607323	1.240277
16	1	0	8.205639	0.373575	1.843371
17	1	0	8.029400	-1.380688	1.709998
18	5	0	2.050590	0.192546	-0.124639
19	8	0	1.383974	1.402418	-0.171062
20	8	0	1.312959	-0.939813	-0.059291
21	1	0	0.342607	-0.790770	-0.061018
22	1	0	1.952889	2.172399	-0.251944
23	6	0	-5.530283	-1.139585	-0.579495
24	6	0	-4.151793	-0.984466	-0.539657
25	6	0	-3.592081	0.222127	-0.117632
26	6	0	-4.432628	1.260520	0.286025
27	6	0	-5.811934	1.094003	0.253636
28	6	0	-6.381097	-0.102897	-0.185856
29	1	0	-5.956094	-2.076663	-0.923922
30	1	0	-3.494898	-1.790192	-0.844128
31	1	0	-4.025119	2.195510	0.654160
32	1	0	-6.456578	1.904771	0.576693
33	6	0	-7.875827	-0.295534	-0.179359
34	6	0	-8.351012	-0.935089	1.130948
35	1	0	-8.163859	-0.929546	-1.021737
36	1	0	-8.367340	0.670752	-0.316306
37	1	0	-9.434305	-1.068636	1.126987
38	1	0	-7.885347	-1.913160	1.272939
39	1	0	-8.084878	-0.306739	1.983995
40	8	0	-1.392674	-0.668795	-0.043254
41	6	0	-2.101524	0.341563	-0.105176
42	7	0	-1.577237	1.574156	-0.164160
43	1	0	-0.565424	1.672226	-0.167649
44	1	0	-2.148493	2.384086	-0.339715

AC-trans: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.419402	-1.287646	0.414107
2	6	0	4.040773	-1.174580	0.295245
3	6	0	3.457043	0.084207	0.141674
4	6	0	4.265061	1.221182	0.108086
5	6	0	5.642173	1.098988	0.227427
6	6	0	6.238941	-0.155647	0.383037
7	1	0	5.869865	-2.267411	0.536732
8	1	0	3.414093	-2.057035	0.324024
9	1	0	3.802743	2.194006	-0.008868
10	1	0	6.266209	1.986408	0.204091
11	6	0	7.737665	-0.291783	0.459029
12	6	0	8.346577	-0.521974	-0.930051
13	1	0	7.994850	-1.128167	1.113777
14	1	0	8.163650	0.612275	0.900805
15	1	0	9.432232	-0.616151	-0.866368
16	1	0	7.948373	-1.435535	-1.377475
17	1	0	8.111856	0.311954	-1.595410
18	8	0	1.450590	1.337577	-0.110608
19	6	0	1.983083	0.247584	0.018990
20	8	0	1.309017	-0.883952	0.063566
21	1	0	0.319941	-0.714604	-0.008641
22	6	0	-5.393850	-1.143757	-0.632856
23	6	0	-4.016894	-0.978973	-0.586192
24	6	0	-3.469027	0.241821	-0.189840
25	6	0	-4.319001	1.284816	0.180819
26	6	0	-5.696638	1.108322	0.141901
27	6	0	-6.254314	-0.103385	-0.270971
28	1	0	-5.810999	-2.091907	-0.956748
29	1	0	-3.352961	-1.787942	-0.865364
30	1	0	-3.920798	2.231096	0.529557
31	1	0	-6.348705	1.922450	0.440308
32	6	0	-7.747464	-0.307280	-0.268179
33	6	0	-8.223028	-0.927977	1.051155
34	1	0	-8.026744	-0.958158	-1.100563
35	1	0	-8.245763	0.652600	-0.423793
36	1	0	-9.305325	-1.069007	1.045415
37	1	0	-7.751233	-1.900294	1.211132
38	1	0	-7.964357	-0.283518	1.894376
39	8	0	-1.271542	-0.640550	-0.070779
40	6	0	-1.982186	0.372785	-0.162969
41	7	0	-1.457186	1.598986	-0.241803
42	1	0	-0.443188	1.693563	-0.218607
43	1	0	-2.027841	2.407656	-0.425659

AC-cis: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.436062	-1.316154	-0.208541
2	6	0	4.052794	-1.197404	-0.188443
3	6	0	3.463946	0.067715	-0.161799
4	6	0	4.271346	1.205817	-0.155816
5	6	0	5.652853	1.077955	-0.175430
6	6	0	6.254953	-0.183421	-0.202562
7	1	0	5.890355	-2.301357	-0.232527
8	1	0	3.426873	-2.080877	-0.195948
9	1	0	3.805215	2.183561	-0.137794
10	1	0	6.276425	1.966069	-0.172678
11	6	0	7.754977	-0.321584	-0.168462
12	6	0	8.272394	-0.410869	1.272862
13	1	0	8.212266	0.535177	-0.669388
14	1	0	8.050305	-1.217803	-0.719723
15	1	0	9.358790	-0.515084	1.289077
16	1	0	8.004575	0.487397	1.833954
17	1	0	7.836723	-1.272107	1.784520
18	8	0	1.449723	1.333089	-0.119419
19	6	0	1.985595	0.237406	-0.141353
20	8	0	1.311797	-0.895150	-0.147833
21	1	0	0.320944	-0.722126	-0.121892
22	6	0	-5.401632	-1.134142	-0.562800
23	6	0	-4.023911	-0.971459	-0.531695
24	6	0	-3.469304	0.243701	-0.127516
25	6	0	-4.313235	1.283039	0.266846
26	6	0	-5.691429	1.108937	0.242460
27	6	0	-6.255994	-0.096913	-0.178423
28	1	0	-5.824054	-2.077877	-0.892710
29	1	0	-3.364530	-1.777520	-0.829459
30	1	0	-3.909766	2.224681	0.622055
31	1	0	-6.338765	1.920394	0.558062
32	6	0	-7.749429	-0.297736	-0.160875
33	6	0	-8.213051	-0.920453	1.161720
34	1	0	-8.038548	-0.945854	-0.992016
35	1	0	-8.247158	0.663646	-0.309052
36	1	0	-9.295596	-1.059658	1.166166
37	1	0	-7.741358	-1.893880	1.315115
38	1	0	-7.945249	-0.278220	2.003786
39	8	0	-1.270674	-0.642088	-0.061967
40	6	0	-1.982000	0.373143	-0.121991
41	7	0	-1.457276	1.600321	-0.185387
42	1	0	-0.442998	1.694033	-0.173445
43	1	0	-2.029898	2.412882	-0.343732

BB-trans: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.761096	1.220837	0.242387
2	6	0	-4.380975	1.219905	0.067684
3	6	0	-3.644146	0.030098	0.098955
4	6	0	-4.349116	-1.162598	0.311877
5	6	0	-5.726947	-1.165323	0.488815

6	6	0	-6.454133	0.027915	0.456606
7	1	0	-6.308829	2.157612	0.214848
8	1	0	-3.888617	2.174654	-0.095563
9	1	0	-3.802348	-2.098925	0.342557
10	1	0	-6.249711	-2.102078	0.656864
11	6	0	-7.955375	0.016540	0.593477
12	6	0	-8.637748	-0.242421	-0.755556
13	1	0	-8.293508	0.973976	0.997478
14	1	0	-8.250065	-0.759140	1.305232
15	1	0	-9.723838	-0.254896	-0.646321
16	1	0	-8.373157	0.535900	-1.475084
17	1	0	-8.322440	-1.204374	-1.166315
18	5	0	-2.091554	-0.019663	-0.090539
19	8	0	-1.315647	1.114122	-0.250510
20	8	0	-1.463097	-1.220356	-0.101972
21	1	0	-0.500574	-1.155565	-0.233602
22	1	0	-1.796877	1.945584	-0.214439
23	6	0	5.754085	-1.195023	-0.298310
24	6	0	4.364313	-1.166210	-0.322136
25	6	0	3.660089	0.042472	-0.256191
26	6	0	4.408030	1.223511	-0.161398
27	6	0	5.797433	1.198652	-0.140022
28	6	0	6.491197	-0.012018	-0.208756
29	1	0	6.276700	-2.145083	-0.352254
30	1	0	3.836906	-2.113798	-0.391681
31	1	0	3.887293	2.173698	-0.108711
32	1	0	6.355229	2.127713	-0.071915
33	6	0	7.996312	-0.046802	-0.131225
34	6	0	8.478209	-0.198354	1.316897
35	1	0	9.568553	-0.225153	1.363658
36	1	0	8.128626	0.637484	1.927423
37	1	0	8.092955	-1.122054	1.755042
38	5	0	2.097734	0.119666	-0.287048
39	8	0	1.297354	-0.988725	-0.495644
40	8	0	1.484867	1.314752	-0.106562
41	1	0	0.514052	1.265261	-0.158790
42	1	0	1.772720	-1.809371	-0.652556
43	1	0	8.404400	0.872725	-0.558369
44	1	0	8.373012	-0.879621	-0.730685

BB-cis: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.763651	-1.242989	0.014093
2	6	0	-4.373830	-1.211759	0.051890
3	6	0	-3.667187	-0.017534	-0.132664
4	6	0	-4.412255	1.148957	-0.351872
5	6	0	-5.800832	1.120640	-0.395036
6	6	0	-6.497450	-0.077025	-0.213410
7	1	0	-6.287141	-2.182539	0.160860
8	1	0	-3.848217	-2.144668	0.236414
9	1	0	-3.890106	2.088684	-0.497151
10	1	0	-6.355926	2.036403	-0.574703
11	6	0	-8.004829	-0.098663	-0.207036
12	6	0	-8.563033	0.185249	1.192878
13	1	0	-8.357108	-1.074408	-0.550923
14	1	0	-8.382821	0.648848	-0.909382
15	1	0	-9.654462	0.166191	1.188345
16	1	0	-8.209098	-0.562756	1.906218
17	1	0	-8.238161	1.167377	1.544296
18	5	0	-2.104598	0.056713	-0.104785
19	8	0	-1.304019	-1.070569	-0.073111
20	8	0	-1.493694	1.266128	-0.114140
21	1	0	-0.521693	1.211378	-0.104901
22	1	0	-1.778142	-1.905939	-0.115572
23	6	0	5.763772	1.242916	0.013692
24	6	0	4.373941	1.211828	0.051304
25	6	0	3.667212	0.017642	-0.133151
26	6	0	4.412195	-1.148959	-0.352074
27	6	0	5.800780	-1.120782	-0.395058
28	6	0	6.497488	0.076847	-0.213529
29	1	0	6.287332	2.182439	0.160378
30	1	0	3.848382	2.144813	0.235592
31	1	0	3.889973	-2.088657	-0.497268
32	1	0	6.355812	-2.036626	-0.574503
33	6	0	8.004868	0.098341	-0.206969
34	6	0	8.562873	-0.185453	1.193047
35	1	0	8.357281	1.074009	-0.550935
36	1	0	8.382874	-0.649293	-0.909178
37	1	0	9.654305	-0.166504	1.188645
38	1	0	8.208926	0.562675	1.906252
39	1	0	8.237861	-1.167505	1.544548
40	5	0	2.104617	-0.056485	-0.105495
41	8	0	1.304077	1.070824	-0.074171
42	8	0	1.493621	-1.265859	-0.114855
43	1	0	0.521617	-1.211015	-0.105616
44	1	0	1.778170	1.906219	-0.116425

BC-trans: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.672289	1.205809	0.258923
2	6	0	4.284183	1.207052	0.166552
3	6	0	3.554113	0.012907	0.165704
4	6	0	4.273483	-1.186605	0.260446
5	6	0	5.659172	-1.191546	0.354126
6	6	0	6.379823	0.006246	0.355144
7	1	0	6.215022	2.145782	0.258533
8	1	0	3.780569	2.167017	0.093111
9	1	0	3.731270	-2.126021	0.263984
10	1	0	6.193980	-2.133529	0.430400
11	6	0	7.886637	-0.005155	0.402794
12	6	0	8.489183	-0.208459	-0.992981
13	1	0	8.223353	-0.807191	1.065048

14	1	0	8.246314	0.936914	0.823920
15	1	0	9.579828	-0.220057	-0.948221
16	1	0	8.153023	-1.155333	-1.421906
17	1	0	8.181009	0.595840	-1.664967
18	5	0	1.994328	-0.039442	0.065975
19	8	0	1.207089	1.102304	0.020994
20	8	0	1.366821	-1.236894	0.020202
21	1	0	0.395026	-1.161319	-0.034339
22	1	0	1.686317	1.934282	0.075220
23	6	0	-5.568717	-1.209770	-0.329829
24	6	0	-4.184308	-1.165252	-0.267145
25	6	0	-3.529427	0.065099	-0.190999
26	6	0	-4.271202	1.247339	-0.178610
27	6	0	-5.657422	1.192296	-0.241530
28	6	0	-6.324650	-0.032857	-0.318501
29	1	0	-6.075184	-2.167418	-0.392425
30	1	0	-3.598413	-2.076338	-0.279379
31	1	0	-3.762578	2.201516	-0.121959
32	1	0	-6.232704	2.112121	-0.233958
33	6	0	-7.830027	-0.091617	-0.332700
34	6	0	-8.392707	-0.254224	1.085241
35	1	0	-8.154828	-0.930427	-0.953475
36	1	0	-8.226773	0.821656	-0.782368
37	1	0	-9.483004	-0.300267	1.065813
38	1	0	-8.018233	-1.171897	1.544459
39	1	0	-8.095052	0.586886	1.715496
40	8	0	-1.374195	-0.938630	-0.136670
41	8	0	-1.516406	1.287331	-0.057815
42	1	0	-0.534020	1.217964	-0.023844
43	6	0	-2.047595	0.077761	-0.127089

BC-cis: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.676486	1.207607	-0.133170
2	6	0	4.285613	1.204497	-0.110749
3	6	0	3.559797	0.008496	-0.152800
4	6	0	4.286495	-1.188606	-0.218219
5	6	0	5.675178	-1.189297	-0.240557
6	6	0	6.391387	0.010361	-0.199325
7	1	0	6.215741	2.149100	-0.102295
8	1	0	3.776170	2.162937	-0.062297
9	1	0	3.748193	-2.129575	-0.255336
10	1	0	6.216331	-2.129178	-0.294602
11	6	0	7.898714	0.003524	-0.173598
12	6	0	8.433819	-0.197907	1.249533
13	1	0	8.275107	0.946800	-0.577143
14	1	0	8.269448	-0.797177	-0.819050
15	1	0	9.525353	-0.205793	1.257575
16	1	0	8.090945	0.605203	1.905978
17	1	0	8.080740	-1.145937	1.662171
18	5	0	1.996980	-0.046795	-0.135016
19	8	0	1.208015	1.092141	-0.060322
20	8	0	1.368319	-1.243118	-0.193470
21	1	0	0.395111	-1.168780	-0.175334
22	6	0	-5.579090	-1.207402	-0.219422
23	6	0	-4.193376	-1.166909	-0.196907
24	6	0	-3.532965	0.062105	-0.153820
25	6	0	-4.270494	1.246824	-0.133752
26	6	0	-5.658139	1.195818	-0.156518
27	6	0	-6.330832	-0.027851	-0.200366
28	1	0	-6.090385	-2.163801	-0.256344
29	1	0	-3.610788	-2.080005	-0.215465
30	1	0	-3.757314	2.199701	-0.102839
31	1	0	-6.230175	2.117573	-0.143409
32	6	0	-7.836174	-0.082560	-0.172493
33	6	0	-8.359690	-0.245819	1.260210
34	1	0	-8.180242	-0.919713	-0.785154
35	1	0	-8.242744	0.832235	-0.610099
36	1	0	-9.450203	-0.289307	1.271036
37	1	0	-7.974907	-1.165000	1.707835
38	1	0	-8.042701	0.593683	1.883155
39	8	0	-1.379030	-0.946676	-0.149778
40	8	0	-1.514488	1.280462	-0.096259
41	1	0	-0.531692	1.209287	-0.083698
42	1	0	1.689074	1.923641	-0.016430
43	6	0	-2.049812	0.071390	-0.133806

CC-trans: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.509182	-1.203684	-0.287988
2	6	0	-4.123780	-1.236567	-0.209042
3	6	0	-3.402689	-0.041479	-0.180504
4	6	0	-4.077410	1.179098	-0.230599
5	6	0	-5.461990	1.201353	-0.308898
6	6	0	-6.196806	0.011972	-0.339935
7	1	0	-6.068424	-2.133082	-0.313210
8	1	0	-3.598376	-2.182563	-0.172791
9	1	0	-3.507747	2.100236	-0.211087
10	1	0	-5.984414	2.151377	-0.350783
11	6	0	-7.702721	0.040656	-0.373596
12	6	0	-8.290549	0.062605	1.043116
13	1	0	-8.071420	-0.837381	-0.909487
14	1	0	-8.037282	0.923948	-0.923114
15	1	0	-9.381240	0.083559	1.008323
16	1	0	-7.981652	-0.823760	1.601916
17	1	0	-7.947262	0.944506	1.588707
18	8	0	-1.268119	0.997506	-0.082443
19	8	0	-1.371742	-1.231576	-0.052525
20	1	0	-0.381871	-1.144800	-0.002671
21	6	0	-1.923143	-0.037309	-0.101006
22	6	0	5.461904	-1.201378	0.309013
23	6	0	4.077332	-1.179058	0.230638

24	6	0	3.402688	0.041555	0.180427
25	6	0	4.123832	1.236611	0.208937
26	6	0	5.509229	1.203659	0.287953
27	6	0	6.196782	-0.012032	0.340012
28	1	0	5.984273	-2.151429	0.350987
29	1	0	3.507619	-2.100166	0.211151
30	1	0	3.598480	2.182634	0.172595
31	1	0	6.068519	2.133029	0.313140
32	6	0	7.702693	-0.040799	0.373751
33	6	0	8.290587	-0.062954	-1.042931
34	1	0	8.037174	-0.924046	0.923392
35	1	0	8.071419	0.837281	0.909554
36	1	0	9.381275	-0.083973	-1.008082
37	1	0	7.947270	-0.944899	-1.588431
38	1	0	7.981772	0.823363	-1.601852
39	8	0	1.268070	-0.997310	0.082341
40	8	0	1.371821	1.231755	0.052384
41	1	0	0.381966	1.144907	0.002584
42	6	0	1.923168	0.037462	0.100835

CC-cis: M062X/6-311+G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.515423	1.211925	-0.169556
2	6	0	-4.127536	1.243578	-0.166814
3	6	0	-3.407108	0.047952	-0.171084
4	6	0	-4.084577	-1.172293	-0.178263
5	6	0	-5.471114	-1.193322	-0.181095
6	6	0	-6.205594	-0.003111	-0.177451
7	1	0	-6.074592	2.141648	-0.168624
8	1	0	-3.599960	2.189030	-0.164280
9	1	0	-3.515277	-2.093814	-0.184743
10	1	0	-5.996221	-2.142760	-0.189474
11	6	0	-7.710880	-0.033099	-0.126229
12	6	0	-8.215488	-0.097675	1.321199
13	1	0	-8.076244	-0.901325	-0.680280
14	1	0	-8.110589	0.858913	-0.614317
15	1	0	-9.306238	-0.123309	1.349672
16	1	0	-7.837452	-0.992621	1.820454
17	1	0	-7.877088	0.774302	1.885522
18	8	0	-1.271734	-0.993729	-0.175316
19	8	0	-1.370644	1.235724	-0.168016
20	1	0	-0.379476	1.147724	-0.168969
21	6	0	-1.925354	0.042165	-0.171546
22	6	0	5.471627	1.196524	-0.174866
23	6	0	4.084990	1.175981	-0.172251
24	6	0	3.407096	-0.043969	-0.171654
25	6	0	4.127100	-1.239935	-0.173793
26	6	0	5.514907	-1.208774	-0.176394
27	6	0	6.205588	0.006082	-0.177661
28	1	0	5.997060	2.145794	-0.177931
29	1	0	3.516041	2.097743	-0.173792
30	1	0	3.599151	-2.185174	-0.176460
31	1	0	6.073760	-2.138700	-0.180525
32	6	0	7.710889	0.034212	-0.125987
33	6	0	8.215585	0.070391	1.322393
34	1	0	8.076987	0.912471	-0.663381
35	1	0	8.109891	-0.848673	-0.631056
36	1	0	9.306377	0.093401	1.351367
37	1	0	7.839164	0.956404	1.838558
38	1	0	7.875487	-0.811471	1.870067
39	8	0	1.271838	0.998149	-0.171098
40	8	0	1.370483	-1.231311	-0.174092
41	1	0	0.379325	-1.143102	-0.174442
42	6	0	1.925350	-0.037822	-0.172146

A'A': MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.592721	0.041313	-0.016998
2	8	0	-1.467108	1.154260	0.021137
3	6	0	-2.082567	0.069231	0.021201
4	7	0	-1.458578	-1.122382	0.019150
5	1	0	-1.985687	-1.977982	0.018244
6	1	0	-0.439258	-1.163505	0.005916
7	1	0	-3.921212	0.241429	-1.035862
8	1	0	-3.973294	0.832328	0.622986
9	1	0	-4.001254	-0.914334	0.301320
10	6	0	3.592716	-0.041311	0.017043
11	8	0	1.467111	-1.154264	-0.021147
12	6	0	2.082564	-0.069232	-0.021433
13	7	0	1.458580	1.122383	-0.019083
14	1	0	0.439265	1.163537	-0.005692
15	1	0	1.985706	1.977973	-0.018007
16	1	0	3.973359	-0.832279	-0.622953
17	1	0	3.921091	-0.241508	1.035933
18	1	0	4.001294	0.914356	-0.301149

A'B': MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.689425	-0.076298	-0.004419
2	5	0	2.111570	-0.060858	0.003920
3	8	0	1.401511	1.138863	0.020039
4	8	0	1.405862	-1.223353	-0.005598
5	1	0	0.430954	-1.089962	-0.000824
6	1	0	1.984302	1.906545	0.025198
7	1	0	4.076600	0.444144	-0.881400
8	1	0	4.084485	-1.089092	-0.008103
9	1	0	4.087150	0.442396	0.868790
10	6	0	-3.562042	-0.185891	0.012577

11	8	0	-1.336326	-1.077199	0.000549
12	6	0	-2.058530	-0.059099	-0.015070
13	7	0	-1.556993	1.187322	-0.021449
14	1	0	-0.550956	1.318067	-0.006801
15	1	0	-2.160700	1.990224	-0.035295
16	1	0	-3.854518	-1.009948	-0.631896
17	1	0	-4.063771	0.724050	-0.306363
18	1	0	-3.873941	-0.422150	1.028797

A'C': MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.505378	-0.066283	0.004465
2	8	0	1.428398	1.161741	0.005517
3	6	0	2.009635	0.075239	0.003026
4	8	0	1.392692	-1.105567	-0.002391
5	1	0	0.396556	-0.982824	-0.004696
6	1	0	3.817956	-0.626163	-0.874558
7	1	0	3.815938	-0.626935	0.883717
8	1	0	3.968501	0.914159	0.005513
9	6	0	-3.490061	-0.215159	0.015480
10	8	0	-1.249186	-1.059315	-0.010970
11	6	0	-1.992476	-0.051538	-0.014380
12	7	0	-1.510313	1.198404	-0.011307
13	1	0	-0.503125	1.334148	-0.003530
14	1	0	-2.123906	1.994157	-0.015486
15	1	0	-3.765232	-1.028891	-0.649411
16	1	0	-4.013708	0.690945	-0.277533
17	1	0	-3.790877	-0.485855	1.026341

B'B': MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.686228	-0.061208	0.000081
2	5	0	-2.116014	0.065216	-0.000143
3	8	0	-1.295901	-1.063243	-0.000063
4	8	0	-1.513077	1.286204	-0.000147
5	1	0	-0.538960	1.216012	-0.000183
6	1	0	-1.800883	-1.884669	0.000042
7	1	0	-4.029377	-0.614162	-0.875095
8	1	0	-4.169850	0.912303	-0.000018
9	1	0	-4.029161	-0.613863	0.875536
10	6	0	3.686239	0.061154	0.000008
11	5	0	2.116025	-0.065214	0.000221
12	8	0	1.295937	1.063261	-0.000162
13	8	0	1.513028	-1.286171	0.000266
14	1	0	0.538909	-1.215945	0.000165
15	1	0	1.800879	1.884710	-0.000375
16	1	0	4.029376	0.614242	0.875102
17	1	0	4.029210	0.613655	-0.875530
18	1	0	4.169835	-0.912370	0.000277

B'C': MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.628784	-0.079803	0.001924
2	5	0	2.061985	0.069830	-0.000353
3	8	0	1.227654	-1.052643	-0.002786
4	8	0	1.467726	1.292837	0.000630
5	1	0	0.491792	1.225372	-0.000715
6	1	0	1.715370	-1.884533	-0.002817
7	1	0	4.125735	0.886882	0.003354
8	1	0	3.964854	-0.636807	-0.873370
9	1	0	3.962209	-0.637989	0.877485
10	6	0	-3.511278	0.062276	0.001643
11	8	0	-1.329253	1.093952	-0.002567
12	8	0	-1.499858	-1.164852	0.001208
13	1	0	-0.512289	-1.106699	-0.000243
14	6	0	-2.011364	0.068441	-0.000227
15	1	0	-3.869822	-0.467707	0.881523
16	1	0	-3.871861	-0.468162	-0.877138
17	1	0	-3.882914	1.080651	0.001753

C'C': MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.442896	-0.070860	0.000114
2	8	0	-1.259066	-1.091297	-0.000044
3	8	0	-1.435548	1.165456	-0.000051
4	1	0	-0.442393	1.108947	-0.000090
5	6	0	-1.944465	-0.063389	-0.000152
6	1	0	-3.806216	0.456733	-0.879195
7	1	0	-3.805950	0.456634	0.879600
8	1	0	-3.806132	-1.092187	0.000123
9	6	0	3.442850	0.070797	0.000219
10	8	0	1.259079	1.091324	0.000020
11	8	0	1.435590	-1.165452	-0.000125
12	1	0	0.442479	-1.108668	-0.000138
13	6	0	1.944455	0.063394	-0.000105
14	1	0	3.806180	-0.456495	-0.879272
15	1	0	3.805874	-0.456999	0.879537
16	1	0	3.806045	1.092132	0.000571

AA-cis: MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.681430	1.245646	0.016254
2	6	0	-4.289609	1.251627	-0.073872
3	6	0	-3.570299	0.069325	0.145314
4	6	0	-4.260011	-1.112498	0.442390
5	6	0	-5.649306	-1.104114	0.539805
6	6	0	-6.381270	0.074721	0.335807
7	1	0	-6.231717	2.163042	-0.160478
8	1	0	-3.774297	2.165134	-0.344384
9	1	0	-3.698097	-2.024074	0.598475
10	1	0	-6.174989	-2.019785	0.787107
11	6	0	-7.886486	0.063362	0.378919
12	6	0	-8.489147	-0.283956	-0.984299
13	1	0	-8.248375	1.041939	0.700464
14	1	0	-8.222675	-0.661873	1.122635
15	1	0	-9.577997	-0.288949	-0.940915
16	1	0	-8.179063	0.443208	-1.734227
17	1	0	-8.154469	-1.268657	-1.309399
18	8	0	-1.508909	-1.032857	-0.326047
19	6	0	-2.080375	0.012463	0.049019
20	7	0	-1.411783	1.135684	0.375783
21	1	0	-1.888434	1.894800	0.831422
22	1	0	-0.391001	1.129459	0.363877
23	1	0	9.577875	0.288564	0.941629
24	8	0	1.508915	1.033052	0.325635
25	7	0	1.411773	-1.135474	-0.376247
26	1	0	1.888444	-1.894588	-0.831871
27	6	0	5.649454	1.104078	-0.539622
28	6	0	4.260145	1.112556	-0.442409
29	6	0	3.570309	-0.069233	-0.145486
30	6	0	4.289502	-1.251596	0.073746
31	6	0	5.681337	-1.245709	-0.016177
32	6	0	6.381306	-0.074819	-0.335572
33	1	0	6.175238	2.019722	-0.786808
34	1	0	3.698318	2.024178	-0.598536
35	1	0	3.774081	-2.165080	0.344129
36	1	0	6.231534	-2.163153	0.160589
37	6	0	7.886529	-0.063564	-0.378467
38	6	0	8.489018	0.283646	0.984856
39	1	0	8.222877	0.661683	-1.122098
40	1	0	8.248395	-1.042151	-0.700006
41	1	0	8.154362	1.268355	1.309955
42	1	0	8.178774	-0.443533	1.734704
43	6	0	2.080376	-0.012280	-0.049408
44	1	0	0.390989	-1.129187	-0.364494

AB-cis: MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.835548	1.104528	0.047033
2	6	0	4.446401	1.214380	0.115108
3	6	0	3.613349	0.101592	-0.095141
4	6	0	4.232955	-1.127970	-0.380511
5	6	0	5.620623	-1.238483	-0.458079
6	6	0	6.443238	-0.122005	-0.251615
7	1	0	6.455435	1.978507	0.216210
8	1	0	4.015945	2.180872	0.357533
9	1	0	3.616866	-2.003993	-0.544875
10	1	0	6.074370	-2.195959	-0.691365
11	6	0	7.943258	-0.255599	-0.272764
12	6	0	8.497712	-0.632680	1.102885
13	1	0	8.388344	0.686212	-0.600304
14	1	0	8.230544	-1.015393	-1.002605
15	1	0	9.583176	-0.726648	1.076561
16	1	0	8.237093	0.126844	1.839510
17	1	0	8.079410	-1.582570	1.434747
18	5	0	2.048585	0.200160	-0.024941
19	8	0	1.382141	1.405617	-0.221626
20	8	0	1.323852	-0.919206	0.234668
21	1	0	0.350592	-0.769544	0.219739
22	1	0	1.973604	2.115894	-0.495954
23	1	0	-8.150641	-0.089495	1.890243
24	7	0	-1.575523	1.505841	-0.312775
25	1	0	-0.565645	1.610468	-0.311599
26	1	0	-2.144593	2.243451	-0.690544
27	6	0	-5.532851	-1.188253	-0.549133
28	6	0	-4.149179	-1.044398	-0.484629
29	6	0	-3.589502	0.184404	-0.114106
30	6	0	-4.429609	1.257825	0.210297
31	6	0	-5.813770	1.098318	0.151591
32	6	0	-6.386255	-0.119122	-0.239935
33	1	0	-5.959431	-2.137717	-0.852914
34	1	0	-3.493066	-1.871295	-0.722744
35	1	0	-4.012200	2.201922	0.538324
36	1	0	-6.458369	1.930959	0.409949
37	6	0	-7.881116	-0.300077	-0.249510
38	6	0	-8.398803	-0.799127	1.101486
39	1	0	-8.155379	-1.010899	-1.031523
40	1	0	-8.360630	0.648878	-0.497456
41	1	0	-9.480846	-0.926678	1.082719
42	1	0	-7.944830	-1.757134	1.353336
43	8	0	-1.404689	-0.704336	0.222560
44	6	0	-2.102740	0.294171	-0.057591

AC-cis: MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.452085	-1.268676	-0.449902
2	6	0	-4.064132	-1.160135	-0.388600
3	6	0	-3.474988	0.094550	-0.186596
4	6	0	-4.283644	1.230296	-0.057824
5	6	0	-5.669215	1.107250	-0.121117
6	6	0	-6.274979	-0.140697	-0.325016
7	1	0	-5.904986	-2.240656	-0.610286

8	1	0	-3.440442	-2.036966	-0.493315
9	1	0	-3.817469	2.194893	0.092473
10	1	0	-6.290744	1.990403	-0.024607
11	6	0	-7.774407	-0.276889	-0.332888
12	6	0	-8.326526	-0.521879	1.073463
13	1	0	-8.060980	-1.102500	-0.987285
14	1	0	-8.219464	0.629659	-0.747756
15	1	0	-9.411779	-0.618626	1.055929
16	1	0	-7.907385	-1.435745	1.493567
17	1	0	-8.066445	0.304506	1.734348
18	8	0	-1.464062	1.363500	0.047491
19	6	0	-1.998496	0.261921	-0.117049
20	8	0	-1.327473	-0.880483	-0.246330
21	1	0	-0.338026	-0.711465	-0.198820
22	8	0	1.299783	-0.707900	-0.167992
23	1	0	0.442521	1.621286	0.184551
24	1	0	2.013079	2.301970	0.546406
25	6	0	5.409628	-1.139580	0.698486
26	6	0	4.027456	-1.000817	0.600537
27	6	0	3.476098	0.204060	0.147848
28	6	0	4.322082	1.257721	-0.222742
29	6	0	5.704619	1.102641	-0.128936
30	6	0	6.269031	-0.089720	0.343351
31	1	0	5.830001	-2.069406	1.065000
32	1	0	3.367047	-1.812749	0.875095
33	1	0	3.911696	2.180567	-0.613915
34	1	0	6.354254	1.919286	-0.423049
35	6	0	7.763336	-0.268837	0.390432
36	6	0	8.305321	-0.841680	-0.921227
37	1	0	8.022904	-0.934996	1.215542
38	1	0	8.238393	0.692796	0.594005
39	1	0	9.386766	-0.967278	-0.875491
40	1	0	7.855679	-1.812459	-1.127842
41	1	0	8.072014	-0.177010	-1.752533
42	6	0	1.993029	0.312321	0.058452
43	7	0	1.454945	1.530351	0.224083

BB-cis: MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.748751	1.205544	0.083848
2	6	0	4.354360	1.169145	0.088386
3	6	0	3.653509	-0.010165	-0.219173
4	6	0	4.409658	-1.152924	-0.534770
5	6	0	5.803243	-1.116214	-0.547950
6	6	0	6.494072	0.065748	-0.245470
7	1	0	6.265585	2.127701	0.326807
8	1	0	3.814399	2.071247	0.357876
9	1	0	3.897271	-2.077017	-0.774414
10	1	0	6.364616	-2.007988	-0.805843
11	6	0	7.999216	0.088910	-0.199187
12	6	0	8.528861	-0.289877	1.185752
13	1	0	8.356368	1.085484	-0.466784
14	1	0	8.396710	-0.603575	-0.944052
15	1	0	9.618263	-0.270140	1.208163
16	1	0	8.157809	0.405257	1.938407
17	1	0	8.198471	-1.291651	1.459006
18	5	0	2.088513	-0.073209	-0.224262
19	8	0	1.306067	1.066381	-0.389554
20	8	0	1.465495	-1.272275	-0.063874
21	1	0	0.493602	-1.196768	-0.130313
22	1	0	1.825634	1.855551	-0.583286
23	1	0	-0.490586	1.276016	-0.082126
24	1	0	-8.276450	-0.730213	1.259377
25	6	0	-5.705014	-1.108403	0.658246
26	6	0	-4.317007	-1.079001	0.522552
27	6	0	-3.645753	0.094228	0.135881
28	6	0	-4.424344	1.240635	-0.102561
29	6	0	-5.812347	1.210874	0.024114
30	6	0	-6.473441	0.037180	0.412817
31	1	0	-6.197788	-2.023164	0.969566
32	1	0	-3.756910	-1.981966	0.743514
33	1	0	-3.933766	2.161995	-0.392879
34	1	0	-6.391587	2.108030	-0.166957
35	6	0	-7.976390	-0.010178	0.495304
36	6	0	-8.604726	-0.395359	-0.845927
37	1	0	-9.691803	-0.426726	-0.775460
38	1	0	-8.331806	0.326152	-1.615565
39	1	0	-8.253243	-1.376840	-1.163037
40	5	0	-2.088146	0.153830	-0.018193
41	8	0	-1.326022	-0.987090	-0.254486
42	8	0	-1.451313	1.352506	0.078717
43	1	0	-1.861725	-1.776475	-0.396363
44	1	0	-8.354604	0.964953	0.809048

BC-cis: MP2/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.672488	1.206324	-0.002077
2	6	0	4.284514	1.172120	-0.135866
3	6	0	3.556769	-0.006161	0.106093
4	6	0	4.278435	-1.149775	0.491653
5	6	0	5.664798	-1.115003	0.633790
6	6	0	6.382427	0.065604	0.395248
7	1	0	6.210917	2.127547	-0.196771
8	1	0	3.773832	2.075141	-0.454706
9	1	0	3.744490	-2.072724	0.683717
10	1	0	6.198484	-2.007331	0.943232
11	6	0	7.885473	0.086300	0.487261
12	6	0	8.539008	-0.290465	-0.844315
13	1	0	8.211863	-0.608602	1.263712
14	1	0	8.218215	1.081637	0.788770
15	1	0	9.625902	-0.272844	-0.766745
16	1	0	8.233248	-1.290987	-1.149014

17	1	0	8.239725	0.407087	-1.626137
18	5	0	1.999373	-0.071033	-0.034659
19	8	0	1.207277	1.076272	0.041721
20	8	0	1.385405	-1.265871	-0.237200
21	1	0	0.410436	-1.177708	-0.264455
22	1	0	1.701977	1.867863	0.285266
23	6	0	-5.598647	-1.183391	-0.423560
24	1	0	-0.527275	1.169877	0.009611
25	6	0	-2.052667	0.046278	-0.169391
26	6	0	-4.207078	-1.159184	-0.388798
27	6	0	-3.536162	0.055134	-0.198715
28	6	0	-4.266364	1.241719	-0.052797
29	6	0	-5.658584	1.201517	-0.089276
30	6	0	-6.345546	-0.005214	-0.281820
31	1	0	-6.114421	-2.124819	-0.575307
32	1	0	-3.632034	-2.068094	-0.504899
33	1	0	-3.748972	2.180167	0.089728
34	1	0	-6.221923	2.121317	0.020243
35	6	0	-7.850301	-0.045720	-0.260317
36	6	0	-8.388640	-0.252790	1.157476
37	1	0	-8.201050	-0.852673	-0.906573
38	1	0	-8.244812	0.886557	-0.669067
39	1	0	-9.477922	-0.280983	1.161200
40	1	0	-8.019727	-1.190467	1.572136
41	1	0	-8.064119	0.556881	1.810467
42	8	0	-1.388496	-0.988039	-0.289321
43	8	0	-1.513340	1.255709	-0.001281

CC-cis: M062X/6-31G(d,p) ,_n,n-DiMethylFormamide:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.522387	-1.211091	0.280282
2	6	0	4.131522	-1.238881	0.205356
3	6	0	3.416504	-0.034481	0.181695
4	6	0	4.099828	1.186374	0.242638
5	6	0	5.489840	1.197662	0.318024
6	6	0	6.221940	0.001995	0.345269
7	1	0	6.074314	-2.143916	0.301793
8	1	0	3.603324	-2.181182	0.162686
9	1	0	3.536337	2.109641	0.228233
10	1	0	6.015670	2.144303	0.369465
11	6	0	7.727045	0.022336	0.366408
12	6	0	8.309863	0.069999	-1.048114
13	1	0	8.095102	-0.865301	0.884483
14	1	0	8.070595	0.889861	0.933202
15	1	0	9.399074	0.083973	-1.021123
16	1	0	7.991861	-0.800687	-1.620867
17	1	0	7.968140	0.962591	-1.571368
18	8	0	1.287844	1.039616	0.076614
19	8	0	1.379486	-1.222506	0.068525
20	1	0	0.388824	-1.122688	0.016085
21	6	0	1.936336	-0.016189	0.104821
22	1	0	-0.388791	1.122769	-0.016077
23	6	0	-5.489835	-1.197668	-0.318028
24	6	0	-4.099819	-1.186358	-0.242667
25	6	0	-3.416505	0.034505	-0.181730
26	6	0	-4.131549	1.238893	-0.205362
27	6	0	-5.522416	1.211081	-0.280262
28	6	0	-6.221953	-0.002014	-0.345248
29	1	0	-6.015652	-2.144316	-0.369468
30	1	0	-3.536316	-2.109617	-0.228281
31	1	0	-3.603368	2.181201	-0.162692
32	1	0	-6.074359	2.143897	-0.301754
33	6	0	-7.727059	-0.022379	-0.366359
34	6	0	-8.309850	-0.070064	1.048174
35	1	0	-8.070607	-0.889904	-0.933154
36	1	0	-8.095140	0.865257	-0.884419
37	1	0	-9.399061	-0.084055	1.021202
38	1	0	-7.968104	-0.962655	1.571413
39	1	0	-7.991852	0.800622	1.620928
40	8	0	-1.287834	-1.039580	-0.076646
41	8	0	-1.379461	1.222538	-0.068534
42	6	0	-1.936323	0.016226	-0.104891

C. DIMERS IN SOLVENT: CCl_4

A'A': M062X/6-311+G(d,p), CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.577538	-0.081986	-0.003061
2	8	0	1.426172	-1.108720	0.004830
3	6	0	2.067047	-0.059373	0.005336
4	7	0	1.474257	1.146230	0.004174
5	1	0	2.020879	1.990212	0.003461
6	1	0	0.452889	1.207081	-0.001156
7	1	0	3.909067	-0.522703	-0.944539
8	1	0	3.918206	-0.728685	0.805332
9	1	0	4.020856	0.907001	0.107443
10	6	0	-3.577538	0.081986	0.003090
11	8	0	-1.426173	1.108720	-0.004855
12	6	0	-2.067047	0.059373	-0.005344
13	7	0	-1.474257	-1.146230	-0.004180
14	1	0	-0.452889	-1.207081	0.001138
15	1	0	-2.020879	-1.990212	-0.003443
16	1	0	-3.918225	0.728693	-0.805288
17	1	0	-3.909045	0.522693	0.944581
18	1	0	-4.020859	-0.907000	-0.107412

A'B': M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.679115	-0.064031	0.012162
2	5	0	-2.105166	-0.072796	-0.008125
3	8	0	-1.392526	1.124463	-0.010890
4	8	0	-1.412759	-1.227095	-0.009848
5	1	0	-0.437537	-1.130993	-0.007516
6	1	0	-1.964912	1.895213	-0.012190
7	1	0	-4.044139	0.296913	0.979467
8	1	0	-4.088679	-1.061730	-0.145197
9	1	0	-4.093504	0.603569	-0.748879
10	6	0	3.554242	-0.209187	0.005505
11	8	0	1.322937	-1.042003	-0.001495
12	6	0	2.053519	-0.054537	0.001840
13	7	0	1.564114	1.197987	0.002177
14	1	0	0.555476	1.329451	-0.001973
15	1	0	2.173995	1.997218	0.004206
16	1	0	3.837190	-0.791107	0.883164
17	1	0	4.083624	0.742667	0.013228
18	1	0	3.842424	-0.779525	-0.878101

A'C': M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.490425	-0.023964	0.000213
2	8	0	1.378029	1.114044	-0.000022
3	6	0	1.990990	0.063029	0.000260
4	8	0	1.408259	-1.119213	0.000025
5	1	0	0.410876	-1.026912	-0.000253
6	1	0	3.818482	-0.577132	-0.881076
7	1	0	3.818469	-0.580492	0.879362
8	1	0	3.920605	0.973630	0.002013
9	6	0	-3.465999	-0.249567	0.000581
10	8	0	-1.214610	-1.016386	-0.000615
11	6	0	-1.973370	-0.042892	-0.000157
12	7	0	-1.519818	1.216853	-0.000329
13	1	0	-0.512223	1.374421	-0.000688
14	1	0	-2.153297	1.997627	0.000142
15	1	0	-3.732128	-0.835504	-0.879718
16	1	0	-4.026435	0.684177	0.000564
17	1	0	-3.731331	-0.834974	0.881475

B'B': M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.681491	0.048465	0.002507
2	5	0	-2.115107	-0.068041	-0.006058
3	8	0	-1.308540	1.064324	-0.005138
4	8	0	-1.496888	-1.269229	-0.004480
5	1	0	-0.525742	-1.207626	-0.000014
6	1	0	-1.800222	1.889271	-0.007768
7	1	0	-4.027927	0.467468	0.952762
8	1	0	-4.157862	-0.923290	-0.127041
9	1	0	-4.040769	0.716727	-0.785347
10	6	0	3.681484	-0.048492	-0.002030
11	5	0	2.115102	0.068040	0.006082
12	8	0	1.308528	-1.064314	0.003964
13	8	0	1.496919	1.269244	0.005213
14	1	0	0.525770	1.207797	0.000260
15	1	0	1.800145	-1.889300	0.006108
16	1	0	4.028236	-0.467917	-0.951979
17	1	0	4.040442	-0.716445	0.786237
18	1	0	4.157851	0.923289	0.127331

B'C': M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.615650	-0.092295	0.000121
2	5	0	-2.055346	0.081755	0.000047
3	8	0	-1.219109	-1.037905	-0.000311
4	8	0	-1.471666	1.295189	0.000231
5	1	0	-0.497273	1.265095	0.000044
6	1	0	-1.696232	-1.871735	-0.000447
7	1	0	-4.128660	0.869049	0.000617
8	1	0	-3.946840	-0.655605	0.878016
9	1	0	-3.946984	-0.654756	-0.878268
10	6	0	3.504288	0.082554	0.000279
11	8	0	1.311344	1.058959	-0.000351
12	8	0	1.505084	-1.163856	0.000042
13	1	0	0.520901	-1.117322	-0.000141
14	6	0	2.005533	0.063354	-0.000064
15	1	0	3.871129	-0.446516	-0.880409
16	1	0	3.870760	-0.446658	0.881034
17	1	0	3.859686	1.108906	0.000420

C'C': M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.426620	0.105566	0.000275
2	8	0	-1.222496	1.046613	0.000808
3	8	0	-1.449408	-1.173452	0.000399
4	1	0	-0.457211	-1.148010	-0.000557
5	6	0	-1.929327	0.052685	0.000971
6	1	0	-3.805062	-0.424708	0.875220
7	1	0	-3.802650	-0.408371	-0.885515
8	1	0	-3.760209	1.139168	0.008729
9	6	0	3.426580	-0.105582	0.001641
10	8	0	1.222527	-1.046613	-0.001882
11	8	0	1.449425	1.173496	-0.001816

12	1	0	0.457206	1.148151	-0.000625
13	6	0	1.929310	-0.052649	-0.001668
14	1	0	3.798389	0.382081	0.904104
15	1	0	3.809324	0.449847	-0.855451
16	1	0	3.760169	-1.138623	-0.033289

AA-trans: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.683894	-1.237160	-0.074000
2	6	0	-4.297017	-1.263036	0.008105
3	6	0	-3.561594	-0.090292	-0.163816
4	6	0	-4.235880	1.106174	-0.403631
5	6	0	-5.620483	1.123192	-0.495445
6	6	0	-6.365300	-0.047145	-0.333590
7	1	0	-6.246525	-2.154037	0.069832
8	1	0	-3.799921	-2.199386	0.236035
9	1	0	-3.657166	2.014290	-0.520774
10	1	0	-6.135146	2.057649	-0.695507
11	6	0	-7.871840	-0.014651	-0.373501
12	6	0	-8.463483	0.258741	1.014708
13	1	0	-8.247516	-0.969054	-0.751529
14	1	0	-8.200802	0.759805	-1.071284
15	1	0	-9.554255	0.282007	0.976720
16	1	0	-8.160179	-0.517096	1.721283
17	1	0	-8.111807	1.218393	1.400225
18	8	0	-1.484047	1.000413	0.189898
19	6	0	-2.065144	-0.049703	-0.081879
20	7	0	-1.404720	-1.197631	-0.314461
21	1	0	-1.881554	-2.005446	-0.676612
22	1	0	-0.382349	-1.193507	-0.284280
23	6	0	5.620302	-1.123332	0.495368
24	6	0	4.235721	-1.106176	0.403279
25	6	0	3.561582	0.090400	0.163596
26	6	0	4.297137	1.263121	-0.007913
27	6	0	5.683996	1.237109	0.074467
28	6	0	6.365250	0.046980	0.333923
29	1	0	6.134845	-2.057879	0.695317
30	1	0	3.656904	-2.014268	0.520096
31	1	0	3.800168	2.199567	-0.235729
32	1	0	6.246733	2.153973	-0.069038
33	6	0	7.871780	0.014339	0.374121
34	6	0	8.463661	-0.258986	-1.014001
35	1	0	8.200533	-0.760215	1.071894
36	1	0	8.247475	0.968670	0.752307
37	1	0	9.554423	-0.282376	-0.975802
38	1	0	8.111954	-1.218563	-1.399676
39	1	0	8.160579	0.516952	-1.720559
40	8	0	1.484034	-1.000105	-0.190699
41	6	0	2.065145	0.049932	0.081353
42	7	0	1.404742	1.197863	0.313981
43	1	0	0.382377	1.193791	0.283632
44	1	0	1.881549	2.005595	0.676355

AA-cis: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.701001	1.206574	0.003356
2	6	0	4.312744	1.254860	0.038360
3	6	0	3.565400	0.089042	-0.129553
4	6	0	4.228831	-1.122645	-0.317388
5	6	0	5.615264	-1.162305	-0.362182
6	6	0	6.372257	0.000745	-0.204383
7	1	0	6.272708	2.118472	0.143092
8	1	0	3.823010	2.203985	0.226326
9	1	0	3.640475	-2.024885	-0.431877
10	1	0	6.121433	-2.108976	-0.522665
11	6	0	7.878639	-0.053857	-0.195391
12	6	0	8.422526	-0.301435	1.216926
13	1	0	8.279529	0.885977	-0.583973
14	1	0	8.217740	-0.849457	-0.863883
15	1	0	9.513514	-0.340055	1.214065
16	1	0	8.108302	0.495188	1.895005
17	1	0	8.045814	-1.246867	1.613868
18	8	0	1.460583	-0.963973	0.174553
19	6	0	2.066492	0.071604	-0.098412
20	7	0	1.431718	1.223901	-0.376913
21	1	0	1.932545	2.016019	-0.741326
22	1	0	0.409072	1.233527	-0.385391
23	6	0	-5.632882	1.209251	0.045519
24	6	0	-4.245491	1.180100	0.051977
25	6	0	-3.566330	-0.017610	-0.165927
26	6	0	-4.297407	-1.179337	-0.415061
27	6	0	-5.686347	-1.140805	-0.432124
28	6	0	-6.374221	0.050608	-0.197053
29	1	0	-6.152032	2.145641	0.223495
30	1	0	-3.668883	2.080820	0.224065
31	1	0	-3.792064	-2.113521	-0.633962
32	1	0	-6.245599	-2.046641	-0.643305
33	6	0	-7.880883	0.076263	-0.159656
34	6	0	-8.411583	-0.209802	1.250322
35	1	0	-8.275682	-0.666037	-0.858302
36	1	0	-8.236503	1.054051	-0.494609
37	1	0	-9.502788	-0.185309	1.269643
38	1	0	-8.083573	-1.193935	1.592651
39	1	0	-8.038168	0.532477	1.959427
40	8	0	-1.462733	1.059311	-0.377245
41	6	0	-2.067532	0.011864	-0.151393
42	7	0	-1.432483	-1.143540	0.113422
43	1	0	-0.410566	-1.146134	0.154576
44	1	0	-1.938594	-1.948270	0.441424

AB-trans: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.826766	1.098904	0.220359
2	6	0	4.447089	1.220647	0.096529
3	6	0	3.608618	0.101327	0.128301
4	6	0	4.212771	-1.152441	0.290142
5	6	0	5.590046	-1.278921	0.413248
6	6	0	6.418500	-0.154409	0.381255
7	1	0	6.453508	1.985175	0.197472
8	1	0	4.035822	2.220560	-0.019922
9	1	0	3.582698	-2.034703	0.322246
10	1	0	6.034565	-2.261595	0.541475
11	6	0	7.916917	-0.299479	0.465337
12	6	0	8.533696	-0.575254	-0.911231
13	1	0	8.165388	-1.117078	1.147421
14	1	0	8.348747	0.612776	0.885301
15	1	0	9.618537	-0.678137	-0.840871
16	1	0	8.128427	-1.496349	-1.336291
17	1	0	8.309005	0.239791	-1.602898
18	5	0	2.046755	0.186569	0.003897
19	8	0	1.390883	1.394392	-0.189029
20	8	0	1.317302	-0.942260	0.085918
21	1	0	0.347537	-0.823573	0.010328
22	1	0	1.980934	2.149007	-0.248433
23	6	0	-5.528343	-1.147059	-0.632132
24	6	0	-4.150398	-0.996928	-0.576593
25	6	0	-3.592309	0.215009	-0.170730
26	6	0	-4.434018	1.262970	0.201865
27	6	0	-5.813309	1.101922	0.153151
28	6	0	-6.380527	-0.100699	-0.270362
29	1	0	-5.953326	-2.089843	-0.961992
30	1	0	-3.488189	-1.809244	-0.850311
31	1	0	-4.026360	2.200857	0.563051
32	1	0	-6.459736	1.920148	0.453465
33	6	0	-7.875908	-0.289957	-0.276534
34	6	0	-8.366153	-0.916124	1.034625
35	1	0	-8.157782	-0.929959	-1.116749
36	1	0	-8.364455	0.675790	-0.429011
37	1	0	-9.449641	-1.048461	1.022760
38	1	0	-7.902553	-1.892690	1.191660
39	1	0	-8.105602	-0.281672	1.884693
40	8	0	-1.401226	-0.685933	-0.066227
41	6	0	-2.100131	0.323065	-0.138478
42	7	0	-1.568310	1.559376	-0.188203
43	1	0	-0.555315	1.644939	-0.201920
44	1	0	-2.133320	2.360753	-0.411334

AB-cis: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.837733	1.077384	-0.151881
2	6	0	4.453617	1.205528	-0.121754
3	6	0	3.615167	0.085760	-0.150598
4	6	0	4.224039	-1.174433	-0.205447
5	6	0	5.606115	-1.307108	-0.237880
6	6	0	6.434353	-0.182550	-0.212734
7	1	0	6.464818	1.963562	-0.130525
8	1	0	4.039063	2.209555	-0.070429
9	1	0	3.594466	-2.057431	-0.226551
10	1	0	6.054100	-2.295160	-0.287283
11	6	0	7.934712	-0.330284	-0.193347
12	6	0	8.466250	-0.474034	1.237969
13	1	0	8.394262	0.539850	-0.669629
14	1	0	8.221235	-1.207271	-0.780028
15	1	0	9.552554	-0.583952	1.243640
16	1	0	8.205571	0.403453	1.834222
17	1	0	8.029399	-1.349725	1.723228
18	5	0	2.048933	0.179252	-0.129613
19	8	0	1.388093	1.398422	-0.186114
20	8	0	1.321585	-0.951674	-0.060548
21	1	0	0.349651	-0.827164	-0.058204
22	1	0	1.976875	2.151663	-0.270281
23	6	0	-5.533040	-1.137837	-0.571876
24	6	0	-4.154598	-0.988614	-0.525881
25	6	0	-3.592849	0.218285	-0.110237
26	6	0	-4.431144	1.261763	0.282205
27	6	0	-5.810805	1.101636	0.242689
28	6	0	-6.381860	-0.095568	-0.191096
29	1	0	-5.960942	-2.076476	-0.909701
30	1	0	-3.494816	-1.797523	-0.815119
31	1	0	-4.020165	2.195192	0.651128
32	1	0	-6.454677	1.916368	0.557708
33	6	0	-7.877406	-0.283545	-0.188842
34	6	0	-8.360061	-0.917744	1.121222
35	1	0	-8.165123	-0.917743	-1.031461
36	1	0	-8.365989	0.683625	-0.332005
37	1	0	-9.443673	-1.049469	1.114950
38	1	0	-7.896079	-1.895512	1.269428
39	1	0	-8.094230	-0.288790	1.973748
40	8	0	-1.400279	-0.682791	-0.039944
41	6	0	-2.100417	0.326561	-0.092150
42	7	0	-1.569945	1.563726	-0.133207
43	1	0	-0.557226	1.650366	-0.156410
44	1	0	-2.138155	2.367376	-0.339242

AC-trans: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.428705	-1.279265	0.415428
2	6	0	4.048891	-1.178867	0.302216
3	6	0	3.454653	0.073600	0.145746
4	6	0	4.251473	1.217024	0.103607

5	6	0	5.629884	1.106988	0.217307
6	6	0	6.237885	-0.141060	0.375479
7	1	0	5.888418	-2.254503	0.541086
8	1	0	3.426451	-2.064044	0.337363
9	1	0	3.775807	2.183111	-0.015437
10	1	0	6.246606	1.999552	0.188023
11	6	0	7.738447	-0.263849	0.444808
12	6	0	8.344851	-0.494838	-0.945063
13	1	0	8.006282	-1.093877	1.103771
14	1	0	8.158713	0.645300	0.882310
15	1	0	9.431750	-0.580031	-0.887159
16	1	0	7.951271	-1.412310	-1.388300
17	1	0	8.099166	0.333114	-1.613715
18	8	0	1.438320	1.308664	-0.103417
19	6	0	1.977935	0.223238	0.028625
20	8	0	1.318698	-0.915448	0.081495
21	1	0	0.330776	-0.760479	0.011625
22	6	0	-5.395912	-1.138242	-0.627313
23	6	0	-4.018725	-0.981965	-0.573126
24	6	0	-3.466215	0.238228	-0.184450
25	6	0	-4.312149	1.288168	0.172711
26	6	0	-5.690527	1.120613	0.125897
27	6	0	-6.252485	-0.090476	-0.280215
28	1	0	-5.816925	-2.087280	-0.943905
29	1	0	-3.353667	-1.795693	-0.835120
30	1	0	-3.909000	2.232913	0.520714
31	1	0	-6.340224	1.940299	0.414630
32	6	0	-7.746854	-0.287039	-0.282879
33	6	0	-8.231801	-0.905027	1.034213
34	1	0	-8.026640	-0.935409	-1.117348
35	1	0	-8.240396	0.674940	-0.442445
36	1	0	-9.314639	-1.042513	1.025113
37	1	0	-7.763454	-1.878171	1.198237
38	1	0	-7.972942	-0.262530	1.878697
39	8	0	-1.278864	-0.661089	-0.058922
40	6	0	-1.976836	0.355141	-0.149209
41	7	0	-1.442327	1.581870	-0.218693
42	1	0	-0.425838	1.665150	-0.201126
43	1	0	-2.007776	2.388124	-0.422095

AC-cis: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.446426	-1.313433	-0.181930
2	6	0	4.062287	-1.207817	-0.170679
3	6	0	3.462531	0.051418	-0.172967
4	6	0	4.257885	1.196749	-0.187035
5	6	0	5.640391	1.081526	-0.197518
6	6	0	6.254111	-0.173657	-0.195358
7	1	0	5.910764	-2.294377	-0.183195
8	1	0	3.441269	-2.094710	-0.163294
9	1	0	3.777574	2.167734	-0.192225
10	1	0	6.256064	1.975264	-0.210313
11	6	0	7.755506	-0.296962	-0.150562
12	6	0	8.267884	-0.356517	1.293894
13	1	0	8.207994	0.554281	-0.665675
14	1	0	8.062663	-1.198955	-0.686262
15	1	0	9.355258	-0.450345	1.318883
16	1	0	7.987583	0.547592	1.838987
17	1	0	7.836390	-1.211396	1.819321
18	8	0	1.438352	1.298586	-0.170288
19	6	0	1.981752	0.207285	-0.162852
20	8	0	1.323162	-0.932993	-0.144578
21	1	0	0.333900	-0.773178	-0.128916
22	6	0	-5.409806	-1.116696	-0.569242
23	6	0	-4.031247	-0.965052	-0.539107
24	6	0	-3.467186	0.241083	-0.124158
25	6	0	-4.302523	1.280945	0.284203
26	6	0	-5.681963	1.118152	0.260339
27	6	0	-6.255832	-0.078112	-0.172758
28	1	0	-5.839894	-2.054411	-0.906731
29	1	0	-3.373910	-1.771170	-0.841056
30	1	0	-3.889631	2.213502	0.653098
31	1	0	-6.323572	1.929968	0.587106
32	6	0	-7.750768	-0.269074	-0.153237
33	6	0	-8.216789	-0.903681	1.162681
34	1	0	-8.046742	-0.904269	-0.992186
35	1	0	-8.242908	0.697024	-0.291090
36	1	0	-9.300075	-1.037880	1.168577
37	1	0	-7.748993	-1.880332	1.306200
38	1	0	-7.943077	-0.273591	2.011846
39	8	0	-1.278724	-0.664407	-0.089525
40	6	0	-1.976953	0.354849	-0.122862
41	7	0	-1.442684	1.583202	-0.160273
42	1	0	-0.426080	1.665260	-0.170444
43	1	0	-2.012348	2.396054	-0.320714

BB-trans: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.763156	1.244558	0.003127
2	6	0	4.373605	1.213233	0.032805
3	6	0	3.667978	0.017522	-0.138299
4	6	0	4.413137	-1.152196	-0.333324
5	6	0	5.801203	-1.124015	-0.368229
6	6	0	6.497044	0.075529	-0.201573
7	1	0	6.286580	2.185811	0.139303
8	1	0	3.847135	2.148956	0.203493
9	1	0	3.887791	-2.091903	-0.464965
10	1	0	6.357409	-2.042578	-0.529434
11	6	0	8.004457	0.095918	-0.185498
12	6	0	8.554547	-0.181513	1.218794
13	1	0	8.360146	1.069108	-0.533785
14	1	0	8.386220	-0.654340	-0.883164

15	1	0	9.646139	-0.164361	1.222272
16	1	0	8.195962	0.569192	1.926725
17	1	0	8.224761	-1.160342	1.574336
18	5	0	2.105654	-0.059682	-0.122747
19	8	0	1.308940	1.074509	-0.129769
20	8	0	1.495173	-1.265199	-0.108001
21	1	0	0.523945	-1.213341	-0.114978
22	1	0	1.795216	1.899872	-0.198131
23	6	0	-5.763190	-1.244524	0.003031
24	6	0	-4.373642	-1.213239	0.032894
25	6	0	-3.667961	-0.017528	-0.137990
26	6	0	-4.413062	1.152229	-0.332991
27	6	0	-5.801125	1.124089	-0.368080
28	6	0	-6.497020	-0.075453	-0.201639
29	1	0	-6.286657	-2.185777	0.139040
30	1	0	-3.847215	-2.148990	0.203565
31	1	0	-3.887673	2.091936	-0.464463
32	1	0	-6.357286	2.042685	-0.529257
33	6	0	-8.004435	-0.095804	-0.185748
34	6	0	-8.554682	0.181413	1.218526
35	1	0	-8.360112	-1.068927	-0.534234
36	1	0	-8.386096	0.654579	-0.883335
37	1	0	-9.646275	0.164306	1.221872
38	1	0	-8.196211	-0.569425	1.926374
39	1	0	-8.224895	1.160170	1.574269
40	5	0	-2.105633	0.059633	-0.122197
41	8	0	-1.308959	-1.074583	-0.129254
42	8	0	-1.495140	1.265137	-0.107139
43	1	0	-0.523912	1.213293	-0.114304
44	1	0	-1.795254	-1.899902	-0.198010

BB-cis: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.763156	1.244558	0.003127
2	6	0	4.373605	1.213233	0.032805
3	6	0	3.667978	0.017522	-0.138299
4	6	0	4.413137	-1.152196	-0.333324
5	6	0	5.801203	-1.124015	-0.368229
6	6	0	6.497044	0.075529	-0.201573
7	1	0	6.286580	2.185811	0.139303
8	1	0	3.847135	2.148956	0.203493
9	1	0	3.887791	-2.091903	-0.464965
10	1	0	6.357409	-2.042578	-0.529434
11	6	0	8.004457	0.095918	-0.185498
12	6	0	8.554547	-0.181513	1.218794
13	1	0	8.360146	1.069108	-0.533785
14	1	0	8.386220	-0.654340	-0.883164
15	1	0	9.646139	-0.164361	1.222272
16	1	0	8.195962	0.569192	1.926725
17	1	0	8.224761	-1.160342	1.574336
18	5	0	2.105654	-0.059682	-0.122747
19	8	0	1.308940	1.074509	-0.129769
20	8	0	1.495173	-1.265199	-0.108001
21	1	0	0.523945	-1.213341	-0.114978
22	1	0	1.795216	1.899872	-0.198131
23	6	0	-5.763190	-1.244524	0.003031
24	6	0	-4.373642	-1.213239	0.032894
25	6	0	-3.667961	-0.017528	-0.137990
26	6	0	-4.413062	1.152229	-0.332991
27	6	0	-5.801125	1.124089	-0.368080
28	6	0	-6.497020	-0.075453	-0.201639
29	1	0	-6.286657	-2.185777	0.139040
30	1	0	-3.847215	-2.148990	0.203565
31	1	0	-3.887673	2.091936	-0.464463
32	1	0	-6.357286	2.042685	-0.529257
33	6	0	-8.004435	-0.095804	-0.185748
34	6	0	-8.554682	0.181413	1.218526
35	1	0	-8.360112	-1.068927	-0.534234
36	1	0	-8.386096	0.654579	-0.883335
37	1	0	-9.646275	0.164306	1.221872
38	1	0	-8.196211	-0.569425	1.926374
39	1	0	-8.224895	1.160170	1.574269
40	5	0	-2.105633	0.059633	-0.122197
41	8	0	-1.308959	-1.074583	-0.129254
42	8	0	-1.495140	1.265137	-0.107139
43	1	0	-0.523912	1.213293	-0.114304
44	1	0	-1.795254	-1.899902	-0.198010

BC-trans: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.669732	1.204398	0.249477
2	6	0	4.282811	1.202488	0.148229
3	6	0	3.553457	0.008994	0.156077
4	6	0	4.272107	-1.188501	0.267257
5	6	0	5.656546	-1.190476	0.370385
6	6	0	6.376457	0.006801	0.363280
7	1	0	6.212511	2.144419	0.241821
8	1	0	3.779829	2.162269	0.058472
9	1	0	3.726614	-2.125759	0.275725
10	1	0	6.191458	-2.131217	0.460286
11	6	0	7.883095	-0.002847	0.418764
12	6	0	8.493996	-0.205902	-0.973314
13	1	0	8.217351	-0.803022	1.084725
14	1	0	8.239896	0.939356	0.842751
15	1	0	9.584604	-0.217023	-0.924296
16	1	0	8.159324	-1.151901	-1.404910
17	1	0	8.187425	0.596791	-1.647730
18	5	0	1.994096	-0.050946	0.048612
19	8	0	1.211373	1.100260	0.014893
20	8	0	1.373121	-1.244702	-0.013313
21	1	0	0.401116	-1.184686	-0.067886
22	1	0	1.707400	1.919001	0.093440

23	6	0	-5.566715	-1.206003	-0.335070
24	6	0	-4.182495	-1.159421	-0.275855
25	6	0	-3.531083	0.071344	-0.191701
26	6	0	-4.274357	1.251404	-0.167708
27	6	0	-5.660422	1.193755	-0.226913
28	6	0	-6.324893	-0.031565	-0.311896
29	1	0	-6.071588	-2.164142	-0.404733
30	1	0	-3.590829	-2.066656	-0.296675
31	1	0	-3.764372	2.204455	-0.105065
32	1	0	-6.238123	2.112132	-0.210745
33	6	0	-7.830518	-0.093444	-0.321744
34	6	0	-8.390348	-0.269066	1.095594
35	1	0	-8.155989	-0.926425	-0.950369
36	1	0	-8.230756	0.822126	-0.764281
37	1	0	-9.480764	-0.316864	1.080299
38	1	0	-8.012259	-1.188910	1.547223
39	1	0	-8.091101	0.565808	1.733130
40	8	0	-1.375434	-0.929226	-0.149493
41	8	0	-1.518859	1.296732	-0.058444
42	1	0	-0.538181	1.222411	-0.027262
43	6	0	-2.048310	0.084382	-0.132548

BC-cis: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.669732	1.204398	0.249477
2	6	0	4.282811	1.202488	0.148229
3	6	0	3.553457	0.008994	0.156077
4	6	0	4.272107	-1.188501	0.267257
5	6	0	5.656546	-1.190476	0.370385
6	6	0	6.376457	0.006801	0.363280
7	1	0	6.212511	2.144419	0.241821
8	1	0	3.779829	2.162269	0.058472
9	1	0	3.726614	-2.125759	0.275725
10	1	0	6.191458	-2.131217	0.460286
11	6	0	7.883095	-0.002847	0.418764
12	6	0	8.493996	-0.205902	-0.973314
13	1	0	8.217351	-0.803022	1.084725
14	1	0	8.239896	0.939356	0.842751
15	1	0	9.584604	-0.217023	-0.924296
16	1	0	8.159324	-1.151901	-1.404910
17	1	0	8.187425	0.596791	-1.647730
18	5	0	1.994096	-0.050946	0.048612
19	8	0	1.211373	1.100260	0.014893
20	8	0	1.373121	-1.244702	-0.013313
21	1	0	0.401116	-1.184686	-0.067886
22	1	0	1.707400	1.919001	0.093440
23	6	0	-5.566715	-1.206003	-0.335070
24	6	0	-4.182495	-1.159421	-0.275855
25	6	0	-3.531083	0.071344	-0.191701
26	6	0	-4.274357	1.251404	-0.167708
27	6	0	-5.660422	1.193755	-0.226913
28	6	0	-6.324893	-0.031565	-0.311896
29	1	0	-6.071588	-2.164142	-0.404733
30	1	0	-3.590829	-2.066656	-0.296675
31	1	0	-3.764372	2.204455	-0.105065
32	1	0	-6.238123	2.112132	-0.210745
33	6	0	-7.830518	-0.093444	-0.321744
34	6	0	-8.390348	-0.269066	1.095594
35	1	0	-8.155989	-0.926425	-0.950369
36	1	0	-8.230756	0.822126	-0.764281
37	1	0	-9.480764	-0.316864	1.080299
38	1	0	-8.012259	-1.188910	1.547223
39	1	0	-8.091101	0.565808	1.733130
40	8	0	-1.375434	-0.929226	-0.149493
41	8	0	-1.518859	1.296732	-0.058444
42	1	0	-0.538181	1.222411	-0.027262
43	6	0	-2.048310	0.084382	-0.132548

CC-trans: M062X/6-311+G(d,p) , CCl_4:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.507310	1.203887	0.287498
2	6	0	-4.122198	1.240992	0.207971
3	6	0	-3.398759	0.048324	0.180136
4	6	0	-4.068734	-1.173897	0.231347
5	6	0	-5.453011	-1.199801	0.309953
6	6	0	-6.190933	-0.013143	0.340236
7	1	0	-6.069806	2.131483	0.312795
8	1	0	-3.595580	2.186267	0.170731
9	1	0	-3.492217	-2.090801	0.212371
10	1	0	-5.973281	-2.151100	0.353107
11	6	0	-7.697176	-0.046351	0.373492
12	6	0	-8.286782	-0.070870	-1.042000
13	1	0	-8.068872	0.829796	0.911030
14	1	0	-8.029375	-0.929317	0.925571
15	1	0	-9.377550	-0.095023	-1.008482
16	1	0	-7.979599	0.814780	-1.602759
17	1	0	-7.940046	-0.950753	-1.588536
18	8	0	-1.263803	-0.986806	0.084784
19	8	0	-1.371824	1.243050	0.048338
20	1	0	-0.381544	1.160277	-0.002062
21	6	0	-1.917526	0.047524	0.100244
22	6	0	5.453070	1.199761	-0.309881
23	6	0	4.068788	1.173915	-0.231339
24	6	0	3.398760	-0.048278	-0.180181
25	6	0	4.122149	-1.240978	-0.208017
26	6	0	5.507266	-1.203931	-0.287487
27	6	0	6.190942	0.013071	-0.340161
28	1	0	5.973385	2.151037	-0.352990
29	1	0	3.492307	2.090842	-0.212370
30	1	0	3.595483	-2.186227	-0.170820
31	1	0	6.069726	-2.131549	-0.312788

32	6	0	7.697188	0.046221	-0.373341
33	6	0	8.286717	0.070745	1.042184
34	1	0	8.029452	0.929163	-0.925418
35	1	0	8.068879	-0.829951	-0.910841
36	1	0	9.377487	0.094855	1.008727
37	1	0	7.939984	0.950653	1.588683
38	1	0	7.979467	-0.814881	1.602943
39	8	0	1.263854	0.986946	-0.084931
40	8	0	1.371812	-1.242940	-0.048535
41	1	0	0.381521	-1.160184	0.001842
42	6	0	1.917529	-0.047416	-0.100319

CC-cis: M062X/6-311+G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.507310	1.203887	0.287498
2	6	0	-4.122198	1.240992	0.207971
3	6	0	-3.398759	0.048324	0.180136
4	6	0	-4.068734	-1.173897	0.231347
5	6	0	-5.453011	-1.199801	0.309953
6	6	0	-6.190933	-0.013143	0.340236
7	1	0	-6.069806	2.131483	0.312795
8	1	0	-3.595580	2.186267	0.170731
9	1	0	-3.492217	-2.090801	0.212371
10	1	0	-5.973281	-2.151100	0.353107
11	6	0	-7.697176	-0.046351	0.373492
12	6	0	-8.286782	-0.070870	-1.042000
13	1	0	-8.068872	0.829796	0.911030
14	1	0	-8.029375	-0.929317	0.925571
15	1	0	-9.377550	-0.095023	-1.008482
16	1	0	-7.979599	0.814780	-1.602759
17	1	0	-7.940046	-0.950753	-1.588536
18	8	0	-1.263803	-0.986806	0.084784
19	8	0	-1.371824	1.243050	0.048338
20	1	0	-0.381544	1.160277	-0.002062
21	6	0	-1.917526	0.047524	0.100244
22	6	0	5.453070	1.199761	-0.309881
23	6	0	4.068788	1.173915	-0.231339
24	6	0	3.398760	-0.048278	-0.180181
25	6	0	4.122149	-1.240978	-0.208017
26	6	0	5.507266	-1.203931	-0.287487
27	6	0	6.190942	0.013071	-0.340161
28	1	0	5.973385	2.151037	-0.352990
29	1	0	3.492307	2.090842	-0.212370
30	1	0	3.595483	-2.186227	-0.170820
31	1	0	6.069726	-2.131549	-0.312788
32	6	0	7.697188	0.046221	-0.373341
33	6	0	8.286717	0.070745	1.042184
34	1	0	8.029452	0.929163	-0.925418
35	1	0	8.068879	-0.829951	-0.910841
36	1	0	9.377487	0.094855	1.008727
37	1	0	7.939984	0.950653	1.588683
38	1	0	7.979467	-0.814881	1.602943
39	8	0	1.263854	0.986946	-0.084931
40	8	0	1.371812	-1.242940	-0.048535
41	1	0	0.381521	-1.160184	0.001842
42	6	0	1.917529	-0.047416	-0.100319

A'A': MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.584154	-0.039299	-0.015146
2	8	0	1.461974	-1.155109	0.018636
3	6	0	2.072430	-0.070467	0.020824
4	7	0	1.448216	1.123311	0.015802
5	1	0	1.975821	1.977569	0.020963
6	1	0	0.428134	1.166669	0.003109
7	1	0	3.915345	-0.215334	-1.037584
8	1	0	3.963430	-0.845092	0.606458
9	1	0	3.992216	0.909122	0.326820
10	6	0	-3.584154	0.039297	0.015147
11	8	0	-1.461974	1.155110	-0.018630
12	6	0	-2.072430	0.070468	-0.020824
13	7	0	-1.448216	-1.123310	-0.015809
14	1	0	-0.428134	-1.166669	-0.003114
15	1	0	-1.975821	-1.977568	-0.020977
16	1	0	-3.963432	0.845119	-0.606417
17	1	0	-3.915344	0.215281	1.037595
18	1	0	-3.992214	-0.909108	-0.326864

A'B': MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.687626	-0.074190	0.006800
2	5	0	-2.108345	-0.065818	-0.005335
3	8	0	-1.402016	1.143310	-0.004897
4	8	0	-1.411871	-1.226552	-0.005887
5	1	0	-0.435940	-1.113491	-0.003940
6	1	0	-1.998605	1.899150	-0.005407
7	1	0	-4.068851	0.355371	0.934675
8	1	0	-4.079392	-1.083856	-0.081821
9	1	0	-4.096482	0.523795	-0.808798
10	6	0	3.564220	-0.183539	0.002751
11	8	0	1.343505	-1.075997	0.000207
12	6	0	2.058755	-0.058699	0.001297
13	7	0	1.553064	1.190643	0.000497
14	1	0	0.545693	1.313325	-0.001388
15	1	0	2.153976	1.994482	0.000829
16	1	0	3.862784	-0.756333	0.877661
17	1	0	4.072351	0.777531	0.010804
18	1	0	3.865705	-0.742911	-0.879889

A'C': MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.501286	-0.052156	-0.000234
2	8	0	1.413267	1.154291	-0.000114
3	6	0	2.002937	0.072389	-0.000218
4	8	0	1.403085	-1.115648	-0.000356
5	1	0	0.407719	-1.007765	-0.000394
6	1	0	3.818731	-0.609232	-0.879275
7	1	0	3.818702	-0.610908	0.877745
8	1	0	3.952009	0.934103	0.000668
9	6	0	-3.488152	-0.208512	0.000886
10	8	0	-1.254588	-1.061018	-0.000295
11	6	0	-1.987771	-0.050793	0.000131
12	7	0	-1.499313	1.200034	0.000062
13	1	0	-0.489886	1.329046	-0.000263
14	1	0	-2.109244	1.997366	0.000530
15	1	0	-3.776212	-0.781406	-0.877488
16	1	0	-4.015087	0.742252	0.000511
17	1	0	-3.775457	-0.780264	0.880261

B'B': MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.690674	-0.058539	-0.000389
2	5	0	-2.119375	0.066915	0.000352
3	8	0	-1.302987	-1.067963	0.000690
4	8	0	-1.515849	1.283339	0.000344
5	1	0	-0.542556	1.214825	0.000441
6	1	0	-1.813151	-1.884939	0.000474
7	1	0	-4.038317	-0.607461	-0.876621
8	1	0	-4.168136	0.917570	-0.000216
9	1	0	-4.038979	-0.608105	0.875183
10	6	0	3.690693	0.058502	0.000489
11	5	0	2.119397	-0.066923	-0.000168
12	8	0	1.303012	1.067967	-0.000594
13	8	0	1.515788	-1.283315	-0.000642
14	1	0	0.542496	-1.214625	-0.000836
15	1	0	1.813220	1.884920	-0.000290
16	1	0	4.038363	0.607188	0.876854
17	1	0	4.038996	0.608282	-0.874952
18	1	0	4.168132	-0.917620	0.000054

B'C': MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.629305	-0.085558	0.000058
2	5	0	-2.062275	0.074636	0.000007
3	8	0	-1.227591	-1.053883	-0.000303
4	8	0	-1.476830	1.295892	0.000198
5	1	0	-0.500630	1.245646	0.000086
6	1	0	-1.724508	-1.879177	-0.000404
7	1	0	-4.127028	0.880248	0.000414
8	1	0	-3.965344	-0.642234	0.875948
9	1	0	-3.965436	-0.641629	-0.876183
10	6	0	3.513967	0.067331	0.000220
11	8	0	1.328232	1.090433	-0.000157
12	8	0	1.508021	-1.168971	-0.000002
13	1	0	0.521766	-1.109898	-0.000141
14	6	0	2.013058	0.068727	-0.000017
15	1	0	3.875769	-0.462148	-0.878687
16	1	0	3.875519	-0.462420	0.879064
17	1	0	3.880293	1.087659	0.000420

C'C': MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.439270	0.078006	0.000776
2	8	0	-1.251799	1.087431	0.000687
3	8	0	-1.440616	-1.170315	0.000097
4	1	0	-0.446959	-1.121602	-0.000645
5	6	0	-1.939613	0.061713	0.000675
6	1	0	-3.806213	-0.455887	0.874745
7	1	0	-3.805308	-0.440657	-0.882787
8	1	0	-3.794783	1.102067	0.009002
9	6	0	3.439290	-0.078158	0.002504
10	8	0	1.251711	-1.087315	-0.001855
11	8	0	1.440662	1.170371	-0.002163
12	1	0	0.447014	1.121688	-0.001049
13	6	0	1.939631	-0.061669	-0.002235
14	1	0	3.801249	0.419816	0.899698
15	1	0	3.810336	0.475706	-0.857023
16	1	0	3.794771	-1.101860	-0.026395

AA-trans: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.673064	-1.244671	-0.022152
2	6	0	-4.281852	-1.250810	0.073042
3	6	0	-3.561401	-0.068164	-0.137829
4	6	0	-4.249508	1.114807	-0.431145
5	6	0	-5.638046	1.106836	-0.533256
6	6	0	-6.371170	-0.072503	-0.338808
7	1	0	-6.224887	-2.162451	0.149064

8	1	0	-3.766168	-2.163656	0.345779
9	1	0	-3.683576	2.025725	-0.575180
10	1	0	-6.163214	2.024095	-0.776422
11	6	0	-7.876350	-0.060124	-0.385315
12	6	0	-8.482891	0.276334	0.978881
13	1	0	-8.238503	-1.035500	-0.716918
14	1	0	-8.210920	0.670282	-1.124952
15	1	0	-9.571778	0.282756	0.934079
16	1	0	-8.174239	-0.456138	1.724055
17	1	0	-8.147387	1.257303	1.313801
18	8	0	-1.501715	1.035854	0.329130
19	6	0	-2.070888	-0.010525	-0.038679
20	7	0	-1.404171	-1.140494	-0.355592
21	1	0	-1.883411	-1.888165	-0.825762
22	1	0	-0.382426	-1.132950	-0.355692
23	6	0	5.637992	-1.106867	0.533281
24	6	0	4.249461	-1.114806	0.431081
25	6	0	3.561397	0.068188	0.137755
26	6	0	4.281886	1.250825	-0.073036
27	6	0	5.673092	1.244654	0.022248
28	6	0	6.371153	0.072462	0.338914
29	1	0	6.163125	-2.024144	0.776455
30	1	0	3.683500	-2.025716	0.575053
31	1	0	3.766239	2.163689	-0.345782
32	1	0	6.224945	2.162427	-0.148908
33	6	0	7.876330	0.060050	0.385518
34	6	0	8.482951	-0.276388	-0.978647
35	1	0	8.210837	-0.670381	1.125159
36	1	0	8.238482	1.035410	0.717167
37	1	0	9.571835	-0.282835	-0.933776
38	1	0	8.147447	-1.257343	-1.313612
39	1	0	8.174363	0.456108	-1.723823
40	8	0	1.501720	-1.035778	-0.329366
41	6	0	2.070889	0.010582	0.038504
42	7	0	1.404171	1.140548	0.355425
43	1	0	0.382426	1.133019	0.355474
44	1	0	1.883397	1.888191	0.825657

AA-cis: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.682740	1.214558	0.101834
2	6	0	4.288841	1.239457	0.134318
3	6	0	3.562659	0.068098	-0.116227
4	6	0	4.247267	-1.122559	-0.385774
5	6	0	5.638920	-1.133330	-0.424947
6	6	0	6.378436	0.034733	-0.190642
7	1	0	6.238732	2.123652	0.303225
8	1	0	3.773841	2.157720	0.389681
9	1	0	3.675856	-2.024522	-0.560982
10	1	0	6.162063	-2.056339	-0.650081
11	6	0	7.883869	0.001555	-0.170064
12	6	0	8.424197	-0.358744	1.215686
13	1	0	8.273720	0.975343	-0.473715
14	1	0	8.241168	-0.725210	-0.902648
15	1	0	9.513812	-0.379943	1.219352
16	1	0	8.092450	0.369507	1.955045
17	1	0	8.060881	-1.338641	1.523659
18	8	0	1.468832	-1.010991	0.246090
19	6	0	2.068486	0.030276	-0.085885
20	7	0	1.432188	1.172220	-0.422384
21	1	0	1.942170	1.915633	-0.866202
22	1	0	0.411716	1.177871	-0.470931
23	6	0	-5.651920	1.210466	0.075081
24	6	0	-4.259846	1.204145	0.052396
25	6	0	-3.568186	0.014406	-0.202517
26	6	0	-4.287597	-1.157841	-0.468270
27	6	0	-5.681823	-1.137700	-0.451966
28	6	0	-6.384954	0.042905	-0.180680
29	1	0	-6.180879	2.135004	0.279187
30	1	0	-3.693339	2.108634	0.230418
31	1	0	-3.766601	-2.073308	-0.721483
32	1	0	-6.232478	-2.045213	-0.674086
33	6	0	-7.888586	0.043745	-0.100003
34	6	0	-8.380143	-0.260819	1.316918
35	1	0	-8.290849	-0.696740	-0.794491
36	1	0	-8.269141	1.016479	-0.418442
37	1	0	-9.468908	-0.257031	1.364662
38	1	0	-8.025940	-1.238877	1.641166
39	1	0	-8.003414	0.482289	2.019057
40	8	0	-1.474486	1.101156	-0.545280
41	6	0	-2.073924	0.057406	-0.220825
42	7	0	-1.437102	-1.083070	0.119480
43	1	0	-0.416999	-1.086339	0.175396
44	1	0	-1.948850	-1.829883	0.555461

AB-cis: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.827527	1.109294	0.015858
2	6	0	4.437972	1.207977	0.084273
3	6	0	3.613861	0.084446	-0.098266
4	6	0	4.242219	-1.146161	-0.355295
5	6	0	5.630216	-1.245871	-0.433039
6	6	0	6.444009	-0.118354	-0.256020
7	1	0	6.440985	1.991712	0.164533
8	1	0	3.999396	2.175067	0.312199
9	1	0	3.630553	-2.029545	-0.492825
10	1	0	6.091831	-2.205018	-0.643331
11	6	0	7.945041	-0.240359	-0.275735
12	6	0	8.504455	-0.580759	1.107409
13	1	0	8.382667	0.696693	-0.626936
14	1	0	8.238068	-1.013853	-0.988947
15	1	0	9.590729	-0.667240	1.083132

16	1	0	8.237594	0.192914	1.826700
17	1	0	8.092794	-1.524855	1.462724
18	5	0	2.047904	0.171509	-0.033032
19	8	0	1.387153	1.378766	-0.271970
20	8	0	1.330901	-0.940189	0.251763
21	1	0	0.356651	-0.809390	0.234754
22	1	0	1.999431	2.063830	-0.562038
23	6	0	-5.539245	-1.171076	-0.559204
24	6	0	-4.155640	-1.036405	-0.485166
25	6	0	-3.591473	0.184531	-0.097727
26	6	0	-4.427494	1.258708	0.233187
27	6	0	-5.812006	1.108388	0.164170
28	6	0	-6.388696	-0.100546	-0.245133
29	1	0	-5.969638	-2.115283	-0.874267
30	1	0	-3.499675	-1.863691	-0.721837
31	1	0	-4.005590	2.193975	0.580763
32	1	0	-6.454196	1.941150	0.428938
33	6	0	-7.884395	-0.274081	-0.264396
34	6	0	-8.410326	-0.802577	1.072140
35	1	0	-8.159539	-0.964030	-1.064846
36	1	0	-8.359030	0.682385	-0.493054
37	1	0	-9.492913	-0.924977	1.047196
38	1	0	-7.961030	-1.767646	1.303979
39	1	0	-8.161087	-0.113967	1.878825
40	8	0	-1.411945	-0.723604	0.213186
41	6	0	-2.103397	0.282391	-0.035486
42	7	0	-1.570081	1.505593	-0.249032
43	1	0	-0.558607	1.591389	-0.273988
44	1	0	-2.132974	2.236636	-0.646544

