

Supporting Information

Aromaticity and Chemical Bonding of Chalcogen-bonded capsules featuring enhanced magnetic anisotropy.

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A. Analysis of the many-body interaction energy terms

The BSSE-corrected interaction energies (ΔE), deformation terms (D), the BSSE-corrected two- ($\Delta^2 E$) and three-body ($\Delta^3 E$) terms are:

$$\Delta E = E_{X_i X_j \dots}^{x_i x_j \dots}(X_i X_j \dots) - \sum_i E_{X_i X_j \dots}^{x_i x_j \dots}(X_i) + \sum_i D_{X_i}$$

$$D_{X_i} = E_{X_i X_j \dots}^{x_i}(X_i) - E_{X_i}^{x_i}(X_i)$$

$$\Delta^2 E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i X_j, BSSE) = E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i X_j) - \{E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i) + E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_j)\}$$

$$\begin{aligned} \Delta^3 E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i X_j X_k, BSSE) = & E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i X_j X_k) - \{E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i) + E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_j) + E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_k)\} \\ & - \{\Delta^2 E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i X_j) + \Delta^2 E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_i X_k) + \Delta^2 E_{X_1 X_2 \dots}^{x_1 x_2 \dots}(X_j X_k)\} \end{aligned}$$

where, $E_G^s(M)$ refers to the total energy of the molecule M computed at the geometry G with basis set s .

B. Dipole moment (μ), linear polarizability (α) and first-order hyperpolarizability (β)

- The total dipole moment is calculated using the following equation:

$$\mu_{tot} = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{\frac{1}{2}}$$

- Linear polarizability (α) is calculated using the following equation:

$$\alpha_{tot} = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$\Delta\alpha = \frac{1}{\sqrt{2}} [(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6\alpha_{xz}^2 + 6\alpha_{xy}^2 + 6\alpha_{yz}^2]^{\frac{1}{2}}$$

where: $\alpha_{xx}, \alpha_{xy}, \alpha_{yy}, \alpha_{xz}, \alpha_{yz}, \alpha_{zz}$, polarizability tensors

- First-order hyperpolarizability (β) is calculated using the following equation:

$$\langle \beta \rangle = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxz})^2 + (\beta_{zzz} + \beta_{zxz} + \beta_{zyy})^2]^{\frac{1}{2}}$$

where: $\beta_{xxx}, \beta_{xyy}, \beta_{xzz}, \beta_{yyy}, \beta_{zxz}, \beta_{yzz}, \beta_{xzz}, \beta_{yzz}, \beta_{zzz}$ hyperpolarizability tensors

C. Properties of the walls of the capsules, furazan and its substituted derivatives with S, Se and Te.

The dipole moments, dipole electric field isotropic and anisotropic polarizabilities, charges via the Mulliken population analysis, charge model 5 (CM5) and natural bond orbital (NBO) analyses, NMR spectra and magnetic isotropy and anisotropy in the plane and out of the plane of **1-4** (see Fig. 1Sa) were calculated. Six methodologies were used, i.e., M06-2X/LAN2LDZ, B3LYP/6-311+G(d,p), M06-2X/6-311+G(d,p), PBE0/6-311+G(d,p), MP2/6-311+G(d,p), and RCCSD/6-311+G(d,p). The magnetic isotropy and anisotropy were calculated, for the **1-4** compounds, at the geometric center of the ring, at the geometric center of the NCCN quadrilateral and in the ring at distance of 1 Å from the chalcogen for the **1-4** systems, see Fig. 1Sb. It should be noted that all six methodologies were used in order to check our results regarding the basis sets and regarding the DFT data *vs* MP2 and CCSD results. We conclude that that all methodologies predict similar results, adding confidence to the DFT results on the larger systems.

The magnetic isotropy and anisotropy in the plane and out of the plane of the **1-4** compounds are given in Tables 1S-6S and they are plotted in Fig.3S-5S. We observe that all six levels of theory present the same trends. Generally, the magnetic anisotropy is larger than isotropy with the exception of the values in the plane at the geometric center of the ring or at 1 Å distance from the Z atom, (X = O, S, Se and Te). Note, while the magnetic isotropy values are the largest ones in the plane, the magnetic anisotropy values are largest at a distance of 1 Å above the plane, see Fig.3S-4S. We found that the replacement of the oxygen atom with a sulfur, selenium or tellurium atom in furazan results in an increase of 6-28 % for the magnetic isotropy and 12-41 % for the magnetic anisotropy in the distance of 3-5 Å perpendicular above the furazan, at all levels of theory, see Table 7S. Moreover, in the substituted furazan compounds, the differences among them are very small, of 0-11 % for magnetic isotropy and 0-13 % for anisotropy in the distance of 3-5 Å from the furazan. It should be noted that, while the magnetic isotropy and anisotropy are small in the distances of 3-5 Å, where the alkane is located in the

capsule, eight furazan or substituted furazan groups are included in the cage, and as a result the total magnetic isotropy and anisotropy are enhanced. Finally, the isotropic polarizabilities are larger than the anisotropic ones, see Table 8S. The replacement of the O atom with S, Se and Te results in an increase of the isotropic and anisotropic polarizabilities as the atomic number increases and an increase of the CM5 positive charges on the chalcogen, see Fig. 7S. On the other hand, the dipole moment decreases, see Fig. 7Sb. It should be noted that while the three Mulliken, CM5 and NBO analyses, predict different charges on the chalcogen atoms, the shape of the curve as the atomic number of the chalcogen is increased is the same, see Tables 1S-6S and Fig. 6S.. We consider that the CM5 charges which are an extension of Hirshfeld population analysis are our best values for the present calculated systems.⁴⁵ Note that CM5 charges are essentially independent of a basis set,⁴³ see also Tables 1S-6S and Fig. 6S.

To sum up, regarding the aromaticity, the three substituted furazans behave similarly, while furazan itself differs. The substituted furazan compounds are much more effective at magnetic anisotropy than furazan because they present similar positive charges which differ from the charge of the O atom, see Fig. 7Sc. Their lone-pair electrons are more diffuse, hence more polarizable. The S, Se, and Te atoms present larger polarizability than O and as a result the corresponding substituted compounds present larger polarizability than furazan. The increase in polarizability in conjunction with the significant decrease of dipole moment, i.e., the molecule is more symmetric in charges, results in an increase in aromaticity. The increased aromaticity is consistent with the observed unusually high magnetic anisotropy within the environment of the chalcogen-bonded capsules.

Table 1S. Magnetic isotropy and anisotropy in the plane and perpendicular out of the plane at the distances R(Å) of **1-4**, charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen of **1-4**, dipole moments μ(Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4** at the M06-2X/LANL2DZ level of theory.

	R	1		2		3		4	
		Mgnatic Isotropy	Mgnatic Anisotropy						
gs C ₂ N ₂ ^a	0	12.1836	22.7648	12.8048	21.9908	11.5845	18.5824	10.7685	18.7454
gs ring ^b	0	10.2450	10.1730	12.5497	4.3138	12.2580	4.3390	13.5638	5.8973
1 Å from X ^c	0	12.1178	6.6780	21.5920	7.3570	23.4505	7.5354	23.0751	6.0916
gs C ₂ N ₂ ^a	1	12.4638	26.6714	12.6194	26.4800	11.9069	24.6643	11.0793	22.4008
gs ring ^b	1	11.6094	25.4182	11.5855	24.6720	11.1388	22.8049	10.4392	20.0696
1 Å from X ^c	1	11.3829	25.3745	12.8653	25.3400	13.4029	22.8431	13.6306	18.6543
gs C ₂ N ₂ ^a	2	4.3355	13.8243	4.7446	15.2349	4.6546	14.8622	4.3290	14.0000
gs ring ^b	2	4.4351	13.7090	4.8789	15.3892	4.8144	15.0411	4.6187	14.2820
1 Å from X ^c	2	4.3977	13.4748	4.6376	15.1914	4.5775	14.8296	4.5488	14.0265
gs C ₂ N ₂ ^a	3	1.6008	6.1450	1.8340	7.1488	1.8405	7.1109	1.7889	6.8771
gs ring ^b	3	1.6395	6.1241	1.8862	7.2657	1.8952	7.2663	1.8753	7.1881
1 Å from X ^c	3	1.6405	6.0450	1.7989	7.1739	1.7766	7.1916	1.7439	7.1692
gs C ₂ N ₂ ^a	4	0.7401	3.0234	0.8527	3.6312	0.8617	3.6557	0.8540	3.6169
gs ring ^b	4	0.7525	3.0176	0.8689	3.6810	0.8787	3.7235	0.8789	3.7621
1 Å from X ^c	4	0.7537	2.9909	0.8439	3.6431	0.8427	3.6889	0.8306	3.7478
gs C ₂ N ₂ ^a	5	0.3970	1.6677	0.4580	2.0380	0.4644	2.0654	0.4651	2.0717
gs ring ^b	5	0.4021	1.6648	0.4645	2.0588	0.4711	2.0946	0.4748	2.1359
1 Å from X ^c	5	0.4031	1.6536	0.4560	2.0427	0.4585	2.0795	0.4571	2.1273
		1	2	3	4				
q _x (Mulliken)		-0.20	0.56	0.61	0.82				
q _x (CM5)		0.00	0.30	0.40	0.49				
q _x (NBO)		-0.20	0.70	0.85	1.06				
μ		4.35	2.27	1.36	0.02				
iso polar.		31.08	41.84	46.05	53.22				
aniso polar.		23.42	39.04	46.47	57.10				

^a In the geometric center of the ring.

^b In the geometric center of the NCCN quadrilateral.

^c In the ring at distance of 1 Å from the chalcogen.

Table 2S. Magnetic isotropy and anisotropy in the plane and perpendicular out of the plane at the distances R(Å) of **1-4**, charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen of **1-4**, dipole moments μ(Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4**, at the M06-2X/6-311+G(d,p) level of theory.

R	1		2		3		4	
	Mgnatic Isotropy	Mgnatic Anisotropy						
gs C ₂ N ₂ ^a	0	14.7467	24.8388	14.2082	24.0710	11.7229	21.1697	9.0023
gs ring ^b	0	12.9850	11.5002	15.9714	10.0459	14.7418	18.7323	14.9968
1 Å from X ^c	0	14.3027	7.6084	24.0690	10.6223	27.6949	30.1470	26.1925
gs C ₂ N ₂ ^a	1	13.7043	30.8606	13.5960	34.2597	12.0139	31.0209	10.1975
gs ring ^b	1	13.0010	30.4644	13.0869	34.3545	11.6897	32.8250	10.5417
1 Å from X ^c	1	12.8609	30.8058	14.2920	35.3988	14.3502	37.4740	14.1157
gs C ₂ N ₂ ^a	2	4.6287	14.7730	5.3063	17.4591	4.8517	17.3012	4.3953
gs ring ^b	2	4.7221	14.7605	5.4855	17.7840	5.1011	18.4486	4.7742
1 Å from X ^c	2	4.6973	14.6458	5.3701	17.6860	4.9905	19.1219	4.8755
gs C ₂ N ₂ ^a	3	1.7193	6.3415	2.1271	7.7183	2.0067	8.0823	1.9141
gs ring ^b	3	1.7510	6.3409	2.1842	7.8383	2.0864	8.4545	2.0226
1 Å from X ^c	3	1.7491	6.3002	2.1376	7.7909	2.0089	8.5575	1.9437
gs C ₂ N ₂ ^a	4	0.7918	3.0867	0.9842	3.8554	0.9458	4.1397	0.9199
gs ring ^b	4	0.8000	3.0888	1.0008	3.8973	0.9701	4.2646	0.9553
1 Å from X ^c	4	0.7988	3.0763	0.9865	3.8770	0.9454	4.2789	0.9260
gs C ₂ N ₂ ^a	5	0.4224	1.6959	0.5228	2.1495	0.5083	2.3365	0.4996
gs ring ^b	5	0.4251	1.6969	0.5289	2.1654	0.5176	2.3835	0.5147
1 Å from X ^c	5	0.4245	1.6922	0.5241	2.1563	0.5091	2.3842	0.5052
	1	2	3	4				
q _x (Mulliken)	0.23	0.38	0.29	0.55				
q _x (CM5)	0.05	0.35	0.42	0.47				
q _x (NBO)	-0.17	0.81	0.85	1.12				
μ	3.57	1.60	1.14	0.05				
iso polar.	35.73	48.84	55.96	67.26				
aniso polar.	18.42	28.42	34.64	45.14				

^a In the geometric center of the ring.

^b In the geometric center of the NCCN quadrilateral.

^c In the ring at distance of 1 Å from the chalcogen.

Table 3S. Magnetic isotropy and anisotropy in the plane and perpendicular out of the plane at the distances R(Å) of **1-4**, charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen of **1-4**, dipole moments μ(Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4** at the B3LYP/6-311+G(d,p) level of theory.

		1	2		3		4	
R	Mgnatic Isotropy	Mgnatic Anisotropy						
gs C ₂ N ₂ ^a	0	15.1116	20.7629	15.0061	21.8477	12.8982	17.7518	10.5982
gs ring ^b	0	13.3264	9.8462	15.9416	8.4245	14.8039	17.4203	15.0971
1 Å from X ^c	0	14.6466	6.4932	23.5911	9.2870	27.0706	28.4807	25.9579
gs C ₂ N ₂ ^a	1	12.9576	29.4540	13.0492	32.5292	11.4811	29.1309	9.8456
gs ring ^b	1	12.3284	29.1359	12.5138	32.6733	11.2005	31.0347	10.1920
1 Å from X ^c	1	12.2082	29.5003	13.7120	33.7823	13.7701	35.9331	13.8332
gs C ₂ N ₂ ^a	2	4.3306	14.4453	4.9777	16.9553	4.5384	16.7669	4.0416
gs ring ^b	2	4.4066	14.4226	5.1708	17.2971	4.7923	17.8619	4.4519
1 Å from X ^c	2	4.3818	14.3100	5.0644	17.2083	4.7075	18.5177	4.5638
gs C ₂ N ₂ ^a	3	1.5971	6.2527	1.9886	7.5685	1.8671	7.9097	1.7401
gs ring ^b	3	1.6238	6.2485	2.0490	7.6945	1.9435	8.2676	1.8538
1 Å from X ^c	3	1.6218	6.2079	2.0039	7.6469	1.8703	8.3656	1.7795
gs C ₂ N ₂ ^a	4	0.7330	3.0537	0.9184	3.7963	0.8776	4.0662	0.8329
gs ring ^b	4	0.7397	3.0546	0.9360	3.8399	0.8999	4.1873	0.8687
1 Å from X ^c	4	0.7384	3.0422	0.9222	3.8190	0.8758	4.2003	0.8406
gs C ₂ N ₂ ^a	5	0.3902	1.6804	0.4871	2.1211	0.4708	2.2990	0.4509
gs ring ^b	5	0.3923	1.6811	0.4936	2.1375	0.4791	2.3447	0.4661
1 Å from X ^c	5	0.3916	1.6765	0.4889	2.1278	0.4706	2.3449	0.4570
	1	2	3	4				
q _x (Mulliken)	0.24	0.37	0.36	0.47				
q _x (CM5)	0.05	0.34	0.40	0.44				
q _x (NBO)	-0.17	0.79	0.82	1.07				
μ	3.60	1.61	1.10	0.11				
iso polar.	37.13	50.43	58.02	69.10				
aniso polar.	19.41	29.15	35.82	47.17				

^a In the geometric center of the ring.

^b In the geometric center of the NCCN quadrilateral.

^c In the ring at distance of 1 Å from the chalcogen.

Table 4S. Magnetic isotropy and anisotropy in the plane and perpendicular out of the plane at the distances R(Å) of **1-4**, charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen of **1-4**, dipole moments μ(Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4** at the PBE0/6-311+G(d,p) level of theory.

R	1		2		3		4		
	Mgnatic Isotropy	Mgnatic Anisotropy							
gs C ₂ N ₂ ^a	0	15.9001	22.3482	15.5658	22.6212	13.1619	17.5073	10.6560	15.6909
gs ring ^b	0	13.6041	10.2320	16.0946	8.9539	14.8540	16.9833	15.1988	6.8345
1 Å from X ^c	0	14.6707	6.2753	24.1423	9.7814	27.2873	28.9070	26.4180	7.0583
gs C ₂ N ₂ ^a	1	13.4598	30.6948	13.4624	33.6608	11.8769	30.6255	10.0789	25.0221
gs ring ^b	1	12.7359	30.3401	12.8410	33.7779	11.5700	32.4085	10.4302	24.4832
1 Å from X ^c	1	12.5633	30.6915	13.4624	33.6608	14.1416	37.3140	14.1332	23.5566
gs C ₂ N ₂ ^a	2	4.4323	14.8372	5.2795	17.7050	4.7158	17.4216	4.1660	14.8508
gs ring ^b	2	4.5176	14.8277	5.0837	17.3514	4.9470	18.4765	4.5525	15.4955
1 Å from X ^c	2	4.4928	14.7144	5.2795	17.7050	4.8502	19.1574	4.6515	15.4409
gs C ₂ N ₂ ^a	3	1.6315	6.3814	2.0207	7.7023	1.9294	8.1489	1.7852	7.1347
gs ring ^b	3	1.6602	6.3818	2.0816	7.8307	1.9981	8.4875	1.8878	7.4643
1 Å from X ^c	3	1.6582	6.3415	2.0207	7.7023	1.9246	8.5915	1.8082	7.4757
gs C ₂ N ₂ ^a	4	0.7488	3.1082	0.9496	3.8970	0.9034	4.1709	0.8507	3.7248
gs ring ^b	4	0.7560	3.1106	0.9319	3.8528	0.9234	4.2838	0.8829	3.8483
1 Å from X ^c	4	0.7546	3.0983	0.9496	3.8970	0.8997	4.2988	0.8537	3.8359
gs C ₂ N ₂ ^a	5	0.3988	1.7081	0.4961	2.1557	0.4838	2.3522	0.4597	2.1249
gs ring ^b	5	0.4010	1.7094	0.4961	2.1557	0.4914	2.3945	0.4736	2.1720
1 Å from X ^c	5	0.4003	1.7048	0.4961	2.1557	0.4832	2.3954	0.4642	2.1606
	1	2	3	4					
q _x (Mulliken)	0.29	0.34	0.33	0.45					
q _x (CM5)	0.06	0.34	0.41	0.44					
q _x (NBO)	-0.15	0.80	0.84	1.07					
μ	3.49	1.63	1.10	0.19					
iso polar.	36.34	49.32	56.73	68.10					
aniso polar.	18.85	28.54	34.95	46.51					

^a In the geometric center of the ring.

^b In the geometric center of the NCCN quadrilateral.

^c In the ring at distance of 1 Å from the chalcogen.

Table 5S. Magnetic isotropy and anisotropy in the plane and perpendicular out of the plane at the distances R(Å) of **1-4**, charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen of **1-4**, dipole moments μ(Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4** at the MP2/6-311+G(d,p) level of theory.

R	1		2		3		4	
	Mgnatic Isotropy	Mgnatic Anisotropy						
gs C ₂ N ₂ ^a	0	18.2252	25.1164	17.3362	25.3072	15.3793	20.3292	12.9531
gs ring ^b	0	15.1039	14.5557	16.6423	13.3462	15.7165	14.7154	15.9527
1 Å from X ^c	0	15.9355	10.9898	24.5545	13.8213	28.0616	26.6386	27.0320
gs C ₂ N ₂ ^a	1	13.8998	33.2518	13.7135	35.8369	12.4097	32.8756	10.5902
gs ring ^b	1	13.1253	32.9735	13.0534	36.0201	12.0602	34.5867	10.9108
1 Å from X ^c	1	12.9415	33.2455	13.7135	35.8369	14.7208	39.1051	14.7249
gs C ₂ N ₂ ^a	2	4.5570	15.6781	5.4057	18.4700	4.9040	18.3481	4.3427
gs ring ^b	2	4.6407	15.6709	5.2017	18.1060	5.1517	19.4220	4.7584
1 Å from X ^c	2	4.6137	15.5484	5.4057	18.4700	5.0656	20.0692	4.8754
gs C ₂ N ₂ ^a	3	1.6666	6.7176	2.0711	8.0256	1.9998	8.5636	1.8538
gs ring ^b	3	1.6961	6.7175	2.1337	8.1572	2.0716	8.9107	1.9603
1 Å from X ^c	3	1.6941	6.6750	2.0711	8.0256	1.9967	9.0127	1.8777
gs C ₂ N ₂ ^a	4	0.7611	3.2704	0.9725	4.0616	0.9330	4.3834	0.8795
gs ring ^b	4	0.7685	3.2727	0.9543	4.0168	0.9536	4.4993	0.9119
1 Å from X ^c	4	0.7673	3.2598	0.9725	4.0616	0.9292	4.5136	0.8810
gs C ₂ N ₂ ^a	5	0.4041	1.7971	0.5072	2.2483	0.4980	2.4728	0.4733
gs ring ^b	5	0.4065	1.7983	0.5072	2.2483	0.5057	2.5163	0.4870
1 Å from X ^c	5	0.4058	1.7935	0.5072	2.2483	0.4973	2.5169	0.4770
	1	2	3	4				
q _x (Mulliken)	0.30	0.39	0.35	0.48				
q _x (CM5)	0.08	0.36	0.43	0.44				
q _x (NBO)	-0.12	0.82	0.85	1.05				
μ	3.40	1.37	0.96	0.06				
iso polar.	36.08	49.46	56.82	67.97				
aniso polar.	18.30	27.91	34.03	44.92				

^a In the geometric center of the ring.

^b In the geometric center of the NCCN quadrilateral.

^c In the ring at distance of 1 Å from the chalcogen.

Table 6S. Charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen of **1-4**, dipole moments μ (Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4** at the CCSD/6-311+G(d,p)// PBE0/6-311+G(d,p) level of theory.

	1	2	3	4
q_x (Mulliken)	0.26	0.38	0.34	0.50
q_x (CM5)	0.05	0.35	0.42	0.44
q_x (NBO)	-0.17	0.81	0.84	1.05
μ	3.54	1.55	1.18	0.23
iso polar.	35.65	48.90	56.01	66.78
aniso polar.	18.17	28.02	33.90	43.95

Table 7S. Ranging of the % differences of magnetic isotropy and anisotropy at different levels of theory at distances of 3-5 Å above the **1-4** compounds.

Methods ^a	Isotr.	Anis.	Isotr.	Anis.	Isotr.	Anis.	Isotr.	Anis.	Isotr.	Anis.	Isotr.	Anis.
	O-S		O-Se		O-Te		S-Se		S-Te		Se-Te	
	O-S	O-Se	O-Te	S-Se	S-Te	Se-Te						
M06-2X/A	9.7–15.5	16.3–23.7	8.3–17.2	15.7–25.8	6.3–18.1	11.9–28.6	-1.4–1.2	-1.8–0.0	-2.2–3.1	-4.1–1.1	-0.8–1.8	-2.3–1.1
M06-2X/B	22.2–25.1	21.7–27.6	14.9–21.8	27.5–40.9	11.1–21.1	12.9–28.1	2.1–6.0	-10.6–(-7.4)	2.7–9.1	-0.4–4.7	0.6–3.2	8.8–12.7
B3LYP/B	23.6–26.5	21.0–27.1	15.3–22.1	26.5–39.9	9.0–18.8	11.8–27.2	2.9–6.7	-10.2–(-7.1)	5.6–11.2	-0.1–4.9	2.7–5.1	8.8–12.4
PBE0/B	21.9–26.8	20.7–26.4	16.1–22.5	27.7–40.5	9.0–18.1	11.8–27.1	0.9–5.3	-11.5–(-7.0)	4.5–10.5	-0.8–4.7	3.6–6.0	9.3–13.0
MP2/B	22.3–27.8	19.5–25.4	17.9–24.4	27.5–40.3	10.8–19.8	12.4–27.9	0.1–4.5	-12.3–(-7.9)	4.0–9.6	-2.3–3.3	3.7–6.0	8.6–12.4

^aA: LANL2DZ, B: 6-311G+(d,p)

Table 8S. CM5 charges q_x on the chalcogen of **1-4**, dipole moments μ (Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au), of **1-4** at different levels of theory.

Methods^a		1	2	3	4
M06-2X/A	q_x	0.00	0.30	0.40	0.49
	μ	4.35	2.27	1.36	0.02
	iso polar.	31.08	41.84	46.05	53.22
	aniso polar.	23.42	39.04	46.47	57.10
M06-2X/B	q_x	0.05	0.35	0.42	0.47
	μ	3.57	1.60	1.14	0.05
	iso polar.	35.73	48.84	55.96	67.26
	aniso polar.	18.42	28.42	34.64	45.14
B3LYP/B	q_x	0.05	0.34	0.40	0.44
	μ	3.60	1.61	1.10	0.11
	iso polar.	37.13	50.43	58.02	69.10
	aniso polar.	19.41	29.15	35.82	47.17
PBE0/B	q_x	0.06	0.34	0.41	0.44
	μ	3.49	1.63	1.10	0.19
	iso polar.	36.34	49.32	56.73	68.10
	aniso polar.	18.85	28.54	34.95	46.51
MP2/B	q_x	0.08	0.36	0.43	0.44
	μ	3.40	1.37	0.96	0.06
	iso polar.	36.08	49.46	56.82	67.97
	aniso polar.	18.30	27.91	34.03	44.92
CCSD/B	q_x	0.05	0.35	0.42	0.44
	μ	3.54	1.55	1.18	0.23
	iso polar.	35.65	48.90	56.01	66.78
	aniso polar.	18.17	28.02	33.90	43.95

^aA: LANL2DZ, B: 6-311G+(d,p).

Table 9S. BSSE corrected ΔE (eV), deformation energy, 2-body(2B), 3-body(3B) terms in eV.

	ΔE_u^a	ΔE_1	Def.	Def ^b	2B ^c	2Bs ^d	3B	ΔE_u^a	ΔE^e	Def. ^e	2B ^e
M06-2X/LANL2DZ											
A_S+A_S_a	-2.06	-1.60	0.14		-1.73						
A_{Se}+A_{Se}_a	-3.78	-3.16	0.29		-3.45						
A_{Te}+A_{Te}_a	-8.09	-7.15	1.36		-8.52						
A_O+A_O_b	-2.39	-1.66	0.32		-1.99						
A_S+A_S_b	-2.52	-1.78	0.20		-1.98						
A_{Se}+A_{Se}_b	-2.71	-1.98	0.19		-2.17						
A_{Te}+A_{Te}_b	-3.25	-2.47	0.20		-2.67						
C ₉ H ₂₀ @A _O +A _O	-3.20	-2.25	0.30	0.05	-1.45	-0.38	-0.72	-0.82	-0.40	0.70	-1.10
C ₉ H ₂₀ @A _S +A _S	-3.23	-2.45	0.21	0.02	-1.70	-0.31	-0.64	-1.16	-0.88	0.07	-0.95
C ₉ H ₂₀ @A _{Se} +A _{Se}	-4.93	-4.01	0.34	0.01	-3.41	-0.12	-0.82	-1.15	-0.88	0.06	-0.95
C ₉ H ₂₀ @A _{Te} +A _{Te}	-9.20	-8.03	1.46	0.01	-8.53	0.18	-1.15	-1.12	-0.91	0.05	-0.96
M06-2X/6-31G(d,p)											
A_S+A_S_a	-1.94	-1.38	0.32		-1.70						
A_{Se}+A_{Se}_a	-3.95	-1.80	0.72		-2.51						
A_{Te}+A_{Te}_a	-5.72	-4.58	2.24		-6.82						
A_O+A_O_b	-2.15	-1.36	0.37		-1.73						
A_S+A_S_b	-2.22	-1.48	0.19		-1.67						
A_{Se}+A_{Se}_b	-3.74	-1.63	0.19		-1.82						
A_{Te}+A_{Te}_b	-3.16	-2.09	0.20		-2.29						
C ₉ H ₂₀ @A _O +A _O	-2.96	-1.85	0.36	0.04	-1.04	-0.50	-0.67	-0.81	-0.23	0.94	-1.17
C ₉ H ₂₀ @A _S +A _S	-3.24	-2.30	0.32	0.03	-1.69	-0.23	-0.70	-1.30	-0.93	0.00	-0.93
C ₉ H ₂₀ @A _{Se} +A _{Se}	-5.95	-2.67	0.71	0.01	-2.44	-0.03	-0.91	-2.00	-0.94	0.00	-0.94
C ₉ H ₂₀ @A _{Te} +A _{Te}	-6.88	-5.33	2.29	0.01	-6.82	0.44	-1.34	-1.16	-0.87	0.03	-0.90

^a Uncorrected BSSE dissociation energy. ^b Deformation energy of alkane. ^c 2B term with respect to the cavitands. ^d Sum of the 2B terms with respect to one cavitand and alkane. ^e ΔE , Def. and 2B with respect to the capsule and alkane.

Table 10S. Relative energies of the A_X+A_X capsules with respect to the a structure in eV.

	M06-2X/1^a	M06-2X/2^a	PBE0/1^a	PBE0/2^a
A_S+A_S	-0.45	-0.28	0.25	0.43
A_{Se}+A_{Se}	1.07	0.20	-1.66	-1.11
A_{Te}+A_{Te}	4.83	2.56	-5.52	-3.63

^a 1:LANL2DZ, 2:6-31G(d,p).

Table 11S. Charges via the Mulliken, CM5 and NBO analyses q_x on the chalcogen (O, S and Te), dipole moments μ (Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au) of \mathbf{A}_x , $\mathbf{A}_x+\mathbf{A}_x$, and $\mathbf{C}_9\mathbf{H}_{20}@\mathbf{A}_x+\mathbf{A}_x$ at the different levels of theory.