AC-trans: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.462544	-1.259587	-0.452853
2	6	0	-4.073623	-1.163670	-0.399681
3	6	0	-3.473537	0.084078	-0.190612
4	6	0	-4.270889	1.225287	-0.046507
5	6	0	-5.657417	1.114255	-0.102210
6	6	0	-6.274936	-0.126336	-0.312762
7	1	0	-5.925169	-2.226232	-0.619047
8	1	0	-3.455287	-2.042767	-0.516038
9	1	0	-3.792087	2.182825	0.108831
10	1	0	-6.271412	2.001666	0.005349
11	6	0	-7.775630	-0.249711	-0.310967
12	6	0	-8.321515	-0.498355	1.097107
13	1	0	-8.074425	-1.068038	-0.969395
14	1	0	-8.216197	0.662542	-0.718703
15	1	0	-9.407783	-0.585949	1.087640
16	1	0	-7.906611	-1.417389	1.509834
17	1	0	-8.049042	0.320929	1.761698
18	8	0	-1.453802	1.334897	0.051399
19	6	0	-1.994908	0.238961	-0.128186
20	8	0	-1.336250	-0.906697	-0.281247
21	1	0	-0.347295	-0.749620	-0.234537
22	6	0	5.409727	-1.131559	0.699481
23	6	0	4.028189	-1.002288	0.587515
24	6	0	3.473479	0.199435	0.132162
25	6	0	4.316366	1.259084	-0.226896
26	6	0	5.698722	1.113723	-0.118675
27	6	0	6.265950	-0.075132	0.357428
28	1	0	5.832835	-2.060018	1.066761
29	1	0	3.367421	-1.818885	0.846571
30	1	0	3.903007	2.177531	-0.625841
31	1	0	6.346597	1.934780	-0.405028
32	6	0	7.760819	-0.245575	0.418694
33	6	0	8.317951	-0.827390	-0.882614
34	1	0	8.017468	-0.901824	1.252871
35	1	0	8.229425	0.720126	0.619043
36	1	0	9.399690	-0.947078	-0.827349
37	1	0	7.874726	-1.801792	-1.085288
38	1	0	8.087416	-0.172600	-1.722348
39	8	0	1.305862	-0.729003	-0.187480
40	6	0	1.989314	0.295452	0.030549
41	7	0	1.443488	1.516698	0.175558
42	1	0	0.428358	1.594748	0.148029
43	1	0	1.994364	2.282551	0.520813

BB-trans: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.769243	1.229521	0.108249
2	6	0	-4.381739	1.197690	-0.027403
3	6	0	-3.661965	-0.002566	0.099365
4	6	0	-4.391549	-1.172812	0.370960
5	6	0	-5.777312	-1.141767	0.514779
6	6	0	-6.486760	0.060938	0.392719
7	1	0	-6.301589	2.168844	0.003010
8	1	0	-3.864715	2.123504	-0.261416
9	1	0	-3.861549	-2.112385	0.468677
10	1	0	-6.317881	-2.056325	0.734915
11	6	0	-7.989818	0.081771	0.484415
12	6	0	-8.643849	-0.177103	-0.874722
13	1	0	-8.318267	1.049171	0.870405
14	1	0	-8.321280	-0.674027	1.199673
15	1	0	-9.730946	-0.160160	-0.798352
16	1	0	-8.338399	0.581438	-1.594768
17	1	0	-8.342222	-1.149152	-1.263591
18	5	0	-2.103326	-0.063844	-0.041973
19	8	0	-1.310178	1.070409	0.136252
20	8	0	-1.501382	-1.243723	-0.339279
21	1	0	-0.528103	-1.173238	-0.362995
22	1	0	-1.820065	1.828401	0.443319
23	6	0	5.752586	-1.242426	-0.076013
24	6	0	4.360052	-1.191652	-0.021922

25	6	0	3.666948	0.022457	-0.165133
26	6	0	4.428080	1.186552	-0.367366
27	6	0	5.819347	1.136438	-0.430493
28	6	0	6.502577	-0.079707	-0.292888
29	1	0	6.264244	-2.191846	0.040728
30	1	0	3.815819	-2.113118	0.162151
31	1	0	3.918596	2.136382	-0.475212
32	1	0	6.385387	2.046610	-0.598642
33	6	0	8.007957	-0.122731	-0.296416
34	6	0	8.584034	0.092368	1.104974
35	1	0	9.673388	0.060014	1.092307
36	1	0	8.273922	1.059289	1.499896
37	1	0	8.225590	-0.678619	1.786326
38	5	0	2.103956	0.103716	-0.112887
39	8	0	1.307790	-1.007025	-0.394880
40	8	0	1.501287	1.276824	0.208586
41	1	0	0.527407	1.219230	0.174243
42	1	0	1.824620	-1.756090	-0.712154
43	1	0	8.392359	0.644723	-0.971637
44	1	0	8.344318	-1.085707	-0.686635

BB-cis: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.749586	1.227710	0.244940
2	6	0	4.356872	1.166024	0.277421
3	6	0	3.666892	0.008759	-0.122054
4	6	0	4.431461	-1.086659	-0.558868
5	6	0	5.823075	-1.023790	-0.600262
6	6	0	6.503136	0.136760	-0.206117
7	1	0	6.258544	2.131806	0.561785
8	1	0	3.809431	2.027875	0.647088
9	1	0	3.924794	-1.993179	-0.867083
10	1	0	6.391990	-1.878144	-0.951652
11	6	0	8.008430	0.180593	-0.190525
12	6	0	8.575910	-0.316224	1.141073
13	1	0	8.345331	1.203292	-0.373144
14	1	0	8.398757	-0.432161	-1.005910
15	1	0	9.665252	-0.281094	1.142633
16	1	0	8.211452	0.298759	1.963340
17	1	0	8.265341	-1.343733	1.327706
18	5	0	2.103559	-0.079841	-0.100382
19	8	0	1.310016	1.066896	-0.149562
20	8	0	1.498253	-1.293223	-0.037450
21	1	0	0.524777	-1.228608	-0.070117
22	1	0	1.830302	1.865482	-0.292550
23	6	0	-5.749613	-1.227737	0.244777
24	6	0	-4.356901	-1.166067	0.277366
25	6	0	-3.666883	-0.008756	-0.121907
26	6	0	-4.431412	1.086727	-0.558631
27	6	0	-5.823024	1.023875	-0.600132
28	6	0	-6.503123	-0.136721	-0.206189
29	1	0	-6.258600	-2.131870	0.561470
30	1	0	-3.809495	-2.027973	0.646957
31	1	0	-3.924716	1.993284	-0.866688
32	1	0	-6.391906	1.878281	-0.951447
33	6	0	-8.008418	-0.180544	-0.190713
34	6	0	-8.575991	0.316107	1.140908
35	1	0	-8.345314	-1.203217	-0.373486
36	1	0	-8.398680	0.432317	-1.006048
37	1	0	-9.665334	0.280984	1.142383
38	1	0	-8.211598	-0.298983	1.963122
39	1	0	-8.265430	1.343590	1.327694
40	5	0	-2.103551	0.079832	-0.100114
41	8	0	-1.310008	-1.066897	-0.149455
42	8	0	-1.498244	1.293206	-0.037008
43	1	0	-0.524770	1.228592	-0.069736
44	1	0	-1.830295	-1.865462	-0.292559

BC-trans: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.666859	1.208312	-0.001043
2	6	0	4.279114	1.167121	-0.131105
3	6	0	3.557563	-0.015156	0.106530
4	6	0	4.284882	-1.157342	0.483101
5	6	0	5.670926	-1.115850	0.621452
6	6	0	6.382386	0.069281	0.388928
7	1	0	6.200996	2.132693	-0.193410
8	1	0	3.763431	2.067860	-0.450402
9	1	0	3.753207	-2.083055	0.666493
10	1	0	6.210129	-2.007514	0.923428
11	6	0	7.885613	0.095720	0.476191
12	6	0	8.537010	-0.278297	-0.857165
13	1	0	8.217169	-0.597256	1.252385
14	1	0	8.215948	1.091897	0.778325
15	1	0	9.624238	-0.257040	-0.783930
16	1	0	8.232987	-1.279115	-1.162054
17	1	0	8.231898	0.417287	-1.638332
18	5	0	1.999594	-0.086824	-0.025222
19	8	0	1.213546	1.069020	0.070021
20	8	0	1.387283	-1.277025	-0.228487
21	1	0	0.411900	-1.200238	-0.252184
22	1	0	1.727958	1.844905	0.320074
23	6	0	-5.597341	-1.181211	-0.419929
24	6	0	-4.206308	-1.156763	-0.379510
25	6	0	-3.537389	0.058977	-0.194719
26	6	0	-4.267793	1.246105	-0.059758
27	6	0	-5.659601	1.204965	-0.101712
28	6	0	-6.345233	-0.002802	-0.288933
29	1	0	-6.112562	-2.123721	-0.568107
30	1	0	-3.627493	-2.064342	-0.486962
31	1	0	-3.748686	2.184293	0.077994
32	1	0	-6.224338	2.125155	-0.001060

33	6	0	-7.850160	-0.044297	-0.272503
34	6	0	-8.394444	-0.255761	1.142317
35	1	0	-8.198830	-0.848771	-0.923320
36	1	0	-8.244336	0.888313	-0.681359
37	1	0	-9.483815	-0.284319	1.143280
38	1	0	-8.026201	-1.193872	1.556342
39	1	0	-8.071609	0.551056	1.799528
40	8	0	-1.390138	-0.984776	-0.271298
41	8	0	-1.514865	1.261156	0.006093
42	1	0	-0.530732	1.170019	0.021206
43	6	0	-2.053722	0.049145	-0.159220

BC-cis: MP2/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.679825	-1.073324	-0.497391
2	6	0	-4.286184	-1.048423	-0.539336
3	6	0	-3.566276	0.115610	-0.220554
4	6	0	-4.301547	1.259940	0.133282
5	6	0	-5.693906	1.234511	0.183748
6	6	0	-6.404535	0.069155	-0.135385
7	1	0	-6.212823	-1.980625	-0.761025
8	1	0	-3.762261	-1.946305	-0.853297
9	1	0	-3.770773	2.174226	0.369162
10	1	0	-6.240483	2.130052	0.459880
11	6	0	-7.905828	0.027635	-0.024863
12	6	0	-8.359635	-0.368096	1.382063
13	1	0	-8.305416	-0.682686	-0.751794
14	1	0	-8.316609	1.006875	-0.279691
15	1	0	-9.446927	-0.394720	1.452360
16	1	0	-7.974762	-1.353424	1.643333
17	1	0	-7.985734	0.343808	2.117261
18	5	0	-2.002627	0.169388	-0.259320
19	8	0	-1.238300	-0.998664	-0.139898
20	8	0	-1.364782	1.354838	-0.403001
21	1	0	-0.390696	1.264972	-0.372836
22	1	0	-1.776562	-1.771672	0.064776
23	6	0	5.619622	1.154269	-0.278317
24	6	0	4.227890	1.151289	-0.294527
25	6	0	3.533740	-0.058131	-0.171604
26	6	0	4.240065	-1.260243	-0.041221
27	6	0	5.632894	-1.240527	-0.025854
28	6	0	6.343703	-0.039358	-0.151266
29	1	0	6.154640	2.092025	-0.378860
30	1	0	3.667687	2.070802	-0.399225
31	1	0	3.701697	-2.193373	0.048606
32	1	0	6.179159	-2.172173	0.071248
33	6	0	7.847220	-0.022748	-0.074141
34	6	0	8.337699	0.145178	1.365950
35	1	0	8.233866	0.791677	-0.690204
36	1	0	8.243140	-0.951323	-0.490432
37	1	0	9.426473	0.155699	1.410766
38	1	0	7.967831	1.078907	1.788341
39	1	0	7.976312	-0.671938	1.989503
40	8	0	1.407253	1.021872	-0.305256
41	8	0	1.486974	-1.232945	-0.090527
42	1	0	0.504566	-1.126463	-0.113846
43	6	0	2.050177	-0.025415	-0.196912

CC-trans: M062X/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.519995	-1.206406	0.287950
2	6	0	4.129635	-1.238164	0.211149
3	6	0	3.412530	-0.035755	0.178788
4	6	0	4.092186	1.186839	0.233397
5	6	0	5.481817	1.201495	0.310089
6	6	0	6.216631	0.008250	0.346207
7	1	0	6.074485	-2.137727	0.317313
8	1	0	3.600815	-2.180311	0.173647
9	1	0	3.523746	2.106954	0.212444
10	1	0	6.005852	2.149595	0.356535
11	6	0	7.721837	0.031791	0.368306
12	6	0	8.307315	0.059036	-1.045619
13	1	0	8.091574	-0.846478	0.901425
14	1	0	8.063706	0.907679	0.923518
15	1	0	9.396585	0.075827	-1.018695
16	1	0	7.991303	-0.820142	-1.606195
17	1	0	7.963627	0.941881	-1.583714
18	8	0	1.282756	1.034149	0.080499
19	8	0	1.380209	-1.228974	0.056046
20	1	0	0.388758	-1.133424	0.005390
21	6	0	1.931643	-0.021233	0.101402
22	6	0	-5.481810	-1.201486	-0.310106
23	6	0	-4.092179	-1.186835	-0.233441
24	6	0	-3.412533	0.035761	-0.178810
25	6	0	-4.129631	1.238173	-0.211119
26	6	0	-5.519993	1.206418	-0.287892
27	6	0	-6.216626	-0.008238	-0.346172
28	1	0	-6.005845	-2.149584	-0.356570
29	1	0	-3.523735	-2.106949	-0.212528
30	1	0	-3.600806	2.180317	-0.173599
31	1	0	-6.074484	2.137739	-0.317215
32	6	0	-7.721832	-0.031783	-0.368241
33	6	0	-8.307281	-0.059142	1.045694
34	1	0	-8.063709	-0.907629	-0.923515
35	1	0	-8.091583	0.846527	-0.901283
36	1	0	-9.396551	-0.075931	1.018791
37	1	0	-7.963581	-0.942030	1.583712
38	1	0	-7.991257	0.819992	1.606333
39	8	0	-1.282748	-1.034116	-0.080583
40	8	0	-1.380258	1.229003	-0.056098
41	1	0	-0.388818	1.133375	-0.005473
42	6	0	-1.931664	0.021250	-0.101455

CC-cis: M062X/6-31G(d,p) , CCl_4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.530099	1.201620	-0.185528
2	6	0	-4.137626	1.234901	-0.182460
3	6	0	-3.418583	0.033333	-0.167398
4	6	0	-4.098887	-1.190115	-0.164770
5	6	0	-5.490617	-1.206287	-0.167751
6	6	0	-6.227572	-0.013932	-0.185412
7	1	0	-6.086333	2.132232	-0.201567
8	1	0	-3.608595	2.177650	-0.189491
9	1	0	-3.529175	-2.109646	-0.158384
10	1	0	-6.015362	-2.155136	-0.169705
11	6	0	-7.731811	-0.038193	-0.127299
12	6	0	-8.241273	-0.043864	1.316008
13	1	0	-8.101785	-0.922542	-0.650142
14	1	0	-8.130263	0.831725	-0.653348
15	1	0	-9.330414	-0.061258	1.347351
16	1	0	-7.868546	-0.918268	1.848521
17	1	0	-7.896699	0.843908	1.845342
18	8	0	-1.285228	-1.034305	-0.165931
19	8	0	-1.383827	1.228863	-0.166736
20	1	0	-0.391361	1.133833	-0.166203
21	6	0	-1.935634	0.020232	-0.167209
22	6	0	5.490564	1.206585	-0.167357
23	6	0	4.098830	1.190343	-0.164365
24	6	0	3.418580	-0.033131	-0.167386
25	6	0	4.137686	-1.234664	-0.182850
26	6	0	5.530153	-1.201312	-0.185918
27	6	0	6.227573	0.014277	-0.185411
28	1	0	6.015264	2.155458	-0.168996
29	1	0	3.529076	2.109846	-0.157667
30	1	0	3.608700	-2.177433	-0.190190
31	1	0	6.086433	-2.131893	-0.202271
32	6	0	7.731812	0.038519	-0.127302
33	6	0	8.241312	0.042095	1.315998
34	1	0	8.101731	0.923647	-0.648859
35	1	0	8.130292	-0.830612	-0.654634
36	1	0	9.330453	0.059539	1.347338
37	1	0	7.868517	0.915679	1.849807
38	1	0	7.896836	-0.846487	1.844037
39	8	0	1.285167	1.034403	-0.165537
40	8	0	1.383842	-1.228750	-0.167151
41	1	0	0.391372	-1.133775	-0.166625
42	6	0	1.935629	-0.020099	-0.167169

D. Encapsulation complexes- capsule a

AA-trans, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.232014	0.863511	3.178539
2	6	0	-11.695069	-0.450849	3.739318
3	6	0	-11.998302	-1.762328	-1.763364
4	6	0	-11.419231	-2.955440	-1.309319
5	6	0	-11.985608	-3.705997	-0.135660
6	6	0	-11.366219	-3.259529	1.157493
7	6	0	-11.809435	-2.108321	1.826406
8	6	0	-11.181062	-1.648440	2.992737
9	6	0	-11.916599	1.517964	2.145208
10	6	0	-12.205397	3.449552	0.527203
11	6	0	-11.640591	2.995149	-0.790240
12	6	0	-12.121008	1.848164	-1.439402
13	6	0	-11.565083	1.401925	-2.647056
14	6	0	-11.497751	-1.084177	-2.885235
15	6	0	-12.109346	0.200218	-3.367873
16	6	0	-10.076491	-2.382422	3.469874
17	6	0	-10.306421	-3.986036	1.731901
18	6	0	-9.634588	-3.564033	2.879280
19	6	0	-10.399874	3.383405	2.300727
20	6	0	-10.103943	1.508977	3.723094
21	6	0	-9.668586	2.767518	3.316659
22	6	0	-10.300854	-3.450377	-2.012318
23	6	0	-10.407771	-1.659092	-3.565770
24	6	0	-9.775291	-2.828884	-3.142513
25	6	0	-10.493615	2.142396	-3.186076
26	6	0	-10.601082	3.714432	-1.412500
27	6	0	-9.994239	3.303036	-2.598563
28	1	0	-8.913164	-3.247328	-3.680527
29	1	0	-12.858265	-1.351211	-1.233686
30	1	0	-11.805796	-4.805012	-0.277993
31	1	0	-13.091331	-3.604048	-0.098603
32	1	0	-12.655268	-1.551166	1.422161
33	1	0	-8.791603	-4.131637	3.298636
34	1	0	-8.793729	3.250923	3.774466
35	1	0	-12.787429	1.040183	1.695452
36	1	0	-12.943609	1.288791	-0.992809
37	1	0	-9.166893	3.867477	-3.052379
38	1	0	-13.216862	0.162908	-3.280509
39	1	0	-11.915938	0.311990	-4.468588
40	1	0	-13.300732	3.273285	0.572392
41	1	0	-12.090399	4.561881	0.620852
42	1	0	-11.369633	-0.523308	4.812552
43	1	0	-12.806711	-0.478989	3.783597
44	8	0	-9.436334	0.851699	4.789156
45	8	0	-9.412409	-1.924859	4.640225
46	8	0	-10.242458	4.952780	-0.832688
47	8	0	-10.095004	4.713814	1.930966
48	8	0	-9.977583	1.725761	-4.436344
49	8	0	-9.996475	-1.041826	-4.774938
50	8	0	-9.940019	-5.214351	1.122431
51	8	0	-9.794466	-4.706458	-1.611750

52	6	0	-8.263453	-1.218684	4.328775
53	6	0	-8.286602	0.209698	4.378272
54	7	0	-7.192567	0.970190	4.070227
55	7	0	-7.133071	-1.920657	4.010722
56	6	0	-6.099169	0.269401	3.750925
57	6	0	-6.061278	-1.165346	3.738245
58	6	0	-4.744516	0.798129	3.319172
59	6	0	-4.660852	-1.607805	3.341326
60	7	0	-3.959046	-0.378783	3.125382
61	8	0	-4.362992	1.919237	3.125156
62	1	0	-2.942049	-0.336649	2.876570
63	8	0	-4.178055	-2.696965	3.212894
64	6	0	-8.928938	4.841760	1.199957
65	6	0	-9.004384	4.954778	-0.221339
66	6	0	-11.503171	2.773276	1.671853
67	7	0	-7.898092	5.144392	-1.001818
68	7	0	-7.746314	4.931502	1.880119
69	6	0	-8.795553	-0.370534	-4.623616
70	6	0	-8.787922	1.032401	-4.359461
71	6	0	-8.707908	-5.102229	0.495374
72	6	0	-8.632814	-4.699342	-0.874633
73	7	0	-7.632126	1.721780	-4.107463
74	7	0	-7.646132	-1.098459	-4.752068
75	7	0	-7.598415	-5.389258	1.236763
76	7	0	-7.440184	-4.426095	-1.487388
77	6	0	-6.672138	5.129663	1.106400
78	6	0	-6.359062	-4.656172	-0.729498
79	6	0	-6.747112	5.228293	-0.324581
80	6	0	-6.522659	-0.402378	-4.554082
81	6	0	-6.516070	0.987787	-4.188788
82	6	0	-6.438351	-5.190780	0.600765
83	6	0	-5.032332	-5.399400	1.141297
84	6	0	-4.892745	-4.396494	-1.051357
85	6	0	-5.215577	5.243607	1.532554
86	6	0	-5.341667	5.392985	-0.883366
87	6	0	-5.093665	-0.915433	-4.594580
88	6	0	-5.081795	1.397908	-3.889239
89	7	0	-4.196837	-4.868379	0.095808
90	7	0	-4.323934	0.223838	-4.170913
91	7	0	-4.512964	5.363360	0.287678
92	8	0	-4.376148	-3.884566	-2.007231
93	8	0	-4.632157	-5.889219	2.151981
94	8	0	-4.632089	-1.970995	-4.903891
95	8	0	-4.616836	2.432348	-3.497421
96	8	0	-4.698826	5.253077	2.609374
97	8	0	-4.939067	5.526932	-1.999624
98	1	0	-3.480584	5.367259	0.227603
99	1	0	-3.301689	0.154945	-3.993595
100	1	0	-3.158394	-4.799528	0.193584
101	1	0	13.293973	3.573802	0.171869
102	6	0	12.191801	3.685585	0.254903
103	6	0	11.522505	3.352712	-1.047923
104	6	0	11.653155	2.847129	1.381610
105	1	0	12.032257	4.771030	0.492055
106	6	0	11.933754	2.254513	-1.821191
107	6	0	10.449320	4.128538	-1.524305
108	6	0	12.223435	1.611903	1.718231
109	6	0	10.563924	3.297447	2.156164
110	6	0	11.259378	1.888762	-2.994088
111	1	0	12.789191	1.663846	-1.491647
112	6	0	9.733892	3.800925	-2.676842
113	8	0	10.107221	5.309428	-0.814432
114	6	0	11.738712	0.847809	2.791181
115	1	0	13.062107	1.233902	1.132683
116	6	0	10.053354	2.589808	3.241361
117	8	0	10.070400	4.589652	1.869266
118	6	0	11.725838	0.754076	-3.861231
119	6	0	10.144254	2.665305	-3.368788
120	1	0	8.878632	4.401387	-3.017436
121	6	0	8.898241	5.155246	-0.151959
122	6	0	12.342565	-0.482085	3.143763
123	6	0	10.674220	1.377646	3.545232
124	1	0	9.210503	2.972205	3.833990
125	6	0	8.878337	4.649315	1.185775
126	1	0	12.836426	0.766391	-3.935888
127	1	0	11.372099	0.932606	-4.913024
128	6	0	11.256164	-0.601890	-3.416893
129	8	0	9.426491	2.281754	-4.534675
130	7	0	7.759902	5.507357	-0.818602
131	6	0	11.747406	-1.607567	2.344060
132	1	0	12.185197	-0.682465	4.237408
133	1	0	13.446631	-0.456282	3.019153
134	8	0	10.286790	0.673064	4.712369
135	7	0	7.712309	4.334056	1.826963
136	6	0	11.949324	-1.343976	-2.449707
137	6	0	10.124753	-1.199814	-4.006800
138	6	0	8.300940	1.548168	-4.209451
139	6	0	6.625822	5.266678	-0.149149
140	6	0	12.252666	-1.964728	1.085779
141	6	0	10.674096	-2.364192	2.855398
142	6	0	9.074737	0.024341	4.564147
143	6	0	6.602533	4.626342	1.135518
144	6	0	11.539995	-2.634863	-2.081265
145	1	0	12.822197	-0.904672	-1.965608
146	6	0	9.698095	-2.491927	-3.709407
147	8	0	9.417957	-0.457482	-4.992314
148	6	0	8.292143	0.141079	-4.458809
149	7	0	7.227906	2.201083	-3.666907
150	6	0	5.196436	5.539097	-0.594502
151	6	0	11.715537	-3.036264	0.357128
152	1	0	13.080962	-1.395148	0.663144
153	6	0	10.107215	-3.443665	2.180265
154	8	0	10.239308	-2.057486	4.166587
155	6	0	9.049973	-1.362628	4.224187
156	7	0	7.935169	0.743269	4.794345
157	6	0	5.154063	4.350368	1.506087
158	6	0	12.245609	-3.405448	-1.000707
159	6	0	10.433542	-3.190679	-2.752534
160	1	0	8.821745	-2.935769	-4.203178
161	7	0	7.202392	-0.641864	-4.193712

162	6	0	6.171832	1.421626	-3.406045
163	7	0	4.404662	4.944064	0.453839
164	8	0	4.751050	6.116353	-1.537659
165	6	0	10.660805	-3.765611	0.941822
166	1	0	9.274035	-4.018867	2.608663
167	7	0	7.881497	-2.047024	4.030620
168	6	0	6.800254	0.052165	4.641307
169	8	0	4.684339	3.741225	2.429673
170	1	0	12.104771	-4.505751	-1.170515
171	1	0	13.343727	-3.249095	-1.054627
172	8	0	10.115098	-4.542276	-2.478416
173	6	0	6.156221	0.012175	-3.676051
174	6	0	4.849721	1.807920	-2.764382
175	1	0	3.362359	4.906853	0.422714
176	8	0	10.243166	-4.936928	0.270351
177	6	0	6.773432	-1.324491	4.232266
178	6	0	5.371929	0.549102	4.801410
179	6	0	8.945019	-4.689742	-1.755211
180	6	0	4.818294	-0.554825	-3.231424
181	7	0	4.126378	0.576733	-2.700660
182	8	0	4.440213	2.859930	-2.359579
183	6	0	9.007925	-4.855407	-0.337694
184	6	0	5.325035	-1.749298	4.051278
185	7	0	4.581345	-0.589099	4.419808
186	8	0	4.925156	1.594569	5.164020
187	7	0	7.766786	-4.731312	-2.446314
188	8	0	4.383537	-1.671246	-3.267807
189	1	0	3.133063	0.531025	-2.381829
190	7	0	7.889277	-5.031450	0.428769
191	8	0	4.845668	-2.786598	3.688051
192	1	0	3.546183	-0.547475	4.334503
193	6	0	6.681772	-4.926974	-1.687451
194	6	0	6.741086	-5.062529	-0.259073
195	6	0	5.228413	-4.993399	-2.131544
196	6	0	5.324682	-5.201814	0.280614
197	7	0	4.509316	-5.120613	-0.895782
198	8	0	4.722281	-4.967291	-3.212883
199	8	0	4.904614	-5.345746	1.389769
200	1	0	3.474257	-5.101898	-0.851720
201	8	0	1.876194	-4.017612	-0.784057
202	6	0	1.236846	-3.817153	-1.819094
203	7	0	-0.047481	-4.330056	-2.105906
204	7	0	1.699623	-3.089440	-2.921272
205	6	0	-0.592610	-3.732109	-3.352820
206	1	0	-0.686668	-4.598099	-1.333212
207	6	0	0.653377	-2.925301	-3.959090
208	1	0	2.659868	-2.753508	-3.039011
209	1	0	-0.997133	-4.537878	-4.013084
210	7	0	-1.600436	-2.673056	-3.119450
211	1	0	1.003186	-3.286654	-4.956505
212	7	0	0.153323	-1.532155	-4.074725
213	6	0	-1.113665	-1.400829	-3.440722
214	1	0	-2.519833	-2.863924	-2.713431
215	1	0	0.827657	-0.744268	-4.007037
216	8	0	-1.711987	-0.337720	-3.297499
217	1	0	1.471129	-5.137816	3.592791
218	6	0	1.024488	-4.285325	3.025158
219	6	0	-0.297860	-3.664440	3.685605
220	7	0	0.565211	-4.764361	1.696406
221	7	0	1.946676	-3.125648	2.930961
222	1	0	-0.635254	-4.176794	4.620436
223	7	0	0.089729	-2.265395	4.003307
224	7	0	-1.308155	-3.793653	2.613075
225	6	0	-0.773659	-4.358133	1.447461
226	1	0	1.237567	-4.803248	0.910641
227	6	0	1.372908	-1.962047	3.489048
228	1	0	2.965889	-3.256118	2.866350
229	1	0	-0.629614	-1.517713	4.027702
230	1	0	-2.276001	-3.475027	2.713352
231	8	0	-1.382836	-4.559937	0.401936
232	8	0	1.925387	-0.871031	3.555904
233	6	0	-0.788667	1.295442	3.496142
234	7	0	0.500849	1.610562	3.991482
235	7	0	-1.484770	2.488167	3.244882
236	8	0	-1.266427	0.167799	3.406439
237	6	0	0.769996	3.070554	3.891039
238	1	0	1.268133	0.927951	3.869942
239	6	0	-0.625502	3.680398	3.390018
240	1	0	-2.473614	2.539039	2.984537
241	1	0	1.116723	3.449151	4.884215
242	7	0	1.710790	3.452370	2.815313
243	1	0	-1.082618	4.432505	4.079504
244	7	0	-0.285718	4.336593	2.098894
245	6	0	1.063199	4.079976	1.741489
246	1	0	2.720984	3.288282	2.865706
247	1	0	-1.010446	4.413296	1.363411
248	8	0	1.596591	4.453637	0.699316
249	1	0	0.797804	5.117737	-3.468904
250	6	0	0.405363	4.233675	-2.909026
251	6	0	-0.848431	3.503503	-3.591157
252	7	0	-0.117149	4.665218	-1.586413
253	7	0	1.421935	3.159920	-2.832611
254	1	0	-1.206917	3.977815	-4.536138
255	7	0	-0.353478	2.130402	-3.874986
256	7	0	-1.880591	3.532393	-2.526887
257	6	0	-1.398168	4.119933	-1.347874
258	1	0	0.546098	4.819998	-0.798830
259	6	0	0.915029	1.924455	-3.265512
260	1	0	2.317587	3.277174	-2.351669
261	1	0	-1.029825	1.341352	-3.867855
262	1	0	-2.864965	3.306550	-2.705958
263	8	0	-2.010618	4.164542	-0.280525
264	8	0	1.517652	0.855978	-3.236194
265	6	0	-6.126663	-0.855448	-1.110387
266	6	0	-4.759518	-0.896665	-0.866184
267	6	0	-4.120888	0.175576	-0.246494
268	6	0	-4.870304	1.293682	0.124965
269	6	0	-6.240109	1.323604	-0.109518
270	6	0	-6.888040	0.251410	-0.728589
271	1	0	-6.611944	-1.695686	-1.604023

272	1	0	-4.159234	-1.755865	-1.150643
273	1	0	-4.396847	2.131468	0.635204
274	1	0	-6.818521	2.192602	0.193426
275	6	0	-8.384381	0.274503	-0.920397
276	6	0	-9.132404	-0.053269	0.376676
277	1	0	-8.666219	-0.446887	-1.694409
278	1	0	-8.692097	1.265403	-1.275009
279	1	0	-10.215021	-0.029138	0.219011
280	1	0	-8.860564	-1.047870	0.738517
281	1	0	-8.887073	0.670970	1.158767
282	8	0	-2.134016	-1.073376	0.080719
283	6	0	5.032256	-1.490200	0.232706
284	6	0	3.648870	-1.439268	0.103921
285	6	0	2.953371	-0.278317	0.450270
286	6	0	3.667751	0.824271	0.918429
287	6	0	5.049140	0.761651	1.056554
288	6	0	5.751146	-0.397236	0.719500
289	1	0	5.562602	-2.399687	-0.035832
290	1	0	3.124884	-2.313076	-0.287899
291	1	0	3.114545	1.720672	1.176990
292	1	0	5.589073	1.619415	1.451961
293	6	0	7.256099	-0.458100	0.822748
294	6	0	7.932845	-0.177996	-0.524428
295	1	0	7.556581	-1.449514	1.182279
296	1	0	7.599892	0.271662	1.562823
297	1	0	9.021313	-0.231961	-0.433098
298	1	0	7.614825	-0.909541	-1.272784
299	1	0	7.665869	0.818094	-0.885643
300	8	0	0.929095	0.963486	0.388297
301	1	0	-2.368616	2.077700	-0.006687
302	1	0	1.201768	-2.186341	0.400755
303	1	0	-0.272529	-1.243649	0.229609
304	1	0	-0.939738	1.124217	0.320608
305	7	0	0.750378	-1.291555	0.274403
306	7	0	-1.958149	1.181899	0.221138
307	6	0	1.456580	-0.154351	0.368531
308	6	0	-2.646196	0.047881	0.018121

AA-cis, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.340707	0.664223	3.195235
2	6	0	-11.854722	-0.667188	3.663032
3	6	0	-12.070456	-1.654224	-1.919803
4	6	0	-11.499241	-2.872779	-1.527517
5	6	0	-12.079550	-3.689951	-0.406030
6	6	0	-11.480804	-3.318659	0.920304
7	6	0	-11.943238	-2.212067	1.650334
8	6	0	-11.334700	-1.819283	2.850292
9	6	0	-11.981633	1.382500	2.174697
10	6	0	-12.217349	3.412363	0.674484
11	6	0	-11.690460	3.055924	-0.686565
12	6	0	-12.165638	1.938645	-1.391136
13	6	0	-11.616215	1.561824	-2.624708
14	6	0	-11.555165	-0.913981	-2.995267
15	6	0	-12.156710	0.398731	-3.409106
16	6	0	-10.230685	-2.573364	3.297031
17	6	0	-10.424057	-4.071260	1.465615
18	6	0	-9.769624	-3.713455	2.645195
19	6	0	-10.369241	3.156024	2.391733
20	6	0	-10.212413	1.251374	3.799483
21	6	0	-9.694612	2.486727	3.411154
22	6	0	-10.373547	-3.328887	-2.244935
23	6	0	-10.462204	-1.454820	-3.698214
24	6	0	-9.837621	-2.648785	-3.335358
25	6	0	-10.554017	2.340321	-3.128713
26	6	0	-10.685381	3.834810	-1.290233
27	6	0	-10.083239	3.490228	-2.500555
28	1	0	-8.969721	-3.038504	-3.885879
29	1	0	-12.934803	-1.271031	-1.376529
30	1	0	-11.894620	-4.778611	-0.608653
31	1	0	-13.185978	-3.592155	-0.379591
32	1	0	-12.786971	-1.637351	1.266999
33	1	0	-8.927257	-4.298366	3.040727
34	1	0	-8.806738	2.918614	3.894184
35	1	0	-12.865489	0.956253	1.698658
36	1	0	-12.974065	1.344691	-0.963684
37	1	0	-9.275663	4.092800	-2.939447
38	1	0	-13.265147	0.361881	-3.330316
39	1	0	-11.956218	0.567972	-4.501313
40	1	0	-13.315761	3.256197	0.727390
41	1	0	-12.076224	4.511001	0.855760
42	1	0	-11.564983	-0.815668	4.738172
43	1	0	-12.966902	-0.673712	3.670272
44	8	0	-9.640859	0.576030	4.909062
45	8	0	-9.610177	-2.179563	4.509976
46	8	0	-10.322053	5.045259	-0.648842
47	8	0	-9.985432	4.471710	2.050943
48	8	0	-10.001020	1.969747	-4.378563
49	8	0	-10.028131	-0.769643	-4.863668
50	8	0	-10.039485	-5.260841	0.792985
51	8	0	-9.862334	-4.600316	-1.902037
52	6	0	-8.448706	-1.459446	4.316678
53	6	0	-8.455429	-0.055743	4.583888
54	7	0	-7.316559	0.699508	4.559768
55	7	0	-7.314840	-2.124269	3.934147
56	6	0	-6.208887	0.027453	4.228708
57	6	0	-6.212041	-1.367218	3.883790
58	6	0	-4.799585	0.569690	4.079777
59	6	0	-4.809938	-1.758993	3.442222
60	7	0	-4.054466	-0.557604	3.600371
61	8	0	-4.332580	1.651809	4.288513
62	1	0	-3.049644	-0.474399	3.333155
63	8	0	-4.358644	-2.795202	3.040776
64	6	0	-8.869194	4.587956	1.251657
65	6	0	-9.047760	4.980884	-0.110613

66	6	0	-11.513539	2.635147	1.752974
67	7	0	-8.002322	5.328848	-0.917501
68	7	0	-7.629893	4.432232	1.808725
69	6	0	-8.826448	-0.118996	-4.640249
70	6	0	-8.820088	1.263534	-4.281968
71	6	0	-8.799102	-5.101245	0.192542
72	6	0	-8.710704	-4.615062	-1.149115
73	7	0	-7.673786	1.916188	-3.915459
74	7	0	-7.678246	-0.847032	-4.772257
75	7	0	-7.695892	-5.417379	0.931552
76	7	0	-7.515029	-4.276780	-1.721967
77	6	0	-6.611007	4.740182	0.995063
78	6	0	-6.441800	-4.529769	-0.960264
79	6	0	-6.798185	5.223552	-0.343856
80	6	0	-6.560032	-0.180487	-4.468582
81	6	0	-6.561186	1.174714	-3.991848
82	6	0	-6.530366	-5.156437	0.328862
83	6	0	-5.128095	-5.379108	0.874297
84	6	0	-4.977280	-4.213254	-1.236079
85	6	0	-5.116541	4.624856	1.261385
86	6	0	-5.440454	5.511658	-0.965502
87	6	0	-5.134989	-0.706160	-4.479074
88	6	0	-5.141109	1.537936	-3.581903
89	7	0	-4.288511	-4.760243	-0.117491
90	7	0	-4.383758	0.374293	-3.892094
91	7	0	-4.516649	5.119417	0.066013
92	8	0	-4.456669	-3.610613	-2.134584
93	8	0	-4.733776	-5.934913	1.852820
94	8	0	-4.663034	-1.726940	-4.874183
95	8	0	-4.690210	2.540984	-3.097199
96	8	0	-4.512152	4.202655	2.206980
97	8	0	-5.126743	5.965831	-2.022789
98	1	0	-3.489200	5.105394	-0.081699
99	1	0	-3.363782	0.281891	-3.687330
100	1	0	-3.250959	-4.693975	-0.008760
101	1	0	13.252684	3.550568	0.437202
102	6	0	12.148158	3.655272	0.496069
103	6	0	11.513322	3.351070	-0.830653
104	6	0	11.587980	2.789107	1.590701
105	1	0	11.977491	4.734272	0.754296
106	6	0	11.949649	2.272375	-1.617650
107	6	0	10.451418	4.135307	-1.318354
108	6	0	12.153557	1.547968	1.912739
109	6	0	10.481276	3.220290	2.351349
110	6	0	11.311627	1.934605	-2.818762
111	1	0	12.796018	1.675022	-1.277027
112	6	0	9.773245	3.836308	-2.500837
113	8	0	10.080817	5.296406	-0.589487
114	6	0	11.649029	0.761024	2.960123
115	1	0	13.003335	1.182570	1.335286
116	6	0	9.955686	2.493459	3.415982
117	8	0	9.981177	4.511864	2.073373
118	6	0	11.802720	0.819163	-3.697208
119	6	0	10.208437	2.720276	-3.209354
120	1	0	8.927095	4.443733	-2.851954
121	6	0	8.856695	5.115021	0.037489
122	6	0	12.240819	-0.580136	3.289813
123	6	0	10.573901	1.276956	3.708242
124	1	0	9.102194	2.863854	4.000850
125	6	0	8.807337	4.569600	1.359078
126	1	0	12.914981	0.830017	-3.737723
127	1	0	11.481399	1.022197	-4.754979
128	6	0	11.316084	-0.544704	-3.297441
129	8	0	9.532536	2.366907	-4.408712
130	7	0	7.732175	5.478940	-0.645787
131	6	0	11.657880	-1.681416	2.448103
132	1	0	12.060006	-0.809074	4.374128
133	1	0	13.347283	-0.555624	3.188665
134	8	0	10.162867	0.549020	4.853619
135	7	0	7.629098	4.216503	1.956742
136	6	0	11.980087	-1.310459	-2.328223
137	6	0	10.199868	-1.125395	-3.931950
138	6	0	8.392275	1.631967	-4.142058
139	6	0	6.583858	5.206453	-0.013508
140	6	0	12.193625	-2.014084	1.195859
141	6	0	10.565244	-2.440840	2.912296
142	6	0	8.947381	-0.082846	4.661155
143	6	0	6.534239	4.518454	1.245566
144	6	0	11.557805	-2.608132	-2.001267
145	1	0	12.840704	-0.885198	-1.810812
146	6	0	9.760120	-2.421710	-3.673632
147	8	0	9.527560	-0.362563	-4.924808
148	6	0	8.385682	0.230910	-4.420141
149	7	0	7.301895	2.280951	-3.630112
150	6	0	5.163600	5.490257	-0.480652
151	6	0	11.668825	-3.065332	0.429549
152	1	0	13.037118	-1.441858	0.808224
153	6	0	10.008161	-3.499969	2.197991
154	8	0	10.099052	-2.160419	4.218498
155	6	0	8.916579	-1.454075	4.263133
156	7	0	7.810420	0.639542	4.892681
157	6	0	5.079532	4.216124	1.567936
158	6	0	12.232808	-3.406846	-0.921660
159	6	0	10.467627	-3.144440	-2.713704
160	1	0	8.896206	-2.851045	-4.201134
161	7	0	7.281344	-0.550571	-4.216647
162	6	0	6.231513	1.503635	-3.430710
163	7	0	4.351155	4.847419	0.523424
164	8	0	4.736388	6.106207	-1.407378
165	6	0	10.593799	-3.800145	0.968768
166	1	0	9.159245	-4.077578	2.590716
167	7	0	7.746886	-2.112135	3.998828
168	6	0	6.672588	-0.028280	4.672868
169	8	0	4.591060	3.565738	2.453386
170	1	0	12.091832	-4.502316	-1.120090
171	1	0	13.332544	-3.254512	-0.944107
172	8	0	10.140260	-4.501130	-2.478826
173	6	0	6.217803	0.099979	-3.731432
174	6	0	4.884591	1.888057	-2.842035
175	1	0	3.308738	4.820114	0.474861

176	8	0	10.190896	-4.956577	0.263953
177	6	0	6.642553	-1.382439	4.194646
178	6	0	5.246610	0.480635	4.809617
179	6	0	8.950784	-4.664170	-1.791900
180	6	0	4.854573	-0.463095	-3.364300
181	7	0	4.147161	0.664014	-2.844120
182	8	0	4.469279	2.934697	-2.429276
183	6	0	8.973445	-4.862092	-0.377388
184	6	0	5.197625	-1.773522	3.935022
185	7	0	4.455497	-0.622093	4.332181
186	8	0	4.798452	1.507218	5.220563
187	7	0	7.792743	-4.690342	-2.517109
188	8	0	4.411971	-1.574178	-3.444550
189	1	0	3.136102	0.625744	-2.585584
190	7	0	7.833719	-5.058753	0.352293
191	8	0	4.720014	-2.784909	3.501854
192	1	0	3.426438	-0.557634	4.206552
193	6	0	6.687010	-4.905130	-1.794487
194	6	0	6.705629	-5.075718	-0.368671
195	6	0	5.246826	-4.958538	-2.281814
196	6	0	5.273572	-5.225659	0.126432
197	7	0	4.492368	-5.113716	-1.070379
198	8	0	4.773316	-4.905952	-3.376608
199	8	0	4.822376	-5.396026	1.219535
200	1	0	3.456694	-5.087235	-1.056483
201	8	0	1.896331	-3.928134	-1.011801
202	6	0	1.244606	-3.694418	-2.032740
203	7	0	-0.059773	-4.165363	-2.300177
204	7	0	1.711908	-2.980611	-3.141983
205	6	0	-0.600997	-3.564467	-3.546668
206	1	0	-0.699305	-4.420475	-1.523377
207	6	0	0.658895	-2.792596	-4.169342
208	1	0	2.672627	-2.646775	-3.259512
209	1	0	-1.027900	-4.366780	-4.197551
210	7	0	-1.587700	-2.482644	-3.325916
211	1	0	0.991586	-3.170842	-5.166705
212	7	0	0.189238	-1.390998	-4.294985
213	6	0	-1.072152	-1.224397	-3.659964
214	1	0	-2.486640	-2.640028	-2.864843
215	1	0	0.876743	-0.613410	-4.258828
216	8	0	-1.646374	-0.144740	-3.538905
217	1	0	1.425656	-5.122342	3.309621
218	6	0	0.962152	-4.258580	2.773036
219	6	0	-0.362308	-3.677423	3.464396
220	7	0	0.498161	-4.700410	1.433701
221	7	0	1.869532	-3.084736	2.704577
222	1	0	-0.675993	-4.215523	4.392902
223	7	0	0.006450	-2.278486	3.808621
224	7	0	-1.384870	-3.801144	2.404294
225	6	0	-0.851347	-4.315336	1.212826
226	1	0	1.164616	-4.701023	0.640457
227	6	0	1.280773	-1.943119	3.292409
228	1	0	2.891993	-3.206200	2.656633
229	1	0	-0.722228	-1.544412	3.857759
230	1	0	-2.358709	-3.513391	2.526562
231	8	0	-1.470275	-4.503477	0.171142
232	8	0	1.815946	-0.844589	3.380625
233	6	0	-0.920052	1.309764	3.483602
234	7	0	0.375942	1.602250	3.962195
235	7	0	-1.607952	2.513108	3.203523
236	8	0	-1.388069	0.182219	3.369952
237	6	0	0.658343	3.061345	3.905707
238	1	0	1.137532	0.913394	3.832145
239	6	0	-0.733249	3.693323	3.422718
240	1	0	-2.629023	2.594200	3.302999
241	1	0	1.008337	3.408245	4.909579
242	7	0	1.602243	3.461156	2.843051
243	1	0	-1.182115	4.425697	4.136943
244	7	0	-0.386534	4.393099	2.156907
245	6	0	0.962624	4.135114	1.791707
246	1	0	2.604372	3.247350	2.869115
247	1	0	-1.106301	4.467223	1.414155
248	8	0	1.509847	4.541177	0.771089
249	1	0	0.836474	5.257121	-3.492376
250	6	0	0.459626	4.339087	-2.978112
251	6	0	-0.802478	3.641522	-3.681886
252	7	0	-0.044084	4.687453	-1.625607
253	7	0	1.484581	3.270697	-2.987136
254	1	0	-1.188695	4.177992	-4.582012
255	7	0	-0.298215	2.300758	-4.071589
256	7	0	-1.814416	3.603968	-2.597828
257	6	0	-1.311806	4.114291	-1.394554
258	1	0	0.617598	4.844335	-0.840110
259	6	0	0.980097	2.062649	-3.496662
260	1	0	2.374399	3.351851	-2.486929
261	1	0	-0.963660	1.505111	-4.136798
262	1	0	-2.764491	3.241670	-2.725121
263	8	0	-1.911565	4.113100	-0.317175
264	8	0	1.592213	1.001041	-3.552065
265	6	0	-5.894415	-0.799343	-0.230345
266	6	0	-4.515646	-0.824970	-0.381993
267	6	0	-3.726151	0.187252	0.166368
268	6	0	-4.340672	1.216811	0.876721
269	6	0	-5.723911	1.227093	1.041558
270	6	0	-6.519728	0.225353	0.489274
271	1	0	-6.499068	-1.588427	-0.671016
272	1	0	-4.018257	-1.627372	-0.918925
273	1	0	-3.749664	2.003573	1.345912
274	1	0	-6.187460	2.021784	1.623689
275	6	0	-8.022319	0.251650	0.636044
276	6	0	-8.721218	0.597315	-0.682722
277	1	0	-8.299857	0.983655	1.402513
278	1	0	-8.374315	-0.725526	0.984516
279	1	0	-9.806972	0.633011	-0.553301
280	1	0	-8.383957	1.568997	-1.055124
281	1	0	-8.495162	-0.151489	-1.446544
282	8	0	-1.732258	-1.028216	-0.236289
283	6	0	5.375040	-1.580717	0.061579
284	6	0	3.999912	-1.480383	-0.114711
285	6	0	3.334795	-0.302622	0.233458

286	6	0	4.065111	0.762008	0.760163
287	6	0	5.437887	0.647754	0.947456
288	6	0	6.112595	-0.524729	0.600220
289	1	0	5.887348	-2.498039	-0.214086
290	1	0	3.453626	-2.318339	-0.551902
291	1	0	3.533897	1.671036	1.025175
292	1	0	5.991705	1.476016	1.383894
293	6	0	7.611033	-0.642195	0.743368
294	6	0	8.332171	-0.394462	-0.587355
295	1	0	7.863477	-1.643024	1.115034
296	1	0	7.964480	0.076170	1.489713
297	1	0	9.414826	-0.500520	-0.471534
298	1	0	7.997470	-1.107791	-1.346269
299	1	0	8.122440	0.613367	-0.953363
300	8	0	1.374528	1.011101	-0.033652
301	1	0	-1.964651	2.094423	0.257861
302	1	0	1.523279	-2.135319	0.231183
303	1	0	0.093596	-1.171409	-0.105506
304	1	0	-0.495727	1.156774	0.051074
305	7	0	1.111597	-1.240581	0.001696
306	7	0	-1.516151	1.196834	0.130045
307	6	0	1.852392	-0.124932	0.062637
308	6	0	-2.235227	0.075495	0.002668

AB-trans, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.185985	0.759350	3.494264
2	6	0	-11.731682	-0.573440	3.921797
3	6	0	-12.106248	-1.374512	-1.682959
4	6	0	-11.606219	-2.642610	-1.354115
5	6	0	-12.200869	-3.454434	-0.235770
6	6	0	-11.539788	-3.138034	1.076151
7	6	0	-11.949056	-2.050369	1.864229
8	6	0	-11.275111	-1.705731	3.044351
9	6	0	-11.821118	1.527458	2.505315
10	6	0	-12.011332	3.609936	1.066970
11	6	0	-11.529087	3.290494	-0.319357
12	6	0	-12.041265	2.199684	-1.040017
13	6	0	-11.537081	1.852709	-2.300718
14	6	0	-11.560267	-0.618732	-2.731099
15	6	0	-12.118168	0.724416	-3.104915
16	6	0	-10.159605	-2.487775	3.407224
17	6	0	-10.469988	-3.923796	1.545196
18	6	0	-9.747243	-3.611502	2.696685
19	6	0	-10.132261	3.226770	2.722565
20	6	0	-10.031336	1.293726	4.096367
21	6	0	-9.471755	2.515647	3.720690
22	6	0	-10.534458	-3.142282	-2.121882
23	6	0	-10.490233	-1.178999	-3.455650
24	6	0	-9.949881	-2.432342	-3.169313
25	6	0	-10.482903	2.632724	-2.817953
26	6	0	-10.534861	4.075060	-0.932926
27	6	0	-9.979951	3.759489	-2.174153
28	1	0	-9.111386	-2.844508	-3.748440
29	1	0	-12.939138	-0.965377	-1.110082
30	1	0	-12.079228	-4.546483	-0.463517
31	1	0	-13.298672	-3.298323	-0.174503
32	1	0	-12.803058	-1.453013	1.543769
33	1	0	-8.890861	-4.216227	3.026358
34	1	0	-8.556441	2.901343	4.191815
35	1	0	-12.729844	1.145921	2.038712
36	1	0	-12.840946	1.601618	-0.602228
37	1	0	-9.181211	4.366612	-2.623205
38	1	0	-13.226861	0.722141	-3.016806
39	1	0	-11.922021	0.912270	-4.195080
40	1	0	-13.113256	3.489648	1.138517
41	1	0	-11.827385	4.695371	1.286313
42	1	0	-11.413171	-0.778242	4.979269
43	1	0	-12.842345	-0.542819	3.964429
44	8	0	-9.451442	0.576159	5.176655
45	8	0	-9.477006	-2.141424	4.599403
46	8	0	-10.112335	5.254126	-0.265075
47	8	0	-9.686022	4.522650	2.382132
48	8	0	-9.968451	2.284338	-4.092072
49	8	0	-10.011735	-0.458129	-4.579392
50	8	0	-10.166461	-5.110134	0.832280
51	8	0	-10.131525	-4.473384	-1.871677
52	6	0	-8.318220	-1.425226	4.383731
53	6	0	-8.282704	-0.054334	4.783826
54	7	0	-7.128038	0.675939	4.794928
55	7	0	-7.226804	-2.058605	3.854509
56	6	0	-6.054760	0.026540	4.330689
57	6	0	-6.116355	-1.311685	3.812972
58	6	0	-4.637009	0.550929	4.181052
59	6	0	-4.762974	-1.656867	3.213991
60	7	0	-3.964650	-0.509110	3.469299
61	8	0	-4.109236	1.554060	4.550401
62	1	0	-2.975094	-0.411168	3.143479
63	8	0	-4.388145	-2.646705	2.642513
64	6	0	-8.604800	4.587929	1.532317
65	6	0	-8.820338	5.105112	0.217996
66	6	0	-11.314075	2.770365	2.102199
67	7	0	-7.792358	5.461826	-0.606773
68	7	0	-7.357744	4.260556	1.990283
69	6	0	-8.807713	0.174830	-4.330943
70	6	0	-8.788617	1.569735	-4.026140
71	6	0	-8.957316	-5.023450	0.163799
72	6	0	-8.933355	-4.616293	-1.205713
73	7	0	-7.629535	2.239537	-3.738391
74	7	0	-7.664077	-0.567584	-4.433186
75	7	0	-7.826314	-5.370100	0.846711
76	7	0	-7.766041	-4.462566	-1.900640
77	6	0	-6.361239	4.551386	1.143582
78	6	0	-6.661454	-4.773105	-1.209345
79	6	0	-6.574112	5.207962	-0.116222
80	6	0	-6.536154	0.109245	-4.193286

81	6	0	-6.519334	1.496690	-3.816605
82	6	0	-6.693898	-5.255524	0.142568
83	6	0	-5.272978	-5.532986	0.607181
84	6	0	-5.210656	-4.658192	-1.649751
85	6	0	-4.873418	4.251350	1.280375
86	6	0	-5.228255	5.470193	-0.775657
87	6	0	-5.111202	-0.414508	-4.206091
88	6	0	-5.082421	1.901634	-3.520914
89	7	0	-4.474187	-5.140187	-0.522931
90	7	0	-4.333377	0.716428	-3.797314
91	7	0	-4.295660	4.844293	0.121743
92	8	0	-4.714376	-4.255342	-2.662243
93	8	0	-4.836290	-5.983405	1.622373
94	8	0	-4.655981	-1.488322	-4.478419
95	8	0	-4.600573	2.932641	-3.143872
96	8	0	-4.267796	3.631653	2.109852
97	8	0	-4.932306	6.058384	-1.770248
98	1	0	-3.270336	4.799299	-0.075858
99	1	0	-3.300451	0.657283	-3.686139
100	1	0	-3.440787	-5.117803	-0.496227
101	1	0	13.410244	3.155942	0.575881
102	6	0	12.313423	3.328908	0.589537
103	6	0	11.697872	2.975688	-0.735371
104	6	0	11.660026	2.561830	1.705814
105	1	0	12.200122	4.429814	0.775635
106	6	0	12.118454	1.845039	-1.453920
107	6	0	10.672561	3.765761	-1.290407
108	6	0	12.127270	1.303153	2.109522
109	6	0	10.550568	3.099900	2.388450
110	6	0	11.509841	1.474583	-2.660674
111	1	0	12.932335	1.236588	-1.057943
112	6	0	10.020954	3.433324	-2.478976
113	8	0	10.349392	4.982212	-0.642451
114	6	0	11.501676	0.587265	3.140592
115	1	0	12.996384	0.871747	1.612071
116	6	0	9.873819	2.423042	3.401617
117	8	0	10.213449	4.435731	2.080203
118	6	0	11.989529	0.302857	-3.468897
119	6	0	10.451653	2.279368	-3.127829
120	1	0	9.206767	4.051475	-2.883212
121	6	0	9.117642	4.945728	-0.010333
122	6	0	12.024644	-0.744186	3.603150
123	6	0	10.377119	1.172650	3.756610
124	1	0	9.000081	2.858266	3.907097
125	6	0	9.042647	4.603050	1.374006
126	1	0	13.101528	0.256146	-3.449697
127	1	0	11.735255	0.478253	-4.549489
128	6	0	11.413356	-1.017075	-3.042250
129	8	0	9.840727	1.907373	-4.355892
130	7	0	8.015644	5.299959	-0.736902
131	6	0	11.437687	-1.880559	2.815280
132	1	0	11.781580	-0.879646	4.690985
133	1	0	13.134696	-0.767016	3.558463
134	8	0	9.832149	0.494754	4.869696
135	7	0	7.855227	4.529202	2.047860
136	6	0	11.970449	-1.759086	-1.991292
137	6	0	10.318822	-1.581969	-3.727663
138	6	0	8.650716	1.237523	-4.154246
139	6	0	6.864413	5.268246	-0.054494
140	6	0	11.984284	-2.279965	1.585766
141	6	0	10.319627	-2.586642	3.298707
142	6	0	8.646039	-0.167712	4.644401
143	6	0	6.782001	4.854965	1.318272
144	6	0	11.468600	-3.020662	-1.633365
145	1	0	12.806692	-1.341428	-1.429209
146	6	0	9.818210	-2.851584	-3.451775
147	8	0	9.734045	-0.837766	-4.787845
148	6	0	8.592665	-0.173536	-4.378963
149	7	0	7.557127	1.961283	-3.766530
150	6	0	5.463533	5.591128	-0.556548
151	6	0	11.420165	-3.322165	0.837595
152	1	0	12.865556	-1.763997	1.203245
153	6	0	9.704145	-3.616716	2.585975
154	8	0	9.865676	-2.276520	4.604226
155	6	0	8.660987	-1.595378	4.598683
156	7	0	7.484735	0.554029	4.585824
157	6	0	5.318767	4.826638	1.736367
158	6	0	12.023086	-3.780018	-0.462008
159	6	0	10.421137	-3.553760	-2.407521
160	1	0	8.983233	-3.274823	-4.027606
161	7	0	7.436989	-0.890400	-4.230822
162	6	0	6.434441	1.247031	-3.628749
163	7	0	4.627124	5.277417	0.567852
164	8	0	5.072936	6.016942	-1.600920
165	6	0	10.274205	-3.954985	1.361603
166	1	0	8.820253	-4.140586	2.975058
167	7	0	7.515404	-2.339546	4.600540
168	6	0	6.369879	-0.186403	4.554390
169	8	0	4.797221	4.499413	2.761514
170	1	0	11.821699	-4.876010	-0.597283
171	1	0	13.131021	-3.699426	-0.430676
172	8	0	9.991112	-4.878849	-2.129079
173	6	0	6.371446	-0.167337	-3.863407
174	6	0	5.066490	1.731996	-3.185595
175	1	0	3.590021	5.294051	0.520572
176	8	0	9.770815	-5.061573	0.638653
177	6	0	6.386535	-1.622111	4.604759
178	6	0	4.922612	0.278121	4.458332
179	6	0	8.742097	-4.874317	-1.528059
180	6	0	4.952346	-0.639257	-3.591338
181	7	0	4.259387	0.549411	-3.210737
182	8	0	4.677402	2.815421	-2.852618
183	6	0	8.636006	-4.828229	-0.101179
184	6	0	4.956030	-2.136085	4.628957
185	7	0	4.172667	-0.934590	4.571649
186	8	0	4.442321	1.364564	4.310900
187	7	0	7.647466	-4.914669	-2.342173
188	8	0	4.453864	-1.730072	-3.638267
189	1	0	3.225241	0.577316	-3.039147
190	7	0	7.436457	-4.659820	0.533197

191	8	0	4.510819	-3.242179	4.696531
192	1	0	3.143394	-0.962467	4.469492
193	6	0	6.474423	-4.825603	-1.702695
194	6	0	6.374578	-4.635280	-0.283910
195	6	0	5.079865	-4.829817	-2.304114
196	6	0	4.917449	-4.387094	0.066158
197	7	0	4.232359	-4.531759	-1.172713
198	8	0	4.679264	-5.039779	-3.406877
199	8	0	4.397714	-4.096314	1.109815
200	1	0	3.204170	-4.402342	-1.268492
201	8	0	1.478348	-3.771545	-1.401824
202	6	0	0.930674	-3.513912	-2.477232
203	7	0	-0.367858	-3.921751	-2.855883
204	7	0	1.536275	-2.837659	-3.542152
205	6	0	-0.754989	-3.320152	-4.162768
206	1	0	-1.090770	-4.089119	-2.130904
207	6	0	0.590710	-2.601601	-4.658979
208	1	0	2.520022	-2.555996	-3.574400
209	1	0	-1.134839	-4.123200	-4.840456
210	7	0	-1.713968	-2.201942	-4.030354
211	1	0	0.996673	-2.989831	-5.625075
212	7	0	0.199453	-1.178031	-4.815488
213	6	0	-1.118967	-0.963203	-4.330005
214	1	0	-2.728589	-2.341897	-3.958982
215	1	0	0.909772	-0.434395	-4.661423
216	8	0	-1.665262	0.129735	-4.252843
217	1	0	0.807810	-5.609534	2.626461
218	6	0	0.525837	-4.614430	2.206394
219	6	0	-0.660529	-3.872509	2.987400
220	7	0	-0.009681	-4.794076	0.825824
221	7	0	1.635142	-3.639313	2.262712
222	1	0	-1.077896	-4.442986	3.852824
223	7	0	-0.039692	-2.611199	3.470005
224	7	0	-1.680067	-3.664601	1.932784
225	6	0	-1.242081	-4.104266	0.682865
226	1	0	0.656332	-4.782730	0.030858
227	6	0	1.262935	-2.453573	2.926404
228	1	0	2.604849	-3.893394	2.050668
229	1	0	-0.634482	-1.761722	3.566829
230	1	0	-2.607530	-3.261871	2.119473
231	8	0	-1.871394	-3.982080	-0.371373
232	8	0	1.975833	-1.467311	3.046770
233	6	0	-0.657431	0.987336	3.122360
234	7	0	0.660834	1.126848	3.638289
235	7	0	-1.240720	2.250480	2.986525
236	8	0	-1.224542	-0.091026	2.944707
237	6	0	1.056276	2.563809	3.685428
238	1	0	1.368167	0.418480	3.381344
239	6	0	-0.273313	3.341259	3.243538
240	1	0	-2.202424	2.424882	2.688191
241	1	0	1.420059	2.806417	4.714293
242	7	0	2.039585	2.952315	2.653085
243	1	0	-0.672084	4.055603	4.005784
244	7	0	0.143250	4.091247	2.030688
245	6	0	1.466330	3.751434	1.651382
246	1	0	3.039796	2.769979	2.751534
247	1	0	-0.563832	4.322331	1.306725
248	8	0	2.046751	4.171961	0.652319
249	1	0	1.300962	5.342640	-3.503118
250	6	0	0.836916	4.460722	-2.996615
251	6	0	-0.503461	3.917287	-3.690237
252	7	0	0.405072	4.836427	-1.629356
253	7	0	1.740175	3.285586	-3.039090
254	1	0	-0.838686	4.502120	-4.581221
255	7	0	-0.143064	2.536700	-4.105703
256	7	0	-1.500597	3.984637	-2.599055
257	6	0	-0.931639	4.420695	-1.390389
258	1	0	1.093339	4.804018	-0.849632
259	6	0	1.110136	2.155460	-3.575471
260	1	0	2.692831	3.302480	-2.667228
261	1	0	-0.875291	1.823951	-4.271302
262	1	0	-2.470020	3.679742	-2.704258
263	8	0	-1.513890	4.529634	-0.317466
264	8	0	1.609239	1.032552	-3.662897
265	6	0	-6.115702	-1.140102	-1.151442
266	6	0	-4.723233	-1.167742	-1.119264
267	6	0	-3.988094	-0.155128	-0.496236
268	6	0	-4.703889	0.886655	0.110044
269	6	0	-6.091656	0.911497	0.092386
270	6	0	-6.818799	-0.099506	-0.545241
271	1	0	-6.662362	-1.929040	-1.665815
272	1	0	-4.209985	-1.990016	-1.624442
273	1	0	-4.146063	1.684423	0.594601
274	1	0	-6.626495	1.726475	0.575278
275	6	0	-8.328232	-0.069049	-0.540195
276	6	0	-8.901662	-0.365399	0.848717
277	1	0	-8.711523	-0.801536	-1.259084
278	1	0	-8.677701	0.915922	-0.870595
279	1	0	-9.995748	-0.342331	0.835826
280	1	0	-8.580844	-1.352303	1.194551
281	1	0	-8.555952	0.374835	1.575620
282	8	0	-1.665429	-1.254904	-0.724502
283	6	0	5.281087	-0.592954	1.034670
284	6	0	3.920592	-0.807589	0.824964
285	6	0	3.112048	0.219896	0.339637
286	6	0	3.680211	1.469651	0.082224
287	6	0	5.038458	1.669409	0.277391
288	6	0	5.860252	0.645441	0.761971
289	1	0	5.892784	-1.400057	1.428830
290	1	0	3.488154	-1.770879	1.097806
291	1	0	3.033947	2.277307	-0.254748
292	1	0	5.469450	2.643234	0.066046
293	6	0	7.332509	0.896635	0.991650
294	6	0	8.096767	1.188199	-0.303996
295	1	0	7.773349	0.027097	1.488220
296	1	0	7.444763	1.740119	1.685982
297	1	0	9.152329	1.385424	-0.097315
298	1	0	8.035480	0.334465	-0.982546
299	1	0	7.682526	2.058829	-0.821233
300	8	0	0.900049	1.047898	0.108525

301	1	0	1.803604	-1.971349	-0.218267
302	1	0	0.187847	-1.309344	-0.292561
303	1	0	-0.821072	1.003948	-0.132962
304	7	0	1.179932	-1.185340	-0.097673
305	6	0	1.639902	0.056073	0.110297
306	1	0	-2.191493	-2.066969	-0.784289
307	8	0	-1.801402	1.045352	-0.210850
308	5	0	-2.414019	-0.122056	-0.472936

AB-cis, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.173391	0.860236	3.328552
2	6	0	-11.703590	-0.462279	3.804372
3	6	0	-12.061813	-1.466970	-1.765087
4	6	0	-11.587920	-2.738422	-1.405351
5	6	0	-12.171068	-3.492207	-0.242200
6	6	0	-11.485342	-3.108107	1.039811
7	6	0	-11.905146	-2.002736	1.795401
8	6	0	-11.232898	-1.615641	2.963413
9	6	0	-11.823184	1.589557	2.320525
10	6	0	-12.040380	3.623115	0.816107
11	6	0	-11.527848	3.270535	-0.551527
12	6	0	-12.004226	2.145727	-1.243547
13	6	0	-11.466840	1.760703	-2.480139
14	6	0	-11.485241	-0.739892	-2.816087
15	6	0	-12.018890	0.595380	-3.250891
16	6	0	-10.109119	-2.372650	3.351212
17	6	0	-10.387650	-3.850768	1.517214
18	6	0	-9.667494	-3.497152	2.657655
19	6	0	-10.169272	3.327342	2.497324
20	6	0	-10.019338	1.423791	3.905774
21	6	0	-9.485732	2.648213	3.502893
22	6	0	-10.537884	-3.288836	-2.166720
23	6	0	-10.403558	-1.330938	-3.498852
24	6	0	-9.914193	-2.601976	-3.207936
25	6	0	-10.417495	2.542764	-3.003380
26	6	0	-10.536828	4.053470	-1.173379
27	6	0	-9.952907	3.703925	-2.391436
28	1	0	-9.077041	-3.039599	-3.770302
29	1	0	-12.893640	-1.032704	-1.209702
30	1	0	-12.055648	-4.594899	-0.413816
31	1	0	-13.266978	-3.329060	-0.171282
32	1	0	-12.769779	-1.427721	1.462807
33	1	0	-8.796350	-4.076278	2.996279
34	1	0	-8.575439	3.060303	3.961426
35	1	0	-12.725911	1.180066	1.866328
36	1	0	-12.802683	1.549149	-0.801138
37	1	0	-9.156920	4.310519	-2.846606
38	1	0	-13.130523	0.598652	-3.198221
39	1	0	-11.788692	0.740095	-4.341349
40	1	0	-13.140067	3.479945	0.875252
41	1	0	-11.883583	4.718476	1.004358
42	1	0	-11.381240	-0.626893	4.867705
43	1	0	-12.814330	-0.443196	3.848038
44	8	0	-9.429616	0.741703	5.000741
45	8	0	-9.461943	-2.005348	4.556333
46	8	0	-10.149231	5.263772	-0.543383
47	8	0	-9.766507	4.630780	2.134006
48	8	0	-9.837012	2.154912	-4.241355
49	8	0	-9.836529	-0.601926	-4.577161
50	8	0	-10.078432	-5.052089	0.837397
51	8	0	-10.178623	-4.631244	-1.904278
52	6	0	-8.288156	-1.305782	4.360673
53	6	0	-8.260602	0.092612	4.646147
54	7	0	-7.105557	0.824360	4.616755
55	7	0	-7.174472	-1.992608	3.960185
56	6	0	-6.017099	0.133728	4.260967
57	6	0	-6.058298	-1.257658	3.903057
58	6	0	-4.594278	0.641260	4.096809
59	6	0	-4.676129	-1.676637	3.432324
60	7	0	-3.884886	-0.504470	3.590000
61	8	0	-4.085847	1.698457	4.318295
62	1	0	-2.880297	-0.447925	3.303460
63	8	0	-4.274149	-2.728217	3.013507
64	6	0	-8.666212	4.714658	1.310602
65	6	0	-8.863732	5.166415	-0.029781
66	6	0	-11.337961	2.829890	1.884178
67	7	0	-7.826049	5.518326	-0.845044
68	7	0	-7.421704	4.462995	1.819527
69	6	0	-8.665110	0.032899	-4.214363
70	6	0	-8.660456	1.452185	-4.051600
71	6	0	-8.899687	-5.002258	0.119370
72	6	0	-8.949880	-4.781276	-1.290922
73	7	0	-7.523965	2.148876	-3.741965
74	7	0	-7.538909	-0.726211	-4.054039
75	7	0	-7.728909	-5.241196	0.782868
76	7	0	-7.829470	-4.793057	-2.074228
77	6	0	-6.413398	4.756560	0.988925
78	6	0	-6.689377	-5.030960	-1.413440
79	6	0	-6.613238	5.335069	-0.310327
80	6	0	-6.437447	-0.031819	-3.749472
81	6	0	-6.425201	1.396722	-3.602585
82	6	0	-6.640148	-5.253254	0.004572
83	6	0	-5.192160	-5.445399	0.426777
84	6	0	-5.273427	-5.072329	-1.967649
85	6	0	-4.920148	4.532501	1.193056
86	6	0	-5.256829	5.611543	-0.943549
87	6	0	-5.044189	-0.565560	-3.474264
88	6	0	-5.012181	1.835106	-3.249841
89	7	0	-4.464352	-5.280574	-0.800691
90	7	0	-4.274646	0.608563	-3.209099
91	7	0	-4.329418	5.081949	0.016697
92	8	0	-4.845668	-4.981517	-3.079496
93	8	0	-4.692881	-5.692497	1.482818
94	8	0	-4.618526	-1.686838	-3.444808
95	8	0	-4.538298	2.914920	-3.036562

96	8	0	-4.320475	3.997549	2.080816
97	8	0	-4.953412	6.148256	-1.965360
98	1	0	-3.298459	5.060761	-0.144187
99	1	0	-3.247077	0.570072	-3.053122
100	1	0	-3.433006	-5.255813	-0.826317
101	1	0	13.383832	3.200007	0.534148
102	6	0	12.286023	3.366450	0.550458
103	6	0	11.670439	3.014570	-0.774807
104	6	0	11.639048	2.591338	1.665008
105	1	0	12.166601	4.465930	0.740950
106	6	0	12.093291	1.885952	-1.495296
107	6	0	10.642903	3.802650	-1.328285
108	6	0	12.118005	1.337065	2.068431
109	6	0	10.523584	3.117821	2.346956
110	6	0	11.484100	1.514972	-2.701546
111	1	0	12.909208	1.279176	-1.100890
112	6	0	9.990758	3.469553	-2.516441
113	8	0	10.315079	5.017381	-0.678553
114	6	0	11.498285	0.614693	3.098591
115	1	0	12.992038	0.914501	1.571994
116	6	0	9.851376	2.433545	3.358100
117	8	0	10.176921	4.451501	2.040122
118	6	0	11.965795	0.344968	-3.510878
119	6	0	10.422823	2.316903	-3.166671
120	1	0	9.175003	4.086331	-2.919598
121	6	0	9.082786	4.971770	-0.047865
122	6	0	12.034915	-0.711043	3.561829
123	6	0	10.366713	1.188025	3.713207
124	1	0	8.972395	2.859500	3.862212
125	6	0	9.006646	4.613395	1.332714
126	1	0	13.078084	0.303901	-3.496965
127	1	0	11.705473	0.517700	-4.590467
128	6	0	11.397961	-0.977056	-3.079698
129	8	0	9.809570	1.943759	-4.393210
130	7	0	7.980629	5.328505	-0.772723
131	6	0	11.456620	-1.853589	2.776578
132	1	0	11.795632	-0.847261	4.650390
133	1	0	13.145014	-0.723791	3.514566
134	8	0	9.829409	0.505449	4.826891
135	7	0	7.817803	4.519722	2.001302
136	6	0	11.966438	-1.717244	-2.033603
137	6	0	10.300241	-1.545774	-3.756895
138	6	0	8.621079	1.271704	-4.187621
139	6	0	6.827659	5.279712	-0.094102
140	6	0	12.000404	-2.245446	1.543352
141	6	0	10.349218	-2.572254	3.265791
142	6	0	8.651103	-0.171971	4.606274
143	6	0	6.744301	4.845022	1.271805
144	6	0	11.473683	-2.981799	-1.673591
145	1	0	12.805066	-1.296262	-1.477621
146	6	0	9.807626	-2.817924	-3.478536
147	8	0	9.707118	-0.803894	-4.813731
148	6	0	8.566168	-0.140980	-4.402464
149	7	0	7.525728	1.995811	-3.805609
150	6	0	5.426114	5.600124	-0.595331
151	6	0	11.443178	-3.292581	0.796922
152	1	0	12.873421	-1.719028	1.156191
153	6	0	9.741966	-3.609173	2.556024
154	8	0	9.896668	-2.266321	4.572963
155	6	0	8.683639	-1.599837	4.569911
156	7	0	7.480741	0.534705	4.546357
157	6	0	5.280222	4.793801	1.682601
158	6	0	12.041612	-3.740577	-0.508212
159	6	0	10.423128	-3.518965	-2.440774
160	1	0	8.969948	-3.244387	-4.048028
161	7	0	7.412651	-0.859813	-4.246132
162	6	0	6.404812	1.280002	-3.661547
163	7	0	4.588092	5.257993	0.520747
164	8	0	5.034609	6.042324	-1.632234
165	6	0	10.308241	-3.939415	1.327715
166	1	0	8.866500	-4.143677	2.949791
167	7	0	7.547487	-2.358018	4.582559
168	6	0	6.374967	-0.219904	4.524713
169	8	0	4.759058	4.439835	2.699731
170	1	0	11.848425	-4.837703	-0.646353
171	1	0	13.149011	-3.650935	-0.483317
172	8	0	10.004960	-4.847805	-2.162926
173	6	0	6.345661	-0.136763	-3.883050
174	6	0	5.035669	1.765162	-3.221737
175	1	0	3.550766	5.268132	0.470920
176	8	0	9.810718	-5.049169	0.605329
177	6	0	6.409654	-1.654666	4.586594
178	6	0	4.921594	0.225843	4.430650
179	6	0	8.761190	-4.855277	-1.551418
180	6	0	4.928142	-0.610331	-3.603948
181	7	0	4.232286	0.580241	-3.235044
182	8	0	4.643538	2.850435	-2.898159
183	6	0	8.667323	-4.821755	-0.123615
184	6	0	4.985754	-2.186405	4.621470
185	7	0	4.186963	-0.995084	4.551783
186	8	0	4.428210	1.306159	4.280382
187	7	0	7.659705	-4.895070	-2.356452
188	8	0	4.432855	-1.702990	-3.639415
189	1	0	3.199315	0.606057	-3.053820
190	7	0	7.472220	-4.667945	0.522859
191	8	0	4.554550	-3.296588	4.705915
192	1	0	3.157925	-1.037242	4.451830
193	6	0	6.491925	-4.818870	-1.706056
194	6	0	6.403128	-4.643126	-0.284526
195	6	0	5.092296	-4.824536	-2.295629
196	6	0	4.947485	-4.408111	0.080666
197	7	0	4.253083	-4.544372	-1.153985
198	8	0	4.683817	-5.024205	-3.397462
199	8	0	4.434470	-4.133278	1.131947
200	1	0	3.223856	-4.416458	-1.239853
201	8	0	1.503845	-3.784677	-1.356085
202	6	0	0.943403	-3.521137	-2.423635
203	7	0	-0.355691	-3.945798	-2.784347
204	7	0	1.518325	-2.818977	-3.487165
205	6	0	-0.775604	-3.327228	-4.072784

206	1	0	-1.064001	-4.129666	-2.048637
207	6	0	0.549157	-2.582862	-4.586250
208	1	0	2.498022	-2.524198	-3.533005
209	1	0	-1.164881	-4.120634	-4.757043
210	7	0	-1.740811	-2.222469	-3.906832
211	1	0	0.943963	-2.954722	-5.563078
212	7	0	0.134052	-1.163904	-4.718230
213	6	0	-1.167144	-0.970143	-4.178559
214	1	0	-2.723037	-2.363426	-3.646834
215	1	0	0.840534	-0.411309	-4.590252
216	8	0	-1.731354	0.110248	-4.056049
217	1	0	0.825655	-5.698049	2.570065
218	6	0	0.526833	-4.698838	2.172506
219	6	0	-0.638457	-3.973435	2.997292
220	7	0	-0.047655	-4.861613	0.805187
221	7	0	1.633073	-3.718115	2.204841
222	1	0	-1.032636	-4.558136	3.864036
223	7	0	-0.005612	-2.719587	3.485382
224	7	0	-1.684215	-3.740646	1.972606
225	6	0	-1.285440	-4.170809	0.706485
226	1	0	0.603093	-4.829076	-0.002619
227	6	0	1.279118	-2.546821	2.905816
228	1	0	2.600222	-3.972023	1.977796
229	1	0	-0.598723	-1.875005	3.616618
230	1	0	-2.631444	-3.417597	2.211499
231	8	0	-1.931271	-4.016919	-0.333735
232	8	0	1.994873	-1.562280	3.020273
233	6	0	-0.573103	0.926403	3.195021
234	7	0	0.766681	1.083016	3.642301
235	7	0	-1.177956	2.183064	3.088996
236	8	0	-1.138724	-0.156319	3.044074
237	6	0	1.144822	2.525838	3.672013
238	1	0	1.469253	0.382943	3.355703
239	6	0	-0.211885	3.286027	3.284846
240	1	0	-2.162145	2.342120	2.867558
241	1	0	1.547622	2.772962	4.685263
242	7	0	2.078691	2.920799	2.598253
243	1	0	-0.580658	4.007447	4.055729
244	7	0	0.139938	4.027049	2.045090
245	6	0	1.456608	3.719398	1.623428
246	1	0	3.089279	2.788425	2.679605
247	1	0	-0.598161	4.241894	1.348098
248	8	0	2.002539	4.159980	0.613833
249	1	0	1.226203	5.354945	-3.526989
250	6	0	0.776476	4.475754	-3.003111
251	6	0	-0.568071	3.912823	-3.672042
252	7	0	0.359440	4.867229	-1.635247
253	7	0	1.689417	3.308086	-3.044959
254	1	0	-0.916407	4.480288	-4.569169
255	7	0	-0.205629	2.526567	-4.069847
256	7	0	-1.551518	3.989656	-2.570406
257	6	0	-0.973366	4.450355	-1.374582
258	1	0	1.055534	4.837547	-0.862677
259	6	0	1.059719	2.165259	-3.553216
260	1	0	2.646458	3.336431	-2.686038
261	1	0	-0.938860	1.805112	-4.195065
262	1	0	-2.525460	3.695220	-2.666588
263	8	0	-1.548999	4.573873	-0.300577
264	8	0	1.568289	1.045791	-3.634910
265	6	0	-6.209840	-1.282009	0.030607
266	6	0	-4.845989	-1.269420	-0.240164
267	6	0	-4.048269	-0.163997	0.077886
268	6	0	-4.674366	0.933121	0.683025
269	6	0	-6.036459	0.922849	0.961889
270	6	0	-6.823977	-0.184709	0.639242
271	1	0	-6.808016	-2.153321	-0.226460
272	1	0	-4.405635	-2.144885	-0.723401
273	1	0	-4.070172	1.799811	0.942326
274	1	0	-6.498487	1.782304	1.445681
275	6	0	-8.312629	-0.179656	0.884799
276	6	0	-9.094208	0.176000	-0.384314
277	1	0	-8.552308	0.541710	1.673668
278	1	0	-8.632342	-1.165931	1.241766
279	1	0	-10.172089	0.180347	-0.193377
280	1	0	-8.806549	1.165403	-0.748992
281	1	0	-8.892362	-0.550705	-1.176615
282	8	0	-1.786924	-1.227822	-0.582535
283	6	0	5.212303	-0.578204	0.994992
284	6	0	3.851426	-0.792373	0.787451
285	6	0	3.046874	0.228278	0.281062
286	6	0	3.620672	1.470472	0.000800
287	6	0	4.978983	1.670229	0.195528
288	6	0	5.796364	0.653008	0.701223
289	1	0	5.820048	-1.379574	1.406359
290	1	0	3.417340	-1.748983	1.081190
291	1	0	2.976727	2.273356	-0.350970
292	1	0	5.412480	2.639105	-0.032574
293	6	0	7.268191	0.903904	0.934827
294	6	0	8.038404	1.194477	-0.357435
295	1	0	7.706535	0.034590	1.434032
296	1	0	7.378238	1.747358	1.629621
297	1	0	9.093519	1.388546	-0.145827
298	1	0	7.977768	0.341434	-1.036895
299	1	0	7.629583	2.067056	-0.875519
300	8	0	0.845012	1.069906	0.008618
301	1	0	1.708633	-1.974934	-0.164616
302	1	0	0.099810	-1.292684	-0.262291
303	1	0	-0.884130	1.036961	-0.117391
304	7	0	1.097401	-1.172696	-0.097134
305	6	0	1.573279	0.070479	0.056526
306	1	0	-2.293897	-2.053360	-0.550773
307	8	0	-1.866528	1.069973	-0.058277
308	5	0	-2.497532	-0.108668	-0.194973

AC-trans, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-11.639863	-0.494446	-2.942057
2	6	0	-12.092870	0.870307	-3.376000
3	6	0	-12.068820	1.857420	2.214095
4	6	0	-11.480752	3.062454	1.806230
5	6	0	-12.072107	3.891997	0.699880
6	6	0	-11.527950	3.497096	-0.643232
7	6	0	-12.051042	2.406833	-1.356467
8	6	0	-11.497767	1.994582	-2.576857
9	6	0	-12.272847	-1.188518	-1.901523
10	6	0	-12.532168	-3.203272	-0.388286
11	6	0	-11.885129	-2.830897	0.916877
12	6	0	-12.310325	-1.721741	1.662908
13	6	0	-11.674764	-1.357271	2.858633
14	6	0	-11.538244	1.101717	3.271262
15	6	0	-12.156956	-0.201271	3.690492
16	6	0	-10.384849	2.711243	-3.061372
17	6	0	-10.464485	4.213004	-1.224002
18	6	0	-9.863049	3.834242	-2.424801
19	6	0	-10.842764	-3.090542	-2.274761
20	6	0	-10.584795	-1.145591	-3.611281
21	6	0	-10.168824	-2.440079	-3.308761
22	6	0	-10.324837	3.490413	2.491760
23	6	0	-10.410715	1.612760	3.941255
24	6	0	-9.771183	2.794307	3.563136
25	6	0	-10.580535	-2.138902	3.281282
26	6	0	-10.819067	-3.597118	1.428302
27	6	0	-10.131346	-3.264746	2.594676
28	1	0	-8.879146	3.162508	4.088730
29	1	0	-12.957410	1.495108	1.695996
30	1	0	-11.848943	4.975539	0.890477
31	1	0	-13.181285	3.826863	0.709610
32	1	0	-12.900237	1.860444	-0.944594
33	1	0	-9.014661	4.389914	-2.848323
34	1	0	-9.351305	-2.926188	-3.860160
35	1	0	-13.087863	-0.708184	-1.358952
36	1	0	-13.151562	-1.128390	1.303647
37	1	0	-9.284436	-3.862848	2.959394
38	1	0	-13.266058	-0.135040	3.659894
39	1	0	-11.914323	-0.397228	4.769255
40	1	0	-13.623522	-3.000017	-0.364199
41	1	0	-12.450808	-4.311513	-0.544479
42	1	0	-11.829512	1.013982	-4.458992
43	1	0	-13.203787	0.931196	-3.349747
44	8	0	-9.969547	-0.454853	-4.689755
45	8	0	-9.808617	2.295913	-4.291605
46	8	0	-10.527286	-4.804323	0.754724
47	8	0	-10.550159	-4.447567	-2.002611
48	8	0	-9.997003	-1.808188	4.526813
49	8	0	-9.957810	0.917764	5.092805
50	8	0	-10.021462	5.390718	-0.566447
51	8	0	-9.794441	4.750629	2.133897
52	6	0	-8.681797	1.518783	-4.102434
53	6	0	-8.763577	0.108298	-4.321582
54	7	0	-7.677634	-0.714147	-4.202863
55	7	0	-7.514406	2.136032	-3.743880
56	6	0	-6.541496	-0.094666	-3.864229
57	6	0	-6.459610	1.319269	-3.630937
58	6	0	-5.177560	-0.712937	-3.612899
59	6	0	-5.035938	1.659452	-3.218165
60	7	0	-4.360750	0.402299	-3.242941
61	8	0	-4.800595	-1.848828	-3.666443
62	1	0	-3.335845	0.299418	-3.055862
63	8	0	-4.526231	2.700957	-2.909797
64	6	0	-9.345249	-4.641731	-1.352195
65	6	0	-9.331507	-4.804340	0.066591
66	6	0	-11.877314	-2.484331	-1.534959
67	7	0	-8.182634	-5.046055	0.766732
68	7	0	-8.213285	-4.748351	-2.111385
69	6	0	-8.773630	0.243808	4.847019
70	6	0	-8.801914	-1.128985	4.449178
71	6	0	-8.772417	5.198934	0.003604
72	6	0	-8.662683	4.733381	1.351728
73	7	0	-7.670786	-1.805014	4.081643
74	7	0	-7.606909	0.933620	5.013667
75	7	0	-7.679738	5.473459	-0.767032
76	7	0	-7.461413	4.381355	1.903703
77	6	0	-7.098345	-5.008566	-1.417254
78	6	0	-6.400964	4.595640	1.112835
79	6	0	-7.081859	-5.142547	0.012283
80	6	0	-6.503187	0.240659	4.711239
81	6	0	-6.538211	-1.100256	4.199340
82	6	0	-6.506185	5.196447	-0.186906
83	6	0	-5.113821	5.376204	-0.769438
84	6	0	-4.939345	4.252545	1.363727
85	6	0	-5.678183	-5.168838	-1.941997
86	6	0	-5.648353	-5.360787	0.472584
87	6	0	-5.060456	0.714181	4.768560
88	6	0	-5.123190	-1.506919	3.813122
89	7	0	-4.264134	4.757335	0.216638
90	7	0	-4.330386	-0.387443	4.197666
91	7	0	-4.899006	-5.339302	-0.748489
92	8	0	-4.410903	3.659592	2.264350
93	8	0	-4.726383	5.902446	-1.766402
94	8	0	-4.563682	1.716192	5.182918
95	8	0	-4.703050	-2.501022	3.289671
96	8	0	-5.235875	-5.177142	-3.050982
97	8	0	-5.179216	-5.512423	1.560983
98	1	0	-3.863533	-5.392741	-0.756697
99	1	0	-3.313787	-0.323354	3.991525
100	1	0	-3.234573	4.656999	0.080696
101	1	0	12.840914	-3.782359	-0.266613
102	6	0	11.729212	-3.774562	-0.304295
103	6	0	11.166183	-3.378455	1.030903
104	6	0	11.253654	-2.907520	-1.436041
105	1	0	11.447444	-4.841187	-0.518125
106	6	0	11.759240	-2.379545	1.815205
107	6	0	10.030983	-4.030141	1.555092
108	6	0	11.893978	-1.704423	-1.764619
109	6	0	10.168788	-3.308971	-2.241470
110	6	0	11.238462	-2.018002	3.069087

111	1	0	12.638660	-1.857271	1.436279
112	6	0	9.506465	-3.749035	2.813481
113	8	0	9.450724	-5.069155	0.784834
114	6	0	11.478397	-0.923459	-2.854477
115	1	0	12.733654	-1.364540	-1.157322
116	6	0	9.727069	-2.582955	-3.345789
117	8	0	9.565928	-4.558232	-1.947410
118	6	0	11.840147	-0.893434	3.863813
119	6	0	10.133220	-2.743352	3.552078
120	1	0	8.635243	-4.293896	3.204903
121	6	0	8.302073	-4.679790	0.122725
122	6	0	12.159296	0.372180	-3.192683
123	6	0	10.408794	-1.400661	-3.636735
124	1	0	8.889223	-2.933024	-3.965498
125	6	0	8.360959	-4.432943	-1.283592
126	1	0	12.949919	-0.940792	3.827142
127	1	0	11.585762	-1.028780	4.949095
128	6	0	11.351707	0.455549	3.409691
129	8	0	9.653268	-2.462375	4.860970
130	7	0	7.133000	-4.606612	0.830267
131	6	0	11.630410	1.520264	-2.379347
132	1	0	12.014406	0.594671	-4.283916
133	1	0	13.259994	0.279162	-3.069602
134	8	0	10.071804	-0.676962	-4.808939
135	7	0	7.249653	-4.126806	-2.019318
136	6	0	12.021450	1.202092	2.429403
137	6	0	10.203890	1.030640	3.992633
138	6	0	8.443649	-1.785073	4.788058
139	6	0	6.051936	-4.312338	0.097526
140	6	0	12.169310	1.849287	-1.128555
141	6	0	10.583766	2.326329	-2.872414
142	6	0	8.886016	0.025198	-4.668317
143	6	0	6.110665	-4.083641	-1.318976
144	6	0	11.573172	2.475570	2.045209
145	1	0	12.909091	0.784398	1.953578
146	6	0	9.726576	2.297767	3.668600
147	8	0	9.591097	0.303517	5.037404
148	6	0	8.433323	-0.357285	4.704901
149	7	0	7.295774	-2.522719	4.776274
150	6	0	4.612425	-4.126601	0.556247
151	6	0	11.692709	2.942303	-0.387702
152	1	0	12.976111	1.240876	-0.718469
153	6	0	10.083462	3.431638	-2.189293
154	8	0	10.116064	2.038108	-4.174245
155	6	0	8.904293	1.387046	-4.236458
156	7	0	7.726719	-0.620595	-4.993572
157	6	0	4.713554	-3.754650	-1.819010
158	6	0	12.258555	3.268050	0.966732
159	6	0	10.446301	3.003700	2.705868
160	1	0	8.833801	2.719635	4.151017
161	7	0	7.302688	0.347536	4.395820
162	6	0	6.181215	-1.810040	4.570715
163	7	0	3.904167	-3.816064	-0.643230
164	8	0	4.110995	-4.185690	1.644220
165	6	0	10.669504	3.725082	-0.957090
166	1	0	9.272807	4.047424	-2.604821
167	7	0	7.757418	2.089234	-3.981681
168	6	0	6.615660	0.101774	-4.810813
169	8	0	4.313164	-3.463880	-2.910896
170	1	0	12.132466	4.364430	1.170822
171	1	0	13.356325	3.101300	0.986878
172	8	0	10.117211	4.349383	2.428295
173	6	0	6.195840	-0.400315	4.296482
174	6	0	4.749835	-2.313545	4.495348
175	1	0	2.866110	-3.657363	-0.671552
176	8	0	10.294640	4.909672	-0.279558
177	6	0	6.626850	1.425764	-4.251546
178	6	0	5.176989	-0.314469	-5.072597
179	6	0	8.954951	4.518597	1.704297
180	6	0	4.798536	0.018642	3.863140
181	7	0	4.021265	-1.160324	4.022570
182	8	0	4.253453	-3.360514	4.773499
183	6	0	9.048440	4.833897	0.314657
184	6	0	5.187819	1.859653	-4.015315
185	7	0	4.413894	0.784523	-4.543227
186	8	0	4.707179	-1.280561	-5.590732
187	7	0	7.759613	4.457232	2.364311
188	8	0	4.388152	1.065867	3.439228
189	1	0	3.012659	-1.211043	3.761095
190	7	0	7.951168	5.130758	-0.444296
191	8	0	4.727167	2.834901	-3.488884
192	1	0	3.370438	0.780781	-4.513554
193	6	0	6.692475	4.739988	1.607616
194	6	0	6.788291	5.087892	0.217651
195	6	0	5.226578	4.716755	2.011207
196	6	0	5.388889	5.331609	-0.327118
197	7	0	4.541051	5.058554	0.800732
198	8	0	4.692689	4.475830	3.053415
199	8	0	4.998082	5.673872	-1.401672
200	1	0	3.507876	5.065654	0.738350
201	8	0	1.998508	3.830088	0.815033
202	6	0	1.350313	3.563714	1.828878
203	7	0	0.083502	4.106254	2.158492
204	7	0	1.784741	2.727804	2.864639
205	6	0	-0.466952	3.450610	3.377442
206	1	0	-0.572989	4.358443	1.389681
207	6	0	0.737877	2.528765	3.894288
208	1	0	2.740403	2.378711	2.975609
209	1	0	-0.800270	4.233228	4.102020
210	7	0	-1.544058	2.477416	3.094338
211	1	0	1.111138	2.779894	4.916774
212	7	0	0.163660	1.158445	3.893609
213	6	0	-1.128220	1.155184	3.300971
214	1	0	-2.482325	2.755824	2.794986
215	1	0	0.787178	0.343359	3.730897
216	8	0	-1.800753	0.152029	3.086257
217	1	0	1.085701	5.226843	-3.389690
218	6	0	0.712306	4.267249	-2.954885
219	6	0	-0.637218	3.713291	-3.620875
220	7	0	0.340765	4.486797	-1.531173

221	7	0	1.674291	3.162039	-3.159361
222	1	0	-1.028599	4.336402	-4.463013
223	7	0	-0.253766	2.372647	-4.139452
224	7	0	-1.592654	3.693677	-2.493246
225	6	0	-0.980115	4.031331	-1.277955
226	1	0	1.064006	4.392251	-0.796285
227	6	0	1.071657	2.044898	-3.764347
228	1	0	2.683160	3.262126	-3.015856
229	1	0	-0.963681	1.616664	-4.196187
230	1	0	-2.552971	3.353597	-2.582742
231	8	0	-1.540555	4.066096	-0.183378
232	8	0	1.638964	0.983729	-4.005478
233	6	0	-1.217796	-1.180102	-3.960011
234	7	0	0.082520	-1.419922	-4.454704
235	7	0	-1.859873	-2.406936	-3.734476
236	8	0	-1.733217	-0.071509	-3.817985
237	6	0	0.434191	-2.859939	-4.353138
238	1	0	0.815751	-0.690632	-4.373629
239	6	0	-0.942909	-3.557480	-3.915732
240	1	0	-2.861975	-2.510391	-3.549875
241	1	0	0.852555	-3.214345	-5.327233
242	7	0	1.343717	-3.181811	-3.232472
243	1	0	-1.349733	-4.293436	-4.651342
244	7	0	-0.601340	-4.253860	-2.649703
245	6	0	0.696577	-3.887446	-2.208449
246	1	0	2.312233	-2.852665	-3.183377
247	1	0	-1.342295	-4.451485	-1.952876
248	8	0	1.208064	-4.230696	-1.144974
249	1	0	0.384894	-5.523312	3.010245
250	6	0	0.079926	-4.602464	2.455172
251	6	0	-1.170840	-3.825467	3.087334
252	7	0	-0.385353	-4.978312	1.092934
253	7	0	1.155312	-3.584883	2.468008
254	1	0	-1.589462	-4.291290	4.012779
255	7	0	-0.626442	-2.479337	3.415881
256	7	0	-2.157226	-3.810730	1.985692
257	6	0	-1.653624	-4.400629	0.817649
258	1	0	0.311133	-5.039975	0.323217
259	6	0	0.703338	-2.344507	2.936272
260	1	0	2.119063	-3.786366	2.186846
261	1	0	-1.254339	-1.654044	3.372781
262	1	0	-3.123037	-3.499384	2.117049
263	8	0	-2.242943	-4.459548	-0.258099
264	8	0	1.377183	-1.319322	3.009726
265	6	0	-4.453277	0.756654	0.340538
266	6	0	-3.119706	0.934470	-0.007687
267	6	0	-2.360118	-0.158345	-0.427953
268	6	0	-2.943259	-1.424019	-0.500261
269	6	0	-4.278060	-1.588637	-0.154893
270	6	0	-5.046823	-0.506966	0.282327
271	1	0	-5.034521	1.602033	0.698440
272	1	0	-2.640218	1.908914	0.060071
273	1	0	-2.343704	-2.275638	-0.810251
274	1	0	-4.722335	-2.580186	-0.198211
275	6	0	-6.498742	-0.702633	0.646713
276	6	0	-7.411141	-0.654868	-0.584261
277	1	0	-6.803941	0.071531	1.357934
278	1	0	-6.617638	-1.668351	1.153307
279	1	0	-8.455375	-0.815565	-0.302851
280	1	0	-7.333657	0.316548	-1.077925
281	1	0	-7.127080	-1.428081	-1.304616
282	8	0	-0.427725	1.179225	-0.741741
283	6	0	6.517585	0.959423	0.320107
284	6	0	5.129606	0.965077	0.301937
285	6	0	4.440884	0.202338	-0.644537
286	6	0	5.154665	-0.580437	-1.546171
287	6	0	6.544163	-0.579404	-1.524132
288	6	0	7.244340	0.200509	-0.601767
289	1	0	7.044679	1.551570	1.065083
290	1	0	4.584197	1.538665	1.051651
291	1	0	4.600857	-1.169033	-2.271193
292	1	0	7.094919	-1.188806	-2.236769
293	6	0	8.752035	0.217255	-0.571540
294	6	0	9.316670	-0.385538	0.715615
295	1	0	9.103008	1.251918	-0.668818
296	1	0	9.141827	-0.328641	-1.436423
297	1	0	10.409796	-0.348235	0.711432
298	1	0	8.966324	0.165821	1.593096
299	1	0	9.006669	-1.427096	0.826883
300	8	0	2.339667	-0.790793	-1.149566
301	1	0	2.857558	2.169950	-0.128293
302	1	0	1.319253	1.398446	-0.469562
303	1	0	0.760584	-0.868321	-1.055499
304	7	0	2.336221	1.338304	-0.372906
305	6	0	2.947633	0.213849	-0.735353
306	6	0	-0.914948	0.054958	-0.718132
307	8	0	-0.231458	-1.048109	-0.930133

AC-cis, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.676291	-0.862461	-2.750536
2	6	0	-12.150346	0.442111	-3.323372
3	6	0	-12.002248	2.075937	2.121612
4	6	0	-11.428321	3.226274	1.563035
5	6	0	-12.041990	3.913963	0.374588
6	6	0	-11.522016	3.359479	-0.921126
7	6	0	-12.061612	2.196654	-1.492849
8	6	0	-11.535966	1.646903	-2.670385
9	6	0	-12.267398	-1.426232	-1.611631
10	6	0	-12.461897	-3.245082	0.139849
11	6	0	-11.780621	-2.704810	1.366856
12	6	0	-12.215306	-1.531282	1.998693
13	6	0	-11.565810	-1.029282	3.136095
14	6	0	-11.448375	1.454229	3.250986
15	6	0	-12.051718	0.209087	3.836085
16	6	0	-10.432004	2.296654	-3.258568

17	6	0	-10.468290	3.997105	-1.602472
18	6	0	-9.890991	3.480158	-2.763119
19	6	0	-10.859998	-3.368314	-1.820741
20	6	0	-10.644623	-1.588666	-3.378274
21	6	0	-10.223542	-2.844312	-2.946891
22	6	0	-10.265428	3.738652	2.174251
23	6	0	-10.307978	2.041121	3.832035
24	6	0	-9.683325	3.172757	3.306289
25	6	0	-10.451795	-1.741292	3.624499
26	6	0	-10.677866	-3.380288	1.927242
27	6	0	-9.979335	-2.915544	3.040118
28	1	0	-8.783244	3.602927	3.767139
29	1	0	-12.897951	1.651646	1.666825
30	1	0	-11.819070	5.012944	0.427470
31	1	0	-13.150607	3.849473	0.412908
32	1	0	-12.903129	1.704731	-1.003861
33	1	0	-9.050683	3.980427	-3.264602
34	1	0	-9.432730	-3.397369	-3.472945
35	1	0	-13.059149	-0.880999	-1.096558
36	1	0	-13.077056	-0.996930	1.597682
37	1	0	-9.110574	-3.452930	3.445840
38	1	0	-13.161369	0.262678	3.814655
39	1	0	-11.791497	0.145110	4.926403
40	1	0	-13.555054	-3.052062	0.175195
41	1	0	-12.369851	-4.363397	0.123316
42	1	0	-11.919159	0.464306	-4.422828
43	1	0	-13.260254	0.503012	-3.271573
44	8	0	-10.072522	-1.032196	-4.552217
45	8	0	-9.905237	1.749819	-4.457493
46	8	0	-10.371492	-4.643277	1.373801
47	8	0	-10.556417	-4.688280	-1.405557
48	8	0	-9.884295	-1.290300	4.837731
49	8	0	-9.844522	1.491135	5.052837
50	8	0	-10.017681	5.244267	-1.096586
51	8	0	-9.757552	4.955792	1.664393
52	6	0	-8.766975	0.995476	-4.251939
53	6	0	-8.852016	-0.430619	-4.315632
54	7	0	-7.750954	-1.233680	-4.201293
55	7	0	-7.580646	1.648350	-4.054135
56	6	0	-6.595568	-0.580412	-4.032303
57	6	0	-6.510459	0.850778	-3.951383
58	6	0	-5.202266	-1.163526	-3.868465
59	6	0	-5.057416	1.238450	-3.717552
60	7	0	-4.368425	-0.013173	-3.709861
61	8	0	-4.809826	-2.296089	-3.846885
62	1	0	-3.329255	-0.090748	-3.590343
63	8	0	-4.532596	2.303181	-3.549802
64	6	0	-9.318392	-4.789151	-0.795688
65	6	0	-9.216159	-4.697648	0.626931
66	6	0	-11.858166	-2.672292	-1.111829
67	7	0	-8.017224	-4.760131	1.280725
68	7	0	-8.235039	-5.030868	-1.592555
69	6	0	-8.660218	0.791026	4.908916
70	6	0	-8.683192	-0.625158	4.719473
71	6	0	-8.762234	5.126518	-0.522578
72	6	0	-8.634553	4.854478	0.875703
73	7	0	-7.542377	-1.355614	4.528052
74	7	0	-7.494702	1.497128	5.007163
75	7	0	-7.680338	5.286451	-1.339775
76	7	0	-7.424050	4.598852	1.459311
77	6	0	-7.073250	-5.138006	-0.936161
78	6	0	-6.374579	4.703445	0.633331
79	6	0	-6.961718	-4.968466	0.484969
80	6	0	-6.385248	0.763009	4.867505
81	6	0	-6.408714	-0.645750	4.589005
82	6	0	-6.498692	5.098915	-0.741073
83	6	0	-5.115295	5.183544	-1.363900
84	6	0	-4.908668	4.414276	0.919154
85	6	0	-5.689421	-5.395764	-1.512748
86	6	0	-5.493504	-5.033567	0.872832
87	6	0	-4.941351	1.236645	4.917420
88	6	0	-4.979329	-1.118578	4.361010
89	7	0	-4.251786	4.720325	-0.307349
90	7	0	-4.193639	0.047592	4.610274
91	7	0	-4.828364	-5.292286	-0.365705
92	8	0	-4.366360	3.995136	1.904158
93	8	0	-4.741614	5.545505	-2.436497
94	8	0	-4.459947	2.300739	5.161861
95	8	0	-4.537555	-2.182922	4.033564
96	8	0	-5.318833	-5.639504	-2.620425
97	8	0	-4.947618	-4.886112	1.928004
98	1	0	-3.793789	-5.345739	-0.430657
99	1	0	-3.171939	0.074219	4.440988
100	1	0	-3.224059	4.605312	-0.442485
101	1	0	12.809238	-3.798504	0.263954
102	6	0	11.698739	-3.793249	0.199275
103	6	0	11.106070	-3.261102	1.473042
104	6	0	11.253605	-3.047342	-1.027189
105	1	0	11.418144	-4.875906	0.090014
106	6	0	11.685542	-2.190842	2.168158
107	6	0	9.953918	-3.852066	2.031108
108	6	0	11.902488	-1.881387	-1.457643
109	6	0	10.191565	-3.531063	-1.817541
110	6	0	11.136290	-1.704507	3.366555
111	1	0	12.577035	-1.711943	1.761294
112	6	0	9.400315	-3.445724	3.241762
113	8	0	9.385109	-4.958072	1.350793
114	6	0	11.516364	-1.214144	-2.630666
115	1	0	12.725474	-1.480171	-0.865059
116	6	0	9.779888	-2.919885	-3.000378
117	8	0	9.576580	-4.744825	-1.416407
118	6	0	11.724831	-0.508295	4.059893
119	6	0	10.015546	-2.374271	3.892284
120	1	0	8.515584	-3.944726	3.662827
121	6	0	8.259195	-4.627706	0.621843
122	6	0	12.207293	0.042425	-3.078390
123	6	0	10.467690	-1.769784	-3.389153
124	1	0	8.959060	-3.332528	-3.604206
125	6	0	8.355016	-4.545336	-0.801515
126	1	0	12.834952	-0.560360	4.052431

127	1	0	11.446470	-0.535688	5.147379
128	6	0	11.250940	0.789765	3.464162
129	8	0	9.507838	-1.964793	5.155737
130	7	0	7.076668	-4.449926	1.287509
131	6	0	11.661166	1.265069	-2.395576
132	1	0	12.089233	0.155960	-4.189450
133	1	0	13.304541	-0.037491	-2.920134
134	8	0	10.158389	-1.166392	-4.635129
135	7	0	7.264955	-4.319256	-1.595493
136	6	0	11.942046	1.432648	2.427007
137	6	0	10.095301	1.423327	3.965309
138	6	0	8.303837	-1.293572	4.991995
139	6	0	6.018321	-4.226264	0.499075
140	6	0	12.171964	1.718700	-1.172286
141	6	0	10.626233	2.015849	-2.990056
142	6	0	8.970155	-0.455561	-4.590709
143	6	0	6.111332	-4.177785	-0.933099
144	6	0	11.507045	2.662844	1.909600
145	1	0	12.836119	0.966873	2.011771
146	6	0	9.630397	2.653358	3.507877
147	8	0	9.459592	0.805003	5.065105
148	6	0	8.303704	0.120221	4.776579
149	7	0	7.152141	-2.024948	5.025032
150	6	0	4.575773	-3.947986	0.898034
151	6	0	11.678533	2.879045	-0.555236
152	1	0	12.969896	1.156616	-0.685875
153	6	0	10.108951	3.181620	-2.431365
154	8	0	10.190034	1.597868	-4.267543
155	6	0	8.979807	0.941929	-4.292878
156	7	0	7.817633	-1.131520	-4.876367
157	6	0	4.731847	-3.891100	-1.502054
158	6	0	12.215973	3.341641	0.770607
159	6	0	10.370929	3.257655	2.493067
160	1	0	8.731237	3.124184	3.929423
161	7	0	7.182642	0.798560	4.384629
162	6	0	6.045524	-1.329862	4.733930
163	7	0	3.899784	-3.774951	-0.346394
164	8	0	4.054739	-3.855636	1.974546
165	6	0	10.666587	3.597584	-1.221469
166	1	0	9.306911	3.750388	-2.923572
167	7	0	7.828152	1.663423	-4.130758
168	6	0	6.703092	-0.396772	-4.787192
169	8	0	4.358595	-3.743203	-2.631879
170	1	0	12.087092	4.453060	0.858993
171	1	0	13.312855	3.178762	0.831024
172	8	0	10.052006	4.569381	2.075547
173	6	0	6.073426	0.049478	4.334704
174	6	0	4.612386	-1.831698	4.676657
175	1	0	2.869835	-3.585428	-0.419195
176	8	0	10.276336	4.842392	-0.673563
177	6	0	6.703291	0.974867	-4.357909
178	6	0	5.269730	-0.838440	-5.035725
179	6	0	8.903000	4.663939	1.317009
180	6	0	4.686212	0.434834	3.842697
181	7	0	3.898732	-0.721197	4.091959
182	8	0	4.104923	-2.848347	5.035840
183	6	0	9.019877	4.825148	-0.096927
184	6	0	5.260277	1.426954	-4.191186
185	7	0	4.496466	0.303814	-4.626697
186	8	0	4.809344	-1.849635	-5.469695
187	7	0	7.697138	4.678511	1.960416
188	8	0	4.290680	1.442534	3.320087
189	1	0	2.892613	-0.786639	3.821626
190	7	0	7.935208	5.033729	-0.902254
191	8	0	4.790029	2.447607	-3.770478
192	1	0	3.452926	0.301056	-4.614862
193	6	0	6.643042	4.876519	1.160014
194	6	0	6.761586	5.064067	-0.258854
195	6	0	5.171045	4.902536	1.541050
196	6	0	5.370865	5.242027	-0.849831
197	7	0	4.505118	5.101007	0.288143
198	8	0	4.621219	4.788231	2.596261
199	8	0	4.997581	5.456995	-1.963077
200	1	0	3.472894	5.098018	0.208703
201	8	0	1.961690	3.875050	0.392190
202	6	0	1.291834	3.737172	1.418226
203	7	0	0.024090	4.325462	1.653706
204	7	0	1.701085	3.033048	2.556202
205	6	0	-0.548218	3.835460	2.940248
206	1	0	-0.619553	4.466952	0.847520
207	6	0	0.637521	2.973796	3.586797
208	1	0	2.648541	2.683086	2.720783
209	1	0	-0.878469	4.708972	3.553851
210	7	0	-1.632001	2.846784	2.766438
211	1	0	1.000692	3.349235	4.574297
212	7	0	0.046758	1.620548	3.754096
213	6	0	-1.242478	1.557131	3.153116
214	1	0	-2.570996	3.101647	2.447618
215	1	0	0.663604	0.787664	3.685660
216	8	0	-1.935114	0.549721	3.071862
217	1	0	1.177138	4.837561	-3.948599
218	6	0	0.781262	3.926284	-3.436531
219	6	0	-0.551914	3.319917	-4.089432
220	7	0	0.368132	4.282012	-2.053021
221	7	0	1.739541	2.800325	-3.503691
222	1	0	-0.915793	3.866341	-4.994723
223	7	0	-0.160399	1.937740	-4.474348
224	7	0	-1.539664	3.402413	-2.992181
225	6	0	-0.961578	3.853912	-1.796367
226	1	0	1.068818	4.253716	-1.290341
227	6	0	1.148230	1.636780	-4.026135
228	1	0	2.744989	2.910185	-3.344111
229	1	0	-0.873910	1.184364	-4.499596
230	1	0	-2.501367	3.070431	-3.085128
231	8	0	-1.548276	3.990032	-0.724726
232	8	0	1.712962	0.554046	-4.150630
233	6	0	-1.143302	-1.586974	-4.055131
234	7	0	0.166919	-1.874462	-4.494997
235	7	0	-1.792888	-2.783638	-3.714795
236	8	0	-1.659514	-0.469687	-4.041296

237	6	0	0.512430	-3.298657	-4.242201
238	1	0	0.900564	-1.141423	-4.452822
239	6	0	-0.871352	-3.944744	-3.750045
240	1	0	-2.801890	-2.870641	-3.565378
241	1	0	0.937415	-3.750434	-5.172079
242	7	0	1.408866	-3.501493	-3.085607
243	1	0	-1.265031	-4.760731	-4.403711
244	7	0	-0.548630	-4.492907	-2.408277
245	6	0	0.748125	-4.087849	-1.996156
246	1	0	2.391011	-3.211909	-3.077331
247	1	0	-1.297113	-4.596093	-1.699057
248	8	0	1.248298	-4.309880	-0.897085
249	1	0	0.355051	-5.125053	3.398659
250	6	0	0.047981	-4.259485	2.761896
251	6	0	-1.241520	-3.466342	3.287233
252	7	0	-0.362512	-4.753861	1.419867
253	7	0	1.098032	-3.218566	2.724698
254	1	0	-1.675689	-3.856900	4.240104
255	7	0	-0.743066	-2.080009	3.508492
256	7	0	-2.194238	-3.564088	2.158254
257	6	0	-1.637398	-4.246938	1.063199
258	1	0	0.357555	-4.874002	0.679790
259	6	0	0.600125	-1.954135	3.067012
260	1	0	2.074137	-3.417667	2.488172
261	1	0	-1.391734	-1.283224	3.359855
262	1	0	-3.200682	-3.422598	2.292621
263	8	0	-2.188578	-4.415876	-0.021472
264	8	0	1.254978	-0.913969	3.078742
265	6	0	-4.584071	0.809235	-0.387004
266	6	0	-3.206413	0.930025	-0.521572
267	6	0	-2.423628	-0.210749	-0.706424
268	6	0	-3.023978	-1.469362	-0.737580
269	6	0	-4.402998	-1.577217	-0.607402
270	6	0	-5.200428	-0.444344	-0.432255
271	1	0	-5.191601	1.696974	-0.235395
272	1	0	-2.714096	1.899853	-0.484617
273	1	0	-2.408543	-2.356852	-0.863342
274	1	0	-4.867679	-2.558885	-0.641028
275	6	0	-6.692202	-0.582089	-0.246330
276	6	0	-7.056828	-0.793565	1.226943
277	1	0	-7.057625	-1.426543	-0.839786
278	1	0	-7.193391	0.316673	-0.619096
279	1	0	-8.136545	-0.902914	1.357718
280	1	0	-6.572422	-1.693548	1.621507
281	1	0	-6.717568	0.055933	1.825605
282	8	0	-0.441175	1.070868	-0.914720
283	6	0	6.488090	0.959978	0.277498
284	6	0	5.100001	0.957135	0.260410
285	6	0	4.414545	0.117499	-0.620871
286	6	0	5.131632	-0.727323	-1.461645
287	6	0	6.521189	-0.717791	-1.441213
288	6	0	7.218236	0.134205	-0.582407
289	1	0	7.012570	1.613416	0.971527
290	1	0	4.550676	1.587958	0.960001
291	1	0	4.579694	-1.370992	-2.139571
292	1	0	7.074983	-1.377733	-2.104565
293	6	0	8.726048	0.160638	-0.555337
294	6	0	9.295758	-0.324286	0.778682
295	1	0	9.071474	1.184724	-0.743141
296	1	0	9.117582	-0.456818	-1.369821
297	1	0	10.388763	-0.282860	0.769012
298	1	0	8.945017	0.300360	1.605362
299	1	0	8.990903	-1.353433	0.981968
300	8	0	2.317470	-0.931965	-1.019156
301	1	0	2.825551	2.117813	-0.302172
302	1	0	1.289672	1.311618	-0.566117
303	1	0	0.728625	-1.003375	-0.972824
304	7	0	2.305606	1.263158	-0.453719
305	6	0	2.920740	0.111674	-0.707663
306	6	0	-0.950241	-0.041367	-0.848195
307	8	0	-0.270631	-1.166093	-0.899659

BB-trans, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.465997	-0.707829	-3.240803
2	6	0	-12.031811	0.624063	-3.645342
3	6	0	-12.158510	1.467772	1.955400
4	6	0	-11.688338	2.743835	1.610870
5	6	0	-12.322049	3.539375	0.503387
6	6	0	-11.703775	3.201283	-0.824363
7	6	0	-12.149925	2.110619	-1.586927
8	6	0	-11.535435	1.762724	-2.798347
9	6	0	-12.052013	-1.474161	-2.221662
10	6	0	-12.177296	-3.548552	-0.770566
11	6	0	-11.621235	-3.208652	0.583018
12	6	0	-12.103142	-2.118774	1.324244
13	6	0	-11.540648	-1.765469	2.559136
14	6	0	-11.556255	0.714384	2.973242
15	6	0	-12.085374	-0.631402	3.380328
16	6	0	-10.447716	2.550838	-3.224058
17	6	0	-10.643735	3.974246	-1.337286
18	6	0	-9.986542	3.665072	-2.527716
19	6	0	-10.398700	-3.194411	-2.541199
20	6	0	-10.345358	-1.248207	-3.900150
21	6	0	-9.782546	-2.480436	-3.566437
22	6	0	-10.600869	3.263686	2.341421
23	6	0	-10.456348	1.285240	3.643279
24	6	0	-9.955420	2.552648	3.352564
25	6	0	-10.465582	-2.544537	3.031757
26	6	0	-10.585784	-3.979412	1.144815
27	6	0	-9.979405	-3.664054	2.360525
28	1	0	-9.098238	2.973483	3.897642
29	1	0	-13.010345	1.051098	1.417058
30	1	0	-12.193062	4.635057	0.709214
31	1	0	-13.421163	3.382833	0.480843
32	1	0	-12.987743	1.514805	-1.223691

33	1	0	-9.143387	4.266762	-2.896270
34	1	0	-8.898494	-2.871807	-4.089905
35	1	0	-12.930106	-1.086575	-1.703747
36	1	0	-12.926621	-1.525931	0.924743
37	1	0	-9.156581	-4.266273	2.771276
38	1	0	-13.197348	-0.634557	3.346652
39	1	0	-11.836071	-0.809709	4.461321
40	1	0	-13.281508	-3.427538	-0.785259
41	1	0	-12.007069	-4.637352	-0.983558
42	1	0	-11.767319	0.823953	-4.718634
43	1	0	-13.143431	0.591814	-3.632835
44	8	0	-9.809070	-0.520087	-4.996509
45	8	0	-9.841988	2.212635	-4.462357
46	8	0	-10.194106	-5.153702	0.453139
47	8	0	-9.958135	-4.503843	-2.242956
48	8	0	-9.897690	-2.200330	4.286284
49	8	0	-9.897566	0.549085	4.720123
50	8	0	-10.297791	5.152549	-0.634823
51	8	0	-10.235923	4.605440	2.088535
52	6	0	-8.665283	1.511019	-4.302017
53	6	0	-8.636574	0.123885	-4.642490
54	7	0	-7.484555	-0.611147	-4.623305
55	7	0	-7.558703	2.173852	-3.844975
56	6	0	-6.404675	0.057429	-4.204408
57	6	0	-6.449103	1.428891	-3.781660
58	6	0	-5.000594	-0.476005	-3.991723
59	6	0	-5.090630	1.804500	-3.212954
60	7	0	-4.317603	0.614680	-3.357631
61	8	0	-4.497544	-1.527014	-4.262791
62	1	0	-3.332488	0.526177	-3.020563
63	8	0	-4.690071	2.827860	-2.732571
64	6	0	-8.815690	-4.596752	-1.478602
65	6	0	-8.940336	-5.022636	-0.119277
66	6	0	-11.534628	-2.723491	-1.850935
67	7	0	-7.858653	-5.344313	0.649764
68	7	0	-7.599000	-4.387445	-2.067797
69	6	0	-8.718654	-0.082395	4.378981
70	6	0	-8.718099	-1.492844	4.150451
71	6	0	-9.078581	5.068310	0.013215
72	6	0	-9.044937	4.762378	1.407327
73	7	0	-7.577911	-2.183362	3.841903
74	7	0	-7.578127	0.669896	4.314813
75	7	0	-7.948822	5.347737	-0.704098
76	7	0	-7.876818	4.706245	2.116098
77	6	0	-6.545038	-4.670626	-1.290270
78	6	0	-6.777688	4.978177	1.402028
79	6	0	-6.676100	-5.183365	0.044474
80	6	0	-6.469600	-0.020208	4.026007
81	6	0	-6.468751	-1.436484	3.787643
82	6	0	-6.813939	5.304289	0.003816
83	6	0	-5.390462	5.523246	-0.489699
84	6	0	-5.327412	4.964983	1.866060
85	6	0	-5.064483	-4.498810	-1.598753
86	6	0	-5.293394	-5.433692	0.623904
87	6	0	-5.055256	0.505649	3.855242
88	6	0	-5.051154	-1.869704	3.451708
89	7	0	-4.590691	5.257293	0.671583
90	7	0	-4.293467	-0.664999	3.533439
91	7	0	-4.413789	-4.957979	-0.410944
92	8	0	-4.840282	4.780839	2.940984
93	8	0	-4.959783	5.856044	-1.552669
94	8	0	-4.600261	1.609460	3.940728
95	8	0	-4.597405	-2.944505	3.168113
96	8	0	-4.492454	-4.080183	-2.563565
97	8	0	-4.931287	-5.918024	1.651998
98	1	0	-3.387597	-4.899334	-0.283979
99	1	0	-3.259538	-0.626963	3.380550
100	1	0	-3.555912	5.213109	0.635777
101	1	0	13.205716	-3.184663	-1.357380
102	6	0	12.099385	-3.287246	-1.342312
103	6	0	11.573888	-3.173524	0.059889
104	6	0	11.461652	-2.284695	-2.263492
105	1	0	11.904700	-4.322604	-1.730739
106	6	0	12.102189	-2.244828	0.969605
107	6	0	10.529207	-4.007391	0.502272
108	6	0	11.988008	-0.995004	-2.420146
109	6	0	10.327587	-2.627003	-3.028695
110	6	0	11.582647	-2.111246	2.264870
111	1	0	12.931114	-1.608224	0.659007
112	6	0	9.962479	-3.905161	1.772666
113	8	0	10.098590	-5.035933	-0.372491
114	6	0	11.421854	-0.075072	-3.315745
115	1	0	12.856955	-0.698760	-1.831747
116	6	0	9.739991	-1.761619	-3.948811
117	8	0	9.860646	-3.957216	-2.930863
118	6	0	12.166865	-1.141388	3.254021
119	6	0	10.503948	-2.944668	2.623879
120	1	0	9.132236	-4.552007	2.090088
121	6	0	8.845264	-4.782794	-0.902857
122	6	0	11.976023	1.312285	-3.472259
123	6	0	10.322209	-0.500683	-4.085088
124	1	0	8.868772	-2.063859	-4.546681
125	6	0	8.723836	-4.140504	-2.173847
126	1	0	13.273578	-1.106911	3.157453
127	1	0	11.984677	-1.521643	4.294891
128	6	0	11.580471	0.235325	3.120025
129	8	0	10.023153	-2.848905	3.951587
130	7	0	7.760821	-5.207259	-0.188573
131	6	0	11.423110	2.269500	-2.453353
132	1	0	11.737997	1.691962	-4.502096
133	1	0	13.086602	1.297119	-3.428599
134	8	0	9.847093	0.381452	-5.088968
135	7	0	7.509144	-3.809706	-2.709480
136	6	0	12.093044	1.166592	2.203675
137	6	0	10.502822	0.638840	3.931590
138	6	0	8.840397	-2.150675	4.077157
139	6	0	6.579372	-4.931527	-0.752453
140	6	0	12.003483	2.414467	-1.186067
141	6	0	10.313108	3.083608	-2.758920
142	6	0	8.634366	0.952006	-4.743067

143	6	0	6.454324	-4.200507	-1.982251
144	6	0	11.535393	2.445627	2.069334
145	1	0	12.943773	0.887606	1.581180
146	6	0	9.893173	1.889349	3.822926
147	8	0	10.085636	-0.251867	4.952306
148	6	0	8.871327	-0.848858	4.663626
149	7	0	7.670533	-2.760123	3.712820
150	6	0	5.190688	-5.265962	-0.228299
151	6	0	11.509374	3.340209	-0.253519
152	1	0	12.854618	1.789180	-0.914536
153	6	0	9.803712	4.041274	-1.885559
154	8	0	9.764013	2.971954	-4.057712
155	6	0	8.598335	2.237699	-4.123489
156	7	0	7.499612	0.251188	-5.041312
157	6	0	4.975948	-3.965286	-2.250795
158	6	0	12.106556	3.461397	1.119204
159	6	0	10.428935	2.765655	2.882546
160	1	0	9.038697	2.172416	4.453624
161	7	0	7.734419	-0.165535	4.992012
162	6	0	6.565133	-2.064463	4.005383
163	7	0	4.316003	-4.635822	-1.182857
164	8	0	4.824484	-5.900540	0.712689
165	6	0	10.434110	4.159037	-0.646408
166	1	0	8.948996	4.673988	-2.163367
167	7	0	7.434346	2.798878	-3.671483
168	6	0	6.364438	0.839006	-4.650850
169	8	0	4.421615	-3.349566	-3.121180
170	1	0	11.915325	4.492395	1.520014
171	1	0	13.213782	3.377873	1.074941
172	8	0	9.934422	4.088294	2.799526
173	6	0	6.597024	-0.794303	4.677129
174	6	0	5.116848	-2.409709	3.695746
175	1	0	3.275778	-4.642464	-1.083742
176	8	0	10.027815	5.188124	0.242505
177	6	0	6.334877	2.079007	-3.923884
178	6	0	4.944060	0.325525	-4.818098
179	6	0	8.760981	4.241191	2.096501
180	6	0	5.172725	-0.311749	4.896796
181	7	0	4.379700	-1.327819	4.262419
182	8	0	4.622707	-3.331058	3.107017
183	6	0	8.806900	4.907045	0.830755
184	6	0	4.899197	2.353725	-3.505220
185	7	0	4.158160	1.290757	-4.096860
186	8	0	4.497331	-0.617480	-5.396332
187	7	0	7.583452	3.846108	2.667877
188	8	0	4.728364	0.647503	5.451286
189	1	0	3.337143	-1.283971	4.224885
190	7	0	7.679491	5.308549	0.173052
191	8	0	4.420928	3.222622	-2.826972
192	1	0	3.127983	1.181975	-3.965123
193	6	0	6.486450	4.199622	1.984307
194	6	0	6.532252	4.970981	0.774846
195	6	0	5.037737	3.856496	2.282616
196	6	0	5.113528	5.250691	0.307345
197	7	0	4.304885	4.525380	1.259008
198	8	0	4.548021	3.157046	3.126964
199	8	0	4.675235	5.905794	-0.586471
200	1	0	3.272058	4.462725	1.184559
201	8	0	1.630698	3.486450	1.250428
202	6	0	1.036967	3.260942	2.310234
203	7	0	-0.272240	3.676742	2.626826
204	7	0	1.606083	2.623086	3.421370
205	6	0	-0.703653	3.120570	3.939398
206	1	0	-0.979949	3.822355	1.875074
207	6	0	0.621043	2.417922	4.510077
208	1	0	2.606712	2.431055	3.526726
209	1	0	-1.113300	3.943243	4.575705
210	7	0	-1.656997	1.998678	3.819238
211	1	0	0.990361	2.828106	5.481483
212	7	0	0.218372	0.999691	4.686338
213	6	0	-1.067461	0.767143	4.138411
214	1	0	-2.638805	2.123323	3.551551
215	1	0	0.929556	0.247267	4.662264
216	8	0	-1.611465	-0.330084	4.041583
217	1	0	0.811460	5.408370	-2.713275
218	6	0	0.417817	4.427571	-2.348838
219	6	0	-0.900239	3.917214	-3.103666
220	7	0	-0.013541	4.571348	-0.931824
221	7	0	1.386719	3.332067	-2.571619
222	1	0	-1.256785	4.591776	-3.920866
223	7	0	-0.491502	2.612202	-3.693710
224	7	0	-1.895811	3.808929	-2.018018
225	6	0	-1.353390	4.121397	-0.762789
226	1	0	0.677835	4.387483	-0.181381
227	6	0	0.817080	2.256956	-3.275539
228	1	0	2.386684	3.420390	-2.365098
229	1	0	-1.190489	1.857593	-3.799659
230	1	0	-2.882747	3.589273	-2.184030
231	8	0	-1.970173	4.112576	0.297389
232	8	0	1.396546	1.213559	-3.557126
233	6	0	-1.166372	-1.084222	-3.509203
234	7	0	0.087559	-1.338040	-4.097568
235	7	0	-1.808949	-2.311756	-3.200990
236	8	0	-1.642246	0.028243	-3.314464
237	6	0	0.390119	-2.791347	-4.141174
238	1	0	0.838342	-0.628531	-4.062491
239	6	0	-0.959611	-3.466055	-3.601298
240	1	0	-2.837300	-2.401779	-3.255335
241	1	0	0.678432	-3.081237	-5.182253
242	7	0	1.406617	-3.242302	-3.167739
243	1	0	-1.467496	-4.136618	-4.336409
244	7	0	-0.517600	-4.266396	-2.428788
245	6	0	0.847709	-3.998350	-2.128571
246	1	0	2.390970	-2.953572	-3.205436
247	1	0	-1.180779	-4.394639	-1.644495
248	8	0	1.456419	-4.452223	-1.164051
249	1	0	0.858372	-5.622777	3.069837
250	6	0	0.498768	-4.610056	2.763392
251	6	0	-0.795556	-4.082504	3.552775
252	7	0	0.046715	-4.641253	1.349515

253	7	0	1.512054	-3.568093	3.043834
254	1	0	-1.207254	-4.799199	4.304871
255	7	0	-0.319192	-2.854893	4.239666
256	7	0	-1.769550	-3.814177	2.468409
257	6	0	-1.228372	-4.064307	1.201525
258	1	0	0.723134	-4.679474	0.564710
259	6	0	0.985401	-2.509455	3.800361
260	1	0	2.486930	-3.631378	2.736150
261	1	0	-0.990385	-2.090341	4.446066
262	1	0	-2.740685	-3.534115	2.644621
263	8	0	-1.810864	-3.868897	0.130736
264	8	0	1.583794	-1.483768	4.108147
265	6	0	-5.165109	1.121885	0.495289
266	6	0	-3.779558	1.110436	0.384594
267	6	0	-3.079969	-0.087052	0.176366
268	6	0	-3.826365	-1.265797	0.076299
269	6	0	-5.213762	-1.257549	0.190238
270	6	0	-5.901591	-0.062908	0.407023
271	1	0	-5.686738	2.060914	0.665472
272	1	0	-3.215372	2.039698	0.467620
273	1	0	-3.323303	-2.227656	-0.069291
274	1	0	-5.770078	-2.188785	0.122819
275	6	0	-7.408330	-0.044673	0.507110
276	6	0	-8.069304	0.230295	-0.848066
277	1	0	-7.716910	0.725738	1.222465
278	1	0	-7.760788	-1.005755	0.895682
279	1	0	-9.159506	0.235009	-0.759445
280	1	0	-7.751704	1.203118	-1.233946
281	1	0	-7.784854	-0.536350	-1.574380
282	8	0	-0.764670	-1.152993	-0.294566
283	8	0	-0.869830	1.085364	0.419482
284	1	0	0.101810	1.030924	0.331314
285	6	0	6.311520	1.053397	0.209004
286	6	0	4.929815	0.956442	0.321490
287	6	0	4.186761	0.124969	-0.525480
288	6	0	4.885514	-0.610289	-1.488757
289	6	0	6.267686	-0.510136	-1.610813
290	6	0	7.000391	0.323476	-0.763554
291	1	0	6.869610	1.694194	0.887040
292	1	0	4.424172	1.520863	1.105935
293	1	0	4.327281	-1.267413	-2.153025
294	1	0	6.786900	-1.091439	-2.371280
295	6	0	8.504961	0.414047	-0.855943
296	6	0	9.198696	-0.251762	0.336834
297	1	0	8.805909	1.467423	-0.906210
298	1	0	8.842645	-0.057286	-1.784765
299	1	0	10.286836	-0.175960	0.249907
300	1	0	8.900411	0.224363	1.275086
301	1	0	8.930973	-1.309760	0.398532
302	8	0	1.862130	0.964781	0.203582
303	8	0	2.019014	-1.124125	-0.861643
304	1	0	1.055063	-1.129779	-0.713858
305	1	0	-1.298262	-1.921358	-0.548966
306	1	0	2.320182	1.794612	0.401755
307	5	0	2.628564	-0.014599	-0.395388
308	5	0	-1.510152	-0.055545	0.091728

BB-cis, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.448838	-1.169949	2.870047
2	6	0	11.939094	0.078686	3.547035
3	6	0	11.991409	2.097830	-1.746340
4	6	0	11.515404	3.279344	-1.155617
5	6	0	12.110433	3.814258	0.116922
6	6	0	11.482076	3.160149	1.316613
7	6	0	11.983896	1.962477	1.846802
8	6	0	11.380982	1.339004	2.949140
9	6	0	12.069829	-1.676209	1.719079
10	6	0	12.282488	-3.388853	-0.138543
11	6	0	11.642722	-2.784935	-1.357438
12	6	0	12.066381	-1.551075	-1.873372
13	6	0	11.438674	-0.963600	-2.981667
14	6	0	11.391687	1.557709	-2.892521
15	6	0	11.928077	0.328803	-3.570768
16	6	0	10.248969	1.960441	3.511965
17	6	0	10.361968	3.738994	1.946695
18	6	0	9.715917	3.156999	3.036074
19	6	0	10.579416	-3.567588	1.726320
20	6	0	10.368310	-1.900511	3.402737
21	6	0	9.913457	-3.100520	2.858780
22	6	0	10.446588	3.946333	-1.784976
23	6	0	10.284254	2.244028	-3.429620
24	6	0	9.800953	3.443956	-2.914821
25	6	0	10.358727	-1.658401	-3.561608
26	6	0	10.587081	-3.445841	-2.016272
27	6	0	9.917316	-2.901326	-3.110978
28	1	0	8.948016	3.964156	-3.373573
29	1	0	12.840596	1.583139	-1.295939
30	1	0	11.951283	4.923731	0.169207
31	1	0	13.213162	3.685010	0.125258
32	1	0	12.860330	1.503094	1.388774
33	1	0	8.832714	3.619664	3.499547
34	1	0	9.076387	-3.654616	3.307237
35	1	0	12.903629	-1.127945	1.279278
36	1	0	12.899567	-1.033033	-1.397168
37	1	0	9.080312	-3.424173	-3.595834
38	1	0	13.040748	0.349987	-3.572031
39	1	0	11.645253	0.361860	-4.657993
40	1	0	13.377286	-3.203205	-0.130964
41	1	0	12.182053	-4.505840	-0.175844
42	1	0	11.664224	0.037163	4.635608
43	1	0	13.050922	0.108166	3.540915
44	8	0	9.776213	-1.417176	4.598042
45	8	0	9.686573	1.366642	4.670845
46	8	0	10.270182	-4.753106	-1.579500
47	8	0	10.262821	-4.842845	1.203065

48	8	0	9.728949	-1.081746	-4.697418
49	8	0	9.669937	1.697615	-4.588133
50	8	0	9.962006	5.016698	1.494794
51	8	0	10.068628	5.211394	-1.273460
52	6	0	8.532144	0.658461	4.402007
53	6	0	8.577842	-0.768207	4.369897
54	7	0	7.461938	-1.531223	4.159573
55	7	0	7.370926	1.359152	4.218563
56	6	0	6.333509	-0.834344	3.989131
57	6	0	6.287681	0.602233	4.015284
58	6	0	4.941394	-1.360198	3.690586
59	6	0	4.863609	1.051756	3.728345
60	7	0	4.153780	-0.178796	3.546173
61	8	0	4.514736	-2.477273	3.589886
62	1	0	3.140776	-0.209889	3.287964
63	8	0	4.362079	2.135507	3.654465
64	6	0	9.063610	-4.897431	0.520211
65	6	0	9.066867	-4.849350	-0.907609
66	6	0	11.639746	-2.867889	1.116747
67	7	0	7.923898	-4.975695	-1.647075
68	7	0	7.917916	-5.079316	1.243657
69	6	0	8.528869	0.985537	-4.273542
70	6	0	8.553205	-0.440172	-4.352316
71	6	0	8.781780	5.039262	0.780588
72	6	0	8.839008	5.191231	-0.638280
73	7	0	7.445380	-1.205325	-4.109845
74	7	0	7.404840	1.679792	-3.916412
75	7	0	7.599117	5.006680	1.466144
76	7	0	7.719831	5.374023	-1.401452
77	6	0	6.807559	-5.212208	0.507719
78	6	0	6.570529	5.371227	-0.715488
79	6	0	6.810039	-5.157494	-0.927245
80	6	0	6.333402	0.918774	-3.668652
81	6	0	6.349922	-0.513242	-3.777930
82	6	0	6.509604	5.165135	0.704604
83	6	0	5.049669	5.125024	1.130504
84	6	0	5.154881	5.522104	-1.255043
85	6	0	5.375484	-5.384568	0.993362
86	6	0	5.379096	-5.284302	-1.428305
87	6	0	4.954261	1.355979	-3.205565
88	6	0	4.974690	-1.044906	-3.412103
89	7	0	4.334368	5.328217	-0.090818
90	7	0	4.227987	0.129625	-3.091170
91	7	0	4.608759	-5.370578	-0.220247
92	8	0	4.740606	5.767152	-2.347022
93	8	0	4.539077	4.961921	2.200664
94	8	0	4.504396	2.438658	-2.954475
95	8	0	4.543414	-2.162584	-3.371423
96	8	0	4.914647	-5.516704	2.086807
97	8	0	4.919358	-5.322991	-2.529952
98	1	0	3.575340	-5.361769	-0.223422
99	1	0	3.211823	0.106526	-2.852557
100	1	0	3.299297	5.280099	-0.131893
101	1	0	-13.257010	-3.429116	0.376194
102	6	0	-12.154779	-3.563015	0.410105
103	6	0	-11.535939	-3.228312	-0.917009
104	6	0	-11.550559	-2.746892	1.519719
105	1	0	-12.006249	-4.653767	0.628947
106	6	0	-11.958409	-2.112419	-1.657824
107	6	0	-10.501069	-4.019164	-1.450346
108	6	0	-12.080727	-1.505048	1.895320
109	6	0	-10.434989	-3.226200	2.237110
110	6	0	-11.332797	-1.746970	-2.857728
111	1	0	-12.783777	-1.507166	-1.281395
112	6	0	-9.835543	-3.693824	-2.632684
113	8	0	-10.148967	-5.214814	-0.770724
114	6	0	-11.529522	-0.761279	2.950236
115	1	0	-12.940018	-1.106121	1.355496
116	6	0	-9.856166	-2.537722	3.300045
117	8	0	-9.985626	-4.526298	1.915727
118	6	0	-11.814926	-0.587949	-3.683539
119	6	0	-10.255573	-2.543746	-3.295117
120	1	0	-9.010239	-4.308091	-3.019825
121	6	0	-8.910090	-5.092512	-0.159096
122	6	0	-12.095358	0.570813	3.352832
123	6	0	-10.437069	-1.316473	3.643658
124	1	0	-8.991492	-2.940314	3.846205
125	6	0	-8.824270	-4.606035	1.183303
126	1	0	-12.927439	-0.577675	-3.709508
127	1	0	-11.510258	-0.752304	-4.752752
128	6	0	-11.296253	0.747850	-3.232070
129	8	0	-9.590416	-2.170967	-4.494442
130	7	0	-7.807935	-5.460510	-0.876131
131	6	0	-11.530944	1.706649	2.545913
132	1	0	-11.880161	0.749676	4.440614
133	1	0	-13.204823	0.560549	3.284507
134	8	0	-9.973363	-0.626551	4.791969
135	7	0	-7.626537	-4.329315	1.781961
136	6	0	-11.941035	1.494881	-2.235573
137	6	0	-10.162095	1.319740	-3.841832
138	6	0	-8.424397	-1.477512	-4.224732
139	6	0	-6.642292	-5.257738	-0.249116
140	6	0	-12.085309	2.082287	1.314041
141	6	0	-10.440137	2.458497	3.027059
142	6	0	-8.764610	0.008618	4.570467
143	6	0	-6.552677	-4.639580	1.043268
144	6	0	-11.479865	2.764465	-1.854980
145	1	0	-12.818657	1.077504	-1.740826
146	6	0	-9.675238	2.585486	-3.522172
147	8	0	-9.529743	0.580310	-4.876635
148	6	0	-8.393585	-0.063998	-4.426644
149	7	0	-7.333463	-2.178471	-3.787360
150	6	0	-5.238322	-5.559679	-0.753104
151	6	0	-11.584051	3.171677	0.585637
152	1	0	-12.922072	1.511534	0.910219
153	6	0	-9.920641	3.566006	2.360156
154	8	0	-9.922108	2.112977	4.298210
155	6	0	-8.742349	1.398963	4.249188
156	7	0	-7.622886	-0.731300	4.706896
157	6	0	-5.085093	-4.410207	1.364555

158	6	0	-12.147297	3.545509	-0.757203
159	6	0	-10.362843	3.289784	-2.534687
160	1	0	-8.791818	3.006348	-4.023573
161	7	0	-7.268310	0.682163	-4.207991
162	6	0	-6.239924	-1.436822	-3.575736
163	7	0	-4.391302	-4.999342	0.271205
164	8	0	-4.844417	-6.136676	-1.719000
165	6	0	-10.526009	3.909354	1.151778
166	1	0	-9.079779	4.142550	2.771775
167	7	0	-7.580494	2.065959	3.968279
168	6	0	-6.492126	-0.057661	4.473730
169	8	0	-4.564823	-3.841328	2.286196
170	1	0	-11.998093	4.643490	-0.934100
171	1	0	-13.248166	3.401978	-0.780128
172	8	0	-9.999183	4.626176	-2.249030
173	6	0	-6.208247	-0.017197	-3.789308
174	6	0	-4.881581	-1.878888	-3.056688
175	1	0	-3.350931	-4.994635	0.205295
176	8	0	-10.138776	5.096623	0.486512
177	6	0	-6.473052	1.322499	4.070996
178	6	0	-5.065158	-0.579522	4.523837
179	6	0	-8.828783	4.757146	-1.527264
180	6	0	-4.829752	0.502450	-3.421017
181	7	0	-4.126747	-0.665914	-2.994938
182	8	0	-4.458741	-2.955256	-2.739367
183	6	0	-8.902382	5.014844	-0.124225
184	6	0	-5.035935	1.717238	3.773602
185	7	0	-4.286545	0.543995	4.079890
186	8	0	-4.607617	-1.630651	4.856420
187	7	0	-7.640413	4.715214	-2.202059
188	8	0	-4.371693	1.609059	-3.446546
189	1	0	-3.113309	-0.652843	-2.745642
190	7	0	-7.792175	5.253436	0.636723
191	8	0	-4.559328	2.744149	3.373699
192	1	0	-3.253869	0.487892	3.939369
193	6	0	-6.560480	4.946479	-1.445147
194	6	0	-6.636489	5.220453	-0.037321
195	6	0	-5.097890	4.918953	-1.861238
196	6	0	-5.228494	5.396745	0.511385
197	7	0	-4.394946	5.155649	-0.634702
198	8	0	-4.572308	4.754582	-2.922460
199	8	0	-4.823520	5.681203	1.597104
200	1	0	-3.365334	5.096772	-0.569940
201	8	0	-1.867907	3.773888	-0.674755
202	6	0	-1.275813	3.662766	-1.753144
203	7	0	-0.001097	4.192249	-2.046435
204	7	0	-1.791136	3.035027	-2.892151
205	6	0	0.473076	3.734941	-3.379666
206	1	0	0.684910	4.385914	-1.289095
207	6	0	-0.802097	2.982401	-3.995823
208	1	0	-2.778114	2.783452	-3.021056
209	1	0	0.835864	4.610664	-3.971932
210	7	0	1.495895	2.668909	-3.317928
211	1	0	-1.203977	3.434527	-4.934978
212	7	0	-0.307748	1.608484	-4.272406
213	6	0	0.986944	1.424056	-3.719222
214	1	0	2.429930	2.811032	-2.921198
215	1	0	-0.972950	0.812383	-4.257198
216	8	0	1.604812	0.363952	-3.694692
217	1	0	-1.056172	4.960392	3.588401
218	6	0	-0.640553	4.090262	3.023409
219	6	0	0.711972	3.484834	3.632702
220	7	0	-0.248748	4.534032	1.659105
221	7	0	-1.568639	2.936675	3.016165
222	1	0	1.075396	3.994953	4.558908
223	7	0	0.350392	2.079130	3.963647
224	7	0	1.681040	3.616519	2.522877
225	6	0	1.094886	4.162072	1.371763
226	1	0	-0.956530	4.499909	0.903712
227	6	0	-0.958948	1.769546	3.520232
228	1	0	-2.586519	3.054041	2.931020
229	1	0	1.072014	1.341626	3.935909
230	1	0	2.690567	3.488466	2.653452
231	8	0	1.659084	4.363650	0.301688
232	8	0	-1.512151	0.681108	3.623676
233	6	0	0.925211	-1.669306	3.435345
234	7	0	-0.362602	-1.987247	3.906543
235	7	0	1.587696	-2.855051	3.025845
236	8	0	1.423811	-0.550608	3.414843
237	6	0	-0.667497	-3.431426	3.739007
238	1	0	-1.107140	-1.272595	3.909790
239	6	0	0.716539	-4.044669	3.210816
240	1	0	2.613818	-2.947033	3.083834
241	1	0	-1.027889	-3.849949	4.711747
242	7	0	-1.612750	-3.741105	2.645972
243	1	0	1.172610	-4.808141	3.886910
244	7	0	0.355848	-4.682253	1.918200
245	6	0	-0.986454	-4.371886	1.563721
246	1	0	-2.607421	-3.487649	2.670575
247	1	0	1.077671	-4.743444	1.177160
248	8	0	-1.526578	-4.701196	0.511385
249	1	0	-0.694002	-5.170549	-3.704199
250	6	0	-0.333404	-4.273565	-3.144150
251	6	0	0.926018	-3.527195	-3.799181
252	7	0	0.161044	-4.678226	-1.804060
253	7	0	-1.367053	-3.213356	-3.101512
254	1	0	1.342838	-4.021494	-4.710109
255	7	0	0.399584	-2.184175	-4.149681
256	7	0	1.913617	-3.499090	-2.691795
257	6	0	1.414695	-4.089144	-1.525787
258	1	0	-0.514042	-4.888531	-1.042611
259	6	0	-0.882438	-1.984074	-3.576862
260	1	0	-2.301886	-3.356028	-2.711566
261	1	0	1.048978	-1.376840	-4.218460
262	1	0	2.879464	-3.176658	-2.817147
263	8	0	1.997492	-4.130855	-0.439170
264	8	0	-1.506721	-0.927777	-3.580261
265	6	0	5.635897	0.679822	0.432881
266	6	0	4.258959	0.755189	0.256505
267	6	0	3.479036	-0.401989	0.126036

268	6	0	4.137055	-1.636341	0.161519
269	6	0	5.514854	-1.714136	0.335860
270	6	0	6.282235	-0.557639	0.483507
271	1	0	6.220124	1.590299	0.545105
272	1	0	3.761706	1.722205	0.229136
273	1	0	3.573252	-2.568980	0.048356
274	1	0	6.004809	-2.683322	0.374230
275	6	0	7.780542	-0.645342	0.644492
276	6	0	8.498066	-0.656669	-0.709210
277	1	0	8.036397	-1.553554	1.202881
278	1	0	8.135373	0.205740	1.235157
279	1	0	9.582234	-0.732335	-0.579242
280	1	0	8.164472	-1.504401	-1.315862
281	1	0	8.282893	0.261383	-1.261698
282	8	0	1.077238	-1.352760	0.145191
283	8	0	1.391240	0.949656	-0.244679
284	1	0	0.417744	0.980785	-0.185440
285	6	0	-5.788901	1.554782	0.168124
286	6	0	-4.411151	1.409822	0.050208
287	6	0	-3.774885	0.214899	0.406662
288	6	0	-4.573021	-0.827548	0.893012
289	6	0	-5.949850	-0.682463	1.021631
290	6	0	-6.577403	0.510931	0.657718
291	1	0	-6.263982	2.490802	-0.113701
292	1	0	-3.827495	2.249329	-0.338943
293	1	0	-4.094106	-1.760550	1.181747
294	1	0	-6.547430	-1.502579	1.415272
295	6	0	-8.077261	0.661275	0.734703
296	6	0	-8.743240	0.415787	-0.624019
297	1	0	-8.325981	1.670079	1.085653
298	1	0	-8.479947	-0.043078	1.469854
299	1	0	-9.828178	0.543362	-0.557844
300	1	0	-8.360844	1.115984	-1.372755
301	1	0	-8.537292	-0.599025	-0.972944
302	8	0	-1.361081	1.074612	0.112014
303	8	0	-1.724618	-1.242930	0.305549
304	1	0	-0.751986	-1.283559	0.248895
305	1	0	1.532205	-2.168110	0.403830
306	1	0	-1.782112	1.944603	0.192917
307	5	0	-2.223777	0.010277	0.276134
308	5	0	1.918485	-0.266216	0.000862

BC-trans, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.304093	1.016188	3.062030
2	6	0	-11.789446	-0.271565	3.666059
3	6	0	-11.974972	-1.812819	-1.785740
4	6	0	-11.407154	-2.986712	-1.270593
5	6	0	-11.994087	-3.686809	-0.075497
6	6	0	-11.402071	-3.187430	1.211275
7	6	0	-11.869149	-2.017360	1.829899
8	6	0	-11.262565	-1.503106	2.985504
9	6	0	-11.958352	1.630346	1.984432
10	6	0	-12.189067	3.491555	0.273868
11	6	0	-11.602033	2.979309	-1.012423
12	6	0	-12.081919	1.810862	-1.623199
13	6	0	-11.508293	1.308589	-2.800103
14	6	0	-11.455918	-1.186677	-2.929515
15	6	0	-12.050617	0.080136	-3.476260
16	6	0	-10.163585	-2.211213	3.511835
17	6	0	-10.345020	-3.880735	1.830727
18	6	0	-9.700485	-3.410089	2.974596
19	6	0	-10.426074	3.486189	2.089376
20	6	0	-10.184337	1.677762	3.604498
21	6	0	-9.727209	2.912599	3.151306
22	6	0	-10.280746	-3.514924	-1.935392
23	6	0	-10.360959	-1.796722	-3.570448
24	6	0	-9.739098	-2.948231	-3.086468
25	6	0	-10.419834	2.016286	-3.350111
26	6	0	-10.544851	3.662575	-1.645161
27	6	0	-9.922068	3.197234	-2.803089
28	1	0	-8.871220	-3.393631	-3.592799
29	1	0	-12.839667	-1.374843	-1.286391
30	1	0	-11.809889	-4.790476	-0.167980
31	1	0	-13.100430	-3.585581	-0.064968
32	1	0	-12.714809	-1.486253	1.391558
33	1	0	-8.860697	-3.953938	3.430507
34	1	0	-8.858624	3.408592	3.607498
35	1	0	-12.822915	1.140102	1.536035
36	1	0	-12.917332	1.277601	-1.168518
37	1	0	-9.079290	3.733145	-3.262939
38	1	0	-13.159450	0.054059	-3.404190
39	1	0	-11.839468	0.142850	-4.577553
40	1	0	-13.286953	3.327541	0.301610
41	1	0	-12.064636	4.605671	0.323951
42	1	0	-11.491797	-0.299291	4.749241
43	1	0	-12.901826	-0.292165	3.682199
44	8	0	-9.546073	1.066980	4.715235
45	8	0	-9.527332	-1.706334	4.677984
46	8	0	-10.177418	4.918469	-1.108777
47	8	0	-10.095053	4.793895	1.663281
48	8	0	-9.880826	1.541451	-4.569138
49	8	0	-9.928758	-1.234655	-4.799292
50	8	0	-9.954499	-5.127648	1.277559
51	8	0	-9.777255	-4.749309	-1.468751
52	6	0	-8.366534	-1.019748	4.368383
53	6	0	-8.385362	0.409499	4.363043
54	7	0	-7.279384	1.154760	4.061350
55	7	0	-7.231142	-1.737146	4.108289
56	6	0	-6.180293	0.438903	3.799163
57	6	0	-6.148903	-0.996052	3.837734
58	6	0	-4.810091	0.947413	3.394744
59	6	0	-4.740817	-1.459029	3.496633
60	7	0	-4.026174	-0.238625	3.264442
61	8	0	-4.408776	2.058970	3.183906
62	1	0	-3.002726	-0.208464	3.056347

63	8	0	-4.253604	-2.550062	3.413093
64	6	0	-8.910590	4.870654	0.955318
65	6	0	-8.952573	4.923536	-0.471165
66	6	0	-11.520937	2.858377	1.463053
67	7	0	-7.825441	5.056607	-1.233315
68	7	0	-7.741766	4.967582	1.657815
69	6	0	-8.721156	-0.572273	-4.657005
70	6	0	-8.700908	0.838533	-4.439159
71	6	0	-8.712966	-5.031531	0.666396
72	6	0	-8.623064	-4.698874	-0.720944
73	7	0	-7.541708	1.520987	-4.185308
74	7	0	-7.579243	-1.317598	-4.744394
75	7	0	-7.610703	-5.271548	1.435085
76	7	0	-7.424951	-4.449949	-1.333615
77	6	0	-6.646453	5.108336	0.901059
78	6	0	-6.351679	-4.633140	-0.552427
79	6	0	-6.687544	5.144024	-0.534309
80	6	0	-6.450643	-0.629848	-4.545509
81	6	0	-6.434348	0.769750	-4.218616
82	6	0	-6.444139	-5.098351	0.803182
83	6	0	-5.042927	-5.273603	1.367820
84	6	0	-4.882563	-4.383602	-0.872016
85	6	0	-5.198263	5.205584	1.355816
86	6	0	-5.266822	5.243990	-1.067476
87	6	0	-5.027879	-1.161790	-4.539472
88	6	0	-5.003378	1.166150	-3.889098
89	7	0	-4.197742	-4.794472	0.306641
90	7	0	-4.253787	-0.025041	-4.112469
91	7	0	-4.463787	5.237955	0.123394
92	8	0	-4.355924	-3.923449	-1.847631
93	8	0	-4.651792	-5.711338	2.406167
94	8	0	-4.570832	-2.225609	-4.825034
95	8	0	-4.536165	2.207923	-3.518091
96	8	0	-4.703210	5.264439	2.441425
97	8	0	-4.832601	5.324194	-2.176870
98	1	0	-3.432924	5.200266	0.089062
99	1	0	-3.238750	-0.105125	-3.895932
100	1	0	-3.161530	-4.713722	0.410682
101	1	0	13.304657	3.662345	0.099405
102	6	0	12.200595	3.760270	0.175939
103	6	0	11.540401	3.375321	-1.117260
104	6	0	11.671953	2.951180	1.328366
105	1	0	12.024666	4.850491	0.376869
106	6	0	11.978006	2.268119	-1.862170
107	6	0	10.450675	4.114069	-1.614995
108	6	0	12.252773	1.729971	1.696594
109	6	0	10.582809	3.414575	2.095041
110	6	0	11.316779	1.860981	-3.029107
111	1	0	12.844989	1.704199	-1.516243
112	6	0	9.745848	3.743625	-2.760879
113	8	0	10.089675	5.307293	-0.936668
114	6	0	11.776629	0.990144	2.790204
115	1	0	13.093032	1.343106	1.118972
116	6	0	10.079787	2.730600	3.198948
117	8	0	10.077753	4.695628	1.776934
118	6	0	11.811630	0.716307	-3.866877
119	6	0	10.186522	2.603394	-3.426788
120	1	0	8.878616	4.316707	-3.117811
121	6	0	8.887352	5.160132	-0.263233
122	6	0	12.396480	-0.322725	3.176233
123	6	0	10.708056	1.529666	3.531514
124	1	0	9.236256	3.122440	3.784464
125	6	0	8.880866	4.723402	1.099041
126	1	0	12.922182	0.747964	-3.934917
127	1	0	11.461731	0.862336	-4.924866
128	6	0	11.363730	-0.636089	-3.390547
129	8	0	9.492530	2.182277	-4.593753
130	7	0	7.740849	5.461483	-0.940818
131	6	0	11.828881	-1.476213	2.396721
132	1	0	12.232000	-0.502026	4.272590
133	1	0	13.501379	-0.281636	3.061760
134	8	0	10.318066	0.848887	4.713040
135	7	0	7.721438	4.442015	1.767399
136	6	0	12.063966	-1.338526	-2.399088
137	6	0	10.246766	-1.269599	-3.970401
138	6	0	8.374575	1.434963	-4.275091
139	6	0	6.613477	5.249019	-0.250932
140	6	0	12.354663	-1.858501	1.154500
141	6	0	10.762465	-2.237203	2.916185
142	6	0	9.114429	0.183919	4.561033
143	6	0	6.603770	4.690014	1.071267
144	6	0	11.674627	-2.625117	-1.996337
145	1	0	12.926866	-0.870966	-1.923655
146	6	0	9.838020	-2.558585	-3.636031
147	8	0	9.541090	-0.569648	-4.987301
148	6	0	8.394758	0.022269	-4.492762
149	7	0	7.278748	2.080963	-3.771892
150	6	0	5.180390	5.477709	-0.705910
151	6	0	11.846719	-2.961436	0.451887
152	1	0	13.175613	-1.284538	0.723701
153	6	0	10.229236	-3.350999	2.270805
154	8	0	10.300712	-1.892474	4.209049
155	6	0	9.106812	-1.205278	4.225921
156	7	0	7.965461	0.893175	4.771707
157	6	0	5.160434	4.433859	1.474149
158	6	0	12.390995	-3.353834	-0.893755
159	6	0	10.579347	-3.217231	-2.655425
160	1	0	8.971875	-3.031578	-4.120878
161	7	0	7.311602	-0.772587	-4.235975
162	6	0	6.229969	1.289489	-3.517383
163	7	0	4.400470	4.941216	0.381715
164	8	0	4.722092	5.986752	-1.681747
165	6	0	10.805396	-3.699425	1.049521
166	1	0	9.403794	-3.930939	2.707530
167	7	0	7.947442	-1.894125	3.997237
168	6	0	6.838366	0.194712	4.593408
169	8	0	4.694572	3.897725	2.442304
170	1	0	12.273186	-4.460731	-1.036645
171	1	0	13.485891	-3.176554	-0.947105
172	8	0	10.284490	-4.565687	-2.345923

173	6	0	6.242827	-0.125680	-3.756897
174	6	0	4.892210	1.666805	-2.905135
175	1	0	3.361081	4.893556	0.359212
176	8	0	10.425303	-4.901245	0.410896
177	6	0	6.830481	-1.177601	4.170885
178	6	0	5.402848	0.680131	4.723490
179	6	0	9.118163	-4.721341	-1.618545
180	6	0	4.907808	-0.707679	-3.321457
181	7	0	4.192388	0.425440	-2.818304
182	8	0	4.458686	2.721158	-2.529738
183	6	0	9.188279	-4.869672	-0.200101
184	6	0	5.390396	-1.603985	3.934254
185	7	0	4.630372	-0.451219	4.287652
186	8	0	4.939118	1.714249	5.097143
187	7	0	7.938655	-4.792844	-2.305781
188	8	0	4.485496	-1.827752	-3.338735
189	1	0	3.196886	0.369245	-2.512742
190	7	0	8.077092	-5.072388	0.570663
191	8	0	4.929789	-2.634202	3.527788
192	1	0	3.592049	-0.418462	4.187524
193	6	0	6.860888	-5.008620	-1.542295
194	6	0	6.928916	-5.139422	-0.113820
195	6	0	5.405569	-5.105494	-1.977769
196	6	0	5.518281	-5.314442	0.432014
197	7	0	4.695712	-5.247705	-0.739609
198	8	0	4.896098	-5.087582	-3.057898
199	8	0	5.112535	-5.472326	1.544299
200	1	0	3.658411	-5.247495	-0.691457
201	8	0	2.036615	-4.223975	-0.653512
202	6	0	1.354625	-3.991504	-1.649394
203	7	0	0.036249	-4.459563	-1.871261
204	7	0	1.796005	-3.304528	-2.790529
205	6	0	-0.525060	-3.895786	-3.124468
206	1	0	-0.591043	-4.634389	-1.061177
207	6	0	0.725219	-3.157096	-3.803241
208	1	0	2.759586	-3.003032	-2.951738
209	1	0	-0.972406	-4.716369	-3.738301
210	7	0	-1.499352	-2.797596	-2.920303
211	1	0	1.034213	-3.578572	-4.790958
212	7	0	0.255111	-1.759620	-3.986114
213	6	0	-0.997873	-1.563380	-3.343219
214	1	0	-2.405939	-2.936508	-2.465112
215	1	0	0.942628	-0.984644	-3.986241
216	8	0	-1.580538	-0.482464	-3.271481
217	1	0	1.490774	-4.992789	3.766037
218	6	0	1.042299	-4.130142	3.214176
219	6	0	-0.282473	-3.522324	3.883919
220	7	0	0.587175	-4.585136	1.875142
221	7	0	1.964709	-2.972612	3.173331
222	1	0	-0.602986	-4.032479	4.825238
223	7	0	0.088843	-2.114427	4.188988
224	7	0	-1.299075	-3.664020	2.820087
225	6	0	-0.759413	-4.204567	1.641647
226	1	0	1.258091	-4.598808	1.082764
227	6	0	1.362657	-1.800995	3.653183
228	1	0	2.958084	-3.055270	2.934293
229	1	0	-0.641673	-1.379571	4.207643
230	1	0	-2.280404	-3.407439	2.945983
231	8	0	-1.382283	-4.411417	0.605215
232	8	0	1.891490	-0.691914	3.680577
233	6	0	-0.844111	1.412986	3.651880
234	7	0	0.439683	1.738269	4.151997
235	7	0	-1.506645	2.595849	3.286089
236	8	0	-1.336709	0.289319	3.617400
237	6	0	0.749695	3.175828	3.936875
238	1	0	1.194303	1.027860	4.120700
239	6	0	-0.624936	3.778268	3.372285
240	1	0	-2.507109	2.657662	3.070273
241	1	0	1.101989	3.628207	4.896299
242	7	0	1.707648	3.428664	2.835718
243	1	0	-1.074267	4.588269	3.997780
244	7	0	-0.254248	4.329603	2.040083
245	6	0	1.087751	4.000902	1.716704
246	1	0	2.718284	3.283270	2.924428
247	1	0	-0.972669	4.349710	1.292402
248	8	0	1.637794	4.257540	0.647498
249	1	0	0.751705	4.972124	-3.504946
250	6	0	0.392590	4.065760	-2.959599
251	6	0	-0.848891	3.313005	-3.639181
252	7	0	-0.123071	4.454017	-1.619623
253	7	0	1.433906	3.015245	-2.904195
254	1	0	-1.241588	3.798006	-4.565367
255	7	0	-0.316015	1.963433	-3.963406
256	7	0	-1.862769	3.285819	-2.556885
257	6	0	-1.381590	3.856866	-1.374499
258	1	0	0.551341	4.600473	-0.841131
259	6	0	0.959318	1.777777	-3.366484
260	1	0	2.370350	3.173049	-2.524283
261	1	0	-0.969363	1.153490	-3.977762
262	1	0	-2.835953	2.998292	-2.717927
263	8	0	-1.980953	3.870193	-0.295406
264	8	0	1.582977	0.721947	-3.336415
265	6	0	-6.486287	-0.774497	-1.131776
266	6	0	-5.114762	-0.850908	-0.928490
267	6	0	-4.418315	0.177771	-0.282298
268	6	0	-5.148694	1.290134	0.149526
269	6	0	-6.524030	1.365840	-0.041742
270	6	0	-7.210349	0.333525	-0.685041
271	1	0	-7.006818	-1.586645	-1.637166
272	1	0	-4.557050	-1.717943	-1.275368
273	1	0	-4.646303	2.110169	0.667435
274	1	0	-7.076626	2.232977	0.311402
275	6	0	-8.709305	0.382743	-0.829181
276	6	0	-9.411672	-0.214220	0.393050
277	1	0	-9.013804	-0.166136	-1.726454
278	1	0	-9.031916	1.421275	-0.962843
279	1	0	-10.498968	-0.174233	0.275553
280	1	0	-9.120397	-1.258180	0.535452
281	1	0	-9.145136	0.338571	1.297850
282	8	0	-2.066774	1.109466	0.235092

283	8	0	-2.332061	-1.208222	-0.105070
284	1	0	-1.357105	-1.222145	-0.011796
285	6	0	4.587588	-1.493652	0.463134
286	6	0	3.209414	-1.409755	0.318309
287	6	0	2.583084	-0.163216	0.348110
288	6	0	3.341942	0.995697	0.522993
289	6	0	4.720844	0.897586	0.668753
290	6	0	5.359802	-0.344772	0.649012
291	1	0	5.070146	-2.467806	0.459523
292	1	0	2.601787	-2.304660	0.192977
293	1	0	2.845015	1.961696	0.555054
294	1	0	5.310038	1.796344	0.828739
295	6	0	6.859932	-0.442312	0.786480
296	6	0	7.568302	-0.326587	-0.567870
297	1	0	7.118783	-1.399937	1.252999
298	1	0	7.216718	0.349884	1.452933
299	1	0	8.651767	-0.412938	-0.448666
300	1	0	7.232804	-1.117455	-1.244788
301	1	0	7.349763	0.638339	-1.032127
302	8	0	0.415845	-1.120066	0.121140
303	8	0	0.596682	1.105656	0.320482
304	1	0	-0.394752	1.069899	0.278517
305	6	0	1.099688	-0.114070	0.248774
306	1	0	-2.491665	1.976755	0.139093
307	5	0	-2.875354	0.019453	-0.052913

BC-cis, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.384425	0.908144	3.033517
2	6	0	-11.904396	-0.390569	3.580140
3	6	0	-12.008002	-1.780948	-1.921195
4	6	0	-11.445875	-2.969045	-1.434001
5	6	0	-12.042470	-3.701122	-0.263622
6	6	0	-11.466092	-3.228272	1.040093
7	6	0	-11.948077	-2.074986	1.679620
8	6	0	-11.365220	-1.594259	2.860011
9	6	0	-12.003764	1.547574	1.949142
10	6	0	-12.215707	3.462929	0.301858
11	6	0	-11.658172	3.005807	-1.016535
12	6	0	-12.126462	1.845966	-1.654099
13	6	0	-11.545623	1.376120	-2.840800
14	6	0	-11.476121	-1.120517	-3.039993
15	6	0	-12.069862	0.160437	-3.553717
16	6	0	-10.267804	-2.308758	3.381532
17	6	0	-10.413336	-3.931090	1.655317
18	6	0	-9.784513	-3.486682	2.819099
19	6	0	-10.416939	3.350744	2.087273
20	6	0	-10.275555	1.545322	3.623620
21	6	0	-9.763485	2.759896	3.167600
22	6	0	-10.311860	-3.478669	-2.100525
23	6	0	-10.375222	-1.713268	-3.686302
24	6	0	-9.759884	-2.879734	-3.229598
25	6	0	-10.462698	2.108690	-3.368941
26	6	0	-10.628852	3.731152	-1.646068
27	6	0	-9.997246	3.296527	-2.811351
28	1	0	-8.885669	-3.309884	-3.738647
29	1	0	-12.878268	-1.357775	-1.418592
30	1	0	-11.851477	-4.801306	-0.379926
31	1	0	-13.149349	-3.605510	-0.262441
32	1	0	-12.787058	-1.534676	1.240263
33	1	0	-8.944942	-4.034918	3.269521
34	1	0	-8.892303	3.232966	3.642490
35	1	0	-12.869952	1.079357	1.480189
36	1	0	-12.953276	1.291564	-1.209240
37	1	0	-9.170385	3.858546	-3.267756
38	1	0	-13.179520	0.126284	-3.494283
39	1	0	-11.847614	0.254994	-4.650651
40	1	0	-13.314732	3.307726	0.342465
41	1	0	-12.079908	4.572567	0.401460
42	1	0	-11.636473	-0.463773	4.668687
43	1	0	-13.016427	-0.400417	3.564924
44	8	0	-9.717713	0.950569	4.784734
45	8	0	-9.680172	-1.827555	4.578787
46	8	0	-10.275086	4.983020	-1.084381
47	8	0	-10.030930	4.642654	1.664061
48	8	0	-9.883071	1.645820	-4.574932
49	8	0	-9.915511	-1.115251	-4.889781
50	8	0	-10.010852	-5.163370	1.077609
51	8	0	-9.807185	-4.722004	-1.659050
52	6	0	-8.514465	-1.120478	4.361727
53	6	0	-8.526503	0.298482	4.524015
54	7	0	-7.385719	1.049935	4.468694
55	7	0	-7.373253	-1.812779	4.057227
56	6	0	-6.271825	0.355163	4.213829
57	6	0	-6.268593	-1.062319	3.975277
58	6	0	-4.857386	0.882034	4.058856
59	6	0	-4.857309	-1.488392	3.599151
60	7	0	-4.102533	-0.277999	3.689986
61	8	0	-4.391221	1.976819	4.196320
62	1	0	-3.088343	-0.220695	3.454651
63	8	0	-4.395891	-2.549877	3.287062
64	6	0	-8.888234	4.698813	0.894697
65	6	0	-9.018471	4.958244	-0.504382
66	6	0	-11.536130	2.773102	1.453286
67	7	0	-7.943862	5.218317	-1.306426
68	7	0	-7.669755	4.604633	1.508015
69	6	0	-8.714002	-0.457171	-4.684545
70	6	0	-8.708858	0.943506	-4.404019
71	6	0	-8.763964	-5.045792	0.481889
72	6	0	-8.661944	-4.679728	-0.896088
73	7	0	-7.568878	1.610484	-4.045197
74	7	0	-7.566840	-1.195088	-4.753622
75	7	0	-7.667943	-5.294319	1.257175
76	7	0	-7.459690	-4.402395	-1.487704
77	6	0	-6.621887	4.826176	0.703196
78	6	0	-6.393780	-4.590081	-0.697529
79	6	0	-6.759906	5.165264	-0.685134

80	6	0	-6.452204	-0.517080	-4.460681
81	6	0	-6.459182	0.860557	-4.053813
82	6	0	-6.496073	-5.091942	0.644274
83	6	0	-5.098861	-5.266158	1.220259
84	6	0	-4.925049	-4.310429	-0.991429
85	6	0	-5.140083	4.733008	1.033842
86	6	0	-5.379712	5.372656	-1.288393
87	6	0	-5.029029	-1.045107	-4.412897
88	6	0	-5.049725	1.238749	-3.625473
89	7	0	-4.247846	-4.749823	0.181203
90	7	0	-4.287152	0.061250	-3.860270
91	7	0	-4.494425	5.084568	-0.191018
92	8	0	-4.393756	-3.805344	-1.941861
93	8	0	-4.714549	-5.727981	2.250537
94	8	0	-4.547880	-2.081483	-4.752268
95	8	0	-4.609056	2.265518	-3.181447
96	8	0	-4.567077	4.423859	2.039582
97	8	0	-5.024461	5.709811	-2.376278
98	1	0	-3.466433	5.038523	-0.301302
99	1	0	-3.275945	-0.026597	-3.615569
100	1	0	-3.212013	-4.668546	0.294122
101	1	0	13.253973	3.670383	0.240448
102	6	0	12.147821	3.761073	0.293484
103	6	0	11.518720	3.373485	-1.014189
104	6	0	11.601071	2.948970	1.435271
105	1	0	11.960681	4.850132	0.490900
106	6	0	11.978895	2.267116	-1.747077
107	6	0	10.438921	4.107915	-1.539107
108	6	0	12.181022	1.732232	1.818796
109	6	0	10.493757	3.407702	2.178469
110	6	0	11.349050	1.856692	-2.929929
111	1	0	12.838554	1.706352	-1.378462
112	6	0	9.766465	3.735345	-2.703699
113	8	0	10.049926	5.298442	-0.870627
114	6	0	11.688255	0.994005	2.906518
115	1	0	13.033081	1.346814	1.257781
116	6	0	9.978381	2.729336	3.279564
117	8	0	9.979323	4.679166	1.837936
118	6	0	11.865970	0.711132	-3.753201
119	6	0	10.228122	2.596604	-3.357494
120	1	0	8.906687	4.305342	-3.082951
121	6	0	8.833029	5.136049	-0.226693
122	6	0	12.300503	-0.319640	3.302100
123	6	0	10.608004	1.534007	3.629998
124	1	0	9.123409	3.120306	3.848769
125	6	0	8.799548	4.685430	1.130895
126	1	0	12.977894	0.743081	-3.792369
127	1	0	11.543607	0.855776	-4.820098
128	6	0	11.406164	-0.640944	-3.287214
129	8	0	9.564993	2.171136	-4.540682
130	7	0	7.699296	5.433962	-0.926661
131	6	0	11.745110	-1.471217	2.510638
132	1	0	12.116152	-0.500516	4.394996
133	1	0	13.407225	-0.279438	3.207321
134	8	0	10.199228	0.858074	4.808364
135	7	0	7.628906	4.372788	1.764874
136	6	0	12.081795	-1.341905	-2.277693
137	6	0	10.304469	-1.276015	-3.893923
138	6	0	8.440510	1.423744	-4.246372
139	6	0	6.558552	5.198642	-0.266318
140	6	0	12.297169	-1.857859	1.281332
141	6	0	10.662819	-2.226232	3.005654
142	6	0	8.993821	0.200479	4.633451
143	6	0	6.525162	4.613762	1.044261
144	6	0	11.682842	-2.627849	-1.882637
145	1	0	12.933003	-0.873694	-1.782174
146	6	0	9.886505	-2.563821	-3.566093
147	8	0	9.624246	-0.580064	-4.930678
148	6	0	8.465407	0.011539	-4.465148
149	7	0	7.334772	2.069081	-3.764461
150	6	0	5.133117	5.428965	-0.744657
151	6	0	11.799901	-2.959373	0.568792
152	1	0	13.130928	-1.288934	0.868799
153	6	0	10.138257	-3.337736	2.349449
154	8	0	10.174169	-1.877620	4.287174
155	6	0	8.984662	-1.183347	4.278117
156	7	0	7.845423	0.913927	4.832026
157	6	0	5.075974	4.334096	1.407703
158	6	0	12.373324	-3.355940	-0.763321
159	6	0	10.602827	-3.220505	-2.565978
160	1	0	9.032551	-3.037654	-4.071419
161	7	0	7.376068	-0.783336	-4.236054
162	6	0	6.280800	1.277321	-3.534441
163	7	0	4.334217	4.867774	0.317125
164	8	0	4.690828	5.954114	-1.719315
165	6	0	10.741346	-3.691527	1.142822
166	1	0	9.299875	-3.912607	2.767766
167	7	0	7.826998	-1.858453	4.004112
168	6	0	6.718328	0.227091	4.613448
169	8	0	4.595567	3.761740	2.348710
170	1	0	12.256424	-4.462900	-0.906493
171	1	0	13.469501	-3.181061	-0.792972
172	8	0	10.299036	-4.567567	-2.259903
173	6	0	6.297116	-0.136894	-3.779604
174	6	0	4.929717	1.654970	-2.953202
175	1	0	3.292527	4.840338	0.287130
176	8	0	10.372817	-4.894263	0.499764
177	6	0	6.711712	-1.135401	4.159949
178	6	0	5.283398	0.719722	4.719155
179	6	0	9.115328	-4.720760	-1.560689
180	6	0	4.949765	-0.717456	-3.382984
181	7	0	4.224206	0.415565	-2.892470
182	8	0	4.490619	2.708712	-2.582242
183	6	0	9.150756	-4.864741	-0.140460
184	6	0	5.276141	-1.543147	3.870446
185	7	0	4.514696	-0.394045	4.233322
186	8	0	4.817255	1.745611	5.111910
187	7	0	7.953327	-4.797063	-2.276429
188	8	0	4.522786	-1.835256	-3.419296
189	1	0	3.219454	0.362323	-2.621915