Methodology ^a	Property	A_O	A_S	A_{Se}	A_{Te}	A_O+A_O	A_S+A_S	$A_{Se}+A_{Se}$	$A_{Te}+A_{Te}$	$C_9\mathbf{H}_{20}@\mathbf{A}_0+A_0$	$C_9\mathbf{H}_{20}@\mathbf{A}_S+A_S$	$C_9\mathbf{H}_{20}@\mathbf{A}_{Se}+A_{Se}$	$C_9\mathbf{H}_{20}@\mathbf{A}_{Te}+A_{Te}$
M06-2X/1	$q_x(\text{Mulliken})$	-0.16	0.61	0.67	0.88	-0.19	0.70	0.77	1.16	-0.20	0.70	0.84	1.17
	$q_x(\text{CM5})$	0.03	0.35	0.45	0.55	0.02	0.35	0.47	0.56	0.02	0.36	0.48	0.57
	$q_x(\text{NBO})$	-0.17	0.21	0.95	0.83	-0.19	0.14	1.04	0.61	-0.19	0.14	1.08	0.61
	μ	9.238	1.848	6.314	12.893	1.050	0.459	0.768	0.367	1.071	0.336	0.420	0.092
	iso polar.	760.71	821.10	846.11	888.12	1483.07	1688.51	1745.88	1884.38	1579.56	1748.89	1813.81	1935.67
	aniso polar.	232.14	351.35	400.84	475.21	643.29	1075.73	1170.19	1324.76	732.70	1118.03	1216.45	1343.82
M06-2X/2	$q_x(\text{Mulliken})$	-0.21	0.58	0.49	0.76	-0.23	0.64	0.53	0.92	-0.22	0.65	0.58	0.93
	$q_x(\text{CM5})$	0.04	0.32	0.43	0.51	0.03	0.31	0.43	0.52	0.03	0.32	0.44	0.53
	$q_x(\text{NBO})$	-0.16	0.22	0.88	0.86	-0.18	0.16	0.93	0.68	-0.18	0.16	0.98	0.68
	μ	7.629	2.096	4.948	10.954	0.866	0.319	0.906	0.227	0.890	0.543	0.517	0.234
	iso polar.	780.09	851.65	880.26	934.93	1520.09	1755.37	1816.44	1980.10	1618.71	1816.53	1886.02	2041.26
	aniso polar.	252.28	382.01	424.14	511.91	681.66	1161.25	1242.05	1358.75	779.14	1204.45	1286.84	1401.95
PBE0/1	$q_x(\text{Mulliken})$	-0.14	0.57	0.62	0.80	-0.17	0.64	0.70	1.07	-0.19	0.65	0.77	1.08
	$q_x(\text{CM5})$	0.04	0.34	0.44	0.52	0.03	0.34	0.44	0.53	0.03	0.35	0.46	0.55
	$q_x(\text{NBO})$	-0.15	0.23	0.93	0.87	0.17	0.16	0.99	0.66	-0.17	0.16	1.04	0.66
	μ	9.207	1.333	5.420	11.419	1.020	0.450	0.761	0.356	1.042	0.364	0.448	0.094
	iso polar.	772.62	834.44	860.06	904.41	1505.19	1723.00	1782.91	1937.88	1601.31	1780.27	1853.73	1984.76
	aniso polar.	240.28	363.05	413.47	492.75	667.79	1125.01	1223.19	1377.19	761.40	1166.30	1270.46	1395.38
PBE0/2	$q_x(\text{Mulliken})$	-0.20	0.57	0.47	0.73	-0.21	0.63	0.52	0.88	-0.21	0.64	0.57	0.89
	$q_x(\text{CM5})$	0.05	0.31	0.42	0.48	0.04	0.31	0.42	0.50	0.04	0.32	0.44	0.51
	$q_x(\text{NBO})$	-0.14	0.23	0.87	0.90	0.16	0.17	0.93	0.71	-0.16	0.17	0.97	0.72
	μ	7.695	1.677	4.840	9.805	0.854	0.308	0.973	0.215	0.879	0.573	0.565	0.206
	iso polar.	792.28	865.03	895.66	949.90	1543.92	1792.94	1858.14	2027.73	1643.00	1851.83	1931.15	2086.61
	aniso polar.	258.92	392.21	438.48	524.86	705.33	1211.30	1303.03	1405.53	808.10	1255.03	1349.90	1449.42

^a 1:LANL2DZ, 2:6-31G(d,p)

Table 12S. % Difference of the isotropic and anisotropic electric field polarizabilities (D1), % Difference of the isotropic electric field polarizabilities of the chalcogen with respect to Te (D2), % Difference of the isotropic electric field polarizabilities of the chalcogen with respect to Te (D3).^a

	D1	D2	D3	D1	D2	D3	D1	D2	D3	D1	D2	D3	D1	D2	D3
	M06-2X ^b			B3LYP ^b			PBE0 ^b			MP2 ^b			CCSD ^b		
	1	94	47	59	91	46	59	93	47	59	97	47	59	96	47
1	94	47	59	91	46	59	93	47	59	97	47	59	96	47	59
2	72	27	37	73	27	38	73	28	39	77	27	38	75	27	36
3	62	17	23	62	16	24	62	17	25	67	16	24	65	16	23
4	49			46			46			51			52		
D1 D2 D3			D1 D2 D3			D1 D2 D3			D1 D2 D3			D1 D2 D3			
			M06-2X/6-31G(d,p)			D1 D2 D3			D1 D2 D3			D1 D2 D3			
A_X			A_X+A_X			C₉H₂₀@A_X+A_X			A_X			A_X+A_X			
O	209	17	51	123	23	50	108	21	44	206	17	51	119	24	50
S	123	9	25	51	11	15	51	11	14	121	9	25	48	12	14
Se	108	6	17	46	8	9	47	8	8	104	6	16	43	8	7
Te	83			46			46			81			44		

^a D1 = 100*(Isotr.- Anisotr.)/Anisotr., D2 = 100* [Isotr(X)- Isotr.(Te)]/ Isotr.(Te), D3 = 100* [Anisotr(X)- Anisotr.(Te)]/Anisotr.(Te)

^b 6-311+G(d,p)

Table 13S. ^1H NMR shifts of $n\text{-C}_9\text{H}_{20}$ inside capsules at different levels of theory.

M06-2X/LANL2DZ				PBE0/LANL2DZ				M06-2X/6-31G(d,p)				PBE0/6-31G(d,p)				
$\text{A}_\text{O}+\text{A}_\text{O}$	$\text{A}_\text{S}+\text{A}_\text{S}$	$\text{A}_\text{Se}+\text{A}_\text{Se}$	$\text{A}_\text{Te}+\text{A}_\text{Te}$													
-4.96	-5.75	-5.94	-5.18	-3.42	-3.99	-4.13	-3.42	-4.26	-4.91	-5.01	-4.30	1	-2.91	-3.40	-3.53	-2.85
-5.28	-5.30	-5.04	-5.34	-3.82	-3.64	-3.34	-3.65	-4.57	-4.57	-4.31	-4.53	1	-3.29	-3.12	-2.85	-3.08
-5.63	-5.27	-5.15	-5.40	-4.27	-3.86	-3.70	-3.69	-4.92	-4.66	-4.54	-4.59	1	-3.75	-3.38	-3.26	-3.13
-3.92	-3.64	-3.42	-4.19	-2.42	-2.11	-1.88	-2.41	-3.25	-3.00	-2.75	-3.39	2	-1.94	-1.63	-1.44	-1.90
-3.46	-4.74	-4.47	-4.29	-2.19	-3.27	-2.95	-2.52	-2.89	-4.05	-3.75	-3.51	2	-1.75	-2.72	-2.44	-2.02
-4.56	-4.53	-4.38	-4.16	-3.28	-3.24	-3.09	-2.34	-3.86	-3.88	-3.70	-3.34	3	-2.73	-2.71	-2.60	-1.83
-5.68	-4.31	-4.65	-4.12	-4.13	-2.89	-3.21	-2.34	-4.90	-3.60	-3.84	-3.29	3	-3.58	-2.33	-2.63	-1.82
-5.89	-5.22	-4.78	-4.14	-4.70	-3.94	-3.49	-2.32	-5.04	-4.38	-3.86	-3.17	4	-4.05	-3.21	-2.79	-1.73
-5.87	-4.19	-3.78	-3.92	-4.58	-2.80	-2.47	-2.08	-5.03	-3.38	-2.91	-2.93	4	-3.94	-2.14	-1.87	-1.51
-6.89	-4.55	-4.35	-3.79	-5.66	-3.32	-3.14	-1.90	-5.99	-3.84	-3.57	-2.80	5	-4.96	-2.71	-2.55	-1.33
-7.22	-4.04	-4.14	-3.70	-5.96	-2.72	-2.88	-1.85	-6.31	-3.21	-3.27	-2.70	5	-5.27	-2.03	-2.25	-1.28
-5.48	-4.21	-5.08	-4.02	-4.15	-2.84	-3.77	-2.26	-4.70	-3.40	-4.16	-3.02	6	-3.57	-2.17	-3.11	-1.66
-6.04	-4.35	-4.21	-3.95	-4.69	-3.06	-2.90	-2.06	-5.24	-3.60	-3.40	-2.99	6	-4.11	-2.40	-2.31	-1.50
-3.65	-5.03	-4.37	-4.19	-2.52	-3.60	-2.92	-2.36	-3.06	-4.27	-3.67	-3.34	7	-2.06	-2.99	-2.41	-1.84
-3.48	-4.53	-4.47	-4.21	-2.27	-3.28	-3.12	-2.40	-2.91	-3.90	-3.79	-3.36	7	-1.79	-2.75	-2.62	-1.87
-4.72	-3.31	-4.20	-4.25	-3.20	-1.77	-2.58	-2.46	-4.04	-2.70	-3.51	-3.42	8	-2.70	-1.30	-2.09	-1.95
-5.36	-4.09	-4.17	-4.25	-3.80	-2.68	-2.69	-2.45	-4.58	-3.45	-3.51	-3.44	8	-3.23	-2.15	-2.19	-1.96
-3.85	-5.64	-5.09	-5.19	-2.50	-3.97	-3.44	-3.42	-3.22	-4.83	-4.31	-4.29	9	-2.07	-3.39	-2.90	-2.84
-5.24	-5.18	-5.25	-5.25	-3.81	-3.83	-3.83	-3.54	-4.57	-4.62	-4.63	-4.44	9	-3.29	-3.36	-3.37	-3.00
-4.95	-5.18	-5.34	-5.36	-3.53	-3.56	-3.78	-3.61	-4.32	-4.47	-4.62	-4.52	9	-3.05	-3.03	-3.26	-3.05

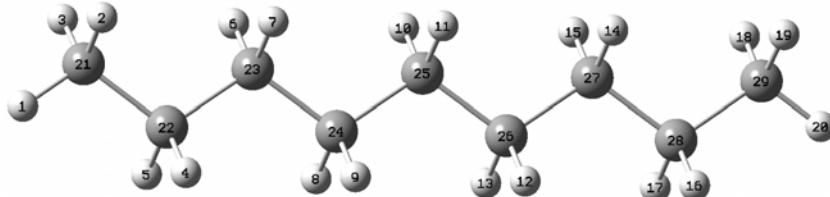


Table 14S. ^1H NMR shifts of $n\text{-C}_9\text{H}_{20}$ free at different levels of theory^a

M06-2X/1	PBE0/1	PBE0/2	M06-2X/2	M06-2X/2 ^b	M06-2X/2 ^c	Expt ^d
0.02	0.17	1.32	1.14	1.14	1.14	0.88
-0.11	0.04	1.11	0.95	0.95	0.95	0.88
-0.11	0.04	1.11	0.94	0.94	0.94	0.88
0.31	0.49	1.60	1.39	1.39	1.39	1.31
0.31	0.49	1.60	1.37	1.37	1.38	1.31
0.28	0.46	1.54	1.34	1.34	1.34	1.29
0.29	0.46	1.54	1.34	1.34	1.34	1.29
0.27	0.44	1.56	1.36	1.36	1.36	1.29
0.26	0.43	1.56	1.36	1.37	1.37	1.29
0.28	0.45	1.57	1.37	1.37	1.37	1.29
0.28	0.45	1.57	1.38	1.38	1.38	1.29
0.27	0.43	1.56	1.37	1.37	1.37	1.29
0.27	0.44	1.56	1.36	1.37	1.37	1.29
0.28	0.46	1.54	1.34	1.35	1.35	1.29
0.28	0.46	1.54	1.34	1.35	1.35	1.29
0.32	0.49	1.60	1.39	1.40	1.40	1.31
0.32	0.49	1.60	1.39	1.39	1.39	1.31
-0.12	0.04	1.11	0.94	0.94	0.94	0.88
-0.12	0.04	1.11	0.93	0.93	0.93	0.88
0.02	0.17	1.32	1.14	1.14	1.14	0.88

^a 1: LANL2DZ, 2: 6-31G(d,p). ^b In Ether solvent. ^c In Ethanol solvent. ^d ^1H NMR: http://www.molbase.com/en/hnmr_111-84-2-moldata-73715.html; https://spectrabase.com/spectrum/1XIYDWGUvtN?a=SPECTRUM_1XIYDWGUvtN

Table 15S: Geometries of the minimum calculated structures at M06-2X/LAN2LDZ level of theory

Atom	Atomic Type	Coordinates (Angstroms)								
		X	Y	Z						
1	6	0	5.115893	-0.682185	-0.338707	9	6	0	6.287865	-0.548718
2	6	0	3.803838	-1.469430	-0.193245	10	6	0	4.381288	0.718452
3	1	0	5.989408	-1.311626	-0.138691	11	8	0	4.002056	3.000608
4	1	0	5.214720	-0.278697	-1.353258	12	6	0	6.319298	2.693302
5	1	0	5.140134	0.162244	0.360051	13	6	0	4.453932	4.101345
6	6	0	2.566920	-0.599798	-0.470698	14	8	0	4.034495	4.454837
7	1	0	3.805436	-2.324232	-0.883031	15	6	0	6.985252	-1.901096
8	1	0	3.731415	-1.886032	0.820503	16	6	0	5.158355	-0.436577
9	1	0	2.563395	0.256616	0.219522	17	1	0	3.520392	0.789697
10	1	0	2.637733	-0.181585	-1.485563	18	6	0	2.803983	3.063841
11	6	0	1.247324	-1.374243	-0.329190	19	6	0	7.021269	1.932404
12	6	0	0.010436	-0.505285	-0.605923	20	6	0	5.230053	3.530842
13	1	0	1.178258	-1.792642	0.685708	21	1	0	3.617367	4.746742
14	1	0	1.252304	-2.230430	-1.019669	22	6	0	2.819987	3.854352
15	6	0	-1.308783	-1.280606	-0.464305	23	1	0	6.822990	-2.458770
16	1	0	0.005276	0.350790	0.084608	24	6	0	6.253712	-2.644647
17	1	0	0.079407	-0.086799	-1.620732	25	8	0	4.892378	-1.504719
18	1	0	-1.303456	-2.136759	-1.154818	26	6	0	6.294059	0.593670
19	1	0	-1.377657	-1.699063	0.550583	27	1	0	6.855323	2.491497
20	6	0	-2.546102	-0.412512	-0.740985	28	8	0	4.982450	3.877140
21	6	0	-3.865490	-1.188552	-0.598854	29	6	0	6.588219	-2.470114
22	1	0	-2.478925	0.005943	-1.756000	30	6	0	5.166551	-3.482846
23	1	0	-2.552867	0.443950	-0.050851	31	6	0	3.687255	-2.199079
24	6	0	-5.093989	-0.308149	-0.878289	32	6	0	0.487015	2.619427
25	1	0	-3.856853	-2.043398	-1.288531	33	6	0	6.661142	-0.547851
26	1	0	-3.930743	-1.605721	0.415146	34	6	0	5.154821	0.496498
27	1	0	-6.027295	-0.871454	-0.774051	35	6	0	3.759708	3.556142
28	1	0	-5.130021	0.538192	-0.182368	36	6	0	0.502147	3.402905
29	1	0	-5.055711	0.097987	-1.895876	37	6	0	5.879816	-3.079028
						38	6	0	4.392854	-4.056402
						39	8	0	4.920438	-3.827170
						40	6	0	3.708620	-3.477792
						41	6	0	5.911981	-1.735681
						42	6	0	4.357888	-0.646468
						43	8	0	4.897846	1.560126
						44	6	0	3.707505	2.278309
						45	6	0	6.358331	-3.011626
						46	6	0	4.742372	-3.824045
						47	1	0	3.556788	-4.702596
						48	6	0	1.431756	-2.607242
						49	6	0	4.729092	-1.734748
						50	1	0	3.491338	-0.705694
						51	6	0	1.514859	4.003342
						52	1	0	5.876269	-3.842753
						53	8	0	3.973642	-4.428424
						54	6	0	1.456811	-3.874744
						55	8	0	3.957099	-2.921825
						56	6	0	1.458188	2.735264
						57	6	0	2.763318	-3.814014
						58	6	0	2.759770	-2.980255
						59	6	0	0.449695	-3.349875
						60	6	0	0.448569	-2.515438
						61	6	0	2.642797	-4.327681
						62	6	0	2.594665	-1.772338
						63	6	0	1.671755	2.459740
						64	6	0	1.702365	4.036059

Atom	Atomic Type	Coordinates (Angstroms)								
		X	Y	Z						
1	6	0	6.395268	3.058129	-1.757668					
2	6	0	5.932915	1.788019	-2.465638					
3	6	0	5.945303	3.124804	-0.301300					
4	1	0	5.903566	3.890998	-2.269916					
5	6	0	6.659883	0.586336	-2.424951					
6	6	0	4.761909	1.805472	-3.236917					
7	6	0	6.663619	2.525896	0.745983					
8	6	0	4.801793	3.862387	0.044441					

65	6	0	1.641159	-4.013743	0.769290	121	1	0	10.471703	2.976335	-2.965909
66	6	0	1.636756	-2.342372	3.167104	122	6	0	10.747794	2.988671	2.854078
67	6	0	2.713518	4.430149	4.298367	123	1	0	11.179779	2.545638	3.751392
68	6	0	2.602192	1.874824	5.724375	124	1	0	11.040922	2.415613	1.973321
69	1	0	2.685539	-5.292529	-3.629748	125	17	0	11.570173	4.651497	2.665274
70	1	0	2.599305	-0.857382	-6.122912	126	17	0	10.391855	3.799065	-5.219103
71	1	0	1.631801	-4.647161	-0.106051	127	17	0	11.399711	-4.730182	-2.085107
72	1	0	1.650268	1.891546	-3.951931	128	17	0	10.700130	-4.423928	3.004410
73	1	0	1.623138	-1.737860	4.061941	129	6	0	-7.020539	-3.074058	1.912426
74	1	0	1.699678	4.636562	0.325723	130	6	0	-6.320560	-3.213583	0.559869
75	1	0	2.780800	5.394761	3.813090	131	6	0	-6.289583	-1.961388	2.663966
76	1	0	2.583823	0.959201	6.300012	132	1	0	-6.859152	-4.005525	2.462656
77	7	0	-0.778006	-2.037204	2.595260	133	6	0	-6.653100	-2.407565	-0.539738
78	7	0	-0.774704	-3.379167	0.678399	134	6	0	-5.248375	-4.103315	0.400815
79	7	0	0.233137	2.554896	6.149720	135	6	0	-6.655171	-0.610062	2.575868
80	7	0	0.324691	4.601461	5.023259	136	6	0	-5.148348	-2.271262	3.423438
81	7	0	-0.721260	3.427778	-0.499578	137	6	0	-5.941686	-2.438689	-1.749119
82	7	0	-0.746069	2.166918	-2.470518	138	6	0	-4.475340	-4.126930	-0.759927
83	7	0	0.213292	-2.400004	-5.982225	139	8	0	-5.009401	-5.061817	1.417606
84	7	0	0.253781	-4.446133	-4.851791	140	6	0	-5.914344	0.417593	3.184119
85	1	0	7.445393	-1.848739	-0.301585	141	6	0	-4.358843	-1.283818	4.007322
86	1	0	7.550345	0.541364	-1.804245	142	8	0	-4.890974	-3.637625	3.683341
87	1	0	7.526934	1.912172	0.501404	143	6	0	-6.380405	-1.655676	-2.982790
88	1	0	7.565068	-0.516847	2.026183	144	6	0	-4.810509	-3.268520	-1.806012
89	6	0	7.887086	-3.216645	2.046394	145	1	0	-3.649525	-4.821683	-0.861319
90	6	0	8.313186	-4.610207	1.558467	146	6	0	-3.782899	-5.065033	2.079343
91	1	0	8.193344	-3.087609	3.090372	147	6	0	-6.371411	1.874133	3.191514
92	1	0	8.431238	-2.455087	1.469325	148	6	0	-4.736958	0.051519	3.852700
93	1	0	7.945782	-5.373813	2.253928	149	1	0	-3.492789	-1.543734	4.604270
94	1	0	7.857011	-4.821459	0.579669	150	6	0	-3.707685	-4.261031	3.304056
95	6	0	8.539529	1.786882	3.017637	151	1	0	-5.908100	-2.138127	-3.844273
96	6	0	9.237658	3.157491	2.957557	152	6	0	-5.885347	-0.213208	-2.973522
97	1	0	8.770222	1.227672	2.100477	153	8	0	-4.039332	-3.287138	-2.995695
98	1	0	8.941518	1.194540	3.850201	154	6	0	-5.924577	2.641239	1.950208
99	1	0	8.874857	3.728580	2.094969	155	1	0	-5.872451	2.347586	4.042869
100	1	0	8.994429	3.741470	3.852950	156	8	0	-3.969958	1.066814	4.476904
101	6	0	7.920369	3.276694	-1.883000	157	6	0	-6.600855	0.823471	-2.356277
102	6	0	8.364144	3.403842	-3.351534	158	6	0	-4.715307	0.134831	-3.663553
103	1	0	8.481852	2.462963	-1.402693	159	6	0	-2.816848	-2.608066	-2.995129
104	1	0	8.175109	4.194049	-1.335411	160	6	0	-1.544353	-5.787808	2.417075
105	1	0	8.169596	2.469962	-3.890880	161	6	0	-6.648610	2.628644	0.745662
106	1	0	7.783531	4.189461	-3.849463	162	6	0	-4.773226	3.442032	1.998701
107	6	0	8.503314	-1.791102	-2.779709	163	6	0	-2.772155	1.467081	3.880378
108	6	0	9.153578	-3.177882	-2.623318	164	6	0	-1.461377	-4.974703	3.612105
109	1	0	8.729012	-1.192208	-1.886760	165	6	0	-6.234410	2.172414	-2.467597
110	1	0	8.944511	-1.257529	-3.631971	166	6	0	-4.328738	1.465588	-3.831853
111	1	0	8.745422	-3.682427	-1.739062	167	8	0	-3.970708	-0.894378	-4.292870
112	1	0	8.913081	-3.807784	-3.487770	168	6	0	-2.781228	-1.317082	-3.693417
113	6	0	10.664877	-3.059484	-2.479390	169	6	0	-6.290155	3.412812	-0.362045
114	1	0	11.151594	-2.734163	-3.398604	170	6	0	-4.416604	4.285353	0.946776
115	1	0	10.953863	-2.411295	-1.650320	171	8	0	-3.998836	3.456109	3.186856
116	6	0	9.818807	-4.749883	1.384385	172	6	0	-2.786328	2.761220	3.187018
117	1	0	10.118532	-5.754304	1.090560	173	6	0	-6.976465	3.283462	-1.721073
118	1	0	10.228289	-4.021530	0.682096	174	6	0	-5.105107	2.466429	-3.248931
119	6	0	9.848010	3.737551	-3.436445	175	1	0	-3.468177	1.715093	-4.441594
120	1	0	10.077776	4.719900	-3.023827	176	6	0	-0.499329	-2.386141	-2.491922

177	6	0	-5.188973	4.270186	-0.212195	233	1	0	-8.879830	-4.101442	0.059395
178	1	0	-3.573148	4.958680	1.044793	234	1	0	-8.993297	-4.957997	1.595057
179	6	0	-0.458449	1.228643	3.371919	235	6	0	-7.913111	-1.742848	-3.177504
180	1	0	-6.809920	4.216828	-2.267610	236	6	0	-8.394737	-0.989711	-4.430238
181	8	0	-4.836638	3.825874	-3.539710	237	1	0	-8.446223	-1.343705	-2.303146
182	6	0	-0.465376	-1.111140	-3.179756	238	1	0	-8.182908	-2.805209	-3.244429
183	8	0	-4.926907	5.205618	-1.243999	239	1	0	-8.193085	0.081322	-4.319012
184	6	0	-0.471557	2.507094	2.689924	240	1	0	-7.844019	-1.325789	-5.316653
185	6	0	-3.645518	4.430362	-3.149050	241	6	0	-9.890542	-1.195063	-4.638405
186	6	0	-3.698995	5.196884	-1.899530	242	1	0	-10.133517	-2.174202	-5.049797
187	6	0	-1.387014	5.107104	-3.449963	243	1	0	-10.463840	-1.020186	-3.726360
188	6	0	-1.444343	5.876257	-2.224568	244	6	0	-10.536496	2.436092	-3.042874
189	6	0	-1.639663	-0.578180	-3.799632	245	1	0	-11.032828	2.538609	-4.005926
190	6	0	-1.708975	-3.147390	-2.408655	246	1	0	-10.507450	1.384707	-2.746947
191	6	0	-2.752527	-5.847635	1.649774	247	6	0	-10.749581	-3.819675	1.087330
192	6	0	-2.590313	-4.228938	4.084736	248	1	0	-11.178147	-3.866362	2.088411
193	6	0	-2.534681	4.401651	-3.938880	249	1	0	-11.046141	-2.893033	0.593855
194	6	0	-2.647973	5.940663	-1.450485	250	6	0	-9.820711	1.654903	4.995031
195	6	0	-1.642073	0.710575	3.986821	251	1	0	-10.049952	2.714743	5.106047
196	6	0	-1.669005	3.286961	2.606533	252	1	0	-10.443851	1.214774	4.215477
197	1	0	-1.604651	0.363534	-4.327289	253	17	0	-10.367137	0.851779	6.586796
198	1	0	-1.721144	-4.107150	-1.912559	254	17	0	-11.571995	-5.186138	0.121309
199	1	0	-2.514245	3.878926	-4.885669	255	17	0	-10.539761	0.047306	-5.874222
200	1	0	-2.839581	-6.479681	0.775940	256	17	0	-11.668498	3.264055	-1.800976
201	1	0	-2.715843	6.550218	-0.559261	257	8	0	-1.511782	2.666188	-1.390427
202	1	0	-2.551828	-3.680693	5.016307	258	8	0	0.557959	5.985526	-3.054869
203	1	0	-1.621264	-0.232495	4.512766	259	8	0	1.522638	-1.586168	-2.436504
204	1	0	-1.665319	4.249625	2.115944	260	8	0	-0.480587	3.705490	5.756711
205	7	0	-0.250121	6.418634	-1.983031	261	8	0	-0.527888	-3.533346	-5.590139
206	7	0	-0.157574	5.178777	-3.962807	262	8	0	1.538226	1.677234	2.634565
207	7	0	0.750243	2.780461	2.233152	263	8	0	0.458322	-5.917626	3.242889
208	7	0	0.771554	0.717876	3.337566	264	8	0	-1.552814	-2.570121	1.537307

C₉H₂₀@A₀+A₀

Atom	Atomic Type	Coordinates (Angstroms)			
		X	Y	Z	
1	6	0	6.582068	3.311659	1.994460
2	6	0	5.932810	3.359831	0.613850
3	6	0	6.326697	1.962018	2.662090
4	1	0	6.075538	4.065311	2.605940
5	6	0	6.533368	2.790486	-0.521933
6	6	0	4.682141	3.967751	0.436699
7	6	0	7.215705	0.879914	2.570022
8	6	0	5.166992	1.778532	3.436155
9	6	0	5.930898	2.803229	-1.791028
10	6	0	4.065643	4.033381	-0.810178
11	8	0	4.024474	4.561055	1.545943
12	6	0	7.010981	-0.336654	3.243781
13	6	0	4.932737	0.598823	4.140157
14	8	0	4.310232	2.887133	3.619647
15	6	0	6.556683	2.136357	-3.008460

16	6	0	4.685067	3.435727	-1.902948	72	1	0	1.523244	4.928079	0.645006
17	1	0	3.123218	4.552666	-0.929409	73	1	0	4.266693	-6.292737	-0.328855
18	6	0	2.864275	3.908405	1.977826	74	1	0	2.068698	1.589302	4.443749
19	6	0	7.970904	-1.521926	3.118668	75	1	0	3.251311	-1.420990	5.922800
20	6	0	5.860407	-0.439848	4.039846	76	1	0	4.318462	-5.611620	3.247721
21	1	0	4.076520	0.509638	4.798175	77	7	0	1.814602	-6.714318	-1.698697
22	6	0	3.028099	2.952375	3.079950	78	7	0	1.541119	-5.795416	-3.828988
23	1	0	6.045804	2.538420	-3.889070	79	7	0	1.709064	-5.301871	4.335227
24	6	0	6.286683	0.632305	-2.999103	80	7	0	1.210878	-3.363550	5.542785
25	8	0	4.040986	3.492839	-3.167933	81	7	0	-0.495775	1.985892	3.316046
26	6	0	7.541641	-2.383937	1.930909	82	7	0	-0.736939	3.456552	1.516705
27	1	0	7.842550	-2.130657	4.019038	83	7	0	-0.742051	2.678482	-2.657323
28	8	0	5.713844	-1.578717	4.866008	84	7	0	-0.554326	0.476229	-3.415003
29	6	0	7.181260	-0.286877	-2.434742	85	1	0	8.054921	0.095224	-1.913913
30	6	0	5.137584	0.114439	-3.623118	86	1	0	7.491318	2.289437	-0.403893
31	6	0	2.863259	2.741677	-3.261114	87	1	0	8.111479	0.991598	1.965512
32	6	0	0.536425	3.430360	1.908558	88	1	0	8.714212	-1.362241	0.445069
33	6	0	8.000131	-2.161718	0.620402	89	6	0	9.475997	-2.182506	-2.005921
34	6	0	6.622750	-3.428546	2.119903	90	6	0	9.962671	-2.135360	-3.463152
35	6	0	4.657059	-2.469594	4.687398	91	1	0	10.107016	-2.871912	-1.434149
36	6	0	0.690877	2.504899	3.010726	92	1	0	9.614529	-1.192359	-1.548862
37	6	0	7.024728	-1.676657	-2.549750	93	1	0	10.045487	-3.154923	-3.857002
38	6	0	4.952254	-1.260018	-3.788804	94	1	0	9.225280	-1.610961	-4.089669
39	8	0	4.256075	1.029038	-4.243582	95	6	0	9.450947	-1.099309	3.040882
40	6	0	2.996092	1.362882	-3.748387	96	6	0	9.894746	-0.332781	4.299825
41	6	0	7.562709	-2.921193	-0.476474	97	1	0	9.647284	-0.479933	2.154985
42	6	0	6.163722	-4.213017	1.061028	98	1	0	10.056056	-2.007747	2.921521
43	8	0	6.272631	-3.780667	3.445166	99	1	0	9.331082	0.602561	4.393405
44	6	0	4.963087	-3.675446	3.909284	100	1	0	9.679305	-0.927137	5.195586
45	6	0	8.013215	-2.654957	-1.912239	101	6	0	8.080687	3.675926	1.948678
46	6	0	5.911000	-2.136467	-3.271155	102	6	0	8.298786	5.106114	1.422642
47	1	0	4.108978	-1.640560	-4.355942	103	1	0	8.643933	2.973253	1.318699
48	6	0	0.525076	2.422145	-2.976295	104	1	0	8.487986	3.582182	2.964656
49	6	0	6.629658	-3.940681	-0.224096	105	1	0	7.950274	5.184302	0.386437
50	1	0	5.497984	-5.048477	1.243330	106	1	0	7.709689	5.816569	2.014482
51	6	0	2.471972	-3.309786	5.112469	107	6	0	8.056708	2.480381	-3.137530
52	1	0	7.927238	-3.599985	-2.457979	108	6	0	8.691071	1.869030	-4.399523
53	8	0	5.849453	-3.511067	-3.608670	109	1	0	8.620115	2.147856	-2.254459
54	6	0	0.649858	1.052696	-3.432684	110	1	0	8.144778	3.574642	-3.164605
55	8	0	6.299805	-4.794680	-1.295145	111	1	0	8.681329	0.775309	-4.333012
56	6	0	2.777423	-4.505762	4.358760	112	1	0	8.105041	2.138112	-5.286236
57	6	0	4.811771	-4.312055	-3.130376	113	6	0	10.127145	2.347198	-4.569810
58	6	0	5.022286	-4.949042	-1.824508	114	1	0	10.191956	3.394049	-4.865499
59	6	0	2.720697	-5.425481	-3.331691	115	1	0	10.733251	2.170751	-3.679477
60	6	0	2.889990	-5.992979	-2.013410	116	6	0	11.287590	-1.407109	-3.634099
61	6	0	1.921152	0.525034	-3.847345	117	1	0	11.657604	-1.435033	-4.656988
62	6	0	1.661645	3.288453	-2.917983	118	1	0	11.241327	-0.373672	-3.284380
63	6	0	1.652718	4.173505	1.409304	119	6	0	9.772087	5.486690	1.490874
64	6	0	1.970656	2.270017	3.610304	120	1	0	10.138350	5.550664	2.515511
65	6	0	3.714796	-4.564293	-3.898768	121	1	0	10.401162	4.813228	0.907201
66	6	0	4.092340	-5.775362	-1.262629	122	6	0	11.384532	-0.020865	4.241736
67	6	0	3.453957	-2.284249	5.302968	123	1	0	12.000173	-0.919244	4.285370
68	6	0	4.066332	-4.693488	3.761342	124	1	0	11.649208	0.574237	3.366681
69	1	0	1.989106	-0.477890	-4.244839	125	17	0	11.884181	1.006425	5.715673
70	1	0	1.559780	4.327642	-2.633932	126	17	0	10.032625	7.179220	0.754307
71	1	0	3.594242	-4.129006	-4.882071	127	17	0	10.958854	1.385230	-5.937967