190	7	0	8.021531	-5.069274	0.603169
191	8	0	4.821568	-2.559914	3.425392
192	1	0	3.480891	-0.348345	4.102364
193	6	0	6.857921	-5.015543	-1.539229
194	6	0	6.890805	-5.143410	-0.109330
195	6	0	5.414736	-5.122781	-2.011621
196	6	0	5.467742	-5.329271	0.401040
197	7	0	4.674768	-5.268333	-0.791704
198	8	0	4.934152	-5.109689	-3.104814
199	8	0	5.035967	-5.492923	1.502377
200	1	0	3.636871	-5.272966	-0.770986
201	8	0	2.029317	-4.206175	-0.799609
202	6	0	1.349094	-3.963307	-1.793788
203	7	0	0.023241	-4.411384	-2.014151
204	7	0	1.800180	-3.289359	-2.939400
205	6	0	-0.530367	-3.843383	-3.268576
206	1	0	-0.606989	-4.581855	-1.205696
207	6	0	0.728706	-3.119298	-3.946678
208	1	0	2.763594	-2.985125	-3.093641
209	1	0	-0.985647	-4.659760	-3.882015
210	7	0	-1.493173	-2.734463	-3.066311
211	1	0	1.028945	-3.540226	-4.937436
212	7	0	0.277375	-1.714336	-4.123527
213	6	0	-0.975222	-1.505424	-3.484207
214	1	0	-2.408688	-2.866960	-2.628377
215	1	0	0.974905	-0.948228	-4.115636
216	8	0	-1.541638	-0.415558	-3.410723
217	1	0	1.456961	-4.916012	3.613995
218	6	0	0.993769	-4.062969	3.059008
219	6	0	-0.339533	-3.473674	3.728334
220	7	0	0.544975	-4.530049	1.722630
221	7	0	1.897660	-2.891102	3.012501
222	1	0	-0.652730	-3.988333	4.669746
223	7	0	0.013925	-2.061514	4.033900
224	7	0	-1.354537	-3.633562	2.665377
225	6	0	-0.807593	-4.172089	1.488736
226	1	0	1.216868	-4.539518	0.930462
227	6	0	1.282484	-1.728852	3.496381
228	1	0	2.889987	-2.959384	2.764057
229	1	0	-0.722766	-1.336042	4.062929
230	1	0	-2.334922	-3.370363	2.781739
231	8	0	-1.427619	-4.398681	0.454784
232	8	0	1.796099	-0.612704	3.524942
233	6	0	-0.935706	1.499337	3.570758
234	7	0	0.351047	1.833769	4.047535
235	7	0	-1.619061	2.673792	3.176871
236	8	0	-1.402386	0.366673	3.540109
237	6	0	0.634373	3.281805	3.872002
238	1	0	1.114862	1.135187	3.996590
239	6	0	-0.751078	3.869473	3.319528
240	1	0	-2.642952	2.758654	3.252807
241	1	0	0.973698	3.714451	4.845577
242	7	0	1.591369	3.587757	2.787147
243	1	0	-1.211593	4.656548	3.964757
244	7	0	-0.387429	4.464210	2.004294
245	6	0	0.962977	4.170090	1.677520
246	1	0	2.597406	3.404940	2.854396
247	1	0	-1.100401	4.469083	1.250587
248	8	0	1.517337	4.469905	0.622813
249	1	0	0.802706	5.001804	-3.638525
250	6	0	0.443458	4.098094	-3.088958
251	6	0	-0.799726	3.342681	-3.765829
252	7	0	-0.072237	4.487940	-1.752224
253	7	0	1.484124	3.045612	-3.032940
254	1	0	-1.203251	3.835795	-4.683137
255	7	0	-0.260255	2.001682	-4.108388
256	7	0	-1.806658	3.310799	-2.677439
257	6	0	-1.319533	3.877890	-1.495862
258	1	0	0.587653	4.691563	-0.975744
259	6	0	1.015306	1.813079	-3.513993
260	1	0	2.422994	3.202798	-2.658854
261	1	0	-0.907990	1.187511	-4.146009
262	1	0	-2.749885	2.921102	-2.792832
263	8	0	-1.917836	3.899092	-0.416389
264	8	0	1.642095	0.758965	-3.496809
265	6	0	-6.259623	-0.847568	-0.096975
266	6	0	-4.882994	-0.861750	-0.265970
267	6	0	-4.082828	0.189767	0.201984
268	6	0	-4.720196	1.257188	0.839582
269	6	0	-6.101428	1.269224	1.023082
270	6	0	-6.888816	0.216414	0.558838
271	1	0	-6.860038	-1.674796	-0.468105
272	1	0	-4.397331	-1.699383	-0.759738
273	1	0	-4.136655	2.092104	1.236517
274	1	0	-6.572189	2.099615	1.546913
275	6	0	-8.388009	0.217537	0.736647
276	6	0	-9.130243	0.319941	-0.598352
277	1	0	-8.676006	1.054834	1.381247
278	1	0	-8.697204	-0.700852	1.249316
279	1	0	-10.213234	0.328733	-0.443219
280	1	0	-8.849196	1.235095	-1.127008
281	1	0	-8.889930	-0.528394	-1.244850
282	8	0	-1.689268	1.174315	0.168654
283	8	0	-1.990402	-1.137189	-0.173616
284	1	0	-1.014051	-1.137882	-0.240918
285	6	0	4.910184	-1.586651	0.193422
286	6	0	3.536272	-1.455064	0.050813
287	6	0	2.932889	-0.214558	0.267478
288	6	0	3.710485	0.882440	0.640657
289	6	0	5.086034	0.735967	0.785682
290	6	0	5.703126	-0.497482	0.566926
291	1	0	5.376558	-2.555700	0.038533
292	1	0	2.912937	-2.306923	-0.217825
293	1	0	3.232334	1.839610	0.824151
294	1	0	5.686764	1.587115	1.095719
295	6	0	7.198918	-0.656004	0.692570
296	6	0	7.901372	-0.558013	-0.666502
297	1	0	7.421269	-1.627731	1.150561
298	1	0	7.592482	0.113335	1.364134
299	1	0	8.981308	-0.691017	-0.557225

300	1	0	7.528480	-1.326384	-1.350231
301	1	0	7.719805	0.419277	-1.120127
302	8	0	0.757286	-1.062351	-0.186738
303	8	0	0.976967	1.098464	0.369436
304	1	0	-0.011216	1.100584	0.275720
305	6	0	1.454930	-0.108876	0.129015
306	1	0	-2.141107	2.028538	0.259392
307	5	0	-2.524997	0.074951	0.052433

CC-trans, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.353177	0.789127	-3.106281
2	6	0	11.847644	-0.547999	-3.579730
3	6	0	12.012636	-1.542869	1.996606
4	6	0	11.480097	-2.774842	1.591926
5	6	0	12.104958	-3.573752	0.481184
6	6	0	11.513289	-3.216828	-0.852397
7	6	0	11.950239	-2.095169	-1.574093
8	6	0	11.339584	-1.711346	-2.776821
9	6	0	12.006102	1.512634	-2.098461
10	6	0	12.222779	3.532605	-0.578798
11	6	0	11.616937	3.147670	0.742984
12	6	0	12.084843	2.044593	1.472628
13	6	0	11.489431	1.659123	2.682433
14	6	0	11.451944	-0.813211	3.055915
15	6	0	12.019994	0.507845	3.490234
16	6	0	10.258496	-2.491214	-3.234836
17	6	0	10.484337	-3.997722	-1.411552
18	6	0	9.828863	-3.650297	-2.592945
19	6	0	10.472685	3.346271	-2.398728
20	6	0	10.227606	1.384914	-3.709774
21	6	0	9.771339	2.661162	-3.391278
22	6	0	10.349571	-3.258716	2.283070
23	6	0	10.345136	-1.371889	3.723383
24	6	0	9.760729	-2.582680	3.349164
25	6	0	10.390427	2.414170	3.139864
26	6	0	10.550121	3.889550	1.288142
27	6	0	9.904224	3.536605	2.472684
28	1	0	8.887588	-2.990265	3.877985
29	1	0	12.883651	-1.141701	1.477325
30	1	0	11.950822	-4.667805	0.679859
31	1	0	13.207983	-3.441858	0.471725
32	1	0	12.776620	-1.500587	-1.183022
33	1	0	9.007813	-4.257402	-3.000143
34	1	0	8.902262	3.105714	-3.897227
35	1	0	12.873339	1.074596	-1.603535
36	1	0	12.928958	1.471330	1.088109
37	1	0	9.056060	4.116404	2.864945
38	1	0	13.130878	0.486412	3.452145
39	1	0	11.777775	0.676231	4.574121
40	1	0	13.320309	3.364994	-0.577064
41	1	0	12.101911	4.636771	-0.738861
42	1	0	11.545268	-0.687303	-4.653218
43	1	0	12.960397	-0.559188	-3.601188
44	8	0	9.583024	0.655014	-4.742542
45	8	0	9.606072	-2.105667	-4.437268
46	8	0	10.200656	5.089426	0.628537
47	8	0	10.147477	4.692981	-2.117989
48	8	0	9.825794	2.054976	4.387090
49	8	0	9.865554	-0.691124	4.871276
50	8	0	10.136501	-5.204461	-0.751195
51	8	0	9.899511	-4.553699	1.944707
52	6	0	8.440900	-1.404931	-4.177946
53	6	0	8.438978	0.018852	-4.307515
54	7	0	7.327209	0.774446	-4.055525
55	7	0	7.320343	-2.108563	-3.831673
56	6	0	6.241647	0.072808	-3.710650
57	6	0	6.231336	-1.359488	-3.615353
58	6	0	4.868431	0.599348	-3.335413
59	6	0	4.835615	-1.808749	-3.212615
60	7	0	4.105719	-0.585685	-3.080636
61	8	0	4.449176	1.715520	-3.218380
62	1	0	3.075971	-0.553359	-2.888579
63	8	0	4.373267	-2.897322	-3.015957
64	6	0	8.955730	4.852022	-1.435123
65	6	0	8.982562	5.043600	-0.021367
66	6	0	11.564691	2.786338	-1.706310
67	7	0	7.848619	5.260006	0.711351
68	7	0	7.795845	4.890348	-2.158374
69	6	0	8.664253	-0.048641	4.626055
70	6	0	8.649811	1.339812	4.294083
71	6	0	8.884396	-5.105310	-0.163607
72	6	0	8.758335	-4.634741	1.180981
73	7	0	7.496628	1.999197	3.962155
74	7	0	7.519840	-0.787285	4.737304
75	7	0	7.806321	-5.475435	-0.914599
76	7	0	7.540724	-4.380937	1.750840
77	6	0	6.694582	5.116313	-1.432505
78	6	0	6.489295	-4.695684	0.981796
79	6	0	6.720429	5.291744	-0.006966
80	6	0	6.396564	-0.117926	4.460598
81	6	0	6.386978	1.254416	4.033164
82	6	0	6.623206	-5.293436	-0.316670
83	6	0	5.240115	-5.588736	-0.876254
84	6	0	5.006582	-4.480984	1.258149
85	6	0	5.250117	5.188583	-1.911236
86	6	0	5.293408	5.464957	0.494602
87	6	0	4.973839	-0.649594	4.464927
88	6	0	4.960040	1.632459	3.661740
89	7	0	4.358410	-5.047248	0.124579
90	7	0	4.207201	0.457535	3.961864
91	7	0	4.505719	5.360419	-0.698007
92	8	0	4.446895	-3.928615	2.165159
93	8	0	4.884201	-6.138777	-1.872554
94	8	0	4.514067	-1.700018	4.795398
95	8	0	4.495049	2.639622	3.207112

96	8	0	4.775463	5.139172	-3.005846
97	8	0	4.855883	5.649557	1.590505
98	1	0	3.467885	5.357407	-0.672136
99	1	0	3.190146	0.371777	3.762929
100	1	0	3.320779	-5.033386	0.008884
101	1	0	-13.429069	3.473796	-0.997193
102	6	0	-12.322488	3.558504	-1.050177
103	6	0	-11.714125	3.450454	0.318981
104	6	0	-11.755663	2.534348	-1.994679
105	1	0	-12.135045	4.585614	-1.462676
106	6	0	-12.190133	2.528746	1.265359
107	6	0	-10.636076	4.275535	0.689784
108	6	0	-12.324608	1.259360	-2.120031
109	6	0	-10.646572	2.838126	-2.811164
110	6	0	-11.577258	2.381954	2.517225
111	1	0	-13.049405	1.905779	1.015369
112	6	0	-9.972967	4.154912	1.911696
113	8	0	-10.249164	5.300110	-0.212700
114	6	0	-11.821147	0.316351	-3.029258
115	1	0	-13.177540	0.992501	-1.495061
116	6	0	-10.118865	1.948491	-3.744230
117	8	0	-10.141273	4.156552	-2.746687
118	6	0	-12.109233	1.436676	3.558160
119	6	0	-10.452711	3.187578	2.789859
120	1	0	-9.112643	4.788036	2.169791
121	6	0	-9.024279	5.017973	-0.795268
122	6	0	-12.425873	-1.052660	-3.155082
123	6	0	-10.739151	0.702602	-3.843004
124	1	0	-9.261944	2.219651	-4.376731
125	6	0	-8.970183	4.318049	-2.041025
126	1	0	-13.221105	1.443496	3.553714
127	1	0	-11.828201	1.816069	4.577303
128	6	0	-11.590514	0.036995	3.392560
129	8	0	-9.843006	3.047307	4.060719
130	7	0	-7.902075	5.439141	-0.141372
131	6	0	-11.864197	-2.027223	-2.157768
132	1	0	-12.245486	-1.442392	-4.192841
133	1	0	-13.532712	-1.000738	-3.063910
134	8	0	-10.325483	-0.201563	-4.855507
135	7	0	-7.788813	3.903441	-2.591652
136	6	0	-12.210036	-0.873962	2.522547
137	6	0	-10.476881	-0.411429	4.127975
138	6	0	-8.695386	2.283684	4.051129
139	6	0	-6.751832	5.083987	-0.725294
140	6	0	-12.385644	-2.142016	-0.861966
141	6	0	-10.808470	-2.891213	-2.513787
142	6	0	-9.123010	-0.811566	-4.546797
143	6	0	-6.696506	4.276357	-1.911054
144	6	0	-11.724648	-2.178497	2.359141
145	1	0	-13.088172	-0.557180	1.958740
146	6	0	-9.939295	-1.691857	3.989788
147	8	0	-9.930395	0.466370	5.101021
148	6	0	-8.724259	1.002049	4.683155
149	7	0	-7.552552	2.799758	3.503117
150	6	0	-5.336438	5.379576	-0.254266
151	6	0	-11.888963	-3.088468	0.048387
152	1	0	-13.189812	-1.474964	-0.549626
153	6	0	-10.309966	-3.878583	-1.668318
154	8	0	-10.304079	-2.793858	-3.833332
155	6	0	-9.115062	-2.103543	-3.935143
156	7	0	-7.973487	-0.147308	-4.869102
157	6	0	-5.241334	3.935405	-2.190800
158	6	0	-12.407274	-3.168551	1.455974
159	6	0	-10.581595	-2.547262	3.098155
160	1	0	-9.057241	-2.012873	4.561625
161	7	0	-7.592008	0.271148	4.907293
162	6	0	-6.460135	2.045322	3.678184
163	7	0	-4.521597	4.628386	-1.175404
164	8	0	-4.914122	6.063239	0.626110
165	6	0	-10.883307	-3.965721	-0.398981
166	1	0	-9.506240	-4.556004	-1.988606
167	7	0	-7.958610	-2.707200	-3.522316
168	6	0	-6.847745	-0.776722	-4.514420
169	8	0	-4.741625	3.229511	-3.023659
170	1	0	-12.246726	-4.205543	1.854883
171	1	0	-13.508970	-3.025749	1.478402
172	8	0	-10.160531	-3.892534	2.995916
173	6	0	-6.470867	0.818302	4.424647
174	6	0	-5.056615	2.263617	3.132821
175	1	0	-3.482403	4.581991	-1.094249
176	8	0	-10.486858	-5.015055	0.469943
177	6	0	-6.841440	-2.024599	-3.804008
178	6	0	-5.414529	-0.309579	-4.712620
179	6	0	-9.046687	-4.115181	2.218720
180	6	0	-5.057647	0.261032	4.484619
181	7	0	-4.310522	1.170773	3.655566
182	8	0	-4.612118	3.112454	2.407843
183	6	0	-9.215248	-4.803362	0.976156
184	6	0	-5.403966	-2.363178	-3.439231
185	7	0	-4.644999	-1.305950	-4.013458
186	8	0	-4.949276	0.618956	-5.298235
187	7	0	-7.813102	-3.772288	2.698945
188	8	0	-4.588522	-0.670955	5.061883
189	1	0	-3.299751	1.022878	3.431701
190	7	0	-8.159905	-5.289362	0.259051
191	8	0	-4.942445	-3.271759	-2.802158
192	1	0	-3.608930	-1.232534	-3.898287
193	6	0	-6.786679	-4.209551	1.957135
194	6	0	-6.958241	-5.010281	0.778429
195	6	0	-5.300280	-3.962148	2.158249
196	6	0	-5.591615	-5.400683	0.237599
197	7	0	-4.680702	-4.709369	1.114351
198	8	0	-4.716918	-3.284626	2.958599
199	8	0	-5.261381	-6.105090	-0.665745
200	1	0	-3.645463	-4.734394	0.984010
201	8	0	-1.868896	-4.262943	0.925190
202	6	0	-1.231776	-3.896724	1.912634
203	7	0	0.075739	-4.321142	2.250872
204	7	0	-1.727913	-3.075725	2.935386
205	6	0	0.582924	-3.580746	3.435806

206	1	0	0.738409	-4.598196	1.499932
207	6	0	-0.692177	-2.750755	3.942421
208	1	0	-2.705868	-2.782395	3.020796
209	1	0	0.997436	-4.303669	4.180670
210	7	0	1.568162	-2.525114	3.108679
211	1	0	-1.033911	-3.000156	4.976761
212	7	0	-0.232424	-1.338544	3.898341
213	6	0	1.041122	-1.240283	3.284949
214	1	0	2.506898	-2.732745	2.763372
215	1	0	-0.920194	-0.573137	3.767708
216	8	0	1.623099	-0.185601	3.032991
217	1	0	-1.250200	-5.593791	-3.302829
218	6	0	-0.852142	-4.670533	-2.814221
219	6	0	0.445623	-4.046390	-3.521233
220	7	0	-0.385268	-4.999114	-1.442869
221	7	0	-1.835059	-3.564953	-2.873157
222	1	0	0.793470	-4.603056	-4.425807
223	7	0	0.013460	-2.679354	-3.920309
224	7	0	1.463128	-4.069271	-2.449292
225	6	0	0.938561	-4.534800	-1.233215
226	1	0	-1.060160	-4.986801	-0.653366
227	6	0	-1.280331	-2.395517	-3.414660
228	1	0	-2.805288	-3.653935	-2.559319
229	1	0	0.712438	-1.911368	-3.950394
230	1	0	2.427095	-3.757202	-2.585455
231	8	0	1.560457	-4.621197	-0.179018
232	8	0	-1.865978	-1.320839	-3.522515
233	6	0	0.865308	0.852051	-3.568792
234	7	0	-0.396213	1.054765	-4.174978
235	7	0	1.496695	2.090276	-3.398010
236	8	0	1.368722	-0.246339	-3.328679
237	6	0	-0.753854	2.496169	-4.188529
238	1	0	-1.132945	0.329423	-4.094832
239	6	0	0.591094	3.223058	-3.701625
240	1	0	2.430061	2.214530	-2.993181
241	1	0	-1.102658	2.786858	-5.209391
242	7	0	-1.737587	2.878789	-3.149056
243	1	0	1.052613	3.912659	-4.450928
244	7	0	0.162877	3.989444	-2.506318
245	6	0	-1.158752	3.656612	-2.134049
246	1	0	-2.734897	2.651125	-3.206234
247	1	0	0.863101	4.277511	-1.794535
248	8	0	-1.736996	4.054693	-1.123800
249	1	0	-0.883364	5.329667	3.023544
250	6	0	-0.511251	4.428099	2.477427
251	6	0	0.790045	3.746564	3.120174
252	7	0	-0.069489	4.820317	1.114702
253	7	0	-1.514597	3.339298	2.504172
254	1	0	1.162399	4.239955	4.051164
255	7	0	0.343619	2.362521	3.442222
256	7	0	1.785970	3.814299	2.030932
257	6	0	1.247628	4.351958	0.853093
258	1	0	-0.765761	4.839133	0.344946
259	6	0	-0.964816	2.129175	2.952028
260	1	0	-2.470477	3.447590	2.155763
261	1	0	1.027025	1.582827	3.424946
262	1	0	2.765402	3.548425	2.158617
263	8	0	1.836345	4.477228	-0.215107
264	8	0	-1.565911	1.057949	3.010299
265	6	0	6.401242	-0.861261	1.087773
266	6	0	5.032375	-0.969072	0.877848
267	6	0	4.334821	0.092265	0.304033
268	6	0	5.004355	1.265577	-0.044117
269	6	0	6.374770	1.356802	0.154626
270	6	0	7.090513	0.296200	0.719385
271	1	0	6.942797	-1.683908	1.551327
272	1	0	4.488642	-1.863000	1.168513
273	1	0	4.436028	2.086482	-0.472853
274	1	0	6.903015	2.265663	-0.120628
275	6	0	8.587260	0.382729	0.869633
276	6	0	9.305370	-0.031529	-0.418630
277	1	0	8.914795	-0.261949	1.691843
278	1	0	8.869971	1.409144	1.129248
279	1	0	10.390721	0.040672	-0.299022
280	1	0	9.058379	-1.062527	-0.684925
281	1	0	9.009675	0.614974	-1.249543
282	8	0	2.217443	0.992515	-0.263875
283	8	0	2.365512	-1.192437	0.225483
284	1	0	1.352743	-1.178728	0.104815
285	6	0	-4.345418	-1.508133	-0.338649
286	6	0	-2.961422	-1.439427	-0.254502
287	6	0	-2.331171	-0.195497	-0.229255
288	6	0	-3.090462	0.976388	-0.268180
289	6	0	-4.476097	0.892934	-0.328396
290	6	0	-5.119945	-0.346711	-0.376361
291	1	0	-4.832719	-2.478114	-0.399082
292	1	0	-2.354961	-2.341344	-0.217550
293	1	0	-2.588826	1.940829	-0.254089
294	1	0	-5.068014	1.803571	-0.349798
295	6	0	-6.626801	-0.430745	-0.419202
296	6	0	-7.239565	-0.322064	0.982024
297	1	0	-6.924566	-1.378948	-0.878624
298	1	0	-7.019585	0.372296	-1.051881
299	1	0	-8.328682	-0.402089	0.941970
300	1	0	-6.857140	-1.113420	1.634246
301	1	0	-6.981100	0.638643	1.434118
302	8	0	-0.177990	-1.174114	-0.021573
303	8	0	-0.329474	1.043106	-0.319492
304	1	0	0.687245	1.003625	-0.295590
305	6	0	2.869122	0.001206	0.072610
306	6	0	-0.848794	-0.148825	-0.176822

CC-cis, capsule a: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.364584	0.779053	-3.102384
2	6	0	11.854451	-0.555540	-3.587599

3	6	0	12.005745	-1.609635	1.979439
4	6	0	11.468175	-2.834852	1.561124
5	6	0	12.089998	-3.624349	0.441935
6	6	0	11.501093	-3.249778	-0.888068
7	6	0	11.945655	-2.123741	-1.598156
8	6	0	11.337909	-1.723617	-2.797054
9	6	0	12.016163	1.488411	-2.083728
10	6	0	12.238476	3.491893	-0.543894
11	6	0	11.631808	3.095656	0.774024
12	6	0	12.095220	1.982956	1.491961
13	6	0	11.499070	1.588177	2.698388
14	6	0	11.447151	-0.888267	3.045600
15	6	0	12.022257	0.425062	3.494028
16	6	0	10.251516	-2.491239	-3.263304
17	6	0	10.467348	-4.018105	-1.455740
18	6	0	9.813884	-3.653801	-2.633189
19	6	0	10.489588	3.330494	-2.367652
20	6	0	10.244848	1.386636	-3.704790
21	6	0	9.790656	2.660035	-3.371753
22	6	0	10.335124	-3.321174	2.246397
23	6	0	10.336442	-1.448459	3.705408
24	6	0	9.747810	-2.653187	3.318430
25	6	0	10.405305	2.345090	3.164920
26	6	0	10.568643	3.836881	1.327082
27	6	0	9.923154	3.475982	2.509336
28	1	0	8.872062	-3.062223	3.841834
29	1	0	12.879284	-1.207132	1.465415
30	1	0	11.930322	-4.719802	0.628218
31	1	0	13.193656	-3.497778	0.434775
32	1	0	12.776082	-1.538871	-1.201075
33	1	0	8.988889	-4.251191	-3.046738
34	1	0	8.925265	3.113736	-3.876006
35	1	0	12.879670	1.041315	-1.590395
36	1	0	12.936049	1.409488	1.100651
37	1	0	9.078108	4.055875	2.908205
38	1	0	13.133046	0.397664	3.456387
39	1	0	11.780299	0.583181	4.579514
40	1	0	13.335525	3.320925	-0.544041
41	1	0	12.121104	4.598043	-0.692784
42	1	0	11.554649	-0.683219	-4.663248
43	1	0	12.967149	-0.571801	-3.605828
44	8	0	9.605007	0.672187	-4.751125
45	8	0	9.605075	-2.091258	-4.463837
46	8	0	10.222331	5.043932	0.678911
47	8	0	10.166587	4.674440	-2.071274
48	8	0	9.839279	1.974886	4.408655
49	8	0	9.855277	-0.776708	4.858194
50	8	0	10.113520	-5.230433	-0.809147
51	8	0	9.879849	-4.610653	1.894503
52	6	0	8.443851	-1.383732	-4.206187
53	6	0	8.452442	0.040194	-4.332007
54	7	0	7.342934	0.802376	-4.090645
55	7	0	7.316079	-2.080669	-3.869130
56	6	0	6.249908	0.107206	-3.757209
57	6	0	6.230000	-1.325040	-3.660981
58	6	0	4.876806	0.643243	-3.395414
59	6	0	4.828148	-1.764674	-3.267831
60	7	0	4.105038	-0.536671	-3.144621
61	8	0	4.464634	1.762326	-3.282970
62	1	0	3.073647	-0.495430	-2.962009
63	8	0	4.357262	-2.849323	-3.069754
64	6	0	8.975612	4.829068	-1.386235
65	6	0	9.003727	5.007597	0.029284
66	6	0	11.578382	2.759419	-1.679176
67	7	0	7.870906	5.221181	0.764610
68	7	0	7.815321	4.878098	-2.108232
69	6	0	8.659915	-0.123038	4.613633
70	6	0	8.657893	1.270357	4.303002
71	6	0	8.861943	-5.132419	-0.220420
72	6	0	8.738198	-4.678189	1.129837
73	7	0	7.512167	1.943736	3.973466
74	7	0	7.509193	-0.855038	4.703107
75	7	0	7.782128	-5.488003	-0.976030
76	7	0	7.521817	-4.426511	1.703252
77	6	0	6.715267	5.101787	-1.379712
78	6	0	6.468966	-4.726637	0.930409
79	6	0	6.742323	5.263831	0.047400
80	6	0	6.393044	-0.173272	4.427446
81	6	0	6.396759	1.206214	4.023542
82	6	0	6.599949	-5.308134	-0.375748
83	6	0	5.215322	-5.589472	-0.938985
84	6	0	4.987311	-4.508348	1.209683
85	6	0	5.271100	5.185761	-1.857322
86	6	0	5.316138	5.437929	0.551083
87	6	0	4.966768	-0.694846	4.406372
88	6	0	4.976444	1.601246	3.645123
89	7	0	4.336428	-5.058010	0.069348
90	7	0	4.213436	0.424984	3.912089
91	7	0	4.527450	5.347041	-0.641988
92	8	0	4.430346	-3.963643	2.122801
93	8	0	4.857015	-6.123739	-1.943003
94	8	0	4.495436	-1.747600	4.712821
95	8	0	4.522322	2.620661	3.207301
96	8	0	4.795685	5.151643	-2.952122
97	8	0	4.879130	5.615459	1.648453
98	1	0	3.489815	5.347675	-0.615930
99	1	0	3.196491	0.351618	3.703153
100	1	0	3.298806	-5.037472	-0.045220
101	1	0	-13.431474	3.419881	-0.996571
102	6	0	-12.324640	3.505870	-1.044158
103	6	0	-11.722164	3.377977	0.325754
104	6	0	-11.754567	2.497117	-2.002856
105	1	0	-12.136521	4.539447	-1.440068
106	6	0	-12.202015	2.441015	1.254797
107	6	0	-10.649311	4.200971	0.716280
108	6	0	-12.320069	1.223089	-2.149832
109	6	0	-10.645072	2.816930	-2.812669
110	6	0	-11.601029	2.281076	2.510800
111	1	0	-13.055459	1.816831	0.988204
112	6	0	-9.999260	4.068981	1.944012

113	8	0	-10.257582	5.238753	-0.168805
114	6	0	-11.813473	0.296562	-3.074440
115	1	0	-13.172295	0.943254	-1.529582
116	6	0	-10.117338	1.946211	-3.762925
117	8	0	-10.139630	4.133614	-2.720782
118	6	0	-12.136903	1.316671	3.531741
119	6	0	-10.485583	3.090805	2.806861
120	1	0	-9.145468	4.703879	2.218952
121	6	0	-9.031120	4.966695	-0.752634
122	6	0	-12.411154	-1.073788	-3.218322
123	6	0	-10.734626	0.700468	-3.883598
124	1	0	-9.261845	2.230947	-4.391378
125	6	0	-8.971876	4.282965	-2.007472
126	1	0	-13.248735	1.318794	3.518743
127	1	0	-11.865603	1.679978	4.559342
128	6	0	-11.610804	-0.077884	3.346772
129	8	0	-9.895336	2.943016	4.086052
130	7	0	-7.911612	5.387022	-0.093889
131	6	0	-11.849552	-2.056911	-2.229134
132	1	0	-12.223826	-1.451347	-4.259350
133	1	0	-13.518625	-1.027860	-3.132072
134	8	0	-10.313618	-0.186034	-4.909426
135	7	0	-7.787972	3.877109	-2.559392
136	6	0	-12.223309	-0.979255	2.462538
137	6	0	-10.498008	-0.532299	4.080126
138	6	0	-8.736225	2.196334	4.085004
139	6	0	-6.758911	5.046312	-0.682008
140	6	0	-12.381724	-2.195398	-0.939867
141	6	0	-10.782276	-2.905534	-2.587720
142	6	0	-9.105413	-0.785957	-4.599061
143	6	0	-6.698073	4.248183	-1.873804
144	6	0	-11.735147	-2.281452	2.286981
145	1	0	-13.098604	-0.657490	1.897136
146	6	0	-9.959232	-1.810810	3.932323
147	8	0	-9.961509	0.335780	5.066529
148	6	0	-8.758710	0.892538	4.670600
149	7	0	-7.588222	2.754145	3.591795
150	6	0	-5.345645	5.355378	-0.213864
151	6	0	-11.884141	-3.150454	-0.039171
152	1	0	-13.195121	-1.540800	-0.625296
153	6	0	-10.281782	-3.900657	-1.752575
154	8	0	-10.266638	-2.783075	-3.900888
155	6	0	-9.086817	-2.075056	-3.981931
156	7	0	-7.961773	-0.107511	-4.911729
157	6	0	-5.240315	3.919923	-2.156443
158	6	0	-12.410821	-3.257565	1.363645
159	6	0	-10.597939	-2.658941	3.030392
160	1	0	-9.079828	-2.136896	4.505431
161	7	0	-7.620802	0.166783	4.883994
162	6	0	-6.487113	2.013040	3.767891
163	7	0	-4.524876	4.616118	-1.139142
164	8	0	-4.928188	6.038912	0.668991
165	6	0	-10.866448	-4.011769	-0.490510
166	1	0	-9.467346	-4.564383	-2.074639
167	7	0	-7.928648	-2.653317	-3.538697
168	6	0	-6.832359	-0.713969	-4.530038
169	8	0	-4.735362	3.223367	-2.993613
170	1	0	-12.249527	-4.300976	1.744995
171	1	0	-13.512904	-3.117953	1.382602
172	8	0	-10.178699	-4.004655	2.922925
173	6	0	-6.497408	0.750032	4.451013
174	6	0	-5.069636	2.291923	3.291792
175	1	0	-3.483775	4.586760	-1.065419
176	8	0	-10.472863	-5.070026	0.367844
177	6	0	-6.819101	-1.950043	-3.799144
178	6	0	-5.404126	-0.222938	-4.703264
179	6	0	-9.054429	-4.220078	2.157288
180	6	0	-5.076987	0.211782	4.520137
181	7	0	-4.319518	1.184938	3.777829
182	8	0	-4.617482	3.192074	2.636849
183	6	0	-9.207310	-4.864829	0.890215
184	6	0	-5.387319	-2.241772	-3.375180
185	7	0	-4.635061	-1.180710	-3.951668
186	8	0	-4.941515	0.695311	-5.306913
187	7	0	-7.826405	-3.907627	2.671638
188	8	0	-4.610477	-0.751855	5.045589
189	1	0	-3.299752	1.067434	3.577245
190	7	0	-8.142663	-5.319506	0.165577
191	8	0	-4.927336	-3.119000	-2.694989
192	1	0	-3.604488	-1.081586	-3.808918
193	6	0	-6.790634	-4.319280	1.928533
194	6	0	-6.947692	-5.061129	0.709583
195	6	0	-5.306690	-4.088238	2.163706
196	6	0	-5.574457	-5.416704	0.160982
197	7	0	-4.675335	-4.770188	1.082509
198	8	0	-4.729636	-3.462512	3.009341
199	8	0	-5.232925	-6.071507	-0.774909
200	1	0	-3.640339	-4.778924	0.957863
201	8	0	-1.890975	-4.204713	0.923628
202	6	0	-1.248165	-3.855412	1.912865
203	7	0	0.064845	-4.276695	2.231170
204	7	0	-1.738851	-3.050378	2.951884
205	6	0	0.579876	-3.552155	3.422544
206	1	0	0.722736	-4.541066	1.470962
207	6	0	-0.694543	-2.736571	3.953963
208	1	0	-2.724749	-2.800595	3.072531
209	1	0	1.006379	-4.283646	4.152036
210	7	0	1.555179	-2.486732	3.098053
211	1	0	-1.023162	-3.000727	4.988712
212	7	0	-0.242870	-1.321341	3.921883
213	6	0	1.021509	-1.207246	3.293539
214	1	0	2.494401	-2.685815	2.750350
215	1	0	-0.935434	-0.556916	3.815700
216	8	0	1.592339	-0.146039	3.043205
217	1	0	-1.329179	-5.472149	-3.303399
218	6	0	-0.903292	-4.565068	-2.807958
219	6	0	0.392614	-3.954460	-3.529916
220	7	0	-0.417739	-4.923784	-1.450884
221	7	0	-1.865771	-3.440402	-2.831544
222	1	0	0.718670	-4.508179	-4.444189

223	7	0	-0.025646	-2.578224	-3.908117
224	7	0	1.426403	-4.003013	-2.473166
225	6	0	0.913737	-4.475755	-1.254999
226	1	0	-1.080828	-4.913184	-0.651172
227	6	0	-1.298407	-2.273317	-3.363687
228	1	0	-2.820691	-3.507333	-2.468889
229	1	0	0.684916	-1.822842	-3.965423
230	1	0	2.391603	-3.700654	-2.619834
231	8	0	1.547234	-4.579240	-0.208988
232	8	0	-1.862801	-1.184093	-3.440548
233	6	0	0.872025	0.938697	-3.604498
234	7	0	-0.393764	1.158826	-4.197978
235	7	0	1.508738	2.170050	-3.407625
236	8	0	1.374074	-0.166614	-3.396103
237	6	0	-0.741876	2.602966	-4.182398
238	1	0	-1.135391	0.439281	-4.108587
239	6	0	0.607480	3.313016	-3.683059
240	1	0	2.443975	2.279441	-3.002418
241	1	0	-1.088683	2.914944	-5.197828
242	7	0	-1.723737	2.975631	-3.137937
243	1	0	1.069977	4.016571	-4.418812
244	7	0	0.185123	4.057550	-2.471450
245	6	0	-1.139905	3.729019	-2.107721
246	1	0	-2.718184	2.733670	-3.187687
247	1	0	0.886127	4.321200	-1.751280
248	8	0	-1.718952	4.116622	-1.093216
249	1	0	-0.850022	5.382183	3.083562
250	6	0	-0.490498	4.469339	2.547924
251	6	0	0.810835	3.786697	3.189429
252	7	0	-0.056738	4.839021	1.176155
253	7	0	-1.501022	3.388055	2.595345
254	1	0	1.193367	4.289861	4.111102
255	7	0	0.357295	2.410324	3.535420
256	7	0	1.798697	3.831027	2.091998
257	6	0	1.257217	4.363970	0.912538
258	1	0	-0.757503	4.851603	0.410163
259	6	0	-0.960175	2.182388	3.065632
260	1	0	-2.474426	3.513573	2.306468
261	1	0	1.033981	1.625089	3.507630
262	1	0	2.781049	3.575346	2.220662
263	8	0	1.844653	4.479540	-0.157080
264	8	0	-1.570693	1.118869	3.148068
265	6	0	6.383735	-0.917839	1.075802
266	6	0	5.017148	-1.008207	0.841105
267	6	0	4.348425	0.053480	0.234898
268	6	0	5.043794	1.210030	-0.120218
269	6	0	6.410536	1.284377	0.105392
270	6	0	7.098160	0.222632	0.702857
271	1	0	6.903319	-1.741199	1.562777
272	1	0	4.454226	-1.888871	1.136026
273	1	0	4.496939	2.031720	-0.574396
274	1	0	6.958066	2.180490	-0.174080
275	6	0	8.592162	0.294182	0.885114
276	6	0	9.334706	-0.092558	-0.397916
277	1	0	8.898101	-0.373014	1.697461
278	1	0	8.876667	1.311868	1.175866
279	1	0	10.417682	-0.030161	-0.253966
280	1	0	9.087277	-1.114994	-0.694954
281	1	0	9.061027	0.575941	-1.218936
282	8	0	2.269495	0.977308	-0.422616
283	8	0	2.344576	-1.182799	0.178929
284	1	0	1.336686	-1.149021	0.035589
285	6	0	-4.404773	-1.153472	0.228745
286	6	0	-3.027484	-1.190840	0.059402
287	6	0	-2.313163	0.003664	-0.053300
288	6	0	-2.982232	1.226888	0.001015
289	6	0	-4.359115	1.249686	0.189056
290	6	0	-5.086217	0.064829	0.311571
291	1	0	-4.961149	-2.082795	0.309719
292	1	0	-2.489631	-2.135707	0.023378
293	1	0	-2.418134	2.152011	-0.087828
294	1	0	-4.872422	2.204676	0.265334
295	6	0	-6.584651	0.090722	0.496778
296	6	0	-7.326358	-0.210388	-0.810239
297	1	0	-6.886792	1.072648	0.873935
298	1	0	-6.869458	-0.647294	1.254880
299	1	0	-8.408630	-0.175486	-0.663268
300	1	0	-7.056200	0.517972	-1.580266
301	1	0	-7.061264	-1.206325	-1.176182
302	8	0	-0.207078	-1.101308	-0.084591
303	8	0	-0.270621	1.118276	-0.395613
304	1	0	0.742292	1.034046	-0.433428
305	6	0	2.886118	-0.012965	-0.023501
306	6	0	-0.835199	-0.042889	-0.183113

AA-trans, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.216604	0.842970	3.207477
2	6	0	-11.680142	-0.472759	3.764699
3	6	0	-12.000039	-1.761572	-1.744186
4	6	0	-11.415313	-2.954456	-1.296879
5	6	0	-11.974523	-3.711343	-0.123862
6	6	0	-11.352318	-3.269067	1.169368
7	6	0	-11.796604	-2.122288	1.845114
8	6	0	-11.166693	-1.667057	3.012454
9	6	0	-11.902293	1.500821	2.177056
10	6	0	-12.195415	3.438614	0.567746
11	6	0	-11.639273	2.989697	-0.755158
12	6	0	-12.123568	1.845529	-1.406230
13	6	0	-11.575476	1.405166	-2.619624
14	6	0	-11.507453	-1.078934	-2.866849
15	6	0	-12.123956	0.206044	-3.341498
16	6	0	-10.060159	-2.401533	3.484230
17	6	0	-10.289357	-3.995793	1.737607
18	6	0	-9.616509	-3.578730	2.886202

19	6	0	-10.380585	3.362230	2.331778
20	6	0	-10.086812	1.485516	3.751938
21	6	0	-9.648527	2.743101	3.345213
22	6	0	-10.298988	-3.443683	-2.007107
23	6	0	-10.420103	-1.649083	-3.555537
24	6	0	-9.781596	-2.817875	-3.138739
25	6	0	-10.507813	2.148331	-3.162449
26	6	0	-10.604292	3.712248	-1.381151
27	6	0	-10.005034	3.306562	-2.573039
28	1	0	-8.921464	-3.232674	-3.682588
29	1	0	-12.858317	-1.354405	-1.208756
30	1	0	-11.791849	-4.809223	-0.271573
31	1	0	-13.080457	-3.613089	-0.082331
32	1	0	-12.644546	-1.564931	1.445609
33	1	0	-8.771484	-4.146828	3.300837
34	1	0	-8.771646	3.224035	3.801753
35	1	0	-12.775133	1.025639	1.728430
36	1	0	-12.942910	1.283714	-0.956726
37	1	0	-9.181189	3.873651	-3.029884
38	1	0	-13.230798	0.167444	-3.246820
39	1	0	-11.938055	0.321846	-4.443043
40	1	0	-13.290763	3.263713	0.618465
41	1	0	-12.078425	4.550394	0.665837
42	1	0	-11.353571	-0.549279	4.837271
43	1	0	-12.791683	-0.500672	3.809999
44	8	0	-9.422953	0.826815	4.819323
45	8	0	-9.397337	-1.949966	4.657362
46	8	0	-10.242784	4.948010	-0.797720
47	8	0	-10.074730	4.693050	1.964621
48	8	0	-10.001198	1.738127	-4.418556
49	8	0	-10.019938	-1.028463	-4.766585
50	8	0	-9.920159	-5.219371	1.120127
51	8	0	-9.785836	-4.698857	-1.612351
52	6	0	-8.247691	-1.241948	4.353256
53	6	0	-8.270831	0.186030	4.413019
54	7	0	-7.174115	0.948205	4.119424
55	7	0	-7.116290	-1.942017	4.034195
56	6	0	-6.079375	0.249226	3.800921
57	6	0	-6.042607	-1.185305	3.773325
58	6	0	-4.723084	0.781543	3.379573
59	6	0	-4.641371	-1.624330	3.374259
60	7	0	-3.938852	-0.393209	3.171058
61	8	0	-4.341390	1.905167	3.200627
62	1	0	-2.923617	-0.349179	2.914314
63	8	0	-4.157873	-2.711932	3.237163
64	6	0	-8.914469	4.823720	1.225309
65	6	0	-9.000681	4.947160	-0.194536
66	6	0	-11.487994	2.756538	1.705728
67	7	0	-7.900728	5.144521	-0.982034
68	7	0	-7.726580	4.909675	1.896855
69	6	0	-8.818575	-0.355923	-4.626189
70	6	0	-8.809938	1.046259	-4.356695
71	6	0	-8.690655	-5.097674	0.489633
72	6	0	-8.622043	-4.688146	-0.878630
73	7	0	-7.652170	1.736627	-4.117444
74	7	0	-7.669746	-1.081001	-4.773256
75	7	0	-7.577215	-5.380945	1.226702
76	7	0	-7.432973	-4.404198	-1.493606
77	6	0	-6.658763	5.116054	1.116496
78	6	0	-6.348475	-4.630581	-0.739606
79	6	0	-6.744822	5.225737	-0.313072
80	6	0	-6.544817	-0.383285	-4.588713
81	6	0	-6.535813	1.005167	-4.217694
82	6	0	-6.420380	-5.171721	0.588489
83	6	0	-5.011380	-5.372476	1.124301
84	6	0	-4.884952	-4.359452	-1.063833
85	6	0	-5.199353	5.232033	1.532226
86	6	0	-5.344221	5.398719	-0.881319
87	6	0	-5.115521	-0.892903	-4.654352
88	6	0	-5.098092	1.417450	-3.938422
89	7	0	-4.182526	-4.828485	0.079565
90	7	0	-4.341446	0.247234	-4.240438
91	7	0	-4.506943	5.367506	0.283451
92	8	0	-4.376206	-3.843827	-2.022449
93	8	0	-4.604897	-5.866149	2.130420
94	8	0	-4.656933	-1.946629	-4.974009
95	8	0	-4.629654	2.450126	-3.546419
96	8	0	-4.674059	5.232020	2.605017
97	8	0	-4.950249	5.538470	-2.000011
98	1	0	-3.475047	5.376538	0.215689
99	1	0	-3.317459	0.179503	-4.077895
100	1	0	-3.144670	-4.748472	0.177889
101	1	0	13.291498	3.574327	0.160065
102	6	0	12.188977	3.684550	0.241008
103	6	0	11.522166	3.339653	-1.059985
104	6	0	11.651370	2.855098	1.374858
105	1	0	12.027035	4.771721	0.468580
106	6	0	11.937315	2.235825	-1.823149
107	6	0	10.449019	4.109720	-1.545733
108	6	0	12.223049	1.623947	1.723643
109	6	0	10.561211	3.311085	2.144703
110	6	0	11.267517	1.860105	-2.995437
111	1	0	12.792493	1.648992	-1.486145
112	6	0	9.737931	3.772025	-2.698166
113	8	0	10.101764	5.295753	-0.846705
114	6	0	11.738756	0.869732	2.803859
115	1	0	13.062163	1.241080	1.141921
116	6	0	10.051877	2.614310	3.237341
117	8	0	10.063768	4.598391	1.842669
118	6	0	11.738015	0.719121	-3.851958
119	6	0	10.152813	2.632226	-3.380375
120	1	0	8.882952	4.368647	-3.046155
121	6	0	8.892421	5.141745	-0.184653
122	6	0	12.341771	-0.457747	3.167025
123	6	0	10.674252	1.406030	3.553307
124	1	0	9.208627	3.001717	3.826060
125	6	0	8.872893	4.644398	1.156259
126	1	0	12.848941	0.730366	-3.921345
127	1	0	11.389444	0.889795	-4.906765
128	6	0	11.265520	-0.633047	-3.399276

129	8	0	9.442966	2.239973	-4.547971
130	7	0	7.753285	5.483960	-0.855078
131	6	0	11.743330	-1.587432	2.375684
132	1	0	12.184816	-0.649579	4.262189
133	1	0	13.445690	-0.434441	3.041342
134	8	0	10.288292	0.713473	4.727902
135	7	0	7.707820	4.322850	1.796072
136	6	0	11.952970	-1.366649	-2.421647
137	6	0	10.137678	-1.236062	-3.990917
138	6	0	8.314368	1.509307	-4.227504
139	6	0	6.619500	5.239532	-0.186467
140	6	0	12.248929	-1.956527	1.120949
141	6	0	10.665323	-2.334582	2.890939
142	6	0	9.074589	0.065568	4.590273
143	6	0	6.597797	4.603128	1.100244
144	6	0	11.542034	-2.654685	-2.045104
145	1	0	12.822444	-0.922780	-1.935579
146	6	0	9.710733	-2.526360	-3.686254
147	8	0	9.436504	-0.502641	-4.986837
148	6	0	8.306530	0.100477	-4.467441
149	7	0	7.236031	2.167350	-3.702029
150	6	0	5.189239	5.503298	-0.634007
151	6	0	11.706537	-3.029695	0.398798
152	1	0	13.082001	-1.395430	0.696351
153	6	0	10.090576	-3.413062	2.220713
154	8	0	10.235516	-2.019755	4.201574
155	6	0	9.046913	-1.324060	4.261263
156	7	0	7.936920	0.786856	4.822260
157	6	0	5.150681	4.316903	1.467553
158	6	0	12.240473	-3.415270	-0.952978
159	6	0	10.440871	-3.217058	-2.719382
160	1	0	8.838424	-2.975090	-4.182683
161	7	0	7.212250	-0.678917	-4.210647
162	6	0	6.175193	1.391502	-3.450003
163	7	0	4.399337	4.904408	0.413892
164	8	0	4.741693	6.077502	-1.577941
165	6	0	10.643855	-3.746212	0.985219
166	1	0	9.252273	-3.979526	2.650760
167	7	0	7.877130	-2.009988	4.082600
168	6	0	6.800698	0.094589	4.683502
169	8	0	4.684090	3.705005	2.391417
170	1	0	12.096781	-4.516990	-1.110992
171	1	0	13.339330	-3.263098	-1.004344
172	8	0	10.120196	-4.566460	-2.435566
173	6	0	6.160245	-0.019595	-3.711524
174	6	0	4.844703	1.785149	-2.830331
175	1	0	3.356421	4.865152	0.383046
176	8	0	10.219780	-4.918725	0.320442
177	6	0	6.770804	-1.285657	4.287399
178	6	0	5.373564	0.592508	4.850950
179	6	0	8.943380	-4.701998	-1.720316
180	6	0	4.813683	-0.580066	-3.284952
181	7	0	4.115868	0.556604	-2.773771
182	8	0	4.432458	2.839802	-2.435818
183	6	0	8.990743	-4.834838	-0.298731
184	6	0	5.321308	-1.713859	4.124812
185	7	0	4.579991	-0.550337	4.490193
186	8	0	4.929525	1.642144	5.205063
187	7	0	7.772865	-4.759333	-2.423001
188	8	0	4.375887	-1.695605	-3.320841
189	1	0	3.118246	0.515332	-2.465726
190	7	0	7.862650	-4.980388	0.460509
191	8	0	4.839805	-2.755093	3.777241
192	1	0	3.545202	-0.510141	4.411959
193	6	0	6.679124	-4.930833	-1.671064
194	6	0	6.721513	-5.022029	-0.238509
195	6	0	5.231359	-5.009439	-2.130782
196	6	0	5.297464	-5.132438	0.288236
197	7	0	4.497232	-5.093150	-0.899984
198	8	0	4.739144	-5.019707	-3.218601
199	8	0	4.862729	-5.228286	1.397241
200	1	0	3.461550	-5.069554	-0.869046
201	8	0	1.872097	-3.991716	-0.820841
202	6	0	1.221466	-3.802000	-1.850354
203	7	0	-0.061798	-4.326126	-2.122074
204	7	0	1.668624	-3.078732	-2.962486
205	6	0	-0.624558	-3.735753	-3.364650
206	1	0	-0.690870	-4.593537	-1.340881
207	6	0	0.609700	-2.925043	-3.988933
208	1	0	2.624806	-2.736010	-3.091541
209	1	0	-1.033316	-4.545638	-4.017089
210	7	0	-1.634067	-2.680411	-3.121647
211	1	0	0.949816	-3.288840	-4.988712
212	7	0	0.100813	-1.534863	-4.104753
213	6	0	-1.158068	-1.407157	-3.453506
214	1	0	-2.548935	-2.875252	-2.706436
215	1	0	0.773444	-0.744598	-4.046480
216	8	0	-1.759889	-0.346834	-3.303392
217	1	0	1.513831	-5.120912	3.565551
218	6	0	1.060052	-4.269095	3.002592
219	6	0	-0.258296	-3.653000	3.674832
220	7	0	0.591237	-4.748224	1.677190
221	7	0	1.978623	-3.106553	2.899689
222	1	0	-0.586914	-4.168139	4.611271
223	7	0	0.128990	-2.253917	3.992813
224	7	0	-1.277027	-3.782600	2.610338
225	6	0	-0.751193	-4.345245	1.440003
226	1	0	1.257223	-4.780149	0.885726
227	6	0	1.407915	-1.946390	3.470467
228	1	0	2.998373	-3.239719	2.844702
229	1	0	-0.591974	-1.508059	4.024058
230	1	0	-2.244993	-3.466845	2.718971
231	8	0	-1.367990	-4.549102	0.399500
232	8	0	1.958766	-0.854759	3.537277
233	6	0	-0.769475	1.302089	3.482317
234	7	0	0.521332	1.626615	3.969241
235	7	0	-1.474144	2.489298	3.231216
236	8	0	-1.239616	0.170819	3.399219
237	6	0	0.779054	3.088668	3.866416
238	1	0	1.292167	0.949420	3.843025

239	6	0	-0.622616	3.687669	3.369603
240	1	0	-2.465892	2.533105	2.980652
241	1	0	1.126099	3.470665	4.858190
242	7	0	1.713038	3.476622	2.787416
243	1	0	-1.081960	4.438579	4.059010
244	7	0	-0.292759	4.343473	2.075524
245	6	0	1.056934	4.097616	1.714385
246	1	0	2.724518	3.318314	2.833687
247	1	0	-1.019985	4.411403	1.341711
248	8	0	1.585445	4.475584	0.671384
249	1	0	0.788989	5.100517	-3.512150
250	6	0	0.395222	4.220074	-2.947399
251	6	0	-0.865692	3.493763	-3.620498
252	7	0	-0.118730	4.658557	-1.623876
253	7	0	1.407518	3.142039	-2.873998
254	1	0	-1.224059	3.964663	-4.567174
255	7	0	-0.380875	2.115481	-3.898625
256	7	0	-1.893443	3.532658	-2.552663
257	6	0	-1.402627	4.124756	-1.378049
258	1	0	0.547667	4.815601	-0.839337
259	6	0	0.892113	1.907595	-3.298230
260	1	0	2.307117	3.256695	-2.399554
261	1	0	-1.062291	1.330955	-3.874058
262	1	0	-2.882311	3.328436	-2.732622
263	8	0	-2.011664	4.177251	-0.309821
264	8	0	1.490114	0.836140	-3.272326
265	6	0	-6.142814	-0.812599	-1.170411
266	6	0	-4.770925	-0.861094	-0.934702
267	6	0	-4.138642	0.172412	-0.237559
268	6	0	-4.895040	1.264774	0.205795
269	6	0	-6.269648	1.298251	-0.024568
270	6	0	-6.913926	0.265994	-0.718424
271	1	0	-6.620156	-1.620380	-1.717759
272	1	0	-4.172131	-1.696135	-1.278070
273	1	0	-4.425329	2.064053	0.771423
274	1	0	-6.849114	2.142059	0.333303
275	6	0	-8.408667	0.289360	-0.902336
276	6	0	-9.153099	-0.104645	0.375099
277	1	0	-8.686351	-0.393143	-1.708125
278	1	0	-8.722130	1.290590	-1.210236
279	1	0	-10.232579	-0.090829	0.216797
280	1	0	-8.866958	-1.106728	0.690403
281	1	0	-8.920909	0.586582	1.184614
282	8	0	-2.156183	-1.090869	0.128321
283	6	0	5.039742	-1.467928	0.122242
284	6	0	3.652625	-1.405304	-0.006218
285	6	0	2.958726	-0.266863	0.426071
286	6	0	3.675135	0.791184	0.995849
287	6	0	5.059626	0.712671	1.130093
288	6	0	5.762515	-0.422698	0.708657
289	1	0	5.563847	-2.355606	-0.212608
290	1	0	3.125442	-2.234742	-0.473320
291	1	0	3.131603	1.667445	1.322384
292	1	0	5.595682	1.531731	1.599554
293	6	0	7.264303	-0.498387	0.811932
294	6	0	7.949954	-0.194754	-0.522611
295	1	0	7.554410	-1.496283	1.152774
296	1	0	7.609195	0.209076	1.568371
297	1	0	9.034667	-0.248181	-0.425059
298	1	0	7.639991	-0.911198	-1.282621
299	1	0	7.684563	0.804159	-0.864630
300	8	0	0.934230	0.992729	0.339862
301	1	0	-2.391214	2.064752	-0.081605
302	1	0	1.222565	-2.166665	0.426498
303	1	0	-0.257553	-1.243948	0.240334
304	1	0	-0.962346	1.135611	0.282090
305	7	0	0.763067	-1.282971	0.267129
306	7	0	-1.979574	1.186463	0.198454
307	6	0	1.467083	-0.136584	0.342993
308	6	0	-2.668975	0.041047	0.027205

AA-cis, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.185416	0.552935	3.413929
2	6	0	-11.694708	-0.790743	3.850980
3	6	0	-12.096350	-1.548362	-1.754925
4	6	0	-11.515709	-2.782115	-1.429113
5	6	0	-12.065690	-3.644105	-0.326089
6	6	0	-11.424407	-3.331994	0.995502
7	6	0	-11.855753	-2.253719	1.784111
8	6	0	-11.208092	-1.914641	2.980125
9	6	0	-11.855174	1.316110	2.445767
10	6	0	-12.124684	3.407258	1.037149
11	6	0	-11.655624	3.110671	-0.358894
12	6	0	-12.160799	2.024379	-1.090719
13	6	0	-11.657763	1.695744	-2.357607
14	6	0	-11.612820	-0.766374	-2.815345
15	6	0	-12.225895	0.560434	-3.162806
16	6	0	-10.097646	-2.694142	3.362353
17	6	0	-10.357204	-4.113193	1.476635
18	6	0	-9.665396	-3.809149	2.649831
19	6	0	-10.209086	3.058193	2.662105
20	6	0	-10.028173	1.104309	3.996582
21	6	0	-9.506278	2.344774	3.631182
22	6	0	-10.412078	-3.210047	-2.196602
23	6	0	-10.541307	-1.279284	-3.570479
24	6	0	-9.906929	-2.486203	-3.273615
25	6	0	-10.614121	2.493748	-2.869996
26	6	0	-10.674333	3.914081	-0.969246
27	6	0	-10.121015	3.619322	-2.215505
28	1	0	-9.056336	-2.853853	-3.864906
29	1	0	-12.943942	-1.187347	-1.171567
30	1	0	-11.892673	-4.723853	-0.580573
31	1	0	-13.170245	-3.543383	-0.261138
32	1	0	-12.706062	-1.657940	1.450651
33	1	0	-8.816448	-4.415979	2.995383

34	1	0	-8.594067	2.747364	4.093517
35	1	0	-12.762810	0.918877	1.989835
36	1	0	-12.954184	1.414470	-0.657540
37	1	0	-9.331321	4.240154	-2.661617
38	1	0	-13.331109	0.521305	-3.048112
39	1	0	-12.061917	0.767069	-4.254694
40	1	0	-13.221559	3.256435	1.126275
41	1	0	-11.967046	4.495511	1.262478
42	1	0	-11.371959	-0.979814	4.910135
43	1	0	-12.806039	-0.791213	3.893432
44	8	0	-9.429969	0.382739	5.061814
45	8	0	-9.436689	-2.356948	4.571260
46	8	0	-10.276188	5.094035	-0.291160
47	8	0	-9.817576	4.379218	2.353546
48	8	0	-10.101761	2.171887	-4.150279
49	8	0	-10.145104	-0.548820	-4.721342
50	8	0	-10.001866	-5.275054	0.742907
51	8	0	-9.897955	-4.496938	-1.924457
52	6	0	-8.273301	-1.641361	4.370936
53	6	0	-8.260593	-0.245978	4.679161
54	7	0	-7.118066	0.502690	4.638669
55	7	0	-7.155745	-2.303639	3.939600
56	6	0	-6.026326	-0.167138	4.254280
57	6	0	-6.048941	-1.552920	3.876940
58	6	0	-4.621526	0.374055	4.066525
59	6	0	-4.663487	-1.941535	3.383556
60	7	0	-3.897733	-0.745011	3.538356
61	8	0	-4.145243	1.451718	4.276934
62	1	0	-2.905146	-0.658468	3.231366
63	8	0	-4.227526	-2.970962	2.949979
64	6	0	-8.739026	4.512513	1.507566
65	6	0	-8.978236	4.991637	0.182546
66	6	0	-11.386483	2.577748	2.052130
67	7	0	-7.968590	5.377514	-0.651680
68	7	0	-7.476783	4.293120	1.986580
69	6	0	-8.936458	0.093806	-4.515032
70	6	0	-8.916879	1.465344	-4.117700
71	6	0	-8.778216	-5.098161	0.113258
72	6	0	-8.724687	-4.554370	-1.207801
73	7	0	-7.757472	2.109419	-3.777566
74	7	0	-7.794188	-0.630341	-4.705838
75	7	0	-7.657096	-5.455472	0.805021
76	7	0	-7.542690	-4.204741	-1.802072
77	6	0	-6.494330	4.633178	1.141227
78	6	0	-6.449972	-4.502350	-1.085451
79	6	0	-6.739637	5.214429	-0.148666
80	6	0	-6.665734	0.028831	-4.425655
81	6	0	-6.647855	1.372220	-3.916572
82	6	0	-6.507227	-5.180626	0.179011
83	6	0	-5.091797	-5.437611	0.673603
84	6	0	-4.989875	-4.191702	-1.393392
85	6	0	-4.991082	4.467964	1.315253
86	6	0	-5.410583	5.526727	-0.817983
87	6	0	-5.243254	-0.497390	-4.503848
88	6	0	-5.210915	1.727456	-3.559924
89	7	0	-4.275042	-4.787091	-0.316594
90	7	0	-4.467908	0.570526	-3.926963
91	7	0	-4.443035	5.039002	0.130735
92	8	0	-4.490904	-3.566014	-2.288170
93	8	0	-4.676198	-6.037090	1.616917
94	8	0	-4.790571	-1.513145	-4.933086
95	8	0	-4.735356	2.717894	-3.073053
96	8	0	-4.347974	3.962086	2.193065
97	8	0	-5.141993	6.058553	-1.850816
98	1	0	-3.423917	5.025428	-0.071470
99	1	0	-3.436735	0.480468	-3.782559
100	1	0	-3.235920	-4.724285	-0.228355
101	1	0	13.283204	3.424318	0.586341
102	6	0	12.179799	3.550589	0.617050
103	6	0	11.569767	3.224612	-0.716422
104	6	0	11.578910	2.722874	1.719954
105	1	0	12.023746	4.638812	0.843888
106	6	0	12.011184	2.123160	-1.468361
107	6	0	10.531018	4.010967	-1.248834
108	6	0	12.109643	1.478733	2.086081
109	6	0	10.464362	3.195397	2.443219
110	6	0	11.401738	1.770184	-2.679544
111	1	0	12.840309	1.522321	-1.093176
112	6	0	9.877809	3.694306	-2.441189
113	8	0	10.163724	5.197530	-0.560831
114	6	0	11.560020	0.727148	3.136755
115	1	0	12.967389	1.082884	1.541447
116	6	0	9.889323	2.501703	3.504567
117	8	0	10.007053	4.493505	2.123312
118	6	0	11.901441	0.632978	-3.523978
119	6	0	10.319407	2.560520	-3.116394
120	1	0	9.049136	4.305050	-2.826461
121	6	0	8.926362	5.054714	0.049007
122	6	0	12.118375	-0.616199	3.513682
123	6	0	10.471138	1.278300	3.839149
124	1	0	9.026924	2.901769	4.055895
125	6	0	8.846862	4.557384	1.387703
126	1	0	13.014397	0.620516	-3.525875
127	1	0	11.621389	0.825273	-4.595394
128	6	0	11.372834	-0.713090	-3.118658
129	8	0	9.689379	2.197075	-4.336162
130	7	0	7.818857	5.409286	-0.666787
131	6	0	11.526931	-1.719859	2.681461
132	1	0	11.908419	-0.815667	4.598340
133	1	0	13.226779	-0.616977	3.436867
134	8	0	10.018289	0.588117	4.990137
135	7	0	7.654037	4.245999	1.978855
136	6	0	11.980052	-1.465975	-2.103505
137	6	0	10.276308	-1.289797	-3.790535
138	6	0	8.524437	1.486120	-4.122365
139	6	0	6.656220	5.176320	-0.044872
140	6	0	12.080552	-2.089881	1.447383
141	6	0	10.401020	-2.435887	3.134100
142	6	0	8.798693	-0.035748	4.804934
143	6	0	6.576840	4.537907	1.238323

144	6	0	11.524728	-2.750515	-1.769074
145	1	0	12.820995	-1.040499	-1.554744
146	6	0	9.812444	-2.577172	-3.529924
147	8	0	9.658610	-0.540297	-4.827329
148	6	0	8.503173	0.083430	-4.393936
149	7	0	7.418525	2.163632	-3.686255
150	6	0	5.246828	5.457525	-0.545247
151	6	0	11.533492	-3.129445	0.681436
152	1	0	12.956475	-1.557381	1.075426
153	6	0	9.809595	-3.471078	2.411384
154	8	0	9.938970	-2.138160	4.437014
155	6	0	8.759567	-1.425287	4.476798
156	7	0	7.665264	0.702451	5.003089
157	6	0	5.115190	4.263520	1.547975
158	6	0	12.132795	-3.530642	-0.637981
159	6	0	10.466231	-3.289800	-2.524615
160	1	0	8.971983	-3.008093	-4.092351
161	7	0	7.366666	-0.667888	-4.269465
162	6	0	6.316235	1.415528	-3.564349
163	7	0	4.410507	4.859127	0.467700
164	8	0	4.840451	6.042080	-1.501000
165	6	0	10.406748	-3.802347	1.196431
166	1	0	8.927332	-4.008301	2.787369
167	7	0	7.585940	-2.098939	4.281242
168	6	0	6.523176	0.024080	4.841140
169	8	0	4.611758	3.650466	2.451730
170	1	0	11.965533	-4.627793	-0.804974
171	1	0	13.237085	-3.412232	-0.624883
172	8	0	10.103792	-4.637138	-2.275574
173	6	0	6.286365	0.012514	-3.867923
174	6	0	4.938139	1.840339	-3.083875
175	1	0	3.368213	4.847256	0.407151
176	8	0	9.967055	-4.942384	0.488206
177	6	0	6.484985	-1.360169	4.460359
178	6	0	5.098511	0.540579	4.966847
179	6	0	8.872766	-4.737940	-1.649726
180	6	0	4.879147	-0.507247	-3.621670
181	7	0	4.161487	0.642593	-3.172866
182	8	0	4.525215	2.892949	-2.686473
183	6	0	8.797148	-4.801747	-0.223804
184	6	0	5.035826	-1.779460	4.278240
185	7	0	4.299019	-0.600394	4.612822
186	8	0	4.656581	1.601626	5.289559
187	7	0	7.765115	-4.809920	-2.445334
188	8	0	4.409842	-1.605310	-3.736446
189	1	0	3.130509	0.636100	-2.995026
190	7	0	7.603680	-4.839252	0.443681
191	8	0	4.549897	-2.821231	3.942869
192	1	0	3.274552	-0.544771	4.487693
193	6	0	6.607317	-4.898708	-1.780771
194	6	0	6.523370	-4.873327	-0.347284
195	6	0	5.205249	-4.979880	-2.362250
196	6	0	5.053779	-4.859441	0.052141
197	7	0	4.363543	-4.929046	-1.197316
198	8	0	4.810285	-5.079211	-3.483489
199	8	0	4.520493	-4.788110	1.121965
200	1	0	3.330117	-4.870554	-1.266978
201	8	0	1.819091	-3.750347	-1.345308
202	6	0	1.146727	-3.525481	-2.354414
203	7	0	-0.168791	-3.981117	-2.581034
204	7	0	1.597148	-2.837531	-3.487537
205	6	0	-0.735828	-3.388838	-3.819256
206	1	0	-0.787026	-4.241109	-1.789047
207	6	0	0.517662	-2.642930	-4.486273
208	1	0	2.554178	-2.500507	-3.622242
209	1	0	-1.194170	-4.190973	-4.448780
210	7	0	-1.701124	-2.290426	-3.585427
211	1	0	0.815572	-3.037404	-5.488084
212	7	0	0.066447	-1.235656	-4.613297
213	6	0	-1.170493	-1.043132	-3.937264
214	1	0	-2.561721	-2.422785	-3.048917
215	1	0	0.767879	-0.469756	-4.602302
216	8	0	-1.719265	0.048507	-3.804230
217	1	0	1.610663	-5.179994	2.912271
218	6	0	1.116584	-4.306905	2.419671
219	6	0	-0.169333	-3.747339	3.192858
220	7	0	0.583974	-4.724551	1.096593
221	7	0	2.018329	-3.128897	2.317329
222	1	0	-0.430020	-4.305878	4.125327
223	7	0	0.212779	-2.354002	3.546199
224	7	0	-1.247300	-3.849750	2.185944
225	6	0	-0.777551	-4.337166	0.956836
226	1	0	1.206545	-4.663389	0.270686
227	6	0	1.463953	-2.005749	2.976371
228	1	0	3.038726	-3.274773	2.276821
229	1	0	-0.518711	-1.624397	3.619889
230	1	0	-2.220869	-3.602045	2.376349
231	8	0	-1.448758	-4.497305	-0.055975
232	8	0	1.999496	-0.909277	3.070951
233	6	0	-0.819341	1.187891	3.264084
234	7	0	0.474900	1.474331	3.758910
235	7	0	-1.525661	2.390927	3.049499
236	8	0	-1.266614	0.058968	3.091464
237	6	0	0.727519	2.941743	3.783500
238	1	0	1.250390	0.819063	3.552733
239	6	0	-0.670568	3.573178	3.321359
240	1	0	-2.548845	2.456080	3.134511
241	1	0	1.061172	3.238978	4.808430
242	7	0	1.671435	3.405735	2.748669
243	1	0	-1.134294	4.267764	4.063447
244	7	0	-0.329505	4.332264	2.087566
245	6	0	1.028172	4.120579	1.725866
246	1	0	2.686547	3.272995	2.814444
247	1	0	-1.043159	4.411417	1.338661
248	8	0	1.577898	4.580507	0.730090
249	1	0	0.926058	5.341415	-3.535353
250	6	0	0.529233	4.407127	-3.067035
251	6	0	-0.757346	3.782077	-3.794733
252	7	0	0.045412	4.695486	-1.693955
253	7	0	1.527247	3.315872	-3.147483

254	1	0	-1.133391	4.374309	-4.663777
255	7	0	-0.293191	2.449974	-4.256496
256	7	0	-1.764401	3.721885	-2.707150
257	6	0	-1.237714	4.152938	-1.482131
258	1	0	0.713135	4.807310	-0.906669
259	6	0	0.983667	2.149114	-3.708816
260	1	0	2.420081	3.343433	-2.646823
261	1	0	-0.981510	1.677793	-4.358726
262	1	0	-2.720044	3.379015	-2.839041
263	8	0	-1.833427	4.119902	-0.403196
264	8	0	1.564783	1.074194	-3.829392
265	6	0	-6.026251	-0.793767	-0.449192
266	6	0	-4.653920	-0.785217	-0.676503
267	6	0	-3.838082	0.150330	-0.029927
268	6	0	-4.417805	1.067017	0.852974
269	6	0	-5.795209	1.044467	1.082562
270	6	0	-6.618621	0.115089	0.440790
271	1	0	-6.645454	-1.523473	-0.960133
272	1	0	-4.191763	-1.502640	-1.343890
273	1	0	-3.801836	1.778066	1.397433
274	1	0	-6.228445	1.751563	1.784785
275	6	0	-8.107711	0.097292	0.674043
276	6	0	-8.892639	0.530018	-0.564575
277	1	0	-8.349124	0.758974	1.509174
278	1	0	-8.421270	-0.907811	0.966032
279	1	0	-9.964800	0.538574	-0.363706
280	1	0	-8.592404	1.529994	-0.876504
281	1	0	-8.711345	-0.151896	-1.394108
282	8	0	-1.836538	-1.013108	-0.582251
283	6	0	5.299215	-1.378029	-0.239285
284	6	0	3.925300	-1.285602	-0.458477
285	6	0	3.222691	-0.156146	-0.017863
286	6	0	3.908319	0.859018	0.657360
287	6	0	5.278009	0.745050	0.888743
288	6	0	5.991950	-0.379446	0.455952
289	1	0	5.837071	-2.251399	-0.588115
290	1	0	3.410112	-2.074692	-1.002458
291	1	0	3.354882	1.726677	0.993425
292	1	0	5.792049	1.522849	1.444051
293	6	0	7.480235	-0.493650	0.667649
294	6	0	8.271615	-0.182561	-0.605301
295	1	0	7.720794	-1.503893	1.010434
296	1	0	7.783773	0.190032	1.462750
297	1	0	9.344588	-0.264659	-0.427868
298	1	0	8.004461	-0.876471	-1.401457
299	1	0	8.056741	0.828965	-0.945832
300	8	0	1.243535	1.136956	-0.339673
301	1	0	-2.131570	2.090924	0.068560
302	1	0	1.467238	-2.014922	-0.030726
303	1	0	0.018869	-1.101785	-0.407552
304	1	0	-0.648792	1.212314	-0.228531
305	7	0	1.033160	-1.138766	-0.284397
306	7	0	-1.664772	1.216827	-0.125060
307	6	0	1.747271	-0.000330	-0.220626
308	6	0	-2.359098	0.076304	-0.265300

AB-trans, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.198382	0.747536	3.490682
2	6	0	-11.745655	-0.586392	3.912747
3	6	0	-12.109948	-1.367305	-1.696526
4	6	0	-11.606892	-2.634968	-1.370525
5	6	0	-12.201839	-3.452273	-0.256240
6	6	0	-11.544683	-3.140661	1.058746
7	6	0	-11.957493	-2.057180	1.850751
8	6	0	-11.285744	-1.715582	3.033053
9	6	0	-11.829314	1.518705	2.501421
10	6	0	-12.013333	3.606185	1.069404
11	6	0	-11.531286	3.290898	-0.317880
12	6	0	-12.045484	2.203814	-1.042654
13	6	0	-11.542766	1.861313	-2.305178
14	6	0	-11.566187	-0.607979	-2.743304
15	6	0	-12.125409	0.735949	-3.112416
16	6	0	-10.169190	-2.496833	3.394758
17	6	0	-10.474846	-3.926748	1.527009
18	6	0	-9.754435	-3.617562	2.680856
19	6	0	-10.137773	3.214360	2.726755
20	6	0	-10.045662	1.279503	4.098474
21	6	0	-9.482318	2.500836	3.726433
22	6	0	-10.533036	-3.129497	-2.138766
23	6	0	-10.496118	-1.164698	-3.470485
24	6	0	-9.951684	-2.416702	-3.186036
25	6	0	-10.488356	2.642372	-2.820329
26	6	0	-10.535892	4.076206	-0.928633
27	6	0	-9.982811	3.765320	-2.171855
28	1	0	-9.112476	-2.825882	-3.766167
29	1	0	-12.943654	-0.961368	-1.122552
30	1	0	-12.077584	-4.543147	-0.488374
31	1	0	-13.300122	-3.298620	-0.196778
32	1	0	-12.812307	-1.460332	1.531478
33	1	0	-8.898018	-4.222477	3.010039
34	1	0	-8.568200	2.884431	4.201514
35	1	0	-12.737084	1.139502	2.031113
36	1	0	-12.845658	1.605051	-0.606697
37	1	0	-9.183491	4.373211	-2.618852
38	1	0	-13.233918	0.733203	-3.022474
39	1	0	-11.931046	0.927375	-4.202234
40	1	0	-13.115623	3.488205	1.139808
41	1	0	-11.827125	4.690473	1.292681
42	1	0	-11.430508	-0.794468	4.970567
43	1	0	-12.856412	-0.555951	3.951844
44	8	0	-9.472295	0.559296	5.180404
45	8	0	-9.489685	-2.155067	4.589721
46	8	0	-10.110218	5.251268	-0.255693
47	8	0	-9.686824	4.509361	2.389009
48	8	0	-9.976678	2.299560	-4.097088

49	8	0	-10.021579	-0.441041	-4.594144
50	8	0	-10.168009	-5.109763	0.809823
51	8	0	-10.124188	-4.459061	-1.890419
52	6	0	-8.330914	-1.436217	4.383302
53	6	0	-8.299935	-0.068009	4.793124
54	7	0	-7.146280	0.663243	4.818872
55	7	0	-7.234941	-2.064391	3.857327
56	6	0	-6.068736	0.018159	4.358559
57	6	0	-6.124869	-1.315938	3.829883
58	6	0	-4.650374	0.545562	4.225465
59	6	0	-4.765914	-1.654497	3.239254
60	7	0	-3.971049	-0.507869	3.510196
61	8	0	-4.127760	1.546063	4.608458
62	1	0	-2.979521	-0.405521	3.192026
63	8	0	-4.385315	-2.639278	2.662854
64	6	0	-8.605315	4.572929	1.539510
65	6	0	-8.818840	5.096194	0.227226
66	6	0	-11.319131	2.761753	2.102698
67	7	0	-7.789518	5.452895	-0.595822
68	7	0	-7.359470	4.238690	1.995955
69	6	0	-8.816701	0.191230	-4.348146
70	6	0	-8.796624	1.584935	-4.037616
71	6	0	-8.956749	-5.017015	0.145766
72	6	0	-8.928090	-4.598721	-1.220263
73	7	0	-7.636639	2.253311	-3.750352
74	7	0	-7.673466	-0.550737	-4.457210
75	7	0	-7.827925	-5.367247	0.830304
76	7	0	-7.758004	-4.432872	-1.907935
77	6	0	-6.361794	4.529772	1.150668
78	6	0	-6.655504	-4.745701	-1.214313
79	6	0	-6.572237	5.192855	-0.106134
80	6	0	-6.544744	0.124918	-4.217557
81	6	0	-6.526739	1.510589	-3.834683
82	6	0	-6.692916	-5.242966	0.132172
83	6	0	-5.273885	-5.523607	0.600055
84	6	0	-5.202574	-4.621324	-1.645477
85	6	0	-4.874947	4.223929	1.285915
86	6	0	-5.225463	5.453509	-0.764168
87	6	0	-5.120172	-0.399884	-4.234341
88	6	0	-5.089259	1.913382	-3.538920
89	7	0	-4.470723	-5.117810	-0.522503
90	7	0	-4.341361	0.728523	-3.820156
91	7	0	-4.295026	4.819810	0.130278
92	8	0	-4.702207	-4.202170	-2.649656
93	8	0	-4.840944	-5.984117	1.612260
94	8	0	-4.665660	-1.472619	-4.511674
95	8	0	-4.605941	2.942403	-3.158509
96	8	0	-4.271869	3.598365	2.113199
97	8	0	-4.927164	6.045611	-1.755697
98	1	0	-3.270038	4.771733	-0.068575
99	1	0	-3.308877	0.667107	-3.706874
100	1	0	-3.437100	-5.095724	-0.490546
101	1	0	13.412364	3.158273	0.546859
102	6	0	12.315550	3.331172	0.561610
103	6	0	11.697241	2.969188	-0.759662
104	6	0	11.664537	2.571335	1.684184
105	1	0	12.202472	4.433285	0.740666
106	6	0	12.118156	1.835227	-1.472715
107	6	0	10.669358	3.754504	-1.316888
108	6	0	12.130963	1.314132	2.093346
109	6	0	10.557858	3.114879	2.366975
110	6	0	11.508275	1.457639	-2.676624
111	1	0	12.933645	1.230127	-1.074910
112	6	0	10.016333	3.414828	-2.502618
113	8	0	10.346530	4.974252	-0.675397
114	6	0	11.506663	0.604391	3.129445
115	1	0	12.998404	0.878992	1.596238
116	6	0	9.882166	2.443877	3.384785
117	8	0	10.222100	4.449689	2.052555
118	6	0	11.988032	0.282214	-3.479425
119	6	0	10.448501	2.258642	-3.146534
120	1	0	9.200441	4.029628	-2.908572
121	6	0	9.117245	4.941685	-0.038419
122	6	0	12.029677	-0.724889	3.598155
123	6	0	10.383903	1.194204	3.744528
124	1	0	9.010312	2.882980	3.890255
125	6	0	9.048608	4.613612	1.349629
126	1	0	13.100048	0.235863	-3.460567
127	1	0	11.733199	0.452193	-4.560735
128	6	0	11.412337	-1.035622	-3.045752
129	8	0	9.838476	1.880007	-4.373018
130	7	0	8.011621	5.286799	-0.764083
131	6	0	11.441629	-1.865222	2.816885
132	1	0	11.787817	-0.854662	4.686969
133	1	0	13.139684	-0.748187	3.552396
134	8	0	9.839292	0.522240	4.861457
135	7	0	7.864421	4.548791	2.030131
136	6	0	11.969894	-1.771473	-1.990720
137	6	0	10.317930	-1.604805	-3.727831
138	6	0	8.648587	1.210872	-4.169504
139	6	0	6.863528	5.262462	-0.076172
140	6	0	11.986911	-2.271680	1.589118
141	6	0	10.323732	-2.568138	3.305303
142	6	0	8.652962	-0.141262	4.640251
143	6	0	6.787843	4.866466	1.302108
144	6	0	11.468596	-3.031175	-1.625535
145	1	0	12.806107	-1.350336	-1.431171
146	6	0	9.817925	-2.873054	-3.444651
147	8	0	9.732748	-0.867260	-4.792435
148	6	0	8.590817	-0.201290	-4.387980
149	7	0	7.554492	1.936310	-3.786591
150	6	0	5.459532	5.576632	-0.575590
151	6	0	11.421506	-3.317683	0.847244
152	1	0	12.868231	-1.758444	1.203056
153	6	0	9.706715	-3.601482	2.598619
154	8	0	9.871982	-2.250775	4.609823
155	6	0	8.667567	-1.569148	4.602367
156	7	0	7.491658	0.580262	4.577972
157	6	0	5.326684	4.843347	1.728206
158	6	0	12.023510	-3.783566	-0.449925

159	6	0	10.421220	-3.569046	-2.396463
160	1	0	8.983230	-3.300023	-4.018120
161	7	0	7.434826	-0.917340	-4.238750
162	6	0	6.431498	1.222746	-3.647756
163	7	0	4.628971	5.276625	0.556254
164	8	0	5.063793	5.987591	-1.624136
165	6	0	10.275384	-3.946657	1.375530
166	1	0	8.822854	-4.122646	2.991356
167	7	0	7.521863	-2.313115	4.609401
168	6	0	6.376674	-0.160129	4.550904
169	8	0	4.810957	4.532202	2.760915
170	1	0	11.821771	-4.880312	-0.578398
171	1	0	13.131501	-3.703124	-0.419738
172	8	0	9.991352	-4.892521	-2.110044
173	6	0	6.368568	-0.192525	-3.876587
174	6	0	5.063166	1.710166	-3.209157
175	1	0	3.591457	5.289580	0.513228
176	8	0	9.770804	-5.056901	0.658991
177	6	0	6.393136	-1.595531	4.610093
178	6	0	4.929412	0.303642	4.450377
179	6	0	8.742370	-4.883841	-1.508915
180	6	0	4.948743	-0.662713	-3.605688
181	7	0	4.255356	0.527818	-3.231189
182	8	0	4.673900	2.794864	-2.880745
183	6	0	8.636298	-4.827331	-0.082325
184	6	0	4.962631	-2.109338	4.637535
185	7	0	4.179315	-0.908360	4.570584
186	8	0	4.449259	1.388943	4.294466
187	7	0	7.647809	-4.929620	-2.322747
188	8	0	4.449398	-1.753272	-3.649053
189	1	0	3.220751	0.557411	-3.062942
190	7	0	7.436860	-4.652955	0.550617
191	8	0	4.517612	-3.214978	4.712871
192	1	0	3.149893	-0.936994	4.468570
193	6	0	6.474769	-4.834964	-1.683997
194	6	0	6.375070	-4.633508	-0.266803
195	6	0	5.080348	-4.842824	-2.285488
196	6	0	4.918237	-4.380655	0.081119
197	7	0	4.232985	-4.534285	-1.156656
198	8	0	4.679519	-5.061299	-3.386493
199	8	0	4.399155	-4.080513	1.122414
200	1	0	3.204896	-4.405864	-1.253799
201	8	0	1.479219	-3.772176	-1.397392
202	6	0	0.925353	-3.520203	-2.470815
203	7	0	-0.376561	-3.925964	-2.839488
204	7	0	1.526297	-2.850132	-3.542725
205	6	0	-0.770081	-3.329144	-4.146777
206	1	0	-1.095741	-4.085588	-2.108714
207	6	0	0.574354	-2.616398	-4.654443
208	1	0	2.511830	-2.576375	-3.584598
209	1	0	-1.156017	-4.134351	-4.818417
210	7	0	-1.725664	-2.207976	-4.012666
211	1	0	0.972730	-3.009263	-5.621779
212	7	0	0.185984	-1.192235	-4.813775
213	6	0	-1.129140	-0.972031	-4.321677
214	1	0	-2.740598	-2.346528	-3.943840
215	1	0	0.898985	-0.450143	-4.665732
216	8	0	-1.670951	0.123023	-4.244767
217	1	0	0.817761	-5.598330	2.650186
218	6	0	0.534107	-4.604221	2.228829
219	6	0	-0.653012	-3.862701	3.009425
220	7	0	-0.001483	-4.786563	0.848479
221	7	0	1.641736	-3.627924	2.284703
222	1	0	-1.066579	-4.430834	3.878169
223	7	0	-0.035093	-2.597290	3.485295
224	7	0	-1.675507	-3.662961	1.956266
225	6	0	-1.236585	-4.101658	0.706289
226	1	0	0.663458	-4.772787	0.052804
227	6	0	1.266415	-2.439097	2.939616
228	1	0	2.609780	-3.875741	2.059761
229	1	0	-0.631685	-1.748567	3.580486
230	1	0	-2.602557	-3.259220	2.142498
231	8	0	-1.866893	-3.982035	-0.347692
232	8	0	1.977027	-1.450013	3.053298
233	6	0	-0.660966	0.998903	3.134648
234	7	0	0.656614	1.140744	3.653294
235	7	0	-1.243008	2.261569	2.988181
236	8	0	-1.230578	-0.079891	2.967127
237	6	0	1.052481	2.578275	3.690848
238	1	0	1.363569	0.432564	3.394631
239	6	0	-0.274427	3.353324	3.237322
240	1	0	-2.198151	2.434292	2.668939
241	1	0	1.411158	2.828048	4.719882
242	7	0	2.041471	2.963314	2.662990
243	1	0	-0.675013	4.074349	3.992307
244	7	0	0.147571	4.092609	2.019990
245	6	0	1.471647	3.746813	1.647945
246	1	0	3.037453	2.758999	2.754085
247	1	0	-0.556393	4.318807	1.291998
248	8	0	2.055253	4.158646	0.646700
249	1	0	1.308608	5.331403	-3.508415
250	6	0	0.840986	4.450882	-3.002774
251	6	0	-0.500875	3.912676	-3.697527
252	7	0	0.410114	4.827159	-1.635402
253	7	0	1.739522	3.271978	-3.044123
254	1	0	-0.832750	4.498449	-4.589150
255	7	0	-0.145547	2.530379	-4.112988
256	7	0	-1.498429	3.983485	-2.607310
257	6	0	-0.929104	4.418103	-1.398099
258	1	0	1.097937	4.788952	-0.855017
259	6	0	1.106491	2.144958	-3.582965
260	1	0	2.696796	3.289256	-2.684192
261	1	0	-0.880723	1.819859	-4.274716
262	1	0	-2.470524	3.688241	-2.714928
263	8	0	-1.512066	4.530071	-0.326118
264	8	0	1.601430	1.020052	-3.669277
265	6	0	-6.113123	-1.119406	-1.193757
266	6	0	-4.717719	-1.146199	-1.149448
267	6	0	-3.989070	-0.159447	-0.467471
268	6	0	-4.716854	0.851120	0.184395

269	6	0	-6.108423	0.874063	0.151280
270	6	0	-6.828203	-0.106402	-0.546621
271	1	0	-6.650272	-1.882654	-1.750371
272	1	0	-4.198486	-1.937934	-1.688834
273	1	0	-4.172428	1.625069	0.713441
274	1	0	-6.645821	1.665441	0.663264
275	6	0	-8.334770	-0.080198	-0.558491
276	6	0	-8.926118	-0.432865	0.806781
277	1	0	-8.703447	-0.784449	-1.308081
278	1	0	-8.683890	0.911630	-0.856340
279	1	0	-10.016724	-0.431501	0.773857
280	1	0	-8.592742	-1.421426	1.121979
281	1	0	-8.610462	0.286758	1.560872
282	8	0	-1.657262	-1.261993	-0.676585
283	6	0	5.310178	-0.570922	1.071866
284	6	0	3.945198	-0.788902	0.871364
285	6	0	3.137391	0.235709	0.363688
286	6	0	3.709287	1.481089	0.075425
287	6	0	5.072749	1.680271	0.265247
288	6	0	5.895292	0.662899	0.771930
289	1	0	5.919073	-1.369304	1.481201
290	1	0	3.507483	-1.738454	1.170347
291	1	0	3.069714	2.284272	-0.275274
292	1	0	5.502675	2.646530	0.032014
293	6	0	7.367615	0.909534	0.987230
294	6	0	8.131523	1.119101	-0.321590
295	1	0	7.796416	0.063130	1.526331
296	1	0	7.494019	1.782891	1.634758
297	1	0	9.191560	1.289586	-0.131069
298	1	0	8.036929	0.239947	-0.956335
299	1	0	7.742520	1.976422	-0.870637
300	8	0	0.904805	1.057692	0.220715
301	1	0	1.864645	-1.933379	-0.290716
302	1	0	0.235309	-1.308934	-0.303235
303	1	0	-0.829931	0.999996	-0.078474
304	7	0	1.226176	-1.170042	-0.126944
305	6	0	1.667391	0.069367	0.150466
306	1	0	-2.197248	-2.066504	-0.732903
307	8	0	-1.807609	1.055519	-0.176418
308	5	0	-2.416906	-0.124747	-0.434408

AB-cis, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.203451	0.903804	3.354729
2	6	0	-11.749759	-0.414452	3.824018
3	6	0	-12.055672	-1.458884	-1.748829
4	6	0	-11.585406	-2.728181	-1.377042
5	6	0	-12.171494	-3.469386	-0.207323
6	6	0	-11.493204	-3.070899	1.074221
7	6	0	-11.924658	-1.964852	1.821910
8	6	0	-11.262653	-1.568378	2.992694
9	6	0	-11.818036	1.626526	2.320258
10	6	0	-11.981729	3.647169	0.794032
11	6	0	-11.473029	3.273379	-0.568958
12	6	0	-11.967474	2.152778	-1.254690
13	6	0	-11.438536	1.754856	-2.490957
14	6	0	-11.479289	-0.744829	-2.808838
15	6	0	-12.006150	0.590480	-3.251838
16	6	0	-10.134733	-2.314666	3.390139
17	6	0	-10.392680	-3.802949	1.561462
18	6	0	-9.680090	-3.438181	2.703195
19	6	0	-10.135922	3.336497	2.501995
20	6	0	-10.063019	1.465309	3.959488
21	6	0	-9.495606	2.670296	3.543676
22	6	0	-10.538047	-3.289213	-2.134286
23	6	0	-10.402912	-1.347262	-3.490020
24	6	0	-9.915934	-2.616091	-3.185520
25	6	0	-10.381108	2.520618	-3.021963
26	6	0	-10.469895	4.037008	-1.195106
27	6	0	-9.895664	3.675659	-2.414222
28	1	0	-9.082826	-3.063326	-3.746293
29	1	0	-12.884438	-1.015855	-1.195790
30	1	0	-12.053488	-4.573816	-0.366086
31	1	0	-13.268101	-3.307530	-0.143526
32	1	0	-12.791663	-1.397761	1.481957
33	1	0	-8.805433	-4.008167	3.047936
34	1	0	-8.592568	3.078736	4.018936
35	1	0	-12.715562	1.223003	1.850712
36	1	0	-12.773737	1.570009	-0.808070
37	1	0	-9.092503	4.269130	-2.874004
38	1	0	-13.117250	0.603140	-3.192783
39	1	0	-11.780931	0.725649	-4.344446
40	1	0	-13.084706	3.527523	0.849458
41	1	0	-11.803782	4.741125	0.972670
42	1	0	-11.449999	-0.579094	4.893778
43	1	0	-12.860871	-0.391683	3.844151
44	8	0	-9.519374	0.796804	5.086808
45	8	0	-9.505138	-1.944447	4.602377
46	8	0	-10.059290	5.240542	-0.565432
47	8	0	-9.686233	4.618690	2.117406
48	8	0	-9.819528	2.124929	-4.265604
49	8	0	-9.844472	-0.634669	-4.583103
50	8	0	-10.076563	-5.007609	0.891553
51	8	0	-10.179605	-4.629234	-1.857439
52	6	0	-8.336903	-1.229469	4.439181
53	6	0	-8.331018	0.157809	4.776443
54	7	0	-7.181932	0.896482	4.823284
55	7	0	-7.207913	-1.886497	4.031247
56	6	0	-6.077790	0.230013	4.470577
57	6	0	-6.098350	-1.138351	4.032942
58	6	0	-4.655249	0.757681	4.383309
59	6	0	-4.703855	-1.510329	3.556361
60	7	0	-3.927821	-0.342834	3.802682
61	8	0	-4.165002	1.793824	4.711686
62	1	0	-2.929405	-0.251501	3.512418
63	8	0	-4.286236	-2.528289	3.075142

64	6	0	-8.587513	4.654109	1.289112
65	6	0	-8.776970	5.113047	-0.050638
66	6	0	-11.303716	2.852458	1.876330
67	7	0	-7.732892	5.439377	-0.867529
68	7	0	-7.348831	4.357305	1.789282
69	6	0	-8.661754	-0.005238	-4.249591
70	6	0	-8.644369	1.415275	-4.095961
71	6	0	-8.898359	-4.961177	0.173402
72	6	0	-8.950953	-4.769892	-1.241039
73	7	0	-7.495840	2.107009	-3.822168
74	7	0	-7.535854	-0.769836	-4.116704
75	7	0	-7.725653	-5.177972	0.841348
76	7	0	-7.831944	-4.799961	-2.025792
77	6	0	-6.335007	4.622145	0.954839
78	6	0	-6.690680	-5.020972	-1.361378
79	6	0	-6.524318	5.218438	-0.338247
80	6	0	-6.421951	-0.079870	-3.848866
81	6	0	-6.397587	1.349363	-3.710087
82	6	0	-6.637915	-5.203797	0.062219
83	6	0	-5.188048	-5.375236	0.486736
84	6	0	-5.276663	-5.080632	-1.918126
85	6	0	-4.847472	4.348145	1.142091
86	6	0	-5.166010	5.463584	-0.977548
87	6	0	-5.024040	-0.619626	-3.612404
88	6	0	-4.972354	1.781970	-3.401461
89	7	0	-4.464553	-5.257068	-0.748325
90	7	0	-4.240671	0.551016	-3.375292
91	7	0	-4.248616	4.890247	-0.030980
92	8	0	-4.852190	-5.021805	-3.033439
93	8	0	-4.684481	-5.575904	1.550754
94	8	0	-4.602544	-1.742815	-3.587195
95	8	0	-4.485227	2.859458	-3.208637
96	8	0	-4.254699	3.782358	2.018166
97	8	0	-4.851674	6.006340	-1.992392
98	1	0	-3.219529	4.843408	-0.205666
99	1	0	-3.208967	0.507031	-3.246075
100	1	0	-3.433167	-5.233130	-0.778512
101	1	0	13.420198	3.127390	0.522973
102	6	0	12.324344	3.306876	0.520906
103	6	0	11.718706	2.913271	-0.797248
104	6	0	11.656225	2.580854	1.655777
105	1	0	12.215909	4.413971	0.669301
106	6	0	12.139277	1.756624	-1.472952
107	6	0	10.704029	3.690073	-1.389428
108	6	0	12.113025	1.334876	2.107762
109	6	0	10.541681	3.146684	2.306938
110	6	0	11.541676	1.350009	-2.673572
111	1	0	12.944678	1.156501	-1.047908
112	6	0	10.063367	3.322098	-2.573512
113	8	0	10.382470	4.930243	-0.787238
114	6	0	11.471331	0.656861	3.154475
115	1	0	12.986712	0.883665	1.636601
116	6	0	9.847543	2.506190	3.331940
117	8	0	10.218605	4.474162	1.951377
118	6	0	12.022643	0.147972	-3.434964
119	6	0	10.494378	2.145229	-3.179860
120	1	0	9.258222	3.931936	-3.007392
121	6	0	9.145300	4.923769	-0.164987
122	6	0	11.985276	-0.658148	3.671023
123	6	0	10.339943	1.265818	3.734216
124	1	0	8.968915	2.961159	3.810703
125	6	0	9.055819	4.627531	1.229245
126	1	0	13.134066	0.095774	-3.403200
127	1	0	11.779808	0.285641	-4.523588
128	6	0	11.433843	-1.151797	-2.965876
129	8	0	9.898280	1.739196	-4.404355
130	7	0	8.052378	5.262936	-0.912173
131	6	0	11.403621	-1.821194	2.919138
132	1	0	11.730258	-0.752837	4.760433
133	1	0	13.095696	-0.685544	3.639205
134	8	0	9.776990	0.627251	4.861508
135	7	0	7.862280	4.584893	1.894747
136	6	0	11.978351	-1.860718	-1.885955
137	6	0	10.339190	-1.731550	-3.638616
138	6	0	8.698410	1.087454	-4.200671
139	6	0	6.895238	5.262888	-0.238955
140	6	0	11.958039	-2.262446	1.707506
141	6	0	10.282117	-2.509874	3.419156
142	6	0	8.594903	-0.044325	4.644186
143	6	0	6.797982	4.894450	1.145416
144	6	0	11.464977	-3.105707	-1.488485
145	1	0	12.814169	-1.430073	-1.333145
146	6	0	9.826595	-2.986768	-3.322148
147	8	0	9.772474	-1.021058	-4.730780
148	6	0	8.632034	-0.331729	-4.364698
149	7	0	7.603014	1.836907	-3.871665
150	6	0	5.501247	5.582048	-0.762042
151	6	0	11.397648	-3.328635	0.991013
152	1	0	12.842080	-1.760074	1.313465
153	6	0	9.671203	-3.563819	2.738168
154	8	0	9.816164	-2.152532	4.708713
155	6	0	8.611177	-1.472950	4.663074
156	7	0	7.434258	0.672121	4.533071
157	6	0	5.331412	4.890210	1.551913
158	6	0	12.007516	-3.829572	-0.289319
159	6	0	10.418485	-3.657286	-2.250979
160	1	0	8.991996	-3.423548	-3.888303
161	7	0	7.467815	-1.032235	-4.205154
162	6	0	6.471106	1.138819	-3.725867
163	7	0	4.653261	5.312591	0.365090
164	8	0	5.122350	5.976136	-1.823098
165	6	0	10.248214	-3.942993	1.529158
166	1	0	8.784608	-4.074137	3.139044
167	7	0	7.466224	-2.217410	4.684865
168	6	0	6.320328	-0.070662	4.518728
169	8	0	4.799979	4.597279	2.582318
170	1	0	11.802349	-4.928486	-0.391417
171	1	0	13.115556	-3.752636	-0.252364
172	8	0	9.979806	-4.970122	-1.931666
173	6	0	6.401510	-0.284903	-3.892629

174	6	0	5.097781	1.654823	-3.337687
175	1	0	3.616746	5.335589	0.308753
176	8	0	9.745363	-5.070870	0.839222
177	6	0	6.336850	-1.501964	4.639394
178	6	0	4.874635	0.386354	4.374361
179	6	0	8.728003	-4.940438	-1.337466
180	6	0	4.973945	-0.733452	-3.624777
181	7	0	4.282732	0.477656	-3.319217
182	8	0	4.708579	2.756206	-3.070085
183	6	0	8.615126	-4.854532	0.086790
184	6	0	4.906649	-2.016472	4.666220
185	7	0	4.123494	-0.820605	4.527293
186	8	0	4.397490	1.464980	4.168679
187	7	0	7.637128	-4.995727	-2.155880
188	8	0	4.467985	-1.821780	-3.626235
189	1	0	3.247099	0.520067	-3.158789
190	7	0	7.413396	-4.662200	0.710381
191	8	0	4.460013	-3.116943	4.788095
192	1	0	3.096007	-0.855559	4.409283
193	6	0	6.461718	-4.881646	-1.525107
194	6	0	6.355723	-4.652987	-0.112274
195	6	0	5.070520	-4.891866	-2.133951
196	6	0	4.898284	-4.386146	0.223345
197	7	0	4.219454	-4.558805	-1.015645
198	8	0	4.674624	-5.127284	-3.233354
199	8	0	4.373949	-4.066587	1.256133
200	1	0	3.193502	-4.421598	-1.121560
201	8	0	1.484526	-3.776101	-1.310289
202	6	0	0.943904	-3.554047	-2.397209
203	7	0	-0.350463	-3.986146	-2.764459
204	7	0	1.539964	-2.892981	-3.475806
205	6	0	-0.746663	-3.412123	-4.080678
206	1	0	-1.071039	-4.143220	-2.034181
207	6	0	0.590189	-2.692692	-4.598520
208	1	0	2.524311	-2.613787	-3.520025
209	1	0	-1.129043	-4.227577	-4.742501
210	7	0	-1.708762	-2.297491	-3.969914
211	1	0	0.998384	-3.100397	-5.555266
212	7	0	0.184884	-1.277043	-4.786589
213	6	0	-1.123576	-1.058383	-4.274807
214	1	0	-2.697016	-2.424747	-3.725874
215	1	0	0.893194	-0.524251	-4.673179
216	8	0	-1.682412	0.029166	-4.197325
217	1	0	0.727872	-5.538726	2.698037
218	6	0	0.446556	-4.554331	2.253242
219	6	0	-0.734757	-3.789255	3.017689
220	7	0	-0.093472	-4.768692	0.878830
221	7	0	1.558607	-3.580625	2.278538
222	1	0	-1.151472	-4.333439	3.900264
223	7	0	-0.109020	-2.516056	3.463975
224	7	0	-1.754979	-3.598673	1.959921
225	6	0	-1.327520	-4.081655	0.723084
226	1	0	0.575670	-4.767325	0.085918
227	6	0	1.192480	-2.377814	2.914652
228	1	0	2.527454	-3.843042	2.070717
229	1	0	-0.700897	-1.662908	3.538093
230	1	0	-2.703376	-3.256650	2.163323
231	8	0	-1.949891	-3.972128	-0.336998
232	8	0	1.912162	-1.392973	3.007537
233	6	0	-0.645400	1.118914	3.068312
234	7	0	0.681720	1.254285	3.561470
235	7	0	-1.209814	2.387910	2.897826
236	8	0	-1.238120	0.047792	2.943664
237	6	0	1.102035	2.684211	3.553509
238	1	0	1.372482	0.523578	3.326436
239	6	0	-0.220924	3.469881	3.106718
240	1	0	-2.151343	2.564627	2.543730
241	1	0	1.486521	2.955088	4.567793
242	7	0	2.075131	3.020391	2.492661
243	1	0	-0.599505	4.209696	3.855301
244	7	0	0.192137	4.182628	1.870844
245	6	0	1.504913	3.813075	1.483978
246	1	0	3.074864	2.833695	2.589757
247	1	0	-0.518507	4.409066	1.149431
248	8	0	2.080976	4.206535	0.471408
249	1	0	1.302440	5.271967	-3.725698
250	6	0	0.850270	4.404000	-3.185537
251	6	0	-0.499103	3.835679	-3.840568
252	7	0	0.439298	4.821209	-1.823164
253	7	0	1.756485	3.230798	-3.206307
254	1	0	-0.847176	4.387883	-4.747243
255	7	0	-0.144557	2.440402	-4.212354
256	7	0	-1.479332	3.936584	-2.737687
257	6	0	-0.895469	4.417062	-1.553418
258	1	0	1.137688	4.799886	-1.051625
259	6	0	1.119716	2.082122	-3.692537
260	1	0	2.723462	3.267214	-2.875104
261	1	0	-0.881023	1.720936	-4.328708
262	1	0	-2.458452	3.658208	-2.829771
263	8	0	-1.465732	4.562707	-0.478631
264	8	0	1.620792	0.957839	-3.749499
265	6	0	-6.281877	-1.301433	-0.135282
266	6	0	-4.918577	-1.253562	-0.424300
267	6	0	-4.114563	-0.189880	0.018335
268	6	0	-4.732467	0.816987	0.777956
269	6	0	-6.093005	0.767986	1.075755
270	6	0	-6.887179	-0.295545	0.629080
271	1	0	-6.880106	-2.134236	-0.489745
272	1	0	-4.487234	-2.050975	-1.027764
273	1	0	-4.129559	1.644099	1.135879
274	1	0	-6.542932	1.557234	1.671608
275	6	0	-8.368751	-0.325635	0.897092
276	6	0	-9.177128	0.171371	-0.302349
277	1	0	-8.594583	0.293206	1.768171
278	1	0	-8.675734	-1.345589	1.144167
279	1	0	-10.247115	0.152641	-0.088400
280	1	0	-8.897236	1.193101	-0.554439
281	1	0	-8.994552	-0.457044	-1.173343
282	8	0	-1.834286	-1.202077	-0.679155
283	6	0	5.147597	-0.479554	1.014500

284	6	0	3.784541	-0.694349	0.798857
285	6	0	2.997134	0.309033	0.220835
286	6	0	3.590292	1.529936	-0.123471
287	6	0	4.951243	1.727303	0.085754
288	6	0	5.752362	0.730899	0.663267
289	1	0	5.738803	-1.260736	1.478763
290	1	0	3.332948	-1.621595	1.143631
291	1	0	2.966430	2.319950	-0.527115
292	1	0	5.394074	2.676889	-0.188389
293	6	0	7.221018	0.975498	0.905337
294	6	0	8.018125	1.145171	-0.389229
295	1	0	7.631268	0.141847	1.477754
296	1	0	7.337696	1.864674	1.532823
297	1	0	9.074540	1.311446	-0.176962
298	1	0	7.931128	0.250837	-1.003463
299	1	0	7.651040	1.991579	-0.969396
300	8	0	0.782183	1.153312	-0.043518
301	1	0	1.693514	-1.889064	-0.255310
302	1	0	0.075613	-1.237263	-0.350834
303	1	0	-0.982903	1.078349	-0.197112
304	7	0	1.067464	-1.101651	-0.179480
305	6	0	1.527949	0.150311	-0.007273
306	1	0	-2.336210	-2.030753	-0.618104
307	8	0	-1.965070	1.107262	-0.144520
308	5	0	-2.571861	-0.095663	-0.275002

AC-trans, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.641931	-0.493267	-2.928518
2	6	0	-12.095629	0.873564	-3.355011
3	6	0	-12.053854	1.845702	2.237764
4	6	0	-11.468697	3.052659	1.831436
5	6	0	-12.064365	3.884376	0.729024
6	6	0	-11.523847	3.493106	-0.616623
7	6	0	-12.048526	2.404305	-1.330996
8	6	0	-11.498329	1.995095	-2.553752
9	6	0	-12.269923	-1.190278	-1.886994
10	6	0	-12.520621	-3.208785	-0.377268
11	6	0	-11.864595	-2.835330	0.923201
12	6	0	-12.291481	-1.731824	1.676402
13	6	0	-11.650949	-1.368979	2.870029
14	6	0	-11.518768	1.087767	3.291029
15	6	0	-12.133739	-0.217729	3.708085
16	6	0	-10.386663	2.713040	-3.039280
17	6	0	-10.462300	4.210869	-1.198627
18	6	0	-9.863626	3.834833	-2.401703
19	6	0	-10.849826	-3.095740	-2.279908
20	6	0	-10.592051	-1.143868	-3.606536
21	6	0	-10.180291	-2.442048	-3.314853
22	6	0	-10.311217	3.480252	2.514532
23	6	0	-10.389683	1.598327	3.958793
24	6	0	-9.752964	2.781815	3.582007
25	6	0	-10.550720	-2.146835	3.283894
26	6	0	-10.789098	-3.595759	1.423746
27	6	0	-10.096974	-3.265237	2.587901
28	1	0	-8.859867	3.149831	4.105916
29	1	0	-12.943662	1.483667	1.721576
30	1	0	-11.841684	4.967678	0.921524
31	1	0	-13.173438	3.818138	0.742049
32	1	0	-12.896619	1.856879	-0.918231
33	1	0	-9.016481	4.391698	-2.826129
34	1	0	-9.368676	-2.928169	-3.874841
35	1	0	-13.079724	-0.710044	-1.336559
36	1	0	-13.138531	-1.141977	1.325074
37	1	0	-9.243978	-3.859641	2.944433
38	1	0	-13.243019	-0.153746	3.681256
39	1	0	-11.887188	-0.417078	4.785315
40	1	0	-13.612108	-3.007282	-0.345244
41	1	0	-12.438656	-4.316924	-0.533800
42	1	0	-11.835798	1.021555	-4.438315
43	1	0	-13.206523	0.934297	-3.325052
44	8	0	-9.976214	-0.448436	-4.681736
45	8	0	-9.813254	2.299883	-4.271623
46	8	0	-10.494894	-4.797920	0.742664
47	8	0	-10.557695	-4.454874	-2.015648
48	8	0	-9.967743	-1.822483	4.531002
49	8	0	-9.933588	0.901283	5.107491
50	8	0	-10.018594	5.387686	-0.540032
51	8	0	-9.783954	4.742289	2.158389
52	6	0	-8.686928	1.521317	-4.085954
53	6	0	-8.769754	0.111644	-4.310168
54	7	0	-7.684451	-0.712053	-4.193752
55	7	0	-7.518987	2.136450	-3.725729
56	6	0	-6.547466	-0.094554	-3.853894
57	6	0	-6.464662	1.318630	-3.616389
58	6	0	-5.182646	-0.713501	-3.608501
59	6	0	-5.040125	1.657736	-3.206031
60	7	0	-4.364921	0.400492	-3.237392
61	8	0	-4.804610	-1.848981	-3.667318
62	1	0	-3.339044	0.298252	-3.056422
63	8	0	-4.529466	2.697940	-2.895273
64	6	0	-9.344020	-4.647353	-1.380274
65	6	0	-9.308117	-4.790839	0.040302
66	6	0	-11.875384	-2.488788	-1.528609
67	7	0	-8.146401	-5.010382	0.726533
68	7	0	-8.224329	-4.764340	-2.155679
69	6	0	-8.748064	0.230258	4.860694
70	6	0	-8.773210	-1.141631	4.459833
71	6	0	-8.767816	5.196322	0.026349
72	6	0	-8.654152	4.728518	1.373360
73	7	0	-7.639627	-1.816854	4.098434
74	7	0	-7.582730	0.920981	5.033373
75	7	0	-7.677422	5.473514	-0.746590
76	7	0	-7.451078	4.377122	1.921757
77	6	0	-7.097456	-5.008178	-1.475098
78	6	0	-6.392940	4.594169	1.128604

79	6	0	-7.056790	-5.111399	-0.043514
80	6	0	-6.476948	0.228925	4.736472
81	6	0	-6.507993	-1.112064	4.224318
82	6	0	-6.502066	5.196957	-0.169877
83	6	0	-5.111289	5.378980	-0.755562
84	6	0	-4.930471	4.251824	1.375083
85	6	0	-5.686087	-5.175254	-2.020617
86	6	0	-5.613755	-5.305582	0.397016
87	6	0	-5.034647	0.702585	4.804729
88	6	0	-5.089573	-1.520034	3.851448
89	7	0	-4.258403	4.760090	0.227933
90	7	0	-4.299690	-0.401165	4.245614
91	7	0	-4.885820	-5.313490	-0.836309
92	8	0	-4.399949	3.656271	2.272929
93	8	0	-4.726849	5.906868	-1.752776
94	8	0	-4.542054	1.707083	5.218437
95	8	0	-4.664070	-2.513384	3.331729
96	8	0	-5.262685	-5.209216	-3.136269
97	8	0	-5.124208	-5.418062	1.481617
98	1	0	-3.850309	-5.364305	-0.859883
99	1	0	-3.281250	-0.338851	4.050076
100	1	0	-3.229534	4.658830	0.088401
101	1	0	12.820773	-3.792106	-0.298836
102	6	0	11.709142	-3.778040	-0.338071
103	6	0	11.146584	-3.401615	1.003031
104	6	0	11.240736	-2.891377	-1.457687
105	1	0	11.422324	-4.839709	-0.569423
106	6	0	11.742818	-2.418881	1.805194
107	6	0	10.007336	-4.056448	1.514441
108	6	0	11.886710	-1.685641	-1.765031
109	6	0	10.158810	-3.276656	-2.274899
110	6	0	11.220209	-2.074968	3.063384
111	1	0	12.625275	-1.894273	1.436778
112	6	0	9.483600	-3.796442	2.777564
113	8	0	9.418624	-5.074761	0.722905
114	6	0	11.480339	-0.888039	-2.846273
115	1	0	12.723741	-1.357205	-1.147909
116	6	0	9.726652	-2.533890	-3.371952
117	8	0	9.545518	-4.525718	-2.000592
118	6	0	11.819369	-0.960404	3.874122
119	6	0	10.113092	-2.805664	3.533754
120	1	0	8.609834	-4.344708	3.158353
121	6	0	8.276541	-4.658000	0.065864
122	6	0	12.167389	0.409771	-3.162754
123	6	0	10.414686	-1.350554	-3.642391
124	1	0	8.891077	-2.872400	-4.001019
125	6	0	8.340547	-4.395232	-1.337015
126	1	0	12.929164	-1.005293	3.838671
127	1	0	11.563151	-1.109900	4.957038
128	6	0	11.328233	0.392890	3.435458
129	8	0	9.633675	-2.545623	4.846918
130	7	0	7.109053	-4.569342	0.774638
131	6	0	11.635785	1.548041	-2.337697
132	1	0	12.030856	0.647151	-4.251896
133	1	0	13.266934	0.312012	-3.033242
134	8	0	10.091482	-0.611183	-4.808961
135	7	0	7.235085	-4.061921	-2.069933
136	6	0	12.001537	1.154806	2.469389
137	6	0	10.174018	0.955493	4.018088
138	6	0	8.421344	-1.871897	4.786559
139	6	0	6.034489	-4.244658	0.045491
140	6	0	12.167022	1.857411	-1.078736
141	6	0	10.594778	2.364073	-2.826594
142	6	0	8.906157	0.092180	-4.672521
143	6	0	6.097379	-4.004330	-1.368963
144	6	0	11.550050	2.430756	2.097689
145	1	0	12.895070	0.747468	1.995607
146	6	0	9.690524	2.222785	3.703147
147	8	0	9.564078	0.216494	5.055677
148	6	0	8.406111	-0.443309	4.721691
149	7	0	7.275896	-2.613395	4.771240
150	6	0	4.600127	-4.027456	0.507137
151	6	0	11.689045	2.941615	-0.325836
152	1	0	12.968255	1.239920	-0.671264
153	6	0	10.096075	3.463315	-2.132907
154	8	0	10.133491	2.094732	-4.134695
155	6	0	8.921613	1.446370	-4.216100
156	7	0	7.750002	-0.544484	-5.025458
157	6	0	4.707184	-3.640756	-1.864578
158	6	0	12.243258	3.242992	1.038906
159	6	0	10.413543	2.943524	2.754125
160	1	0	8.791357	2.633912	4.182911
161	7	0	7.271059	0.262187	4.431380
162	6	0	6.157692	-1.901762	4.582453
163	7	0	3.899378	-3.686064	-0.687462
164	8	0	4.100157	-4.088469	1.596018
165	6	0	10.674963	3.737665	-0.892723
166	1	0	9.291694	4.088675	-2.546119
167	7	0	7.772725	2.144612	-3.959498
168	6	0	6.637849	0.175927	-4.841294
169	8	0	4.313797	-3.341598	-2.957048
170	1	0	12.114625	4.335355	1.262026
171	1	0	13.340996	3.076687	1.064867
172	8	0	10.081464	4.291207	2.490885
173	6	0	6.165966	-0.487955	4.329800
174	6	0	4.727047	-2.408890	4.508421
175	1	0	2.869863	-3.483600	-0.710738
176	8	0	10.298042	4.913797	-0.201011
177	6	0	6.644213	1.487583	-4.253685
178	6	0	5.202023	-0.233809	-5.127311
179	6	0	8.929668	4.470945	1.754093
180	6	0	4.763897	-0.066491	3.914671
181	7	0	3.991170	-1.250079	4.062058
182	8	0	4.236936	-3.462433	4.772726
183	6	0	9.044012	4.828358	0.376156
184	6	0	5.202882	1.915399	-4.019506
185	7	0	4.433661	0.851911	-4.577055
186	8	0	4.737319	-1.185715	-5.675021
187	7	0	7.723739	4.383294	2.391673
188	8	0	4.347354	0.986022	3.510913

189	1	0	2.981825	-1.298176	3.803568
190	7	0	7.958952	5.151602	-0.389273
191	8	0	4.737335	2.878079	-3.474310
192	1	0	3.390395	0.843868	-4.551405
193	6	0	6.668307	4.688461	1.627226
194	6	0	6.785975	5.086960	0.252624
195	6	0	5.195821	4.645718	2.003819
196	6	0	5.395897	5.352121	-0.305239
197	7	0	4.529984	5.038140	0.798513
198	8	0	4.645168	4.357171	3.025481
199	8	0	5.022227	5.735440	-1.371865
200	1	0	3.498034	5.045908	0.719939
201	8	0	1.999830	3.800698	0.800209
202	6	0	1.357872	3.539871	1.819476
203	7	0	0.095345	4.089537	2.154891
204	7	0	1.793512	2.702855	2.853729
205	6	0	-0.451902	3.438556	3.377945
206	1	0	-0.564817	4.341852	1.389380
207	6	0	0.751078	2.511697	3.889736
208	1	0	2.754596	2.371209	2.974060
209	1	0	-0.777952	4.223703	4.102894
210	7	0	-1.534267	2.470202	3.099395
211	1	0	1.130574	2.761226	4.910243
212	7	0	0.170481	1.143896	3.892238
213	6	0	-1.122615	1.145724	3.303427
214	1	0	-2.474417	2.753048	2.810834
215	1	0	0.790591	0.326208	3.728116
216	8	0	-1.800907	0.146972	3.087060
217	1	0	1.078946	5.241788	-3.378792
218	6	0	0.710502	4.278020	-2.949063
219	6	0	-0.636003	3.720553	-3.618031
220	7	0	0.338048	4.487581	-1.524130
221	7	0	1.678237	3.179112	-3.159864
222	1	0	-1.029651	4.344999	-4.458119
223	7	0	-0.246188	2.383422	-4.141329
224	7	0	-1.592299	3.692831	-2.491244
225	6	0	-0.980979	4.024647	-1.273781
226	1	0	1.062011	4.389144	-0.789972
227	6	0	1.080877	2.060721	-3.767227
228	1	0	2.685757	3.280705	-3.008921
229	1	0	-0.953713	1.624817	-4.198899
230	1	0	-2.549348	3.343829	-2.581389
231	8	0	-1.540808	4.049914	-0.178647
232	8	0	1.654459	1.003546	-4.012442
233	6	0	-1.217810	-1.157480	-3.992614
234	7	0	0.081267	-1.382671	-4.496095
235	7	0	-1.850313	-2.390627	-3.775932
236	8	0	-1.738663	-0.053597	-3.832841
237	6	0	0.445258	-2.820733	-4.405995
238	1	0	0.810226	-0.648602	-4.414124
239	6	0	-0.925298	-3.533349	-3.972630
240	1	0	-2.851330	-2.502773	-3.591724
241	1	0	0.866268	-3.164368	-5.382654
242	7	0	1.357059	-3.139732	-3.287139
243	1	0	-1.328958	-4.263646	-4.715351
244	7	0	-0.575905	-4.239751	-2.714861
245	6	0	0.717855	-3.860649	-2.268401
246	1	0	2.321239	-2.796098	-3.232326
247	1	0	-1.315436	-4.446391	-2.018583
248	8	0	1.232397	-4.200922	-1.206508
249	1	0	0.376283	-5.542534	2.927564
250	6	0	0.072667	-4.613871	2.384843
251	6	0	-1.185659	-3.851035	3.019433
252	7	0	-0.380591	-4.969652	1.013037
253	7	0	1.144357	-3.593964	2.423066
254	1	0	-1.607693	-4.330650	3.936262
255	7	0	-0.649541	-2.506834	3.369946
256	7	0	-2.165195	-3.824984	1.911608
257	6	0	-1.650898	-4.397214	0.739135
258	1	0	0.322326	-5.015772	0.247516
259	6	0	0.684564	-2.361802	2.905246
260	1	0	2.108584	-3.783125	2.133686
261	1	0	-1.279780	-1.683787	3.329542
262	1	0	-3.140245	-3.546532	2.049199
263	8	0	-2.233320	-4.445415	-0.341302
264	8	0	1.359330	-1.339396	3.003865
265	6	0	-4.476125	0.755258	0.392570
266	6	0	-3.136749	0.922416	0.046206
267	6	0	-2.399997	-0.171283	-0.424322
268	6	0	-3.005535	-1.429237	-0.526885
269	6	0	-4.346752	-1.577084	-0.183244
270	6	0	-5.094113	-0.498602	0.306653
271	1	0	-5.032940	1.595312	0.791970
272	1	0	-2.647291	1.886634	0.136108
273	1	0	-2.429963	-2.280445	-0.871275
274	1	0	-4.804298	-2.557941	-0.250119
275	6	0	-6.545753	-0.677657	0.669513
276	6	0	-7.464208	-0.584624	-0.551108
277	1	0	-6.831397	0.082326	1.399377
278	1	0	-6.678953	-1.648758	1.155169
279	1	0	-8.507256	-0.722325	-0.265469
280	1	0	-7.364796	0.390430	-1.024648
281	1	0	-7.206269	-1.349860	-1.283127
282	8	0	-0.450362	1.153936	-0.769431
283	6	0	6.510137	0.952907	0.422469
284	6	0	5.117879	0.914899	0.388711
285	6	0	4.464890	0.191290	-0.618206
286	6	0	5.215629	-0.503529	-1.568124
287	6	0	6.606877	-0.459811	-1.524152
288	6	0	7.273973	0.287368	-0.544964
289	1	0	7.006535	1.513897	1.208211
290	1	0	4.544874	1.413681	1.166553
291	1	0	4.695467	-1.059491	-2.338298
292	1	0	7.183823	-1.000791	-2.266407
293	6	0	8.777062	0.344014	-0.493195
294	6	0	9.342742	-0.424397	0.698749
295	1	0	9.099282	1.387217	-0.437101
296	1	0	9.189860	-0.060187	-1.419628
297	1	0	10.431973	-0.370286	0.711827
298	1	0	8.973771	-0.009866	1.636369

299	1	0	9.050920	-1.472121	0.653572
300	8	0	2.380399	-0.866510	-1.116776
301	1	0	2.864914	2.139050	-0.170152
302	1	0	1.336899	1.354339	-0.500900
303	1	0	0.698432	-0.925196	-1.014373
304	7	0	2.349439	1.302538	-0.401817
305	6	0	2.976326	0.166760	-0.725682
306	6	0	-0.955479	0.027946	-0.709591
307	8	0	-0.278797	-1.106414	-0.880323

AC-cis, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.674691	-0.792294	-2.767594
2	6	0	-12.150297	0.526910	-3.304497
3	6	0	-11.992484	2.015746	2.181067
4	6	0	-11.420690	3.180948	1.651868
5	6	0	-12.038088	3.899786	0.483949
6	6	0	-11.520508	3.380665	-0.827282
7	6	0	-12.059934	2.232641	-1.428377
8	6	0	-11.535787	1.714484	-2.620805
9	6	0	-12.263378	-1.386578	-1.643043
10	6	0	-12.453627	-3.251403	0.059840
11	6	0	-11.769821	-2.743600	1.299246
12	6	0	-12.203336	-1.587362	1.962927
13	6	0	-11.551445	-1.115545	3.111841
14	6	0	-11.434868	1.364187	3.291582
15	6	0	-12.036077	0.103773	3.845329
16	6	0	-10.433398	2.380597	-3.193444
17	6	0	-10.468933	4.037378	-1.493659
18	6	0	-9.893059	3.551547	-2.668391
19	6	0	-10.856023	-3.322051	-1.906878
20	6	0	-10.644131	-1.501208	-3.416553
21	6	0	-10.222091	-2.767920	-3.019957
22	6	0	-10.256187	3.677342	2.273121
23	6	0	-10.292719	1.935648	3.884501
24	6	0	-9.670142	3.081325	3.387534
25	6	0	-10.436332	-1.840038	3.578895
26	6	0	-10.665708	-3.433405	1.839139
27	6	0	-9.964998	-2.998308	2.962535
28	1	0	-8.768789	3.499334	3.857043
29	1	0	-12.889533	1.603530	1.717907
30	1	0	-11.816154	4.997184	0.565816
31	1	0	-13.146536	3.833111	0.523163
32	1	0	-12.900091	1.727185	-0.950970
33	1	0	-9.054299	4.065797	-3.158169
34	1	0	-9.432309	-3.306556	-3.562301
35	1	0	-13.054269	-0.855597	-1.111985
36	1	0	-13.066095	-1.042785	1.578162
37	1	0	-9.095399	-3.546171	3.352187
38	1	0	-13.145812	0.157282	3.828263
39	1	0	-11.772966	0.011354	4.932930
40	1	0	-13.546769	-3.059789	0.102704
41	1	0	-12.361304	-4.368865	0.013498
42	1	0	-11.921007	0.578561	-4.403370
43	1	0	-13.260188	0.585672	-3.249304
44	8	0	-10.073333	-0.913033	-4.575713
45	8	0	-9.907174	1.865218	-4.406566
46	8	0	-10.359830	-4.680847	1.251183
47	8	0	-10.550602	-4.652378	-1.527607
48	8	0	-9.866125	-1.421559	4.802387
49	8	0	-9.825692	1.353245	5.088662
50	8	0	-10.018984	5.271489	-0.956248
51	8	0	-9.751046	4.908388	1.795039
52	6	0	-8.768616	1.106306	-4.220834
53	6	0	-8.853015	-0.317643	-4.323111
54	7	0	-7.751760	-1.123074	-4.229379
55	7	0	-7.582800	1.753943	-4.003849
56	6	0	-6.596785	-0.474237	-4.041348
57	6	0	-6.512434	0.954211	-3.921376
58	6	0	-5.203630	-1.061172	-3.890911
59	6	0	-5.060144	1.335950	-3.674326
60	7	0	-4.370690	0.084832	-3.698080
61	8	0	-4.810171	-2.193499	-3.899883
62	1	0	-3.331785	0.004209	-3.579185
63	8	0	-4.535940	2.396033	-3.477451
64	6	0	-9.311014	-4.767931	-0.923401
65	6	0	-9.205906	-4.713931	0.500919
66	6	0	-11.852803	-2.645442	-1.177524
67	7	0	-8.005456	-4.791309	1.150295
68	7	0	-8.228949	-4.986387	-1.728677
69	6	0	-8.641757	0.657335	4.923373
70	6	0	-8.665085	-0.753649	4.698978
71	6	0	-8.761781	5.140653	-0.388831
72	6	0	-8.629977	4.830371	1.001100
73	7	0	-7.524577	-1.479415	4.488609
74	7	0	-7.476035	1.360929	5.036405
75	7	0	-7.682347	5.325389	-1.203999
76	7	0	-7.417520	4.560732	1.574247
77	6	0	-7.065533	-5.108618	-1.077791
78	6	0	-6.370402	4.690136	0.748781
79	6	0	-6.951303	-4.976586	0.347078
80	6	0	-6.366890	0.630323	4.877530
81	6	0	-6.390706	-0.771521	4.565936
82	6	0	-6.498796	5.123644	-0.613704
83	6	0	-5.117162	5.228589	-1.237402
84	6	0	-4.903237	4.395644	1.022642
85	6	0	-5.682266	-5.347778	-1.663836
86	6	0	-5.482136	-5.049002	0.730083
87	6	0	-4.922864	1.102509	4.937951
88	6	0	-4.961262	-1.239601	4.328575
89	7	0	-4.250042	4.738265	-0.196170
90	7	0	-4.175422	-0.079590	4.605387
91	7	0	-4.818984	-5.272071	-0.516370
92	8	0	-4.357656	3.948598	1.993432
93	8	0	-4.747088	5.621256	-2.300395
94	8	0	-4.441706	2.161253	5.205225

95	8	0	-4.519172	-2.296306	3.977912
96	8	0	-5.313669	-5.561518	-2.778354
97	8	0	-4.934688	-4.929732	1.788001
98	1	0	-3.784318	-5.321381	-0.584744
99	1	0	-3.153340	-0.049571	4.438808
100	1	0	-3.222894	4.627582	-0.337340
101	1	0	12.790998	-3.819213	0.143474
102	6	0	11.680440	-3.805556	0.080185
103	6	0	11.092474	-3.313099	1.371964
104	6	0	11.239367	-3.018078	-1.121570
105	1	0	11.393648	-4.882505	-0.064271
106	6	0	11.677852	-2.269683	2.102081
107	6	0	9.937962	-3.916738	1.911313
108	6	0	11.892949	-1.840792	-1.512423
109	6	0	10.178063	-3.472484	-1.930116
110	6	0	11.131575	-1.821108	3.316537
111	1	0	12.570883	-1.781183	1.710392
112	6	0	9.389629	-3.551497	3.137237
113	8	0	9.358294	-4.991697	1.191040
114	6	0	11.513069	-1.135789	-2.665187
115	1	0	12.714852	-1.460967	-0.904482
116	6	0	9.773345	-2.823626	-3.095259
117	8	0	9.553020	-4.693789	-1.567881
118	6	0	11.720843	-0.646499	4.045489
119	6	0	10.010710	-2.505499	3.822711
120	1	0	8.503632	-4.061108	3.542553
121	6	0	8.237431	-4.620504	0.473899
122	6	0	12.208891	0.132169	-3.071167
123	6	0	10.466637	-1.664597	-3.445393
124	1	0	8.953254	-3.214590	-3.714264
125	6	0	8.333685	-4.498456	-0.946296
126	1	0	12.830899	-0.696427	4.033537
127	1	0	11.445105	-0.707522	5.132205
128	6	0	11.242278	0.667750	3.490011
129	8	0	9.509443	-2.138267	5.101276
130	7	0	7.059494	-4.436401	1.146427
131	6	0	11.662002	1.334238	-2.353527
132	1	0	12.096376	0.279970	-4.178740
133	1	0	13.305214	0.044996	-2.910361
134	8	0	10.168015	-1.023488	-4.675315
135	7	0	7.247230	-4.230272	-1.732286
136	6	0	11.932676	1.344559	2.474033
137	6	0	10.083008	1.280845	4.008083
138	6	0	8.302349	-1.465884	4.967985
139	6	0	6.005840	-4.166936	0.366416
140	6	0	12.168423	1.747997	-1.114497
141	6	0	10.631107	2.105521	-2.928753
142	6	0	8.980646	-0.312510	-4.619249
143	6	0	6.097843	-4.083035	-1.064189
144	6	0	11.492876	2.587267	1.992141
145	1	0	12.830483	0.895930	2.048094
146	6	0	9.610591	2.519809	3.582886
147	8	0	9.454838	0.631886	5.093997
148	6	0	8.296793	-0.046127	4.797658
149	7	0	7.152942	-2.201463	4.989072
150	6	0	4.572074	-3.857836	0.775332
151	6	0	11.674963	2.889702	-0.463479
152	1	0	12.962380	1.168595	-0.642060
153	6	0	10.116206	3.255938	-2.337360
154	8	0	10.198402	1.728086	-4.219957
155	6	0	8.988287	1.073977	-4.272599
156	7	0	7.830672	-0.976651	-4.940470
157	6	0	4.725103	-3.745603	-1.621579
158	6	0	12.205037	3.306622	0.880235
159	6	0	10.350016	3.156878	2.587673
160	1	0	8.707329	2.973007	4.014845
161	7	0	7.169261	0.642287	4.443934
162	6	0	6.041394	-1.500279	4.733789
163	7	0	3.900651	-3.627325	-0.461336
164	8	0	4.057713	-3.785884	1.856953
165	6	0	10.669588	3.632508	-1.112470
166	1	0	9.318723	3.842568	-2.815649
167	7	0	7.835247	1.788986	-4.092392
168	6	0	6.715475	-0.245312	-4.833436
169	8	0	4.355451	-3.568270	-2.748783
170	1	0	12.073380	4.413999	1.006987
171	1	0	13.302038	3.143993	0.939826
172	8	0	10.026435	4.478757	2.207736
173	6	0	6.061106	-0.107559	4.383374
174	6	0	4.608741	-2.004575	4.674644
175	1	0	2.883650	-3.377920	-0.525578
176	8	0	10.277778	4.859930	-0.526890
177	6	0	6.712074	1.108910	-4.352011
178	6	0	5.284508	-0.677869	-5.109432
179	6	0	8.884872	4.594990	1.442161
180	6	0	4.666304	0.291768	3.924934
181	7	0	3.884618	-0.874563	4.143439
182	8	0	4.109734	-3.036405	5.001049
183	6	0	9.016164	4.820796	0.038270
184	6	0	5.267552	1.552191	-4.174588
185	7	0	4.507307	0.445831	-4.656800
186	8	0	4.827960	-1.669350	-5.589915
187	7	0	7.671551	4.571936	2.071355
188	8	0	4.261278	1.316520	3.445046
189	1	0	2.877443	-0.932500	3.877327
190	7	0	7.940074	5.066493	-0.767886
191	8	0	4.793805	2.554745	-3.715723
192	1	0	3.464169	0.438960	-4.646274
193	6	0	6.625657	4.803673	1.269213
194	6	0	6.759455	5.063501	-0.136835
195	6	0	5.149164	4.803287	1.632892
196	6	0	5.375466	5.269918	-0.733833
197	7	0	4.497161	5.069737	0.385877
198	8	0	4.587448	4.625935	2.673373
199	8	0	5.014089	5.541881	-1.838437
200	1	0	3.465918	5.068500	0.295370
201	8	0	1.961713	3.839834	0.464503
202	6	0	1.297571	3.684647	1.491838
203	7	0	0.030875	4.269830	1.742229
204	7	0	1.710086	2.960085	2.615499

205	6	0	-0.538255	3.756183	3.020916
206	1	0	-0.615867	4.426261	0.941398
207	6	0	0.649040	2.882527	3.647897
208	1	0	2.662954	2.624602	2.780181
209	1	0	-0.867368	4.617733	3.651591
210	7	0	-1.622036	2.770765	2.829203
211	1	0	1.014656	3.238070	4.641774
212	7	0	0.058741	1.526034	3.789357
213	6	0	-1.229982	1.473376	3.187253
214	1	0	-2.562772	3.032375	2.521919
215	1	0	0.676906	0.695206	3.704823
216	8	0	-1.921048	0.467072	3.081210
217	1	0	1.172615	4.927566	-3.834056
218	6	0	0.779186	4.003070	-3.344286
219	6	0	-0.550483	3.407265	-4.013590
220	7	0	0.362648	4.324063	-1.953405
221	7	0	1.741768	2.882439	-3.436141
222	1	0	-0.915039	3.973407	-4.906354
223	7	0	-0.153167	2.035822	-4.429959
224	7	0	-1.540062	3.459067	-2.916098
225	6	0	-0.966088	3.885141	-1.709241
226	1	0	1.062735	4.277506	-1.190486
227	6	0	1.155510	1.728971	-3.985408
228	1	0	2.746307	2.991466	-3.270592
229	1	0	-0.865161	1.281275	-4.471783
230	1	0	-2.501525	3.128993	-3.018786
231	8	0	-1.554739	3.992939	-0.635611
232	8	0	1.724411	0.651052	-4.132509
233	6	0	-1.146418	-1.482370	-4.091015
234	7	0	0.158900	-1.753941	-4.554142
235	7	0	-1.789477	-2.688781	-3.775140
236	8	0	-1.662902	-0.366068	-4.036854
237	6	0	0.511687	-3.183361	-4.340562
238	1	0	0.891951	-1.020779	-4.500099
239	6	0	-0.865147	-3.846870	-3.852683
240	1	0	-2.798100	-2.783515	-3.628781
241	1	0	0.930305	-3.609775	-5.284975
242	7	0	1.417493	-3.407840	-3.196293
243	1	0	-1.263664	-4.645188	-4.524708
244	7	0	-0.528284	-4.429234	-2.529494
245	6	0	0.769287	-4.024822	-2.115490
246	1	0	2.398968	-3.113666	-3.188602
247	1	0	-1.271913	-4.551432	-1.817573
248	8	0	1.279176	-4.263738	-1.025794
249	1	0	0.375268	-5.212918	3.234268
250	6	0	0.063442	-4.327036	2.628401
251	6	0	-1.228986	-3.558631	3.182758
252	7	0	-0.346211	-4.776308	1.270281
253	7	0	1.108444	-3.281106	2.627795
254	1	0	-1.659514	-3.984150	4.122223
255	7	0	-0.737145	-2.178350	3.451745
256	7	0	-2.183224	-3.622660	2.052502
257	6	0	-1.624993	-4.266267	0.934552
258	1	0	0.374240	-4.867195	0.525556
259	6	0	0.605715	-2.031747	3.014388
260	1	0	2.082646	-3.462333	2.367874
261	1	0	-1.388835	-1.380274	3.328103
262	1	0	-3.190382	-3.492773	2.193972
263	8	0	-2.179363	-4.404644	-0.153238
264	8	0	1.259601	-0.992312	3.066134
265	6	0	-4.627346	0.832613	-0.333749
266	6	0	-3.242625	0.940428	-0.445558
267	6	0	-2.472633	-0.207489	-0.669248
268	6	0	-3.092250	-1.458897	-0.759974
269	6	0	-4.478317	-1.547828	-0.649978
270	6	0	-5.265749	-0.409980	-0.437002
271	1	0	-5.220163	1.722047	-0.155482
272	1	0	-2.743266	1.900781	-0.369060
273	1	0	-2.494084	-2.349332	-0.917665
274	1	0	-4.954548	-2.517961	-0.732734
275	6	0	-6.758353	-0.533093	-0.269551
276	6	0	-7.145082	-0.805558	1.185675
277	1	0	-7.129649	-1.340116	-0.904413
278	1	0	-7.240175	0.386502	-0.606616
279	1	0	-8.224751	-0.902469	1.298370
280	1	0	-6.680916	-1.727108	1.540951
281	1	0	-6.801661	0.008084	1.823078
282	8	0	-0.467943	1.063103	-0.854755
283	6	0	6.483779	0.970126	0.398509
284	6	0	5.091567	0.920750	0.377272
285	6	0	4.436826	0.125719	-0.572938
286	6	0	5.185733	-0.619792	-1.484888
287	6	0	6.577054	-0.564263	-1.453971
288	6	0	7.245840	0.246593	-0.527999
289	1	0	6.981415	1.586422	1.140854
290	1	0	4.518957	1.469466	1.121299
291	1	0	4.664300	-1.222606	-2.217883
292	1	0	7.152821	-1.145784	-2.165564
293	6	0	8.749081	0.313881	-0.489543
294	6	0	9.327485	-0.371299	0.746466
295	1	0	9.065745	1.360203	-0.504590
296	1	0	9.158305	-0.148272	-1.390093
297	1	0	10.416633	-0.312943	0.747104
298	1	0	8.964779	0.103338	1.657640
299	1	0	9.039582	-1.420743	0.773792
300	8	0	2.353930	-0.989558	-0.942895
301	1	0	2.832455	2.095965	-0.301530
302	1	0	1.304601	1.277223	-0.539545
303	1	0	0.655696	-1.038148	-0.895059
304	7	0	2.317627	1.238108	-0.437860
305	6	0	2.947118	0.080514	-0.660850
306	6	0	-0.999044	-0.049804	-0.789875
307	8	0	-0.330549	-1.201672	-0.825507

BB-trans, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-11.465634	-0.666469	-3.245602
2	6	0	-12.029491	0.668743	-3.641888
3	6	0	-12.156413	1.476403	1.963219
4	6	0	-11.684744	2.754371	1.627568
5	6	0	-12.316620	3.557993	0.524886
6	6	0	-11.697645	3.227211	-0.804432
7	6	0	-12.145740	2.142548	-1.574371
8	6	0	-11.531457	1.801336	-2.787786
9	6	0	-12.052567	-1.438256	-2.231178
10	6	0	-12.181668	-3.521941	-0.794116
11	6	0	-11.624096	-3.191725	0.561214
12	6	0	-12.103445	-2.105967	1.309806
13	6	0	-11.540454	-1.762590	2.547370
14	6	0	-11.553954	0.714978	2.974820
15	6	0	-12.083932	-0.632609	3.374889
16	6	0	-10.442294	2.590261	-3.208214
17	6	0	-10.635227	4.000859	-1.311470
18	6	0	-9.978521	3.698434	-2.503929
19	6	0	-10.403345	-3.160238	-2.563386
20	6	0	-10.346202	-1.204719	-3.908736
21	6	0	-9.785756	-2.440309	-3.583629
22	6	0	-10.596794	3.268150	2.361638
23	6	0	-10.451842	1.279238	3.646902
24	6	0	-9.950317	2.548523	3.366127
25	6	0	-10.467541	-2.547428	3.015219
26	6	0	-10.589849	-3.968176	1.117457
27	6	0	-9.983122	-3.662757	2.335422
28	1	0	-9.091928	2.964073	3.913341
29	1	0	-13.009344	1.064838	1.422740
30	1	0	-12.186124	4.652147	0.737691
31	1	0	-13.415926	3.403228	0.500476
32	1	0	-12.984972	1.546142	-1.215399
33	1	0	-9.133821	4.300729	-2.867926
34	1	0	-8.902908	-2.830070	-4.110314
35	1	0	-12.929601	-1.052326	-1.710199
36	1	0	-12.925568	-1.508458	0.914447
37	1	0	-9.161894	-4.269857	2.742204
38	1	0	-13.195921	-0.634749	3.341710
39	1	0	-11.834283	-0.816947	4.454803
40	1	0	-13.285638	-3.398556	-0.807407
41	1	0	-12.013872	-4.609728	-1.014133
42	1	0	-11.764757	0.874936	-4.713921
43	1	0	-13.141162	0.637970	-3.629591
44	8	0	-9.809030	-0.470104	-5.000282
45	8	0	-9.838194	2.259783	-4.449514
46	8	0	-10.201762	-5.138552	0.417469
47	8	0	-9.966936	-4.473293	-2.275701
48	8	0	-9.899985	-2.215903	4.273364
49	8	0	-9.892820	0.532480	4.716007
50	8	0	-10.287303	5.173792	-0.601251
51	8	0	-10.232181	4.611960	2.119298
52	6	0	-8.662251	1.555629	-4.295083
53	6	0	-8.635781	0.170078	-4.642333
54	7	0	-7.485104	-0.567185	-4.626149
55	7	0	-7.554078	2.214891	-3.836790
56	6	0	-6.403930	0.097697	-4.204802
57	6	0	-6.445648	1.467876	-3.777592
58	6	0	-5.001123	-0.439398	-3.993392
59	6	0	-5.086184	1.839517	-3.209290
60	7	0	-4.315128	0.648822	-3.358432
61	8	0	-4.500434	-1.491439	-4.265040
62	1	0	-3.330193	0.557385	-3.021794
63	8	0	-4.683322	2.860301	-2.725425
64	6	0	-8.823940	-4.576773	-1.513456
65	6	0	-8.948539	-5.008425	-0.155976
66	6	0	-11.537749	-2.691239	-1.869313
67	7	0	-7.867176	-5.339338	0.609606
68	7	0	-7.607146	-4.373396	-2.104649
69	6	0	-8.716320	-0.099881	4.369396
70	6	0	-8.717948	-1.510693	4.143700
71	6	0	-9.069559	5.084261	0.048650
72	6	0	-9.039617	4.773872	1.441868
73	7	0	-7.577766	-2.204786	3.843188
74	7	0	-7.575166	0.651123	4.299700
75	7	0	-7.937634	5.364553	-0.664937
76	7	0	-7.873670	4.717264	2.154126
77	6	0	-6.553306	-4.667730	-1.331149
78	6	0	-6.772525	4.991201	1.443980
79	6	0	-6.685003	-5.183877	0.002254
80	6	0	-6.467559	-0.041752	4.014625
81	6	0	-6.467074	-1.460194	3.788760
82	6	0	-6.804704	5.318958	0.046042
83	6	0	-5.379606	5.536884	-0.443194
84	6	0	-5.323742	4.977861	1.912702
85	6	0	-5.072022	-4.508282	-1.643578
86	6	0	-5.302924	-5.446789	0.577474
87	6	0	-5.053248	0.482441	3.838752
88	6	0	-5.047991	-1.897808	3.464217
89	7	0	-4.583310	5.269701	0.719993
90	7	0	-4.290503	-0.691805	3.535039
91	7	0	-4.422159	-4.977978	-0.459138
92	8	0	-4.839868	4.795437	2.989253
93	8	0	-4.945601	5.869554	-1.504940
94	8	0	-4.599946	1.588242	3.907907
95	8	0	-4.592018	-2.975320	3.195397
96	8	0	-4.498885	-4.091789	-2.608535
97	8	0	-4.942418	-5.933539	1.605045
98	1	0	-3.394950	-4.930968	-0.334879
99	1	0	-3.255627	-0.656105	3.386156
100	1	0	-3.548833	5.223374	0.686190
101	1	0	13.204145	-3.167854	-1.396495
102	6	0	12.097566	-3.267938	-1.381084
103	6	0	11.574548	-3.170036	0.023199
104	6	0	11.461335	-2.253265	-2.289981
105	1	0	11.899897	-4.298174	-1.781530
106	6	0	12.105581	-2.253165	0.943277
107	6	0	10.529129	-4.007477	0.456946
108	6	0	11.991245	-0.963435	-2.432832
109	6	0	10.326068	-2.583898	-3.058612
110	6	0	11.587351	-2.133629	2.240476

111	1	0	12.935236	-1.614334	0.639296
112	6	0	9.964577	-3.919909	1.729371
113	8	0	10.094183	-5.023520	-0.430263
114	6	0	11.428496	-0.032869	-3.319585
115	1	0	12.860517	-0.675624	-1.840739
116	6	0	9.742566	-1.707971	-3.971305
117	8	0	9.853232	-3.912835	-2.973904
118	6	0	12.172595	-1.174514	3.239507
119	6	0	10.508212	-2.970072	2.591080
120	1	0	9.133818	-4.569335	2.040207
121	6	0	8.840284	-4.759197	-0.954033
122	6	0	11.985165	1.355192	-3.459887
123	6	0	10.329355	-0.447919	-4.095237
124	1	0	8.871251	-2.002036	-4.573011
125	6	0	8.717665	-4.099400	-2.215816
126	1	0	13.279178	-1.138820	3.142218
127	1	0	11.991407	-1.565938	4.276385
128	6	0	11.585675	0.203437	3.120718
129	8	0	10.028295	-2.888687	3.920072
130	7	0	7.756288	-5.189364	-0.242498
131	6	0	11.430799	2.301179	-2.431328
132	1	0	11.749960	1.746680	-4.485893
133	1	0	13.095599	1.338102	-3.413854
134	8	0	9.859900	0.444651	-5.092754
135	7	0	7.502766	-3.755549	-2.742957
136	6	0	12.097425	1.144810	2.214203
137	6	0	10.508096	0.597649	3.936926
138	6	0	8.845631	-2.191683	4.053566
139	6	0	6.574435	-4.901163	-0.799039
140	6	0	12.009395	2.431800	-1.161711
141	6	0	10.321075	3.118546	-2.729106
142	6	0	8.646133	1.012492	-4.746154
143	6	0	6.448543	-4.152018	-2.017936
144	6	0	11.538416	2.424570	2.093109
145	1	0	12.948515	0.873217	1.588958
146	6	0	9.896529	1.848256	3.840556
147	8	0	10.092259	-0.303528	4.948978
148	6	0	8.877294	-0.896835	4.655084
149	7	0	7.675459	-2.795752	3.681333
150	6	0	5.186179	-5.239277	-0.276217
151	6	0	11.513967	3.346873	-0.219350
152	1	0	12.860166	1.803476	-0.896067
153	6	0	9.810658	4.066371	-1.845802
154	8	0	9.774197	3.021930	-4.030040
155	6	0	8.608587	2.289191	-4.107862
156	7	0	7.512201	0.317467	-5.059954
157	6	0	4.970004	-3.909100	-2.279025
158	6	0	12.109423	3.451959	1.155407
159	6	0	10.430786	2.734384	2.908684
160	1	0	9.041577	2.123843	4.473884
161	7	0	7.740870	-0.216655	4.991509
162	6	0	6.570553	-2.102418	3.981207
163	7	0	4.310932	-4.593001	-1.219492
164	8	0	4.820576	-5.887036	0.655934
165	6	0	10.439429	4.170257	-0.604514
166	1	0	8.956422	4.702311	-2.117588
167	7	0	7.443506	2.843201	-3.650073
168	6	0	6.375927	0.899752	-4.664103
169	8	0	4.415118	-3.281048	-3.140574
170	1	0	11.916871	4.477950	1.568301
171	1	0	13.216789	3.369953	1.111330
172	8	0	9.933024	4.056526	2.837469
173	6	0	6.603113	-0.840630	4.668515
174	6	0	5.122262	-2.441600	3.664704
175	1	0	3.270610	-4.599794	-1.117842
176	8	0	10.030739	5.189039	0.295272
177	6	0	6.344649	2.127267	-3.916615
178	6	0	4.956185	0.388931	-4.843589
179	6	0	8.761311	4.213455	2.132670
180	6	0	5.179089	-0.359086	4.892386
181	7	0	4.385740	-1.365399	4.243083
182	8	0	4.628059	-3.355142	3.064150
183	6	0	8.808825	4.898316	0.877154
184	6	0	4.908241	2.393676	-3.494981
185	7	0	4.168588	1.340586	-4.105999
186	8	0	4.510958	-0.543495	-5.439719
187	7	0	7.583502	3.803486	2.692855
188	8	0	4.735386	0.592958	5.459658
189	1	0	3.343533	-1.318416	4.201873
190	7	0	7.682239	5.306607	0.222364
191	8	0	4.429015	3.249763	-2.801391
192	1	0	3.138961	1.227409	-3.975522
193	6	0	6.487573	4.162932	2.010643
194	6	0	6.534278	4.955214	0.814858
195	6	0	5.039350	3.807534	2.296617
196	6	0	5.115960	5.237857	0.347992
197	7	0	4.306982	4.493129	1.284410
198	8	0	4.550647	3.088520	3.125343
199	8	0	4.677896	5.906961	-0.535514
200	1	0	3.274321	4.428395	1.206012
201	8	0	1.623814	3.478508	1.268513
202	6	0	1.033066	3.243099	2.327747
203	7	0	-0.276450	3.653385	2.650821
204	7	0	1.606434	2.598700	3.432709
205	6	0	-0.702948	3.086221	3.960491
206	1	0	-0.985982	3.802713	1.901956
207	6	0	0.624293	2.380343	4.521301
208	1	0	2.606337	2.398831	3.530012
209	1	0	-1.111144	3.903593	4.604621
210	7	0	-1.656218	1.964860	3.837639
211	1	0	0.995165	2.781951	5.495691
212	7	0	0.224649	0.959755	4.684853
213	6	0	-1.062712	0.730798	4.138621
214	1	0	-2.633513	2.088265	3.553289
215	1	0	0.936618	0.208560	4.650494
216	8	0	-1.605344	-0.366489	4.033874
217	1	0	0.818868	5.424479	-2.678967
218	6	0	0.425288	4.442143	-2.318671
219	6	0	-0.888760	3.931303	-3.079878
220	7	0	-0.011934	4.581097	-0.903045

221	7	0	1.397041	3.348967	-2.540991
222	1	0	-1.243234	4.607022	-3.896880
223	7	0	-0.475575	2.628057	-3.671327
224	7	0	-1.887869	3.815926	-1.998240
225	6	0	-1.351053	4.127141	-0.739878
226	1	0	0.677323	4.397651	-0.150288
227	6	0	0.831530	2.273648	-3.247368
228	1	0	2.395291	3.436853	-2.326819
229	1	0	-1.173768	1.872643	-3.778526
230	1	0	-2.876565	3.609135	-2.170491
231	8	0	-1.970785	4.109727	0.318021
232	8	0	1.413786	1.231129	-3.527561
233	6	0	-1.167414	-1.057938	-3.497827
234	7	0	0.084998	-1.306113	-4.091241
235	7	0	-1.813046	-2.287984	-3.206061
236	8	0	-1.639748	0.053183	-3.286418
237	6	0	0.384628	-2.759440	-4.154332
238	1	0	0.837379	-0.598458	-4.047655
239	6	0	-0.966140	-3.438692	-3.622623
240	1	0	-2.841466	-2.374813	-3.264294
241	1	0	0.671590	-3.035991	-5.199409
242	7	0	1.400760	-3.224663	-3.187588
243	1	0	-1.476146	-4.098070	-4.366390
244	7	0	-0.524890	-4.255468	-2.461520
245	6	0	0.840984	-3.994264	-2.158436
246	1	0	2.385404	-2.935576	-3.221146
247	1	0	-1.187805	-4.395778	-1.679056
248	8	0	1.449759	-4.463295	-1.201447
249	1	0	0.871372	-5.653970	3.031110
250	6	0	0.506398	-4.642561	2.726566
251	6	0	-0.784862	-4.119355	3.523690
252	7	0	0.045938	-4.676187	1.315440
253	7	0	1.517924	-3.597295	3.001028
254	1	0	-1.189624	-4.837427	4.278235
255	7	0	-0.308276	-2.890390	4.207905
256	7	0	-1.766408	-3.854383	2.445220
257	6	0	-1.231956	-4.103240	1.174890
258	1	0	0.718513	-4.708936	0.527071
259	6	0	0.992550	-2.540604	3.761054
260	1	0	2.490296	-3.655830	2.684748
261	1	0	-0.980591	-2.128374	4.419905
262	1	0	-2.737207	-3.578520	2.628318
263	8	0	-1.821099	-3.909507	0.107678
264	8	0	1.589967	-1.513540	4.066347
265	6	0	-5.223241	1.054780	0.443693
266	6	0	-3.831964	1.058596	0.355429
267	6	0	-3.111622	-0.140099	0.203252
268	6	0	-3.844902	-1.335945	0.140817
269	6	0	-5.237141	-1.340452	0.233661
270	6	0	-5.945983	-0.145138	0.396424
271	1	0	-5.755675	1.991180	0.572458
272	1	0	-3.286301	1.996555	0.412445
273	1	0	-3.328925	-2.293174	0.045134
274	1	0	-5.777186	-2.280026	0.201066
275	6	0	-7.451555	-0.145859	0.469923
276	6	0	-8.096938	0.048636	-0.903809
277	1	0	-7.782334	0.650460	1.140660
278	1	0	-7.792431	-1.089291	0.901450
279	1	0	-9.185049	0.029886	-0.832112
280	1	0	-7.798513	1.007231	-1.326082
281	1	0	-7.783463	-0.741365	-1.586006
282	8	0	-0.784599	-1.190620	-0.278457
283	8	0	-0.905218	1.033618	0.521491
284	1	0	0.065922	0.981175	0.418316
285	6	0	6.311988	0.998253	0.295763
286	6	0	4.927197	0.888960	0.412528
287	6	0	4.178762	0.104513	-0.481178
288	6	0	4.876187	-0.569122	-1.496120
289	6	0	6.260555	-0.455028	-1.619636
290	6	0	6.998862	0.333807	-0.728704
291	1	0	6.866673	1.600844	1.006449
292	1	0	4.427097	1.399408	1.232218
293	1	0	4.322620	-1.187772	-2.195225
294	1	0	6.774572	-0.988976	-2.413792
295	6	0	8.499374	0.437416	-0.830968
296	6	0	9.211228	-0.285273	0.313712
297	1	0	8.794950	1.490073	-0.833373
298	1	0	8.826157	0.016967	-1.784356
299	1	0	10.294682	-0.214600	0.207439
300	1	0	8.937857	0.148300	1.274835
301	1	0	8.936502	-1.339010	0.329462
302	8	0	1.842474	0.943980	0.238631
303	8	0	2.024059	-1.182278	-0.779821
304	1	0	1.057962	-1.177380	-0.638614
305	1	0	-1.329607	-1.936706	-0.575047
306	1	0	2.311466	1.774198	0.413041
307	5	0	2.623680	-0.046409	-0.342504
308	5	0	-1.541903	-0.102166	0.140259

BB-cis, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.454973	-1.168779	2.876867
2	6	0	11.943485	0.079149	3.556512
3	6	0	11.995554	2.106606	-1.734314
4	6	0	11.517877	3.286906	-1.142439
5	6	0	12.109935	3.819725	0.132310
6	6	0	11.481036	3.162217	1.329876
7	6	0	11.984870	1.965117	1.859250
8	6	0	11.383088	1.339662	2.961186
9	6	0	12.076676	-1.673023	1.725458
10	6	0	12.289318	-3.382147	-0.135535
11	6	0	11.648876	-2.776021	-1.353011
12	6	0	12.072499	-1.541408	-1.867011
13	6	0	11.445698	-0.952810	-2.975257
14	6	0	11.397913	1.568045	-2.882271
15	6	0	11.935651	0.340489	-3.561873

16	6	0	10.250535	1.958985	3.525159
17	6	0	10.358929	3.737743	1.959551
18	6	0	9.714561	3.154274	3.049060
19	6	0	10.587136	-3.565248	1.729418
20	6	0	10.374399	-1.900634	3.407722
21	6	0	9.920452	-3.100199	2.862295
22	6	0	10.450209	3.954665	-1.772821
23	6	0	10.290782	2.254500	-3.419878
24	6	0	9.806518	3.453700	-2.904442
25	6	0	10.366610	-1.647146	-3.557271
26	6	0	10.593263	-3.435848	-2.013009
27	6	0	9.924389	-2.890206	-3.107659
28	1	0	8.954169	3.974243	-3.363875
29	1	0	12.844260	1.591631	-1.283343
30	1	0	11.949021	4.928854	0.186847
31	1	0	13.212877	3.692190	0.142032
32	1	0	12.862227	1.507646	1.401034
33	1	0	8.830507	3.615092	3.512746
34	1	0	9.083295	-3.655190	3.309485
35	1	0	12.910430	-1.123825	1.286763
36	1	0	12.905206	-1.023743	-1.389552
37	1	0	9.087742	-3.412592	-3.593656
38	1	0	13.048304	0.362004	-3.561652
39	1	0	11.654211	0.375122	-4.649403
40	1	0	13.384075	-3.196211	-0.128143
41	1	0	12.189183	-4.499089	-0.175077
42	1	0	11.668879	0.034933	4.645029
43	1	0	13.055251	0.110428	3.550229
44	8	0	9.781306	-1.417965	4.602710
45	8	0	9.690074	1.365219	4.685138
46	8	0	10.276101	-4.743678	-1.578112
47	8	0	10.270998	-4.839770	1.204013
48	8	0	9.739038	-1.070493	-4.694320
49	8	0	9.678030	1.708631	-4.579384
50	8	0	9.955564	5.014338	1.507636
51	8	0	10.070200	5.218628	-1.259757
52	6	0	8.535397	0.656856	4.417046
53	6	0	8.582843	-0.769545	4.374855
54	7	0	7.468535	-1.532361	4.155573
55	7	0	7.372631	1.357163	4.242719
56	6	0	6.339156	-0.835694	3.990624
57	6	0	6.290299	0.600317	4.033959
58	6	0	4.948785	-1.360922	3.683051
59	6	0	4.864613	1.050092	3.755762
60	7	0	4.157950	-0.179901	3.556205
61	8	0	4.525783	-2.477592	3.563814
62	1	0	3.145015	-0.209931	3.297614
63	8	0	4.359451	2.133048	3.698528
64	6	0	9.071192	-4.893053	0.522014
65	6	0	9.073245	-4.840795	-0.905641
66	6	0	11.647043	-2.863902	1.121070
67	7	0	7.929517	-4.964204	-1.644422
68	7	0	7.926161	-5.077095	1.246009
69	6	0	8.537174	0.995303	-4.267094
70	6	0	8.561939	-0.430071	-4.351338
71	6	0	8.777534	5.034333	0.789963
72	6	0	8.838839	5.194550	-0.627868
73	7	0	7.453473	-1.196303	-4.115440
74	7	0	7.412856	1.687813	-3.907381
75	7	0	7.592615	4.992347	1.471113
76	7	0	7.721782	5.379845	-1.393478
77	6	0	6.815083	-5.207295	0.510753
78	6	0	6.570226	5.369363	-0.711391
79	6	0	6.816295	-5.147726	-0.924059
80	6	0	6.341205	0.925545	-3.664447
81	6	0	6.357368	-0.505804	-3.782320
82	6	0	6.505169	5.152011	0.706810
83	6	0	5.043907	5.103129	1.126998
84	6	0	5.156064	5.521278	-1.254503
85	6	0	5.383529	-5.382023	0.997089
86	6	0	5.384898	-5.272490	-1.424182
87	6	0	4.961886	1.360361	-3.199349
88	6	0	4.981181	-1.039084	-3.422347
89	7	0	4.332122	5.316148	-0.094342
90	7	0	4.235058	0.133699	-3.093510
91	7	0	4.615735	-5.363499	-0.215975
92	8	0	4.744732	5.774553	-2.345645
93	8	0	4.530597	4.926917	2.193952
94	8	0	4.512623	2.441768	-2.941659
95	8	0	4.548807	-2.156593	-3.390424
96	8	0	4.923640	-5.519819	2.090166
97	8	0	4.924078	-5.305906	-2.525636
98	1	0	3.582162	-5.355938	-0.218757
99	1	0	3.218135	0.109180	-2.857897
100	1	0	3.297395	5.265956	-0.138985
101	1	0	-13.251403	-3.422325	0.383588
102	6	0	-12.148860	-3.553875	0.417964
103	6	0	-11.530702	-3.219782	-0.909541
104	6	0	-11.547085	-2.735625	1.527221
105	1	0	-11.998272	-4.644143	0.638071
106	6	0	-11.955141	-2.106134	-1.652405
107	6	0	-10.495025	-4.010379	-1.441770
108	6	0	-12.079700	-1.494122	1.900310
109	6	0	-10.432565	-3.212847	2.247690
110	6	0	-11.331774	-1.743444	-2.854368
111	1	0	-12.780551	-1.500683	-1.276408
112	6	0	-9.831888	-3.687891	-2.626158
113	8	0	-10.140956	-5.203369	-0.758619
114	6	0	-11.532929	-0.749244	2.956774
115	1	0	-12.937554	-1.096317	1.357363
116	6	0	-9.859185	-2.523876	3.313232
117	8	0	-9.978878	-4.511788	1.927916
118	6	0	-11.815828	-0.586116	-3.681446
119	6	0	-10.255002	-2.540716	-3.291866
120	1	0	-9.006528	-4.302443	-3.012803
121	6	0	-8.902629	-5.077540	-0.146728
122	6	0	-12.100378	0.583529	3.354746
123	6	0	-10.443304	-1.303606	3.655164
124	1	0	-8.996498	-2.925784	3.862898
125	6	0	-8.817572	-4.589270	1.195052

126	1	0	-12.928338	-0.575762	-3.705259
127	1	0	-11.513200	-0.752119	-4.750961
128	6	0	-11.295610	0.749906	-3.232418
129	8	0	-9.594859	-2.172491	-4.495235
130	7	0	-7.799931	-5.445286	-0.863050
131	6	0	-11.533227	1.717073	2.546458
132	1	0	-11.888501	0.765131	4.442696
133	1	0	-13.209603	0.572979	3.283052
134	8	0	-9.985440	-0.613953	4.806101
135	7	0	-7.620146	-4.310284	1.793518
136	6	0	-11.938757	1.498962	-2.236371
137	6	0	-10.160837	1.319246	-3.843397
138	6	0	-8.426172	-1.480271	-4.233913
139	6	0	-6.634731	-5.240877	-0.235925
140	6	0	-12.085228	2.091570	1.313207
141	6	0	-10.441525	2.467620	3.027691
142	6	0	-8.774605	0.019320	4.589897
143	6	0	-6.545755	-4.620836	1.055672
144	6	0	-11.475023	2.767924	-1.856866
145	1	0	-12.817169	1.083745	-1.741234
146	6	0	-9.670965	2.583967	-3.524256
147	8	0	-9.532687	0.578681	-4.879701
148	6	0	-8.395056	-0.066690	-4.435281
149	7	0	-7.332640	-2.183033	-3.806122
150	6	0	-5.230696	-5.543582	-0.739042
151	6	0	-11.580780	3.178684	0.583548
152	1	0	-12.922632	1.521842	0.909290
153	6	0	-9.918836	3.572824	2.359614
154	8	0	-9.927026	2.123321	4.300453
155	6	0	-8.748624	1.407181	4.257659
156	7	0	-7.634730	-0.720415	4.740631
157	6	0	-5.078058	-4.391229	1.376823
158	6	0	-12.141611	3.551707	-0.760516
159	6	0	-10.356707	3.290179	-2.536828
160	1	0	-8.786904	3.002827	-4.026208
161	7	0	-7.267500	0.678076	-4.223707
162	6	0	-6.236548	-1.442950	-3.602441
163	7	0	-4.383977	-4.981181	0.284548
164	8	0	-4.836495	-6.122572	-1.703552
165	6	0	-10.521954	3.915146	1.149779
166	1	0	-9.077064	4.148192	2.771055
167	7	0	-7.584671	2.069305	3.974194
168	6	0	-6.501781	-0.050267	4.507566
169	8	0	-4.558004	-3.822575	2.299178
170	1	0	-11.989822	4.649143	-0.938754
171	1	0	-13.242790	3.410600	-0.784390
172	8	0	-9.989757	4.625949	-2.252165
173	6	0	-6.205111	-0.022908	-3.813715
174	6	0	-4.874478	-1.887599	-3.095445
175	1	0	-3.343240	-4.975873	0.217446
176	8	0	-10.130996	5.100153	0.482693
177	6	0	-6.478942	1.324892	4.088671
178	6	0	-5.075813	-0.572907	4.573061
179	6	0	-8.819844	4.754082	-1.529071
180	6	0	-4.823603	0.494749	-3.454193
181	7	0	-4.118137	-0.675168	-3.036995
182	8	0	-4.449630	-2.964773	-2.784069
183	6	0	-8.894120	5.013411	-0.126466
184	6	0	-5.040166	1.713157	3.790987
185	7	0	-4.293109	0.544324	4.120081
186	8	0	-4.621992	-1.620918	4.920112
187	7	0	-7.630767	4.707346	-2.202364
188	8	0	-4.364793	1.601185	-3.478081
189	1	0	-3.102625	-0.663234	-2.794581
190	7	0	-7.783971	5.248338	0.635837
191	8	0	-4.561458	2.732106	3.373893
192	1	0	-3.259938	0.485363	3.985982
193	6	0	-6.550988	4.935079	-1.444212
194	6	0	-6.627603	5.210190	-0.036577
195	6	0	-5.088055	4.901852	-1.858462
196	6	0	-5.219506	5.381490	0.513551
197	7	0	-4.385682	5.138136	-0.631874
198	8	0	-4.561966	4.732953	-2.918856
199	8	0	-4.814603	5.664715	1.599626
200	1	0	-3.356210	5.075272	-0.566266
201	8	0	-1.866850	3.754857	-0.688145
202	6	0	-1.271004	3.647674	-1.764647
203	7	0	0.005475	4.177101	-2.050577
204	7	0	-1.783127	3.026303	-2.908972
205	6	0	0.483256	3.727587	-3.385252
206	1	0	0.689659	4.363230	-1.289657
207	6	0	-0.789976	2.978356	-4.009232
208	1	0	-2.771237	2.783269	-3.045304
209	1	0	0.847199	4.606946	-3.971460
210	7	0	1.506737	2.662123	-3.328022
211	1	0	-1.188015	3.434720	-4.947936
212	7	0	-0.295093	1.605478	-4.290185
213	6	0	0.997897	1.418406	-3.733729
214	1	0	2.436159	2.800710	-2.919307
215	1	0	-0.960383	0.809546	-4.279867
216	8	0	1.615701	0.358238	-3.711561
217	1	0	-1.062518	4.947606	3.578079
218	6	0	-0.646713	4.074964	3.017045
219	6	0	0.703696	3.469876	3.631207
220	7	0	-0.251592	4.513737	1.651918
221	7	0	-1.576166	2.922860	3.012909
222	1	0	1.064067	3.980611	4.558218
223	7	0	0.340849	2.064358	3.962413
224	7	0	1.676449	3.599196	2.524231
225	6	0	1.093541	4.143114	1.370208
226	1	0	-0.956965	4.474030	0.894386
227	6	0	-0.967926	1.755317	3.516320
228	1	0	-2.593101	3.039592	2.918873
229	1	0	1.062670	1.326871	3.933548
230	1	0	2.686592	3.482359	2.661534
231	8	0	1.661527	4.343534	0.302071
232	8	0	-1.522540	0.667247	3.618892
233	6	0	0.932690	-1.673551	3.423170
234	7	0	-0.353826	-1.993813	3.896161
235	7	0	1.597481	-2.857945	3.015331

236	8	0	1.428291	-0.553364	3.400219
237	6	0	-0.655467	-3.438951	3.730282
238	1	0	-1.099919	-1.280544	3.900209
239	6	0	0.729412	-4.049534	3.200945
240	1	0	2.624170	-2.946964	3.065926
241	1	0	-1.013684	-3.857499	4.703802
242	7	0	-1.601120	-3.751635	2.638615
243	1	0	1.187981	-4.811655	3.876908
244	7	0	0.368937	-4.688415	1.908937
245	6	0	-0.974362	-4.381520	1.555770
246	1	0	-2.595668	-3.497526	2.662589
247	1	0	1.089824	-4.748497	1.166825
248	8	0	-1.515564	-4.712888	0.504742
249	1	0	-0.682361	-5.177884	-3.717976
250	6	0	-0.322611	-4.279394	-3.159794
251	6	0	0.939093	-3.535974	-3.813887
252	7	0	0.168210	-4.680541	-1.817289
253	7	0	-1.355489	-3.218358	-3.122943
254	1	0	1.356836	-4.032585	-4.723160
255	7	0	0.415118	-2.192956	-4.168380
256	7	0	1.924681	-3.506872	-2.704877
257	6	0	1.422732	-4.093844	-1.538374
258	1	0	-0.508539	-4.888010	-1.056653
259	6	0	-0.868565	-1.990782	-3.600277
260	1	0	-2.293223	-3.360377	-2.739651
261	1	0	1.065408	-1.386275	-4.236138
262	1	0	2.892076	-3.189312	-2.830632
263	8	0	2.004444	-4.135242	-0.451263
264	8	0	-1.492290	-0.934093	-3.608537
265	6	0	5.608527	0.694529	0.467756
266	6	0	4.227258	0.765175	0.293290
267	6	0	3.456060	-0.395982	0.109466
268	6	0	4.128088	-1.629370	0.103792
269	6	0	5.510289	-1.699830	0.275782
270	6	0	6.268833	-0.540892	0.477117
271	1	0	6.179880	1.603640	0.622678
272	1	0	3.726992	1.727093	0.301756
273	1	0	3.575319	-2.558385	-0.050735
274	1	0	6.004718	-2.664501	0.281732
275	6	0	7.765301	-0.622730	0.633056
276	6	0	8.484039	-0.618045	-0.717530
277	1	0	8.024337	-1.532216	1.181785
278	1	0	8.115177	0.220537	1.232000
279	1	0	9.565130	-0.689310	-0.587400
280	1	0	8.156241	-1.459865	-1.327870
281	1	0	8.265403	0.301370	-1.258115
282	8	0	1.051002	-1.364148	0.138836
283	8	0	1.362404	0.947278	-0.282538
284	1	0	0.388065	0.965085	-0.213905
285	6	0	-5.845295	1.513535	0.066163
286	6	0	-4.463764	1.363287	-0.047299
287	6	0	-3.819961	0.197100	0.399464
288	6	0	-4.614913	-0.805084	0.979723
289	6	0	-5.994787	-0.651105	1.104231
290	6	0	-6.630227	0.511692	0.650755
291	1	0	-6.320076	2.422431	-0.285693
292	1	0	-3.886524	2.164040	-0.509520
293	1	0	-4.138847	-1.710924	1.339159
294	1	0	-6.584254	-1.436428	1.567800
295	6	0	-8.127629	0.662423	0.722202
296	6	0	-8.798894	0.344969	-0.615829
297	1	0	-8.376987	1.683897	1.022475
298	1	0	-8.524132	-0.000643	1.493764
299	1	0	-9.881677	0.461652	-0.548626
300	1	0	-8.431889	1.011618	-1.395957
301	1	0	-8.583018	-0.679652	-0.913961
302	8	0	-1.400393	1.058006	0.092773
303	8	0	-1.772508	-1.271789	0.288952
304	1	0	-0.798183	-1.300297	0.235546
305	1	0	1.523676	-2.167059	0.408215
306	1	0	-1.833008	1.923088	0.178013
307	5	0	-2.270977	-0.009461	0.263825
308	5	0	1.895694	-0.270902	-0.017443