128	17	0	12.620983	-2.217689	-2.597155	184	6	0	-0.460612	-1.293604	3.306011
129	6	0	-6.589739	-3.278338	-1.917621	185	6	0	-4.901033	4.839404	2.212407
130	6	0	-6.353763	-1.901042	-2.533625	186	6	0	-4.582192	4.035223	3.397867
131	6	0	-5.885851	-3.388968	-0.568454	187	6	0	-2.725440	5.802349	2.301919
132	1	0	-6.113344	-4.004627	-2.583621	188	6	0	-2.427101	5.035163	3.490874
133	6	0	-7.231296	-0.823055	-2.339456	189	6	0	-4.074013	4.759379	-3.323111
134	6	0	-5.228519	-1.679827	-3.345381	190	6	0	-3.607228	2.482204	-5.096500
135	6	0	-6.432902	-2.880233	0.619788	191	6	0	-2.034430	-2.294438	-3.791683
136	6	0	-4.633895	-4.015713	-0.476023	192	6	0	-1.654043	-4.252489	-1.649470
137	6	0	-7.053079	0.428036	-2.950388	193	6	0	-4.011134	5.721143	1.671758
138	6	0	-5.015271	-0.458140	-3.985243	194	6	0	-3.394695	4.145003	4.059019
139	8	0	-4.396668	-2.784708	-3.639063	195	6	0	-1.456006	-3.541416	2.796275
140	6	0	-5.788123	-2.980838	1.866237	196	6	0	-1.729505	-0.783111	3.744272
141	6	0	-3.974139	-4.164076	0.738162	197	1	0	-4.273360	5.638499	-2.725033
142	8	0	-4.039518	-4.551744	-1.646072	198	1	0	-3.459582	1.664796	-5.789750
143	6	0	-7.997181	1.607879	-2.714477	199	1	0	-4.266542	6.358743	0.835948
144	6	0	-5.935993	0.573325	-3.788677	200	1	0	-2.161129	-1.596912	-4.607486
145	1	0	-4.182301	-0.331330	-4.667252	201	1	0	-3.187954	3.591867	4.965821
146	6	0	-3.085908	-2.923078	-3.187147	202	1	0	-1.508540	-5.030697	-0.911991
147	6	0	-6.396478	-2.387176	3.133437	203	1	0	-1.349630	-4.576321	2.497833
148	6	0	-4.547943	-3.633049	1.891928	204	1	0	-1.800658	0.221525	4.134505
149	1	0	-3.030760	-4.693658	0.792210	205	7	0	-1.176455	5.283170	3.879799
150	6	0	-2.889488	-3.914519	-2.119798	206	7	0	-1.660689	6.528539	1.962626
151	1	0	-7.918559	2.262161	-3.588373	207	7	0	0.736209	-0.702800	3.280371
152	6	0	-7.507231	2.414135	-1.509783	208	7	0	0.938549	-2.899700	2.503683
153	8	0	-5.835233	1.755140	-4.560612	209	7	0	0.759979	-3.699777	-1.964995
154	6	0	-6.165796	-0.876949	3.185423	210	7	0	0.464774	-2.189541	-3.722170
155	1	0	-5.847265	-2.817839	3.977027	211	7	0	-1.368578	3.551541	-5.401605
156	8	0	-3.830525	-3.775052	3.112343	212	7	0	-1.734030	5.363430	-3.972708
157	6	0	-7.894439	2.113107	-0.194071	213	1	0	-8.568404	1.275254	-0.034906
158	6	0	-6.621119	3.487935	-1.685948	214	1	0	-8.095525	-0.972271	-1.698582
159	6	0	-4.766041	2.633233	-4.392988	215	1	0	-7.392676	-2.369722	0.576318
160	6	0	-0.723706	-2.623097	-3.310280	216	1	0	-8.054045	-0.278380	2.350517
161	6	0	-7.118369	0.070040	2.777310	217	6	0	-9.362986	2.041596	2.425702
162	6	0	-4.950619	-0.390893	3.701162	218	6	0	-10.325105	3.173674	2.028933
163	6	0	-2.654949	-3.014013	3.175528	219	1	0	-9.584563	1.715209	3.447782
164	6	0	-0.537394	-3.572173	-2.232432	220	1	0	-9.551125	1.171669	1.780645
165	6	0	-7.457271	2.841797	0.923856	221	1	0	-10.342235	3.937072	2.815167
166	6	0	-6.156327	4.240659	-0.607401	222	1	0	-9.967627	3.666131	1.112249
167	8	0	-6.302923	3.892841	-3.003212	223	6	0	-7.882158	-2.767695	3.297056
168	6	0	-5.009214	3.783638	-3.515119	224	6	0	-8.068493	-4.292627	3.394931
169	6	0	-6.914960	1.454552	2.907499	225	1	0	-8.486846	-2.386874	2.462266
170	6	0	-4.727537	0.971327	3.904818	226	1	0	-8.263243	-2.282848	4.205881
171	8	0	-4.044428	-1.349620	4.195518	227	1	0	-7.753577	-4.772778	2.461200
172	6	0	-2.791564	-1.638724	3.670483	228	1	0	-7.435892	-4.697406	4.193860
173	6	0	-7.891620	2.491393	2.352516	229	6	0	-8.083350	-3.651449	-1.808850
174	6	0	-6.575700	3.908255	0.680826	230	6	0	-8.777547	-3.682298	-3.182375
175	1	0	-5.522058	5.103954	-0.772188	231	1	0	-8.620821	-2.961046	-1.143628
176	6	0	-2.596302	3.474527	-4.887981	232	1	0	-8.145750	-4.641649	-1.338159
177	6	0	-5.724338	1.872099	3.522878	233	1	0	-8.764409	-2.686992	-3.640579
178	1	0	-3.827165	1.318633	4.399302	234	1	0	-8.235812	-4.353507	-3.859166
179	6	0	-0.327610	-2.660011	2.840176	235	6	0	-9.469889	1.169073	-2.577242
180	1	0	-7.779946	3.399701	2.953591	236	6	0	-10.412630	2.366386	-2.360061
181	8	0	-6.217135	4.750650	1.758753	237	1	0	-9.601617	0.465079	-1.743919
182	6	0	-2.821745	4.593804	-4.001608	238	1	0	-9.749000	0.624882	-3.489454
183	8	0	-5.613806	3.236332	3.881989	239	1	0	-10.164470	2.868610	-1.417896

240 1 0 -10.280148 3.105871 -3.158484
 241 6 0 -11.865459 1.910607 -2.314998
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 248 1 0 -10.286396 -5.193420 -2.717142
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 253 17 0 -9.757664 -6.486755 3.697203
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 257 8 0 -1.387920 2.556389 2.384030
 258 8 0 -0.692234 6.212129 2.933108
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 261 8 0 -1.422851 1.474995 -2.926164
 262 8 0 1.611281 -1.689604 2.772678
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 264 8 0 0.969066 -6.594491 -2.818125
 265 6 0 4.906394 -0.351629 0.330055
 266 6 0 3.603499 -0.936164 -0.220127
 267 1 0 5.772545 -0.979098 0.096945
 268 1 0 5.089991 0.646837 -0.089243
 269 1 0 4.839087 -0.250810 1.421415
 270 6 0 2.421025 0.005445 0.037718
 271 1 0 3.688323 -1.130024 -1.299987
 272 1 0 3.396986 -1.905189 0.257942
 273 1 0 2.403298 0.276283 1.106698
 274 1 0 2.564405 0.946437 -0.525354
 275 6 0 1.087687 -0.640415 -0.340950
 276 6 0 -0.128903 0.207035 0.029338
 277 1 0 1.016077 -1.619446 0.157395
 278 1 0 1.076171 -0.847323 -1.422398
 279 6 0 -1.439154 -0.552454 -0.185111
 280 1 0 -0.055177 0.509090 1.085935
 281 1 0 -0.144048 1.141217 -0.554148
 282 1 0 -1.484756 -0.915789 -1.225741
 283 1 0 -1.457913 -1.449806 0.461091
 284 6 0 -2.667254 0.310131 0.094202
 285 6 0 -3.965750 -0.490863 -0.010058
 286 1 0 -2.688344 1.148276 -0.617835
 287 1 0 -2.592047 0.754517 1.098713
 288 6 0 -5.180247 0.432060 0.043637
 289 1 0 -3.967507 -1.066893 -0.949195
 290 1 0 -4.006053 -1.224005 0.810577
 291 1 0 -6.126672 -0.119801 0.076031
 292 1 0 -5.129341 1.069980 0.935512
 293 1 0 -5.198570 1.086904 -0.837338

As+As

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	-8.374509	-3.421684
2	6	0	-7.789833	-2.347272
3	6	0	-7.781042	-3.299308
4	1	0	-8.046911	-4.386740
5	6	0	-8.334490	-1.055962
6	6	0	-6.665991	-2.629482
7	6	0	-8.320827	-2.457336
8	6	0	-6.651584	-4.057162
9	6	0	-7.808101	-0.065351
10	6	0	-6.115925	-1.679022
11	8	0	-6.136847	-3.942261
12	6	0	-7.788168	-2.360874
13	6	0	-6.097608	-4.001296
14	8	0	-6.127770	-4.972652
15	6	0	-8.403221	1.336526
16	6	0	-6.679865	-0.405636
17	1	0	-5.291455	-1.941425
18	6	0	-4.881721	-4.165554
19	6	0	-8.392214	-1.457117
20	6	0	-6.661056	-3.144412
21	1	0	-5.271547	-4.647615
22	6	0	-4.876928	-4.720605
23	1	0	-8.096476	1.742257
24	6	0	-7.797575	2.243593
25	8	0	-6.167875	0.546898
26	6	0	-7.814224	-0.048028
27	1	0	-8.067121	-1.856796
28	8	0	-6.141401	-3.133645
29	6	0	-8.321514	2.323670
30	6	0	-6.693434	3.055543
31	6	0	-4.917587	1.127480
32	6	0	-2.478659	-4.238828
33	6	0	-8.363902	0.936186
34	6	0	-6.686651	0.308928
35	6	0	-4.891693	-2.546109
36	6	0	-2.473995	-4.795361
37	6	0	-7.807779	3.186417
38	6	0	-6.148387	3.926471
39	8	0	-6.182020	3.056176
40	6	0	-4.926100	2.482681
41	6	0	-7.830882	2.231585
42	6	0	-6.137821	1.589289
43	8	0	-6.157397	-0.630768
44	6	0	-4.900391	-1.193614
45	6	0	-8.425585	3.296584
46	6	0	-6.701096	3.973266
47	1	0	-5.339173	4.592922
48	6	0	-2.514855	1.177436
49	6	0	-6.702512	2.528306
				3.196472

50	1	0	-5.313838	1.862637	4.705302	106	1	0	-10.093372	-4.602900	-3.084757
51	6	0	-2.488823	-2.567395	4.317642	107	6	0	-9.946725	1.322890	-3.202994
52	1	0	-8.125367	4.268913	1.902697	108	6	0	-10.540237	2.737263	-3.333390
53	8	0	-6.193970	4.906969	0.683979	109	1	0	-10.319245	0.869694	-2.273909
54	6	0	-2.524036	2.536149	-4.115978	110	1	0	-10.301004	0.684219	-4.023166
55	8	0	-6.191630	3.848238	3.175795	111	1	0	-10.252186	3.342971	-2.466174
56	6	0	-2.497409	-1.211667	4.871058	112	1	0	-10.135711	3.239737	-4.219908
57	6	0	-4.940532	4.666427	1.260300	113	6	0	-12.059818	2.681492	-3.421412
58	6	0	-4.938867	4.092307	2.603801	114	1	0	-12.414563	2.293921	-4.376128
59	6	0	-2.538762	4.768996	1.297150	115	1	0	-12.503433	2.117027	-2.599342
60	6	0	-2.536585	4.196901	2.645082	116	6	0	-12.020622	4.287825	0.346146
61	6	0	-3.773275	3.183531	-3.823321	117	1	0	-12.448726	5.171701	-0.122722
62	6	0	-3.755202	0.493336	-4.906086	118	1	0	-12.191245	3.413593	-0.285744
63	6	0	-3.726072	-3.948653	-3.098404	119	6	0	-12.025963	-3.786992	-2.596073
64	6	0	-3.716528	-5.050630	-0.415756	120	1	0	-12.354566	-4.663873	-2.038301
65	6	0	-3.784788	5.018407	0.625690	121	1	0	-12.487000	-2.886581	-2.187650
66	6	0	-3.779976	3.882207	3.293877	122	6	0	-12.028635	-2.816528	3.792655
67	6	0	-3.729767	-3.230568	4.023842	123	1	0	-12.374200	-2.265577	4.667316
68	6	0	-3.746446	-0.545641	5.120396	124	1	0	-12.485276	-2.411529	2.888574
69	1	0	-3.780367	4.207043	-3.471740	125	17	0	-12.720928	-4.538655	3.974749
70	1	0	-3.746812	-0.486683	-5.364957	126	17	0	-12.738743	-3.980888	-4.308244
71	1	0	-3.786920	5.494821	-0.346045	127	17	0	-12.769365	4.403757	-3.282062
72	1	0	-3.728814	-3.592743	-4.120419	128	17	0	-13.047139	3.990842	1.884857
73	1	0	-3.776891	3.513298	4.311189	129	6	0	8.374510	3.426620	-1.275231
74	1	0	-3.711813	-5.515931	0.561274	130	6	0	7.789282	2.355906	-2.193957
75	1	0	-3.722962	-4.253110	3.669538	131	6	0	7.781403	3.298789	0.126009
76	1	0	-3.751123	0.431997	5.584379	132	1	0	8.046988	4.393285	-1.669979
77	7	0	-1.320839	4.005153	3.158795	133	6	0	8.333536	1.064778	-2.291826
78	7	0	-1.324971	5.004403	0.797192	134	6	0	6.665576	2.641315	-2.983933
79	7	0	-1.285689	-0.699918	5.091081	135	6	0	8.321617	2.453472	1.108589
80	7	0	-1.270606	-3.073527	4.121420	136	6	0	6.651514	4.054715	0.479236
81	7	0	-1.257469	-5.012774	-0.590151	137	6	0	7.807067	0.077397	-3.139470
82	7	0	-1.265464	-4.037417	-2.961897	138	6	0	6.115248	1.694028	-3.847642
83	7	0	-1.296424	0.681090	-4.880504	139	8	0	6.136669	3.954191	-2.970207
84	7	0	-1.312766	3.060228	-3.924237	140	6	0	7.788807	2.351872	2.404798
85	1	0	-9.178874	1.704159	-0.625633	141	6	0	6.097435	3.993877	1.756256
86	1	0	-9.206890	-0.819873	-1.692465	142	8	0	6.127643	4.973436	-0.461430
87	1	0	-9.197236	-1.862912	0.855287	143	6	0	8.402164	-1.324109	-3.248725
88	1	0	-9.243489	0.689401	1.932489	144	6	0	6.678876	0.420696	-3.902797
89	6	0	-9.966943	3.251726	1.459280	145	1	0	5.290709	1.958928	-4.497742
90	6	0	-10.553040	4.459437	0.709491	146	6	0	4.881540	4.175419	-2.390907
91	1	0	-10.347827	3.239823	2.486320	147	6	0	8.392760	1.444212	3.475628
92	1	0	-10.331116	2.327476	0.988596	148	6	0	6.661272	3.133762	2.698491
93	1	0	-10.421106	5.366831	1.309893	149	1	0	5.271059	4.638807	2.028060
94	1	0	-10.007743	4.617634	-0.233117	150	6	0	4.876734	4.724102	-1.036693
95	6	0	-9.935052	-1.459649	3.456536	151	1	0	8.094957	-1.726350	-4.219001
96	6	0	-10.509079	-2.866995	3.700186	152	6	0	7.797042	-2.235053	-2.183193
97	1	0	-10.329212	-1.070072	2.507817	153	8	0	6.166563	-0.528269	-4.819161
98	1	0	-10.280961	-0.772210	4.239784	154	6	0	7.814619	0.035568	3.358711
99	1	0	-10.216142	-3.542164	2.888053	155	1	0	8.067707	1.840437	4.442561
100	1	0	-10.098637	-3.283845	4.627519	156	8	0	6.141765	3.117710	4.015287
101	6	0	-9.917453	-3.421182	-1.269073	157	6	0	8.321613	-2.320175	-0.884390
102	6	0	-10.508305	-3.677986	-2.667104	158	6	0	6.692622	-3.045651	-2.485070
103	1	0	-10.314291	-2.473176	-0.879737	159	6	0	4.916338	-1.109694	-4.578599
104	1	0	-10.247011	-4.203958	-0.572576	160	6	0	2.478531	4.249549	-2.431391
105	1	0	-10.232979	-2.866142	-3.349958	161	6	0	8.364135	-0.945406	2.516192

$$\mathbf{A_S}^+ \mathbf{A_S}^- \mathbf{b}$$

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z

1	6	0	-6.409474	-0.917252	3.566361	57	6	0	-3.315316	1.002853	-4.741410
2	6	0	-5.210664	-1.575256	2.888418	58	6	0	-4.125235	2.208680	-4.595815
3	6	0	-6.668468	0.471740	2.989511	59	6	0	-1.321289	2.319331	-4.821168
4	1	0	-6.134357	-0.774033	4.615839	60	6	0	-2.129488	3.537799	-4.677293
5	6	0	-5.320071	-2.273975	1.675963	61	6	0	-0.028797	-1.557653	-1.393202
6	6	0	-3.939928	-1.511394	3.478510	62	6	0	0.244477	-2.359387	1.386238
7	6	0	-7.509225	0.697219	1.888922	63	6	0	-1.739554	0.380065	4.815867
8	6	0	-6.080280	1.598116	3.590408	64	6	0	-3.331413	2.815841	4.719701
9	6	0	-4.231835	-2.920946	1.065753	65	6	0	-1.958935	1.033925	-4.875172
10	6	0	-2.828918	-2.126240	2.906220	66	6	0	-3.561637	3.450229	-4.582160
11	8	0	-3.802703	-0.850547	4.724742	67	6	0	-5.841115	6.033454	1.868150
12	6	0	-7.798761	1.983149	1.403175	68	6	0	-5.831603	6.180671	-1.031585
13	6	0	-6.354663	2.892979	3.153801	69	1	0	-0.102027	-1.291822	-2.441267
14	8	0	-5.289564	1.405145	4.746136	70	1	0	0.335095	-2.665049	2.419568
15	6	0	-4.387709	-3.680370	-0.249777	71	1	0	-1.383072	0.125269	-5.027232
16	6	0	-2.986775	-2.822579	1.709450	72	1	0	-1.165953	-0.539876	4.895969
17	1	0	-1.858497	-2.062930	3.389535	73	1	0	-4.151199	4.355874	-4.529457
18	6	0	-3.100951	0.358349	4.734056	74	1	0	-3.914968	3.726366	4.743284
19	6	0	-8.700515	2.217928	0.193310	75	1	0	-5.889188	6.022550	2.949252
20	6	0	-7.207637	3.069965	2.063626	76	1	0	-5.873539	6.284414	-2.107861
21	1	0	-5.958714	3.749579	3.685932	77	7	0	-1.427069	4.673892	-4.653505
22	6	0	-3.904697	1.577849	4.698718	78	7	0	-0.003134	2.536223	-4.895729
23	1	0	-3.521529	-4.343216	-0.340796	79	7	0	-4.084544	7.898519	-0.779110
24	6	0	-4.325612	-2.705201	-1.423295	80	7	0	-4.097578	7.772440	1.802993
25	8	0	-1.859541	-3.504718	1.173200	81	7	0	-1.187954	4.023720	4.729621
26	6	0	-7.851301	2.135618	-1.072545	82	7	0	0.223937	1.871947	4.818569
27	1	0	-9.071438	3.244673	0.266043	83	7	0	2.441868	-1.241158	1.326399
28	8	0	-7.582339	4.380244	1.681913	84	7	0	2.161097	-0.466144	-1.127011
29	6	0	-5.454251	-2.068262	-1.960073	85	1	0	-6.427326	-2.272979	-1.520986
30	6	0	-3.083386	-2.399668	-1.999174	86	1	0	-6.293160	-2.323379	1.194286
31	6	0	-0.833805	-2.720243	0.635339	87	1	0	-7.972756	-0.156402	1.401929
32	6	0	-1.097440	1.664185	4.800842	88	1	0	-8.064376	0.019092	-1.365629
33	6	0	-7.607644	0.928131	-1.745212	89	6	0	-7.854211	-1.370815	-3.640459
34	6	0	-7.260535	3.295720	-1.597649	90	6	0	-7.682237	-2.589244	-4.562906
35	6	0	-6.641530	5.236627	1.103288	91	1	0	-8.712915	-0.777864	-3.973521
36	6	0	-1.897800	2.891790	4.746296	92	1	0	-8.101217	-1.721454	-2.628368
37	6	0	-5.378083	-1.190236	-3.056039	93	1	0	-7.707718	-2.266568	-5.610017
38	6	0	-2.958563	-1.563099	-3.102898	94	1	0	-6.698067	-3.051621	-4.394299
39	8	0	-1.946883	-3.040904	-1.468994	95	6	0	-9.920655	1.276800	0.153130
40	6	0	-0.945498	-2.363928	-0.778201	96	6	0	-10.822207	1.456291	1.387916
41	6	0	-6.815600	0.844334	-2.902485	97	1	0	-9.616079	0.223690	0.081302
42	6	0	-6.461441	3.260326	-2.739198	98	1	0	-10.487487	1.496729	-0.761207
43	8	0	-7.597560	4.540268	-1.016628	99	1	0	-10.276361	1.184482	2.298816
44	6	0	-6.640155	5.313046	-0.357256	100	1	0	-11.112413	2.508647	1.490058
45	6	0	-6.597304	-0.477707	-3.637968	101	6	0	-7.669847	-1.807669	3.531681
46	6	0	-4.111768	-0.974623	-3.616951	102	6	0	-7.441789	-3.146248	4.256874
47	1	0	-1.997965	-1.388433	-3.574532	103	1	0	-7.990675	-2.008972	2.500023
48	6	0	1.281454	-1.585455	0.759816	104	1	0	-8.489842	-1.255776	4.011091
49	6	0	-6.234322	2.035970	-3.369111	105	1	0	-6.668412	-3.728144	3.742387
50	1	0	-6.066085	4.175412	-3.163906	106	1	0	-7.081384	-2.962814	5.275965
51	6	0	-4.949153	6.940240	1.198270	107	6	0	-5.660598	-4.554026	-0.267188
52	1	0	-6.354252	-0.228525	-4.676183	108	6	0	-5.798357	-5.352366	-1.576144
53	8	0	-4.024857	-0.196845	-4.793259	109	1	0	-6.563760	-3.943808	-0.127906
54	6	0	1.121543	-1.145275	-0.632350	110	1	0	-5.614200	-5.236942	0.591362
55	8	0	-5.508868	2.018178	-4.583965	111	1	0	-5.888086	-4.664837	-2.424967
56	6	0	-4.941810	7.011666	-0.267083	112	1	0	-4.899702	-5.955881	-1.749635

113	6	0	-7.024502	-6.255149	-1.534277	169	6	0	6.687699	-0.447965	-3.055623
114	1	0	-6.901338	-7.106832	-0.865766	170	6	0	6.362109	-2.865838	-3.239721
115	1	0	-7.934212	-5.707937	-1.280973	171	8	0	7.568700	-4.369711	-1.766630
116	6	0	-8.723661	-3.673920	-4.329653	172	6	0	6.619331	-5.225356	-1.202468
117	1	0	-8.640831	-4.500085	-5.033242	173	6	0	6.418842	0.950370	-3.602265
118	1	0	-8.703635	-4.054979	-3.306508	174	6	0	3.938453	1.527645	-3.505675
119	6	0	-8.732037	-3.953899	4.310784	175	1	0	1.861333	2.097192	-3.419871
120	1	0	-9.497317	-3.475121	4.921708	176	6	0	-1.085889	1.144373	0.654661
121	1	0	-9.125712	-4.172377	3.317109	177	6	0	6.094709	-1.565576	-3.665841
122	6	0	-12.070982	0.592374	1.269247	178	1	0	5.962670	-3.716254	-3.778928
123	1	0	-12.716815	0.905440	0.448925	179	6	0	4.907327	-7.008958	0.142227
124	1	0	-11.833542	-0.468293	1.177167	180	1	0	6.151991	0.832073	-4.657532
125	17	0	-13.107180	0.741360	2.812513	181	8	0	3.800579	0.886860	-4.762397
126	17	0	-8.420444	-5.613636	5.101516	182	6	0	-1.263400	1.578592	-0.737036
127	17	0	-7.337987	-6.982839	-3.225881	183	8	0	5.300511	-1.359103	-4.817788
128	17	0	-10.450480	-2.987518	-4.565987	184	6	0	4.916865	-6.917625	-1.322028
129	6	0	6.607456	0.435040	3.604563	185	6	0	3.106316	-0.326200	-4.780171
130	6	0	5.404727	1.189178	3.043037	186	6	0	3.917428	-1.541313	-4.767889
131	6	0	6.801450	-0.873263	2.837750	187	6	0	1.108881	-1.641455	-4.837441
132	1	0	6.356113	0.162543	4.634286	188	6	0	1.916489	-2.865300	-4.813237
133	6	0	5.490888	2.081924	1.958202	189	6	0	-0.237301	2.355730	-1.377269
134	6	0	4.138121	0.976650	3.602418	190	6	0	0.071558	1.561769	1.401438
135	6	0	7.586195	-0.950560	1.675812	191	6	0	1.963507	-1.020661	4.861696
136	6	0	6.212457	-2.066082	3.293921	192	6	0	3.527257	-3.454712	4.509703
137	6	0	4.364056	2.720546	1.418691	193	6	0	1.744022	-0.353952	-4.843986
138	6	0	2.988139	1.577541	3.093743	194	6	0	3.349976	-2.781884	-4.802113
139	8	0	4.045505	0.182781	4.767308	195	6	0	5.800316	-6.192712	0.918840
140	6	0	7.830376	-2.154879	0.997094	196	6	0	5.815198	-6.007470	-1.978661
141	6	0	6.431768	-3.285328	2.652670	197	1	0	-0.338127	2.653781	-2.412110
142	8	0	5.494576	-2.053298	4.512332	198	1	0	0.158398	1.293226	2.447449
143	6	0	4.411144	3.675764	0.228789	199	1	0	1.165043	0.564108	-4.904567
144	6	0	3.118614	2.414114	1.991940	200	1	0	1.401309	-0.106903	5.033597
145	1	0	2.027116	1.401698	3.563871	201	1	0	3.937696	-3.689014	-4.843707
146	6	0	3.317896	-1.006055	4.706765	202	1	0	4.103686	-4.367396	4.436658
147	6	0	8.692606	-2.229281	-0.261928	203	1	0	5.839980	-6.310029	1.993838
148	6	0	7.236031	-3.316169	1.513525	204	1	0	5.865292	-5.983761	-3.059430
149	1	0	6.031174	-4.202016	3.069036	205	7	0	1.212669	-4.001085	-4.803568
150	6	0	4.107849	-2.221477	4.533986	206	7	0	-0.211390	-1.855822	-4.838350
151	1	0	3.550571	4.345829	0.319322	207	7	0	4.061667	-7.737049	-1.938979
152	6	0	4.228807	2.898406	-1.073061	208	7	0	4.044560	-7.897888	0.641195
153	8	0	1.988277	3.051721	1.446239	209	7	0	1.378278	-4.650596	4.601941
154	6	0	7.806047	-1.976326	-1.477930	210	7	0	-0.011317	-2.497960	4.901130
155	1	0	9.057445	-3.257967	-0.338273	211	7	0	-2.116901	0.463136	1.163415
156	8	0	7.572307	-4.559539	0.929856	212	7	0	-2.427739	1.226038	-1.289885
157	6	0	5.313029	2.246539	-1.684113	213	1	0	6.282153	2.290074	-1.193386
158	6	0	2.987480	2.822830	-1.722897	214	1	0	6.467641	2.278141	1.524543
159	6	0	0.976619	2.372117	0.774815	215	1	0	8.045803	-0.041531	1.297645
160	6	0	1.307788	-2.297009	4.802726	216	1	0	8.001901	0.163934	-1.472822
161	6	0	7.531763	-0.685593	-1.959384	217	6	0	7.658551	1.866102	-3.524848
162	6	0	7.207224	-3.055022	-2.146511	218	6	0	7.440942	3.179938	-4.293553
163	6	0	6.614216	-5.320681	0.256915	219	1	0	8.521471	1.336352	-3.943105
164	6	0	2.096090	-3.524108	4.626450	220	1	0	7.918580	2.101661	-2.483018
165	6	0	5.208643	1.574487	-2.910629	221	1	0	7.448875	2.983725	-5.371857
166	6	0	2.829492	2.140912	-2.929244	222	1	0	6.451606	3.596608	-4.051526
167	8	0	1.862409	3.512274	-1.190925	223	6	0	9.918845	-1.295986	-0.214316
168	6	0	0.845427	2.726290	-0.637756	224	6	0	10.857492	-1.647367	0.953954

225	1	0	9.620779	-0.241729	-0.132215	8	6	0	6.693133	4.116811	-0.388599
226	1	0	10.454160	-1.391430	-1.168191	9	6	0	7.839813	-0.587264	-3.032559
227	1	0	10.339513	-1.512228	1.910442	10	6	0	6.130897	0.833290	-4.055497
228	1	0	11.149862	-2.702347	0.894224	11	8	0	6.158652	3.229802	-3.700529
229	6	0	7.892143	1.287413	3.644149	12	6	0	7.825702	2.872745	1.863339
230	6	0	7.726505	2.522799	4.547623	13	6	0	6.147039	4.346885	0.872311
231	1	0	8.189182	1.615409	2.638180	14	8	0	6.161639	4.805945	-1.505433
232	1	0	8.709214	0.655699	4.018099	15	6	0	8.433562	-1.983326	-2.853599
233	1	0	6.946052	3.181317	4.149425	16	6	0	6.695211	-0.419436	-3.828943
234	1	0	7.404470	2.212884	5.548724	17	1	0	5.301169	0.948233	-4.740848
235	6	0	5.688631	4.542332	0.218400	18	6	0	4.905135	3.569314	-3.179166
236	6	0	5.729567	5.494900	-0.990064	19	6	0	8.428139	2.209432	3.100553
237	1	0	6.594065	3.920050	0.204116	20	6	0	6.708708	3.713954	1.980760
238	1	0	5.718663	5.113430	1.156093	21	1	0	5.326904	5.043240	0.996463
239	1	0	5.808866	4.914322	-1.916811	22	6	0	4.906920	4.425048	-1.995585
240	1	0	4.798300	6.070137	-1.054487	23	1	0	8.129120	-2.573044	-3.724063
241	6	0	6.916010	6.444688	-0.890729	24	6	0	7.823161	-2.659124	-1.628859
242	1	0	6.786064	7.204332	-0.120277	25	8	0	6.160602	-1.552651	-4.479542
243	1	0	7.859836	5.917183	-0.741684	26	6	0	7.835553	0.813804	3.278998
244	6	0	8.465513	4.252309	-3.954355	27	1	0	8.108683	2.802550	3.963056
245	1	0	8.347517	5.156544	-4.548343	28	8	0	6.192101	4.000150	3.267774
246	1	0	8.464376	4.503992	-2.891596	29	6	0	8.333535	-2.455241	-0.337231
247	6	0	9.036115	3.293714	4.650476	30	6	0	6.727185	-3.525309	-1.754894
248	1	0	9.814858	2.725074	5.158660	31	6	0	4.917685	-2.060137	-4.091089
249	1	0	9.393253	3.635655	3.678078	32	6	0	2.502257	3.616030	-3.210959
250	6	0	12.103175	-0.771368	0.925916	33	6	0	8.379282	-0.333326	2.675085
251	1	0	12.725013	-0.959478	0.050717	34	6	0	6.693210	0.642496	4.076480
252	1	0	11.864560	0.290700	0.996572	35	6	0	4.934184	3.492677	3.615235
253	17	0	13.182165	-1.141526	2.401228	36	6	0	2.503254	4.477103	-2.026553
254	17	0	8.794754	4.838786	5.666163	37	6	0	7.808827	-3.080281	0.804962
255	17	0	7.118094	7.382620	-2.493171	38	6	0	6.171051	-4.164268	-0.648285
256	17	0	10.199395	3.640638	-4.313531	39	8	0	6.215796	-3.829909	-3.041862
257	16	0	3.216772	-8.644570	-0.705967	40	6	0	4.948361	-3.323812	-3.360988
258	16	0	-0.479888	-3.587256	-4.818703	41	6	0	7.821732	-1.613039	2.835835
259	16	0	-0.303170	-4.225231	4.797588	42	6	0	6.118359	-0.610579	4.277185
260	16	0	3.374767	-0.359955	0.133039	43	8	0	6.178266	1.760652	4.774352
261	16	0	0.501761	3.601632	4.777638	44	6	0	4.926652	2.277102	4.425377
262	16	0	-3.259334	8.668003	0.556790	45	6	0	8.411106	-2.866801	2.192801
263	16	0	-3.343349	0.344910	-0.083098	46	6	0	6.703906	-3.926580	0.617177
264	16	0	0.263544	4.268668	-4.809112	47	1	0	5.358849	-4.869833	-0.775817

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Atom	Atomic Type		Coordinates (Angstroms)			X	Y	Z
	Type							
1	6	0	8.408404	3.095617	-1.961850	53	8	0
2	6	0	7.824432	1.843532	-2.612241	54	6	0
3	6	0	7.814164	3.289965	-0.569096	55	8	0
4	1	0	8.080242	3.946581	-2.566799	56	6	0
5	6	0	8.376061	0.563083	-2.432476	57	6	0
6	6	0	6.690557	1.947244	-3.431030	58	6	0
7	6	0	8.349782	2.676926	0.574723	59	6	0
						60	6	0
						61	6	0
						62	6	0
						63	6	0

64	6	0	3.749514	4.889485	-1.440806	120	1	0	12.394002	4.136417	-2.951028
65	6	0	3.747268	-4.692271	1.617544	121	1	0	12.519307	2.365881	-2.731177
66	6	0	3.717957	-2.896112	3.895493	122	6	0	12.073568	3.580315	3.130814
67	6	0	3.781576	4.141983	3.278627	123	1	0	12.417446	3.211735	4.097260
68	6	0	3.765642	1.727916	4.887325	124	1	0	12.526662	3.001642	2.324768
69	1	0	3.836601	-4.973982	-2.562682	125	17	0	12.775314	5.300555	2.968310
70	1	0	3.706180	-0.562841	-5.044186	126	17	0	12.771616	2.999286	-5.031991
71	1	0	3.757351	-5.399987	0.798651	127	17	0	12.793342	-4.997534	-2.239017
72	1	0	3.741209	2.604672	-4.701325	128	17	0	13.038432	-3.461204	2.711257
73	1	0	3.696840	-2.278599	4.783605	129	6	0	-8.457714	-3.589174	-0.439345
74	1	0	3.749933	5.570107	-0.599415	130	6	0	-7.863426	-2.774637	-1.585933
75	1	0	3.789233	5.073859	2.728278	131	6	0	-7.848776	-3.131259	0.885195
76	1	0	3.757767	0.863967	5.538929	132	1	0	-8.141365	-4.625905	-0.591251
77	7	0	1.265524	-2.991075	3.726968	133	6	0	-8.387424	-1.527641	-1.970959
78	7	0	1.281878	-4.586185	1.721707	134	6	0	-6.743220	-3.245496	-2.286680
79	7	0	1.308504	1.917419	4.844746	135	6	0	-8.382402	-2.087333	1.659556
80	7	0	1.319069	4.049982	3.421684	136	6	0	-6.702023	-3.775206	1.378155
81	7	0	1.288375	4.802446	-1.582785	137	6	0	-7.831505	-0.751320	-2.998831
82	7	0	1.287300	3.295014	-3.656086	138	6	0	-6.161543	-2.507955	-3.317897
83	7	0	1.292789	-1.673679	-4.364554	139	8	0	-6.238943	-4.539869	-2.007243
84	7	0	1.340574	-3.937838	-3.165474	140	6	0	-7.822104	-1.685971	2.884739
85	1	0	9.182327	-1.786652	-0.218758	141	6	0	-6.124276	-3.421217	2.594953
86	1	0	9.259658	0.465268	-1.807821	142	8	0	-6.190175	-4.881316	0.663610
87	1	0	9.215754	2.029855	0.462128	143	6	0	-8.395299	0.601613	-3.424924
88	1	0	9.273352	-0.229552	2.067039	144	6	0	-6.693577	-1.263949	-3.643652
89	6	0	9.953210	-2.844036	2.157683	145	1	0	-5.332902	-2.917960	-3.881883
90	6	0	10.533735	-4.194230	1.705195	146	6	0	-4.972549	-4.640670	-1.416484
91	1	0	10.328090	-2.601541	3.158032	147	6	0	-8.403900	-0.563005	3.742335
92	1	0	10.327767	-2.053294	1.492342	148	6	0	-6.679035	-2.370670	3.323577
93	1	0	10.408774	-4.936734	2.501618	149	1	0	-5.291784	-3.986643	2.993128
94	1	0	9.979956	-4.566883	0.830481	150	6	0	-4.945334	-4.788162	0.034791
95	6	0	9.970450	2.196956	3.083657	151	1	0	-8.074944	0.768146	-4.458210
96	6	0	10.554202	3.620296	3.030915	152	6	0	-7.780718	1.723179	-2.590478
97	1	0	10.359123	1.617146	2.235226	153	8	0	-6.136650	-0.528502	-4.713855
98	1	0	10.314089	1.683707	3.991553	154	6	0	-7.813850	0.781156	3.322147
99	1	0	10.263570	4.115540	2.097241	155	1	0	-8.070368	-0.747324	4.768303
100	1	0	10.148500	4.221962	3.852850	156	8	0	-6.137644	-2.043023	4.587972
101	6	0	9.951235	3.101829	-1.942056	157	6	0	-8.303986	2.098209	-1.342904
102	6	0	10.542923	3.049684	-3.362172	158	6	0	-6.678489	2.447706	-3.066489
103	1	0	10.349158	2.262671	-1.354538	159	6	0	-4.886091	0.077688	-4.558455
104	1	0	10.278675	4.018392	-1.433055	160	6	0	-2.572968	-4.777216	-1.480919
105	1	0	10.263665	2.111850	-3.855943	161	6	0	-8.351985	1.543497	2.271822
106	1	0	10.132116	3.865783	-3.968184	162	6	0	-6.696227	1.307340	3.989227
107	6	0	9.976726	-1.963460	-2.809293	163	6	0	-4.889418	-1.416480	4.656366
108	6	0	10.567727	-3.374946	-2.641544	164	6	0	-2.546630	-4.895491	-0.021979
109	1	0	10.345311	-1.329303	-1.991172	165	6	0	-7.790814	3.163536	-0.587304
110	1	0	10.336786	-1.507732	-3.741414	166	6	0	-6.129214	3.507708	-2.345176
111	1	0	10.275262	-3.786953	-1.668551	167	8	0	-6.152092	2.147426	-4.347615
112	1	0	10.165254	-4.049971	-3.406054	168	6	0	-4.895988	1.528582	-4.396255
113	6	0	12.087715	-3.340458	-2.733405	169	6	0	-7.821530	2.782807	1.880121
114	1	0	12.446358	-3.158468	-3.746196	170	6	0	-6.146508	2.541066	3.641932
115	1	0	12.529636	-2.619066	-2.043780	171	8	0	-6.161066	0.609181	5.101012
116	6	0	11.997230	-4.112760	1.296910	172	6	0	-4.902220	0.012382	4.958027
117	1	0	12.423123	-5.082059	1.045039	173	6	0	-8.411654	3.601832	0.737552
118	1	0	12.158836	-3.411885	0.475061	174	6	0	-6.680194	3.844587	-1.110503
119	6	0	12.061077	3.164746	-3.315905	175	1	0	-5.317674	4.091251	-2.762156

176	6	0	-2.482526	0.095238	-4.554225	232	1	0	-10.333916	-4.153683	0.449308
177	6	0	-6.701803	3.255736	2.582568	233	1	0	-10.320794	-3.524402	-2.568579
178	1	0	-5.326803	2.956128	4.215352	234	1	0	-10.192357	-5.147431	-1.893983
179	6	0	-2.486987	-1.396458	4.661644	235	6	0	-9.939025	0.626356	-3.397915
180	1	0	-8.109790	4.641569	0.900690	236	6	0	-10.503509	1.984922	-3.850994
181	8	0	-6.172713	4.963909	-0.409149	237	1	0	-10.325610	0.402552	-2.393983
182	6	0	-2.494011	1.552214	-4.411085	238	1	0	-10.301486	-0.175070	-4.055569
183	8	0	-6.187943	4.536378	2.264911	239	1	0	-10.220115	2.763594	-3.133093
184	6	0	-2.498072	0.031302	4.986468	240	1	0	-10.073716	2.272912	-4.817674
185	6	0	-4.923374	4.865617	0.214666	241	6	0	-12.021934	1.931504	-3.957967
186	6	0	-4.931517	4.639586	1.658134	242	1	0	-12.365265	1.347049	-4.811233
187	6	0	-2.522163	4.989270	0.245303	243	1	0	-12.491028	1.568517	-3.041773
188	6	0	-2.529479	4.771767	1.693635	244	6	0	-11.992568	4.291216	-0.645883
189	6	0	-3.743623	2.257207	-4.345325	245	1	0	-12.419140	5.044895	-1.304945
190	6	0	-3.720585	-0.628367	-4.645923	246	1	0	-12.145090	3.297030	-1.071723
191	6	0	-3.831637	-4.664795	-2.166425	247	6	0	-12.117010	-4.223478	-1.611351
192	6	0	-3.774339	-4.926844	0.722118	248	1	0	-12.449211	-4.934479	-0.854921
193	6	0	-3.762452	5.053700	-0.477916	249	1	0	-12.571053	-3.247222	-1.435659
194	6	0	-3.778193	4.614350	2.388557	250	6	0	-12.051064	-1.765395	4.398707
195	6	0	-3.723938	-2.114243	4.527620	251	1	0	-12.380654	-1.021012	5.123484
196	6	0	-3.750089	0.719029	5.148497	252	1	0	-12.515128	-1.577833	3.429509
197	1	0	-3.750983	3.337548	-4.281932	253	17	0	-12.756471	-3.388853	4.985973
198	1	0	-3.703332	-1.696408	-4.819169	254	17	0	-12.836318	-4.826902	-3.222366
199	1	0	-3.756348	5.276476	-1.536960	255	17	0	-12.703489	3.650829	-4.218237
200	1	0	-3.856960	-4.621089	-3.247801	256	17	0	-13.043508	4.328561	0.904482
201	1	0	-3.785236	4.507772	3.465519	257	16	0	0.094766	4.061335	-2.628952
202	1	0	-3.747674	-5.098288	1.790217	258	16	0	-0.119662	4.972497	0.993879
203	1	0	-3.706788	-3.183053	4.360317	259	16	0	-0.080239	0.846588	-4.491959
204	1	0	-3.759657	1.763932	5.430176	260	16	0	0.122026	3.009478	4.164598
205	7	0	-1.316919	4.732104	2.248781	261	16	0	0.126080	-2.843106	-3.790196
206	7	0	-1.305256	5.109956	-0.286636	262	16	0	-0.084179	-0.659011	4.789517
207	7	0	-1.286749	0.580232	5.085724	263	16	0	-0.158317	-4.946427	-0.799366
208	7	0	-1.269704	-1.917942	4.512950	264	16	0	0.080202	-3.802432	2.728924
209	7	0	-1.323051	-4.991604	0.500826	265	6	0	5.096363	-0.615208	-0.290408
210	7	0	-1.366178	-4.784821	-2.053956	266	6	0	3.797023	-1.395197	-0.035853
211	7	0	-1.263216	-0.441061	-4.606572	267	1	0	5.969711	-1.121723	0.138147
212	7	0	-1.283766	2.108166	-4.350319	268	1	0	5.272049	-0.490548	-1.368879
213	1	0	-9.161387	1.552227	-0.957746	269	1	0	5.041253	0.387948	0.153617
214	1	0	-9.260152	-1.151695	-1.444002	270	6	0	2.560380	-0.659165	-0.573352
215	1	0	-9.273966	-1.576942	1.304782	271	1	0	3.859828	-2.392029	-0.500902
216	1	0	-9.221109	1.161827	1.743712	272	1	0	3.671905	-1.565152	1.046099
217	6	0	-9.952903	3.551426	0.704343	273	1	0	2.490747	0.326471	-0.088297
218	6	0	-10.532885	4.554628	-0.306701	274	1	0	2.687978	-0.465323	-1.651272
219	1	0	-10.337749	3.776868	1.704829	275	6	0	1.251372	-1.430223	-0.342842
220	1	0	-10.317289	2.544056	0.458097	276	6	0	0.014890	-0.608147	-0.737281
221	1	0	-10.416923	5.574875	0.076565	277	1	0	1.176453	-1.709481	0.721888
222	1	0	-9.971978	4.502540	-1.252047	278	1	0	1.274583	-2.376910	-0.906114
223	6	0	-9.946691	-0.546399	3.745702	279	6	0	-1.315248	-1.365719	-0.599985
224	6	0	-10.533295	-1.854637	4.306159	280	1	0	-0.021157	0.297818	-0.112864
225	1	0	-10.349173	-0.372599	2.738209	281	1	0	0.126801	-0.263379	-1.777687
226	1	0	-10.273768	0.303650	4.358912	282	1	0	-1.378703	-2.141366	-1.379545
227	1	0	-10.256986	-2.700595	3.666428	283	1	0	-1.349721	-1.885983	0.371691
228	1	0	-10.117022	-2.055215	5.300442	284	6	0	-2.527708	-0.427797	-0.719497
229	6	0	-9.999490	-3.565831	-0.416227	285	6	0	-3.870480	-1.173720	-0.719902
230	6	0	-10.598995	-4.146051	-1.709856	286	1	0	-2.441459	0.165129	-1.646007
231	1	0	-10.384444	-2.547464	-0.266443	287	1	0	-2.510599	0.292837	0.111790

288	6	0	-5.076577	-0.222067	-0.684429	42	6	0	6.618975	-2.692023	3.515014
289	1	0	-3.926149	-1.809532	-1.617108	43	8	0	6.689213	-0.838613	5.074362
290	1	0	-3.908761	-1.851416	0.148187	44	6	0	5.408643	-0.269449	5.001624
291	1	0	-6.027870	-0.769530	-0.680470	45	6	0	8.690772	-3.540984	0.408468
292	1	0	-5.049760	0.410476	0.212909	46	6	0	6.842276	-3.722236	-1.338769
293	1	0	-5.073139	0.445462	-1.559150	47	1	0	5.348789	-3.866108	-2.891527

A_{Se}+A_{Se}_a

Atom	Atomic		Coordinates (Angstroms)								
	Type		X	Y	Z						
1	6	0	8.496825	3.670272	-0.396129	53	8	0	6.401408	-4.891901	-0.659193
2	6	0	7.866542	2.890440	-1.546607	54	6	0	2.457919	-1.295657	-4.539025
3	6	0	7.978246	3.154926	0.943701	55	8	0	6.588206	-4.605687	2.024316
4	1	0	8.154067	4.705739	-0.493324	56	6	0	3.002793	-0.368584	4.975859
5	6	0	8.399358	1.684138	-2.030618	57	6	0	5.187596	-4.866010	0.054092
6	6	0	6.697827	3.369796	-2.151623	58	6	0	5.290179	-4.698537	1.501711
7	6	0	8.588766	2.087250	1.621449	59	6	0	2.786233	-5.029248	0.255091
8	6	0	6.849426	3.738453	1.542892	60	6	0	2.893095	-4.846228	1.715946
9	6	0	7.817101	0.960665	-3.083518	61	6	0	3.713842	-1.983270	-4.447367
10	6	0	6.088753	2.687276	-3.205512	62	6	0	3.672393	0.892499	-4.785180
11	8	0	6.185281	4.629648	-1.742081	63	6	0	3.772885	4.677088	-1.790477
12	6	0	8.138596	1.611060	2.864651	64	6	0	3.811883	4.890348	1.095106
13	6	0	6.378198	3.304265	2.776197	65	6	0	3.979376	-5.059899	-0.554000
14	8	0	6.239256	4.869994	0.946929	66	6	0	4.194172	-4.710969	2.312495
15	6	0	8.392051	-0.355564	-3.610056	67	6	0	4.182964	1.839554	4.687380
16	6	0	6.648067	1.489870	-3.650554	68	6	0	4.276732	-1.016128	5.148245
17	1	0	5.212152	3.095718	-3.689977	69	1	0	3.725154	-3.063249	-4.372692
18	6	0	4.940853	4.659438	-1.090005	70	1	0	3.659005	1.960233	-4.961529
19	6	0	8.811177	0.463351	3.618587	71	1	0	3.893214	-5.246041	-1.616250
20	6	0	7.021788	2.246835	3.417510	72	1	0	3.756522	4.658763	-2.872504
21	1	0	5.546563	3.812173	3.245976	73	1	0	4.279203	-4.632310	3.388827
22	6	0	4.962473	4.771403	0.366514	74	1	0	3.829263	5.030073	2.169115
23	1	0	8.019508	-0.480859	-4.631886	75	1	0	4.127888	2.910405	4.559078
24	6	0	7.844721	-1.529069	-2.792993	76	1	0	4.312443	-2.077128	5.357941
25	8	0	6.085974	0.828068	-4.773675	77	7	0	1.743621	-4.811407	2.391459
26	6	0	8.225320	-0.879771	3.181146	78	7	0	1.550658	-5.151178	-0.233676
27	1	0	8.557166	0.590378	4.675827	79	7	0	1.823761	-0.986656	4.985536
28	8	0	6.582121	1.855249	4.709895	80	7	0	1.781001	1.622521	4.515039
29	6	0	8.451798	-1.964753	-1.605886	81	7	0	1.343982	4.943033	0.988948
30	6	0	6.703597	-2.223441	-3.216748	82	7	0	1.339129	4.764378	-1.642874
31	6	0	4.839083	0.196476	-4.659523	83	7	0	1.230108	0.724765	-4.776806
32	6	0	2.535119	4.765151	-1.065976	84	7	0	1.276321	-1.897637	-4.498736
33	6	0	8.701223	-1.576711	2.058552	85	1	0	9.336530	-1.438335	-1.258702
34	6	0	7.171396	-1.469473	3.893404	86	1	0	9.301701	1.295405	-1.566414
35	6	0	5.363652	1.169294	4.781724	87	1	0	9.458673	1.616787	1.171361
36	6	0	2.543581	4.868999	0.404307	88	1	0	9.521369	-1.147173	1.489693
37	6	0	7.987016	-3.061481	-0.862372	89	6	0	10.226031	-3.438254	0.294269
38	6	0	6.200460	-3.316905	-2.508899	90	6	0	10.786275	-4.391193	-0.777323
39	8	0	6.114995	-1.868192	-4.457077	91	1	0	10.672796	-3.673642	1.265951
40	6	0	4.858688	-1.250189	-4.486546	92	1	0	10.543018	-2.412352	0.060959
41	6	0	8.165424	-2.802278	1.633303	93	1	0	10.834005	-5.411220	-0.380529
						94	1	0	10.111854	-4.416932	-1.646250
						95	6	0	10.348720	0.490347	3.494575
						96	6	0	10.947077	1.778085	4.088886
						97	1	0	10.667975	0.393071	2.447262

98	1	0	10.748190	-0.387679	4.019279	154	6	0	-5.264083	-4.529480	-1.994038
99	1	0	10.583202	2.655258	3.541274	155	1	0	-7.911360	2.732368	-3.809976
100	1	0	10.623655	1.896345	5.129894	156	6	0	-7.754545	2.783974	-1.696376
101	6	0	10.038956	3.675650	-0.457248	157	8	0	-5.977343	1.611367	-4.472528
102	6	0	10.555507	4.343442	-1.744620	158	6	0	-8.150455	-0.653488	3.207634
103	1	0	10.448018	2.657676	-0.392111	159	1	0	-8.563328	-2.639883	3.826198
104	1	0	10.413613	4.214855	0.423381	160	8	0	-6.684302	-3.864148	3.203008
105	1	0	10.223264	3.779725	-2.624097	161	6	0	-8.353042	2.599836	-0.439499
106	1	0	10.137228	5.352674	-1.837252	162	6	0	-6.610685	3.589538	-1.746355
107	6	0	9.934343	-0.330637	-3.674037	163	6	0	-4.734488	2.121133	-4.078024
108	6	0	10.508321	-1.629440	-4.268701	164	6	0	-2.748912	-4.083133	-3.158695
109	1	0	10.377871	-0.162172	-2.682405	165	6	0	-8.602046	0.510810	2.568925
110	1	0	10.228819	0.527564	-4.292945	166	6	0	-7.057801	-0.527362	4.079548
111	1	0	10.229286	-2.486670	-3.644060	167	6	0	-5.424823	-3.424835	3.626330
112	1	0	10.079461	-1.810381	-5.261504	168	6	0	-2.904058	-4.964126	-1.982186
113	6	0	12.027553	-1.548293	-4.377354	169	6	0	-7.864093	3.197322	0.732849
114	1	0	12.354033	-0.869023	-5.164808	170	6	0	-6.084060	4.199673	-0.608988
115	1	0	12.496860	-1.262638	-3.433690	171	8	0	-6.036635	3.883441	-3.003951
116	6	0	12.154799	-3.968029	-1.294336	172	6	0	-4.775162	3.364228	-3.317182
117	1	0	12.603149	-4.701310	-1.962148	173	6	0	-8.025683	1.771286	2.783285
118	1	0	12.120093	-2.998262	-1.795741	174	6	0	-6.453066	0.707176	4.323886
119	6	0	12.078074	4.420290	-1.735718	175	8	0	-6.634568	-1.670831	4.809424
120	1	0	12.453672	5.083343	-0.956082	176	6	0	-5.400377	-2.267088	4.515955
121	1	0	12.538797	3.436388	-1.634023	177	6	0	-8.545060	3.026779	2.090767
122	6	0	12.469931	1.737065	4.027956	178	6	0	-6.710473	3.990332	0.615453
123	1	0	12.888007	0.959200	4.667220	179	1	0	-5.226639	4.858052	-0.690001
124	1	0	12.837312	1.610357	3.008441	180	6	0	-2.328251	2.237511	-4.122519
125	17	0	13.186732	3.348752	4.637270	181	6	0	-6.942183	1.839770	3.670018
126	17	0	12.701064	5.115241	-3.351501	182	1	0	-5.643682	0.790007	5.040855
127	17	0	12.731983	-3.221921	-4.817691	183	6	0	-3.031445	-3.633859	3.828141
128	17	0	13.360444	-3.762508	0.126528	184	1	0	-8.243121	3.882290	2.703127
129	34	0	0.493071	0.289641	4.656620	185	8	0	-6.245717	4.679150	1.764107
130	34	0	0.025756	4.932349	-0.337114	186	6	0	-2.376479	3.507057	-3.375209
131	34	0	0.347739	-5.035266	1.176579	187	8	0	-6.412266	3.118684	3.978292
132	34	0	-0.059188	-0.616255	-4.659453	188	6	0	-3.013443	-2.494885	4.761612
133	6	0	-8.645558	-2.904520	-2.110929	189	6	0	-5.030470	4.301321	2.352188
134	6	0	-7.932947	-1.699752	-2.727333	190	6	0	-5.128505	3.475293	3.549368
135	6	0	-8.138087	-3.120980	-0.686539	191	6	0	-2.625279	4.355730	2.565042
136	1	0	-8.346405	-3.782164	-2.690727	192	6	0	-2.736368	3.536469	3.784661
137	6	0	-8.411129	-0.389235	-2.572783	193	6	0	-3.647086	4.049607	-2.987721
138	6	0	-6.749759	-1.869229	-3.465648	194	6	0	-3.553475	1.567309	-4.476205
139	6	0	-8.687201	-2.475593	0.432202	195	6	0	-3.905795	-3.464792	-3.751226
140	6	0	-7.064411	-3.994051	-0.456374	196	6	0	-4.209127	-5.170377	-1.425356
141	6	0	-7.767320	0.726492	-3.126797	197	6	0	-3.827891	4.749156	1.878319
142	6	0	-6.069093	-0.786931	-4.030386	198	6	0	-4.024298	3.126962	4.266068
143	8	0	-6.305500	-3.185651	-3.726678	199	6	0	-4.285284	-4.104613	3.300440
144	6	0	-8.209431	-2.684638	1.738346	200	6	0	-4.247289	-1.836793	5.099248
145	6	0	-6.554570	-4.228121	0.814332	201	1	0	-3.691006	4.998345	-2.466913
146	8	0	-6.559315	-4.740466	-1.535563	202	1	0	-3.515127	0.678615	-5.094525
147	6	0	-8.305263	2.148577	-2.972196	203	1	0	-3.761550	5.400932	1.016782
148	6	0	-6.579790	0.497030	-3.842065	204	1	0	-3.800924	-2.877309	-4.654217
149	1	0	-5.186164	-0.948767	-4.638627	205	1	0	-4.093226	2.557311	5.183682
150	6	0	-5.121307	-3.678049	-3.169036	206	1	0	-4.335137	-5.846626	-0.588609
151	6	0	-8.811131	-2.007712	2.968121	207	1	0	-4.299804	-4.985584	2.672558
152	6	0	-7.127747	-3.562226	1.893416	208	1	0	-4.241430	-1.017382	5.806808
153	1	0	-5.752802	-4.943636	0.962860	209	7	0	-1.588528	3.192924	4.368391