BC-trans, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.316042	1.013449	3.041908
2	6	0	-11.803284	-0.273368	3.646383
3	6	0	-11.969069	-1.825621	-1.804240
4	6	0	-11.398283	-2.996423	-1.285292
5	6	0	-11.984706	-3.696112	-0.089669
6	6	0	-11.398148	-3.192222	1.197865
7	6	0	-11.872117	-2.023250	1.813428
8	6	0	-11.271104	-1.504906	2.970035
9	6	0	-11.965790	1.623338	1.959124
10	6	0	-12.193628	3.481131	0.244561
11	6	0	-11.603598	2.966790	-1.039447
12	6	0	-12.081984	1.797392	-1.649453
13	6	0	-11.505657	1.293447	-2.824314
14	6	0	-11.450676	-1.201168	-2.949273
15	6	0	-12.046723	0.063675	-3.499068
16	6	0	-10.171362	-2.208062	3.501447
17	6	0	-10.340071	-3.880031	1.821617
18	6	0	-9.701343	-3.405510	2.967229
19	6	0	-10.436647	3.481426	2.066043
20	6	0	-10.200267	1.678252	3.588600
21	6	0	-9.742108	2.911975	3.133028
22	6	0	-10.269431	-3.522651	-1.947492
23	6	0	-10.354239	-1.810398	-3.588342
24	6	0	-9.729141	-2.958427	-3.100405
25	6	0	-10.415856	2.000207	-3.372939
26	6	0	-10.545047	3.649150	-1.670886
27	6	0	-9.919279	3.181930	-2.826493
28	1	0	-8.859883	-3.403190	-3.604816
29	1	0	-12.835469	-1.388743	-1.306901
30	1	0	-11.795830	-4.799237	-0.179488

31	1	0	-13.091506	-3.599410	-0.081947
32	1	0	-12.718647	-1.496313	1.371787
33	1	0	-8.860884	-3.945419	3.426572
34	1	0	-8.876773	3.410832	3.592260
35	1	0	-12.827277	1.130306	1.507863
36	1	0	-12.918447	1.264798	-1.195911
37	1	0	-9.075422	3.717198	-3.285060
38	1	0	-13.155546	0.036584	-3.427609
39	1	0	-11.834972	0.124738	-4.600297
40	1	0	-13.291518	3.316677	0.270201
41	1	0	-12.069906	4.595433	0.292759
42	1	0	-11.510852	-0.298815	4.731024
43	1	0	-12.915658	-0.295183	3.657111
44	8	0	-9.569998	1.074288	4.707437
45	8	0	-9.544475	-1.699599	4.670718
46	8	0	-10.179929	4.906202	-1.135893
47	8	0	-10.106123	4.788618	1.637850
48	8	0	-9.875891	1.524711	-4.591219
49	8	0	-9.924497	-1.251516	-4.819543
50	8	0	-9.941696	-5.125729	1.270999
51	8	0	-9.760547	-4.752875	-1.475543
52	6	0	-8.382685	-1.010543	4.371518
53	6	0	-8.403660	0.418689	4.370050
54	7	0	-7.294176	1.166442	4.088327
55	7	0	-7.243564	-1.725610	4.121202
56	6	0	-6.190534	0.452990	3.838801
57	6	0	-6.158815	-0.982245	3.867672
58	6	0	-4.814877	0.965015	3.457859
59	6	0	-4.746680	-1.442440	3.538837
60	7	0	-4.029774	-0.219806	3.325550
61	8	0	-4.410342	2.078349	3.263023
62	1	0	-3.004703	-0.188100	3.124487
63	8	0	-4.258053	-2.532365	3.451150
64	6	0	-8.920012	4.865518	0.932761
65	6	0	-8.957389	4.913710	-0.494018
66	6	0	-11.528185	2.850763	1.436751
67	7	0	-7.827953	5.045645	-1.253001
68	7	0	-7.753722	4.967917	1.638689
69	6	0	-8.716653	-0.588805	-4.681602
70	6	0	-8.695910	0.822017	-4.462601
71	6	0	-8.699340	-5.022826	0.662580
72	6	0	-8.608470	-4.692245	-0.725161
73	7	0	-7.536022	1.504029	-4.211001
74	7	0	-7.575011	-1.333739	-4.774172
75	7	0	-7.597200	-5.252990	1.434482
76	7	0	-7.410918	-4.434352	-1.335228
77	6	0	-6.656375	5.108943	0.885028
78	6	0	-6.338388	-4.607066	-0.550702
79	6	0	-6.692594	5.138147	-0.550622
80	6	0	-6.445761	-0.646089	-4.578074
81	6	0	-6.428686	0.752751	-4.248460
82	6	0	-6.430504	-5.071227	0.805323
83	6	0	-5.029335	-5.233800	1.373756
84	6	0	-4.870715	-4.345222	-0.866188
85	6	0	-5.210257	5.214173	1.344435
86	6	0	-5.270207	5.238947	-1.079080
87	6	0	-5.023037	-1.178169	-4.577656
88	6	0	-4.997014	1.148357	-3.920928
89	7	0	-4.185454	-4.747181	0.314451
90	7	0	-4.247791	-0.042385	-4.149630
91	7	0	-4.471694	5.245893	0.114523
92	8	0	-4.346397	-3.884048	-1.843066
93	8	0	-4.636853	-5.668653	2.412690
94	8	0	-4.566868	-2.241030	-4.867906
95	8	0	-4.529023	2.188709	-3.547362
96	8	0	-4.719379	5.277834	2.431639
97	8	0	-4.831959	5.309865	-2.187662
98	1	0	-3.440374	5.212986	0.084211
99	1	0	-3.233919	-0.124139	-3.931775
100	1	0	-3.149986	-4.656420	0.422404
101	1	0	13.297004	3.677059	0.063135
102	6	0	12.192970	3.773288	0.142184
103	6	0	11.530184	3.383180	-1.148153
104	6	0	11.668696	2.966897	1.298520
105	1	0	12.015640	4.863820	0.340160
106	6	0	11.967653	2.274099	-1.890404
107	6	0	10.438160	4.118588	-1.645775
108	6	0	12.252890	1.748200	1.669698
109	6	0	10.580266	3.430581	2.066038
110	6	0	11.304033	1.861800	-3.054144
111	1	0	12.836430	1.712771	-1.544752
112	6	0	9.731002	3.743017	-2.788572
113	8	0	10.076466	5.313488	-0.970662
114	6	0	11.780556	1.011142	2.766834
115	1	0	13.092788	1.361136	1.091688
116	6	0	10.080918	2.749348	3.173295
117	8	0	10.071862	4.709437	1.744455
118	6	0	11.798397	0.715003	-3.889281
119	6	0	10.171513	2.600983	-3.451425
120	1	0	8.861980	4.313509	-3.145304
121	6	0	8.875887	5.165746	-0.294152
122	6	0	12.403785	-0.299134	3.156138
123	6	0	10.712352	1.550838	3.508552
124	1	0	9.237794	3.141427	3.759241
125	6	0	8.873474	4.732093	1.069115
126	1	0	12.908687	0.748466	-3.960823
127	1	0	11.445025	0.856588	-4.946723
128	6	0	11.354484	-0.636517	-3.406797
129	8	0	9.474417	2.174113	-4.614479
130	7	0	7.727157	5.462871	-0.969839
131	6	0	11.836755	-1.456359	2.381798
132	1	0	12.241967	-0.474970	4.253458
133	1	0	13.508364	-0.256344	3.039206
134	8	0	10.326416	0.873148	4.693140
135	7	0	7.716274	4.448493	1.740388
136	6	0	12.059171	-1.334088	-2.415047
137	6	0	10.237002	-1.274253	-3.980954
138	6	0	8.359143	1.425795	-4.288762
139	6	0	6.601831	5.248743	-0.277109
140	6	0	12.360551	-1.841505	1.139617

141	6	0	10.773212	-2.217972	2.906263
142	6	0	9.123751	0.205262	4.546440
143	6	0	6.596513	4.691829	1.046004
144	6	0	11.673759	-2.620070	-2.006675
145	1	0	12.922615	-0.863136	-1.943955
146	6	0	9.831853	-2.562870	-3.640765
147	8	0	9.526770	-0.579290	-4.998175
148	6	0	8.381133	0.012426	-4.501762
149	7	0	7.264389	2.071350	-3.782621
150	6	0	5.167116	5.473138	-0.729083
151	6	0	11.853754	-2.948120	0.442002
152	1	0	13.179013	-1.266933	0.704912
153	6	0	10.241620	-3.335578	2.266149
154	8	0	10.313299	-1.869932	4.198860
155	6	0	9.118017	-1.185139	4.216331
156	7	0	7.973938	0.912890	4.758004
157	6	0	5.154842	4.432209	1.452323
158	6	0	12.395239	-3.343466	-0.903905
159	6	0	10.577626	-3.216698	-2.660308
160	1	0	8.965145	-3.039280	-4.121239
161	7	0	7.300501	-0.783553	-4.237925
162	6	0	6.218363	1.278716	-3.520538
163	7	0	4.391018	4.936346	0.361261
164	8	0	4.705188	5.979681	-1.704488
165	6	0	10.816081	-3.686952	1.044894
166	1	0	9.418905	-3.916291	2.706970
167	7	0	7.959353	-1.877291	3.993979
168	6	0	6.847777	0.211344	4.586128
169	8	0	4.692851	3.895650	2.422180
170	1	0	12.279880	-4.451108	-1.042954
171	1	0	13.489511	-3.163551	-0.960973
172	8	0	10.287027	-4.564852	-2.345829
173	6	0	6.232754	-0.137132	-3.755960
174	6	0	4.883377	1.654968	-2.901609
175	1	0	3.351535	4.887564	0.342040
176	8	0	10.438270	-4.892230	0.411517
177	6	0	6.841389	-1.162631	4.168969
178	6	0	5.411671	0.694143	4.719721
179	6	0	9.123656	-4.721893	-1.614103
180	6	0	4.901379	-0.720548	-3.311462
181	7	0	4.186490	0.412567	-2.807559
182	8	0	4.449809	2.709379	-2.526297
183	6	0	9.199172	-4.866766	-0.195601
184	6	0	5.401242	-1.593312	3.940316
185	7	0	4.640003	-0.440821	4.291952
186	8	0	4.947229	1.728955	5.090536
187	7	0	7.941961	-4.798854	-2.297038
188	8	0	4.481303	-1.841526	-3.323434
189	1	0	3.193547	0.354829	-2.493175
190	7	0	8.091466	-5.071945	0.579483
191	8	0	4.941185	-2.626345	3.540329
192	1	0	3.600912	-0.410971	4.196951
193	6	0	6.867652	-5.016914	-1.529325
194	6	0	6.941212	-5.144736	-0.100851
195	6	0	5.411090	-5.120228	-1.959324
196	6	0	5.533284	-5.324417	0.450429
197	7	0	4.706330	-5.263753	-0.718438
198	8	0	4.897747	-5.105690	-3.037673
199	8	0	5.132430	-5.481467	1.564575
200	1	0	3.669277	-5.267039	-0.666347
201	8	0	2.049861	-4.237584	-0.624937
202	6	0	1.363824	-4.009351	-1.618833
203	7	0	0.049197	-4.489357	-1.839235
204	7	0	1.795921	-3.314178	-2.758656
205	6	0	-0.520342	-3.925815	-3.089024
206	1	0	-0.574887	-4.667364	-1.027105
207	6	0	0.721637	-3.174727	-3.768966
208	1	0	2.757705	-3.009180	-2.924082
209	1	0	-0.962507	-4.748090	-3.704220
210	7	0	-1.502626	-2.836138	-2.877661
211	1	0	1.031987	-3.591065	-4.758380
212	7	0	0.239073	-1.780841	-3.947036
213	6	0	-1.013350	-1.596662	-3.298825
214	1	0	-2.410892	-2.985398	-2.428107
215	1	0	0.921385	-1.000993	-3.945059
216	8	0	-1.604728	-0.521013	-3.220421
217	1	0	1.489965	-4.981552	3.805630
218	6	0	1.046016	-4.120453	3.247731
219	6	0	-0.280248	-3.506457	3.908959
220	7	0	0.595635	-4.581107	1.908915
221	7	0	1.971575	-2.965510	3.206538
222	1	0	-0.605418	-4.010835	4.851800
223	7	0	0.092942	-2.097785	4.207538
224	7	0	-1.293249	-3.652643	2.842244
225	6	0	-0.749649	-4.199119	1.668515
226	1	0	1.269299	-4.596573	1.119093
227	6	0	1.368612	-1.789427	3.674099
228	1	0	2.964387	-3.050201	2.966623
229	1	0	-0.636028	-1.361246	4.223153
230	1	0	-2.273963	-3.391150	2.962226
231	8	0	-1.368689	-4.411762	0.630828
232	8	0	1.898738	-0.680561	3.695382
233	6	0	-0.838973	1.430851	3.675563
234	7	0	0.449869	1.755851	4.162370
235	7	0	-1.503082	2.613218	3.311582
236	8	0	-1.332952	0.307507	3.650166
237	6	0	0.759771	3.192261	3.940361
238	1	0	1.202841	1.043913	4.130068
239	6	0	-0.618438	3.794240	3.383693
240	1	0	-2.505266	2.675021	3.103713
241	1	0	1.119303	3.647517	4.895750
242	7	0	1.710048	3.440329	2.831618
243	1	0	-1.061157	4.608333	4.008638
244	7	0	-0.257045	4.338713	2.046015
245	6	0	1.083000	4.010232	1.715229
246	1	0	2.721364	3.295958	2.914562
247	1	0	-0.980256	4.357077	1.302961
248	8	0	1.626984	4.265478	0.642664
249	1	0	0.740783	4.942896	-3.517684
250	6	0	0.381701	4.044559	-2.959151

251	6	0	-0.861909	3.283791	-3.625867
252	7	0	-0.131156	4.451873	-1.623765
253	7	0	1.422467	2.994168	-2.892107
254	1	0	-1.253062	3.753955	-4.560271
255	7	0	-0.333002	1.927039	-3.927200
256	7	0	-1.875312	3.275678	-2.543217
257	6	0	-1.391160	3.862291	-1.369030
258	1	0	0.544054	4.607418	-0.847788
259	6	0	0.944269	1.750027	-3.331570
260	1	0	2.358219	3.155143	-2.511798
261	1	0	-0.988345	1.118509	-3.922005
262	1	0	-2.851517	2.998839	-2.703366
263	8	0	-1.988880	3.889810	-0.289817
264	8	0	1.566511	0.693664	-3.288004
265	6	0	-6.491569	-0.734272	-1.158624
266	6	0	-5.118036	-0.818305	-0.946201
267	6	0	-4.428671	0.183909	-0.244247
268	6	0	-5.167280	1.282487	0.223862
269	6	0	-6.544671	1.362584	0.022865
270	6	0	-7.224513	0.357439	-0.675678
271	1	0	-7.002353	-1.523168	-1.703301
272	1	0	-4.561620	-1.668810	-1.324761
273	1	0	-4.672764	2.076662	0.780735
274	1	0	-7.098255	2.213954	0.403600
275	6	0	-8.719972	0.407606	-0.826934
276	6	0	-9.433094	-0.239387	0.360002
277	1	0	-9.014508	-0.100858	-1.747329
278	1	0	-9.042269	1.447199	-0.921626
279	1	0	-10.515971	-0.196502	0.233521
280	1	0	-9.142020	-1.284096	0.459227
281	1	0	-9.177700	0.274678	1.285612
282	8	0	-2.071065	1.119464	0.273803
283	8	0	-2.356663	-1.219247	0.011943
284	1	0	-1.381875	-1.222219	0.109264
285	6	0	4.620319	-1.511635	0.477562
286	6	0	3.235606	-1.433820	0.354922
287	6	0	2.606378	-0.183843	0.373371
288	6	0	3.366735	0.980577	0.539959
289	6	0	4.751798	0.883173	0.663722
290	6	0	5.396545	-0.360076	0.655388
291	1	0	5.099748	-2.484398	0.482788
292	1	0	2.633860	-2.330123	0.239229
293	1	0	2.875179	1.945495	0.566036
294	1	0	5.336749	1.782701	0.817378
295	6	0	6.896190	-0.453245	0.770613
296	6	0	7.589619	-0.342875	-0.589094
297	1	0	7.162112	-1.404503	1.238969
298	1	0	7.258072	0.339693	1.428434
299	1	0	8.671549	-0.422890	-0.481718
300	1	0	7.251417	-1.137447	-1.253634
301	1	0	7.361511	0.615161	-1.053293
302	8	0	0.425933	-1.155446	0.229275
303	8	0	0.627952	1.101257	0.320570
304	1	0	-0.361939	1.060031	0.295202
305	6	0	1.122879	-0.138499	0.299423
306	1	0	-2.501955	1.979487	0.139366
307	5	0	-2.891338	0.023375	0.009379

BC-cis, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.406013	0.889290	3.025431
2	6	0	-11.924896	-0.410837	3.569753
3	6	0	-12.012145	-1.795604	-1.933286
4	6	0	-11.445438	-2.981620	-1.446333
5	6	0	-12.039888	-3.717733	-0.277364
6	6	0	-11.468326	-3.244101	1.028144
7	6	0	-11.957000	-2.093868	1.668051
8	6	0	-11.379316	-1.612215	2.850594
9	6	0	-12.023097	1.527841	1.939177
10	6	0	-12.234552	3.444716	0.293186
11	6	0	-11.675224	2.990338	-1.025364
12	6	0	-12.141867	1.831017	-1.665186
13	6	0	-11.558618	1.362697	-2.851287
14	6	0	-11.483035	-1.133191	-3.052269
15	6	0	-12.080374	0.146478	-3.565103
16	6	0	-10.280501	-2.322871	3.374398
17	6	0	-10.414060	-3.943081	1.645150
18	6	0	-9.790537	-3.497807	2.811466
19	6	0	-10.439077	3.332855	2.081938
20	6	0	-10.300343	1.528317	3.619399
21	6	0	-9.788206	2.743226	3.164408
22	6	0	-10.309099	-3.486196	-2.112703
23	6	0	-10.381145	-1.722582	-3.699844
24	6	0	-9.760793	-2.886325	-3.242998
25	6	0	-10.475802	2.097004	-3.377366
26	6	0	-10.645630	3.717254	-1.652609
27	6	0	-10.012386	3.284713	-2.817870
28	1	0	-8.885420	-3.313529	-3.752401
29	1	0	-12.883559	-1.375433	-1.430170
30	1	0	-11.843384	-4.816846	-0.394725
31	1	0	-13.147255	-3.627531	-0.277878
32	1	0	-12.797073	-1.556489	1.227145
33	1	0	-8.949935	-4.043172	3.263430
34	1	0	-8.919323	3.217821	3.641946
35	1	0	-12.887158	1.058261	1.467654
36	1	0	-12.968972	1.275483	-1.222235
37	1	0	-9.185731	3.848315	-3.272691
38	1	0	-13.189891	0.109451	-3.505183
39	1	0	-11.858784	0.242427	-4.662017
40	1	0	-13.333489	3.288376	0.332268
41	1	0	-12.099973	4.554360	0.394544
42	1	0	-11.660845	-0.483948	4.659218
43	1	0	-13.036790	-0.423695	3.550256
44	8	0	-9.746981	0.936046	4.783860
45	8	0	-9.699363	-1.841387	4.574588
46	8	0	-10.292596	4.968068	-1.088324

47	8	0	-10.052681	4.624887	1.659615
48	8	0	-9.894763	1.636737	-4.583603
49	8	0	-9.925099	-1.123362	-4.904237
50	8	0	-10.003543	-5.172341	1.066320
51	8	0	-9.796768	-4.725812	-1.669361
52	6	0	-8.534715	-1.130509	4.365077
53	6	0	-8.551943	0.288041	4.530714
54	7	0	-7.412903	1.042868	4.486516
55	7	0	-7.389455	-1.818437	4.066042
56	6	0	-6.294997	0.352070	4.238296
57	6	0	-6.286426	-1.064497	3.994333
58	6	0	-4.880433	0.883126	4.096833
59	6	0	-4.871537	-1.485472	3.625885
60	7	0	-4.120202	-0.274094	3.729829
61	8	0	-4.417428	1.978277	4.241411
62	1	0	-3.105614	-0.212681	3.498650
63	8	0	-4.405814	-2.543771	3.309588
64	6	0	-8.908603	4.681060	0.892364
65	6	0	-9.036741	4.942024	-0.506516
66	6	0	-11.556032	2.754207	1.444918
67	7	0	-7.960917	5.203192	-1.306554
68	7	0	-7.691090	4.586014	1.507661
69	6	0	-8.723834	-0.464310	-4.700526
70	6	0	-8.719762	0.935429	-4.414860
71	6	0	-8.756265	-5.045549	0.473209
72	6	0	-8.653922	-4.674610	-0.903507
73	7	0	-7.580088	1.601809	-4.054049
74	7	0	-7.576101	-1.200748	-4.774429
75	7	0	-7.660144	-5.288846	1.249939
76	7	0	-7.452662	-4.384144	-1.490872
77	6	0	-6.642044	4.809396	0.704991
78	6	0	-6.387207	-4.565965	-0.698699
79	6	0	-6.778087	5.150138	-0.683211
80	6	0	-6.461765	-0.522920	-4.479850
81	6	0	-6.469730	0.852737	-4.066608
82	6	0	-6.488521	-5.075178	0.640405
83	6	0	-5.091247	-5.242879	1.218027
84	6	0	-4.920112	-4.273529	-0.987503
85	6	0	-5.160440	4.719387	1.038365
86	6	0	-5.397178	5.361033	-1.283429
87	6	0	-5.038241	-1.050399	-4.435245
88	6	0	-5.060470	1.229708	-3.636353
89	7	0	-4.241874	-4.714366	0.183330
90	7	0	-4.297140	0.053547	-3.876509
91	7	0	-4.513510	5.075787	-0.184184
92	8	0	-4.390997	-3.759233	-1.934648
93	8	0	-4.705353	-5.708160	2.246054
94	8	0	-4.556692	-2.084303	-4.781316
95	8	0	-4.620559	2.254853	-3.188147
96	8	0	-4.588975	4.410732	2.045253
97	8	0	-5.040584	5.698828	-2.370729
98	1	0	-3.484894	5.033117	-0.292911
99	1	0	-3.287793	-0.036600	-3.627245
100	1	0	-3.205894	-4.630052	0.297422
101	1	0	13.229243	3.698978	0.238587
102	6	0	12.122624	3.784764	0.290705
103	6	0	11.496710	3.394747	-1.017758
104	6	0	11.578814	2.970628	1.432490
105	1	0	11.930533	4.873026	0.487886
106	6	0	11.961773	2.288828	-1.748459
107	6	0	10.416133	4.125582	-1.545974
108	6	0	12.164277	1.757628	1.819213
109	6	0	10.467968	3.424800	2.173294
110	6	0	11.335844	1.875056	-2.932132
111	1	0	12.822148	1.730961	-1.377103
112	6	0	9.747907	3.749855	-2.712102
113	8	0	10.019298	5.315170	-0.879841
114	6	0	11.673705	1.019257	2.907991
115	1	0	13.018736	1.375038	1.259937
116	6	0	9.955795	2.747458	3.276307
117	8	0	9.945305	4.691186	1.826636
118	6	0	11.857021	0.729369	-3.752563
119	6	0	10.214000	2.611521	-3.363283
120	1	0	8.887497	4.317063	-3.094101
121	6	0	8.801647	5.144574	-0.238978
122	6	0	12.289793	-0.292063	3.305221
123	6	0	10.591231	1.556206	3.630302
124	1	0	9.098529	3.135718	3.843866
125	6	0	8.767869	4.686272	1.116144
126	1	0	12.968906	0.764145	-3.790114
127	1	0	11.535896	0.871143	-4.820221
128	6	0	11.399849	-0.622925	-3.284606
129	8	0	9.554002	2.181802	-4.546699
130	7	0	7.667554	5.439332	-0.939527
131	6	0	11.738350	-1.445975	2.514328
132	1	0	12.105241	-0.472601	4.398138
133	1	0	13.396449	-0.248646	3.211147
134	8	0	10.184237	0.881232	4.809964
135	7	0	7.598504	4.355598	1.743212
136	6	0	12.076682	-1.320451	-2.273492
137	6	0	10.300012	-1.261709	-3.890745
138	6	0	8.431061	1.432178	-4.252046
139	6	0	6.526950	5.189665	-0.284028
140	6	0	12.292826	-1.832405	1.286062
141	6	0	10.657607	-2.203588	3.008812
142	6	0	8.980108	0.221148	4.634158
143	6	0	6.494990	4.590921	1.020320
144	6	0	11.680745	-2.606619	-1.876361
145	1	0	12.926880	-0.849480	-1.778813
146	6	0	9.883813	-2.549287	-3.559438
147	8	0	9.620262	-0.570364	-4.930816
148	6	0	8.459184	0.019840	-4.468933
149	7	0	7.323734	2.075590	-3.771088
150	6	0	5.100768	5.415755	-0.762204
151	6	0	11.800072	-2.936741	0.574752
152	1	0	13.124896	-1.261109	0.873370
153	6	0	10.138299	-3.318557	2.354357
154	8	0	10.164758	-1.853826	4.288324
155	6	0	8.974148	-1.161623	4.275119
156	7	0	7.830043	0.931847	4.833055

157	6	0	5.047545	4.292750	1.375303
158	6	0	12.374457	-3.331994	-0.757255
159	6	0	10.601315	-3.202477	-2.557942
160	1	0	9.030794	-3.025862	-4.063786
161	7	0	7.371092	-0.777071	-4.240864
162	6	0	6.271474	1.281757	-3.540799
163	7	0	4.303768	4.836446	0.291602
164	8	0	4.656353	5.949607	-1.731100
165	6	0	10.744563	-3.672701	1.149429
166	1	0	9.301958	-3.896007	2.773174
167	7	0	7.818468	-1.837276	3.993814
168	6	0	6.704747	0.243962	4.608862
169	8	0	4.570033	3.700252	2.305636
170	1	0	12.261399	-4.439402	-0.900037
171	1	0	13.469999	-3.153298	-0.787518
172	8	0	10.301491	-4.549807	-2.250137
173	6	0	6.290519	-0.132525	-3.785724
174	6	0	4.919791	1.656854	-2.959411
175	1	0	3.261804	4.807050	0.262294
176	8	0	10.382763	-4.878817	0.509011
177	6	0	6.701690	-1.116341	4.148506
178	6	0	5.268747	0.733578	4.713473
179	6	0	9.119911	-4.708400	-1.548913
180	6	0	4.943945	-0.715460	-3.390162
181	7	0	4.216325	0.416418	-2.899594
182	8	0	4.478802	2.709607	-2.587795
183	6	0	9.159472	-4.857504	-0.129354
184	6	0	5.267788	-1.524368	3.851629
185	7	0	4.503258	-0.378589	4.218492
186	8	0	4.799739	1.755940	5.111884
187	7	0	7.956522	-4.788348	-2.262080
188	8	0	4.518217	-1.833628	-3.427923
189	1	0	3.211750	0.361538	-2.627547
190	7	0	8.033764	-5.075079	0.615871
191	8	0	4.816481	-2.539427	3.399168
192	1	0	3.469635	-0.333745	4.085321
193	6	0	6.864564	-5.018608	-1.523322
194	6	0	6.902069	-5.155380	-0.094353
195	6	0	5.420935	-5.134268	-1.992628
196	6	0	5.482115	-5.358670	0.418435
197	7	0	4.685635	-5.297102	-0.772228
198	8	0	4.937514	-5.114938	-3.084505
199	8	0	5.055122	-5.534802	1.519570
200	1	0	3.648044	-5.309873	-0.749437
201	8	0	2.046803	-4.223903	-0.794438
202	6	0	1.361618	-3.979416	-1.784512
203	7	0	0.037366	-4.434240	-2.002473
204	7	0	1.803563	-3.295392	-2.927941
205	6	0	-0.524419	-3.863420	-3.251988
206	1	0	-0.589205	-4.610627	-1.192365
207	6	0	0.727686	-3.128746	-3.931222
208	1	0	2.765869	-2.990548	-3.087453
209	1	0	-0.976738	-4.679784	-3.867618
210	7	0	-1.493455	-2.761397	-3.041666
211	1	0	1.027169	-3.543782	-4.924661
212	7	0	0.266771	-1.726071	-4.100986
213	6	0	-0.985031	-1.527327	-3.456361
214	1	0	-2.407376	-2.901137	-2.602225
215	1	0	0.959874	-0.956040	-4.091944
216	8	0	-1.557945	-0.441489	-3.376385
217	1	0	1.456186	-4.895697	3.628340
218	6	0	0.993165	-4.046842	3.066724
219	6	0	-0.343704	-3.456387	3.728042
220	7	0	0.550318	-4.522667	1.731367
221	7	0	1.895137	-2.873809	3.018774
222	1	0	-0.657370	-3.963947	4.673165
223	7	0	0.004515	-2.040409	4.022061
224	7	0	-1.355763	-3.629451	2.664574
225	6	0	-0.803400	-4.171973	1.492340
226	1	0	1.224301	-4.532047	0.940982
227	6	0	1.273429	-1.708736	3.486143
228	1	0	2.884912	-2.938223	2.759880
229	1	0	-0.733971	-1.316751	4.047361
230	1	0	-2.335858	-3.362953	2.774716
231	8	0	-1.420012	-4.409447	0.458611
232	8	0	1.784014	-0.590429	3.505829
233	6	0	-0.955825	1.520367	3.580244
234	7	0	0.335728	1.852013	4.045213
235	7	0	-1.640134	2.696453	3.192292
236	8	0	-1.424069	0.388423	3.553859
237	6	0	0.620190	3.299571	3.869556
238	1	0	1.097541	1.151459	3.991339
239	6	0	-0.768678	3.890577	3.328993
240	1	0	-2.663097	2.782868	3.276765
241	1	0	0.968186	3.730579	4.840875
242	7	0	1.569148	3.606310	2.778096
243	1	0	-1.222485	4.677326	3.979397
244	7	0	-0.413911	4.487712	2.012518
245	6	0	0.933612	4.192671	1.674597
246	1	0	2.572706	3.405884	2.830395
247	1	0	-1.131477	4.498142	1.263703
248	8	0	1.481224	4.495964	0.617590
249	1	0	0.783744	4.987903	-3.662642
250	6	0	0.425465	4.092053	-3.099742
251	6	0	-0.819880	3.327885	-3.763092
252	7	0	-0.086957	4.499918	-1.767385
253	7	0	1.466279	3.040112	-3.032967
254	1	0	-1.224656	3.808008	-4.686704
255	7	0	-0.282258	1.981425	-4.087364
256	7	0	-1.824279	3.311696	-2.672343
257	6	0	-1.333438	3.893576	-1.499274
258	1	0	0.572788	4.717527	-0.995117
259	6	0	0.995194	1.801201	-3.494572
260	1	0	2.404509	3.200369	-2.658747
261	1	0	-0.930244	1.166817	-4.110266
262	1	0	-2.768647	2.922952	-2.781117
263	8	0	-1.926698	3.924958	-0.417602
264	8	0	1.621587	0.746913	-3.466285
265	6	0	-6.201404	-0.794903	-0.134005
266	6	0	-4.819239	-0.817658	-0.292326

267	6	0	-4.010566	0.211440	0.220607
268	6	0	-4.646698	1.267616	0.889576
269	6	0	-6.032544	1.285721	1.061084
270	6	0	-6.828016	0.251297	0.558225
271	1	0	-6.801867	-1.603446	-0.536631
272	1	0	-4.344236	-1.642558	-0.810533
273	1	0	-4.060904	2.080164	1.318639
274	1	0	-6.497499	2.100668	1.608997
275	6	0	-8.325434	0.262607	0.724203
276	6	0	-9.052656	0.466703	-0.604648
277	1	0	-8.604776	1.058265	1.418621
278	1	0	-8.653002	-0.678718	1.172327
279	1	0	-10.132876	0.501541	-0.456895
280	1	0	-8.738164	1.399514	-1.072038
281	1	0	-8.833511	-0.346403	-1.295052
282	8	0	-1.602721	1.186995	0.191237
283	8	0	-1.921318	-1.144707	-0.082494
284	1	0	-0.944374	-1.137894	-0.142691
285	6	0	5.016141	-1.647681	0.151891
286	6	0	3.636605	-1.505616	0.036319
287	6	0	3.046251	-0.259182	0.278434
288	6	0	3.839123	0.824307	0.674531
289	6	0	5.219306	0.661288	0.793843
290	6	0	5.826854	-0.575410	0.546888
291	1	0	5.467623	-2.616980	-0.024282
292	1	0	3.008143	-2.346408	-0.243105
293	1	0	3.377818	1.780676	0.884693
294	1	0	5.826422	1.498128	1.121562
295	6	0	7.320758	-0.748027	0.644303
296	6	0	8.003296	-0.661919	-0.723004
297	1	0	7.542011	-1.715691	1.104155
298	1	0	7.731262	0.017600	1.305055
299	1	0	9.081612	-0.794517	-0.629858
300	1	0	7.620641	-1.431985	-1.392872
301	1	0	7.815951	0.309484	-1.177014
302	8	0	0.846768	-1.107220	-0.107838
303	8	0	1.112128	1.093998	0.366442
304	1	0	0.124703	1.094485	0.288238
305	6	0	1.568765	-0.143260	0.163575
306	1	0	-2.067137	2.037198	0.264493
307	5	0	-2.452368	0.086874	0.097333

CC-trans, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.357589	0.748359	-3.111553
2	6	0	11.854689	-0.592693	-3.571541
3	6	0	12.009178	-1.522020	2.020340
4	6	0	11.472150	-2.755836	1.627140
5	6	0	12.096036	-3.569659	0.526486
6	6	0	11.509483	-3.228953	-0.813607
7	6	0	11.953279	-2.119789	-1.550347
8	6	0	11.344879	-1.748036	-2.758175
9	6	0	12.008522	1.482401	-2.109881
10	6	0	12.223101	3.519105	-0.611751
11	6	0	11.618378	3.151255	0.715345
12	6	0	12.086533	2.056982	1.458047
13	6	0	11.491705	1.686135	2.672630
14	6	0	11.451853	-0.780758	3.073446
15	6	0	12.022499	0.543907	3.493057
16	6	0	10.262142	-2.530069	-3.208522
17	6	0	10.478530	-4.013024	-1.364670
18	6	0	9.827344	-3.679196	-2.552322
19	6	0	10.471496	3.309978	-2.427595
20	6	0	10.231577	1.336629	-3.721483
21	6	0	9.771974	2.614520	-3.414083
22	6	0	10.339653	-3.228094	2.323102
23	6	0	10.344370	-1.329597	3.748009
24	6	0	9.754748	-2.540992	3.384318
25	6	0	10.392538	2.446342	3.121370
26	6	0	10.552901	3.900528	1.252844
27	6	0	9.907057	3.561412	2.441605
28	1	0	8.881055	-2.941301	3.917593
29	1	0	12.881274	-1.128621	1.496936
30	1	0	11.938083	-4.660729	0.738570
31	1	0	13.199561	-3.441396	0.518075
32	1	0	12.782587	-1.524427	-1.166650
33	1	0	9.005398	-4.289121	-2.953561
34	1	0	8.902403	3.052864	-3.924576
35	1	0	12.876258	1.050477	-1.610490
36	1	0	12.930282	1.478961	1.079886
37	1	0	9.059183	4.146066	2.827287
38	1	0	13.133265	0.520817	3.453839
39	1	0	11.781790	0.724691	4.575232
40	1	0	13.320679	3.351710	-0.608482
41	1	0	12.102048	4.621206	-0.785710
42	1	0	11.554869	-0.742443	-4.644278
43	1	0	12.967421	-0.603143	-3.590254
44	8	0	9.592014	0.597656	-4.750729
45	8	0	9.614591	-2.158820	-4.417896
46	8	0	10.203985	5.093281	0.580263
47	8	0	10.145434	4.659038	-2.160300
48	8	0	9.828471	2.101772	4.372738
49	8	0	9.869854	-0.637694	4.891315
50	8	0	10.123388	-5.209022	-0.688741
51	8	0	9.882279	-4.523428	1.996393
52	6	0	8.446798	-1.456975	-4.174125
53	6	0	8.444902	-0.034468	-4.318231
54	7	0	7.330173	0.722582	-4.084811
55	7	0	7.323621	-2.158068	-3.831259
56	6	0	6.241935	0.023391	-3.743183
57	6	0	6.231840	-1.407844	-3.633037
58	6	0	4.865556	0.552739	-3.384168
59	6	0	4.832861	-1.853911	-3.237635
60	7	0	4.101530	-0.629540	-3.122482
61	8	0	4.445382	1.669912	-3.278920
62	1	0	3.071113	-0.595311	-2.932964

63	8	0	4.368190	-2.940290	-3.035349
64	6	0	8.954926	4.826621	-1.477660
65	6	0	8.984744	5.040329	-0.067257
66	6	0	11.564918	2.758973	-1.730017
67	7	0	7.852742	5.270772	0.664270
68	7	0	7.793451	4.854197	-2.198966
69	6	0	8.667470	0.002804	4.645507
70	6	0	8.652124	1.386077	4.291788
71	6	0	8.869897	-5.095085	-0.106668
72	6	0	8.742581	-4.604768	1.230677
73	7	0	7.497816	2.040232	3.953660
74	7	0	7.523069	-0.732090	4.777847
75	7	0	7.791988	-5.469479	-0.855634
76	7	0	7.524998	-4.333137	1.792541
77	6	0	6.694166	5.093690	-1.474513
78	6	0	6.474116	-4.652287	1.024569
79	6	0	6.723189	5.292858	-0.052082
80	6	0	6.398565	-0.066071	4.497374
81	6	0	6.387920	1.297579	4.043345
82	6	0	6.608356	-5.271043	-0.264077
83	6	0	5.225474	-5.567623	-0.822951
84	6	0	4.991689	-4.425386	1.292691
85	6	0	5.248914	5.162147	-1.951513
86	6	0	5.297386	5.477223	0.449260
87	6	0	4.975224	-0.595758	4.522124
88	6	0	4.959682	1.668437	3.669153
89	7	0	4.343739	-5.005353	0.166847
90	7	0	4.206884	0.500791	3.998428
91	7	0	4.507454	5.357857	-0.740562
92	8	0	4.433453	-3.858368	2.192102
93	8	0	4.868929	-6.132383	-1.810670
94	8	0	4.516955	-1.638189	4.878623
95	8	0	4.493860	2.665098	3.193108
96	8	0	4.772425	5.094164	-3.044436
97	8	0	4.862279	5.678913	1.543072
98	1	0	3.469446	5.358342	-0.713572
99	1	0	3.189938	0.410713	3.803162
100	1	0	3.306662	-4.987113	0.046311
101	1	0	-13.430058	3.477670	-0.999629
102	6	0	-12.323425	3.559069	-1.056890
103	6	0	-11.710995	3.460141	0.311114
104	6	0	-11.762597	2.526391	-1.995666
105	1	0	-12.134718	4.582528	-1.477855
106	6	0	-12.185974	2.546661	1.265944
107	6	0	-10.630225	4.285892	0.672392
108	6	0	-12.335407	1.252077	-2.109864
109	6	0	-10.655710	2.821262	-2.818381
110	6	0	-11.569624	2.408168	2.517053
111	1	0	-13.047219	1.923512	1.023293
112	6	0	-9.963731	4.173252	1.893231
113	8	0	-10.243344	5.302504	-0.239188
114	6	0	-11.838162	0.301532	-3.014656
115	1	0	-13.186392	0.991751	-1.479509
116	6	0	-10.134734	1.924189	-3.748080
117	8	0	-10.145348	4.138216	-2.764113
118	6	0	-12.100349	1.471752	3.566601
119	6	0	-10.442659	3.213556	2.780167
120	1	0	-9.101406	4.806633	2.143929
121	6	0	-9.020846	5.011681	-0.822683
122	6	0	-12.445759	-1.067316	-3.127592
123	6	0	-10.759080	0.679533	-3.836088
124	1	0	-9.279845	2.188889	-4.386006
125	6	0	-8.972201	4.300086	-2.062025
126	1	0	-13.212208	1.480509	3.565288
127	1	0	-11.815710	1.858238	4.582065
128	6	0	-11.584438	0.070022	3.409818
129	8	0	-9.829350	3.081858	4.050189
130	7	0	-7.895576	5.434797	-0.175364
131	6	0	-11.880689	-2.034913	-2.125409
132	1	0	-12.270765	-1.465214	-4.163163
133	1	0	-13.552070	-1.012999	-3.031697
134	8	0	-10.353009	-0.232394	-4.844667
135	7	0	-7.793736	3.874261	-2.610406
136	6	0	-12.207976	-0.846272	2.548258
137	6	0	-10.469218	-0.374625	4.145093
138	6	0	-8.683085	2.316190	4.043245
139	6	0	-6.748050	5.069021	-0.758029
140	6	0	-12.397037	-2.139441	-0.826722
141	6	0	-10.827010	-2.902404	-2.479092
142	6	0	-9.149480	-0.841841	-4.538995
143	6	0	-6.698528	4.248658	-1.935303
144	6	0	-11.724750	-2.152519	2.392532
145	1	0	-13.087478	-0.532315	1.985017
146	6	0	-9.933717	-1.656701	4.014284
147	8	0	-9.918536	0.509262	5.110199
148	6	0	-8.712466	1.039582	4.685351
149	7	0	-7.540774	2.826053	3.488393
150	6	0	-5.330448	5.363807	-0.293202
151	6	0	-11.897678	-3.079469	0.088829
152	1	0	-13.199421	-1.469353	-0.516274
153	6	0	-10.326026	-3.883706	-1.628064
154	8	0	-10.328576	-2.816275	-3.801589
155	6	0	-9.139366	-2.128368	-3.915878
156	7	0	-8.001248	-0.182513	-4.875508
157	6	0	-5.245406	3.897467	-2.213380
158	6	0	-12.411158	-3.148491	1.498771
159	6	0	-10.579800	-2.517388	3.130573
160	1	0	-9.050249	-1.974864	4.585549
161	7	0	-7.580823	0.308720	4.912705
162	6	0	-6.449146	2.071237	3.666775
163	7	0	-4.520731	4.598548	-1.207163
164	8	0	-4.903500	6.055553	0.578611
165	6	0	-10.894577	-3.960963	-0.355880
166	1	0	-9.524139	-4.564262	-1.946311
167	7	0	-7.981039	-2.730006	-3.505404
168	6	0	-6.874051	-0.810633	-4.523136
169	8	0	-4.750411	3.179634	-3.038881
170	1	0	-12.250188	-4.182684	1.904744
171	1	0	-13.512654	-3.004525	1.523862
172	8	0	-10.160109	-3.863623	3.035351

173	6	0	-6.459948	0.850278	4.423125
174	6	0	-5.046584	2.283086	3.116597
175	1	0	-3.481070	4.550230	-1.128298
176	8	0	-10.495470	-5.004387	0.518986
177	6	0	-6.864748	-2.051809	-3.801163
178	6	0	-5.441614	-0.347950	-4.736652
179	6	0	-9.049070	-4.091083	2.255526
180	6	0	-5.047350	0.291578	4.484678
181	7	0	-4.300643	1.193804	3.646739
182	8	0	-4.602616	3.125704	2.383966
183	6	0	-9.221983	-4.788991	1.019060
184	6	0	-5.425172	-2.389694	-3.444202
185	7	0	-4.668483	-1.339918	-4.034887
186	8	0	-4.979220	0.574280	-5.334261
187	7	0	-7.813980	-3.742168	2.727512
188	8	0	-4.577958	-0.635790	5.069007
189	1	0	-3.291286	1.041764	3.420164
190	7	0	-8.169062	-5.279832	0.301705
191	8	0	-4.960559	-3.292736	-2.801485
192	1	0	-3.631749	-1.267636	-3.928410
193	6	0	-6.790157	-4.183664	1.984683
194	6	0	-6.965636	-4.994968	0.813789
195	6	0	-5.303285	-3.931129	2.176402
196	6	0	-5.600695	-5.388242	0.270787
197	7	0	-4.687223	-4.687655	1.137114
198	8	0	-4.717720	-3.244252	2.967023
199	8	0	-5.273366	-6.100263	-0.627712
200	1	0	-3.652408	-4.712616	1.002923
201	8	0	-1.878153	-4.247841	0.936784
202	6	0	-1.237499	-3.875774	1.919882
203	7	0	0.067601	-4.307103	2.260293
204	7	0	-1.726965	-3.044783	2.937496
205	6	0	0.581846	-3.558877	3.437061
206	1	0	0.726887	-4.592598	1.509817
207	6	0	-0.687006	-2.717181	3.939417
208	1	0	-2.701232	-2.739099	3.018480
209	1	0	0.993841	-4.277396	4.187566
210	7	0	1.572885	-2.511954	3.099117
211	1	0	-1.028498	-2.956743	4.976239
212	7	0	-0.218267	-1.308144	3.884931
213	6	0	1.055383	-1.222438	3.269265
214	1	0	2.507348	-2.728404	2.746721
215	1	0	-0.902234	-0.540718	3.746188
216	8	0	1.646879	-0.173995	3.013078
217	1	0	-1.264213	-5.627661	-3.278433
218	6	0	-0.868153	-4.698247	-2.800045
219	6	0	0.427614	-4.078409	-3.514478
220	7	0	-0.399739	-5.010969	-1.425380
221	7	0	-1.853561	-3.595552	-2.869085
222	1	0	0.774967	-4.642407	-4.414640
223	7	0	-0.007143	-2.715360	-3.925009
224	7	0	1.446384	-4.088741	-2.443638
225	6	0	0.923501	-4.542131	-1.222221
226	1	0	-1.074116	-4.988283	-0.635202
227	6	0	-1.301546	-2.429954	-3.421472
228	1	0	-2.825157	-3.685383	-2.559567
229	1	0	0.690895	-1.946452	-3.958661
230	1	0	2.412044	-3.785049	-2.586316
231	8	0	1.545795	-4.614287	-0.167277
232	8	0	-1.889162	-1.357269	-3.536976
233	6	0	0.854129	0.813650	-3.581225
234	7	0	-0.409390	1.014479	-4.183593
235	7	0	1.488415	2.051735	-3.421880
236	8	0	1.355964	-0.284462	-3.335621
237	6	0	-0.763840	2.456528	-4.208460
238	1	0	-1.147384	0.291319	-4.096621
239	6	0	0.584394	3.184291	-3.732137
240	1	0	2.425327	2.177154	-3.026202
241	1	0	-1.115122	2.739129	-5.230817
242	7	0	-1.743759	2.852057	-3.170452
243	1	0	1.045245	3.866298	-4.488748
244	7	0	0.161457	3.961470	-2.542312
245	6	0	-1.159482	3.635018	-2.162497
246	1	0	-2.739456	2.615687	-3.216229
247	1	0	0.863984	4.260293	-1.837703
248	8	0	-1.733480	4.043712	-1.154038
249	1	0	-0.869872	5.347925	2.989316
250	6	0	-0.502320	4.445353	2.441800
251	6	0	0.801132	3.761813	3.078235
252	7	0	-0.067079	4.835959	1.076479
253	7	0	-1.507278	3.358232	2.473953
254	1	0	1.177562	4.253316	4.008605
255	7	0	0.355029	2.377316	3.399748
256	7	0	1.792477	3.830662	1.985351
257	6	0	1.248951	4.367233	0.809434
258	1	0	-0.766540	4.852582	0.309677
259	6	0	-0.957014	2.147169	2.918308
260	1	0	-2.466267	3.469122	2.134727
261	1	0	1.037462	1.596575	3.377053
262	1	0	2.771025	3.559316	2.107195
263	8	0	1.833053	4.492022	-0.261183
264	8	0	-1.559688	1.076908	2.979140
265	6	0	6.476913	-0.789982	1.186219
266	6	0	5.103065	-0.908347	0.989105
267	6	0	4.416406	0.093730	0.297397
268	6	0	5.097798	1.224953	-0.164052
269	6	0	6.472891	1.320828	0.025343
270	6	0	7.180988	0.320928	0.706452
271	1	0	7.006372	-1.564879	1.733184
272	1	0	4.558815	-1.763435	1.370915
273	1	0	4.543436	2.001374	-0.677950
274	1	0	7.004709	2.192045	-0.339826
275	6	0	8.676038	0.406111	0.843621
276	6	0	9.389758	-0.140244	-0.393194
277	1	0	8.996992	-0.153372	1.724546
278	1	0	8.968793	1.446928	1.001686
279	1	0	10.472615	-0.073866	-0.277807
280	1	0	9.127324	-1.184374	-0.557312
281	1	0	9.106705	0.426695	-1.279180
282	8	0	2.283378	0.985490	-0.271230

283	8	0	2.463988	-1.220643	0.233833
284	1	0	1.469341	-1.198300	0.130774
285	6	0	-4.383792	-1.510981	-0.342907
286	6	0	-2.995144	-1.452678	-0.263267
287	6	0	-2.356843	-0.208741	-0.218029
288	6	0	-3.111574	0.971091	-0.244723
289	6	0	-4.501754	0.892196	-0.300843
290	6	0	-5.156564	-0.344286	-0.370824
291	1	0	-4.872224	-2.476366	-0.420319
292	1	0	-2.398074	-2.357634	-0.234263
293	1	0	-2.611863	1.932330	-0.218235
294	1	0	-5.084703	1.805760	-0.313948
295	6	0	-6.661405	-0.419815	-0.406481
296	6	0	-7.271808	-0.317708	0.993473
297	1	0	-6.963634	-1.360461	-0.871352
298	1	0	-7.051107	0.385395	-1.033007
299	1	0	-8.358001	-0.395435	0.955616
300	1	0	-6.890675	-1.111609	1.636393
301	1	0	-7.011723	0.636909	1.447588
302	8	0	-0.197274	-1.195117	0.034852
303	8	0	-0.356843	1.030110	-0.371066
304	1	0	0.640128	0.977605	-0.327886
305	6	0	2.952138	0.000945	0.071976
306	6	0	-0.875377	-0.175929	-0.167003

CC-cis, capsule a: oniom(mp2/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.374902	0.703936	-3.102573
2	6	0	11.870452	-0.639572	-3.557009
3	6	0	11.998986	-1.560870	2.039131
4	6	0	11.456261	-2.791970	1.645164
5	6	0	12.079389	-3.610192	0.547280
6	6	0	11.499444	-3.268084	-0.795372
7	6	0	11.952770	-2.163446	-1.533075
8	6	0	11.350426	-1.790276	-2.743505
9	6	0	12.020573	1.436497	-2.096456
10	6	0	12.234167	3.474994	-0.601270
11	6	0	11.627661	3.111232	0.726005
12	6	0	12.091894	2.016856	1.471101
13	6	0	11.496180	1.651311	2.686894
14	6	0	11.442642	-0.815222	3.089745
15	6	0	12.019850	0.506834	3.508902
16	6	0	10.263770	-2.565901	-3.195755
17	6	0	10.465315	-4.046549	-1.348351
18	6	0	9.819317	-3.710594	-2.538290
19	6	0	10.487565	3.266084	-2.422264
20	6	0	10.255495	1.295130	-3.721670
21	6	0	9.794476	2.572798	-3.414779
22	6	0	10.318927	-3.257246	2.338034
23	6	0	10.329986	-1.357278	3.761360
24	6	0	9.734853	-2.565771	3.396912
25	6	0	10.401770	2.418545	3.135056
26	6	0	10.564814	3.865651	1.261506
27	6	0	9.919736	3.533401	2.452509
28	1	0	8.857307	-2.960728	3.927841
29	1	0	12.875109	-1.173060	1.518245
30	1	0	11.914789	-4.700177	0.759993
31	1	0	13.183614	-3.487942	0.542555
32	1	0	12.785027	-1.572937	-1.148310
33	1	0	8.994728	-4.316050	-2.940862
34	1	0	8.929326	3.013180	-3.931116
35	1	0	12.884164	1.002759	-1.591490
36	1	0	12.932935	1.434411	1.093725
37	1	0	9.074524	4.122593	2.837188
38	1	0	13.130527	0.477829	3.471000
39	1	0	11.778819	0.689668	4.590644
40	1	0	13.331584	3.306178	-0.596112
41	1	0	12.115051	4.576970	-0.777708
42	1	0	11.576762	-0.790908	-4.631206
43	1	0	12.983161	-0.654194	-3.568663
44	8	0	9.626806	0.559465	-4.759707
45	8	0	9.626712	-2.195933	-4.410496
46	8	0	10.217404	5.056348	0.584363
47	8	0	10.160622	4.615133	-2.155487
48	8	0	9.836068	2.078225	4.387183
49	8	0	9.854583	-0.661713	4.902275
50	8	0	10.102393	-5.239728	-0.671754
51	8	0	9.855145	-4.550301	2.011769
52	6	0	8.460956	-1.485495	-4.183933
53	6	0	8.469031	-0.064801	-4.343579
54	7	0	7.353804	0.700104	-4.141194
55	7	0	7.329123	-2.176732	-3.848673
56	6	0	6.256404	0.010325	-3.810614
57	6	0	6.237807	-1.418984	-3.678006
58	6	0	4.876367	0.552159	-3.486041
59	6	0	4.830226	-1.851441	-3.296277
60	7	0	4.103312	-0.621911	-3.214152
61	8	0	4.460848	1.673113	-3.409411
62	1	0	3.069362	-0.577031	-3.043137
63	8	0	4.357123	-2.931267	-3.078781
64	6	0	8.969880	4.784227	-1.473923
65	6	0	8.998624	5.001954	-0.063980
66	6	0	11.577286	2.714032	-1.719666
67	7	0	7.866200	5.235604	0.665931
68	7	0	7.808928	4.811849	-2.196088
69	6	0	8.657862	-0.012947	4.650986
70	6	0	8.654319	1.371722	4.302475
71	6	0	8.847487	-5.119132	-0.094263
72	6	0	8.717704	-4.626693	1.241976
73	7	0	7.506871	2.035663	3.960352
74	7	0	7.507406	-0.740530	4.771490
75	7	0	7.770638	-5.488985	-0.847005
76	7	0	7.499379	-4.348758	1.799173
77	6	0	6.709385	5.055677	-1.473375
78	6	0	6.449857	-4.663655	1.027586
79	6	0	6.737155	5.257814	-0.051340

80	6	0	6.389475	-0.065647	4.485556
81	6	0	6.391324	1.300458	4.039069
82	6	0	6.585885	-5.284066	-0.260120
83	6	0	5.203776	-5.573716	-0.824537
84	6	0	4.967478	-4.429025	1.289571
85	6	0	5.265104	5.127739	-1.952577
86	6	0	5.310981	5.445081	0.447869
87	6	0	4.962591	-0.586379	4.493090
88	6	0	4.968885	1.683291	3.655435
89	7	0	4.321137	-5.007091	0.161702
90	7	0	4.206550	0.516840	3.965831
91	7	0	4.522138	5.325024	-0.742492
92	8	0	4.408411	-3.857532	2.185527
93	8	0	4.848550	-6.136059	-1.814113
94	8	0	4.493910	-1.627655	4.839403
95	8	0	4.513043	2.687363	3.185428
96	8	0	4.789596	5.062144	-3.045958
97	8	0	4.873985	5.649905	1.540516
98	1	0	3.484367	5.324949	-0.716578
99	1	0	3.189782	0.436288	3.761421
100	1	0	3.284923	-4.982101	0.036475
101	1	0	-13.429779	3.414197	-1.034598
102	6	0	-12.322570	3.492510	-1.087400
103	6	0	-11.716848	3.390770	0.283221
104	6	0	-11.762035	2.460400	-2.026633
105	1	0	-12.129685	4.516321	-1.505841
106	6	0	-12.200031	2.476956	1.233390
107	6	0	-10.638666	4.216081	0.653639
108	6	0	-12.334850	1.186680	-2.145006
109	6	0	-10.654462	2.757542	-2.847662
110	6	0	-11.598138	2.341719	2.491810
111	1	0	-13.057087	1.851480	0.981783
112	6	0	-9.987766	4.108100	1.883310
113	8	0	-10.241986	5.231993	-0.254420
114	6	0	-11.837718	0.239305	-3.053529
115	1	0	-13.185070	0.923632	-1.514760
116	6	0	-10.137394	1.866187	-3.784430
117	8	0	-10.139249	4.071980	-2.782044
118	6	0	-12.136725	1.401604	3.533852
119	6	0	-10.478478	3.152482	2.768632
120	1	0	-9.130201	4.744412	2.142775
121	6	0	-9.019150	4.938497	-0.835541
122	6	0	-12.439784	-1.132140	-3.164847
123	6	0	-10.762463	0.621970	-3.877569
124	1	0	-9.284233	2.134226	-4.423267
125	6	0	-8.968569	4.226097	-2.074775
126	1	0	-13.248493	1.405779	3.520632
127	1	0	-11.864642	1.786650	4.553241
128	6	0	-11.613012	0.002516	3.378599
129	8	0	-9.889508	3.031594	4.051045
130	7	0	-7.894649	5.365973	-0.190143
131	6	0	-11.872781	-2.094791	-2.158709
132	1	0	-12.260465	-1.532157	-4.198839
133	1	0	-13.546475	-1.081942	-3.071845
134	8	0	-10.353760	-0.286756	-4.888644
135	7	0	-7.789468	3.797268	-2.619576
136	6	0	-12.226740	-0.916131	2.513024
137	6	0	-10.500348	-0.437711	4.120630
138	6	0	-8.732333	2.282437	4.069427
139	6	0	-6.746237	5.003500	-0.773766
140	6	0	-12.397675	-2.204648	-0.863727
141	6	0	-10.808297	-2.952078	-2.504995
142	6	0	-9.143657	-0.882625	-4.577888
143	6	0	-6.694810	4.176274	-1.945967
144	6	0	-11.738484	-2.221313	2.362119
145	1	0	-13.102910	-0.605563	1.942755
146	6	0	-9.960405	-1.718235	3.995682
147	8	0	-9.964596	0.448290	5.091391
148	6	0	-8.759139	0.993832	4.687771
149	7	0	-7.582046	2.824826	3.564739
150	6	0	-5.329267	5.315015	-0.318725
151	6	0	-11.896171	-3.140516	0.054750
152	1	0	-13.208632	-1.542449	-0.558879
153	6	0	-10.304116	-3.929175	-1.650964
154	8	0	-10.301405	-2.860880	-3.823943
155	6	0	-9.121001	-2.157513	-3.932014
156	7	0	-8.002286	-0.214093	-4.918807
157	6	0	-5.240128	3.831823	-2.225770
158	6	0	-12.416574	-3.217115	1.461853
159	6	0	-10.598916	-2.583067	3.109792
160	1	0	-9.080104	-2.033082	4.573616
161	7	0	-7.623195	0.272537	4.924963
162	6	0	-6.482935	2.086334	3.763420
163	7	0	-4.516500	4.549749	-1.229567
164	8	0	-4.904163	6.016080	0.546674
165	6	0	-10.881830	-4.012413	-0.383491
166	1	0	-9.492199	-4.600706	-1.963058
167	7	0	-7.959012	-2.728791	-3.489646
168	6	0	-6.869973	-0.814772	-4.536832
169	8	0	-4.743024	3.111140	-3.047043
170	1	0	-12.253102	-4.252050	1.864881
171	1	0	-13.518720	-3.077825	1.482234
172	8	0	-10.176143	-3.929290	3.024346
173	6	0	-6.497304	0.842606	4.480836
174	6	0	-5.063939	2.349386	3.283309
175	1	0	-3.474953	4.516749	-1.159657
176	8	0	-10.483266	-5.052190	0.495327
177	6	0	-6.850838	-2.034504	-3.779008
178	6	0	-5.442987	-0.330866	-4.738353
179	6	0	-9.056414	-4.154905	2.255219
180	6	0	-5.077853	0.304901	4.570405
181	7	0	-4.316470	1.256269	3.803082
182	8	0	-4.609681	3.229834	2.603263
183	6	0	-9.215231	-4.832437	1.006087
184	6	0	-5.414213	-2.321339	-3.368182
185	7	0	-4.666556	-1.275520	-3.977684
186	8	0	-4.986519	0.573803	-5.366559
187	7	0	-7.826424	-3.819431	2.750088
188	8	0	-4.613988	-0.643011	5.125556
189	1	0	-3.297170	1.131650	3.607656

190	7	0	-8.153648	-5.301879	0.286520
191	8	0	-4.947082	-3.185322	-2.675934
192	1	0	-3.634088	-1.176236	-3.851032
193	6	0	-6.794042	-4.243780	2.009411
194	6	0	-6.956151	-5.022218	0.814153
195	6	0	-5.309824	-3.993896	2.223340
196	6	0	-5.585168	-5.386602	0.265905
197	7	0	-4.682952	-4.705650	1.159116
198	8	0	-4.730633	-3.336045	3.042865
199	8	0	-5.247076	-6.068599	-0.651627
200	1	0	-3.648538	-4.713053	1.026296
201	8	0	-1.900425	-4.161325	0.958453
202	6	0	-1.250997	-3.798139	1.938666
203	7	0	0.061310	-4.222292	2.257015
204	7	0	-1.733110	-2.979337	2.970462
205	6	0	0.586502	-3.481635	3.433424
206	1	0	0.713303	-4.501335	1.497238
207	6	0	-0.682278	-2.656505	3.963124
208	1	0	-2.714089	-2.708543	3.082962
209	1	0	1.017712	-4.202917	4.170389
210	7	0	1.561776	-2.422348	3.088357
211	1	0	-1.006841	-2.909935	5.001916
212	7	0	-0.225641	-1.243497	3.916088
213	6	0	1.034947	-1.139253	3.277968
214	1	0	2.489828	-2.627711	2.714218
215	1	0	-0.916430	-0.477749	3.808433
216	8	0	1.611211	-0.082803	3.019454
217	1	0	-1.346902	-5.554288	-3.234407
218	6	0	-0.921926	-4.631689	-2.767804
219	6	0	0.370710	-4.040106	-3.511253
220	7	0	-0.432403	-4.947954	-1.401401
221	7	0	-1.886564	-3.510055	-2.821190
222	1	0	0.694680	-4.619167	-4.410358
223	7	0	-0.050806	-2.675633	-3.927149
224	7	0	1.407666	-4.055296	-2.456567
225	6	0	0.898829	-4.491782	-1.223371
226	1	0	-1.093764	-4.909969	-0.600507
227	6	0	-1.322491	-2.357538	-3.387610
228	1	0	-2.843111	-3.570756	-2.461295
229	1	0	0.659045	-1.921080	-4.005556
230	1	0	2.374585	-3.765964	-2.617336
231	8	0	1.534585	-4.559949	-0.175901
232	8	0	-1.887905	-1.271130	-3.489890
233	6	0	0.861798	0.843117	-3.672732
234	7	0	-0.407142	1.063143	-4.259543
235	7	0	1.502391	2.073861	-3.486099
236	8	0	1.362633	-0.262482	-3.461815
237	6	0	-0.749915	2.508657	-4.254560
238	1	0	-1.150665	0.346929	-4.161593
239	6	0	0.604211	3.217900	-3.767079
240	1	0	2.442492	2.182984	-3.092233
241	1	0	-1.099460	2.813060	-5.271481
242	7	0	-1.726840	2.897500	-3.211553
243	1	0	1.066020	3.913544	-4.510781
244	7	0	0.189497	3.974255	-2.560398
245	6	0	-1.135439	3.655361	-2.188884
246	1	0	-2.718129	2.640823	-3.244296
247	1	0	0.893423	4.247478	-1.847250
248	8	0	-1.709969	4.057594	-1.177271
249	1	0	-0.846804	5.439492	2.972379
250	6	0	-0.490049	4.514159	2.456748
251	6	0	0.811876	3.844168	3.110230
252	7	0	-0.059279	4.852222	1.075739
253	7	0	-1.501540	3.435327	2.529617
254	1	0	1.195245	4.365175	4.021574
255	7	0	0.359056	2.474382	3.483955
256	7	0	1.798222	3.865496	2.011144
257	6	0	1.254759	4.372606	0.820981
258	1	0	-0.761047	4.844142	0.310496
259	6	0	-0.961330	2.239635	3.025229
260	1	0	-2.479073	3.559501	2.253734
261	1	0	1.035728	1.688279	3.461575
262	1	0	2.781801	3.617698	2.145644
263	8	0	1.840895	4.463688	-0.251453
264	8	0	-1.573670	1.179477	3.132003
265	6	0	6.473382	-0.815878	1.192588
266	6	0	5.103985	-0.932245	0.964040
267	6	0	4.444652	0.044788	0.212735
268	6	0	5.147880	1.151722	-0.274940
269	6	0	6.517104	1.247387	-0.049977
270	6	0	7.198617	0.270904	0.689950
271	1	0	6.982092	-1.573656	1.781872
272	1	0	4.543762	-1.767922	1.365042
273	1	0	4.613400	1.910690	-0.833678
274	1	0	7.064879	2.100661	-0.433573
275	6	0	8.689135	0.357322	0.867966
276	6	0	9.438296	-0.191883	-0.346228
277	1	0	8.985374	-0.199190	1.759190
278	1	0	8.976668	1.398897	1.030981
279	1	0	10.517275	-0.124999	-0.199341
280	1	0	9.180876	-1.236495	-0.515303
281	1	0	9.181840	0.372221	-1.242064
282	8	0	2.355985	0.913815	-0.524526
283	8	0	2.458200	-1.225377	0.226013
284	1	0	1.470452	-1.193776	0.077474
285	6	0	-4.436220	-1.144565	0.184492
286	6	0	-3.054896	-1.205797	0.019224
287	6	0	-2.318856	-0.019455	-0.084047
288	6	0	-2.966997	1.218950	-0.003482
289	6	0	-4.347037	1.259891	0.183162
290	6	0	-5.099282	0.085216	0.292720
291	1	0	-5.004483	-2.064501	0.254329
292	1	0	-2.538706	-2.158744	-0.028404
293	1	0	-2.393078	2.135006	-0.082697
294	1	0	-4.839699	2.221040	0.281995
295	6	0	-6.595617	0.140205	0.465941
296	6	0	-7.334564	-0.051828	-0.860179
297	1	0	-6.871353	1.101321	0.903904
298	1	0	-6.907631	-0.632703	1.171927
299	1	0	-8.413328	0.012695	-0.721017

300	1	0	-7.031956	0.710654	-1.577906
301	1	0	-7.100835	-1.028197	-1.282325
302	8	0	-0.210472	-1.147619	-0.041816
303	8	0	-0.277739	1.067593	-0.522012
304	1	0	0.715114	0.962935	-0.548217
305	6	0	2.986688	-0.041766	-0.052078
306	6	0	-0.843714	-0.094620	-0.212830

AA-trans, capsule b: oniom(m062x/6-31g(d,p):pm6):

1	6	0	11.826594	0.955417	-2.719737
2	6	0	12.372483	-0.307299	-3.325423
3	6	0	11.880364	-2.144186	2.040185
4	6	0	11.330215	-3.295124	1.455510
5	6	0	11.935526	-3.907117	0.224554
6	6	0	11.465007	-3.236667	-1.035687
7	6	0	12.118239	-2.118261	-1.569977
8	6	0	11.688930	-1.522795	-2.766192
9	6	0	12.350172	1.483623	-1.530596
10	6	0	12.412559	3.250307	0.292149
11	6	0	11.725022	2.694567	1.507029
12	6	0	12.125744	1.474517	2.073813
13	6	0	11.476685	0.938020	3.194001
14	6	0	11.319310	-1.561956	3.185211
15	6	0	11.925548	-0.347468	3.829045
16	6	0	10.595649	-2.104573	-3.436270
17	6	0	10.354976	-3.744383	-1.741347
18	6	0	9.896326	-3.205303	-2.940560
19	6	0	10.803202	3.321461	-1.656604
20	6	0	10.778428	1.658899	-3.346295
21	6	0	10.235818	2.836823	-2.833547
22	6	0	10.202918	-3.871274	2.072697
23	6	0	10.180503	-2.178507	3.740630
24	6	0	9.602490	-3.330560	3.210252
25	6	0	10.401128	1.669225	3.737376
26	6	0	10.663003	3.386542	2.119854
27	6	0	9.972836	2.892461	3.226961
28	1	0	8.720138	-3.796269	3.672331
29	1	0	12.762618	-1.688847	1.588909
30	1	0	11.670863	-4.997798	0.184037
31	1	0	13.045208	-3.890094	0.286072
32	1	0	12.976843	-1.699052	-1.044672
33	1	0	9.034096	-3.631479	-3.472390
34	1	0	9.416989	3.364574	-3.342556
35	1	0	13.165101	0.960990	-1.028563
36	1	0	12.958949	0.929732	1.628421
37	1	0	9.137859	3.444521	3.681420
38	1	0	13.035308	-0.417986	3.819432
39	1	0	11.653228	-0.334105	4.918976
40	1	0	13.509407	3.082868	0.350120
41	1	0	12.296575	4.366578	0.274076
42	1	0	12.233082	-0.278043	-4.438747
43	1	0	13.472177	-0.371379	-3.181377
44	8	0	10.368706	1.193208	-4.615779
45	8	0	10.272417	-1.591317	-4.715112
46	8	0	10.349273	4.680440	1.632969
47	8	0	10.420730	4.586482	-1.152878
48	8	0	9.798275	1.158411	4.912669
49	8	0	9.658579	-1.630052	4.940095
50	8	0	9.769100	-4.926056	-1.232679
51	8	0	9.713194	-5.096590	1.552200
52	6	0	9.098127	-0.864882	-4.742296
53	6	0	9.143986	0.560869	-4.649604
54	7	0	8.017660	1.333566	-4.707575
55	7	0	7.931502	-1.549697	-4.938973
56	6	0	6.882294	0.649209	-4.895386
57	6	0	6.840444	-0.779846	-5.027490
58	6	0	5.465193	1.185840	-4.988024
59	6	0	5.398293	-1.215001	-5.243299
60	7	0	4.665375	0.024467	-5.193054
61	8	0	5.041005	2.306683	-4.908150
62	1	0	3.624195	0.065543	-5.266719
63	8	0	4.905007	-2.285147	-5.426726
64	6	0	9.202940	4.617800	-0.512089
65	6	0	9.168990	4.718674	0.914732
66	6	0	11.849788	2.669065	-0.974705
67	7	0	8.006460	4.911844	1.606986
68	7	0	8.068667	4.643232	-1.273596
69	6	0	8.511865	-0.887257	4.728465
70	6	0	8.586671	0.537741	4.682820
71	6	0	8.572911	-4.747867	-0.574243
72	6	0	8.535476	-4.933347	0.842488
73	7	0	7.484968	1.323931	4.480020
74	7	0	7.326222	-1.560242	4.615152
75	7	0	7.446753	-4.496687	-1.309216
76	7	0	7.360974	-5.004071	1.537289
77	6	0	6.937083	4.813708	-0.579115
78	6	0	6.261169	-4.831126	0.794420
79	6	0	6.905623	4.971895	0.846651
80	6	0	6.253743	-0.779083	4.450142
81	6	0	6.333824	0.652794	4.364911
82	6	0	6.307455	-4.524953	-0.607475
83	6	0	4.891459	-4.249961	-1.089401
84	6	0	4.806821	-4.882015	1.240233
85	6	0	5.514636	4.829749	-1.104341
86	6	0	5.461400	5.147664	1.291111
87	6	0	4.802581	-1.203329	4.278040
88	6	0	4.940913	1.200217	4.097639
89	7	0	4.082794	-4.496301	0.056348
90	7	0	4.112991	0.041202	4.083491
91	7	0	4.715824	5.005232	0.062991
92	8	0	4.304265	-5.171174	2.281532
93	8	0	4.484985	-3.877685	-2.155948
94	8	0	4.284192	-2.278289	4.276973
95	8	0	4.551575	2.320910	3.914688
96	8	0	5.090031	4.712772	-2.221346
97	8	0	4.968172	5.365123	2.354158
98	1	0	3.675449	4.990160	0.033552
99	1	0	3.082828	0.093808	3.910937

100	1	0	3.036292	-4.443319	0.026269
101	1	0	-13.041011	3.877902	-0.242628
102	6	0	-11.931126	3.901032	-0.188089
103	6	0	-11.448214	3.224982	1.064623
104	6	0	-11.329262	3.298811	-1.425497
105	1	0	-11.672474	4.992887	-0.142272
106	6	0	-12.095065	2.103387	1.600030
107	6	0	-10.331916	3.730831	1.761708
108	6	0	-11.873558	2.143896	-2.008686
109	6	0	-10.209929	3.885169	-2.047285
110	6	0	-11.654930	1.504908	2.790677
111	1	0	-12.957428	1.684810	1.080573
112	6	0	-9.862527	3.188917	2.955624
113	8	0	-9.755465	4.916432	1.252175
114	6	0	-11.311710	1.565881	-3.155150
115	1	0	-12.751123	1.682507	-1.554469
116	6	0	-9.608330	3.347906	-3.186193
117	8	0	-9.728454	5.116041	-1.531588
118	6	0	-12.330017	0.285983	3.352620
119	6	0	-10.557903	2.086962	3.454501
120	1	0	-8.996198	3.614132	3.481526
121	6	0	-8.565112	4.752926	0.581119
122	6	0	-11.909103	0.348351	-3.801584
123	6	0	-10.177902	2.190189	-3.712068
124	1	0	-8.730819	3.819756	-3.651107
125	6	0	-8.542220	4.963069	-0.832910
126	1	0	-13.430673	0.344678	3.213699
127	1	0	-12.185239	0.257308	4.465420
128	6	0	-11.781867	-0.974831	2.744838
129	8	0	-10.229674	1.571702	4.731002
130	7	0	-7.430020	4.497656	1.300250
131	6	0	-11.449348	-0.936305	-3.172874
132	1	0	-11.639586	0.340887	-4.892285
133	1	0	-13.019459	0.410064	-3.789137
134	8	0	-9.653105	1.637222	-4.908398
135	7	0	-7.374922	5.066564	-1.535499
136	6	0	-12.304376	-1.499236	1.553648
137	6	0	-10.734847	-1.680729	3.370808
138	6	0	-9.054096	0.846673	4.753682
139	6	0	-6.297806	4.552184	0.588586
140	6	0	-12.091305	-1.475748	-2.049705
141	6	0	-10.374883	-1.663601	-3.723668
142	6	0	-8.504906	0.899108	-4.692787
143	6	0	-6.266208	4.893861	-0.805376
144	6	0	-11.805402	-2.684378	0.995748
145	1	0	-13.118203	-0.974421	1.052170
146	6	0	-10.195481	-2.859976	2.856899
147	8	0	-10.320528	-1.215782	4.639143
148	6	0	-9.097418	-0.579143	4.665488
149	7	0	-7.887887	1.534938	4.941977
150	6	0	-4.876070	4.275733	1.051559
151	6	0	-11.685642	-2.695476	-1.486862
152	1	0	-12.924061	-0.933660	-1.600054
153	6	0	-9.939196	-2.885350	-3.214115
154	8	0	-9.780349	-1.153772	-4.904964
155	6	0	-8.570315	-0.527083	-4.678260
156	7	0	-7.326831	1.578287	-4.541282
157	6	0	-4.815747	4.977525	-1.259309
158	6	0	-12.368879	-3.259582	-0.273434
159	6	0	-10.762087	-3.341544	1.677989
160	1	0	-9.378424	-3.390389	3.366017
161	7	0	-7.968800	-1.349135	4.718956
162	6	0	-6.794757	0.767997	5.025410
163	7	0	-4.077967	4.562722	-0.092964
164	8	0	-4.461009	3.871968	2.102869
165	6	0	-10.622450	-3.382293	-2.103984
166	1	0	-9.105013	-3.435072	-3.672789
167	7	0	-7.461847	-1.309835	-4.498516
168	6	0	-6.250456	0.801888	-4.382420
169	8	0	-4.323640	5.310998	-2.292330
170	1	0	-12.250175	-4.375739	-0.262056
171	1	0	-13.466398	-3.094625	-0.327948
172	8	0	-10.380492	-4.606583	1.173057
173	6	0	-6.833986	-0.661802	4.897286
174	6	0	-5.352044	1.207510	5.230294
175	1	0	-3.031669	4.510332	-0.075540
176	8	0	-10.307401	-4.675864	-1.618111
177	6	0	-6.316998	-0.633182	-4.354386
178	6	0	-4.810510	1.234311	-4.151455
179	6	0	-9.163464	-4.636637	0.529689
180	6	0	-5.414210	-1.193890	4.980607
181	7	0	-4.617070	-0.029884	5.180796
182	8	0	-4.862327	2.280116	5.409512
183	6	0	-9.128660	-4.718311	-0.898121
184	6	0	-4.922218	-1.176484	-4.090606
185	7	0	-4.110365	-0.009508	-3.995504
186	8	0	-4.305432	2.313911	-4.084724
187	7	0	-8.029593	-4.680375	1.291701
188	8	0	-4.987060	-2.313397	4.899411
189	1	0	-3.574185	-0.067310	5.243027
190	7	0	-7.965678	-4.903011	-1.592201
191	8	0	-4.518668	-2.300552	-3.964134
192	1	0	-3.084321	-0.054881	-3.799517
193	6	0	-6.897886	-4.845640	0.596536
194	6	0	-6.866114	-4.979191	-0.832024
195	6	0	-5.474992	-4.877532	1.121468
196	6	0	-5.422492	-5.152831	-1.279391
197	7	0	-4.677244	-5.037634	-0.050255
198	8	0	-5.046440	-4.781883	2.238394
199	8	0	-4.931350	-5.346354	-2.348487
200	1	0	-3.635613	-5.031464	-0.021295
201	8	0	-2.067316	-4.016554	0.302853
202	6	0	-1.563219	-3.903307	1.424842
203	7	0	-0.319964	-3.346575	1.722459
204	7	0	-2.164006	-4.351600	2.623832
205	6	0	-0.115266	-3.179084	3.182255
206	1	0	0.399362	-3.097503	1.028247
207	6	0	-1.418217	-3.867950	3.814506
208	1	0	-3.168580	-4.569928	2.683977
209	1	0	0.862098	-3.610694	3.510143

210	7	0	-0.251046	-1.765665	3.598382
211	1	0	-1.209884	-4.716378	4.510654
212	7	0	-2.085730	-2.757706	4.535401
213	6	0	-1.455183	-1.516670	4.264298
214	1	0	0.435248	-1.037083	3.355988
215	1	0	-3.080363	-2.816447	4.793568
216	8	0	-1.878657	-0.418032	4.614294
217	1	0	-1.152099	-4.807805	-4.040086
218	6	0	-0.730338	-4.010323	-3.382913
219	6	0	0.686736	-3.430268	-3.863657
220	7	0	-0.447264	-4.567841	-2.037113
221	7	0	-1.605372	-2.807874	-3.310759
222	1	0	1.107598	-3.906329	-4.782571
223	7	0	0.393106	-1.998395	-4.122098
224	7	0	1.556627	-3.649137	-2.690269
225	6	0	0.855828	-4.193115	-1.601096
226	1	0	-1.210425	-4.596169	-1.338500
227	6	0	-0.902160	-1.646746	-3.720209
228	1	0	-2.624119	-2.889289	-3.446631
229	1	0	1.136450	-1.293114	-4.262738
230	1	0	2.561219	-3.445920	-2.688418
231	8	0	1.300315	-4.386551	-0.478341
232	8	0	-1.370187	-0.511497	-3.727299
233	6	0	1.490774	1.540378	-4.346341
234	7	0	0.277031	1.806291	-3.702546
235	7	0	2.145846	2.772334	-4.596672
236	8	0	1.900996	0.436453	-4.694547
237	6	0	0.164865	3.214119	-3.264201
238	1	0	-0.420103	1.083416	-3.471637
239	6	0	1.486912	3.886700	-3.874994
240	1	0	3.144745	2.817536	-4.842508
241	1	0	-0.800280	3.669704	-3.594710
242	7	0	0.363132	3.345267	-1.797921
243	1	0	1.301333	4.744679	-4.566029
244	7	0	2.227229	4.347468	-2.671712
245	6	0	1.607335	3.899409	-1.484576
246	1	0	-0.399725	3.218448	-1.117228
247	1	0	3.238176	4.544494	-2.719521
248	8	0	2.097483	3.989376	-0.355492
249	1	0	-1.160019	3.946339	4.683145
250	6	0	-0.712090	3.460733	3.781721
251	6	0	0.708588	4.051101	3.324728
252	7	0	-1.560090	3.662659	2.588522
253	7	0	-0.409788	2.036764	4.066879
254	1	0	1.102998	4.867984	3.975039
255	7	0	1.597126	2.860163	3.306099
256	7	0	0.450079	4.578369	1.960712
257	6	0	-0.840491	4.184945	1.504757
258	1	0	-2.545477	3.382346	2.546270
259	6	0	0.900483	1.694310	3.703087
260	1	0	-1.148242	1.323081	4.191692
261	1	0	2.616719	2.947463	3.397844
262	1	0	1.227153	4.611212	1.281244
263	8	0	-1.265888	4.364053	0.369591
264	8	0	1.380568	0.564997	3.735831
265	1	0	-1.811787	-2.038975	-0.714300
266	7	0	-1.400343	-1.168625	-0.405450
267	6	0	-2.129989	-0.054313	-0.275840
268	1	0	-0.407132	-1.155599	-0.160402
269	6	0	-3.612270	-0.166319	-0.500884
270	8	0	-1.636723	1.040264	0.020406
271	6	0	-4.300085	-1.380565	-0.464719
272	6	0	-4.324476	1.011765	-0.724538
273	6	0	-5.675740	-1.408364	-0.666107
274	1	0	-3.776354	-2.313218	-0.254354
275	6	0	-5.698430	0.975644	-0.928835
276	1	0	-3.772217	1.945815	-0.737123
277	6	0	-6.394612	-0.235043	-0.901307
278	1	0	-6.205172	-2.356145	-0.638006
279	1	0	-6.242167	1.898579	-1.111133
280	6	0	-7.895105	-0.279716	-1.061843
281	6	0	-8.609148	-0.304981	0.294728
282	1	0	-8.175447	-1.169240	-1.637948
283	1	0	-8.229444	0.592710	-1.632536
284	1	0	-9.694971	-0.345494	0.168393
285	1	0	-8.298525	-1.175259	0.880251
286	1	0	-8.362265	0.589361	0.873230
287	8	0	1.380216	-1.115487	0.396112
288	6	0	1.909587	0.000579	0.476809
289	6	0	3.404502	0.110555	0.596652
290	7	0	1.205191	1.138118	0.450613
291	6	0	4.118150	-1.045009	0.912438
292	6	0	4.103674	1.298881	0.371145
293	1	0	0.190963	1.103116	0.296943
294	1	0	1.647135	2.037569	0.583408
295	6	0	5.504847	-1.012037	1.015255
296	1	0	3.559964	-1.961052	1.076149
297	6	0	5.489019	1.323993	0.473142
298	1	0	3.581252	2.213672	0.090319
299	6	0	6.211101	0.172737	0.796575
300	1	0	6.047895	-1.919529	1.265398
301	1	0	6.023517	2.251609	0.290220
302	6	0	7.719961	0.221646	0.852608
303	6	0	8.339491	0.287697	-0.548963
304	1	0	8.097497	-0.660521	1.379220
305	1	0	8.033167	1.098879	1.430843
306	1	0	9.429899	0.358144	-0.497802
307	1	0	8.076152	-0.603328	-1.125116
308	1	0	7.966951	1.159006	-1.096379

AA-cis, capsule b: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.651117	-2.874483	1.014315
2	6	0	-12.189913	-3.510426	-0.236575
3	6	0	-11.815916	1.836999	-2.174433
4	6	0	-11.192818	1.234099	-3.276222

5	6	0	-11.737889	-0.022339	-3.892802
6	6	0	-11.268034	-1.269305	-3.199465
7	6	0	-11.927539	-1.785406	-2.075770
8	6	0	-11.505666	-2.974612	-1.461968
9	6	0	-12.184836	-1.678764	1.515541
10	6	0	-12.269177	0.182177	3.237461
11	6	0	-11.627885	1.396614	2.627487
12	6	0	-12.089002	1.938202	1.418432
13	6	0	-11.500484	3.079276	0.855757
14	6	0	-11.335692	3.034401	-1.624235
15	6	0	-11.997582	3.669168	-0.434093
16	6	0	-10.416219	-3.659927	-2.033116
17	6	0	-10.159227	-1.985467	-3.693539
18	6	0	-9.712448	-3.182827	-3.139042
19	6	0	-10.648784	-1.756492	3.365392
20	6	0	-10.600053	-3.478377	1.734054
21	6	0	-10.072125	-2.940734	2.907104
22	6	0	-10.058168	1.871234	-3.817162
23	6	0	-10.215797	3.634236	-2.232335
24	6	0	-9.548216	3.069645	-3.319401
25	6	0	-10.429617	3.676398	1.551074
26	6	0	-10.554515	2.045218	3.268989
27	6	0	-9.927327	3.178493	2.752112
28	1	0	-8.671040	3.552704	-3.772697
29	1	0	-12.693629	1.363030	-1.733689
30	1	0	-11.432010	-0.064491	-4.973153
31	1	0	-12.849240	0.010566	-3.919025
32	1	0	-12.784605	-1.249755	-1.666652
33	1	0	-8.853657	-3.726202	-3.557889
34	1	0	-9.254379	-3.434269	3.450785
35	1	0	-13.000804	-1.192927	0.979416
36	1	0	-12.923808	1.460143	0.904775
37	1	0	-9.089426	3.663604	3.272793
38	1	0	-13.102996	3.583522	-0.506855
39	1	0	-11.797605	4.773950	-0.440307
40	1	0	-13.371032	0.207585	3.093806
41	1	0	-12.128617	0.207107	4.351102
42	1	0	-12.045334	-4.622234	-0.182066
43	1	0	-13.290125	-3.373134	-0.307141
44	8	0	-10.173032	-4.750171	1.290384
45	8	0	-10.095609	-4.930495	-1.495853
46	8	0	-10.182578	1.567334	4.549265
47	8	0	-10.261259	-1.225089	4.619761
48	8	0	-9.939883	4.898634	1.036709
49	8	0	-9.824840	4.911094	-1.758345
50	8	0	-9.543781	-1.488460	-4.868065
51	8	0	-9.479553	1.303996	-4.980375
52	6	0	-8.918507	-4.937005	-0.771652
53	6	0	-8.953340	-4.784991	0.649892
54	7	0	-7.818242	-4.792076	1.412186
55	7	0	-7.757514	-5.163447	-1.456407
56	6	0	-6.687246	-5.000746	0.726106
57	6	0	-6.658877	-5.210282	-0.693739
58	6	0	-5.262421	-5.046004	1.248951
59	6	0	-5.220916	-5.446315	-1.132131
60	7	0	-4.473511	-5.313280	0.093486
61	8	0	-4.825937	-4.888040	2.357108
62	1	0	-3.431078	-5.379785	0.125969
63	8	0	-4.739973	-5.697143	-2.193748
64	6	0	-9.044506	-0.575886	4.602490
65	6	0	-9.002462	0.853181	4.562623
66	6	0	-11.693021	-1.093699	2.691221
67	7	0	-7.828718	1.553021	4.615989
68	7	0	-7.914000	-1.337457	4.700261
69	6	0	-8.657889	4.880838	-1.017025
70	6	0	-8.715190	4.816435	0.408478
71	6	0	-8.356070	-0.825975	-4.633128
72	6	0	-8.318445	0.599391	-4.723340
73	7	0	-7.589731	4.764039	1.185273
74	7	0	-7.474922	4.970551	-1.697363
75	7	0	-7.236566	-1.575167	-4.393476
76	7	0	-7.150933	1.305615	-4.628673
77	6	0	-6.774755	-0.638481	4.762603
78	6	0	-6.058429	0.557541	-4.437187
79	6	0	-6.729793	0.795838	4.719391
80	6	0	-6.383995	4.962625	-0.924038
81	6	0	-6.439556	4.827362	0.505168
82	6	0	-6.103505	-0.870758	-4.296545
83	6	0	-4.697281	-1.374683	-4.011071
84	6	0	-4.614766	1.018148	-4.296189
85	6	0	-5.357117	-1.171354	4.838323
86	6	0	-5.276930	1.243666	4.767817
87	6	0	-4.927373	5.034495	-1.358174
88	6	0	-5.018192	4.733480	1.038940
89	7	0	-3.894825	-0.197669	-4.049937
90	7	0	-4.205640	4.886972	-0.123564
91	7	0	-4.548005	0.004824	4.823971
92	8	0	-4.122030	2.105801	-4.337780
93	8	0	-4.288418	-2.477218	-3.770386
94	8	0	-4.423427	5.185912	-2.428664
95	8	0	-4.603155	4.562714	2.150833
96	8	0	-4.932657	-2.292386	4.885192
97	8	0	-4.766126	2.322692	4.757922
98	1	0	-3.505044	-0.036169	4.808480
99	1	0	-3.171052	4.795582	-0.090631
100	1	0	-2.850702	-0.224047	-3.941729
101	1	0	12.865631	0.032481	3.905205
102	6	0	11.754008	0.056953	3.882806
103	6	0	11.272047	1.302087	3.194432
104	6	0	11.216301	-1.201669	3.264129
105	1	0	11.451388	0.093657	4.964251
106	6	0	11.924478	1.826903	2.070621
107	6	0	10.158325	2.007368	3.693042
108	6	0	11.840208	-1.796529	2.158425
109	6	0	10.087876	-1.848609	3.806448
110	6	0	11.490599	3.013726	1.460649
111	1	0	12.785501	1.300036	1.658411
112	6	0	9.698870	3.201453	3.141756
113	8	0	9.551646	1.503107	4.868965
114	6	0	11.366281	-2.995080	1.605272

115	1	0	12.713462	-1.315159	1.716836
116	6	0	9.584032	-3.048271	3.305435
117	8	0	9.509875	-1.289960	4.974047
118	6	0	12.168354	3.559429	0.235998
119	6	0	10.395546	3.687261	2.035162
120	1	0	8.836021	3.736005	3.563628
121	6	0	8.367992	0.832055	4.638202
122	6	0	12.029688	-3.622037	0.411902
123	6	0	10.251754	-3.604167	2.214011
124	1	0	8.711433	-3.538828	3.759525
125	6	0	8.342002	-0.593820	4.724713
126	1	0	13.269871	3.432129	0.304890
127	1	0	12.013420	4.670007	0.184956
128	6	0	11.633956	2.922197	-1.016089
129	8	0	10.061885	4.955755	1.501118
130	7	0	7.241417	1.573094	4.406640
131	6	0	11.527874	-3.031485	-0.875790
132	1	0	11.836124	-4.728002	0.415015
133	1	0	13.134745	-3.530307	0.483340
134	8	0	9.866727	-4.881305	1.735598
135	7	0	7.179644	-1.308943	4.634147
136	6	0	12.177959	1.732718	-1.521247
137	6	0	10.576595	3.518592	-1.732787
138	6	0	8.884236	4.953384	0.777891
139	6	0	6.113404	0.860031	4.313857
140	6	0	12.108793	-1.885172	-1.435593
141	6	0	10.460968	-3.633852	-1.572718
142	6	0	8.698468	-4.853508	0.996222
143	6	0	6.080303	-0.568916	4.450566
144	6	0	11.689816	1.146333	-2.697732
145	1	0	12.999165	1.253057	-0.987577
146	6	0	10.051439	2.978943	-2.906209
147	8	0	10.139359	4.785715	-1.285680
148	6	0	8.919753	4.808537	-0.644380
149	7	0	7.721464	5.165507	1.464237
150	6	0	4.701672	1.353678	4.037731
151	6	0	11.645138	-1.344404	-2.644111
152	1	0	12.939541	-1.402095	-0.920041
153	6	0	9.957731	-3.138203	-2.774201
154	8	0	9.976757	-4.858996	-1.059762
155	6	0	8.752987	-4.782604	-0.429136
156	7	0	7.517095	-4.951338	1.678203
157	6	0	4.639478	-1.040541	4.316379
158	6	0	12.276887	-0.122461	-3.249006
159	6	0	10.638149	1.801183	-3.368216
160	1	0	9.228167	3.466173	-3.447248
161	7	0	7.784451	4.810802	-1.406388
162	6	0	6.622179	5.206877	0.702158
163	7	0	3.908554	0.170394	4.078158
164	8	0	4.283174	2.453553	3.801645
165	6	0	10.578369	-2.000305	-3.289092
166	1	0	9.124053	-3.628467	-3.296794
167	7	0	7.625826	-4.729572	-1.203489
168	6	0	6.424715	-4.943673	0.906966
169	8	0	4.156005	-2.132254	4.357108
170	1	0	12.136987	-0.143973	-4.362787
171	1	0	13.378823	-0.139408	-3.104902
172	8	0	10.254271	1.269051	-4.623214
173	6	0	6.651943	5.006449	-0.718980
174	6	0	5.182247	5.427088	1.142370
175	1	0	2.863226	0.189183	3.977892
176	8	0	10.205554	-1.524333	-4.569953
177	6	0	6.477120	-4.799935	-0.521542
178	6	0	4.969193	-5.023649	1.343421
179	6	0	9.044361	0.607613	-4.608134
180	6	0	5.226691	5.043455	-1.241457
181	7	0	4.435755	5.295527	-0.083798
182	8	0	4.699372	5.666343	2.205827
183	6	0	9.017964	-0.822170	-4.583552
184	6	0	5.054363	-4.706208	-1.051351
185	7	0	4.244493	-4.868519	0.111171
186	8	0	4.467761	-5.185194	2.413495
187	7	0	7.905348	1.357822	-4.694559
188	8	0	4.791123	4.890421	-2.350571
189	1	0	3.392727	5.352737	-0.115608
190	7	0	7.852411	-1.534354	-4.649598
191	8	0	4.636661	-4.528473	-2.161488
192	1	0	3.208403	-4.783975	0.080477
193	6	0	6.773975	0.646940	-4.765534
194	6	0	6.745260	-0.788182	-4.745296
195	6	0	5.350171	1.164634	-4.829443
196	6	0	5.297876	-1.251947	-4.805037
197	7	0	4.554274	-0.020224	-4.834527
198	8	0	4.914352	2.282117	-4.855644
199	8	0	4.800161	-2.336671	-4.821975
200	1	0	3.511274	0.008406	-4.814165
201	8	0	1.986105	0.341111	-3.847154
202	6	0	1.451822	1.454073	-3.793565
203	7	0	0.194614	1.744032	-3.267671
204	7	0	2.029793	2.646797	-4.281728
205	6	0	-0.048392	3.203681	-3.164967
206	1	0	-0.494248	1.039304	-2.965237
207	6	0	1.248910	3.838092	-3.863079
208	1	0	3.021798	2.720081	-4.542231
209	1	0	-1.027512	3.487020	-3.623839
210	7	0	0.056491	3.683305	-1.768829
211	1	0	1.036596	4.495400	-4.740772
212	7	0	1.885224	4.620223	-2.774573
213	6	0	1.246036	4.379185	-1.530824
214	1	0	-0.640502	3.460049	-1.042867
215	1	0	2.882561	4.871715	-2.826354
216	8	0	1.652087	4.772404	-0.439924
217	1	0	1.430414	-4.140147	-4.775093
218	6	0	0.990300	-3.515981	-3.961142
219	6	0	-0.404297	-4.059145	-3.383859
220	7	0	0.654204	-2.169683	-4.491754
221	7	0	1.868787	-3.434963	-2.762765
222	1	0	-0.795444	-4.979988	-3.880551
223	7	0	-0.092841	-4.342919	-1.961097
224	7	0	-1.316444	-2.910478	-3.564217

225	6	0	-0.660232	-1.787883	-4.097459
226	1	0	1.387358	-1.443615	-4.503095
227	6	0	1.190621	-3.896401	-1.606506
228	1	0	2.889076	-3.543035	-2.855028
229	1	0	-0.836056	-4.488064	-1.254916
230	1	0	-2.324256	-2.961373	-3.386809
231	8	0	-1.148588	-0.679596	-4.263020
232	8	0	1.663365	-3.910542	-0.474676
233	6	0	-1.275865	-4.430319	1.543681
234	7	0	-0.082094	-3.742862	1.783612
235	7	0	-1.918026	-4.669595	2.786865
236	8	0	-1.684288	-4.818098	0.451765
237	6	0	0.027286	-3.269331	3.181491
238	1	0	0.622251	-3.532668	1.060809
239	6	0	-1.277253	-3.892542	3.876592
240	1	0	-2.919693	-4.904974	2.835317
241	1	0	1.002891	-3.564340	3.640325
242	7	0	-0.199461	-1.807607	3.290360
243	1	0	-1.072574	-4.551911	4.754516
244	7	0	-2.048617	-2.694414	4.292517
245	6	0	-1.456700	-1.506667	3.810183
246	1	0	0.490592	-1.108702	2.977594
247	1	0	-3.038878	-2.757522	4.560637
248	8	0	-1.979983	-0.388679	3.864755
249	1	0	0.776100	4.930500	3.893315
250	6	0	0.389987	4.005189	3.401123
251	6	0	-0.999359	3.454708	3.983498
252	7	0	1.310225	2.863161	3.582789
253	7	0	0.072979	4.281050	1.978051
254	1	0	-1.442375	4.079733	4.795158
255	7	0	-1.880380	3.359580	2.787324
256	7	0	-0.652706	2.113419	4.520131
257	6	0	0.662827	1.738092	4.122073
258	1	0	2.317820	2.921842	3.407024
259	6	0	-1.207380	3.822615	1.627716
260	1	0	0.813463	4.430738	1.270066
261	1	0	-2.899682	3.474649	2.883934
262	1	0	-1.381242	1.382479	4.531534
263	8	0	1.158255	0.633273	4.288897
264	8	0	-1.681285	3.826335	0.496484
265	1	0	8.072796	0.326773	1.253894
266	6	0	8.405680	-0.084169	0.297751
267	6	0	7.718795	-1.426019	0.018887
268	1	0	9.492976	-0.198643	0.329391
269	1	0	8.160689	0.644806	-0.479759
270	6	0	6.215360	-1.290662	-0.015889
271	1	0	8.074786	-1.824609	-0.938902
272	1	0	8.002031	-2.144925	0.794203
273	6	0	5.583921	-0.718518	-1.122834
274	6	0	5.429409	-1.678197	1.071943
275	6	0	4.206794	-0.526647	-1.141337
276	1	0	6.182101	-0.412289	-1.976422
277	6	0	4.053640	-1.481386	1.063857
278	1	0	5.903221	-2.137635	1.937373
279	6	0	3.432301	-0.902737	-0.041532
280	1	0	3.742645	-0.051192	-2.004927
281	1	0	3.438649	-1.769721	1.911159
282	6	0	1.954080	-0.651125	0.029630
283	8	0	1.402729	-0.538139	1.132807
284	7	0	1.292981	-0.534946	-1.127350
285	1	0	1.751568	-0.705740	-2.013788
286	1	0	0.312587	-0.242374	-1.127801
287	8	0	-1.428774	0.476227	-1.125566
288	6	0	-1.981155	0.592896	-0.023213
289	6	0	-3.455980	0.863823	0.044737
290	7	0	-1.325709	0.460929	1.135220
291	6	0	-4.064424	1.467689	-1.054260
292	6	0	-4.239941	0.481886	1.135591
293	1	0	-0.345383	0.168361	1.136810
294	1	0	-1.780509	0.648043	2.020460
295	6	0	-5.437439	1.682669	-1.065222
296	1	0	-3.441973	1.761043	-1.894393
297	6	0	-5.614339	0.692065	1.114215
298	1	0	-3.784590	-0.011992	1.993140
299	6	0	-6.233199	1.289378	0.013345
300	1	0	-5.901501	2.160439	-1.926029
301	1	0	-6.220348	0.380681	1.960362
302	6	0	-7.734342	1.447139	-0.025232
303	6	0	-8.441040	0.118361	-0.316626
304	1	0	-8.003795	2.176122	-0.796011
305	1	0	-8.087442	1.844289	0.934268
306	1	0	-9.526300	0.250268	-0.351445
307	1	0	-8.111172	-0.290573	-1.274633
308	1	0	-8.210838	-0.620287	0.456215

AB-trans, capsule b: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.925079	-2.069288	-1.830301
2	6	0	-12.461499	-1.252321	-2.972650
3	6	0	-11.845160	3.042475	0.729594
4	6	0	-11.299554	3.743052	-0.357869
5	6	0	-11.909467	3.642108	-1.726529
6	6	0	-11.460556	2.408323	-2.459162
7	6	0	-12.149771	1.192127	-2.362694
8	6	0	-11.745918	0.063641	-3.093085
9	6	0	-12.418290	-1.911886	-0.526964
10	6	0	-12.449775	-2.502273	1.938998
11	6	0	-11.720473	-1.414984	2.677506
12	6	0	-12.103113	-0.069801	2.570667
13	6	0	-11.423154	0.944258	3.261011
14	6	0	-11.270575	3.105962	2.005832
15	6	0	-11.862138	2.378673	3.179760
16	6	0	-10.644479	0.200568	-3.959469
17	6	0	-10.333920	2.456792	-3.306008
18	6	0	-9.902084	1.376525	-4.070991
19	6	0	-10.929234	-3.630593	0.258238

20	6	0	-10.918494	-3.033816	-2.039165
21	6	0	-10.397377	-3.825094	-1.015979
22	6	0	-10.170165	4.550232	-0.122070
23	6	0	-10.124054	3.909318	2.165561
24	6	0	-9.557290	4.646208	1.128432
25	6	0	-10.333633	0.568256	4.071977
26	6	0	-10.635881	-1.721163	3.522422
27	6	0	-9.915803	-0.753293	4.221539
28	1	0	-8.669691	5.275242	1.287772
29	1	0	-12.731317	2.426403	0.573676
30	1	0	-11.629491	4.549381	-2.326186
31	1	0	-13.018420	3.678494	-1.663021
32	1	0	-13.017309	1.119676	-1.706479
33	1	0	-9.029183	1.451434	-4.734181
34	1	0	-9.613965	-4.571910	-1.207711
35	1	0	-13.199724	-1.174682	-0.339009
36	1	0	-12.948814	0.194054	1.934578
37	1	0	-9.067292	-1.018428	4.867828
38	1	0	-12.971902	2.444519	3.155411
39	1	0	-11.568597	2.906986	4.126697
40	1	0	-13.542951	-2.303134	1.927603
41	1	0	-12.343135	-3.469113	2.499286
42	1	0	-12.346983	-1.828676	-3.929019
43	1	0	-13.556490	-1.098339	-2.865979
44	8	0	-10.519719	-3.271635	-3.374429
45	8	0	-10.362477	-0.890998	-4.814847
46	8	0	-10.340988	-3.091149	3.727334
47	8	0	-10.541215	-4.484812	1.318130
48	8	0	-9.707462	1.579532	4.841058
49	8	0	-9.579057	4.008403	3.471287
50	8	0	-9.710644	3.715758	-3.452387
51	8	0	-9.675285	5.345493	-1.188975
52	6	0	-9.204763	-1.568821	-4.488412
53	6	0	-9.280924	-2.768590	-3.715327
54	7	0	-8.171824	-3.499691	-3.391801
55	7	0	-8.026667	-1.093212	-4.992788
56	6	0	-7.023953	-3.018421	-3.885843
57	6	0	-6.953276	-1.833912	-4.694358
58	6	0	-5.618297	-3.562015	-3.704090
59	6	0	-5.505378	-1.588783	-5.092383
60	7	0	-4.797038	-2.665327	-4.446419
61	8	0	-5.215082	-4.512867	-3.089907
62	1	0	-3.758082	-2.756956	-4.488787
63	8	0	-4.993995	-0.754462	-5.773317
64	6	0	-9.295156	-4.212194	1.842905
65	6	0	-9.193434	-3.512080	3.085741
66	6	0	-11.926721	-2.676586	0.540888
67	7	0	-7.997008	-3.301944	3.712630
68	7	0	-8.199902	-4.704262	1.189953
69	6	0	-8.434856	3.249668	3.627978
70	6	0	-8.499309	2.003364	4.322149
71	6	0	-8.527757	3.883824	-2.770708
72	6	0	-8.493265	4.829927	-1.699430
73	7	0	-7.389912	1.237043	4.557028
74	7	0	-7.259817	3.758195	3.146851
75	7	0	-7.406839	3.228937	-3.201425
76	7	0	-7.320762	5.276680	-1.159270
77	6	0	-7.036009	-4.494198	1.817121
78	6	0	-6.221273	4.696180	-1.655445
79	6	0	-6.934727	-3.805326	3.072287
80	6	0	-6.183193	3.004303	3.391057
81	6	0	-6.244975	1.753064	4.094369
82	6	0	-6.272139	3.628579	-2.614106
83	6	0	-4.866328	3.075989	-2.792840
84	6	0	-4.765030	4.973579	-1.305845
85	6	0	-5.642073	-4.875865	1.358227
86	6	0	-5.471760	-3.733112	3.478869
87	6	0	-4.746157	3.266032	2.968258
88	6	0	-4.843737	1.165979	4.156998
89	7	0	-4.050584	3.940135	-2.012726
90	7	0	-4.037804	2.124285	3.476438
91	7	0	-4.789886	-4.390747	2.396394
92	8	0	-4.256148	5.826847	-0.647776
93	8	0	-4.482573	2.107327	-3.391509
94	8	0	-4.245781	4.162588	2.360104
95	8	0	-4.426413	0.147798	4.638851
96	8	0	-5.259528	-5.445136	0.373025
97	8	0	-4.925494	-3.268841	4.433719
98	1	0	-3.750749	-4.458367	2.348582
99	1	0	-3.013694	1.992193	3.333367
100	1	0	-3.010111	3.831382	-1.955384
101	1	0	13.093642	-3.658729	1.581683
102	6	0	11.983983	-3.640082	1.645834
103	6	0	11.519369	-2.452376	2.441146
104	6	0	11.376644	-3.676029	0.272552
105	1	0	11.716918	-4.581753	2.195959
106	6	0	12.185042	-1.220252	2.390379
107	6	0	10.404258	-2.558377	3.297062
108	6	0	11.922408	-2.930523	-0.783369
109	6	0	10.249796	-4.474592	-0.001741
110	6	0	11.764230	-0.128826	3.165557
111	1	0	13.047877	-1.105754	1.733447
112	6	0	9.950593	-1.513930	4.098916
113	8	0	9.813544	-3.838480	3.408429
114	6	0	11.356358	-2.950382	-2.065624
115	1	0	12.804112	-2.315309	-0.599901
116	6	0	9.646084	-4.530113	-1.258194
117	8	0	9.764106	-5.313419	1.035644
118	6	0	12.466838	1.197631	3.099937
119	6	0	10.663343	-0.316823	4.023509
120	1	0	9.084026	-1.630528	4.764327
121	6	0	8.619518	-4.000266	2.745236
122	6	0	11.955284	-2.170655	-3.200975
123	6	0	10.218531	-3.756837	-2.267191
124	1	0	8.766215	-5.161077	-1.448181
125	6	0	8.586553	-4.840222	1.586128
126	1	0	13.565081	1.057518	3.005145
127	1	0	12.333320	1.740051	4.073713
128	6	0	11.940665	2.048837	1.978353
129	8	0	10.349112	0.739580	4.911719

130	7	0	7.489479	-3.441207	3.274273
131	6	0	11.518910	-0.733096	-3.217379
132	1	0	11.666505	-2.653562	-4.173559
133	1	0	13.064906	-2.239438	-3.174347
134	8	0	9.691956	-3.832076	-3.581653
135	7	0	7.414468	-5.242935	1.012723
136	6	0	12.457701	1.949850	0.678853
137	6	0	10.920917	2.993898	2.208401
138	6	0	9.192593	1.418674	4.582612
139	6	0	6.350964	-3.810370	2.672917
140	6	0	12.200001	0.252914	-2.490845
141	6	0	10.426438	-0.325118	-4.009446
142	6	0	8.538684	-3.082016	-3.732747
143	6	0	6.310879	-4.746433	1.586259
144	6	0	11.977907	2.756234	-0.362873
145	1	0	13.250845	1.229908	0.473907
146	6	0	10.402837	3.817994	1.209794
147	8	0	10.510444	3.173127	3.549809
148	6	0	9.273461	2.647739	3.856637
149	7	0	8.007560	0.913642	5.040663
150	6	0	4.934973	-3.347323	2.966585
151	6	0	11.819423	1.601889	-2.552975
152	1	0	13.044144	-0.033827	-1.862878
153	6	0	10.015735	1.001725	-4.121435
154	8	0	9.805216	-1.317682	-4.803946
155	6	0	8.603210	-1.776394	-4.307728
156	7	0	7.355920	-3.657705	-3.358804
157	6	0	4.862801	-5.012642	1.212820
158	6	0	12.535081	2.654888	-1.755141
159	6	0	10.960773	3.684047	-0.061153
160	1	0	9.608663	4.548575	1.418185
161	7	0	8.165031	3.382563	3.539798
162	6	0	6.933912	1.657409	4.749343
163	7	0	4.130316	-4.106929	2.066442
164	8	0	4.513418	-2.517339	3.724601
165	6	0	10.745180	1.944731	-3.396682
166	1	0	9.171281	1.290412	-4.762755
167	7	0	7.494219	-0.988677	-4.461987
168	6	0	6.275319	-2.895599	-3.558510
169	8	0	4.356739	-5.761433	0.436448
170	1	0	12.437770	3.647258	-2.270530
171	1	0	13.628033	2.457361	-1.730308
172	8	0	10.603999	4.587771	-1.087017
173	6	0	7.012430	2.874936	3.992905
174	6	0	5.477744	1.385580	5.097089
175	1	0	3.091098	-4.053633	2.065543
176	8	0	10.483745	3.323641	-3.578924
177	6	0	6.346179	-1.559908	-4.081272
178	6	0	4.821650	-3.228915	-3.255774
179	6	0	9.378533	4.366400	-1.677211
180	6	0	5.608687	3.419619	3.803127
181	7	0	4.777218	2.483749	4.485399
182	8	0	4.954184	0.510073	5.716379
183	6	0	9.323141	3.760880	-2.971654
184	6	0	4.945169	-0.963784	-4.079470
185	7	0	4.119478	-2.033157	-3.615676
186	8	0	4.313973	-4.212172	-2.805344
187	7	0	8.262974	4.839929	-1.044732
188	8	0	5.214867	4.392051	3.219382
189	1	0	3.734509	2.568320	4.505974
190	7	0	8.161904	3.665126	-3.686307
191	8	0	4.557582	0.137445	-4.347645
192	1	0	3.078108	-1.944572	-3.522455
193	6	0	7.132150	4.730895	-1.753151
194	6	0	7.084648	4.169584	-3.072923
195	6	0	5.722454	5.114892	-1.338283
196	6	0	5.650511	4.219643	-3.581967
197	7	0	4.921802	4.769977	-2.465503
198	8	0	5.308588	5.581319	-0.312431
199	8	0	5.164622	3.911995	-4.625395
200	1	0	3.880123	4.837189	-2.454437
201	8	0	2.294391	4.116588	-1.699445
202	6	0	1.817017	4.449139	-0.616115
203	7	0	0.578295	4.060808	-0.099844
204	7	0	2.430343	5.338548	0.300742
205	6	0	0.364917	4.537721	1.284306
206	1	0	-0.145251	3.565892	-0.646604
207	6	0	1.682567	5.403614	1.578238
208	1	0	3.428567	5.579386	0.252654
209	1	0	-0.601806	5.089047	1.386756
210	7	0	0.461156	3.437347	2.273424
211	1	0	1.490755	6.466608	1.864112
212	7	0	2.329767	4.682916	2.704368
213	6	0	1.661828	3.467125	2.987727
214	1	0	-0.259399	2.714432	2.388913
215	1	0	3.331516	4.811076	2.903264
216	8	0	2.054048	2.611862	3.781177
217	1	0	1.067008	2.110300	-5.582145
218	6	0	0.701055	1.657021	-4.627376
219	6	0	-0.739314	0.954961	-4.728379
220	7	0	0.497112	2.716559	-3.609162
221	7	0	1.598416	0.546681	-4.224141
222	1	0	-1.174760	0.918555	-5.756608
223	7	0	-0.479774	-0.414132	-4.215041
224	7	0	-1.582853	1.777944	-3.837700
225	6	0	-0.807755	2.678706	-3.076556
226	1	0	1.281070	3.140231	-3.088580
227	6	0	0.851953	-0.591892	-3.833686
228	1	0	2.523918	0.739955	-3.828631
229	1	0	-1.207580	-1.135163	-4.109026
230	1	0	-2.523015	1.483005	-3.550835
231	8	0	-1.233462	3.405185	-2.182360
232	8	0	1.330417	-1.614496	-3.336902
233	6	0	-1.627603	-3.693113	-3.023786
234	7	0	-0.403988	-3.677099	-2.343579
235	7	0	-2.325606	-4.878753	-2.673487
236	8	0	-2.018042	-2.861103	-3.836334
237	6	0	-0.302128	-4.757389	-1.338520
238	1	0	0.335432	-2.972077	-2.509704
239	6	0	-1.679000	-5.560113	-1.530040

240	1	0	-3.339120	-4.976679	-2.838498
241	1	0	0.626765	-5.361985	-1.477851
242	7	0	-0.407621	-4.247963	0.051173
243	1	0	-1.560865	-6.651122	-1.739571
244	7	0	-2.380248	-5.360180	-0.233169
245	6	0	-1.671805	-4.476104	0.603358
246	1	0	0.352161	-3.769464	0.543644
247	1	0	-3.395372	-5.518057	-0.146360
248	8	0	-2.085408	-4.013365	1.671022
249	1	0	1.154020	-1.127357	5.952293
250	6	0	0.738208	-1.080639	4.916961
251	6	0	-0.669878	-1.824343	4.712883
252	7	0	1.624168	-1.749895	3.932686
253	7	0	0.439087	0.319701	4.543300
254	1	0	-1.095913	-2.283221	5.636670
255	7	0	-1.548971	-0.778813	4.127919
256	7	0	-0.355599	-2.888733	3.721960
257	6	0	0.931978	-2.709848	3.177800
258	1	0	2.646016	-1.662734	3.953899
259	6	0	-0.845855	0.448645	3.983364
260	1	0	1.192890	0.999402	4.326532
261	1	0	-2.563063	-0.782816	4.315023
262	1	0	-1.110904	-3.315386	3.156109
263	8	0	1.395605	-3.305874	2.204310
264	8	0	-1.292761	1.464244	3.468535
265	1	0	-8.740700	-0.465223	-0.977535
266	6	0	-8.936324	-0.763157	0.056193
267	6	0	-8.123942	0.096201	1.028605
268	1	0	-10.009884	-0.658379	0.240664
269	1	0	-8.666960	-1.818443	0.151287
270	6	0	-6.637332	-0.038823	0.802536
271	1	0	-8.418218	1.145224	0.909554
272	1	0	-8.362045	-0.186283	2.060140
273	6	0	-5.820357	-0.679369	1.732637
274	6	0	-6.050617	0.462807	-0.364775
275	6	0	-4.452237	-0.807912	1.503040
276	1	0	-6.254664	-1.061271	2.655490
277	6	0	-4.685712	0.338667	-0.584361
278	1	0	-6.675184	0.959741	-1.104312
279	6	0	-3.854284	-0.298558	0.347379
280	1	0	-3.844585	-1.291717	2.270865
281	1	0	-4.237573	0.744169	-1.488418
282	5	0	-2.302673	-0.358468	0.095776
283	8	0	-1.489911	-1.213740	0.815230
284	8	0	-1.760376	0.448816	-0.834444
285	1	0	-1.971191	-1.818367	1.396450
286	1	0	-0.781499	0.427615	-0.907841
287	8	0	0.991806	0.569784	-1.059397
288	6	0	1.771671	-0.214269	-0.505491
289	6	0	3.252601	-0.072266	-0.692169
290	7	0	1.352665	-1.218647	0.277468
291	6	0	3.747819	1.162634	-1.115431
292	6	0	4.142188	-1.123219	-0.465207
293	1	0	0.357013	-1.298817	0.478404
294	1	0	2.000475	-1.741344	0.849339
295	6	0	5.113547	1.339009	-1.284734
296	1	0	3.045275	1.971141	-1.307170
297	6	0	5.509627	-0.939477	-0.649062
298	1	0	3.773691	-2.107673	-0.185187
299	6	0	6.015385	0.294940	-1.056528
300	1	0	5.493578	2.300261	-1.615208
301	1	0	6.191830	-1.767478	-0.479035
302	6	0	7.498501	0.518884	-1.226295
303	6	0	8.105350	1.257418	-0.028321
304	1	0	7.676011	1.089406	-2.145972
305	1	0	8.000577	-0.445212	-1.352254
306	1	0	9.178920	1.414839	-0.162718
307	1	0	7.628213	2.231709	0.116056
308	1	0	7.956040	0.679951	0.887960

BB-cis, capsule b: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.999958	-1.745010	2.127730
2	6	0	12.536881	-0.747408	3.115440
3	6	0	11.956401	2.833406	-1.276360
4	6	0	11.471797	3.739962	-0.319346
5	6	0	12.113006	3.861551	1.033745
6	6	0	11.628957	2.793163	1.975347
7	6	0	12.282377	1.558682	2.090750
8	6	0	11.843521	0.580213	2.995663
9	6	0	12.498156	-1.819050	0.818648
10	6	0	12.541045	-2.841894	-1.502568
11	6	0	11.797549	-1.917643	-2.425113
12	6	0	12.153816	-0.566292	-2.549474
13	6	0	11.440367	0.307079	-3.382531
14	6	0	11.322755	2.665956	-2.514809
15	6	0	11.860405	1.737377	-3.565913
16	6	0	10.733880	0.885331	3.807592
17	6	0	10.506375	3.017800	2.798650
18	6	0	10.031068	2.086987	3.719507
19	6	0	11.002758	-3.642664	0.341309
20	6	0	10.989030	-2.653863	2.497956
21	6	0	10.463800	-3.607707	1.626297
22	6	0	10.358742	4.528671	-0.665250
23	6	0	10.172741	3.440757	-2.767950
24	6	0	9.681132	4.391526	-1.877955
25	6	0	10.339656	-0.217621	-4.089217
26	6	0	10.717970	-2.385714	-3.198823
27	6	0	9.959505	-1.556750	-4.025255
28	1	0	8.798330	5.000168	-2.119349
29	1	0	12.838882	2.236604	-1.043506
30	1	0	11.881971	4.870370	1.468343
31	1	0	13.220393	3.838731	0.947043
32	1	0	13.150727	1.353231	1.464093
33	1	0	9.155754	2.293734	4.350693
34	1	0	9.676735	-4.306730	1.942389

35	1	0	13.282841	-1.128446	0.507725
36	1	0	13.002974	-0.185615	-1.980828
37	1	0	9.107646	-1.939833	-4.604618
38	1	0	12.969975	1.809210	-3.607778
39	1	0	11.517452	2.091075	-4.575999
40	1	0	13.631103	-2.628993	-1.524749
41	1	0	12.449390	-3.896696	-1.874866
42	1	0	12.403838	-1.145083	4.156760
43	1	0	13.635535	-0.630767	2.997425
44	8	0	10.587346	-2.652037	3.854463
45	8	0	10.409030	-0.042727	4.824804
46	8	0	10.464023	-3.778945	-3.187628
47	8	0	10.632834	-4.674631	-0.550968
48	8	0	9.643601	0.651763	-4.968194
49	8	0	9.529063	3.270886	-4.021545
50	8	0	9.938253	4.310140	2.749601
51	8	0	9.939293	5.533075	0.247212
52	6	0	9.254726	-0.761813	4.592472
53	6	0	9.345905	-2.095048	4.084485
54	7	0	8.244967	-2.885274	3.905822
55	7	0	8.063655	-0.191245	4.946667
56	6	0	7.086977	-2.315750	4.261914
57	6	0	6.995932	-0.981355	4.783486
58	6	0	5.688943	-2.900853	4.179054
59	6	0	5.535562	-0.661668	5.068908
60	7	0	4.847042	-1.862432	4.674018
61	8	0	5.306292	-3.972260	3.795007
62	1	0	3.805916	-1.951798	4.709627
63	8	0	5.002044	0.309141	5.512234
64	6	0	9.393961	-4.533268	-1.136821
65	6	0	9.312893	-4.121386	-2.503961
66	6	0	12.008425	-2.758735	-0.099103
67	7	0	8.136250	-4.116083	-3.199154
68	7	0	8.290178	-4.895328	-0.416544
69	6	0	8.409820	2.465230	-3.929195
70	6	0	8.465179	1.126155	-4.423762
71	6	0	8.750086	4.425826	2.068019
72	6	0	8.742760	5.182374	0.853810
73	7	0	7.374626	0.300001	-4.423296
74	7	0	7.267692	3.002292	-3.400871
75	7	0	7.606129	3.913454	2.613936
76	7	0	7.585763	5.589817	0.254520
77	6	0	7.143689	-4.873907	-1.107630
78	6	0	6.468102	5.150554	0.846261
79	6	0	7.068779	-4.508953	-2.493356
80	6	0	6.209163	2.184522	-3.408740
81	6	0	6.258863	0.845964	-3.925411
82	6	0	6.482471	4.261654	1.973361
83	6	0	5.057988	3.809605	2.249014
84	6	0	5.026396	5.421455	0.445803
85	6	0	5.743287	-5.183368	-0.610681
86	6	0	5.622323	-4.612537	-2.954823
87	6	0	4.807781	2.455562	-2.881060
88	6	0	4.884003	0.216042	-3.771575
89	7	0	4.274974	4.553200	1.320377
90	7	0	4.096660	1.247734	-3.176677
91	7	0	4.917316	-4.994802	-1.756778
92	8	0	4.543650	6.169749	-0.345817
93	8	0	4.628204	2.994070	3.018202
94	8	0	4.342983	3.404477	-2.321614
95	8	0	4.478468	-0.879130	-4.046754
96	8	0	5.351998	-5.504278	0.478131
97	8	0	5.109847	-4.448807	-4.018676
98	1	0	3.876806	-5.077934	-1.718530
99	1	0	3.077173	1.129579	-2.972775
100	1	0	3.243964	4.446735	1.250719
101	1	0	-13.088432	-3.799209	-0.644080
102	6	0	-11.982475	-3.826144	-0.747037
103	6	0	-11.509563	-2.774846	-1.712626
104	6	0	-11.321312	-3.684487	0.594054
105	1	0	-11.760472	-4.842615	-1.168414
106	6	0	-12.164651	-1.542739	-1.845013
107	6	0	-10.396113	-3.017556	-2.543233
108	6	0	-11.786128	-2.754685	1.537990
109	6	0	-10.210402	-4.476232	0.941222
110	6	0	-11.738562	-0.584973	-2.777591
111	1	0	-13.024819	-1.323973	-1.211705
112	6	0	-9.934340	-2.108332	-3.491577
113	8	0	-9.829575	-4.308648	-2.474674
114	6	0	-11.139921	-2.569432	2.768126
115	1	0	-12.663435	-2.151697	1.301171
116	6	0	-9.530644	-4.332650	2.150900
117	8	0	-9.796874	-5.492608	0.039738
118	6	0	-12.429689	0.741781	-2.921738
119	6	0	-10.641194	-0.910780	-3.598170
120	1	0	-9.068659	-2.329304	-4.131039
121	6	0	-8.629033	-4.420267	-1.815080
122	6	0	-11.652583	-1.598078	3.793196
123	6	0	-10.005291	-3.362809	3.031035
124	1	0	-8.654362	-4.949391	2.397521
125	6	0	-8.607166	-5.156145	-0.587923
126	1	0	-13.525738	0.633851	-2.775304
127	1	0	-12.318617	1.106961	-3.977470
128	6	0	-11.866750	1.767115	-1.977739
129	8	0	-10.332146	-0.004552	-4.638699
130	7	0	-7.489745	-3.940494	-2.399241
131	6	0	-11.223863	-0.176937	3.558405
132	1	0	-11.296993	-1.920291	4.809576
133	1	0	-12.761931	-1.658604	3.853901
134	8	0	-9.334611	-3.180743	4.270885
135	7	0	-7.443087	-5.573799	-0.009857
136	6	0	-12.330906	1.875499	-0.658579
137	6	0	-10.865303	2.665379	-2.396019
138	6	0	-9.171141	0.712776	-4.436167
139	6	0	-6.356361	-4.305543	-1.784732
140	6	0	-11.949186	0.689966	2.728689
141	6	0	-10.093868	0.348086	4.217473
142	6	0	-8.202294	-2.400251	4.103137
143	6	0	-6.331938	-5.171775	-0.640309
144	6	0	-11.813293	2.832796	0.225240

145	1	0	-13.111142	1.197028	-0.311814
146	6	0	-10.310281	3.632500	-1.558012
147	8	0	-10.492989	2.633651	-3.761240
148	6	0	-9.254373	2.067340	-3.991098
149	7	0	-7.983188	0.113713	-4.752376
150	6	0	-4.927237	-3.912406	-2.120444
151	6	0	-11.573646	2.032291	2.562812
152	1	0	-12.822106	0.312327	2.195573
153	6	0	-9.696674	1.679316	4.117591
154	8	0	-9.372554	-0.520121	5.076763
155	6	0	-8.233601	-1.023906	4.479739
156	7	0	-7.086461	-2.988548	3.574870
157	6	0	-4.885932	-5.481894	-0.283543
158	6	0	-12.319137	2.950639	1.636131
159	6	0	-10.809817	3.696694	-0.258264
160	1	0	-9.526175	4.318609	-1.909239
161	7	0	-8.149831	2.862258	-3.859795
162	6	0	-6.911389	0.903754	-4.625929
163	7	0	-4.136132	-4.657755	-1.205579
164	8	0	-4.497579	-3.137531	-2.934266
165	6	0	-10.466569	2.501648	3.295710
166	1	0	-8.819155	2.059339	4.659712
167	7	0	-7.163778	-0.189722	4.298198
168	6	0	-6.041117	-2.168033	3.423910
169	8	0	-4.399508	-6.232555	0.502441
170	1	0	-12.203460	4.010769	1.986183
171	1	0	-13.411907	2.756449	1.681083
172	8	0	-10.393435	4.739824	0.599854
173	6	0	-6.995785	2.268649	-4.185894
174	6	0	-5.451927	0.554151	-4.873518
175	1	0	-3.099506	-4.585861	-1.179560
176	8	0	-10.190310	3.889271	3.241919
177	6	0	-6.084377	-0.774557	3.766749
178	6	0	-4.675836	-2.487816	2.836303
179	6	0	-9.143433	4.578723	1.159087
180	6	0	-5.594510	2.848798	-4.136983
181	7	0	-4.758832	1.773730	-4.565053
182	8	0	-4.922329	-0.453831	-5.234270
183	6	0	-9.043706	4.191251	2.531209
184	6	0	-4.758026	-0.138529	3.381873
185	7	0	-3.988498	-1.230821	2.874900
186	8	0	-4.221994	-3.501308	2.394179
187	7	0	-8.046287	4.901067	0.409469
188	8	0	-5.200444	3.939487	-3.827299
189	1	0	-3.716106	1.848527	-4.594015
190	7	0	-7.853544	4.171656	3.203165
191	8	0	-4.387576	1.001081	3.418910
192	1	0	-2.981611	-1.138341	2.613318
193	6	0	-6.885644	4.862695	1.076101
194	6	0	-6.791850	4.523396	2.468209
195	6	0	-5.487504	5.135358	0.549685
196	6	0	-5.336185	4.610936	2.903617
197	7	0	-4.646049	4.959723	1.686824
198	8	0	-5.103727	5.429650	-0.549490
199	8	0	-4.809428	4.466476	3.963222
200	1	0	-3.609416	5.066355	1.639532
201	8	0	-1.835262	4.886345	1.040310
202	6	0	-1.492563	4.926880	-0.139098
203	7	0	-0.277495	4.449714	-0.652014
204	7	0	-2.224588	5.531722	-1.187816
205	6	0	-0.220261	4.524810	-2.129301
206	1	0	0.509906	4.135839	-0.068612
207	6	0	-1.590331	5.270888	-2.506073
208	1	0	-3.244095	5.673463	-1.117179
209	1	0	0.710070	5.035547	-2.477635
210	7	0	-0.372919	3.199192	-2.772499
211	1	0	-1.460745	6.231839	-3.061915
212	7	0	-2.305527	4.282003	-3.344990
213	6	0	-1.630030	3.038449	-3.365802
214	1	0	0.330305	2.447375	-2.719402
215	1	0	-3.317540	4.362717	-3.519828
216	8	0	-2.058367	2.012246	-3.888649
217	1	0	-1.014283	2.998345	4.744234
218	6	0	-0.566611	2.392920	3.918828
219	6	0	0.818469	1.660880	4.280715
220	7	0	-0.204284	3.247150	2.761290
221	7	0	-1.467593	1.273644	3.554635
222	1	0	1.171633	1.797311	5.330328
223	7	0	0.530329	0.239055	3.987743
224	7	0	1.770887	2.250776	3.309070
225	6	0	1.118460	3.046148	2.357748
226	1	0	-0.894698	3.815457	2.235424
227	6	0	-0.741455	0.062645	3.429277
228	1	0	-2.308692	1.450355	2.984017
229	1	0	1.230645	-0.517119	4.072439
230	1	0	2.775294	2.050804	3.302477
231	8	0	1.631559	3.488407	1.321968
232	8	0	-1.194786	-0.987529	2.979529
233	6	0	1.717606	-3.178497	3.448028
234	7	0	0.484489	-3.317706	2.799698
235	7	0	2.427717	-4.397074	3.337935
236	8	0	2.094578	-2.194185	4.082499
237	6	0	0.408266	-4.564862	2.004301
238	1	0	-0.209772	-2.556004	2.722341
239	6	0	1.777816	-5.314952	2.371342
240	1	0	3.432578	-4.468613	3.548686
241	1	0	-0.524654	-5.132420	2.242383
242	7	0	0.534212	-4.333494	0.547168
243	1	0	1.649791	-6.328289	2.823942
244	7	0	2.476432	-5.420922	1.066417
245	6	0	1.788259	-4.709473	0.054445
246	1	0	-0.181195	-3.851745	-0.010893
247	1	0	3.491426	-5.588747	1.021577
248	8	0	2.204104	-4.526298	-1.089235
249	1	0	-1.164510	-1.949534	-5.483391
250	6	0	-0.751762	-1.800295	-4.457313
251	6	0	0.660052	-2.514318	-4.192656
252	7	0	-1.643233	-2.353205	-3.398502
253	7	0	-0.456218	-0.364324	-4.236854
254	1	0	1.077081	-3.074658	-5.064857

255	7	0	1.538745	-1.395349	-3.792809
256	7	0	0.367618	-3.457718	-3.083371
257	6	0	-0.930543	-3.275744	-2.574995
258	1	0	-2.641145	-2.515773	-3.605530
259	6	0	0.839328	-0.179267	-3.708548
260	1	0	-1.213312	0.313414	-4.037072
261	1	0	2.548433	-1.496574	-3.653001
262	1	0	1.134568	-3.808158	-2.473719
263	8	0	-1.396659	-3.822154	-1.584795
264	8	0	1.310252	0.884412	-3.312263
265	1	0	2.877720	-2.163602	-1.043971
266	6	0	3.501879	-1.340719	-0.699331
267	6	0	2.885054	-0.190144	-0.189416
268	6	0	4.885875	-1.437880	-0.774013
269	6	0	3.712200	0.845592	0.260634
270	5	0	1.318730	-0.092246	-0.181534
271	6	0	5.704271	-0.393746	-0.335576
272	1	0	5.344401	-2.331732	-1.188050
273	6	0	5.098658	0.747908	0.191688
274	1	0	3.277612	1.755750	0.682916
275	8	0	0.664369	1.103827	0.052321
276	8	0	0.580742	-1.196264	-0.429300
277	6	0	7.207469	-0.525110	-0.383094
278	1	0	5.720560	1.563069	0.553051
279	1	0	1.261219	1.865052	0.095221
280	1	0	-0.359421	-0.972904	-0.562657
281	6	0	7.757104	-1.206804	0.874920
282	1	0	7.659174	0.467184	-0.484036
283	1	0	7.495649	-1.100057	-1.269562
284	1	0	8.845650	-1.300846	0.830968
285	1	0	7.493963	-0.625890	1.762920
286	1	0	7.329847	-2.208117	0.991997
287	1	0	-1.151648	1.337435	0.417938
288	8	0	-2.122357	1.362535	0.518578
289	5	0	-2.730627	0.530765	-0.360562
290	6	0	-4.296993	0.491643	-0.448347
291	8	0	-1.928519	-0.271572	-1.142683
292	6	0	-4.986254	-0.322671	-1.353527
293	6	0	-5.060506	1.291443	0.413379
294	1	0	-2.401749	-0.833703	-1.768720
295	6	0	-6.376746	-0.347276	-1.398775
296	1	0	-4.446170	-0.965623	-2.054273
297	6	0	-6.448474	1.266442	0.376030
298	1	0	-4.544268	1.929795	1.126867
299	6	0	-7.127492	0.446912	-0.531373
300	1	0	-6.883016	-0.996411	-2.112563
301	1	0	-7.021645	1.887870	1.059616
302	6	0	-8.635414	0.386087	-0.525375
303	6	0	-9.164717	-0.457376	0.639364
304	1	0	-8.990515	-0.035430	-1.471784
305	1	0	-9.044070	1.400636	-0.453669
306	1	0	-10.258372	-0.495397	0.631069
307	1	0	-8.785090	-1.480426	0.577052
308	1	0	-8.846054	-0.035970	1.596803

BC-trans, capsule b: oniom(m062x/6-31g(d,p):pm6):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.738227	-1.192351	-2.077987
2	6	0	-12.260950	0.001797	-2.824780
3	6	0	-11.464240	2.590118	2.160435
4	6	0	-11.012240	3.662353	1.374979
5	6	0	-11.745623	4.090097	0.134396
6	6	0	-11.321779	3.262573	-1.047851
7	6	0	-11.961484	2.055811	-1.366381
8	6	0	-11.548175	1.271782	-2.453180
9	6	0	-12.209341	-1.522531	-0.798206
10	6	0	-12.241069	-3.006030	1.260248
11	6	0	-11.445968	-2.329523	2.340631
12	6	0	-11.723389	-1.011203	2.737433
13	6	0	-10.930586	-0.347129	3.683821
14	6	0	-10.742779	2.141279	3.275891
15	6	0	-11.253530	1.040194	4.161208
16	6	0	-10.457117	1.734279	-3.216073
17	6	0	-10.261551	3.682131	-1.876442
18	6	0	-9.793406	2.931658	-2.954190
19	6	0	-10.746680	-3.432259	-0.740305
20	6	0	-10.771262	-2.035562	-2.658809
21	6	0	-10.246869	-3.154320	-2.010701
22	6	0	-9.834128	4.321067	1.776860
23	6	0	-9.535936	2.803674	3.577509
24	6	0	-9.066890	3.903777	2.864131
25	6	0	-9.835359	-1.053010	4.221459
26	6	0	-10.383604	-2.998524	2.977234
27	6	0	-9.552717	-2.380434	3.911686
28	1	0	-8.132155	4.411528	3.142141
29	1	0	-12.393922	2.088542	1.890081
30	1	0	-11.535904	5.172850	-0.072122
31	1	0	-12.844487	4.037412	0.284083
32	1	0	-12.798375	1.718572	-0.754094
33	1	0	-8.950140	3.270360	-3.573150
34	1	0	-9.486132	-3.791323	-2.483747
35	1	0	-12.967639	-0.892671	-0.331911
36	1	0	-12.568025	-0.487949	2.288178
37	1	0	-8.706549	-2.908632	4.373834
38	1	0	-12.352618	1.145774	4.302326
39	1	0	-10.823796	1.176975	5.190913
40	1	0	-13.321135	-2.764176	1.353143
41	1	0	-12.185047	-4.118925	1.393686
42	1	0	-12.148938	-0.173988	-3.928427
43	1	0	-13.356170	0.110283	-2.668322
44	8	0	-10.390560	-1.765755	-3.996759
45	8	0	-10.106541	0.983530	-4.362620
46	8	0	-10.187706	-4.371418	2.680994
47	8	0	-10.363481	-4.621241	-0.079962
48	8	0	-8.997335	-0.380171	5.151682
49	8	0	-8.785142	2.348588	4.695440

50	8	0	-9.744358	4.975612	-1.640988
51	8	0	-9.462494	5.492301	1.073608
52	6	0	-8.978072	0.204316	-4.218912
53	6	0	-9.127606	-1.210413	-4.092607
54	7	0	-8.061005	-2.064947	-4.121846
55	7	0	-7.751601	0.806584	-4.301250
56	6	0	-6.871871	-1.466697	-4.248218
57	6	0	-6.714515	-0.038474	-4.304825
58	6	0	-5.501906	-2.114533	-4.322543
59	6	0	-5.228675	0.282833	-4.349926
60	7	0	-4.603407	-1.003412	-4.393580
61	8	0	-5.162195	-3.264019	-4.337218
62	1	0	-3.566048	-1.128488	-4.445469
63	8	0	-4.633625	1.322654	-4.343729
64	6	0	-9.118147	-4.608485	0.507504
65	6	0	-9.038796	-4.578123	1.934955
66	6	0	-11.726015	-2.641096	-0.105119
67	7	0	-7.867768	-4.778216	2.609428
68	7	0	-8.008595	-4.733619	-0.280858
69	6	0	-7.754253	1.516807	4.297235
70	6	0	-7.865039	0.112641	4.527510
71	6	0	-8.478632	5.007428	-1.093665
72	6	0	-8.333243	5.316209	0.292906
73	7	0	-6.887789	-0.769870	4.154701
74	7	0	-6.658559	2.075918	3.697610
75	7	0	-7.404584	4.828834	-1.920331
76	7	0	-7.112105	5.499159	0.879411
77	6	0	-6.862177	-4.890723	0.394472
78	6	0	-6.068832	5.344172	0.055181
79	6	0	-6.795892	-4.954413	1.826456
80	6	0	-5.708557	1.203515	3.343875
81	6	0	-5.824087	-0.210785	3.567216
82	6	0	-6.214853	4.994438	-1.329992
83	6	0	-4.833809	4.818938	-1.942928
84	6	0	-4.586329	5.438973	0.387408
85	6	0	-5.453479	-5.012755	-0.158879
86	6	0	-5.351847	-5.195045	2.245558
87	6	0	-4.399065	1.479943	2.622704
88	6	0	-4.595181	-0.896294	2.993760
89	7	0	-3.946434	5.080214	-0.847423
90	7	0	-3.814103	0.181212	2.476160
91	7	0	-4.637113	-5.197174	0.990729
92	8	0	-4.011239	5.752986	1.385653
93	8	0	-4.488244	4.540370	-3.052211
94	8	0	-3.909974	2.493085	2.214178
95	8	0	-4.285545	-2.053256	2.926086
96	8	0	-5.053013	-4.958153	-1.291177
97	8	0	-4.850391	-5.379189	3.310729
98	1	0	-3.598602	-5.278165	0.931589
99	1	0	-2.851793	0.039476	2.093486
100	1	0	-2.929759	4.923578	-0.924241
101	1	0	13.424082	-3.127281	0.588527
102	6	0	12.325598	-3.287615	0.628494
103	6	0	11.698718	-2.447879	1.706511
104	6	0	11.696960	-3.012577	-0.707882
105	1	0	12.206041	-4.373976	0.884317
106	6	0	12.193621	-1.177245	2.030301
107	6	0	10.596905	-2.931352	2.441669
108	6	0	12.103357	-1.922952	-1.493188
109	6	0	10.675913	-3.842206	-1.209710
110	6	0	11.614985	-0.405402	3.048271
111	1	0	13.049079	-0.781456	1.481889
112	6	0	9.974995	-2.203575	3.454817
113	8	0	10.228730	-4.272671	2.203811
114	6	0	11.488280	-1.631821	-2.718530
115	1	0	12.912087	-1.283495	-1.137433
116	6	0	10.018201	-3.588183	-2.413916
117	8	0	10.371271	-5.021262	-0.485678
118	6	0	12.157909	0.947135	3.414250
119	6	0	10.517679	-0.951472	3.743105
120	1	0	9.116875	-2.604436	4.011915
121	6	0	9.063342	-4.478312	1.502161
122	6	0	11.956995	-0.498830	-3.586180
123	6	0	10.437658	-2.473025	-3.136596
124	1	0	9.212316	-4.239427	-2.780711
125	6	0	9.146783	-4.954805	0.156564
126	1	0	13.266182	0.961213	3.332243
127	1	0	11.952115	1.149505	4.499273
128	6	0	11.551460	2.038804	2.578850
129	8	0	10.050563	-0.224435	4.862398
130	7	0	7.869710	-4.339558	2.155072
131	6	0	11.380830	0.833782	-3.200415
132	1	0	11.685238	-0.719139	-4.654175
133	1	0	13.068640	-0.451497	-3.586476
134	8	0	9.832259	-2.196727	-4.390775
135	7	0	8.054917	-5.413421	-0.524637
136	6	0	12.067246	2.366575	1.316388
137	6	0	10.452921	2.782267	3.052563
138	6	0	8.847782	0.422518	4.681677
139	6	0	6.804266	-4.759883	1.461700
140	6	0	11.967691	1.635808	-2.211861
141	6	0	10.247709	1.342924	-3.865949
142	6	0	8.625193	-1.536997	-4.251254
143	6	0	6.902202	-5.336853	0.151183
144	6	0	11.505248	3.388590	0.538774
145	1	0	12.923167	1.811795	0.930421
146	6	0	9.850851	3.805147	2.319738
147	8	0	10.026640	2.530223	4.379187
148	6	0	8.836375	1.835389	4.461758
149	7	0	7.698752	-0.305373	4.826185
150	6	0	5.335914	-4.701591	1.857139
151	6	0	11.454270	2.902981	-1.895649
152	1	0	12.840352	1.265510	-1.672912
153	6	0	9.712438	2.603968	-3.612072
154	8	0	9.687505	0.546914	-4.897907
155	6	0	8.554279	-0.130650	-4.493806
156	7	0	7.525175	-2.276018	-3.912142
157	6	0	5.515370	-5.770166	-0.305041
158	6	0	12.061955	3.746555	-0.810955
159	6	0	10.403959	4.088364	1.072005

160	1	0	8.994464	4.370301	2.713184
161	7	0	7.676930	2.557622	4.411508
162	6	0	6.571918	0.414608	4.779306
163	7	0	4.661149	-5.324137	0.766181
164	8	0	4.804157	-4.226727	2.821255
165	6	0	10.347578	3.367420	-2.632523
166	1	0	8.836809	2.978369	-4.160774
167	7	0	7.386575	0.573262	-4.382458
168	6	0	6.387209	-1.578136	-3.823451
169	8	0	5.146388	-6.352443	-1.276834
170	1	0	11.861305	4.830496	-1.022234
171	1	0	13.169522	3.659349	-0.816503
172	8	0	9.939143	5.200294	0.333013
173	6	0	6.562571	1.837299	4.585068
174	6	0	5.135945	-0.075283	4.897252
175	1	0	3.622144	-5.386898	0.717841
176	8	0	9.937047	4.705094	-2.414757
177	6	0	6.320110	-0.162386	-4.048792
178	6	0	5.003501	-2.081476	-3.439486
179	6	0	8.739326	5.017513	-0.319526
180	6	0	5.123284	2.320452	4.588719
181	7	0	4.362245	1.130302	4.787212
182	8	0	4.673336	-1.167280	5.035614
183	6	0	8.738974	4.813910	-1.735396
184	6	0	4.893412	0.300581	-3.807136
185	7	0	4.194912	-0.894509	-3.468818
186	8	0	4.610345	-3.169674	-3.144825
187	7	0	7.583948	5.149804	0.399141
188	8	0	4.654725	3.417010	4.454250
189	1	0	3.316303	1.132259	4.803541
190	7	0	7.588059	4.797793	-2.472522
191	8	0	4.404563	1.396602	-3.845090
192	1	0	3.162486	-0.910017	-3.303266
193	6	0	6.464418	5.120898	-0.334958
194	6	0	6.466492	4.969520	-1.762209
195	6	0	5.025882	5.220017	0.140157
196	6	0	5.031346	5.009591	-2.266135
197	7	0	4.257894	5.149843	-1.057441
198	8	0	4.567427	5.314977	1.246413
199	8	0	4.566155	4.954667	-3.362640
200	1	0	3.214360	5.181221	-1.056433
201	8	0	1.497105	4.673584	-0.546853
202	6	0	1.064741	4.567662	0.598624
203	7	0	-0.113759	3.909039	0.970333
204	7	0	1.650048	5.151238	1.749069
205	6	0	-0.283907	3.847101	2.442242
206	1	0	-0.813439	3.558384	0.303738
207	6	0	0.978721	4.676006	2.986783
208	1	0	2.650525	5.399373	1.764402
209	1	0	-1.284646	4.238059	2.755405
210	7	0	-0.059943	2.490140	2.993316
211	1	0	0.720587	5.545010	3.639309
212	7	0	1.759092	3.662786	3.732565
213	6	0	1.198215	2.375165	3.606836
214	1	0	-0.589381	1.662007	2.673399
215	1	0	2.708556	3.838101	4.079430
216	8	0	1.702069	1.340799	4.036363
217	1	0	0.970740	3.648614	-4.617362
218	6	0	0.515093	2.890954	-3.937133
219	6	0	-0.763664	2.126259	-4.529132
220	7	0	-0.015037	3.549056	-2.717166
221	7	0	1.451904	1.788544	-3.592560
222	1	0	-1.114536	2.488852	-5.524660
223	7	0	-0.306499	0.719764	-4.626644
224	7	0	-1.792643	2.320617	-3.475546
225	6	0	-1.289871	3.043524	-2.387058
226	1	0	0.640354	3.877869	-1.981193
227	6	0	0.913673	0.528971	-3.941281
228	1	0	2.464528	1.949893	-3.527470
229	1	0	-0.997339	-0.054310	-4.678507
230	1	0	-2.780695	2.087176	-3.614871
231	8	0	-1.876951	3.228558	-1.315327
232	8	0	1.431543	-0.555354	-3.700284
233	6	0	-1.496996	-2.713958	-3.916670
234	7	0	-0.242759	-2.986544	-3.355562
235	7	0	-2.241441	-3.912499	-3.982843
236	8	0	-1.869221	-1.633387	-4.372662
237	6	0	-0.171997	-4.357268	-2.795466
238	1	0	0.462234	-2.261596	-3.165255
239	6	0	-1.572018	-5.004668	-3.236897
240	1	0	-3.254114	-3.921605	-4.162310
241	1	0	0.735723	-4.889591	-3.172066
242	7	0	-0.235905	-4.398347	-1.316850
243	1	0	-1.479616	-5.913933	-3.880537
244	7	0	-2.220265	-5.364215	-1.950348
245	6	0	-1.470609	-4.866998	-0.850162
246	1	0	0.515133	-4.030590	-0.720049
247	1	0	-3.249865	-5.406812	-1.894486
248	8	0	-1.824514	-4.938346	0.324426
249	1	0	1.440978	-2.845196	4.830511
250	6	0	1.051743	-2.696592	3.795652
251	6	0	-0.288811	-3.507711	3.445104
252	7	0	2.009198	-3.156934	2.761355
253	7	0	0.652742	-1.285924	3.582264
254	1	0	-0.711830	-4.108024	4.286626
255	7	0	-1.232513	-2.441863	3.027518
256	7	0	0.124632	-4.399397	2.336365
257	6	0	1.415505	-4.065807	1.861982
258	1	0	3.021357	-3.057004	2.871134
259	6	0	-0.613079	-1.181284	2.990014
260	1	0	1.309999	-0.496827	3.641964
261	1	0	-2.168660	-2.636367	2.666869
262	1	0	-0.594319	-4.782856	1.690376
263	8	0	1.935426	-4.512402	0.847132
264	8	0	-1.124921	-0.147917	2.559354
265	1	0	-8.935385	-0.801345	-1.075606
266	6	0	-8.446626	0.082541	-0.652278
267	6	0	-6.950578	-0.047690	-0.789763
268	6	0	-8.862948	0.242038	0.814365
269	1	0	-8.795031	0.951134	-1.222928

270	6	0	-6.140779	1.090485	-0.799705
271	6	0	-6.337551	-1.301602	-0.843416
272	1	0	-9.949735	0.335344	0.905684
273	1	0	-8.541892	-0.622085	1.402032
274	1	0	-8.407134	1.136847	1.247717
275	6	0	-4.756581	0.972946	-0.834519
276	1	0	-6.604030	2.074502	-0.784528
277	6	0	-4.952549	-1.414992	-0.876606
278	1	0	-6.956529	-2.196564	-0.858839
279	6	0	-4.132290	-0.279869	-0.859085
280	1	0	-4.162079	1.891266	-0.848598
281	1	0	-4.484884	-2.395623	-0.912475
282	5	0	-2.574011	-0.453136	-0.804885
283	8	0	-1.739574	0.631185	-0.599497
284	8	0	-2.030560	-1.680315	-0.914012
285	1	0	-2.191127	1.487869	-0.523388
286	1	0	-1.057241	-1.686796	-0.807784
287	1	0	-0.103613	0.577327	-0.222464
288	8	0	0.873770	0.598448	-0.052298
289	6	0	1.389044	-0.601765	-0.229419
290	6	0	2.859851	-0.656249	-0.015870
291	8	0	0.728358	-1.586129	-0.539655
292	6	0	3.525082	-1.871393	-0.191068
293	6	0	3.576120	0.479661	0.363281
294	6	0	4.896520	-1.937885	0.009026
295	1	0	2.953262	-2.753853	-0.471350
296	6	0	4.947486	0.394802	0.578706
297	1	0	3.051890	1.420127	0.493728
298	6	0	5.625292	-0.813973	0.412060
299	1	0	5.412435	-2.880668	-0.143748
300	1	0	5.499183	1.278185	0.886358
301	6	0	7.112151	-0.920829	0.658513
302	6	0	7.905331	-1.236234	-0.613514
303	1	0	7.292390	-1.701157	1.408946
304	1	0	7.473581	0.016241	1.092523
305	1	0	8.973716	-1.320275	-0.396071
306	1	0	7.574992	-2.178407	-1.061986
307	1	0	7.768221	-0.444714	-1.353662

AA-trans, capsule a: M062X/6-31g(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.870315	-0.162012	0.222239
2	7	0	-2.186533	-1.300468	0.381449
3	1	0	-1.164963	-1.287453	0.291261
4	1	0	-2.645204	-2.174145	0.593286
5	6	0	-6.455357	0.821724	0.842877
6	6	0	-5.072708	0.872358	0.720243
7	6	0	-4.367286	-0.253313	0.283511
8	6	0	-5.060538	-1.404394	-0.085657
9	6	0	-6.448960	-1.439715	0.018016
10	6	0	-7.157111	-0.343034	0.506205
11	1	0	-6.997416	1.680351	1.238105
12	1	0	-4.513211	1.759720	0.998985
13	1	0	-4.518557	-2.252778	-0.492361
14	1	0	-7.001904	-2.326219	-0.280523
15	6	0	-8.654267	-0.394490	0.617220
16	6	0	-9.329454	0.387529	-0.503422
17	1	0	-8.969788	0.023773	1.578548
18	1	0	-8.992316	-1.437878	0.590443
19	1	0	-10.417099	0.308713	-0.424208
20	1	0	-9.059937	1.451059	-0.470020
21	1	0	-9.027099	-0.012260	-1.477866
22	8	0	-2.339090	0.939339	0.028289
23	6	0	4.885295	1.176965	-0.290444
24	6	0	3.498907	1.202279	-0.158156
25	6	0	2.780657	0.004467	-0.039785
26	6	0	3.487182	-1.203133	-0.022646
27	6	0	4.876188	-1.211833	-0.140031
28	6	0	5.600402	-0.025954	-0.301559
29	1	0	5.426263	2.109454	-0.428367
30	1	0	2.997644	2.169738	-0.167388
31	1	0	2.924306	-2.130676	0.057894
32	1	0	5.404778	-2.161347	-0.169582
33	6	0	7.099665	-0.022625	-0.532424
34	6	0	7.925964	0.404113	0.687182
35	1	0	7.326358	0.668001	-1.356320
36	1	0	7.419889	-1.020225	-0.859805
37	1	0	8.990826	0.460328	0.436930
38	1	0	7.609807	1.390506	1.046794
39	1	0	7.810160	-0.314994	1.505986
40	8	0	0.719307	-1.176677	0.055648
41	1	0	1.024244	1.974109	-0.082576
42	1	0	-0.437417	1.036845	0.056453
43	7	0	0.584687	1.084266	0.113179
44	6	0	1.270947	-0.071699	0.037290
45	6	0	-10.995900	-0.667151	-3.264486
46	6	0	-11.528503	0.678798	-3.721821
47	6	0	-11.708410	1.632426	1.934678
48	6	0	-11.160534	2.836190	1.493484
49	6	0	-11.824016	3.656054	0.398827
50	6	0	-11.237538	3.360074	-0.967328
51	6	0	-11.681585	2.280447	-1.737266
52	6	0	-11.044469	1.870282	-2.910213
53	6	0	-11.665718	-1.420652	-2.298893
54	6	0	-11.939513	-3.412737	-0.751207
55	6	0	-11.378997	-3.105554	0.623343
56	6	0	-11.806204	-2.000513	1.363716
57	6	0	-11.227244	-1.636613	2.579978
58	6	0	-11.133953	0.866129	2.950367
59	6	0	-11.740153	-0.452633	3.377829
60	6	0	-9.929631	2.611386	-3.306708
61	6	0	-10.174221	4.108185	-1.474758
62	6	0	-9.514838	3.751649	-2.641516
63	6	0	-10.016683	-3.141628	-2.399580

64	6	0	-9.817049	-1.208896	-3.779593
65	6	0	-9.318256	-2.439763	-3.370718
66	6	0	-9.977958	3.257837	2.110985
67	6	0	-9.969335	1.354877	3.543585
68	6	0	-9.375237	2.543521	3.138564
69	6	0	-10.156926	-2.412779	3.032262
70	6	0	-10.372064	-3.892109	1.182427
71	6	0	-9.745525	-3.560884	2.376505
72	1	0	-8.473358	2.910075	3.616955
73	1	0	-12.632846	1.281733	1.478906
74	1	0	-11.708633	4.718531	0.622522
75	1	0	-12.892592	3.422652	0.389691
76	1	0	-12.536517	1.706442	-1.381307
77	1	0	-8.667832	4.325518	-2.998794
78	1	0	-8.408071	-2.842452	-3.800376
79	1	0	-12.595242	-1.029465	-1.888495
80	1	0	-12.622482	-1.395153	0.972136
81	1	0	-8.941536	-4.170384	2.772910
82	1	0	-12.825119	-0.396635	3.248675
83	1	0	-11.534359	-0.619827	4.436540
84	1	0	-12.995357	-3.128915	-0.779966
85	1	0	-11.867968	-4.484878	-0.943297
86	1	0	-11.254596	0.833047	-4.767535
87	1	0	-12.620825	0.650211	-3.663135
88	8	0	-9.122127	-0.484353	-4.750140
89	8	0	-9.189967	2.169914	-4.403614
90	8	0	-9.983130	-5.047459	0.507628
91	8	0	-9.604593	-4.422961	-2.047653
92	8	0	-9.500971	-2.027286	4.198694
93	8	0	-9.417108	0.626402	4.597454
94	8	0	-9.737958	5.237426	-0.782154
95	8	0	-9.473177	4.498297	1.749510
96	6	0	-8.050208	1.521246	-4.046030
97	6	0	-8.001762	0.117393	-4.271801
98	7	0	-6.938164	-0.611826	-4.005237
99	7	0	-7.057546	2.189161	-3.492115
100	6	0	-5.933916	0.083431	-3.479588
101	6	0	-5.998414	1.434443	-3.207294
102	6	0	-4.577394	-0.420173	-3.076180
103	6	0	-4.689420	1.847808	-2.583640
104	7	0	-3.905704	0.712079	-2.610774
105	8	0	-4.155588	-1.544599	-3.129987
106	1	0	-2.981488	0.627885	-2.178725
107	8	0	-4.365116	2.938684	-2.170564
108	6	0	-8.491410	-4.601992	-1.292905
109	6	0	-8.702645	-5.003189	0.056630
110	6	0	-11.199147	-2.650396	-1.834215
111	7	0	-7.722289	-5.299631	0.881147
112	7	0	-7.287642	-4.467463	-1.815175
113	6	0	-8.252105	-0.009987	4.303651
114	6	0	-8.303241	-1.405922	4.024913
115	6	0	-8.473158	5.104158	-0.295303
116	6	0	-8.331082	4.594933	1.025422
117	7	0	-7.248618	-2.092784	3.630242
118	7	0	-7.133546	0.681936	4.271924
119	7	0	-7.447146	5.420356	-1.054628
120	7	0	-7.160932	4.308100	1.559167
121	6	0	-6.300147	-4.752851	-0.961592
122	6	0	-6.128158	4.598840	0.763372
123	6	0	-6.515098	-5.164150	0.340190
124	6	0	-6.070428	-0.038232	3.926014
125	6	0	-6.125825	-1.374682	3.581821
126	6	0	-6.268425	5.172003	-0.485888
127	6	0	-4.896776	5.456503	-1.040029
128	6	0	-4.649355	4.437249	1.038773
129	6	0	-4.805298	-4.627357	-1.162890
130	6	0	-5.186668	-5.359254	1.019467
131	6	0	-4.657957	0.442504	3.760776
132	6	0	-4.736877	-1.801781	3.156889
133	7	0	-4.022518	5.002905	-0.049246
134	7	0	-3.946997	-0.689900	3.361514
135	7	0	-4.252234	-4.979971	0.055737
136	8	0	-4.118647	3.921563	1.997396
137	8	0	-4.595094	5.975419	-2.078408
138	8	0	-4.212541	1.549393	3.908208
139	8	0	-4.368972	-2.872314	2.723046
140	8	0	-4.203084	-4.265219	-2.145964
141	8	0	-4.959048	-5.757046	2.128010
142	1	0	-3.236633	-4.947834	0.247305
143	1	0	-2.967978	-0.573677	3.063396
144	1	0	-2.994955	5.034917	-0.166528
145	1	0	13.149054	-3.316001	0.154600
146	6	0	12.083890	-3.563798	0.137071
147	6	0	11.408102	-2.897663	1.319904
148	6	0	11.483865	-3.090769	-1.170402
149	1	0	11.982470	-4.647308	0.218203
150	6	0	11.902779	-1.713054	1.862251
151	6	0	10.253486	-3.433782	1.897231
152	6	0	11.912952	-1.911802	-1.782399
153	6	0	10.436476	-3.782265	-1.778327
154	6	0	11.297006	-1.062856	2.938237
155	1	0	12.808386	-1.284010	1.437206
156	6	0	9.624464	-2.840221	2.982099
157	8	0	9.793610	-4.651788	1.409348
158	6	0	11.301163	-1.385528	-2.919787
159	1	0	12.755825	-1.376609	-1.348158
160	6	0	9.785014	-3.296440	-2.903636
161	8	0	10.034511	-4.998351	-1.227937
162	6	0	11.866454	0.224870	3.498410
163	6	0	10.160169	-1.660074	3.483670
164	1	0	8.741250	-3.285064	3.426025
165	6	0	8.645926	-4.688130	0.685403
166	6	0	11.809374	-0.120408	-3.585606
167	6	0	10.207971	-2.087676	-3.431292
168	1	0	8.955952	-3.836213	-3.346711
169	6	0	8.779291	-4.958594	-0.705183
170	1	0	12.951413	0.211222	3.358194
171	1	0	11.667269	0.268872	4.571077
172	6	0	11.321640	1.481175	2.844017
173	8	0	9.568363	-1.055589	4.595884

174	7	0	7.476456	-4.532737	1.272703
175	6	0	11.224866	1.153825	-3.011944
176	1	0	11.589192	-0.168141	-4.653947
177	1	0	12.896411	-0.085527	-3.467093
178	8	0	9.537043	-1.559422	-4.533331
179	7	0	7.749395	-5.133088	-1.504028
180	6	0	11.899996	2.021074	1.695440
181	6	0	10.227538	2.163728	3.379107
182	6	0	8.398479	-0.428336	4.314203
183	6	0	6.439864	-4.685528	0.445559
184	6	0	11.839337	1.816425	-1.948527
185	6	0	10.061158	1.722463	-3.530689
186	6	0	8.352713	-0.957799	-4.253791
187	6	0	6.574661	-4.996992	-0.894264
188	6	0	11.434751	3.191189	1.092179
189	1	0	12.745776	1.504482	1.244718
190	6	0	9.768847	3.363034	2.859358
191	8	0	9.584497	1.618803	4.489718
192	6	0	8.416101	0.990518	4.201207
193	7	0	7.314885	-1.146651	4.107795
194	6	0	4.961576	-4.559060	0.744100
195	6	0	11.328204	2.988413	-1.394935
196	1	0	12.763834	1.408199	-1.544255
197	6	0	9.507725	2.888838	-3.016520
198	8	0	9.468018	1.110203	-4.636180
199	6	0	8.308318	0.461209	-4.362874
200	7	0	7.307508	-1.679710	-3.899620
201	6	0	5.203472	-5.112084	-1.505981
202	6	0	12.006707	3.673076	-0.224615
203	6	0	10.384259	3.860888	1.719642
204	1	0	8.938181	3.886362	3.318504
205	7	0	7.369098	1.688703	3.808261
206	6	0	6.261002	-0.424029	3.740617
207	7	0	4.335086	-4.773664	-0.468797
208	8	0	4.424941	-4.320820	1.799979
209	6	0	10.148920	3.496140	-1.946584
210	1	0	8.605785	3.314093	-3.441901
211	7	0	7.205224	1.156963	-4.184827
212	6	0	6.204094	-0.959961	-3.698575
213	8	0	4.900153	-5.437595	-2.620777
214	1	0	11.881630	4.754024	-0.307368
215	1	0	13.076445	3.447458	-0.255717
216	8	0	9.942718	5.070003	1.182857
217	6	0	6.291874	0.945134	3.566259
218	6	0	4.899305	-0.922249	3.355352
219	1	0	3.299834	-4.814443	-0.578740
220	8	0	9.678205	4.703734	-1.445414
221	6	0	6.152632	0.410153	-3.862631
222	6	0	4.840100	-1.428186	-3.247507
223	6	0	8.681943	5.006363	0.676533
224	6	0	4.953900	1.377104	3.016813
225	7	0	4.211771	0.220332	2.948767
226	8	0	4.476750	-2.046470	3.380187
227	6	0	8.538856	4.722640	-0.710992
228	6	0	4.761340	0.877503	-3.546275
229	7	0	4.069608	-0.283729	-3.214197
230	8	0	4.483780	-2.550113	-2.969955
231	7	0	7.656669	5.178129	1.482546
232	8	0	4.594017	2.490036	2.699693
233	1	0	3.244715	0.122475	2.625984
234	7	0	7.367133	4.541807	-1.285563
235	8	0	4.324882	1.998326	-3.565160
236	1	0	3.114452	-0.201462	-2.854731
237	6	0	6.477767	5.023515	0.883795
238	6	0	6.337361	4.693951	-0.450763
239	6	0	5.108040	5.135758	1.501887
240	6	0	4.863018	4.535118	-0.738763
241	7	0	4.237940	4.800947	0.462957
242	8	0	4.805827	5.457494	2.617260
243	8	0	4.325103	4.227840	-1.776668
244	1	0	3.216058	4.688398	0.570986
245	8	0	1.589068	4.264091	0.528331
246	6	0	1.050693	3.951678	1.603582
247	7	0	-0.170050	4.374641	2.017698
248	7	0	1.587667	3.132880	2.542346
249	6	0	-0.635626	3.611294	3.150136
250	1	0	-0.790779	4.768826	1.313967
251	6	0	0.674438	2.898811	3.644924
252	1	0	2.584311	2.926913	2.560602
253	1	0	-1.104655	4.255760	3.896222
254	7	0	-1.483745	2.494673	2.804244
255	1	0	1.071080	3.301806	4.579276
256	7	0	0.256654	1.526961	3.795332
257	6	0	-0.939810	1.308073	3.161865
258	1	0	-2.471794	2.594209	2.593035
259	1	0	0.926622	0.758889	3.709811
260	8	0	-1.429977	0.188663	2.984680
261	1	0	1.219922	4.581270	-3.857222
262	6	0	0.777179	4.057762	-3.006926
263	6	0	-0.575897	3.345583	-3.343912
264	7	0	0.401657	4.985777	-1.966422
265	7	0	1.615049	2.950511	-2.583256
266	1	0	-1.044306	3.706729	-4.262976
267	7	0	-0.185787	1.964900	-3.461253
268	7	0	-1.381611	3.671613	-2.183312
269	6	0	-0.812227	4.642452	-1.426080
270	1	0	1.095129	5.275034	-1.285034
271	6	0	1.057921	1.755365	-2.935278
272	1	0	2.630356	3.030872	-2.558908
273	1	0	-0.836320	1.184702	-3.349471
274	1	0	-2.369457	3.443447	-2.091839
275	8	0	-1.309290	5.172743	-0.427460
276	8	0	1.582482	0.647622	-2.815732
277	6	0	-0.956137	-1.492915	-2.762459
278	7	0	0.175415	-1.699657	-3.505238
279	7	0	-1.503008	-2.699666	-2.433188
280	8	0	-1.410149	-0.384442	-2.478036
281	6	0	0.540115	-3.090987	-3.546102
282	1	0	0.853285	-0.939546	-3.492831
283	6	0	-0.753027	-3.795214	-3.004658

284	1	0	-2.510614	-2.760521	-2.321645
285	1	0	0.822171	-3.399726	-4.555594
286	7	0	1.540806	-3.500870	-2.579476
287	1	0	-1.330549	-4.313673	-3.772771
288	7	0	-0.228562	-4.727163	-2.032189
289	6	0	1.058807	-4.415813	-1.705498
290	1	0	2.533128	-3.293560	-2.659541
291	1	0	-0.819597	-5.030973	-1.259870
292	8	0	1.683280	-4.934000	-0.767841
293	1	0	1.420735	-4.857304	3.539086
294	6	0	0.909711	-4.145715	2.887098
295	6	0	-0.359955	-3.482837	3.535298
296	7	0	0.361029	-4.812892	1.726369
297	7	0	1.753127	-3.012510	2.592151
298	1	0	-0.650469	-3.928862	4.489522
299	7	0	0.045110	-2.108621	3.699557
300	7	0	-1.379753	-3.697208	2.529932
301	6	0	-0.921647	-4.440071	1.486144
302	1	0	0.939623	-5.060779	0.922507
303	6	0	1.219873	-1.849824	3.044666
304	1	0	2.753867	-3.099168	2.433988
305	1	0	-0.631881	-1.344019	3.686618
306	1	0	-2.375134	-3.556908	2.681736
307	8	0	-1.578886	-4.744016	0.480919
308	8	0	1.711874	-0.723194	2.938830

AB-trans, capsule a: M062X/6-31g(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.693881	1.836187	1.212489
2	8	0	1.976391	-1.091802	0.150887
3	5	0	2.675239	0.039692	0.371399
4	1	0	1.026535	-1.009808	0.389956
5	6	0	6.298313	1.110226	-0.574813
6	6	0	4.948605	1.167714	-0.240506
7	6	0	4.226000	0.010937	0.079796
8	6	0	4.912563	-1.209072	0.082808
9	6	0	6.267785	-1.269933	-0.233656
10	6	0	6.972970	-0.114523	-0.577585
11	1	0	6.837314	2.011531	-0.868370
12	1	0	4.429707	2.123769	-0.261515
13	1	0	4.357689	-2.115627	0.314216
14	1	0	6.795590	-2.221145	-0.241197
15	6	0	8.441048	-0.177313	-0.904321
16	6	0	9.295846	0.256818	0.284259
17	1	0	8.659874	0.480798	-1.754362
18	1	0	8.713811	-1.198359	-1.201201
19	1	0	10.360811	0.214253	0.034371
20	1	0	9.053281	1.283923	0.584383
21	1	0	9.117134	-0.401127	1.142893
22	8	0	2.072274	1.177835	0.872673
23	6	0	-5.096513	1.099667	0.804020
24	6	0	-3.707663	1.262093	0.774478
25	6	0	-2.870791	0.152719	0.615406
26	6	0	-3.446402	-1.115744	0.470264
27	6	0	-4.826202	-1.261580	0.488933
28	6	0	-5.678629	-0.164634	0.671208
29	1	0	-5.724108	1.967405	0.997473
30	1	0	-3.310508	2.265004	0.924603
31	1	0	-2.787110	-1.970917	0.344785
32	1	0	-5.264594	-2.247976	0.367409
33	6	0	-7.175127	-0.392139	0.757520
34	6	0	-7.843254	-0.731624	-0.582177
35	1	0	-7.658390	0.489504	1.198628
36	1	0	-7.355847	-1.230693	1.443182
37	1	0	-8.888849	-1.024111	-0.430164
38	1	0	-7.832066	0.129319	-1.261282
39	1	0	-7.329557	-1.563821	-1.080869
40	8	0	-0.707642	-0.817344	0.750468
41	1	0	-1.331424	2.263705	0.309648
42	1	0	0.225911	1.478273	0.509031
43	7	0	-0.789410	1.420841	0.420967
44	6	0	-1.363730	0.216728	0.607032
45	6	0	11.216575	-0.856585	2.910662
46	6	0	11.725065	0.473778	3.434148
47	6	0	11.502787	2.017226	-2.094274
48	6	0	10.957229	3.180121	-1.548774
49	6	0	11.622176	3.871194	-0.371041
50	6	0	11.098496	3.353229	0.953842
51	6	0	11.665718	2.251227	1.597855
52	6	0	11.109701	1.680760	2.745161
53	6	0	11.819105	-1.471461	1.810680
54	6	0	12.005563	-3.284474	0.040029
55	6	0	11.347945	-2.843837	-1.252144
56	6	0	11.723706	-1.658697	-1.887481
57	6	0	11.099910	-1.189065	-3.043391
58	6	0	10.929840	1.341175	-3.170933
59	6	0	11.556453	0.082462	-3.731649
60	6	0	9.944046	2.268995	3.239404
61	6	0	9.974260	3.929358	1.545463
62	6	0	9.384913	3.408762	2.685810
63	6	0	10.232553	-3.249679	1.855072
64	6	0	10.119913	-1.508405	3.477164
65	6	0	9.619017	-2.702324	2.970269
66	6	0	9.785829	3.665817	-2.137404
67	6	0	9.757872	1.874452	-3.710793
68	6	0	9.177018	3.033697	-3.214797
69	6	0	10.048789	-1.954163	-3.551630
70	6	0	10.331377	-3.592547	-1.848416
71	6	0	9.673373	-3.166103	-2.994674
72	1	0	8.270725	3.435591	-3.654015
73	1	0	12.424638	1.626529	-1.666158
74	1	0	11.453058	4.947556	-0.438049
75	1	0	12.699542	3.690873	-0.425443
76	1	0	12.563222	1.803126	1.173880
77	1	0	8.497964	3.858837	3.114856
78	1	0	8.768021	-3.188933	3.433171

79	1	0	12.688473	-0.994626	1.360343
80	1	0	12.540641	-1.077487	-1.461764
81	1	0	8.867439	-3.750183	-3.424464
82	1	0	12.642430	0.159493	-3.622221
83	1	0	11.329574	0.012107	-4.797001
84	1	0	13.058728	-2.989519	0.019335
85	1	0	11.957439	-4.372091	0.119299
86	1	0	11.525029	0.538584	4.505703
87	1	0	12.808960	0.511054	3.289664
88	8	0	9.502077	-0.949076	4.598158
89	8	0	9.334850	1.694589	4.348650
90	8	0	9.975992	-4.813120	-1.279522
91	8	0	9.808614	-4.475701	1.358926
92	8	0	9.355497	-1.472169	-4.662337
93	8	0	9.173115	1.212687	-4.791792
94	8	0	9.444254	5.077103	0.961105
95	8	0	9.258299	4.871637	-1.678552
96	6	0	8.208536	0.981339	4.090018
97	6	0	8.281626	-0.420024	4.313050
98	7	0	7.235527	-1.212458	4.216796
99	7	0	7.115440	1.584447	3.666844
100	6	0	6.126263	-0.582510	3.839199
101	6	0	6.073676	0.764264	3.533311
102	6	0	4.750401	-1.158777	3.661038
103	6	0	4.667443	1.086653	3.081638
104	7	0	3.970708	-0.091131	3.223057
105	8	0	4.363713	-2.280470	3.859592
106	1	0	2.951308	-0.244592	3.042976
107	8	0	4.230068	2.143126	2.674115
108	6	0	8.638205	-4.555954	0.676377
109	6	0	8.735479	-4.818720	-0.718211
110	6	0	11.348887	-2.659505	1.254825
111	7	0	7.687446	-5.054568	-1.477580
112	7	0	7.483789	-4.459815	1.305697
113	6	0	8.055418	0.510445	-4.462598
114	6	0	8.158374	-0.904099	-4.355426
115	6	0	8.200153	4.944283	0.440786
116	6	0	8.099461	4.821043	-0.975008
117	7	0	7.160842	-1.662200	-3.941962
118	7	0	6.941577	1.165016	-4.205694
119	7	0	7.153355	4.949190	1.238206
120	7	0	6.945350	4.707705	-1.600639
121	6	0	6.427828	-4.676919	0.519131
122	6	0	5.892383	4.717181	-0.780502
123	6	0	6.529894	-4.990553	-0.823744
124	6	0	5.938876	0.383203	-3.820968
125	6	0	6.046750	-0.985977	-3.674349
126	6	0	5.995602	4.828186	0.593002
127	6	0	4.610431	4.809574	1.178182
128	6	0	4.428175	4.621110	-1.133413
129	6	0	4.957524	-4.611151	0.870993
130	6	0	5.144512	-5.207983	-1.375590
131	6	0	4.569220	0.807233	-3.373258
132	6	0	4.743769	-1.500975	-3.110179
133	7	0	3.767976	4.611582	0.089943
134	7	0	3.931840	-0.382030	-3.027319
135	7	0	4.298612	-4.922052	-0.304525
136	8	0	3.911224	4.571338	-2.222213
137	8	0	4.267335	4.947364	2.325431
138	8	0	4.110224	1.918153	-3.307282
139	8	0	4.445844	-2.627530	-2.791937
140	8	0	4.448309	-4.336521	1.930824
141	8	0	4.817802	-5.564978	-2.474049
142	1	0	3.266255	-5.033812	-0.368056
143	1	0	3.046527	-0.340654	-2.520384
144	1	0	2.739362	4.707820	0.208123
145	1	0	-12.844289	-3.615477	-0.555498
146	6	0	-11.767655	-3.801472	-0.505518
147	6	0	-11.101466	-3.138532	-1.694640
148	6	0	-11.232258	-3.251020	0.801505
149	1	0	-11.604495	-4.879799	-0.545129
150	6	0	-11.611312	-1.951943	-2.224926
151	6	0	-9.944198	-3.655823	-2.281855
152	6	0	-11.800715	-2.141560	1.424552
153	6	0	-10.113075	-3.820530	1.410067
154	6	0	-10.997393	-1.265322	-3.271527
155	1	0	-12.529683	-1.547387	-1.803123
156	6	0	-9.299119	-3.015640	-3.330729
157	8	0	-9.442836	-4.874430	-1.828927
158	6	0	-11.282867	-1.585844	2.596117
159	1	0	-12.687877	-1.690635	0.983110
160	6	0	-9.558290	-3.312155	2.575106
161	8	0	-9.587346	-4.968306	0.826704
162	6	0	-11.588960	0.005165	-3.847450
163	6	0	-9.828424	-1.820479	-3.792313
164	1	0	-8.394851	-3.430133	-3.760905
165	6	0	-8.270748	-4.819955	-1.142046
166	6	0	-11.936739	-0.379322	3.241432
167	6	0	-10.147325	-2.188988	3.141030
168	1	0	-8.691907	-3.775485	3.033758
169	6	0	-8.353672	-4.856262	0.278494
170	1	0	-12.678809	-0.068408	-3.783272
171	1	0	-11.322146	0.070636	-4.904272
172	6	0	-11.167668	1.288570	-3.157786
173	8	0	-9.170075	-1.125371	-4.810450
174	7	0	-7.125097	-4.759303	-1.791456
175	6	0	-11.420478	0.933675	2.688652
176	1	0	-11.768019	-0.411086	4.319440
177	1	0	-13.014887	-0.433848	3.064910
178	8	0	-9.623008	-1.679336	4.327197
179	7	0	-7.296251	-4.807033	1.059351
180	6	0	-11.857876	1.782357	-2.051643
181	6	0	-10.097336	2.054820	-3.624939
182	6	0	-8.084090	-0.456503	-4.348302
183	6	0	-6.057946	-4.728975	-0.990334
184	6	0	-12.025604	1.559177	1.598310
185	6	0	-10.309072	1.561460	3.251747
186	6	0	-8.453924	-0.995912	4.209107
187	6	0	-6.148587	-4.744517	0.389167
188	6	0	-11.529005	2.986919	-1.425738