210	7	0	-1.378539	4.655945	2.174362
211	7	0	-1.820215	-2.143246	5.239486
212	7	0	-1.845893	-4.167625	3.526063
213	7	0	-1.796394	-5.528136	-1.503452
214	7	0	-1.509551	-3.926398	-3.619793
215	7	0	-1.111354	1.807404	-4.446791
216	7	0	-1.203710	4.069160	-3.091558
217	1	0	-9.241725	1.978288	-0.377474
218	1	0	-9.325187	-0.236978	-2.005981
219	1	0	-9.520342	-1.794263	0.285564
220	1	0	-9.444450	0.436278	1.887443
221	6	0	-10.083863	3.035290	1.980768
222	6	0	-10.615616	4.403908	1.517526
223	1	0	-10.512388	2.783998	2.956717
224	1	0	-10.441779	2.260043	1.288905
225	1	0	-10.623558	5.104967	2.359340
226	1	0	-9.945975	4.827772	0.754274
227	6	0	-10.349898	-1.895409	2.897290
228	6	0	-11.021123	-3.278700	2.820315
229	1	0	-10.671649	-1.291144	2.037878
230	1	0	-10.692886	-1.360025	3.792621
231	1	0	-10.713628	-3.800873	1.906856
232	1	0	-10.699555	-3.899487	3.665021
233	6	0	-10.182524	-2.794408	-2.183129
234	6	0	-10.679179	-2.729517	-3.638716
235	1	0	-10.550600	-1.912720	-1.639354
236	1	0	-10.611032	-3.669479	-1.675855
237	1	0	-10.290708	-1.830789	-4.132051
238	1	0	-10.301254	-3.590360	-4.202816
239	6	0	-9.848585	2.195919	-3.058717
240	6	0	-10.388573	3.634588	-2.968654
241	1	0	-10.319387	1.588324	-2.273630
242	1	0	-10.142994	1.744207	-4.015807
243	1	0	-10.109722	4.083243	-2.007558
244	1	0	-9.935871	4.256931	-3.749779
245	6	0	-11.906100	3.650646	-3.120380
246	1	0	-12.225706	3.439728	-4.140928
247	1	0	-12.399623	2.958330	-2.435267
248	6	0	-12.001565	4.325008	0.891340
249	1	0	-12.426060	5.302947	0.671970
250	1	0	-12.004372	3.718862	-0.017282
251	6	0	-12.202964	-2.716475	-3.685179
252	1	0	-12.635112	-3.651007	-3.326811
253	1	0	-12.624106	-1.879320	-3.126149
254	6	0	-12.539068	-3.137596	2.837779
255	1	0	-12.906571	-2.745259	3.786203
256	1	0	-12.903793	-2.516375	2.018277
257	17	0	-13.348071	-4.805334	2.619035
258	17	0	-12.796238	-2.510983	-5.442500
259	17	0	-12.577130	5.345686	-2.710904
260	17	0	-13.207507	3.492709	2.061004
261	34	0	-0.526516	-3.242426	4.462364
262	34	0	-0.384859	-4.946941	-2.552022
263	34	0	-0.190694	3.904308	3.393392
264	34	0	0.157741	3.032833	-3.828749

$\mathbf{A}_{\text{Se}^+}\mathbf{A}_{\text{Se}^-}\mathbf{b}$

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	6.284858	0.955506
2	6	0	5.038775	1.578876
3	6	0	6.581794	-0.392196
4	1	0	6.041926	0.747525
5	6	0	5.078200	2.383629
6	6	0	3.782303	1.341913
7	6	0	7.397451	-0.513482
8	6	0	6.064060	-1.580203
9	6	0	3.924068	2.942657
10	6	0	2.605339	1.848403
11	8	0	3.738419	0.637087
12	6	0	7.730210	-1.752654
13	6	0	6.366050	-2.830569
14	8	0	5.338554	-1.512653
15	6	0	3.963636	3.812709
16	6	0	2.691408	2.636238
17	1	0	1.651765	1.661567
18	6	0	3.099301	-0.601981
19	6	0	8.618785	-1.872563
20	6	0	7.193555	-2.903525
21	1	0	6.011683	-3.733904
22	6	0	3.965959	-1.772301
23	1	0	3.052049	4.417917
24	6	0	3.904753	2.916015
25	8	0	1.526931	3.261354
26	6	0	7.738699	-1.747754
27	1	0	9.033939	-2.884751
28	8	0	7.608138	-4.167686
29	6	0	5.058736	2.347939
30	6	0	2.676223	2.623717
31	6	0	0.497405	2.543708
32	6	0	1.170370	-2.011657
33	6	0	7.414472	-0.508251
34	6	0	7.197349	-2.897725
35	6	0	6.693146	-5.022433
36	6	0	2.038199	-3.201660
37	6	0	5.027993	1.559323
38	6	0	2.595671	1.838618
39	8	0	1.508722	3.259277
40	6	0	0.487324	2.544422
41	6	0	6.594841	-0.386141
42	6	0	6.374106	-2.823755
43	8	0	7.606150	-4.161696
44	6	0	6.690153	-5.017196
45	6	0	6.286471	0.965600
46	6	0	3.773676	1.332418
47	1	0	1.644598	1.662847
48	6	0	-1.667366	1.465679
				0.732230

49	6	0	6.074034	-1.572068	-3.515089	105	1	0	6.419793	3.752520	3.900118
50	1	0	6.018270	-3.726395	-3.459992	106	1	0	6.931547	2.935007	5.375864
51	6	0	5.064557	-6.800356	0.713245	107	6	0	5.171974	4.772461	-0.041501
52	1	0	6.054324	0.772228	-4.660840	108	6	0	5.200304	5.639658	-1.312953
53	8	0	3.733400	0.641728	-4.793913	109	1	0	6.121137	4.223725	0.030255
54	6	0	-1.676145	1.464266	-0.744179	110	1	0	5.113597	5.407484	0.852601
55	8	0	5.343123	-1.500975	-4.720576	111	1	0	5.344910	5.002128	-2.193010
56	6	0	5.060495	-6.794443	-0.762549	112	1	0	4.239959	6.151818	-1.445909
57	6	0	3.101269	-0.601106	-4.830453	113	6	0	6.325673	6.663738	-1.246926
58	6	0	3.972543	-1.767765	-4.747650	114	1	0	6.125459	7.468532	-0.540013
59	6	0	1.176465	-2.017143	-5.004257	115	1	0	7.292280	6.205938	-1.029747
60	6	0	2.048548	-3.203743	-4.904578	116	6	0	8.167465	4.346812	-4.066157
61	6	0	-0.548693	2.009060	-1.459870	117	1	0	8.028760	5.210342	-4.713868
62	6	0	-0.530374	2.009388	1.433766	118	1	0	8.097598	4.652428	-3.019797
63	6	0	1.751237	-0.695800	4.941311	119	6	0	8.490492	4.056568	4.401563
64	6	0	3.465885	-3.037974	4.764849	120	1	0	9.303160	3.588397	4.956952
65	6	0	1.753445	-0.699625	-4.990697	121	1	0	8.831789	4.345830	3.406655
66	6	0	3.475814	-3.035212	-4.804124	122	6	0	11.934727	-0.164647	1.094293
67	6	0	5.925027	-5.890425	1.425732	123	1	0	12.579368	-0.403775	0.248531
68	6	0	5.917799	-5.879667	-1.472626	124	1	0	11.650149	0.887961	1.064056
69	1	0	-0.565724	2.043914	-2.542401	125	17	0	13.003316	-0.350811	2.611476
70	1	0	-0.534755	2.044518	2.516240	126	17	0	8.128371	5.656149	5.290121
71	1	0	1.145386	0.192271	-5.112735	127	17	0	6.531250	7.492718	-2.908670
72	1	0	1.145755	0.198032	5.062050	128	17	0	9.949438	3.821751	-4.307191
73	1	0	4.112109	-3.910340	-4.794003	129	34	0	3.379570	-8.634900	-0.027315
74	1	0	4.100159	-3.914654	4.758784	130	34	0	-0.405426	-4.090395	5.004742
75	1	0	5.971662	-5.937355	2.506043	131	34	0	-0.392188	-4.101011	-5.038503
76	1	0	5.959358	-5.919684	-2.553392	132	34	0	-3.992256	0.531769	0.008153
77	7	0	1.432767	-4.386965	-4.910950	133	6	0	-6.285430	-0.954807	3.575339
78	7	0	-0.134159	-2.261535	-5.078618	134	6	0	-5.039344	-1.578341	2.950343
79	7	0	4.252881	-7.674954	-1.354135	135	6	0	-6.582174	0.392853	2.919591
80	7	0	4.260072	-7.685398	1.302292	136	1	0	-6.042557	-0.746723	4.621927
81	7	0	1.418470	-4.382741	4.877307	137	6	0	-5.078696	-2.383553	1.799635
82	7	0	-0.141021	-2.251755	5.035944	138	6	0	-3.782885	-1.340942	3.523475
83	7	0	-2.776337	1.017109	1.328971	139	6	0	-7.397558	0.513962	1.782963
84	7	0	-2.791066	1.012654	-1.327289	140	6	0	-6.064574	1.580957	3.466638
85	1	0	6.017625	2.549219	-1.346509	141	6	0	-3.924484	-2.942533	1.227737
86	1	0	6.042555	2.586304	1.341028	142	6	0	-2.605848	-1.847348	2.974316
87	1	0	7.810799	0.388371	1.339791	143	8	0	-3.739128	-0.635868	4.746172
88	1	0	7.831303	0.394614	-1.398112	144	6	0	-7.730199	1.753034	1.212009
89	6	0	7.481318	1.938574	-3.551496	145	6	0	-6.366419	2.831227	2.928133
90	6	0	7.223891	3.199275	-4.393973	146	8	0	-5.339348	1.513700	4.675405
91	1	0	8.377483	1.428036	-3.920590	147	6	0	-3.963813	-3.812985	-0.023172
92	1	0	7.706457	2.239623	-2.518532	148	6	0	-2.691841	-2.635610	1.829232
93	1	0	7.291504	2.952403	-5.459597	149	1	0	-1.652291	-1.660121	3.457331
94	1	0	6.202302	3.566945	-4.214680	150	6	0	-3.100026	0.603187	4.780358
95	6	0	9.795647	-0.877282	-0.024220	151	6	0	-8.618522	1.872711	-0.022542
96	6	0	10.726714	-1.087944	1.183388	152	6	0	-7.193674	2.904008	1.807697
97	1	0	9.443945	0.163535	-0.028370	153	1	0	-6.012106	3.734641	3.410089
98	1	0	10.354495	-1.017216	-0.959001	154	6	0	-3.966774	1.773449	4.703415
99	1	0	10.186726	-0.892555	2.117060	155	1	0	-3.052236	-4.418212	-0.024916
100	1	0	11.063375	-2.130694	1.220072	156	6	0	-3.904631	-2.916609	-1.255192
101	6	0	7.505088	1.898590	3.554455	157	8	0	-1.527327	-3.260750	1.326515
102	6	0	7.241159	3.186801	4.354723	158	6	0	-7.738240	1.747620	-1.261202
103	1	0	7.789494	2.166329	2.527132	159	1	0	-9.033653	2.884909	-0.021868
104	1	0	8.360770	1.359296	3.982964	160	8	0	-7.608135	4.168100	1.330170

C₉H₂₀@A_{Se}+A_{Se_a}

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z

1	6	0	8.364964	3.223322	-1.771107	57	6	0	4.913312	-4.424193	1.894284
2	6	0	7.777011	2.016796	-2.499395	58	6	0	4.884718	-3.570664	3.078017
3	6	0	7.772334	3.331393	-0.368536	59	6	0	2.501999	-4.526060	1.892569
4	1	0	8.039276	4.111929	-2.320682	60	6	0	2.476264	-3.644604	3.071775
5	6	0	8.324397	0.726375	-2.401875	61	6	0	3.757254	-3.737496	-3.235908
6	6	0	6.644407	2.176353	-3.310926	62	6	0	3.698490	-1.171082	-4.574824
7	6	0	8.304456	2.642653	0.732669	63	6	0	3.705837	3.458117	-3.582393
8	6	0	6.656349	4.151889	-0.134071	64	6	0	3.718207	5.023928	-1.147538
9	6	0	7.788002	-0.380454	-3.079022	65	6	0	3.771117	-4.909446	1.327111
10	6	0	6.084499	1.107431	-4.009756	66	6	0	3.710110	-3.195874	3.660703
11	8	0	6.118222	3.476186	-3.494177	67	6	0	3.741577	3.939381	3.523791
12	6	0	7.783511	2.758541	2.032337	68	6	0	3.717375	1.389638	4.894295
13	6	0	6.112557	4.302258	1.139669	69	1	0	3.781859	-4.720040	-2.781330
14	8	0	6.129790	4.916992	-1.202801	70	1	0	3.667686	-0.243908	-5.132667
15	6	0	8.383909	-1.783660	-2.992515	71	1	0	3.799176	-5.590324	0.485396
16	6	0	6.647401	-0.158749	-3.867830	72	1	0	3.699324	2.930016	-4.527485
17	1	0	5.255258	1.268740	-4.686488	73	1	0	3.679256	-2.616462	4.574569
18	6	0	4.867619	3.791738	-2.951355	74	1	0	3.725691	5.657369	-0.269435
19	6	0	8.388797	2.013278	3.220868	75	1	0	3.754399	4.918514	3.061557
20	6	0	6.671926	3.597333	2.205601	76	1	0	3.704719	0.470488	5.466046
21	1	0	5.294558	4.991879	1.308877	77	7	0	1.267054	-3.338075	3.528543
22	6	0	4.873498	4.577920	-1.720080	78	7	0	1.309810	-4.904563	1.437095
23	1	0	8.075137	-2.317228	-3.896932	79	7	0	1.268549	1.527950	4.821307
24	6	0	7.784683	-2.539215	-1.809917	80	7	0	1.283105	3.842796	3.598117
25	8	0	6.115045	-1.244162	-4.600804	81	7	0	1.261783	4.989655	-1.280417
26	6	0	7.806767	0.603999	3.300079	82	7	0	1.256221	3.564569	-3.474548
27	1	0	8.063917	2.541843	4.122401	83	7	0	1.254922	-1.321212	-4.454064
28	8	0	6.152695	3.803541	3.507796	84	7	0	1.297077	-3.651942	-3.270325
29	6	0	8.300056	-2.415731	-0.510877	85	1	0	9.141130	-1.745821	-0.351682
30	6	0	6.694667	-3.403728	-1.986956	86	1	0	9.206420	0.585560	-1.783141
31	6	0	4.873286	-1.775556	-4.237420	87	1	0	9.166225	1.998603	0.577752
32	6	0	2.457351	3.866199	-2.992194	88	1	0	9.265202	-0.352270	2.041155
33	6	0	8.364375	-0.498860	2.630042	89	6	0	9.947002	-2.961771	1.936397
34	6	0	6.656789	0.375847	4.071793	90	6	0	10.530522	-4.277689	1.395855
35	6	0	4.893581	3.266535	3.809141	91	1	0	10.328840	-2.780012	2.947017
36	6	0	2.461534	4.667581	-1.756395	92	1	0	10.311852	-2.129358	1.318068
37	6	0	7.792856	-3.126531	0.588660	93	1	0	10.405551	-5.071925	2.140743
38	6	0	6.157022	-4.127996	-0.924958	94	1	0	9.978435	-4.591977	0.497398
39	8	0	6.166974	-3.604426	-3.286369	95	6	0	9.931205	2.015157	3.204741
40	6	0	4.901061	-3.064666	-3.552425	96	6	0	10.502371	3.444088	3.244843
41	6	0	7.810668	-1.788167	2.701792	97	1	0	10.325268	1.496179	2.320154
42	6	0	6.086288	-0.890308	4.186405	98	1	0	10.279144	1.446435	4.077301
43	8	0	6.132041	1.447068	4.831156	99	1	0	10.214080	3.992852	2.340888
44	6	0	4.882291	1.983201	4.506372	100	1	0	10.084970	3.990859	4.098689
45	6	0	8.405622	-2.996417	1.982079	101	6	0	9.907886	3.222850	-1.752480
46	6	0	6.701580	-3.977320	0.349345	102	6	0	10.498565	3.251436	-3.173753
47	1	0	5.351404	-4.832188	-1.094090	103	1	0	10.303145	2.348953	-1.215995
48	6	0	2.463287	-1.818359	-4.217655	104	1	0	10.238953	4.106625	-1.190599
49	6	0	6.655083	-1.949416	3.482068	105	1	0	10.219971	2.342209	-3.718677
50	1	0	5.247876	-1.057320	4.850044	106	1	0	10.086236	4.099391	-3.733232
51	6	0	2.481216	3.334116	3.874662	107	6	0	9.927547	-1.763191	-2.956492
52	1	0	8.102124	-3.884463	2.546407	108	6	0	10.522744	-3.180908	-2.883819
53	8	0	6.181100	-4.767919	1.403379	109	1	0	10.299741	-1.182327	-2.101263
54	6	0	2.488621	-3.128439	-3.545886	110	1	0	10.280759	-1.247144	-3.859363
55	8	0	6.126622	-3.250829	3.631102	111	1	0	10.236161	-3.656079	-1.938276
56	6	0	2.471612	2.032416	4.565006	112	1	0	10.118201	-3.805874	-3.688723

113	6	0	12.042188	-3.136306	-2.980407	169	6	0	-7.760668	3.210668	-0.405945
114	1	0	12.395479	-2.889395	-3.981213	170	6	0	-6.100164	3.679856	-2.134871
115	1	0	12.485495	-2.458897	-2.248384	171	8	0	-6.116681	2.460678	-4.225722
116	6	0	11.994411	-4.167488	0.995961	172	6	0	-4.857008	1.853886	-4.319258
117	1	0	12.420198	-5.116711	0.676432	173	6	0	-7.787025	2.638692	2.017976
118	1	0	12.157370	-3.410319	0.226017	174	6	0	-6.088677	2.266801	3.733243
119	6	0	12.016668	3.365014	-3.122178	175	8	0	-6.082325	0.219528	5.026594
120	1	0	12.349399	4.318483	-2.712044	176	6	0	-4.828951	-0.366847	4.820865
121	1	0	12.475187	2.539659	-2.575729	177	6	0	-8.384360	3.544260	0.947065
122	6	0	12.021294	3.411018	3.353558	178	6	0	-6.654434	3.932351	-0.881598
123	1	0	12.361887	2.996020	4.302136	179	1	0	-5.291094	4.294242	-2.510317
124	1	0	12.484438	2.878258	2.521986	180	6	0	-2.430937	0.441037	-4.581476
125	17	0	12.710191	5.142777	3.284277	181	6	0	-6.658885	3.059197	2.739684
126	17	0	12.727234	3.280233	-4.844192	182	1	0	-5.266173	2.641257	4.329282
127	17	0	12.754469	-4.819469	-2.595451	183	6	0	-2.415810	-1.782250	4.448119
128	17	0	13.034433	-3.618563	2.454132	184	1	0	-8.086406	4.569051	1.191553
129	34	0	-0.051290	2.693689	4.211918	185	8	0	-6.150838	5.006938	-0.110558
130	34	0	-0.067262	4.309385	-2.397284	186	6	0	-2.445931	1.891795	-4.328553
131	34	0	-0.035785	-4.181191	2.505245	187	8	0	-6.153345	4.362294	2.517138
132	34	0	-0.052248	-2.510840	-3.867549	188	6	0	-2.419739	-0.342143	4.758708
133	6	0	-8.375652	-3.562617	-0.724549	189	6	0	-4.897888	4.872049	0.500179
134	6	0	-7.780487	-2.645729	-1.790693	190	6	0	-4.898725	4.524544	1.919420
135	6	0	-7.772732	-3.221516	0.635087	191	6	0	-2.489388	5.027577	0.530947
136	1	0	-8.054716	-4.580376	-0.967467	192	6	0	-2.489553	4.685902	1.963961
137	6	0	-8.316355	-1.381366	-2.088941	193	6	0	-3.706805	2.578625	-4.215849
138	6	0	-6.646749	-3.050460	-2.510154	194	6	0	-3.673457	-0.270643	-4.730448
139	6	0	-8.301385	-2.226623	1.473788	195	6	0	-3.727547	-4.436289	-2.437816
140	6	0	-6.637226	-3.911695	1.090920	196	6	0	-3.717840	-5.123839	0.374588
141	6	0	-7.768650	-0.533562	-3.064224	197	6	0	-3.741314	5.133197	-0.174391
142	6	0	-6.072020	-2.242479	-3.490662	198	6	0	-3.741583	4.453325	2.639258
143	8	0	-6.137930	-4.354372	-2.307376	199	6	0	-3.665411	-2.491800	4.350793
144	6	0	-7.750095	-1.913089	2.727836	200	6	0	-3.671281	0.337725	4.968127
145	6	0	-6.067040	-3.642543	2.332713	201	1	0	-3.719653	3.652062	-4.074924
146	8	0	-6.129309	-4.980995	0.316340	202	1	0	-3.653960	-1.322070	-4.986958
147	6	0	-8.348592	0.836890	-3.403933	203	1	0	-3.744986	5.447494	-1.210553
148	6	0	-6.626910	-0.990295	-3.742660	204	1	0	-3.733554	-4.244655	-3.503457
149	1	0	-5.240347	-2.605507	-4.080855	205	1	0	-3.743702	4.261378	3.704856
150	6	0	-4.881350	-4.513801	-1.713050	206	1	0	-3.716619	-5.439769	1.410279
151	6	0	-8.336628	-0.839833	3.643492	207	1	0	-3.659715	-3.559909	4.174458
152	6	0	-6.619602	-2.640768	3.129821	208	1	0	-3.667325	1.380926	5.256791
153	1	0	-5.235315	-4.234671	2.693424	209	7	0	-1.288987	4.603204	2.531559
154	6	0	-4.876578	-4.855258	-0.294403	210	7	0	-1.289216	5.204903	-0.014974
155	1	0	-8.033537	1.071837	-4.425502	211	7	0	-1.225664	0.236953	4.776939
156	6	0	-7.740864	1.906833	-2.500182	212	7	0	-1.218359	-2.320659	4.248039
157	8	0	-6.088974	-0.185427	-4.772083	213	7	0	-1.268021	-5.233515	0.194772
158	6	0	-7.758169	0.531484	3.299629	214	7	0	-1.275967	-4.590221	-2.342835
159	1	0	-8.000759	-1.076937	4.657917	215	7	0	-1.226158	-0.113126	-4.652026
160	8	0	-6.077631	-2.412770	4.418060	216	7	0	-1.252341	2.462125	-4.202444
161	6	0	-8.265839	2.194431	-1.230795	217	1	0	-9.118491	1.617349	-0.882379
162	6	0	-6.642741	2.667972	-2.926624	218	1	0	-9.196143	-1.052364	-1.542673
163	6	0	-4.841381	0.418795	-4.587337	219	1	0	-9.179748	-1.678409	1.142747
164	6	0	-2.475312	-4.671453	-1.767660	220	1	0	-9.191507	1.032462	1.777574
165	6	0	-8.313311	1.371608	2.319799	221	6	0	-9.925270	3.491012	0.911557
166	6	0	-6.631012	1.007970	3.987129	222	6	0	-10.509066	4.564965	-0.020975
167	6	0	-4.825841	-1.792101	4.503025	223	1	0	-10.308977	3.641212	1.926601
168	6	0	-2.470993	-5.027998	-0.339473	224	1	0	-10.287333	2.503783	0.591102

225	1	0	-10.366683	5.556849	0.423297		281	1	0	-0.236591	-0.379334	-1.482117
226	1	0	-9.969171	4.563589	-0.979883		282	1	0	-1.612213	-2.255025	-0.579389
227	6	0	-9.879555	-0.836030	3.649183		283	1	0	-1.512712	-1.575365	1.048812
228	6	0	-10.453277	-2.177616	4.139714		284	6	0	-2.785504	-0.447519	-0.298373
229	1	0	-10.284931	-0.612705	2.652667		285	6	0	-4.105227	-1.127833	0.103195
230	1	0	-10.212996	-0.022783	4.307346		286	1	0	-2.821337	-0.191847	-1.369903
231	1	0	-10.174781	-2.984521	3.452241		287	1	0	-2.693087	0.504501	0.246854
232	1	0	-10.028856	-2.429502	5.118772		288	6	0	-5.324780	-0.210432	-0.093362
233	6	0	-9.917619	-3.547752	-0.704998		289	1	0	-4.237485	-2.044353	-0.493468
234	6	0	-10.509285	-4.027705	-2.042631		290	1	0	-4.046073	-1.447204	1.155644
235	1	0	-10.308044	-2.546170	-0.476821		291	1	0	-6.259848	-0.714711	0.183645
236	1	0	-10.252095	-4.203708	0.110023		292	1	0	-5.238847	0.697233	0.520585
237	1	0	-10.224329	-3.344113	-2.850623		293	1	0	-5.412211	0.103133	-1.144277

$$A_{Te} + A_{Te} \rightarrow a$$

Atom	Atomic Type	Coordinates (Angstroms)			
		X	Y	Z	
1	6	0	8.273999	3.398154	-1.393747
2	6	0	7.690065	2.296744	-2.277348
3	6	0	7.684715	3.316900	0.012146
4	1	0	7.943275	4.350499	-1.819708
5	6	0	8.238858	1.005684	-2.343366
6	6	0	6.561992	2.555422	-3.070815
7	6	0	8.222630	2.495479	1.017059
8	6	0	6.561025	4.089826	0.346634
9	6	0	7.716350	-0.004702	-3.167277
10	6	0	6.023581	1.589281	-3.919625
11	8	0	6.013037	3.858858	-3.071187
12	6	0	7.686482	2.425128	2.313815
13	6	0	6.000576	4.054826	1.621723
14	8	0	6.036462	4.991257	-0.611074
15	6	0	8.309549	-1.409568	-3.229480
16	6	0	6.594548	0.318507	-3.948096
17	1	0	5.200578	1.835009	-4.578929
18	6	0	4.765211	4.076224	-2.475508
19	6	0	8.291309	1.552988	3.414119
20	6	0	6.553955	3.209548	2.582110
21	1	0	5.175195	4.708238	1.875306
22	6	0	4.777695	4.712898	-1.160984
23	1	0	8.001875	-1.843285	-4.186093
24	6	0	7.704590	-2.286603	-2.134922
25	8	0	6.082959	-0.648105	-4.846989
26	6	0	7.719978	0.138943	3.343607
27	1	0	7.962667	1.979179	4.367120
28	8	0	6.015126	3.207042	3.890129
29	6	0	8.231643	-2.339194	-0.835522
30	6	0	6.597085	-3.102454	-2.411624
31	6	0	4.825120	-1.206020	-4.578957
32	6	0	2.341835	4.106053	-2.481069
33	6	0	8.269291	-0.863397	2.525331
34	6	0	6.599633	-0.204381	4.116412

35	6	0	4.773879	2.600985	4.115557	91	1	0	10.252963	-3.164745	2.554578
36	6	0	2.350271	4.777679	-1.154969	92	1	0	10.240294	-2.294414	1.031734
37	6	0	7.720811	-3.182021	0.164705	93	1	0	10.325185	-5.324690	1.434920
38	6	0	6.063176	-3.962040	-1.453151	94	1	0	9.926690	-4.613540	-0.129880
39	8	0	6.066871	-3.113836	-3.723274	95	6	0	9.834230	1.561729	3.402552
40	6	0	4.817216	-2.525025	-3.951859	96	6	0	10.402316	2.976849	3.612957
41	6	0	7.736334	-2.160629	2.448892	97	1	0	10.231143	1.150486	2.464161
42	6	0	6.047894	-1.484125	4.082004	98	1	0	10.181672	0.895200	4.203004
43	8	0	6.068081	0.748360	5.019529	99	1	0	10.105673	3.632039	2.785965
44	6	0	4.802489	1.284978	4.748598	100	1	0	9.990902	3.412776	4.531049
45	6	0	8.333945	-3.250578	1.562482	101	6	0	9.817055	3.400937	-1.379522
46	6	0	6.621397	-3.985702	-0.175570	102	6	0	10.404039	3.623459	-2.785055
47	1	0	5.256448	-4.637527	-1.709514	103	1	0	10.216319	2.463766	-0.967080
48	6	0	2.397528	-1.216526	-4.658511	104	1	0	10.146941	4.201856	-0.704132
49	6	0	6.604503	-2.437547	3.232340	105	1	0	10.125681	2.796058	-3.447667
50	1	0	5.225960	-1.743402	4.737426	106	1	0	9.988939	4.538825	-3.223086
51	6	0	2.350649	2.585373	4.161192	107	6	0	9.853155	-1.395631	-3.189335
52	1	0	8.032982	-4.211135	1.993431	108	6	0	10.447555	-2.812579	-3.281778
53	8	0	6.114607	-4.905028	0.774736	109	1	0	10.224885	-0.917683	-2.272385
54	6	0	2.394285	-2.547964	-3.997441	110	1	0	10.207688	-0.778847	-4.025972
55	8	0	6.078073	-3.750423	3.222427	111	1	0	10.153157	-3.397786	-2.402792
56	6	0	2.375454	1.256731	4.827812	112	1	0	10.050019	-3.335741	-4.159411
57	6	0	4.852492	-4.641605	1.326566	113	6	0	11.967741	-2.758041	-3.359235
58	6	0	4.832406	-3.991854	2.634580	114	1	0	12.329888	-2.391740	-4.319561
59	6	0	2.426227	-4.740486	1.321662	115	1	0	12.404452	-2.174997	-2.546468
60	6	0	2.409405	-4.061958	2.644419	116	6	0	11.935694	-4.274704	0.457451
61	6	0	3.653011	-3.180958	-3.680352	117	1	0	12.364431	-5.171133	0.013593
62	6	0	3.668185	-0.584745	-4.943140	118	1	0	12.114427	-3.416627	-0.193921
63	6	0	3.598022	3.792307	-3.121181	119	6	0	11.922003	3.732321	-2.721227
64	6	0	3.623250	5.074770	-0.534341	120	1	0	12.253243	4.620138	-2.182622
65	6	0	3.703249	-5.024129	0.702829	121	1	0	12.383545	2.839958	-2.296045
66	6	0	3.661319	-3.722360	3.279815	122	6	0	11.922128	2.935196	3.705236
67	6	0	3.599236	3.237400	3.841338	123	1	0	12.270735	2.402560	4.589991
68	6	0	3.655850	0.646759	5.115280	124	1	0	12.380136	2.515292	2.808680
69	1	0	3.656573	-4.186218	-3.275384	125	17	0	12.606633	4.663687	3.854350
70	1	0	3.676015	0.360204	-5.473982	126	17	0	12.629422	3.890583	-4.439388
71	1	0	3.722642	-5.567356	-0.234952	127	17	0	12.677308	-4.476200	-3.175467
72	1	0	3.596509	3.382541	-4.124470	128	17	0	12.951051	-3.943979	1.996769
73	1	0	3.654145	-3.304017	4.279460	129	6	0	-8.273907	-3.396983	-1.395924
74	1	0	3.634871	5.611829	0.407048	130	6	0	-7.689924	-2.294991	-2.278755
75	1	0	3.586621	4.241680	3.434189	131	6	0	-7.684690	-3.316748	0.010050
76	1	0	3.679206	-0.295618	5.650221	132	1	0	-7.943202	-4.349042	-1.822540
77	7	0	1.213451	-3.785755	3.133686	133	6	0	-8.238610	-1.003826	-2.343749
78	7	0	1.251596	-4.998774	0.774002	134	6	0	-6.561990	-2.553162	-3.072564
79	7	0	1.204219	0.695889	5.072311	135	6	0	-8.222689	-2.496140	1.015578
80	7	0	1.152072	3.063578	3.876938	136	6	0	-6.560956	-4.089861	0.343966
81	7	0	1.172619	5.017377	-0.605250	137	6	0	-7.716160	0.007113	-3.167006
82	7	0	1.149694	3.812388	-2.969656	138	6	0	-6.023570	-1.586415	-3.920691
83	7	0	1.216957	-0.674197	-4.901080	139	8	0	-6.013083	-3.856649	-3.074060
84	7	0	1.204261	-3.047624	-3.714469	140	6	0	-7.686579	-2.426778	2.312408
85	1	0	9.087865	-1.712539	-0.599723	141	6	0	-6.000585	-4.055888	1.619114
86	1	0	9.110334	0.784005	-1.733498	142	8	0	-6.036304	-4.990440	-0.614485
87	1	0	9.099013	1.895475	0.786207	143	6	0	-8.309435	1.411987	-3.228180
88	1	0	9.147471	-0.628063	1.930861	144	6	0	-6.594430	-0.315574	-3.948166
89	6	0	9.875480	-3.205492	1.527015	145	1	0	-5.200638	-1.831737	-4.580240
90	6	0	10.464687	-4.433087	0.812936	146	6	0	-4.765244	-4.074378	-2.478495

147	6	0	-8.291375	-1.555426	3.413354	203	1	0	-3.586863	-4.244407	3.431528
148	6	0	-6.554065	-3.211400	2.580142	204	1	0	-3.679039	0.291513	5.650395
149	1	0	-5.175209	-4.709485	1.872235	205	7	0	-1.213643	3.783051	3.136900
150	6	0	-4.777596	-4.711645	-1.164271	206	7	0	-1.251518	4.998321	0.778296
151	1	0	-8.001744	1.846435	-4.184453	207	7	0	-1.204089	-0.699799	5.071545
152	6	0	-7.704592	2.288245	-2.132948	208	7	0	-1.152329	-3.066771	3.874667
153	8	0	-6.082809	0.651654	-4.846406	209	7	0	-1.172409	-5.016191	-0.609050
154	6	0	-7.720018	-0.141347	3.343833	210	7	0	-1.149808	-3.810040	-2.972851
155	1	0	-7.962705	-1.982290	4.366046	211	7	0	-1.216753	0.678172	-4.900299
156	8	0	-6.015307	-3.209872	3.888187	212	7	0	-1.204332	3.050558	-3.711635
157	6	0	-8.231676	2.339892	-0.833530	213	1	0	-9.087918	1.713078	-0.598224
158	6	0	-6.597071	3.104279	-2.409035	214	1	0	-9.109982	-0.782516	-1.733596
159	6	0	-4.825006	1.209460	-4.577862	215	1	0	-9.099091	-1.895995	0.785160
160	6	0	-2.341864	-4.104064	-2.484271	216	1	0	-9.147523	0.626667	1.931644
161	6	0	-8.269343	0.861587	2.526279	217	6	0	-9.875515	3.204306	1.529532
162	6	0	-6.599662	0.201425	4.116862	218	6	0	-10.464775	4.432290	0.816132
163	6	0	-4.774009	-2.604054	4.113977	219	1	0	-10.253098	3.162865	2.557027
164	6	0	-2.350168	-4.776339	-1.158479	220	1	0	-10.240205	2.293498	1.033670
165	6	0	-7.720820	3.181953	0.167335	221	1	0	-10.326479	5.323338	1.439175
166	6	0	-6.063165	3.963158	-1.449937	222	1	0	-9.925951	4.614073	-0.125957
167	8	0	-6.066886	3.116532	-3.720693	223	6	0	-9.834296	-1.564149	3.401824
168	6	0	-4.817200	2.527957	-3.949688	224	6	0	-10.402379	-2.979392	3.611425
169	6	0	-7.736398	2.158875	2.450780	225	1	0	-10.231243	-1.152343	2.463695
170	6	0	-6.047960	1.481215	4.083398	226	1	0	-10.181710	-0.898099	4.202686
171	8	0	-6.068019	-0.751943	5.019283	227	1	0	-10.105801	-3.634096	2.784025
172	6	0	-4.802473	-1.288442	4.747857	228	1	0	-9.990904	-3.415869	4.529229
173	6	0	-8.333995	3.249463	1.565147	229	6	0	-9.816966	-3.399728	-1.381787
174	6	0	-6.621394	3.985880	-0.172331	230	6	0	-10.403863	-3.621124	-2.787534
175	1	0	-5.256444	4.638854	-1.705766	231	1	0	-10.216228	-2.462863	-0.968647
176	6	0	-2.397380	1.220149	-4.657309	232	1	0	-10.146921	-4.201162	-0.707042
177	6	0	-6.604581	2.435248	3.234442	233	1	0	-10.125467	-2.793181	-3.449455
178	1	0	-5.226002	1.739990	4.738985	234	1	0	-9.988728	-4.536130	-3.226285
179	6	0	-2.350789	-2.588609	4.159409	235	6	0	-9.853048	1.397919	-3.188158
180	1	0	-8.033081	4.209725	1.996793	236	6	0	-10.447531	2.814896	-3.279650
181	8	0	-6.114596	4.904539	0.778616	237	1	0	-10.224842	0.919255	-2.271608
182	6	0	-2.394274	2.551063	-3.995123	238	1	0	-10.207455	0.781733	-4.025291
183	8	0	-6.078191	3.748135	3.225460	239	1	0	-10.153813	3.399332	-2.399915
184	6	0	-2.375413	-1.260375	4.826867	240	1	0	-10.049435	3.338920	-4.156519
185	6	0	-4.852489	4.640713	1.330316	241	6	0	-11.967655	2.760264	-3.358268
186	6	0	-4.832494	3.989965	2.637839	242	1	0	-12.329021	2.394535	-4.319109
187	6	0	-2.426184	4.739559	1.325627	243	1	0	-12.404930	2.176640	-2.546219
188	6	0	-2.409503	4.059884	2.647811	244	6	0	-11.935319	4.273283	0.459022
189	6	0	-3.653047	3.183714	-3.677574	245	1	0	-12.364307	5.169891	0.015769
190	6	0	-3.668016	0.588544	-4.942497	246	1	0	-12.112763	3.415796	-0.193490
191	6	0	-3.598123	-3.790134	-3.124133	247	6	0	-11.921830	-3.730044	-2.723895
192	6	0	-3.623070	-5.073740	-0.537866	248	1	0	-12.253102	-4.618322	-2.186072
193	6	0	-3.703201	5.023726	0.706960	249	1	0	-12.383399	-2.838046	-2.297974
194	6	0	-3.661457	3.719903	3.282912	250	6	0	-11.922186	-2.937785	3.703839
195	6	0	-3.599443	-3.240370	3.839277	251	1	0	-12.270725	-2.405721	4.588964
196	6	0	-3.655761	-0.650515	5.114837	252	1	0	-12.380253	-2.517295	2.807588
197	1	0	-3.656670	4.188635	-3.271769	253	17	0	-12.606687	-4.666369	3.851899
198	1	0	-3.675811	-0.355987	-5.474086	254	17	0	-12.629137	-3.886838	-4.442236
199	1	0	-3.722538	5.567686	-0.230399	255	17	0	-12.677524	4.478225	-3.173980
200	1	0	-3.596725	-3.379902	-4.127234	256	17	0	-12.951909	3.940024	1.996976
201	1	0	-3.654331	3.300830	4.282249	257	52	0	0.343456	1.887247	-4.351509
202	1	0	-3.634638	-5.611282	0.403248	258	52	0	0.392474	-4.449030	-1.801711

259	52	0	0.321205	4.449884	1.971950	42	6	0	6.503159	-2.499768	-2.935257
260	52	0	0.376549	-1.880011	4.519087	43	8	0	7.847295	-3.759363	-1.358299
261	52	0	-0.376589	1.876174	4.520824	44	6	0	6.996036	-4.680157	-0.737957
262	52	0	-0.321188	-4.451695	1.967903	45	6	0	6.229118	1.273161	-3.605050
263	52	0	-0.392460	4.450795	-1.797973	46	6	0	3.699999	1.515630	-3.539857
264	52	0	-0.343343	-1.883480	-4.353368	47	1	0	1.557146	1.735326	-3.463092

A_{Te}+A_{Te}_b

Atom	Atomic		Coordinates (Angstroms)								
	Type		X	Y	Z						
1	6	0	6.237153	1.271476	3.572346	53	8	0	3.681824	0.814265	-4.763072
2	6	0	4.970588	1.836707	2.932570	54	6	0	-1.792671	1.555940	-0.787814
3	6	0	6.609602	-0.056930	2.914570	55	8	0	5.391265	-1.242743	-4.675787
4	1	0	5.986994	1.044495	4.613399	56	6	0	5.498931	-6.582970	-0.743052
5	6	0	4.983452	2.667227	1.798021	57	6	0	3.106701	-0.459606	-4.793159
6	6	0	3.719759	1.510701	3.476036	58	6	0	4.033656	-1.580696	-4.701913
7	6	0	7.445576	-0.130669	1.787049	59	6	0	1.243421	-1.969835	-4.970307
8	6	0	6.145247	-1.273685	3.449957	60	6	0	2.180905	-3.121716	-4.861954
9	6	0	3.808733	3.170327	1.216471	61	6	0	-0.677252	2.152002	-1.489824
10	6	0	2.523858	1.955786	2.911551	62	6	0	-0.625043	2.069799	1.395810
11	8	0	3.699871	0.799547	4.692345	63	6	0	1.782151	-0.638203	4.881308
12	6	0	7.850851	-1.348020	1.215567	64	6	0	3.622374	-2.880319	4.747924
13	6	0	6.520437	-2.503347	2.908315	65	6	0	1.768140	-0.625381	-4.956811
14	8	0	5.411242	-1.254020	4.651884	66	6	0	3.599993	-2.868839	-4.755080
15	6	0	3.810248	4.049593	-0.030387	67	6	0	6.316957	-5.608449	1.444296
16	6	0	2.584648	2.783349	1.791707	68	6	0	6.284612	-5.595989	-1.449914
17	1	0	1.574346	1.692440	3.367640	69	1	0	-0.707499	2.213784	-2.570778
18	6	0	3.122134	-0.472009	4.730913	70	1	0	-0.621079	2.070606	2.479001
19	6	0	8.744033	-1.417125	-0.020397	71	1	0	1.116202	0.235709	-5.081687
20	6	0	7.371762	-2.528587	1.804100	72	1	0	1.126182	0.222500	4.985168
21	1	0	6.200908	-3.426011	3.378104	73	1	0	4.277386	-3.712934	-4.738083
22	6	0	4.052354	-1.592315	4.673335	74	1	0	4.303222	-3.721862	4.755396
23	1	0	2.874903	4.617507	-0.026469	75	1	0	6.373899	-5.652569	2.524577
24	6	0	3.778465	3.149879	-1.262428	76	1	0	6.318388	-5.632886	-2.531402
25	8	0	1.405353	3.375729	1.295235	77	7	0	1.664174	-4.348297	-4.867867
26	6	0	7.850339	-1.344025	-1.254508	78	7	0	-0.059586	-2.239161	-5.052136
27	1	0	9.214594	-2.404860	-0.020437	79	7	0	4.771119	-7.505327	-1.365383
28	8	0	7.868214	-3.764264	1.337009	80	7	0	4.803289	-7.518196	1.377413
29	6	0	4.951423	2.620549	-1.823122	81	7	0	1.688811	-4.362570	4.870435
30	6	0	2.558690	2.801244	-1.864758	82	7	0	-0.041950	-2.255196	4.988169
31	6	0	0.382980	2.643227	0.679815	83	7	0	-2.828541	1.012286	1.330713
32	6	0	1.261069	-1.983697	4.915228	84	7	0	-2.880079	1.092283	-1.406629
33	6	0	7.457203	-0.126592	-1.834028	85	1	0	5.903768	2.866479	-1.359230
34	6	0	7.356616	-2.524411	-1.833078	86	1	0	5.942420	2.934274	1.361300
35	6	0	7.011272	-4.686139	0.724220	87	1	0	7.813784	0.794374	1.350574
36	6	0	2.202708	-3.135142	4.843546	88	1	0	7.839153	0.799304	-1.413360
37	6	0	4.948106	1.813617	-2.972139	89	6	0	7.375468	2.303643	-3.570750
38	6	0	2.504548	1.978021	-2.990472	90	6	0	7.049012	3.540936	-4.423887
39	8	0	1.373887	3.417519	-1.404026	91	1	0	8.292204	1.833392	-3.942910
40	6	0	0.358143	2.680658	-0.779344	92	1	0	7.595024	2.627203	-2.543348
41	6	0	6.609711	-0.054387	-2.953070	93	1	0	7.124676	3.287744	-5.487478
						94	1	0	6.010247	3.855575	-4.242229
						95	6	0	9.861776	-0.356502	-0.026165
						96	6	0	10.808707	-0.519337	1.176506
						97	1	0	9.451358	0.662767	-0.024312

98	1	0	10.423264	-0.460836	-0.963988	154	6	0	-4.041357	1.564854	4.674071
99	1	0	10.260357	-0.369063	2.113683	155	1	0	-2.875559	-4.617802	-0.057303
100	1	0	11.211141	-1.538839	1.200621	156	6	0	-3.791965	-3.142160	-1.274899
101	6	0	7.409764	2.273107	3.576710	157	8	0	-1.392118	-3.416760	1.306791
102	6	0	7.067889	3.540114	4.381284	158	6	0	-7.849370	1.351439	-1.238011
103	1	0	7.696863	2.562424	2.555929	159	1	0	-9.212563	2.408704	0.000431
104	1	0	8.284305	1.774011	4.015554	160	8	0	-7.875593	3.761463	1.376036
105	1	0	6.223698	4.064003	3.918549	161	6	0	-4.967541	-2.623309	-1.839286
106	1	0	6.758462	3.264694	5.396355	162	6	0	-2.572281	-2.771007	-1.863906
107	6	0	4.980634	5.054237	-0.054007	163	6	0	-0.370348	-2.676237	0.697864
108	6	0	4.965363	5.921706	-1.325512	164	6	0	-1.249298	1.959342	4.897127
109	1	0	5.950807	4.542471	0.010056	165	6	0	-7.463518	0.137049	-1.828326
110	1	0	4.904712	5.686380	0.840912	166	6	0	-7.347981	2.534106	-1.805749
111	1	0	5.130061	5.289585	-2.206010	167	6	0	-7.014610	4.686187	0.772622
112	1	0	3.983362	6.393138	-1.451598	168	6	0	-2.191396	3.109882	4.825596
113	6	0	6.047042	6.992020	-1.268895	169	6	0	-4.964823	-1.803285	-2.979565
114	1	0	5.823414	7.783380	-0.553841	170	6	0	-2.518944	-1.940575	-2.983733
115	1	0	7.035610	6.574844	-1.069625	171	8	0	-1.388577	-3.378082	-1.393636
116	6	0	7.932375	4.739436	-4.110915	172	6	0	-0.373094	-2.648769	-0.761680
117	1	0	7.746199	5.588905	-4.765413	173	6	0	-6.618021	0.069200	-2.949613
118	1	0	7.850991	5.050157	-3.066856	174	6	0	-6.496536	2.513998	-2.909260
119	6	0	8.267560	4.475591	4.450960	175	8	0	-7.832179	3.766348	-1.318785
120	1	0	9.095413	4.050476	5.018264	176	6	0	-6.981603	4.681117	-0.689255
121	1	0	8.608467	4.787085	3.462692	177	6	0	-6.244869	-1.257047	-3.609952
122	6	0	11.955144	0.479864	1.094269	178	6	0	-3.716549	-1.489054	-3.537813
123	1	0	12.607533	0.294941	0.240862	179	1	0	-1.572141	-1.686260	-3.450924
124	1	0	11.604244	1.512642	1.082535	180	6	0	1.780455	-1.551156	0.728137
125	17	0	13.044495	0.338505	2.601655	181	6	0	-6.135974	1.286176	-3.466303
126	17	0	7.804811	6.050412	5.338249	182	1	0	-6.164593	3.438702	-3.365986
127	17	0	6.191111	7.839471	-2.928366	183	6	0	-5.517748	6.588021	0.815321
128	17	0	9.738361	4.306547	-4.355598	184	1	0	-6.012229	-1.034464	-4.656603
129	52	0	-0.331742	-4.228393	-5.012480	185	8	0	-3.699505	-0.785428	-4.758931
130	52	0	-4.203038	0.463970	-0.029035	186	6	0	1.772462	-1.514785	-0.760266
131	52	0	3.880211	-8.666958	0.011288	187	8	0	-5.403136	1.269119	-4.668504
132	52	0	-0.309208	-4.245402	4.991062	188	6	0	-5.478914	6.579608	-0.674133
133	6	0	-6.223865	-1.286956	3.565903	189	6	0	-3.120178	0.485936	-4.793931
134	6	0	-4.956411	-1.846733	2.923527	190	6	0	-4.046001	1.607761	-4.703901
135	6	0	-6.602445	0.043866	2.917827	191	6	0	-1.256804	1.993167	-4.989712
136	1	0	-5.973805	-1.065746	4.608197	192	6	0	-2.193811	3.146329	-4.885239
137	6	0	-4.970076	-2.664931	1.780686	193	6	0	0.644191	-2.079545	-1.467393
138	6	0	-3.705549	-1.537103	3.476731	194	6	0	0.655125	-2.142096	1.418997
139	6	0	-7.440109	0.124110	1.792417	195	6	0	-1.769591	0.613505	4.872730
140	6	0	-6.141900	1.257350	3.463479	196	6	0	-3.611265	2.853557	4.740179
141	6	0	-3.797770	-3.179560	1.203762	197	6	0	-1.782225	0.648980	-4.964620
142	6	0	-2.511747	-1.993539	2.917337	198	6	0	-3.612607	2.895188	-4.768548
143	8	0	-3.684418	-0.828661	4.695340	199	6	0	-6.328774	5.607438	1.501987
144	6	0	-7.850254	1.345210	1.232086	200	6	0	-6.258033	5.594982	-1.391575
145	6	0	-6.523979	2.490289	2.935071	201	1	0	0.653728	-2.087698	-2.550566
146	8	0	-5.400553	1.227130	4.660753	202	1	0	0.671574	-2.196018	2.500581
147	6	0	-3.811199	-4.050414	-0.048963	203	1	0	-1.131370	-0.213048	-5.088615
148	6	0	-2.573315	-2.814622	1.792209	204	1	0	-1.112497	-0.246417	4.975956
149	1	0	-1.561375	-1.741852	3.378696	205	1	0	-4.289710	3.739561	-4.753519
150	6	0	-3.110197	0.444992	4.730176	206	1	0	-4.292435	3.694824	4.748106
151	6	0	-8.743110	1.420449	-0.003686	207	1	0	-6.399281	5.650219	2.581547
152	6	0	-7.376446	2.522086	1.831644	208	1	0	-6.277842	5.633270	-2.473334
153	1	0	-6.208496	3.410195	3.412906	209	7	0	-1.676836	4.372610	-4.904891

210 7 0 0.045640 2.261479 -5.081933
 211 7 0 -4.740114 7.499867 -1.286571
 212 7 0 -4.811638 7.514952 1.455429
 213 7 0 -1.677845 4.337696 4.841534
 214 7 0 0.054168 2.231650 4.958948
 215 7 0 2.860418 -1.085924 1.358605
 216 7 0 2.844314 -1.016807 -1.379391
 217 1 0 -5.920274 -2.885014 -1.385029
 218 1 0 -5.928913 -2.916262 1.334263
 219 1 0 -7.805361 -0.798337 1.347964
 220 1 0 -7.849972 -0.790197 -1.414929
 221 6 0 -7.395219 -2.282800 -3.578942
 222 6 0 -7.074170 -3.518421 -4.436630
 223 1 0 -8.310226 -1.807497 -3.948892
 224 1 0 -7.615867 -2.609156 -2.552689
 225 1 0 -7.150654 -3.261519 -5.499264
 226 1 0 -6.036198 -3.837109 -4.257648
 227 6 0 -9.862112 0.361203 -0.013163
 228 6 0 -10.808243 0.521156 1.190520
 229 1 0 -9.452944 -0.658567 -0.014752
 230 1 0 -10.423804 0.469463 -0.950433
 231 1 0 -10.259787 0.365598 2.126780
 232 1 0 -11.208236 1.541507 1.219135
 233 6 0 -7.393122 -2.292903 3.565363
 234 6 0 -7.044829 -3.565096 4.358924
 235 1 0 -7.681700 -2.575137 2.543020
 236 1 0 -8.268187 -1.800152 4.010315
 237 1 0 -6.201669 -4.083570 3.888278
 238 1 0 -6.731258 -3.296643 5.374611
 239 6 0 -4.981413 -5.055475 -0.065904
 240 6 0 -4.976684 -5.919823 -1.339658
 241 1 0 -5.951065 -4.544031 0.008093
 242 1 0 -4.897881 -5.689982 0.826599
 243 1 0 -5.140748 -5.284815 -2.218112
 244 1 0 -3.998284 -6.397361 -1.470516
 245 6 0 -6.065126 -6.983228 -1.281588
 246 1 0 -5.843649 -7.778514 -0.570248
 247 1 0 -7.049918 -6.560039 -1.076427
 248 6 0 -7.960982 -4.715060 -4.126199
 249 1 0 -7.778646 -5.562864 -4.783937
 250 1 0 -7.878914 -5.029746 -3.083404
 251 6 0 -8.241967 -4.503926 4.427037
 252 1 0 -9.067461 -4.086152 5.003147
 253 1 0 -8.587936 -4.807141 3.437949
 254 6 0 -11.957120 -0.474922 1.104557
 255 1 0 -12.609183 -0.285021 0.251991
 256 1 0 -11.608790 -1.508509 1.088718
 257 17 0 -13.045898 -0.336716 2.612639
 258 17 0 -7.770081 -6.085797 5.296931
 259 17 0 -6.222676 -7.823886 -2.943343
 260 17 0 -9.765863 -4.275330 -4.366564
 261 52 0 0.318321 4.251156 -5.061695
 262 52 0 4.201153 -0.463051 -0.003756
 263 52 0 -3.866418 8.660557 0.101911
 264 52 0 0.320854 4.221663 4.947132

C₉H₂₀@A_{Te}+A_{Te}

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	8.283023	3.335989 -1.518603
2	6	0	7.690899	2.204251 -2.355454
3	6	0	7.698613	3.309122 -0.109879
4	1	0	7.953470	4.272749 -1.978850
5	6	0	8.239121	0.911233 -2.378882
6	6	0	6.555402	2.434371 -3.147071
7	6	0	8.236678	2.525535 0.924919
8	6	0	6.576910	4.095817 0.196173
9	6	0	7.710330	-0.126926 -3.162967
10	6	0	6.008116	1.437743 -3.952606
11	8	0	6.006391	3.736413 -3.197810
12	6	0	7.700424	2.505761 2.223424
13	6	0	6.013974	4.106112 1.469684
14	8	0	6.051831	4.964210 -0.790070
15	6	0	8.303343	-1.532181 -3.185576
16	6	0	6.580267	0.168226 -3.941817
17	1	0	5.179593	1.659331 -4.613269
18	6	0	4.762576	3.969652 -2.598396
19	6	0	8.304750	1.677968 3.356337
20	6	0	6.565953	3.297057 2.460247
21	1	0	5.188020	4.767884 1.697913
22	6	0	4.787593	4.659009 -1.311952
23	1	0	7.987381	-1.997619 -4.124498
24	6	0	7.702061	-2.365512 -2.056642
25	8	0	6.061286	-0.825865 -4.804108
26	6	0	7.730237	0.264340 3.333217
27	1	0	7.974381	2.138885 4.292489
28	8	0	6.022719	3.345652 3.764694
29	6	0	8.229307	-2.364157 -0.756321
30	6	0	6.593433	-3.190492 -2.298507
31	6	0	4.806743	-1.371395 -4.504656
32	6	0	2.339501	3.993222 -2.575554
33	6	0	8.274935	-0.766584 2.548233
34	6	0	6.609722	-0.048927 4.117954
35	6	0	4.783299	2.744404 4.006133
36	6	0	2.362086	4.717466 -1.279276
37	6	0	7.719355	-3.167306 0.276504
38	6	0	6.059599	-4.009808 -1.306329
39	8	0	6.055293	-3.251548 -3.604965
40	6	0	4.803705	-2.669187 -3.837131
41	6	0	7.739075	-2.064488 2.519561
42	6	0	6.054059	-1.326681 4.129098
43	8	0	6.079379	0.935598 4.985799
44	6	0	4.813171	1.456240 4.692166
45	6	0	8.334212	-3.186241 1.674076
46	6	0	6.619955	-3.983057 -0.030778
47	1	0	5.251656	-4.693806 -1.533948
48	6	0	2.380900	-1.383793 -4.568905
49	6	0	6.607711	-2.310581 3.313868

50	1	0	5.232167	-1.560487	4.793844	106	1	0	9.994581	4.401087	-3.395591
51	6	0	2.361545	2.723711	4.044755	107	6	0	9.846974	-1.520668	-3.157285
52	1	0	8.032095	-4.129930	2.140247	108	6	0	10.436930	-2.941449	-3.209090
53	8	0	6.112379	-4.863802	0.954012	109	1	0	10.226685	-1.014991	-2.258679
54	6	0	2.381475	-2.690020	-3.861155	110	1	0	10.196715	-0.931618	-4.015668
55	8	0	6.075970	-3.620332	3.353047	111	1	0	10.149158	-3.496906	-2.308816
56	6	0	2.387349	1.425240	4.766831	112	1	0	10.029952	-3.491722	-4.065554
57	6	0	4.850115	-4.571565	1.489414	113	6	0	11.956419	-2.893611	-3.302560
58	6	0	4.829693	-3.873034	2.771106	114	1	0	12.310183	-2.558535	-4.277294
59	6	0	2.425158	-4.658253	1.480074	115	1	0	12.402333	-2.286558	-2.512689
60	6	0	2.406744	-3.932225	2.776152	116	6	0	11.932879	-4.258392	0.605549
61	6	0	3.641296	-3.313600	-3.531507	117	1	0	12.359412	-5.172228	0.196421
62	6	0	3.648169	-0.760282	-4.879501	118	1	0	12.112857	-3.426564	-0.078711
63	6	0	3.588193	3.655302	-3.217946	119	6	0	11.926257	3.604523	-2.873049
64	6	0	3.639828	5.041043	-0.684806	120	1	0	12.263997	4.509602	-2.368271
65	6	0	3.701269	-4.969189	0.874659	121	1	0	12.385806	2.725891	-2.418153
66	6	0	3.657779	-3.572084	3.401757	122	6	0	11.935260	3.068482	3.604488
67	6	0	3.608404	3.365144	3.700472	123	1	0	12.282056	2.567143	4.508045
68	6	0	3.667534	0.829215	5.081007	124	1	0	12.394969	2.617422	2.724088
69	1	0	3.646590	-4.305440	-3.094847	125	17	0	12.619610	4.801064	3.694511
70	1	0	3.652846	0.165666	-5.442870	126	17	0	12.626213	3.697743	-4.598962
71	1	0	3.721117	-5.547194	-0.042120	127	17	0	12.663619	-4.607038	-3.071965
72	1	0	3.574911	3.208191	-4.205067	128	17	0	12.950244	-3.870435	2.130067
73	1	0	3.649050	-3.118319	4.385816	129	6	0	-8.285456	-3.444918	-1.253222
74	1	0	3.660856	5.617304	0.232921	130	6	0	-7.700687	-2.382868	-2.181787
75	1	0	3.594083	4.352105	3.252964	131	6	0	-7.694167	-3.302593	0.146239
76	1	0	3.691913	-0.089855	5.654994	132	1	0	-7.955613	-4.414876	-1.638348
77	7	0	1.209125	-3.641224	3.253225	133	6	0	-8.246310	-1.094424	-2.298132
78	7	0	1.250806	-4.934154	0.941389	134	6	0	-6.574404	-2.675297	-2.965850
79	7	0	1.216151	0.876101	5.034738	135	6	0	-8.228920	-2.440089	1.117391
80	7	0	1.162736	3.187556	3.741918	136	6	0	-6.572119	-4.062847	0.510844
81	7	0	1.189413	4.987643	-0.732856	137	6	0	-7.723755	-0.120094	-3.164113
82	7	0	1.140212	3.691416	-3.043308	138	6	0	-6.035672	-1.746108	-3.854235
83	7	0	1.198803	-0.855330	-4.829796	139	8	0	-6.021382	-3.975257	-2.911119
84	7	0	1.192741	-3.178310	-3.556671	140	6	0	-7.691948	-2.321553	2.410264
85	1	0	9.084896	-1.727523	-0.546020	141	6	0	-6.008438	-3.977841	1.781431
86	1	0	9.116032	0.711344	-1.769150	142	8	0	-6.050253	-5.002293	-0.409213
87	1	0	9.112317	1.916111	0.716720	143	6	0	-8.313411	1.281507	-3.282720
88	1	0	9.151767	-0.554032	1.943169	144	6	0	-6.604609	-0.476949	-3.933373
89	6	0	9.875667	-3.144876	1.635123	145	1	0	-5.213708	-2.019893	-4.503500
90	6	0	10.461858	-4.399939	0.967935	146	6	0	-4.775290	-4.158534	-2.301270
91	1	0	10.254461	-3.065620	2.659976	147	6	0	-8.295418	-1.408250	3.475594
92	1	0	10.241309	-2.253951	1.105064	148	6	0	-6.559325	-3.094918	2.707944
93	1	0	10.321080	-5.266838	1.623657	149	1	0	-5.183783	-4.621990	2.059096
94	1	0	9.922744	-4.615231	0.033105	150	6	0	-4.791013	-4.742918	-0.963769
95	6	0	9.847548	1.685358	3.347640	151	1	0	-8.005744	1.676059	-4.256229
96	6	0	10.415641	3.106997	3.507898	152	6	0	-7.703080	2.196791	-2.224774
97	1	0	10.246215	1.240146	2.425666	153	8	0	-6.090726	0.450661	-4.870608
98	1	0	10.193003	1.048156	4.172476	154	6	0	-7.721305	-0.000867	3.346082
99	1	0	10.120657	3.732107	2.657340	155	1	0	-7.966447	-1.796639	4.444579
100	1	0	10.002664	3.575697	4.408987	156	8	0	-6.016076	-3.041870	4.012996
101	6	0	9.825972	3.332776	-1.510682	157	6	0	-8.230111	2.304033	-0.928742
102	6	0	10.407544	3.500504	-2.926025	158	6	0	-6.589651	2.992697	-2.533676
103	1	0	10.223162	2.409869	-1.065361	159	6	0	-4.829185	1.009195	-4.621658
104	1	0	10.162074	4.156859	-0.866950	160	6	0	-2.353172	-4.181345	-2.293493
105	1	0	10.122359	2.650623	-3.556512	161	6	0	-8.268445	0.967752	2.486970