189	1	0	-12.683269	1.197132	-1.649555
190	6	0	-9.781196	3.292030	-3.092617
191	8	0	-9.314372	1.551050	-4.667178
192	6	0	-8.168098	0.961271	-4.239759
193	7	0	-7.029141	-1.140536	-3.958447
194	6	0	-4.589420	-4.684127	-1.358130
195	6	0	-11.551919	2.755805	1.062643
196	1	0	-12.908604	1.101417	1.155924
197	6	0	-9.794749	2.753683	2.758534
198	8	0	-9.752220	0.983126	4.388776
199	6	0	-8.526124	0.423765	4.239852
200	7	0	-7.317131	-1.652108	4.082087
201	6	0	-4.760782	-4.671586	0.959462
202	6	0	-12.209025	3.408056	-0.139304
203	6	0	-10.508215	3.744388	-1.999497
204	1	0	-8.964357	3.877319	-3.499049
205	7	0	-7.204439	1.693628	-3.713825
206	6	0	-6.064176	-0.385279	-3.448279
207	7	0	-3.925691	-4.568761	-0.143084
208	8	0	-4.073584	-4.753381	-2.445498
209	6	0	-10.423933	3.323113	1.661030
210	1	0	-8.936625	3.228004	3.220781
211	7	0	-7.464381	1.197464	4.146123
212	6	0	-6.249847	-0.859447	3.990015
213	8	0	-4.422591	-4.692742	2.116646
214	1	0	-12.165358	4.493874	-0.038238
215	1	0	-13.260342	3.108021	-0.173652
216	8	0	-10.184097	4.984002	-1.446967
217	6	0	-6.147682	0.985117	-3.318768
218	6	0	-4.780197	-0.848859	-2.829298
219	1	0	-2.899000	-4.704020	0.003554
220	8	0	-10.002215	4.553494	1.174495
221	6	0	-6.326241	0.520786	4.022693
222	6	0	-4.796423	-1.243720	3.811704
223	6	0	-8.941984	4.987185	-0.887020
224	6	0	-4.892317	1.462679	-2.632568
225	7	0	-4.144845	0.320488	-2.421911
226	8	0	-4.389693	-1.977928	-2.682936
227	6	0	-8.837070	4.644591	0.489488
228	6	0	-4.935753	1.075407	3.893511
229	7	0	-4.121447	-0.031451	3.777888
230	8	0	-4.305160	-2.340115	3.728149
231	7	0	-7.898618	5.255998	-1.641074
232	8	0	-4.580973	2.595169	-2.337138
233	1	0	-3.232794	0.264894	-1.965257
234	7	0	-7.680428	4.481255	1.098670
235	8	0	-4.586416	2.233147	3.895383
236	1	0	-3.106577	0.087351	3.597176
237	6	0	-6.736988	5.129680	-1.003158
238	6	0	-6.629720	4.724001	0.313081
239	6	0	-5.353481	5.368692	-1.548978
240	6	0	-5.162107	4.636505	0.656828
241	7	0	-4.508790	5.072074	-0.480536
242	8	0	-5.026522	5.742136	-2.642196
243	8	0	-4.648532	4.260167	1.683329
244	1	0	-3.479745	5.083037	-0.536908
245	8	0	-1.791775	4.899320	-0.393317
246	6	0	-1.210252	4.420535	-1.374397
247	7	0	-0.006729	4.837065	-1.856645
248	7	0	-1.674571	3.398201	-2.141570
249	6	0	0.527665	3.888173	-2.808883
250	1	0	0.593938	5.286880	-1.172199
251	6	0	-0.732731	3.028397	-3.178894
252	1	0	-2.662248	3.153156	-2.159511
253	1	0	0.987211	4.396984	-3.658064
254	7	0	1.425914	2.910060	-2.230559
255	1	0	-1.134814	3.234846	-4.173495
256	7	0	-0.237524	1.678461	-3.076718
257	6	0	0.965472	1.638624	-2.430501
258	1	0	2.431999	3.056208	-2.271340
259	1	0	-0.858685	0.880396	-2.915215
260	8	0	1.548369	0.606334	-2.096720
261	1	0	-1.122051	4.634025	4.161102
262	6	0	-0.796328	3.936167	3.385825
263	6	0	0.609743	3.281992	3.667255
264	7	0	-0.556678	4.627147	2.137486
265	7	0	-1.686774	2.808100	3.299744
266	1	0	1.040314	3.571505	4.629237
267	7	0	0.296417	1.873839	3.638003
268	7	0	1.436984	3.755312	2.581541
269	6	0	0.723598	4.532208	1.707655
270	1	0	-1.275230	4.962083	1.504155
271	6	0	-1.019039	1.626373	3.444551
272	1	0	-2.696478	2.854710	3.425893
273	1	0	0.946933	1.098850	3.523537
274	1	0	2.438543	3.906867	2.684350
275	8	0	1.182088	5.071345	0.694423
276	8	0	-1.533204	0.503192	3.423687
277	6	0	0.916139	-1.811318	3.156516
278	7	0	-0.311273	-2.087018	3.670092
279	7	0	1.526145	-2.969489	2.790779
280	8	0	1.401064	-0.674395	3.080246
281	6	0	-0.648513	-3.482550	3.554241
282	1	0	-0.987635	-1.329623	3.667451
283	6	0	0.717982	-4.124301	3.117650
284	1	0	2.538216	-3.022648	2.712471
285	1	0	-1.035967	-3.870775	4.499076
286	7	0	-1.531093	-3.827190	2.460139
287	1	0	1.193755	-4.723490	3.897496
288	7	0	0.334451	-4.944721	1.995329
289	6	0	-0.937129	-4.686793	1.587492
290	1	0	-2.544458	-3.813166	2.551796
291	1	0	0.993251	-5.269575	1.291839
292	8	0	-1.464988	-5.191789	0.587727
293	1	0	-1.124410	-4.409709	-3.731495
294	6	0	-0.666816	-3.949221	-2.853366
295	6	0	0.635851	-3.131374	-3.170151
296	7	0	-0.190277	-4.954348	-1.933598
297	7	0	-1.551691	-2.950446	-2.281581
298	1	0	1.014982	-3.282511	-4.184189

299	7	0	0.204297	-1.767566	-2.978291
300	7	0	1.570248	-3.628864	-2.188915
301	6	0	1.061334	-4.659719	-1.468608
302	1	0	-0.811461	-5.392789	-1.260656
303	6	0	-1.038651	-1.692987	-2.423078
304	1	0	-2.561339	-3.063035	-2.317704
305	1	0	0.840072	-0.994050	-2.778639
306	1	0	2.555413	-3.379397	-2.182035
307	8	0	1.631564	-5.273592	-0.559411
308	8	0	-1.614383	-0.636036	-2.147280

AC-trans, capsule a: M062X/6-31g(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.067993	0.817632	0.241266
2	6	0	-2.731577	-0.166859	0.154726
3	8	0	-2.071506	0.960885	0.124594
4	6	0	-6.320529	-0.977697	-0.644631
5	6	0	-4.961193	-1.113181	-0.393166
6	6	0	-4.205365	0.002909	-0.027105
7	6	0	-4.819553	1.245832	0.123414
8	6	0	-6.187565	1.366650	-0.107295
9	6	0	-6.949199	0.266384	-0.505554
10	1	0	-6.903523	-1.831686	-0.985692
11	1	0	-4.450672	-2.064961	-0.497309
12	1	0	-4.212444	2.104598	0.391629
13	1	0	-6.677069	2.332207	-0.008931
14	6	0	-8.426761	0.400918	-0.761629
15	6	0	-9.256441	-0.290210	0.317979
16	1	0	-8.669345	-0.047271	-1.732262
17	1	0	-8.701834	1.462282	-0.814560
18	1	0	-10.325681	-0.163576	0.123303
19	1	0	-9.043959	-1.365971	0.356239
20	1	0	-9.034965	0.138865	1.301420
21	8	0	-2.242258	-1.279946	0.316494
22	6	0	4.903302	-1.073979	0.554202
23	6	0	3.521932	-1.254191	0.446248
24	6	0	2.669667	-0.148016	0.355523
25	6	0	3.225972	1.137410	0.344524
26	6	0	4.601821	1.300465	0.435754
27	6	0	5.466147	0.205843	0.562665
28	1	0	5.543530	-1.944050	0.685979
29	1	0	3.131955	-2.271013	0.466037
30	1	0	2.559361	1.992958	0.267747
31	1	0	5.022744	2.300976	0.421715
32	6	0	6.952306	0.449334	0.739909
33	6	0	7.681204	0.838154	-0.552996
34	1	0	7.424723	-0.441864	1.174258
35	1	0	7.085899	1.263262	1.464972
36	1	0	8.718820	1.123407	-0.343965
37	1	0	7.699284	0.001999	-1.261782
38	1	0	7.186542	1.686922	-1.042024
39	8	0	0.485698	0.782592	0.387269
40	1	0	1.157906	-2.311529	0.188141
41	1	0	-0.405379	-1.520828	0.206111
42	7	0	0.614666	-1.460098	0.128701
43	6	0	1.167906	-0.251849	0.298710
44	6	0	-11.051683	0.508371	3.131742
45	6	0	-11.599461	-0.862218	3.479780
46	6	0	-11.609680	-1.506646	-2.218671
47	6	0	-11.085649	-2.746808	-1.855698
48	6	0	-11.777352	-3.606706	-0.812536
49	6	0	-11.218111	-3.361204	0.574285
50	6	0	-11.684293	-2.327604	1.391198
51	6	0	-11.077278	-1.988176	2.602314
52	6	0	-11.678052	1.318850	2.183645
53	6	0	-11.864950	3.396854	0.738688
54	6	0	-11.268275	3.156171	-0.633681
55	6	0	-11.690636	2.095424	-1.437696
56	6	0	-11.105495	1.800642	-2.669521
57	6	0	-11.016005	-0.682979	-3.175082
58	6	0	-11.610435	0.661595	-3.534092
59	6	0	-9.963379	-2.741837	2.979428
60	6	0	-10.154011	-4.123458	1.055684
61	6	0	-9.516450	-3.831466	2.251872
62	6	0	-10.007574	3.004051	2.428161
63	6	0	-9.892585	1.010497	3.724843
64	6	0	-9.360558	2.251400	3.396424
65	6	0	-9.908535	-3.151791	-2.494642
66	6	0	-9.852401	-1.150027	-3.787158
67	6	0	-9.284088	-2.375440	-3.463027
68	6	0	-10.044248	2.610995	-3.079005
69	6	0	-10.249693	3.967578	-1.134738
70	6	0	-9.626743	3.712242	-2.349298
71	1	0	-8.380790	-2.720595	-3.953819
72	1	0	-12.532292	-1.173618	-1.745995
73	1	0	-11.661001	-4.660390	-1.073092
74	1	0	-12.844848	-3.368493	-0.818009
75	1	0	-12.540056	-1.743347	1.055291
76	1	0	-8.670697	-4.417846	2.591230
77	1	0	-8.462006	2.620001	3.878299
78	1	0	-12.594770	0.961133	1.717346
79	1	0	-12.510578	1.470245	-1.086782
80	1	0	-8.818319	4.342207	-2.702490
81	1	0	-12.697050	0.601535	-3.421333
82	1	0	-11.391786	0.884921	-4.579736
83	1	0	-12.926400	3.133836	0.716670
84	1	0	-11.780268	4.455394	0.991784
85	1	0	-11.361944	-1.089254	4.520922
86	1	0	-12.688904	-0.832103	3.382545
87	8	0	-9.253201	0.230841	4.690329
88	8	0	-9.278600	-2.384520	4.138891
89	8	0	-9.847055	5.071412	-0.387120
90	8	0	-9.557572	4.285217	2.135078
91	8	0	-9.386604	2.292780	-4.267092
92	8	0	-9.268799	-0.350927	-4.771854
93	8	0	-9.713033	-5.207955	0.299326

94	8	0	-9.420118	-4.424501	-2.221580
95	6	0	-8.119524	-1.711774	3.912395
96	6	0	-8.096966	-0.329970	4.250344
97	7	0	-7.020609	0.417479	4.128351
98	7	0	-7.079721	-2.338565	3.398874
99	6	0	-5.971613	-0.237376	3.639876
100	6	0	-6.002971	-1.565698	3.266123
101	6	0	-4.585293	0.289468	3.405751
102	6	0	-4.631234	-1.942633	2.761925
103	7	0	-3.862585	-0.810133	2.945284
104	8	0	-4.168730	1.405781	3.568315
105	1	0	-2.882545	-0.686441	2.661196
106	8	0	-4.264275	-3.005751	2.315972
107	6	0	-8.418381	4.468059	1.420513
108	6	0	-8.580392	4.968516	0.097909
109	6	0	-11.178116	2.563116	1.802269
110	7	0	-7.568662	5.314746	-0.667533
111	7	0	-7.235686	4.258974	1.964567
112	6	0	-8.127825	0.274717	-4.380447
113	6	0	-8.194037	1.664555	-4.082848
114	6	0	-8.444464	-5.063528	-0.166780
115	6	0	-8.285438	-4.565537	-1.490347
116	7	0	-7.163481	2.343066	-3.616538
117	7	0	-7.022284	-0.429442	-4.252450
118	7	0	-7.429727	-5.360271	0.615559
119	7	0	-7.105346	-4.308291	-2.018607
120	6	0	-6.215859	4.595602	1.170295
121	6	0	-6.084069	-4.589083	-1.204376
122	6	0	-6.381308	5.126573	-0.096061
123	6	0	-5.986759	0.276516	-3.811134
124	6	0	-6.055198	1.617576	-3.488286
125	6	0	-6.243651	-5.115709	0.063276
126	6	0	-4.882774	-5.337327	0.670337
127	6	0	-4.602296	-4.403199	-1.447239
128	6	0	-4.728199	4.458972	1.423383
129	6	0	-5.024968	5.403697	-0.688155
130	6	0	-4.603094	-0.219416	-3.502475
131	6	0	-4.711758	2.037988	-2.940712
132	7	0	-3.995814	-4.836569	-0.284447
133	7	0	-3.925512	0.905877	-3.034003
134	7	0	-4.128784	4.927309	0.268246
135	8	0	-4.050222	-3.963805	-2.429075
136	8	0	-4.597748	-5.845158	1.718917
137	8	0	-4.155827	-1.329813	-3.616875
138	8	0	-4.374023	3.117242	-2.511848
139	8	0	-4.165330	4.024847	2.400099
140	8	0	-4.752101	5.929168	-1.731816
141	1	0	-3.101887	5.031868	0.146655
142	1	0	-2.989890	0.788897	-2.633506
143	1	0	-2.971103	-4.878665	-0.144474
144	1	0	12.968709	3.448895	-0.166424
145	6	0	11.896768	3.660683	-0.118368
146	6	0	11.232158	3.097118	-1.358209
147	6	0	11.325427	3.038399	1.139456
148	1	0	11.762846	4.743186	-0.087108
149	6	0	11.722637	1.935075	-1.954785
150	6	0	10.099333	3.682599	-1.930579
151	6	0	11.846774	1.870166	1.693183
152	6	0	10.214772	3.602475	1.766896
153	6	0	11.121027	1.337508	-3.061718
154	1	0	12.618665	1.477724	-1.538761
155	6	0	9.469858	3.134842	-3.039066
156	8	0	9.620537	4.880533	-1.404670
157	6	0	11.288652	1.252188	2.813778
158	1	0	12.727162	1.421920	1.235863
159	6	0	9.621991	3.034771	2.884642
160	8	0	9.739012	4.804849	1.255755
161	6	0	11.695653	0.086471	-3.697001
162	6	0	9.985315	1.963574	-3.575498
163	1	0	8.590024	3.603463	-3.464827
164	6	0	8.440399	4.823449	-0.731389
165	6	0	11.890960	-0.016951	3.387167
166	6	0	10.163951	1.856386	3.380273
167	1	0	8.763085	3.495619	3.359216
168	6	0	8.508211	4.774541	0.689606
169	1	0	12.783519	0.117277	-3.584094
170	1	0	11.471143	0.097292	-4.765670
171	6	0	11.201359	-1.221596	-3.107076
172	8	0	9.346420	1.377802	-4.672356
173	7	0	7.299978	4.847753	-1.391825
174	6	0	11.337426	-1.277889	2.753276
175	1	0	11.712943	-0.045138	4.463886
176	1	0	12.972212	0.009996	3.223406
177	8	0	9.600114	1.281280	4.517901
178	7	0	7.441265	4.724431	1.457385
179	6	0	11.838421	-1.822200	-2.021585
180	6	0	10.107859	-1.900719	-3.649326
181	6	0	8.211405	0.726167	-4.314717
182	6	0	6.223409	4.813052	-0.602943
183	6	0	11.928660	-1.855249	1.628639
184	6	0	10.206933	-1.908198	3.273751
185	6	0	8.416604	0.642810	4.326288
186	6	0	6.298344	4.745387	0.776555
187	6	0	11.431155	-3.044939	-1.483702
188	1	0	12.685403	-1.311736	-1.566152
189	6	0	9.707520	-3.147431	-3.200075
190	8	0	9.393099	-1.297495	-4.686345
191	6	0	8.245480	-0.696915	-4.281494
192	7	0	7.157604	1.423566	-3.946311
193	6	0	4.757928	4.840715	-0.988777
194	6	0	11.421232	-3.000706	1.017219
195	1	0	12.826658	-1.397662	1.217246
196	6	0	9.660479	-3.052079	2.706295
197	8	0	9.651639	-1.381803	4.438123
198	6	0	8.445502	-0.779433	4.293119
199	7	0	7.307395	1.339003	4.179256
200	6	0	4.901529	4.696103	1.330923
201	6	0	12.065558	-3.592844	-0.221745
202	6	0	10.379317	-3.703975	-2.120397
203	1	0	8.870977	-3.659962	-3.660538

204	7	0	7.235802	-1.424037	-3.843061
205	6	0	6.144069	0.674601	-3.527808
206	7	0	4.079511	4.698508	0.211268
207	8	0	4.260357	4.969283	-2.080499
208	6	0	10.274131	-3.570282	1.575582
209	1	0	8.785183	-3.526723	3.134588
210	7	0	7.366069	-1.513384	4.123320
211	6	0	6.222771	0.584972	4.002817
212	8	0	4.542654	4.657652	2.479082
213	1	0	11.967886	-4.679595	-0.202812
214	1	0	13.130619	-3.343909	-0.218743
215	8	0	9.981120	-4.954775	-1.648064
216	6	0	6.182189	-0.702550	-3.463805
217	6	0	4.851235	1.145294	-2.931003
218	1	0	3.047927	4.732383	0.356563
219	8	0	9.805914	-4.748225	1.005273
220	6	0	6.254415	-0.796564	3.979815
221	6	0	4.801177	1.028295	3.739257
222	6	0	8.737874	-4.938296	-1.093880
223	6	0	4.890097	-1.174924	-2.846570
224	7	0	4.169342	-0.023139	-2.604293
225	8	0	4.489499	2.276381	-2.735640
226	6	0	8.642050	-4.731588	0.311063
227	6	0	4.861552	-1.299471	3.722903
228	7	0	4.094903	-0.151130	3.595345
229	8	0	4.358275	2.147764	3.668572
230	7	0	7.686221	-5.073105	-1.872192
231	8	0	4.540592	-2.310492	-2.613555
232	1	0	3.242617	0.038351	-2.177972
233	7	0	7.490550	-4.581354	0.933091
234	8	0	4.472075	-2.436141	3.639728
235	1	0	3.118877	-0.245215	3.297297
236	6	0	6.528086	-4.955525	-1.226471
237	6	0	6.433630	-4.692217	0.126563
238	6	0	5.137352	-5.046358	-1.799002
239	6	0	4.970429	-4.555465	0.473226
240	7	0	4.302943	-4.787147	-0.711200
241	8	0	4.795756	-5.297250	-2.921578
242	8	0	4.469223	-4.288147	1.540660
243	1	0	3.272467	-4.714467	-0.774847
244	8	0	1.624918	-4.437403	-0.719277
245	6	0	1.080764	-3.982848	-1.739935
246	7	0	-0.144243	-4.341466	-2.200158
247	7	0	1.615998	-3.047897	-2.562023
248	6	0	-0.621268	-3.409409	-3.197643
249	1	0	-0.765060	-4.793315	-1.532181
250	6	0	0.682085	-2.617162	-3.580998
251	1	0	2.605614	-2.814305	-2.538668
252	1	0	-1.092866	-3.930669	-4.032524
253	7	0	-1.477999	-2.374445	-2.668601
254	1	0	1.057666	-2.838590	-4.582430
255	7	0	0.263951	-1.240785	-3.465365
256	6	0	-0.939597	-1.139051	-2.823897
257	1	0	-2.483330	-2.495128	-2.579638
258	1	0	0.922286	-0.477752	-3.291444
259	8	0	-1.447706	-0.072174	-2.464563
260	1	0	1.219348	-5.052935	3.678990
261	6	0	0.789799	-4.413406	2.904897
262	6	0	-0.554793	-3.728420	3.332334
263	7	0	0.397350	-5.189262	1.751280
264	7	0	1.651617	-3.275873	2.628066
265	1	0	-1.018738	-4.183248	4.211161
266	7	0	-0.147782	-2.373460	3.597471
267	7	0	-1.375567	-3.908490	2.153976
268	6	0	-0.820163	-4.773695	1.271995
269	1	0	1.078680	-5.415246	1.033901
270	6	0	1.095035	-2.117902	3.100851
271	1	0	2.668058	-3.361999	2.616309
272	1	0	-0.783528	-1.575902	3.589839
273	1	0	-2.356100	-3.637785	2.096897
274	8	0	-1.326205	-5.165274	0.215687
275	8	0	1.617796	-1.004008	3.089940
276	6	0	-0.849363	1.237937	3.077859
277	7	0	0.341430	1.477022	3.699458
278	7	0	-1.449083	2.424944	2.790533
279	8	0	-1.305560	0.111808	2.850591
280	6	0	0.671792	2.878122	3.719640
281	1	0	1.018031	0.720927	3.683218
282	6	0	-0.686281	3.544132	3.298029
283	1	0	-2.460574	2.466969	2.704170
284	1	0	1.026399	3.185700	4.706420
285	7	0	1.583003	3.327093	2.683787
286	1	0	-1.212608	4.037605	4.118217
287	7	0	-0.268394	4.497674	2.302466
288	6	0	1.009424	4.277831	1.892928
289	1	0	2.593021	3.293144	2.803394
290	1	0	-0.905199	4.927736	1.636453
291	8	0	1.550623	4.878094	0.957179
292	1	0	1.312651	5.000291	-3.403313
293	6	0	0.823294	4.412075	-2.624499
294	6	0	-0.483555	3.684291	-3.102275
295	7	0	0.340006	5.262742	-1.561259
296	7	0	1.672228	3.313427	-2.201882
297	1	0	-0.846182	4.026753	-4.074631
298	7	0	-0.073079	2.303362	-3.155835
299	7	0	-1.426174	4.007779	-2.052994
300	6	0	-0.917900	4.900064	-1.164725
301	1	0	0.956775	5.543071	-0.804797
302	6	0	1.140786	2.107299	-2.562026
303	1	0	2.684743	3.409913	-2.188455
304	1	0	-0.727646	1.521768	-3.097106
305	1	0	-2.419791	3.796944	-2.101089
306	8	0	-1.492365	5.351555	-0.167684
307	8	0	1.676423	1.004927	-2.422903

BB-trans, capsule a: M062X/6-31g(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	-2.500792	0.126052	0.158666
2	1	0	-2.006454	2.099469	0.067595
3	6	0	-6.150435	-0.857974	-0.640724
4	6	0	-4.780139	-0.908045	-0.411835
5	6	0	-4.052272	0.248956	-0.087309
6	6	0	-4.751465	1.456976	0.001424
7	6	0	-6.129734	1.507923	-0.212450
8	6	0	-6.847095	0.352838	-0.531593
9	1	0	-6.694041	-1.755969	-0.931789
10	1	0	-4.245755	-1.854297	-0.471672
11	1	0	-4.212522	2.380448	0.212729
12	1	0	-6.666481	2.454025	-0.158130
13	6	0	-8.340755	0.388390	-0.742110
14	6	0	-9.107735	-0.360110	0.350855
15	1	0	-8.583689	-0.069599	-1.709802
16	1	0	-8.685107	1.429666	-0.779394
17	1	0	-10.186259	-0.305902	0.170121
18	1	0	-8.823334	-1.420142	0.385580
19	1	0	-8.906013	0.082107	1.332764
20	8	0	-1.650582	1.201156	0.169985
21	8	0	-2.017352	-1.122056	0.386450
22	1	0	-1.046079	-1.141335	0.503089
23	6	0	5.200207	-1.419905	0.610190
24	6	0	3.810505	-1.355683	0.588433
25	6	0	3.138664	-0.131693	0.740664
26	6	0	3.921930	1.018411	0.917362
27	6	0	5.316187	0.952947	0.934042
28	6	0	5.978148	-0.268193	0.775753
29	1	0	5.707415	-2.379503	0.554998
30	1	0	3.251433	-2.283032	0.462808
31	1	0	3.425501	1.977701	1.053740
32	1	0	5.905313	1.849917	1.114231
33	6	0	7.487767	-0.386709	0.805288
34	6	0	8.108460	-0.640567	-0.577106
35	1	0	7.760442	-1.228028	1.456418
36	1	0	7.924792	0.517848	1.248523
37	1	0	9.186510	-0.823450	-0.496794
38	1	0	7.649549	-1.515620	-1.057675
39	1	0	7.960287	0.221662	-1.239838
40	8	0	0.751936	-1.109101	0.449663
41	8	0	1.001644	1.196037	0.903118
42	1	0	0.036676	1.196598	0.740070
43	1	0	1.198254	-1.965077	0.337273
44	5	0	1.561329	-0.023998	0.724731
45	6	0	-11.025612	0.201885	3.224949
46	6	0	-11.542651	-1.195657	3.502259
47	6	0	-11.647410	-1.502130	-2.198680
48	6	0	-11.061382	-2.737200	-1.924821
49	6	0	-11.694973	-3.692609	-0.931373
50	6	0	-11.124426	-3.513255	0.459185
51	6	0	-11.605460	-2.535719	1.333258
52	6	0	-11.004141	-2.260156	2.562175
53	6	0	-11.682084	1.052516	2.334364
54	6	0	-11.938227	3.219695	1.037476
55	6	0	-11.355922	3.070529	-0.353323
56	6	0	-11.780750	2.053677	-1.209277
57	6	0	-11.224494	1.841520	-2.470887
58	6	0	-11.114917	-0.602904	-3.122681
59	6	0	-11.748912	0.747159	-3.381127
60	6	0	-9.882529	-3.020628	2.897725
61	6	0	-10.041133	-4.279096	0.888163
62	6	0	-9.411419	-4.051777	2.102830
63	6	0	-10.059202	2.764670	2.681147
64	6	0	-9.874027	0.695293	3.839876
65	6	0	-9.379607	1.969921	3.590935
66	6	0	-9.880956	-3.053233	-2.606817
67	6	0	-9.963755	-0.995934	-3.802725
68	6	0	-9.329873	-2.208353	-3.560382
69	6	0	-10.184006	2.690906	-2.856092
70	6	0	-10.351805	3.918552	-0.820994
71	6	0	-9.753914	3.743838	-2.062456
72	1	0	-8.431640	-2.488412	-4.097938
73	1	0	-12.566640	-1.235444	-1.679532
74	1	0	-11.536736	-4.720611	-1.262929
75	1	0	-12.771919	-3.502868	-0.906313
76	1	0	-12.470159	-1.946007	1.031847
77	1	0	-8.550984	-4.636989	2.405190
78	1	0	-8.485792	2.329509	4.087951
79	1	0	-12.594052	0.701888	1.853533
80	1	0	-12.584892	1.397855	-0.878717
81	1	0	-8.961248	4.403972	-2.397190
82	1	0	-12.828344	0.661081	-3.224813
83	1	0	-11.579518	1.034221	-4.420384
84	1	0	-12.995261	2.939970	1.012491
85	1	0	-11.868025	4.261901	1.354199
86	1	0	-11.293544	-1.472431	4.528487
87	1	0	-12.633095	-1.181757	3.412915
88	8	0	-9.207751	-0.126875	4.750510
89	8	0	-9.203021	-2.717909	4.077307
90	8	0	-9.958234	4.988465	-0.019734
91	8	0	-9.654077	4.076622	2.463570
92	8	0	-9.567982	2.481992	-4.089830
93	8	0	-9.455454	-0.118629	-4.761102
94	8	0	-9.571042	-5.295365	0.058981
95	8	0	-9.321623	-4.307806	-2.400929
96	6	0	-8.058256	-2.015144	3.869166
97	6	0	-8.051710	-0.648447	4.263443
98	7	0	-6.991831	0.123754	4.144445
99	7	0	-7.022105	-2.600965	3.302458
100	6	0	-5.945734	-0.490725	3.600379
101	6	0	-5.965587	-1.802155	3.172450
102	6	0	-4.579234	0.074084	3.335540
103	6	0	-4.610999	-2.127840	2.599151
104	7	0	-3.854291	-0.993861	2.805700
105	8	0	-4.185906	1.193810	3.525541
106	1	0	-2.894657	-0.861731	2.479602
107	8	0	-4.244695	-3.161825	2.087529
108	6	0	-8.521094	4.334538	1.766167
109	6	0	-8.693168	4.894356	0.466340

110	6	0	-11.221412	2.333510	2.035918
111	7	0	-7.687742	5.315248	-0.269183
112	7	0	-7.337152	4.139450	2.309706
113	6	0	-8.302449	0.490234	-4.386227
114	6	0	-8.360212	1.860145	-4.009968
115	6	0	-8.313188	-5.068367	-0.405662
116	6	0	-8.179306	-4.447702	-1.679873
117	7	0	-7.306572	2.526708	-3.577689
118	7	0	-7.193438	-0.217181	-4.341690
119	7	0	-7.283357	-5.411690	0.335612
120	7	0	-7.010837	-4.103760	-2.185413
121	6	0	-6.324057	4.547832	1.542475
122	6	0	-5.972383	-4.426721	-1.407269
123	6	0	-6.499025	5.140424	0.305563
124	6	0	-6.142549	0.471715	-3.916923
125	6	0	-6.190984	1.800444	-3.545740
126	6	0	-6.109604	-5.084359	-0.198606
127	6	0	-4.742994	-5.362829	0.365119
128	6	0	-4.489606	-4.200396	-1.645468
129	6	0	-4.837220	4.435390	1.800847
130	6	0	-5.150720	5.465604	-0.277109
131	6	0	-4.742714	-0.027259	-3.731159
132	6	0	-4.803127	2.208177	-3.110004
133	7	0	-3.869817	-4.768573	-0.545049
134	7	0	-4.034278	1.071493	-3.261175
135	7	0	-4.246529	5.025049	0.692335
136	8	0	-3.940458	-3.657795	-2.573693
137	8	0	-4.444433	-5.979588	1.350221
138	8	0	-4.306363	-1.129800	-3.942653
139	8	0	-4.418416	3.292065	-2.731653
140	8	0	-4.261300	3.939523	2.737033
141	8	0	-4.882530	5.991305	-1.320962
142	1	0	-3.248867	4.933265	0.494947
143	1	0	-3.007513	1.006900	-3.171948
144	1	0	-2.848518	-4.813204	-0.407422
145	1	0	13.031708	3.325380	0.119896
146	6	0	11.968239	3.566747	0.205509
147	6	0	11.276003	3.203818	-1.092397
148	6	0	11.382553	2.797959	1.373913
149	1	0	11.873185	4.638996	0.386745
150	6	0	11.681731	2.084045	-1.821964
151	6	0	10.188896	3.927586	-1.586354
152	6	0	11.897796	1.571368	1.789088
153	6	0	10.270723	3.288033	2.060312
154	6	0	11.022755	1.642817	-2.968323
155	1	0	12.550959	1.528029	-1.474793
156	6	0	9.500792	3.533102	-2.724957
157	8	0	9.771370	5.084067	-0.925716
158	6	0	11.345063	0.837237	2.840908
159	1	0	12.772301	1.170880	1.279441
160	6	0	9.690440	2.609728	3.121556
161	8	0	9.793144	4.537713	1.682100
162	6	0	11.522599	0.447238	-3.757356
163	6	0	9.911567	2.382781	-3.377334
164	1	0	8.642788	4.094552	-3.076021
165	6	0	8.567469	4.958157	-0.300928
166	6	0	11.934381	-0.497766	3.254901
167	6	0	10.237267	1.386954	3.489127
168	1	0	8.836996	3.019706	3.649551
169	6	0	8.583525	4.595864	1.075111
170	1	0	12.614530	0.432040	-3.687722
171	1	0	11.259711	0.586302	-4.808123
172	6	0	11.006196	-0.904052	-3.300747
173	8	0	9.174387	1.929223	-4.474806
174	7	0	7.453580	5.149347	-0.978467
175	6	0	11.318850	-1.665718	2.509127
176	1	0	11.793044	-0.639049	4.327950
177	1	0	13.009412	-0.480395	3.053304
178	8	0	9.708674	0.713444	4.587959
179	7	0	7.487493	4.352042	1.761355
180	6	0	11.653718	-1.644861	-2.311846
181	6	0	9.876688	-1.481704	-3.882280
182	6	0	8.062832	1.249520	-4.091277
183	6	0	6.347902	4.936651	-0.263354
184	6	0	11.836601	-2.116918	1.295181
185	6	0	10.201897	-2.333444	3.011412
186	6	0	8.511803	0.099718	4.394127
187	6	0	6.371709	4.526657	1.056718
188	6	0	11.210822	-2.903867	-1.900563
189	1	0	12.534643	-1.220120	-1.833902
190	6	0	9.432245	-2.751756	-3.555476
191	8	0	9.160039	-0.732450	-4.817332
192	6	0	8.055254	-0.160987	-4.272943
193	7	0	7.069359	1.901262	-3.518080
194	6	0	4.901101	5.054482	-0.693859
195	6	0	11.270621	-3.172190	0.580866
196	1	0	12.726076	-1.634210	0.894440
197	6	0	9.592864	-3.385746	2.337380
198	8	0	9.724011	-1.941712	4.258887
199	6	0	8.521749	-1.311472	4.236616
200	7	0	7.402824	0.814582	4.369953
201	6	0	4.955807	4.302251	1.510664
202	6	0	11.858710	-3.626395	-0.739672
203	6	0	10.108688	-3.443735	-2.562044
204	1	0	8.562865	-3.180747	-4.039570
205	7	0	7.055653	-0.925473	-3.880529
206	6	0	6.064309	1.117610	-3.142289
207	7	0	4.179221	4.620178	0.412376
208	8	0	4.441545	5.443625	-1.735840
209	6	0	10.130146	-3.775289	1.119114
210	1	0	8.727728	-3.890472	2.752904
211	7	0	7.427185	-2.019418	4.050040
212	6	0	6.303056	0.088350	4.183530
213	8	0	4.562398	3.910232	2.581564
214	1	0	11.722601	-4.703179	-0.852952
215	1	0	12.931784	-3.414400	-0.738600
216	8	0	9.676182	-4.721994	-2.213175
217	6	0	6.061752	-0.250744	-3.315515
218	6	0	4.791300	1.505233	-2.441244
219	1	0	3.156017	4.613329	0.515708

220	8	0	9.599029	-4.872523	0.447983
221	6	0	6.320044	-1.286494	4.026185
222	6	0	4.866386	0.551995	4.083351
223	6	0	8.453111	-4.748292	-1.619349
224	6	0	4.793998	-0.799587	-2.729247
225	7	0	4.105833	0.305499	-2.275341
226	8	0	4.440457	2.594800	-2.070146
227	6	0	8.410643	-4.756577	-0.195278
228	6	0	4.915400	-1.756067	3.778264
229	7	0	4.148574	-0.612805	3.841478
230	8	0	4.409069	1.658762	4.203605
231	7	0	7.372675	-4.751454	-2.370341
232	8	0	4.443447	-1.957094	-2.671163
233	1	0	3.152796	0.292226	-1.929728
234	7	0	7.280250	-4.726620	0.481473
235	8	0	4.523780	-2.880032	3.569630
236	1	0	3.143670	-0.649535	3.610880
237	6	0	6.237268	-4.741570	-1.674292
238	6	0	6.192634	-4.718205	-0.293510
239	6	0	4.827311	-4.721810	-2.208258
240	6	0	4.741648	-4.648101	0.126196
241	7	0	4.032054	-4.654151	-1.062649
242	8	0	4.444897	-4.771161	-3.344353
243	8	0	4.269477	-4.585728	1.235270
244	1	0	3.028947	-4.439769	-1.067532
245	8	0	1.471160	-3.601694	-0.731719
246	6	0	0.956264	-3.212493	-1.796709
247	7	0	-0.259721	-3.564890	-2.261641
248	7	0	1.550975	-2.364713	-2.682509
249	6	0	-0.616251	-2.866505	-3.468401
250	1	0	-0.889933	-4.085474	-1.660421
251	6	0	0.743419	-2.190977	-3.875264
252	1	0	2.567278	-2.297314	-2.688619
253	1	0	-1.020205	-3.553480	-4.214737
254	7	0	-1.484809	-1.728978	-3.277748
255	1	0	1.221557	-2.651239	-4.743471
256	7	0	0.357186	-0.828544	-4.144633
257	6	0	-0.901602	-0.571882	-3.681787
258	1	0	-2.498157	-1.810694	-3.233088
259	1	0	1.028602	-0.057015	-4.109483
260	8	0	-1.419715	0.552246	-3.664077
261	1	0	1.207461	-5.076933	3.534497
262	6	0	0.805885	-4.393665	2.783095
263	6	0	-0.578593	-3.772701	3.175158
264	7	0	0.504094	-5.096662	1.558929
265	7	0	1.652854	-3.219830	2.643298
266	1	0	-1.080476	-4.297999	3.991430
267	7	0	-0.222871	-2.432353	3.558484
268	7	0	-1.325056	-3.890347	1.941422
269	6	0	-0.702323	-4.689424	1.039372
270	1	0	1.240463	-5.246228	0.880904
271	6	0	1.043568	-2.118803	3.175901
272	1	0	2.670674	-3.291570	2.695407
273	1	0	-0.868676	-1.645785	3.615796
274	1	0	-2.319154	-3.678063	1.866089
275	8	0	-1.151419	-5.043193	-0.053393
276	8	0	1.552716	-1.001177	3.310533
277	6	0	-0.914781	1.205453	3.316339
278	7	0	0.259629	1.449991	3.967300
279	7	0	-1.545956	2.388331	3.072579
280	8	0	-1.344565	0.089877	3.014141
281	6	0	0.551189	2.861330	4.067629
282	1	0	0.968558	0.725121	3.913581
283	6	0	-0.777714	3.513805	3.536490
284	1	0	-2.558949	2.410264	2.994923
285	1	0	0.800707	3.137351	5.094462
286	7	0	1.544545	3.370220	3.147550
287	1	0	-1.323851	4.084947	4.289762
288	7	0	-0.315337	4.373678	2.464699
289	6	0	1.001023	4.133616	2.175033
290	1	0	2.539701	3.167554	3.185916
291	1	0	-0.926187	4.503083	1.659247
292	8	0	1.582349	4.604838	1.188173
293	1	0	1.134188	5.587703	-2.830646
294	6	0	0.714154	4.651879	-2.457693
295	6	0	-0.459911	4.070202	-3.320742
296	7	0	0.090435	4.842714	-1.162513
297	7	0	1.677980	3.580998	-2.492238
298	1	0	-0.853303	4.769041	-4.061467
299	7	0	0.132513	2.911189	-3.947969
300	7	0	-1.460511	3.753218	-2.316477
301	6	0	-1.092456	4.188672	-1.086787
302	1	0	0.653023	4.933372	-0.309478
303	6	0	1.298716	2.556413	-3.303527
304	1	0	2.632325	3.647373	-2.155048
305	1	0	-0.478285	2.125314	-4.171376
306	1	0	-2.448270	3.600138	-2.517811
307	8	0	-1.755361	4.011642	-0.042630
308	8	0	1.906306	1.498686	-3.465290

BC-trans, capsule a: M062X/6-31g(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.672259	-1.872886	0.804171
2	5	0	-2.214548	-0.078637	0.027554
3	6	0	-5.784052	1.159089	0.798293
4	6	0	-4.408333	1.111394	0.596913
5	6	0	-3.746804	-0.107372	0.381578
6	6	0	-4.511748	-1.276419	0.380138
7	6	0	-5.896202	-1.230502	0.553848
8	6	0	-6.550983	-0.014323	0.759554
9	1	0	-6.276092	2.107281	1.011455
10	1	0	-3.819434	2.025545	0.607590
11	1	0	-4.023915	-2.233396	0.205384
12	1	0	-6.486638	-2.144989	0.544944
13	6	0	-8.052751	0.033669	0.900285
14	6	0	-8.760928	0.292885	-0.435078

15	1	0	-8.331592	0.826577	1.605399
16	1	0	-8.413354	-0.915479	1.317162
17	1	0	-9.847624	0.271546	-0.304067
18	1	0	-8.486303	1.273433	-0.845571
19	1	0	-8.491607	-0.475785	-1.171991
20	8	0	-1.360144	-1.144075	0.245132
21	8	0	-1.780522	1.000880	-0.672157
22	1	0	-0.805875	1.022826	-0.781527
23	6	0	5.197433	1.205161	-0.948498
24	6	0	3.803276	1.193727	-0.920825
25	6	0	3.122783	-0.017842	-0.779880
26	6	0	3.841111	-1.211952	-0.673909
27	6	0	5.230691	-1.186262	-0.696409
28	6	0	5.931561	0.019525	-0.827240
29	1	0	5.724256	2.138678	-1.125849
30	1	0	3.235258	2.116003	-1.024167
31	1	0	3.299289	-2.147009	-0.575631
32	1	0	5.794358	-2.115652	-0.648312
33	6	0	7.445306	0.011730	-0.871550
34	6	0	8.105918	-0.269441	0.486431
35	1	0	7.806862	0.970194	-1.264112
36	1	0	7.771835	-0.765840	-1.575972
37	1	0	9.192113	-0.358351	0.376015
38	1	0	7.905274	0.541017	1.197848
39	1	0	7.732012	-1.204600	0.922543
40	8	0	0.981973	1.009852	-0.616331
41	8	0	1.106486	-1.231324	-0.754168
42	1	0	0.149571	-1.189862	-0.495205
43	6	0	1.631767	-0.021010	-0.713328
44	6	0	-11.074064	-1.216602	-2.868685
45	6	0	-11.645758	0.057728	-3.461454
46	6	0	-11.650261	1.864765	1.917738
47	6	0	-11.150620	3.020563	1.320546
48	6	0	-11.834791	3.649795	0.122099
49	6	0	-11.261799	3.127705	-1.177791
50	6	0	-11.715785	1.932076	-1.738202
51	6	0	-11.122971	1.348746	-2.858117
52	6	0	-11.656752	-1.828695	-1.758791
53	6	0	-11.785600	-3.589690	0.056041
54	6	0	-11.143099	-3.004443	1.297439
55	6	0	-11.626943	-1.841138	1.893294
56	6	0	-11.024763	-1.258522	3.009313
57	6	0	-11.047408	1.269219	3.026545
58	6	0	-11.595897	-0.002919	3.639834
59	6	0	-10.037005	2.024891	-3.416589
60	6	0	-10.218791	3.786935	-1.829528
61	6	0	-9.598650	3.252743	-2.949397
62	6	0	-10.076401	-3.612573	-1.828820
63	6	0	-9.960812	-1.849598	-3.423883
64	6	0	-9.464299	-3.050454	-2.938503
65	6	0	-9.989279	3.574548	1.867489
66	6	0	-9.912887	1.890516	3.548084
67	6	0	-9.367611	3.040254	2.987563
68	6	0	-9.886418	-1.885930	3.520895
69	6	0	-10.018520	-3.596831	1.873364
70	6	0	-9.378144	-3.060558	2.981335
71	1	0	-8.481926	3.502395	3.409148
72	1	0	-12.555737	1.416771	1.511723
73	1	0	-11.721981	4.734470	0.164892
74	1	0	-12.902075	3.414180	0.164149
75	1	0	-12.555567	1.423299	-1.267187
76	1	0	-8.768125	3.762166	-3.423760
77	1	0	-8.607266	-3.524667	-3.402376
78	1	0	-12.528113	-1.360777	-1.303358
79	1	0	-12.518015	-1.373421	1.477765
80	1	0	-8.503575	-3.536884	3.409940
81	1	0	-12.681874	-0.014600	3.508178
82	1	0	-11.384204	-0.009074	4.710704
83	1	0	-12.854405	-3.357955	0.066856
84	1	0	-11.671092	-4.674807	0.059098
85	1	0	-11.446549	0.066470	-4.535261
86	1	0	-12.731134	0.036492	-3.323860
87	8	0	-9.314148	-1.243193	-4.502393
88	8	0	-9.354132	1.429931	-4.477572
89	8	0	-9.580434	-4.798499	1.323289
90	8	0	-9.612670	-4.834309	-1.342786
91	8	0	-9.274930	-1.337382	4.644398
92	8	0	-9.339086	1.336857	4.691130
93	8	0	-9.784486	5.015842	-1.335973
94	8	0	-9.523969	4.758402	1.307814
95	6	0	-8.206834	0.819322	-4.081733
96	6	0	-8.178665	-0.600863	-4.120465
97	7	0	-7.126066	-1.305357	-3.756824
98	7	0	-7.191908	1.542484	-3.650734
99	6	0	-6.103577	-0.560958	-3.347810
100	6	0	-6.139082	0.816960	-3.283718
101	6	0	-4.751112	-1.025183	-2.881360
102	6	0	-4.805990	1.294719	-2.771718
103	7	0	-4.039172	0.149386	-2.653424
104	8	0	-4.371659	-2.156518	-2.720827
105	1	0	-3.087509	0.136427	-2.285190
106	8	0	-4.457103	2.426303	-2.530015
107	6	0	-8.397499	-4.813429	-0.736153
108	6	0	-8.384573	-4.776711	0.688197
109	6	0	-11.170654	-3.012498	-1.202275
110	7	0	-7.273589	-4.744707	1.391640
111	7	0	-7.297893	-4.847500	-1.461416
112	6	0	-8.136559	0.737520	4.491332
113	6	0	-8.102998	-0.682140	4.428981
114	6	0	-8.522676	4.976677	-0.825479
115	6	0	-8.383949	4.747359	0.572604
116	7	0	-6.998949	-1.363137	4.189670
117	7	0	-7.062119	1.483449	4.346212
118	7	0	-7.495305	5.123092	-1.634387
119	7	0	-7.213079	4.591247	1.154666
120	6	0	-6.178077	-4.831007	-0.737244
121	6	0	-6.182089	4.712940	0.316275
122	6	0	-6.172955	-4.773662	0.644151
123	6	0	-5.955011	0.782885	4.125826
124	6	0	-5.919820	-0.597083	4.036431

125	6	0	-6.316101	4.994833	-1.028029
126	6	0	-4.938339	5.099946	-1.635230
127	6	0	-4.712526	4.560691	0.617162
128	6	0	-4.741513	-4.859577	-1.211124
129	6	0	-4.750294	-4.708644	1.116800
130	6	0	-4.575528	1.316451	3.873574
131	6	0	-4.498450	-1.007973	3.711456
132	7	0	-4.071201	4.808072	-0.577099
133	7	0	-3.791642	0.181841	3.689672
134	7	0	-3.992840	-4.726156	-0.047180
135	8	0	-4.199171	4.272669	1.674621
136	8	0	-4.631467	5.390096	-2.757521
137	8	0	-4.195420	2.456767	3.834421
138	8	0	-4.042532	-2.109557	3.519760
139	8	0	-4.300662	-4.983734	-2.325233
140	8	0	-4.328804	-4.638480	2.243660
141	1	0	-2.972487	-4.845487	0.036112
142	1	0	-2.864845	0.295584	3.265048
143	1	0	-3.040278	4.725873	-0.675983
144	1	0	12.806297	-3.499703	0.697233
145	6	0	11.731164	-3.695847	0.654273
146	6	0	11.061240	-3.009817	1.827426
147	6	0	11.191373	-3.184251	-0.667054
148	1	0	11.577964	-4.774314	0.721180
149	6	0	11.545496	-1.790477	2.307557
150	6	0	9.923803	-3.534181	2.445241
151	6	0	11.766422	-2.102424	-1.331046
152	6	0	10.067957	-3.769442	-1.252842
153	6	0	10.916238	-1.073574	3.324336
154	1	0	12.451968	-1.381489	1.864796
155	6	0	9.267131	-2.865431	3.468436
156	8	0	9.434685	-4.777109	2.043646
157	6	0	11.259148	-1.598243	-2.530513
158	1	0	12.651142	-1.635052	-0.902161
159	6	0	9.531062	-3.320639	-2.450373
160	8	0	9.534931	-4.884555	-0.613765
161	6	0	11.474106	0.233576	3.852375
162	6	0	9.760864	-1.634847	3.867557
163	1	0	8.374324	-3.282880	3.918450
164	6	0	8.250486	-4.742240	1.375031
165	6	0	11.903699	-0.409107	-3.215980
166	6	0	10.136038	-2.231466	-3.066466
167	1	0	8.668832	-3.803281	-2.896642
168	6	0	8.312064	-4.759288	-0.048136
169	1	0	12.565519	0.184862	3.790487
170	1	0	11.205691	0.329189	4.906533
171	6	0	11.022869	1.482671	3.119405
172	8	0	9.068949	-0.899797	4.832979
173	7	0	7.115141	-4.700418	2.043665
174	6	0	11.345998	0.912450	-2.726670
175	1	0	11.757363	-0.489315	-4.294571
176	1	0	12.978842	-0.431862	-3.015828
177	8	0	9.646382	-1.787144	-4.292327
178	7	0	7.241295	-4.693271	-0.808358
179	6	0	11.699334	1.945508	1.991739
180	6	0	9.943414	2.250340	3.562980
181	6	0	7.993015	-0.265023	4.303950
182	6	0	6.032766	-4.665501	1.262811
183	6	0	11.912861	1.586006	-1.644335
184	6	0	10.238236	1.500779	-3.337943
185	6	0	8.462399	-1.119942	-4.245634
186	6	0	6.104956	-4.651172	-0.116879
187	6	0	11.343470	3.115516	1.317173
188	1	0	12.537913	1.363626	1.612701
189	6	0	9.592808	3.452161	2.973454
190	8	0	9.169817	1.775800	4.627428
191	6	0	8.043011	1.152798	4.194694
192	7	0	6.983010	-0.980437	3.853274
193	6	0	4.567124	-4.638599	1.651461
194	6	0	11.403514	2.789641	-1.160515
195	1	0	12.795478	1.161840	-1.169039
196	6	0	9.686474	2.696353	-2.893409
197	8	0	9.725662	0.878484	-4.472305
198	6	0	8.507695	0.297135	-4.334092
199	7	0	7.335922	-1.793974	-4.116757
200	6	0	4.714562	-4.561686	-0.669710
201	6	0	12.027346	3.502973	0.023072
202	6	0	10.300228	3.869500	1.854312
203	1	0	8.763357	4.035768	3.356058
204	7	0	7.075152	1.859452	3.641741
205	6	0	6.020324	-0.252814	3.302312
206	7	0	3.888596	-4.510807	0.441880
207	8	0	4.054732	-4.723143	2.738095
208	6	0	10.274543	3.311275	-1.797442
209	1	0	8.829893	3.137318	-3.390918
210	7	0	7.429345	1.052720	-4.290939
211	6	0	6.252878	-1.020290	-4.082141
212	8	0	4.368226	-4.525125	-1.824278
213	1	0	11.958485	4.582822	-0.120631
214	1	0	13.085184	3.231014	0.081695
215	8	0	9.938698	5.071008	1.246226
216	6	0	6.058418	1.122803	3.202214
217	6	0	4.768576	-0.744506	2.641178
218	1	0	2.878589	-4.691133	0.297292
219	8	0	9.813568	4.544701	-1.357751
220	6	0	6.302428	0.359751	-4.165205
221	6	0	4.806196	-1.428662	-3.918478
222	6	0	8.704878	5.021558	0.669222
223	6	0	4.810258	1.572632	2.487256
224	7	0	4.109306	0.405874	2.235645
225	8	0	4.410043	-1.884837	2.476399
226	6	0	8.632571	4.637230	-0.699414
227	6	0	4.899641	0.891122	-4.056218
228	7	0	4.106267	-0.229463	-3.923044
229	8	0	4.335963	-2.532199	-3.817032
230	7	0	7.642056	5.295071	1.393637
231	8	0	4.471626	2.696504	2.198881
232	1	0	3.187282	0.338052	1.800709
233	7	0	7.490732	4.447280	-1.328195
234	8	0	4.528835	2.041322	-4.077716

235	1	0	3.083107	-0.145411	-3.752577
236	6	0	6.494304	5.147094	0.733133
237	6	0	6.419949	4.710981	-0.575264
238	6	0	5.094720	5.399231	1.235337
239	6	0	4.960168	4.621686	-0.957651
240	7	0	4.274934	5.065157	0.158754
241	8	0	4.739855	5.801712	2.309923
242	8	0	4.476625	4.235254	-1.994189
243	1	0	3.242024	5.177956	0.167074
244	8	0	1.568863	5.288941	0.211633
245	6	0	1.074023	4.771727	1.218305
246	7	0	-0.134973	5.122272	1.759355
247	7	0	1.648498	3.813145	1.989703
248	6	0	-0.514461	4.212539	2.818954
249	1	0	-0.827135	5.390171	1.066430
250	6	0	0.805039	3.403821	3.086372
251	1	0	2.628917	3.560469	1.912537
252	1	0	-0.875721	4.761167	3.691396
253	7	0	-1.451612	3.178473	2.439194
254	1	0	1.271379	3.628148	4.048521
255	7	0	0.352461	2.030827	3.036327
256	6	0	-0.927703	1.942357	2.573846
257	1	0	-2.454519	3.335248	2.358350
258	1	0	0.961900	1.242095	2.818798
259	8	0	-1.516969	0.870197	2.355971
260	1	0	0.858337	4.323032	-4.152294
261	6	0	0.628146	3.525512	-3.441713
262	6	0	-0.745684	2.820922	-3.705799
263	7	0	0.424811	4.044858	-2.105233
264	7	0	1.571548	2.443174	-3.562920
265	1	0	-1.140550	2.989334	-4.711470
266	7	0	-0.388606	1.429295	-3.509688
267	7	0	-1.604671	3.399257	-2.712262
268	6	0	-0.879746	4.012888	-1.728858
269	1	0	1.091373	4.583893	-1.562545
270	6	0	0.947808	1.236701	-3.498688
271	1	0	2.584505	2.537301	-3.562531
272	1	0	-1.005595	0.621645	-3.440399
273	1	0	-2.532718	3.036541	-2.507856
274	8	0	-1.354278	4.498901	-0.697899
275	8	0	1.500451	0.124421	-3.471394
276	6	0	-1.047599	-2.152498	-2.875624
277	7	0	0.131947	-2.417878	-3.503346
278	7	0	-1.598726	-3.328694	-2.425714
279	8	0	-1.547729	-1.035337	-2.750909
280	6	0	0.513646	-3.798563	-3.371756
281	1	0	0.796129	-1.649021	-3.583265
282	6	0	-0.811565	-4.468502	-2.864088
283	1	0	-2.614890	-3.376757	-2.408213
284	1	0	0.879622	-4.200490	-4.319373
285	7	0	1.439480	-4.086208	-2.294322
286	1	0	-1.341042	-5.043124	-3.626788
287	7	0	-0.336052	-5.324200	-1.802761
288	6	0	0.919472	-4.963206	-1.396900
289	1	0	2.446560	-3.964962	-2.371927
290	1	0	-0.951055	-5.676698	-1.078375
291	8	0	1.478767	-5.398825	-0.383518
292	1	0	1.228450	-4.072587	3.863534
293	6	0	0.726619	-3.705331	2.965915
294	6	0	-0.605456	-2.923921	3.242825
295	7	0	0.273877	-4.795033	2.141571
296	7	0	1.537896	-2.718627	2.278504
297	1	0	-1.013722	-3.082141	4.242634
298	7	0	-0.201616	-1.558798	3.044478
299	7	0	-1.522328	-3.449848	2.227846
300	6	0	-0.972331	-4.588927	1.648630
301	1	0	0.899449	-5.349147	1.564306
302	6	0	1.001589	-1.467945	2.409847
303	1	0	2.551469	-2.792708	2.244362
304	1	0	-0.838680	-0.769326	2.927868
305	1	0	-2.515286	-3.515720	2.469208
306	8	0	-1.525762	-5.307214	0.819883
307	8	0	1.524472	-0.412053	2.045341

CC-trans, capsule a: M062X/6-31g(d,p):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.183685	1.163660	2.651570
2	6	0	-11.625597	-0.122468	3.322795
3	6	0	-11.430886	-2.197129	-2.018678
4	6	0	-10.883928	-3.318857	-1.391312
5	6	0	-11.516536	-3.855768	-0.121804
6	6	0	-10.959966	-3.176784	1.113366
7	6	0	-11.526672	-2.030776	1.666328
8	6	0	-10.972013	-1.370034	2.765405
9	6	0	-11.809760	1.668944	1.512764
10	6	0	-12.021136	3.298780	-0.418873
11	6	0	-11.280277	2.691962	-1.597533
12	6	0	-11.672167	1.484521	-2.170515
13	6	0	-11.000161	0.900945	-3.247578
14	6	0	-10.884742	-1.629007	-3.168105
15	6	0	-11.488043	-0.408417	-3.833986
16	6	0	-9.806189	-1.909173	3.315358
17	6	0	-9.812424	-3.677852	1.726720
18	6	0	-9.222473	-3.069487	2.823480
19	6	0	-10.410759	3.600335	1.527724
20	6	0	-10.118080	1.903027	3.165068
21	6	0	-9.746620	3.134253	2.653712
22	6	0	-9.750075	-3.891551	-1.978387
23	6	0	-9.743995	-2.234911	-3.691052
24	6	0	-9.176463	-3.369393	-3.129847
25	6	0	-9.889368	1.580136	-3.755963
26	6	0	-10.165252	3.323075	-2.153615
27	6	0	-9.463932	2.794335	-3.228981
28	1	0	-8.293444	-3.826164	-3.561199
29	1	0	-12.325777	-1.749523	-1.589082
30	1	0	-11.349178	-4.932198	-0.054644

31	1	0	-12.595037	-3.680212	-0.169360
32	1	0	-12.437414	-1.629808	1.224225
33	1	0	-8.328889	-3.479100	3.280466
34	1	0	-8.942181	3.703529	3.104767
35	1	0	-12.626073	1.101129	1.068587
36	1	0	-12.550286	0.979031	-1.771604
37	1	0	-8.603981	3.308791	-3.643256
38	1	0	-12.575129	-0.452121	-3.718691
39	1	0	-11.260625	-0.433854	-4.901287
40	1	0	-13.065825	2.976774	-0.458036
41	1	0	-11.995532	4.387292	-0.493803
42	1	0	-11.414348	-0.053965	4.391769
43	1	0	-12.708579	-0.218769	3.199661
44	8	0	-9.423447	1.376523	4.248600
45	8	0	-9.217829	-1.283867	4.416082
46	8	0	-9.820466	4.562603	-1.629338
47	8	0	-10.061113	4.847719	1.010138
48	8	0	-9.210578	1.045777	-4.854432
49	8	0	-9.160998	-1.644986	-4.811509
50	8	0	-9.298228	-4.861281	1.211906
51	8	0	-9.202611	-5.055648	-1.438143
52	6	0	-8.090947	-0.580673	4.115257
53	6	0	-8.219160	0.825607	3.948253
54	7	0	-7.224651	1.589667	3.544197
55	7	0	-6.940553	-1.211273	3.989086
56	6	0	-6.076487	0.933758	3.389783
57	6	0	-5.926615	-0.416689	3.647990
58	6	0	-4.729311	1.492898	3.009935
59	6	0	-4.457845	-0.756956	3.527644
60	7	0	-3.850631	0.443143	3.173594
61	8	0	-4.447225	2.608686	2.633500
62	1	0	-2.818804	0.551605	3.063696
63	8	0	-3.896387	-1.802611	3.730172
64	6	0	-8.805596	4.885294	0.487594
65	6	0	-8.676358	4.652196	-0.910180
66	6	0	-11.418284	2.862935	0.901744
67	7	0	-7.510700	4.551164	-1.509962
68	7	0	-7.775089	5.095931	1.279962
69	6	0	-8.014211	-0.980944	-4.516702
70	6	0	-8.026160	0.439115	-4.566082
71	6	0	-8.076575	-4.795310	0.634722
72	6	0	-8.017182	-4.926459	-0.781697
73	7	0	-6.953280	1.168615	-4.318743
74	7	0	-6.959942	-1.672153	-4.137681
75	7	0	-7.009164	-4.639768	1.386488
76	7	0	-6.878540	-4.963544	-1.447057
77	6	0	-6.599495	5.027322	0.655176
78	6	0	-5.798334	-4.837949	-0.671208
79	6	0	-6.480038	4.740178	-0.688514
80	6	0	-5.903596	-0.922586	-3.856137
81	6	0	-5.881197	0.454038	-3.977207
82	6	0	-5.872840	-4.659890	0.697195
83	6	0	-4.486916	-4.479679	1.238591
84	6	0	-4.328012	-4.852574	-1.048889
85	6	0	-5.208306	5.202686	1.226065
86	6	0	-5.024457	4.637892	-1.024637
87	6	0	-4.597619	-1.380100	-3.279142
88	6	0	-4.502859	0.928828	-3.564675
89	7	0	-3.657532	-4.557778	0.134141
90	7	0	-3.836509	-0.232508	-3.183182
91	7	0	-4.358548	4.910212	0.152976
92	8	0	-3.811765	-5.095726	-2.109989
93	8	0	-4.155150	-4.287361	2.382859
94	8	0	-4.271672	-2.496322	-2.953223
95	8	0	-4.042731	2.040994	-3.563911
96	8	0	-4.880752	5.546860	2.326842
97	8	0	-4.535117	4.347444	-2.090955
98	1	0	-3.330281	5.008647	0.144725
99	1	0	-2.927971	-0.272476	-2.704610
100	1	0	-2.621769	-4.553820	0.274290
101	1	0	12.791766	3.643474	-0.975535
102	6	0	11.718291	3.842491	-0.909045
103	6	0	11.023503	3.166193	-2.076081
104	6	0	11.204236	3.325985	0.422924
105	1	0	11.567277	4.921894	-0.966461
106	6	0	11.492666	1.940789	-2.557900
107	6	0	9.882792	3.694586	-2.686153
108	6	0	11.797596	2.258304	1.093894
109	6	0	10.076876	3.898113	1.012210
110	6	0	10.843126	1.216619	-3.555948
111	1	0	12.403514	1.529831	-2.126065
112	6	0	9.201799	3.013371	-3.686419
113	8	0	9.396853	4.945072	-2.296597
114	6	0	11.295366	1.752179	2.295225
115	1	0	12.690950	1.803280	0.669829
116	6	0	9.539284	3.442946	2.207167
117	8	0	9.530534	4.998303	0.361007
118	6	0	11.388449	-0.097396	-4.081461
119	6	0	9.675565	1.773336	-4.078564
120	1	0	8.301926	3.430727	-4.122591
121	6	0	8.221790	4.888271	-1.609796
122	6	0	11.962633	0.583883	2.993188
123	6	0	10.155083	2.361848	2.823768
124	1	0	8.667522	3.912576	2.647544
125	6	0	8.305783	4.842110	-0.190054
126	1	0	12.481022	-0.046920	-4.049802
127	1	0	11.090900	-0.208548	-5.126157
128	6	0	10.955486	-1.332445	-3.315370
129	8	0	8.955975	1.027602	-5.015834
130	7	0	7.076109	4.853477	-2.260888
131	6	0	11.415907	-0.754525	2.539547
132	1	0	11.830531	0.683124	4.072080
133	1	0	13.034613	0.615371	2.777934
134	8	0	9.672383	1.915402	4.052114
135	7	0	7.256296	4.668982	0.581855
136	6	0	11.668089	-1.779638	-2.202323
137	6	0	9.854153	-2.095842	-3.708855
138	6	0	7.890192	0.394291	-4.463238
139	6	0	6.011624	4.727363	-1.465423
140	6	0	11.950190	-1.422937	1.438704

141	6	0	10.351192	-1.365639	3.201885
142	6	0	8.511697	1.209002	4.048859
143	6	0	6.113122	4.607047	-0.093534
144	6	0	11.321627	-2.931021	-1.493517
145	1	0	12.530252	-1.203781	-1.870437
146	6	0	9.499229	-3.274329	-3.073289
147	8	0	9.071566	-1.646995	-4.778273
148	6	0	7.941825	-1.024246	-4.353517
149	7	0	6.890358	1.107692	-3.986290
150	6	0	4.540867	4.669466	-1.825617
151	6	0	11.458632	-2.648000	0.988893
152	1	0	12.792540	-0.974517	0.914842
153	6	0	9.824933	-2.586891	2.800623
154	8	0	9.851911	-0.736162	4.338979
155	6	0	8.611957	-0.201100	4.209744
156	7	0	7.355421	1.834585	3.935716
157	6	0	4.745906	4.391409	0.475729
158	6	0	12.050907	-3.331751	-0.227738
159	6	0	10.241864	-3.673283	-1.971452
160	1	0	8.648907	-3.854568	-3.411931
161	7	0	6.979931	-1.732478	-3.794175
162	6	0	5.935624	0.378092	-3.420074
163	7	0	3.899384	4.412470	-0.615791
164	8	0	4.000364	4.820276	-2.890283
165	6	0	10.386013	-3.204542	1.691479
166	1	0	9.009033	-3.051820	3.343459
167	7	0	7.562506	-0.994677	4.239496
168	6	0	6.299261	1.021157	3.979314
169	8	0	4.444373	4.211060	1.630503
170	1	0	12.000173	-4.414875	-0.102349
171	1	0	13.102881	-3.045356	-0.315220
172	8	0	9.908935	-4.857670	-1.321218
173	6	0	5.971076	-0.998313	-3.335500
174	6	0	4.725211	0.865752	-2.679672
175	1	0	2.891576	4.487832	-0.436489
176	8	0	9.938925	-4.464309	1.309689
177	6	0	6.406332	-0.350363	4.117608
178	6	0	4.826042	1.362147	3.885092
179	6	0	8.710775	-4.831149	-0.679099
180	6	0	4.771775	-1.451027	-2.542677
181	7	0	4.093230	-0.285566	-2.235690
182	8	0	4.379167	2.003063	-2.476412
183	6	0	8.721265	-4.575182	0.720793
184	6	0	5.028293	-0.945903	4.046752
185	7	0	4.180864	0.134901	3.936954
186	8	0	4.297304	2.441755	3.800268
187	7	0	7.606654	-5.043492	-1.361599
188	8	0	4.463568	-2.575680	-2.224416
189	1	0	3.208820	-0.211456	-1.728981
190	7	0	7.621001	-4.512203	1.443727
191	8	0	4.713240	-2.113450	4.062317
192	1	0	3.152106	-0.001032	3.811719
193	6	0	6.503595	-4.995797	-0.616917
194	6	0	6.507792	-4.735579	0.741444
195	6	0	5.082017	-5.219713	-1.061477
196	6	0	5.075645	-4.780386	1.232400
197	7	0	4.325397	-5.035513	0.092913
198	8	0	4.666199	-5.507599	-2.151338
199	8	0	4.651902	-4.624493	2.349229
200	1	0	3.299461	-5.202459	0.096707
201	8	0	1.660488	-5.440215	-0.138342
202	6	0	1.161163	-4.811537	-1.075575
203	7	0	-0.012409	-5.137669	-1.699775
204	7	0	1.693631	-3.712365	-1.681016
205	6	0	-0.431851	-4.104482	-2.618332
206	1	0	-0.693570	-5.606351	-1.116223
207	6	0	0.867546	-3.236191	-2.768949
208	1	0	2.688343	-3.509878	-1.644828
209	1	0	-0.787126	-4.538181	-3.555331
210	7	0	-1.394494	-3.153841	-2.094044
211	1	0	1.373432	-3.358857	-3.729895
212	7	0	0.365533	-1.895638	-2.607783
213	6	0	-0.910033	-1.880264	-2.143253
214	1	0	-2.395904	-3.294657	-2.209822
215	1	0	0.940140	-1.065087	-2.451192
216	8	0	-1.540726	-0.855125	-1.848573
217	1	0	1.213098	-4.429149	4.398329
218	6	0	0.862914	-3.754152	3.613843
219	6	0	-0.535093	-3.095786	3.917471
220	7	0	0.600780	-4.470520	2.392120
221	7	0	1.742206	-2.609677	3.498100
222	1	0	-1.010944	-3.473210	4.825901
223	7	0	-0.202885	-1.698625	4.055861
224	7	0	-1.316937	-3.420424	2.753260
225	6	0	-0.649659	-4.245419	1.899886
226	1	0	1.291877	-4.918338	1.802389
227	6	0	1.090138	-1.442302	3.743038
228	1	0	2.757465	-2.667532	3.553909
229	1	0	-0.871272	-0.944105	3.934983
230	1	0	-2.332952	-3.380831	2.751958
231	8	0	-1.099394	-4.739006	0.862630
232	8	0	1.594544	-0.309019	3.720963
233	6	0	-0.751633	1.947629	3.251737
234	7	0	0.407855	2.278993	3.878773
235	7	0	-1.346225	3.072928	2.780633
236	8	0	-1.202880	0.797203	3.151811
237	6	0	0.752024	3.661194	3.653346
238	1	0	1.086110	1.533182	4.002376
239	6	0	-0.600598	4.267413	3.140243
240	1	0	-2.327663	3.069384	2.514265
241	1	0	1.126881	4.124456	4.568802
242	7	0	1.636685	3.908768	2.535523
243	1	0	-1.137126	4.856312	3.887705
244	7	0	-0.183580	5.080017	2.029913
245	6	0	1.072457	4.730472	1.610713
246	1	0	2.643840	3.768449	2.562517
247	1	0	-0.836728	5.383718	1.309875
248	8	0	1.594450	5.138004	0.570508
249	1	0	0.893092	4.305013	-3.682101
250	6	0	0.517004	3.838363	-2.769279

251	6	0	-0.792970	2.988562	-2.969962
252	7	0	0.091380	4.836826	-1.813425
253	7	0	1.471979	2.875169	-2.260168
254	1	0	-1.202984	3.027834	-3.981452
255	7	0	-0.342894	1.651736	-2.646033
256	7	0	-1.714184	3.558175	-2.022907
257	6	0	-1.162029	4.593191	-1.332499
258	1	0	0.741905	5.289553	-1.176987
259	6	0	0.945748	1.614444	-2.228359
260	1	0	2.473583	2.980319	-2.390886
261	1	0	-0.952410	0.881052	-2.376624
262	1	0	-2.721981	3.498185	-2.146959
263	8	0	-1.700576	5.238164	-0.424189
264	8	0	1.553408	0.586564	-1.906360
265	6	0	-6.019812	-1.183245	-0.236671
266	6	0	-4.682002	-1.126935	0.135365
267	6	0	-3.998299	0.089950	0.079721
268	6	0	-4.652915	1.244737	-0.352895
269	6	0	-5.990915	1.175635	-0.732285
270	6	0	-6.689516	-0.036819	-0.676979
271	1	0	-6.561361	-2.127891	-0.208457
272	1	0	-4.142255	-2.012456	0.454489
273	1	0	-4.096437	2.177763	-0.399902
274	1	0	-6.498026	2.060249	-1.115296
275	6	0	-8.149393	-0.114956	-1.042727
276	6	0	-9.054348	0.068536	0.178152
277	1	0	-8.359659	-1.089734	-1.502816
278	1	0	-8.386333	0.659445	-1.780793
279	1	0	-10.105969	-0.055972	-0.099885
280	1	0	-8.817665	-0.672636	0.952335
281	1	0	-8.928929	1.069330	0.610051
282	8	0	-1.893198	1.175772	0.285622
283	8	0	-2.110426	-0.943668	1.009735
284	1	0	-1.106763	-0.913824	1.079140
285	6	0	-2.558900	0.156317	0.459115
286	6	0	4.626291	-1.452874	0.801922
287	6	0	3.245061	-1.317613	0.811475
288	6	0	2.674245	-0.039846	0.827343
289	6	0	3.499656	1.087241	0.807163
290	6	0	4.887991	0.933050	0.809607
291	6	0	5.473374	-0.338538	0.821927
292	1	0	5.069278	-2.442152	0.792213
293	1	0	2.593008	-2.186991	0.816873
294	1	0	3.054328	2.078376	0.808878
295	1	0	5.521953	1.816964	0.849257
296	6	0	6.971226	-0.562958	0.892772
297	6	0	7.606026	-1.005452	-0.431689
298	1	0	7.164504	-1.346408	1.637337
299	1	0	7.468723	0.347977	1.253038
300	1	0	8.663463	-1.257828	-0.288732
301	1	0	7.098885	-1.891232	-0.837801
302	1	0	7.552139	-0.209589	-1.183432
303	8	0	0.485328	-0.951132	0.904997
304	8	0	0.699283	1.278531	0.792565
305	1	0	-0.298588	1.240337	0.668357
306	6	0	1.183969	0.059711	0.845909

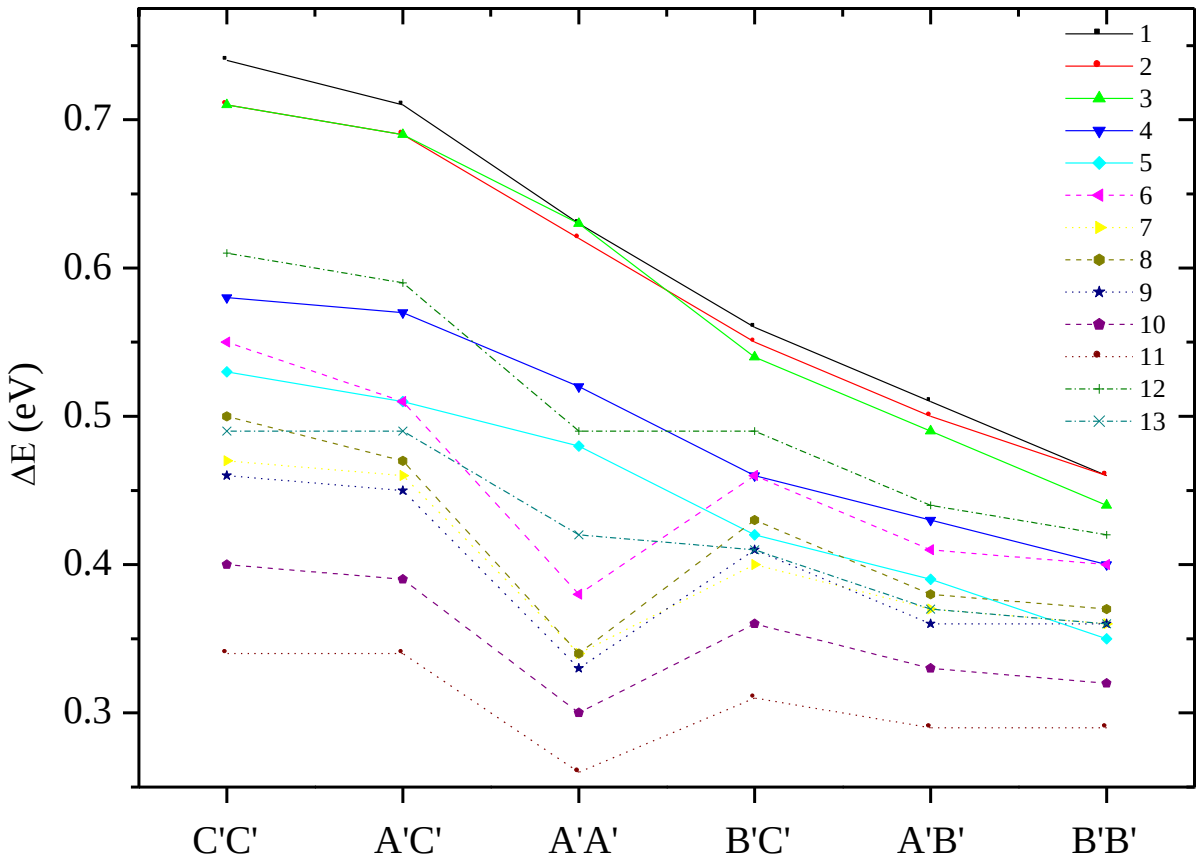

Figure 1S. Dimerization energies of the **C'C'**, **A'C'**, **A'A'**, **B'C'**, **A'B'**, and **B'B'** dimers at 1: M06-2X/6-31G(d,p), 2: M06-2X/6-311+G(d,p), 3: M06-L/6-311+G(d,p), 4: MP2/6-31G(d,p), 5: MP2/6-311+G(d,p), 6: M06-2X/6-31G(d,p) in n,n-DiMethylFormamide solvent using the PCM model, 7: M06-2X/6-31G(d,p) in n,n-DiMethylFormamide solvent using the SCI-PCM model, 8: M06-2X/6-311+G(d,p) in n,n-DiMethyl Formamide solvent using the PCM model, 9: M06-2X/6-311+G(d,p) in n,n-DiMethylFormamide solvent using the SCI-PCM model, 10: MP2/6-31G(d,p) in n,n-DiMethylFormamide solvent using the PCM model, 11: MP2/6-31G(d,p) in n,n-DiMethylFormamide solvent using the SCI-PCM model, 12: M06-2X/6-311+G(d,p) in CCl_4 solvent using the PCM model, and 13: MP2/6-31G(d,p) in CCl_4 solvent using the PCM model

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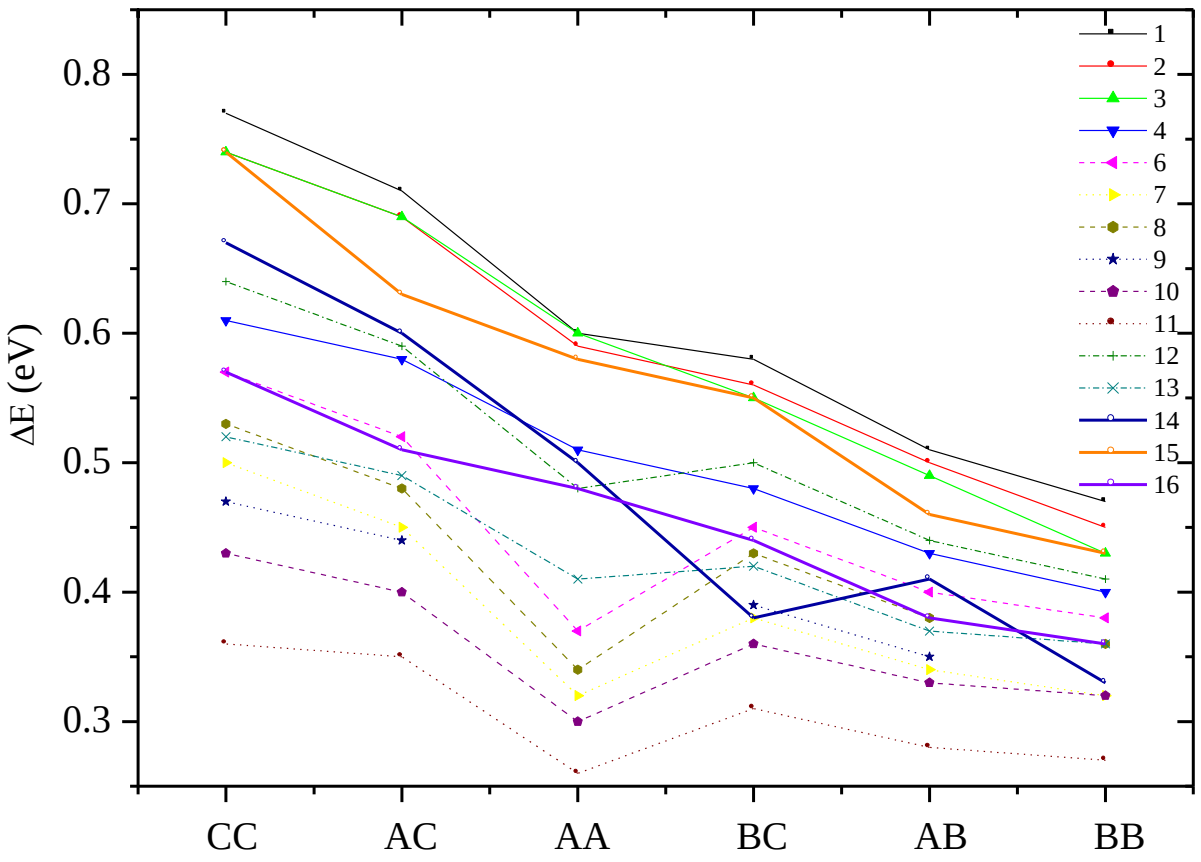

Figure 2S. Dimerization energies of the **CC**, **AC**, **AA**, **BC**, **AB**, and **BB** dimers at 1: M06-2X/6-31G(d,p), 2: M06-2X/6-311+G(d,p), 3: M06-L/6-311+G(d,p), 4: MP2/6-31G(d,p), 6: M06-2X/6-31G(d,p) in n,n-DiMethylFormamide solvent using the PCM model, 7: M06-2X/6-31G(d,p) in n,n-DiMethyl Formamide solvent using the SCI-PCM model, 8: M06-2X/6-311+G(d,p) in n,n-DiMethyl Formamide solvent using the PCM model, 9: M06-2X/6-311+G(d,p) in n,n-DiMethylFormamide solvent using the SCI-PCM model, 10: MP2/6-31G(d,p) in n,n-DiMethylFormamide solvent using the PCM model, 11: MP2/6-31G(d,p) in n,n-DiMethylFormamide solvent using the SCI-PCM model, 12: M06-2X/6-311+G(d,p) in CCl_4 solvent using the PCM model, 13: MP2/6-31G(d,p) in CCl_4 solvent using the PCM model, 14: M06-2X/6-31G(d,p) in the capsule **a**, 15: Oniom-M06-2X/6-31G(d,p) in the capsule **a**, 16: Oniom-MP2/6-31G(d,p) in the capsule **a**.

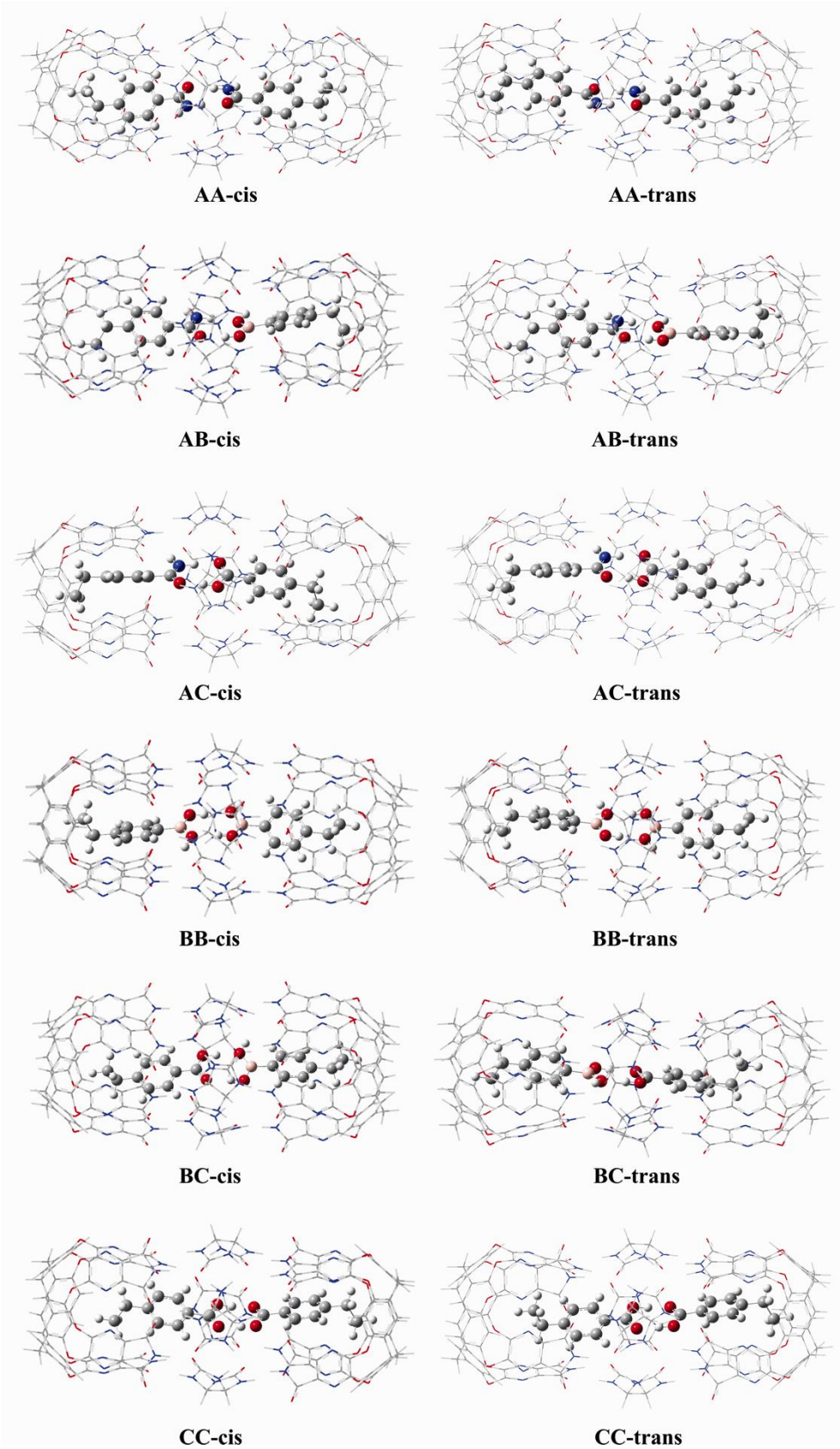

Figure 3S: Structures of the encapsulated dimers in the capsule **1.2$_4$.1a**. The atoms of the capsule are designed with stick bonds for clarity. (H atoms = white spheres, C = grey spheres, O = red spheres and N = blue spheres).

Complete Reference 36

36. Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.