162	6	0	-6.599027	0.370150	4.102124	218	6	0	-10.451740	4.473501	0.630412
163	6	0	-4.773255	-2.426996	4.203481	219	1	0	-10.244803	3.281187	2.425637
164	6	0	-2.366094	-4.803855	-0.945205	220	1	0	-10.237707	2.345251	0.942304
165	6	0	-7.713342	3.182759	0.036723	221	1	0	-10.308761	5.390505	1.213467
166	6	0	-6.048239	3.883505	-1.609396	222	1	0	-9.912550	4.610879	-0.318960
167	8	0	-6.062123	2.954125	-3.845736	223	6	0	-9.838197	-1.415219	3.465007
168	6	0	-4.814219	2.352716	-4.050603	224	6	0	-10.407666	-2.820551	3.729819
169	6	0	-7.732046	2.259173	2.357733	225	1	0	-10.234928	-1.040165	2.511529
170	6	0	-6.042525	1.644411	4.013719	226	1	0	-10.184561	-0.717785	4.239191
171	8	0	-6.065516	-0.544708	5.041874	227	1	0	-10.111795	-3.507270	2.928503
172	6	0	-4.800248	-1.087191	4.783320	228	1	0	-9.996556	-3.221311	4.663925
173	6	0	-8.326445	3.314434	1.429329	229	6	0	-9.828416	-3.445862	-1.237622
174	6	0	-6.607090	3.962322	-0.334935	230	6	0	-10.416551	-3.726841	-2.632092
175	1	0	-5.236916	4.542778	-1.891635	231	1	0	-10.226637	-2.491820	-0.864797
176	6	0	-2.402330	1.001707	-4.697454	232	1	0	-10.158460	-4.217291	-0.528770
177	6	0	-6.598200	2.563673	3.127439	233	1	0	-10.138251	-2.928089	-3.329018
178	1	0	-5.218523	1.927340	4.656425	234	1	0	-10.002376	-4.660055	-3.031635
179	6	0	-2.350018	-2.402526	4.228000	235	6	0	-9.856817	1.273860	-3.238836
180	1	0	-8.020055	4.290612	1.819552	236	6	0	-10.446555	2.688367	-3.383403
181	8	0	-6.094606	4.917603	0.574328	237	1	0	-10.227975	0.832049	-2.303712
182	6	0	-2.391263	2.362204	-4.100755	238	1	0	-10.215166	0.627132	-4.050873
183	8	0	-6.066001	3.871795	3.064745	239	1	0	-10.148460	3.305033	-2.527459
184	6	0	-2.373861	-1.047861	4.839060	240	1	0	-10.048818	3.176898	-4.280699
185	6	0	-4.834455	4.666559	1.134008	241	6	0	-11.967045	2.636469	-3.456256
186	6	0	-4.818589	4.075439	2.468272	242	1	0	-12.332169	2.236230	-4.401789
187	6	0	-2.410065	4.751573	1.126820	243	1	0	-12.404451	2.085481	-2.621802
188	6	0	-2.396996	4.128977	2.475805	244	6	0	-11.923203	4.306117	0.281062
189	6	0	-3.646206	3.014921	-3.809405	245	1	0	-12.347922	5.184338	-0.201352
190	6	0	-3.675567	0.364244	-4.954499	246	1	0	-12.105168	3.421506	-0.332877
191	6	0	-3.606040	-3.893401	-2.951199	247	6	0	-11.934503	-3.832069	-2.562570
192	6	0	-3.639321	-5.076590	-0.317107	248	1	0	-12.265811	-4.696436	-1.987115
193	6	0	-3.683399	5.012917	0.493257	249	1	0	-12.395161	-2.922479	-2.174598
194	6	0	-3.649822	3.823513	3.124725	250	6	0	-11.927401	-2.773856	3.820642
195	6	0	-3.598860	-3.071131	3.944981	251	1	0	-12.275350	-2.207540	4.684500
196	6	0	-3.653066	-0.429777	5.112275	252	1	0	-12.385086	-2.387948	2.908789
197	1	0	-3.643528	4.037359	-3.450187	253	17	0	-12.613677	-4.494687	4.035483
198	1	0	-3.688272	-0.602198	-5.444916	254	17	0	-12.643556	-4.061397	-4.271983
199	1	0	-3.699209	5.516345	-0.466558	255	17	0	-12.670034	4.362825	-3.334915
200	1	0	-3.600320	-3.523659	-3.969958	256	17	0	-12.940896	4.046386	1.832384
201	1	0	-3.644877	3.450578	4.142171	257	52	0	0.345159	1.670385	-4.434594
202	1	0	-3.654407	-5.577753	0.643812	258	52	0	0.382700	-4.510262	-1.592189
203	1	0	-3.585735	-4.091482	3.580222	259	52	0	0.336961	4.495141	1.794273
204	1	0	-3.675309	0.533643	5.608433	260	52	0	0.380098	-1.672195	4.534857
205	7	0	-1.202266	3.875237	2.979178	261	52	0	-0.367826	2.030180	4.436921
206	7	0	-1.233450	4.990002	0.575575	262	52	0	-0.325889	-4.346819	2.109852
207	7	0	-1.202197	-0.476215	5.051358	263	52	0	-0.388383	4.382940	-1.886027
208	7	0	-1.151747	-2.889898	3.958837	264	52	0	-0.361755	-2.044500	-4.236052
209	7	0	-1.189780	-5.027833	-0.387175	265	6	0	-5.136371	-0.351496	-0.006934
210	7	0	-1.158750	-3.910137	-2.787682	266	6	0	-3.855521	0.498423	-0.058138
211	7	0	-1.224369	0.446104	-4.919680	267	1	0	-6.038095	0.276205	-0.029033
212	7	0	-1.197062	2.872419	-3.854592	268	1	0	-5.188558	-1.039788	-0.863642
213	1	0	-9.090969	1.693489	-0.668611	269	1	0	-5.179340	-0.961428	0.908103
214	1	0	-9.114561	-0.845565	-1.694088	270	6	0	-2.569083	-0.345212	-0.030881
215	1	0	-9.103972	-1.847295	0.863747	271	1	0	-3.862080	1.118607	-0.968877
216	1	0	-9.147190	0.710141	1.902591	272	1	0	-3.845249	1.200781	0.790778
217	6	0	-9.868049	3.275328	1.397013	273	1	0	-2.558166	-0.961187	0.883735

274 1 0 -2.578655 -1.052603 -0.877391
 275 6 0 -1.286659 0.502064 -0.090520
 276 6 0 -0.001121 -0.339181 -0.036859
 277 1 0 -1.285771 1.222552 0.745897
 278 1 0 -1.288995 1.105153 -1.014883
 279 6 0 1.283477 0.505086 -0.057475
 280 1 0 -0.010129 -0.961447 0.874124
 281 1 0 0.008604 -1.041779 -0.887770
 282 1 0 1.290042 1.139465 -0.961041
 283 1 0 1.277529 1.196157 0.802603
 284 6 0 2.566118 -0.343280 -0.020262
 285 6 0 3.853021 0.499835 -0.038002
 286 1 0 2.571907 -1.035162 -0.879505
 287 1 0 2.558556 -0.976532 0.882762
 288 6 0 5.132920 -0.351709 0.002600
 289 1 0 3.859307 1.128312 -0.943229
 290 1 0 3.844592 1.193628 0.817466
 291 1 0 6.035792 0.274372 -0.020438
 292 1 0 5.178553 -0.965967 0.914746
 293 1 0 5.180130 -1.036729 -0.857488

SeN₂C₂H₂

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	1.611698	0.733895 0.000821
2	6	0	1.611700	-0.733893 -0.000829
3	1	0	2.508837	1.339280 0.000751
4	1	0	2.508841	-1.339275 -0.000796
5	7	0	0.434638	-1.326096 0.000518
6	7	0	0.434635	1.326096 -0.000488
7	34	0	-0.895382	-0.000000 -0.000003

TeN₂C₂H₂

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	-1.906370	-0.740112 -0.000073
2	6	0	-1.906371	0.740114 -0.000083
3	1	0	-2.824321	-1.318168 -0.000064
4	1	0	-2.824324	1.318166 -0.000074
5	7	0	-0.753048	1.370198 0.000145
6	7	0	-0.753050	-1.370199 0.000139
7	52	0	0.751303	-0.000000 -0.000017

ON₂C₂H₂

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	-0.721503	0.894011 0.000070
2	6	0	0.721504	0.894010 -0.000128
3	1	0	-1.404821	1.726019 0.000112
4	1	0	1.404821	1.726019 -0.000160
5	7	0	1.161531	-0.351555 0.000152
6	7	0	-1.161531	-0.351555 -0.000001
7	8	0	-0.000000	-1.157300 -0.000083

SN₂C₂H₂

Atom	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
1	6	0	1.214418	0.729902 -0.000551
2	6	0	1.214420	-0.729898 0.000599
3	16	0	-1.188404	-0.000001 0.000046
4	1	0	2.094560	1.356914 -0.000500
5	1	0	2.094565	-1.356906 0.000758
6	7	0	0.018024	-1.289509 -0.000465
7	7	0	0.018019	1.289508 0.000282

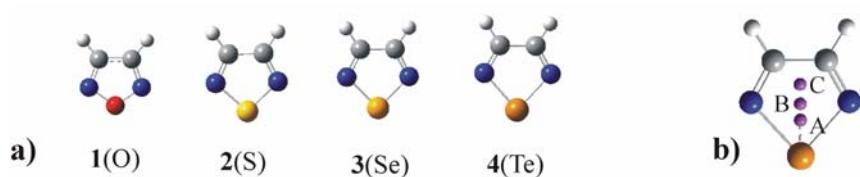


Figure 1S. **a)** Calculated Compounds, parts of the walls of the capsules. **b)** Magnetic isotropy and anisotropy were calculated at the geometric center of the ring (point B), at the geometric center of the NCCN quadrilateral (point C) and in the ring at distance of 1 Å (point A) from the chalcogen.

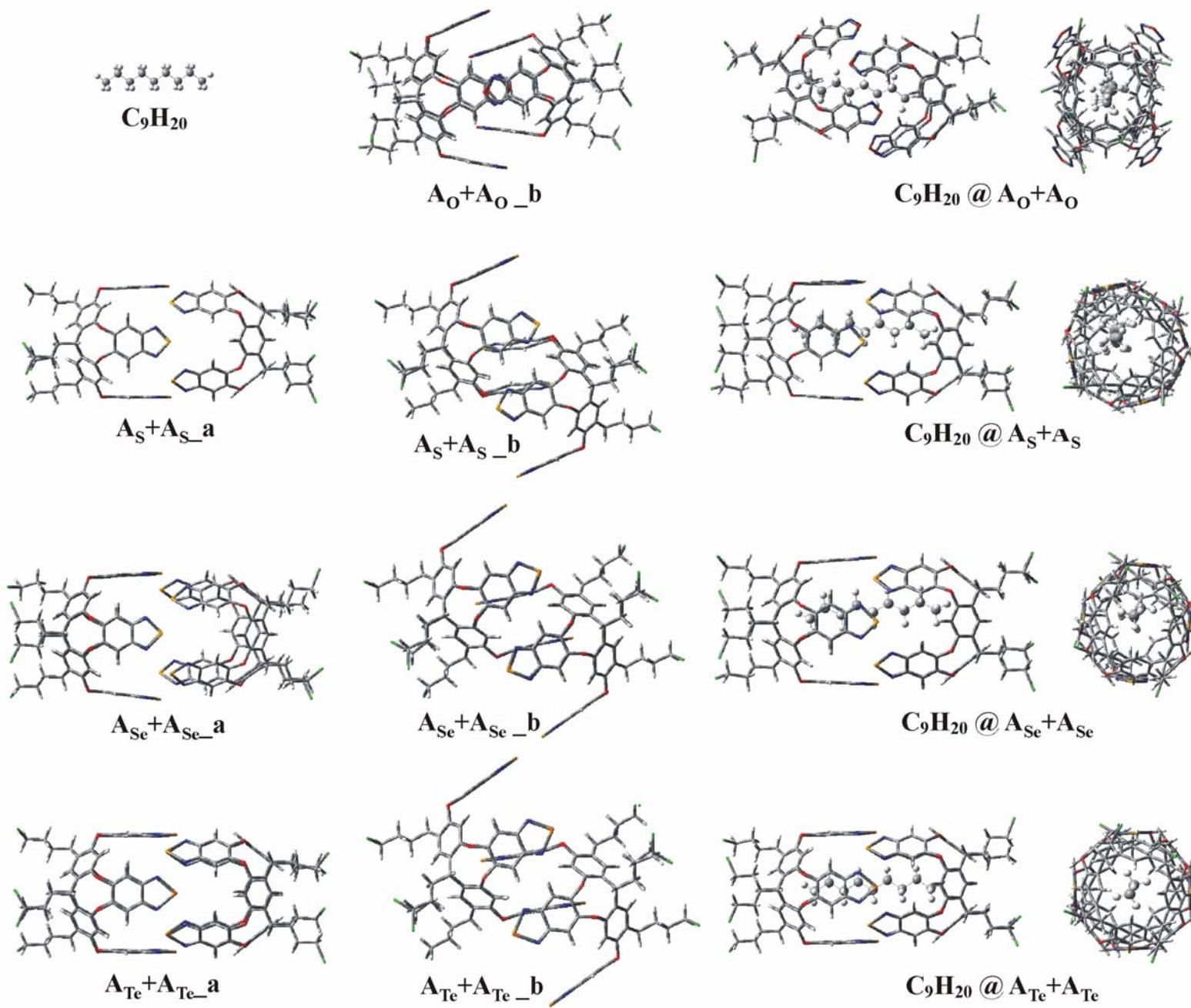


Fig. 2S: Calculated cages, **A_X+A_X**, **B+B**, and **C+C**, and encapsulated complexes **C₉H₂₀@A_X+A_X**, **C₉H₂₀@B+B**, and **C₉H₂₀@C+C**.

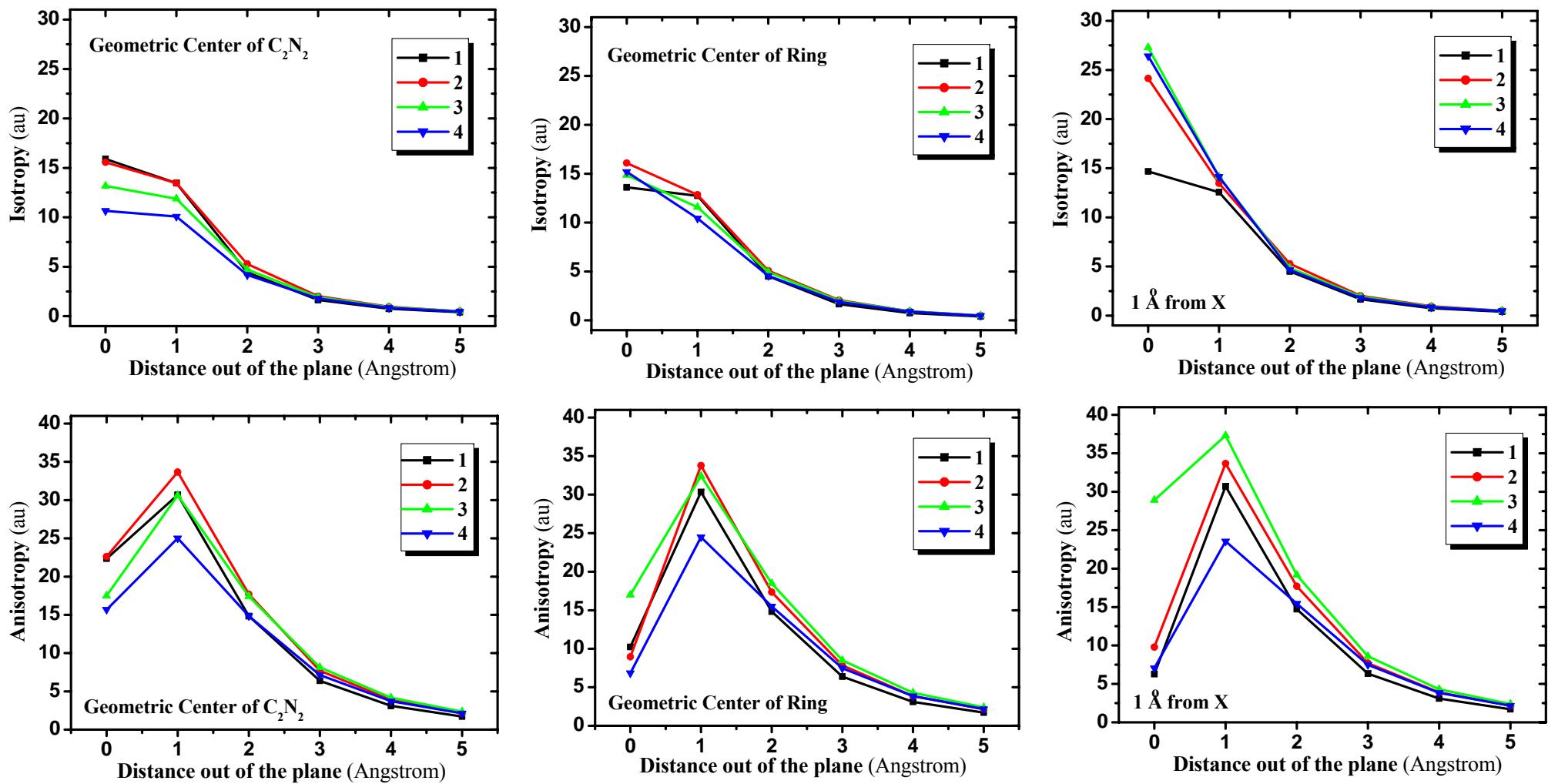


Fig. 3S: Magnetic isotropy and anisotropy perpendicular out of the plane of the compounds **1**, **2**, **3**, and **4** at the PBE0/6-311+G(d,p) levels of theory.

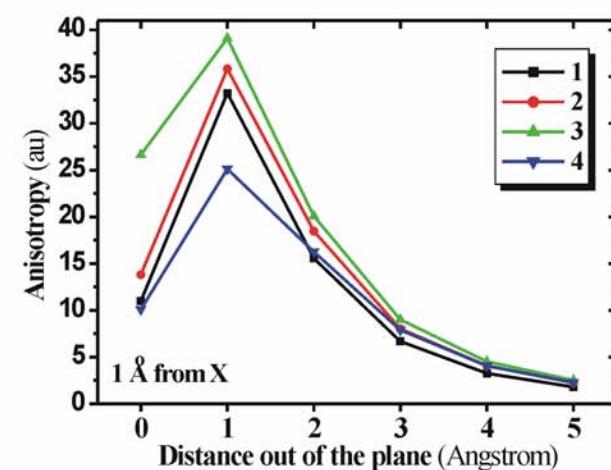
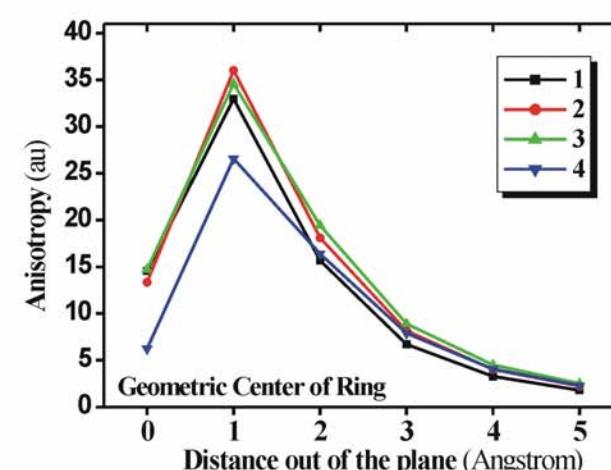
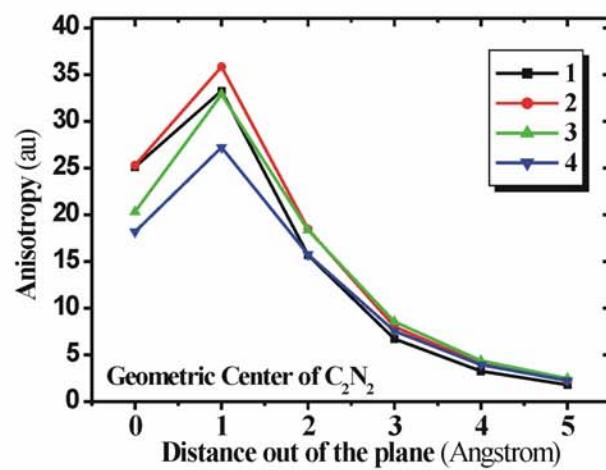
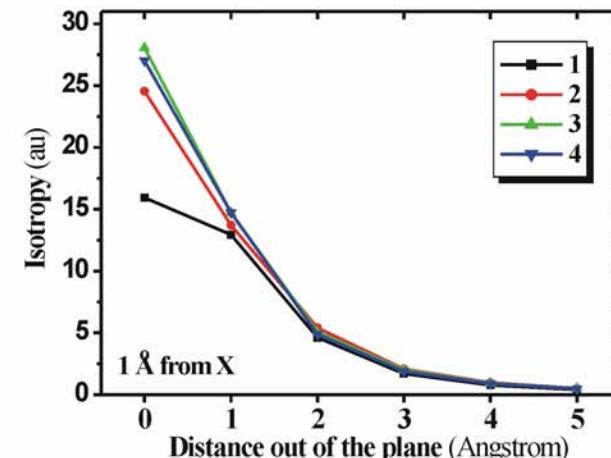
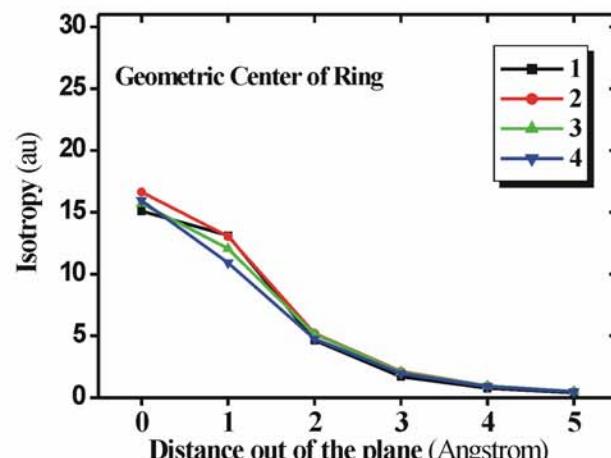
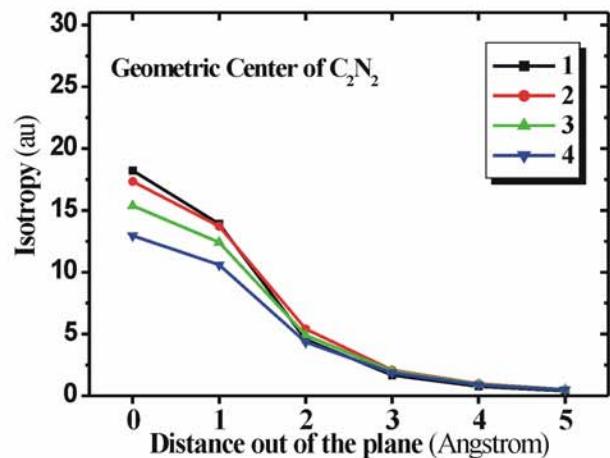


Fig. 4S. Magnetic isotropy and anisotropy in the plane (0 Å) and out of the plane of the compounds **1**, **2**, **3**, and **4** at the MP2/6-311+G(d,p) levels of theory.

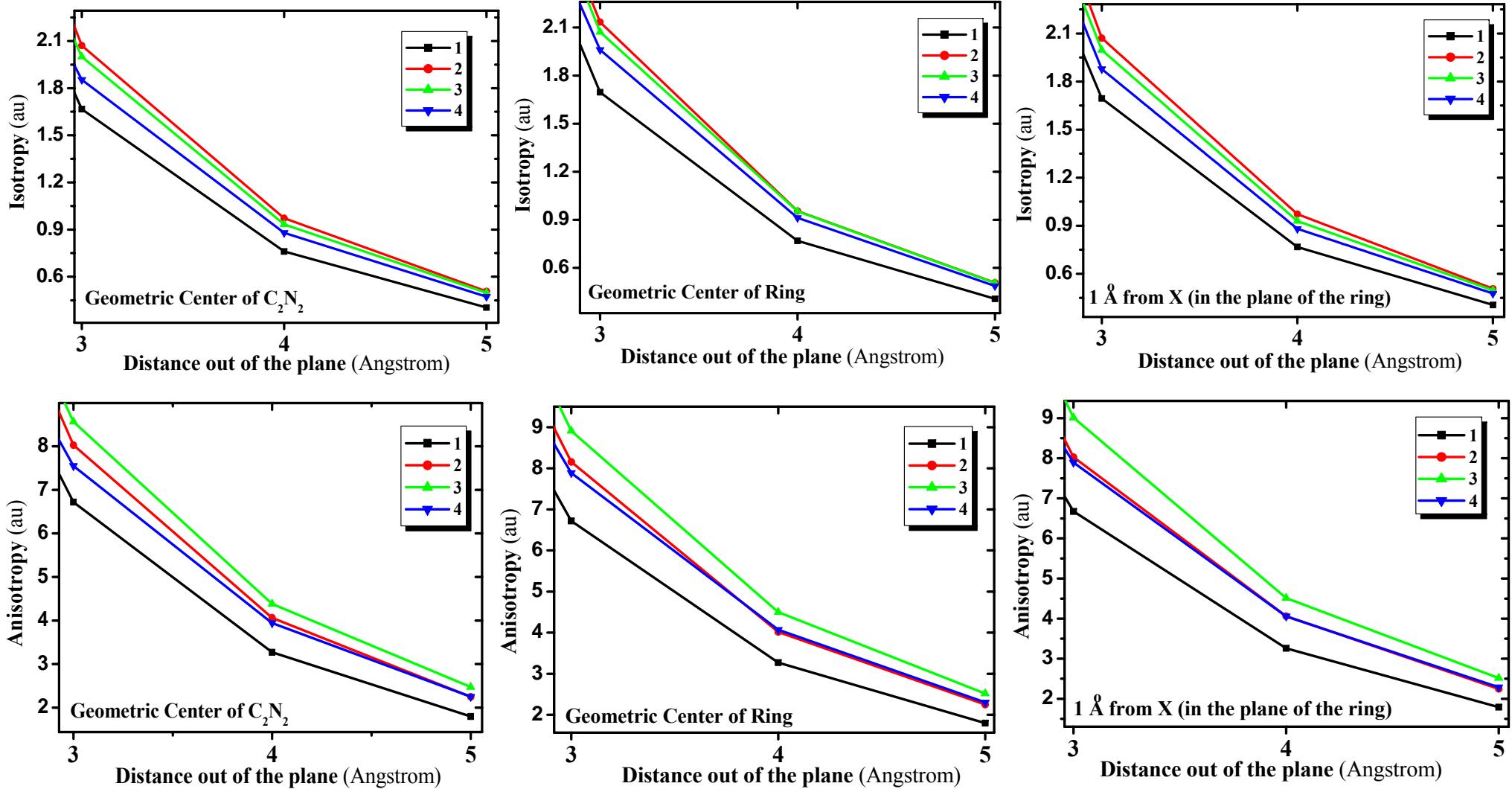
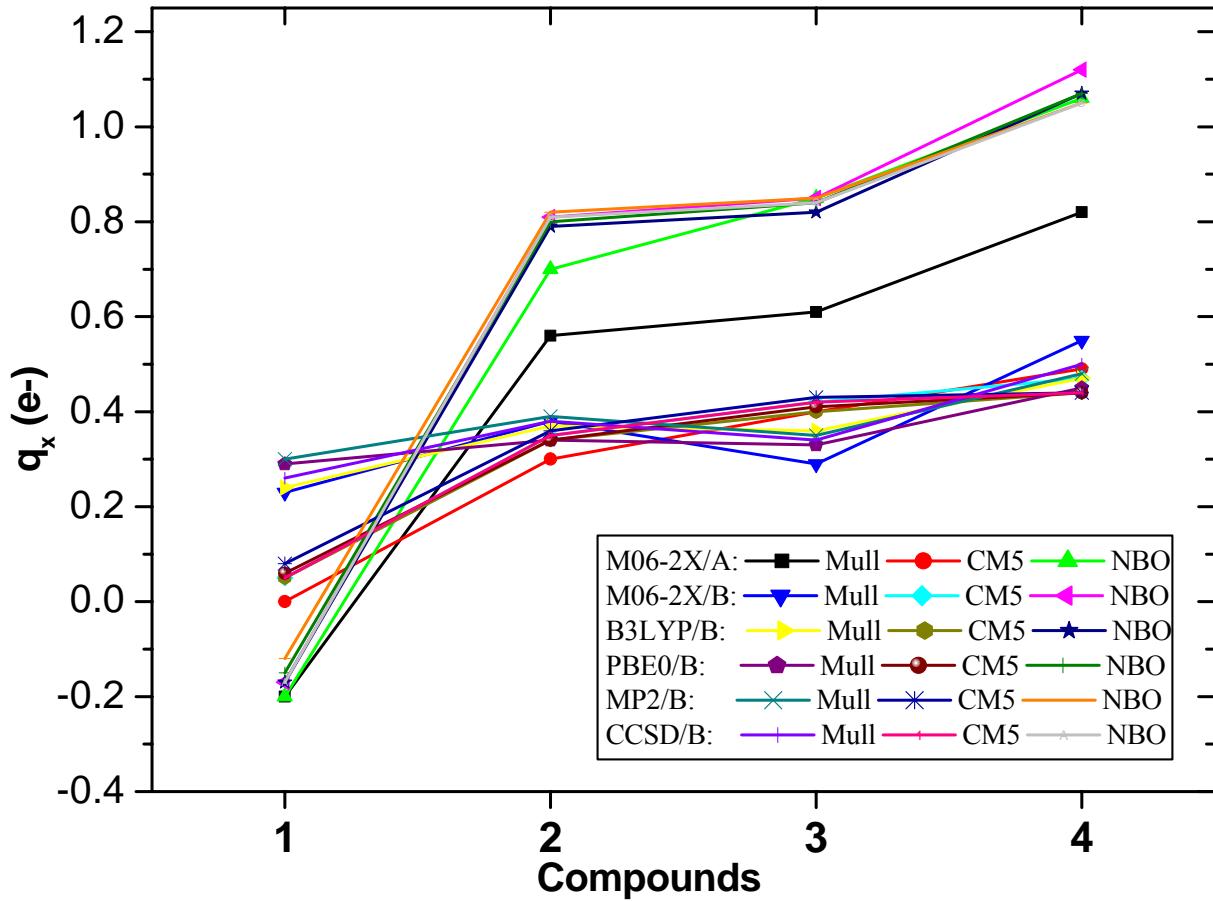


Fig. 5S: Magnetic isotropy and anisotropy perpendicular out of the plane of the compounds **1**, **2**, **3**, and **4** at the MP2/6-311+G(d,p) levels of theory at distances of 3-5 Å.



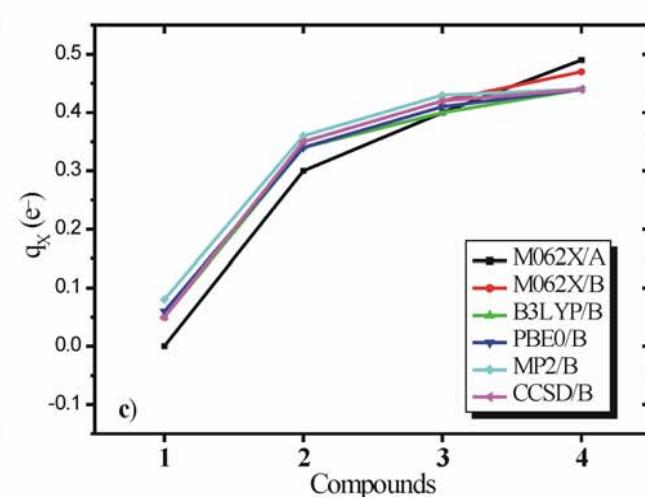
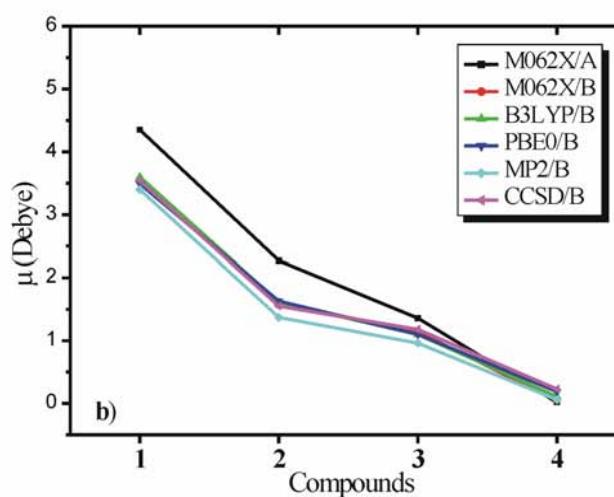
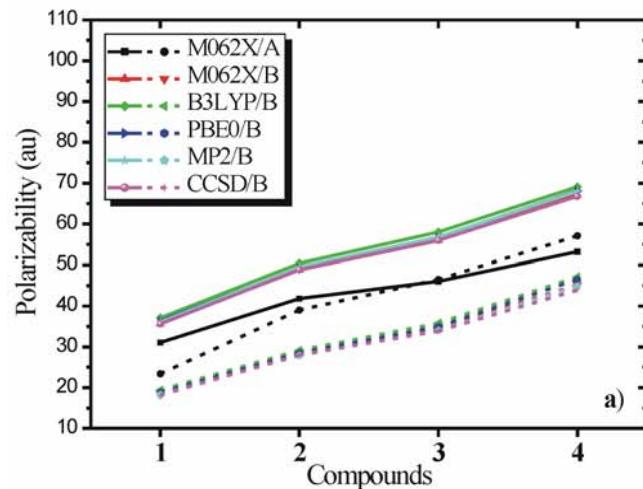


Fig. 7S. **a)** Isotropic (Solid lines) and Anisotropic (Dot lines) polarizabilities; **b)** CM5 charges q_x on the chalcogen; **c)** Dipole moments μ of **1-4**. [A: LANL2DZ, B: 6-311G+(d,p)].

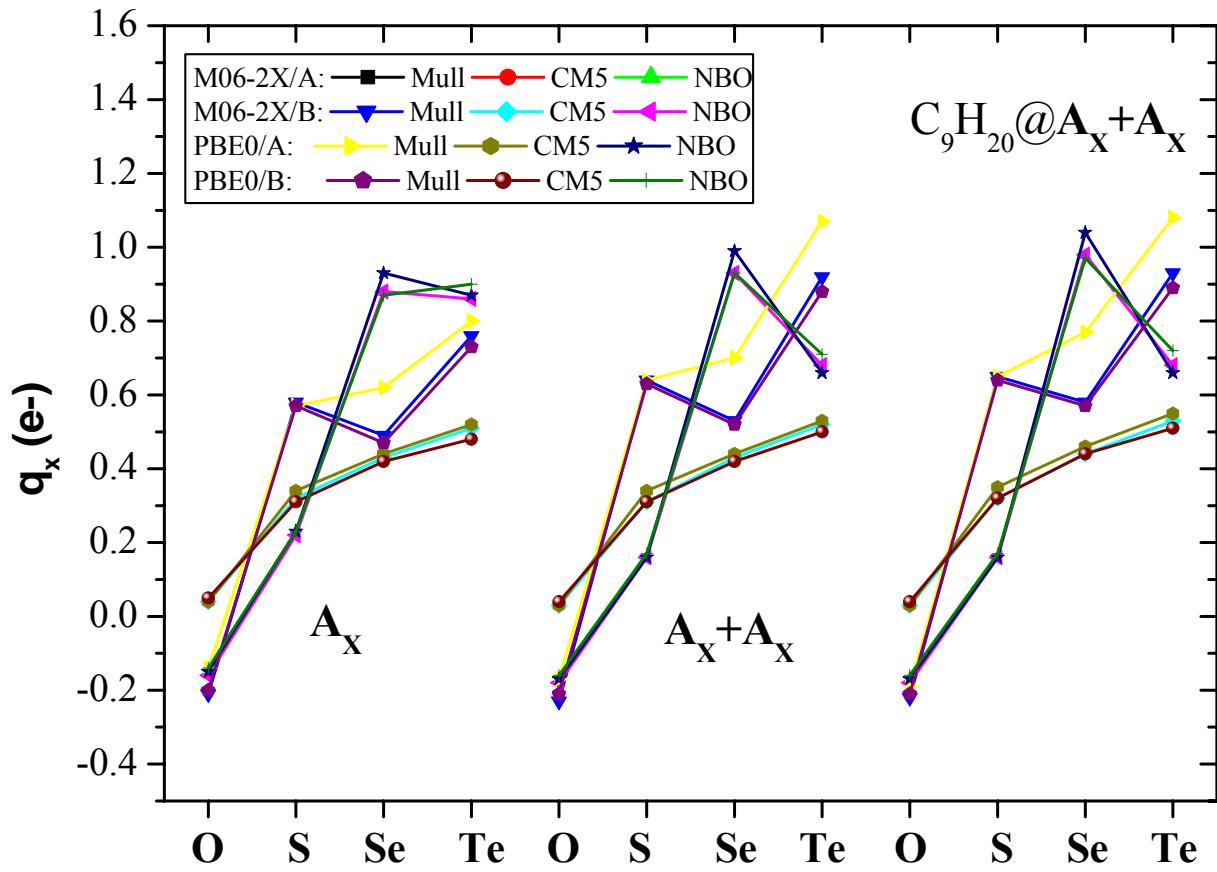
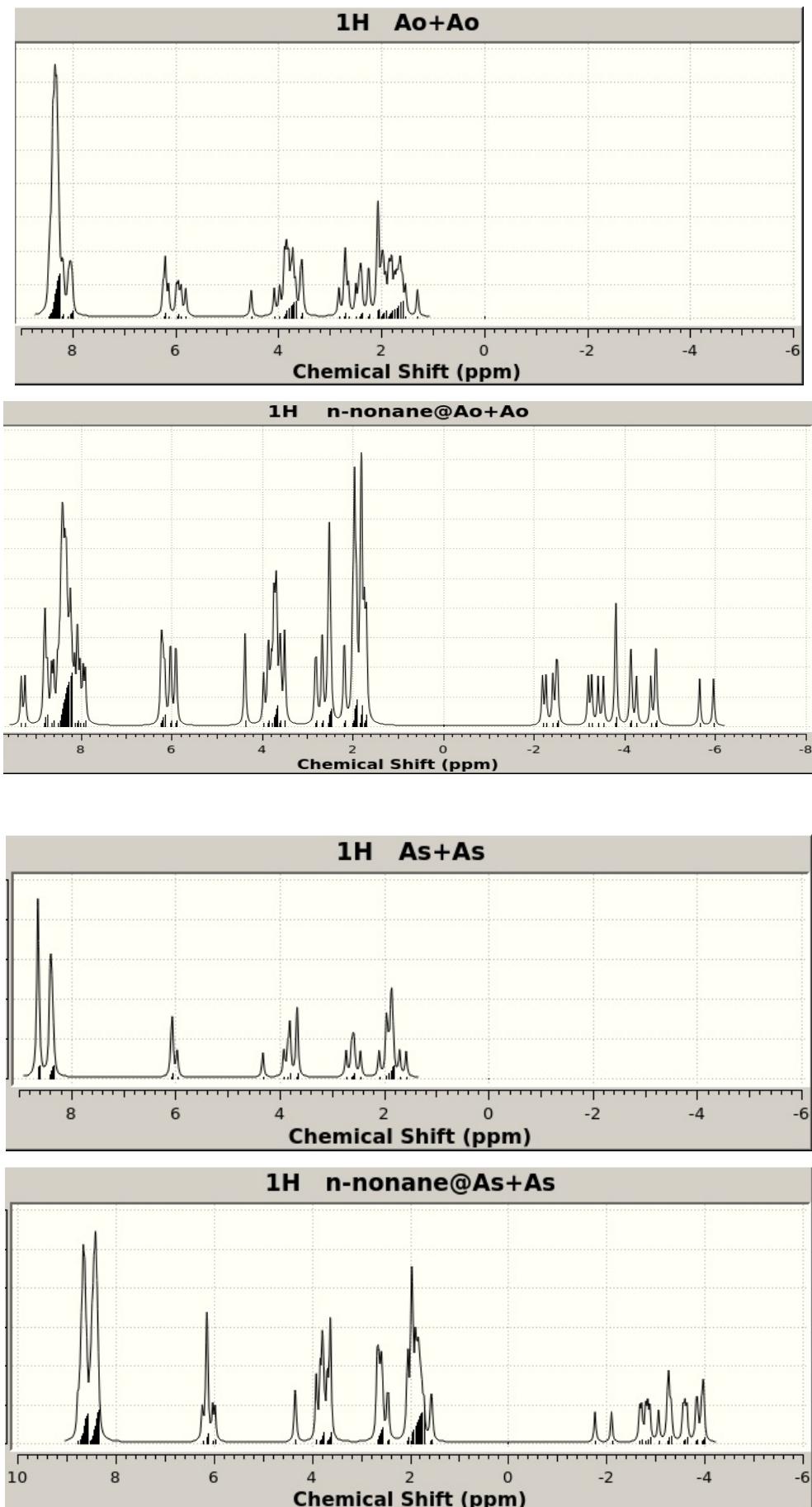


Fig 8S. Mulliken, CM5 and NBO charges q_x on the chalcogen of A_X , $A_X + A_X$, and $C_9H_{20} @ A_X + A_X$, where $X = O, S, Se$ and Te , at different levels of theory. A: LANL2DZ, B: 6-311G+(d,p).

^1H NMR spectra



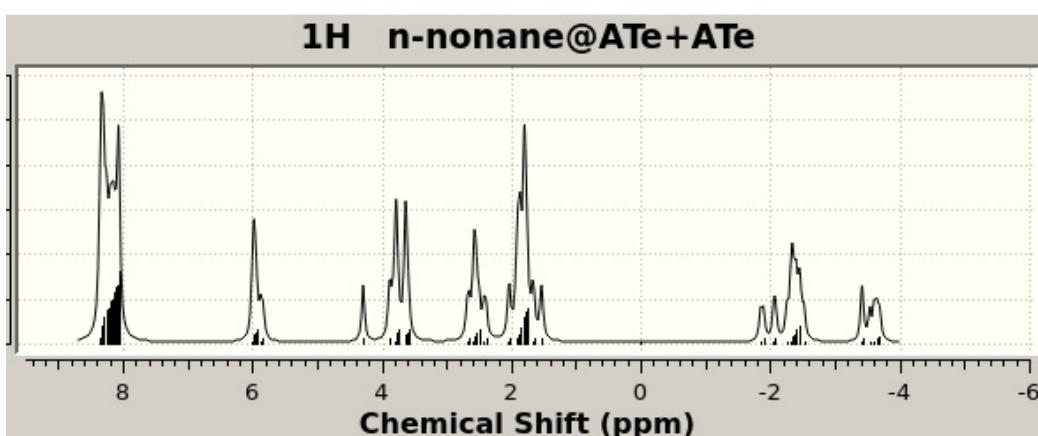
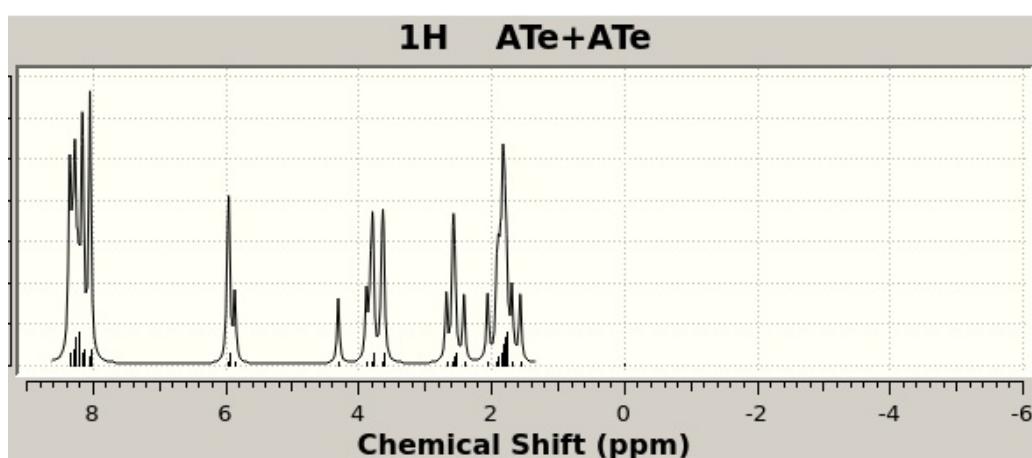
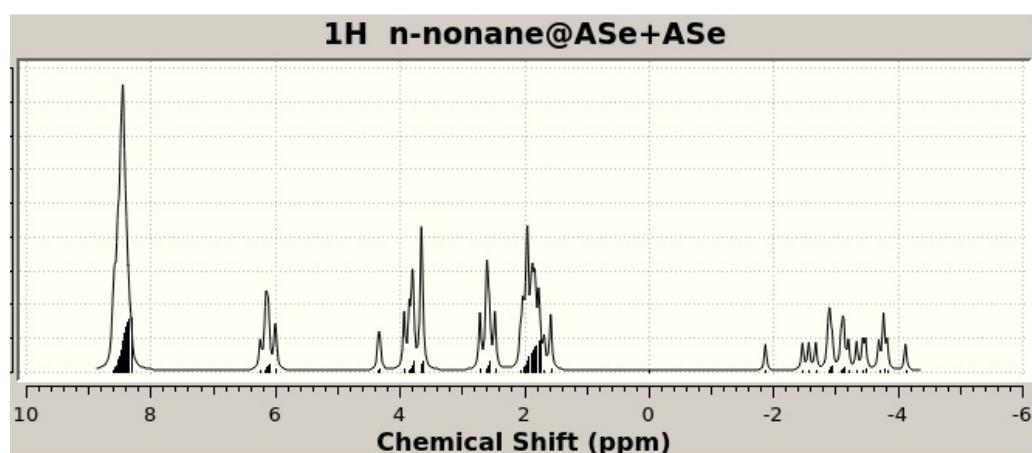
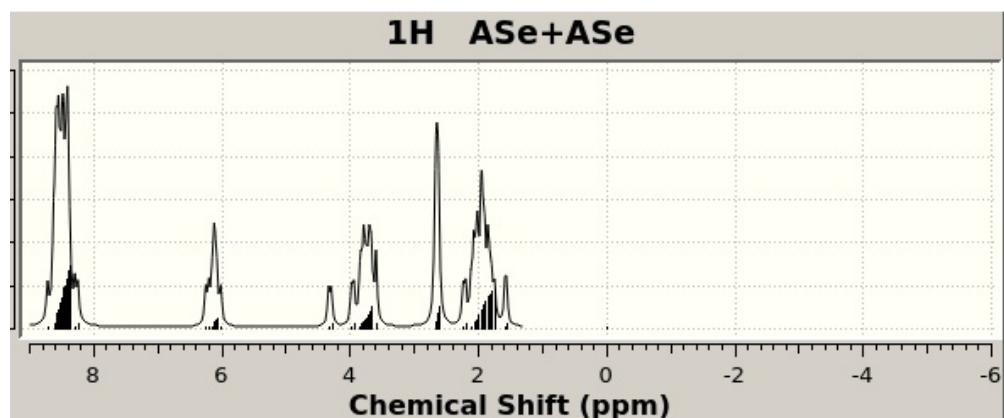
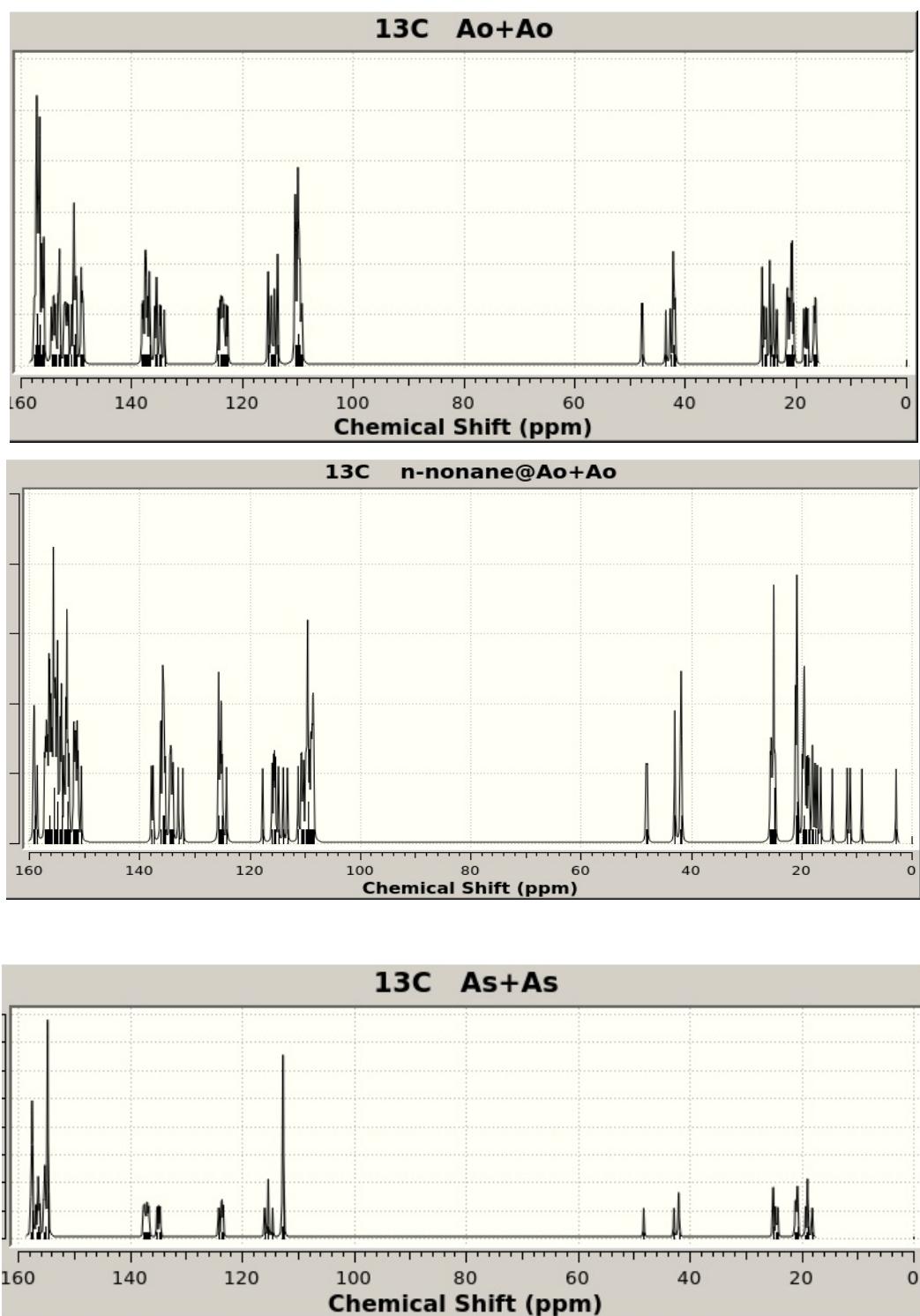
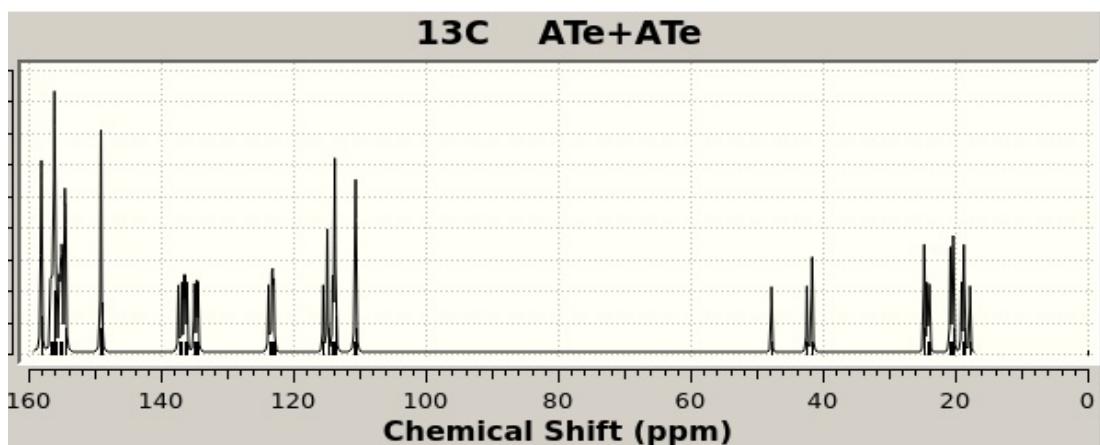
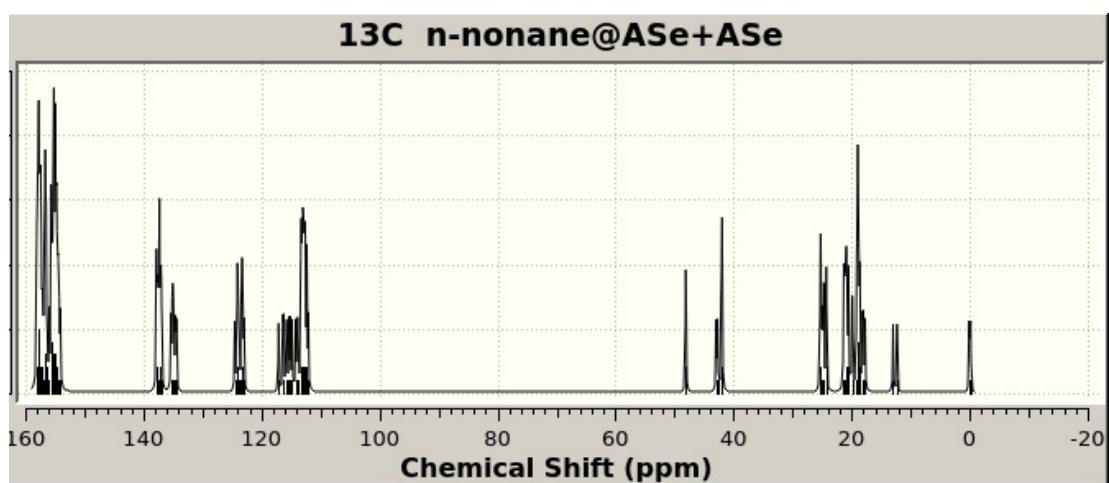
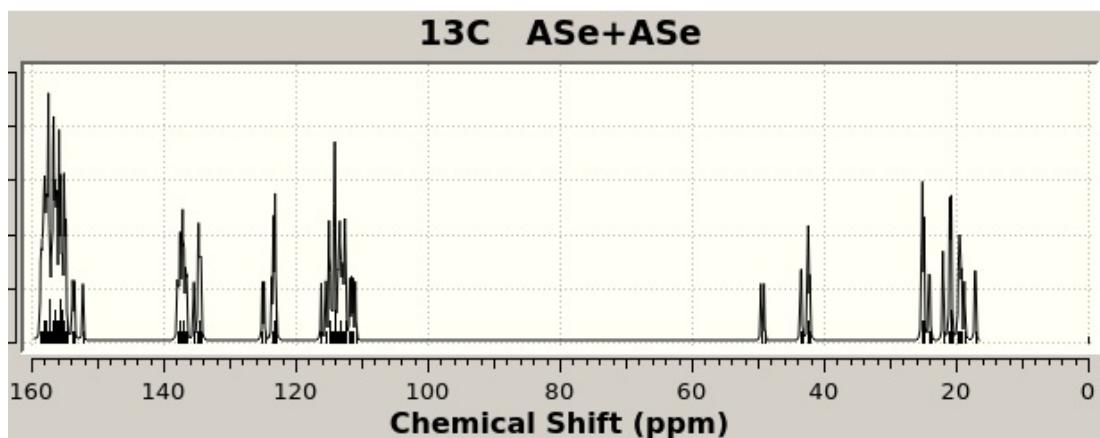
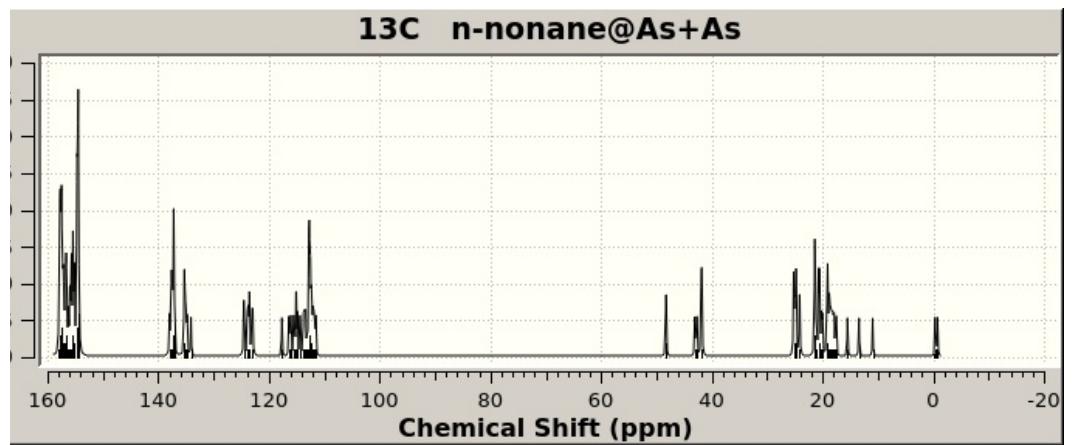


Figure 9S. ^1H NMR spectra of the capsular complexes at the M06-2X/6-31G(d,p) level of theory. NMR shielding tensors have been computed with the Gauge-Independent Atomic Orbital (GIAO) method. Relative shifts for protons are calculated with respect to the tetramethylsilane (TMS).





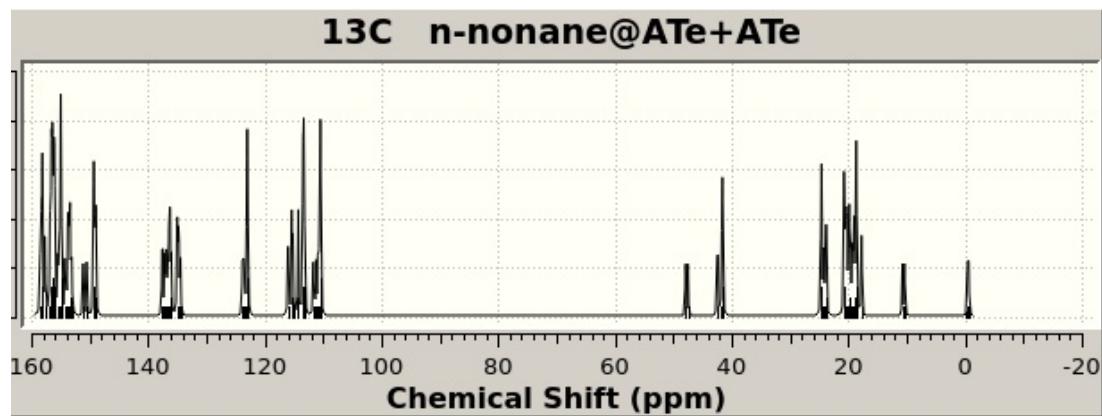
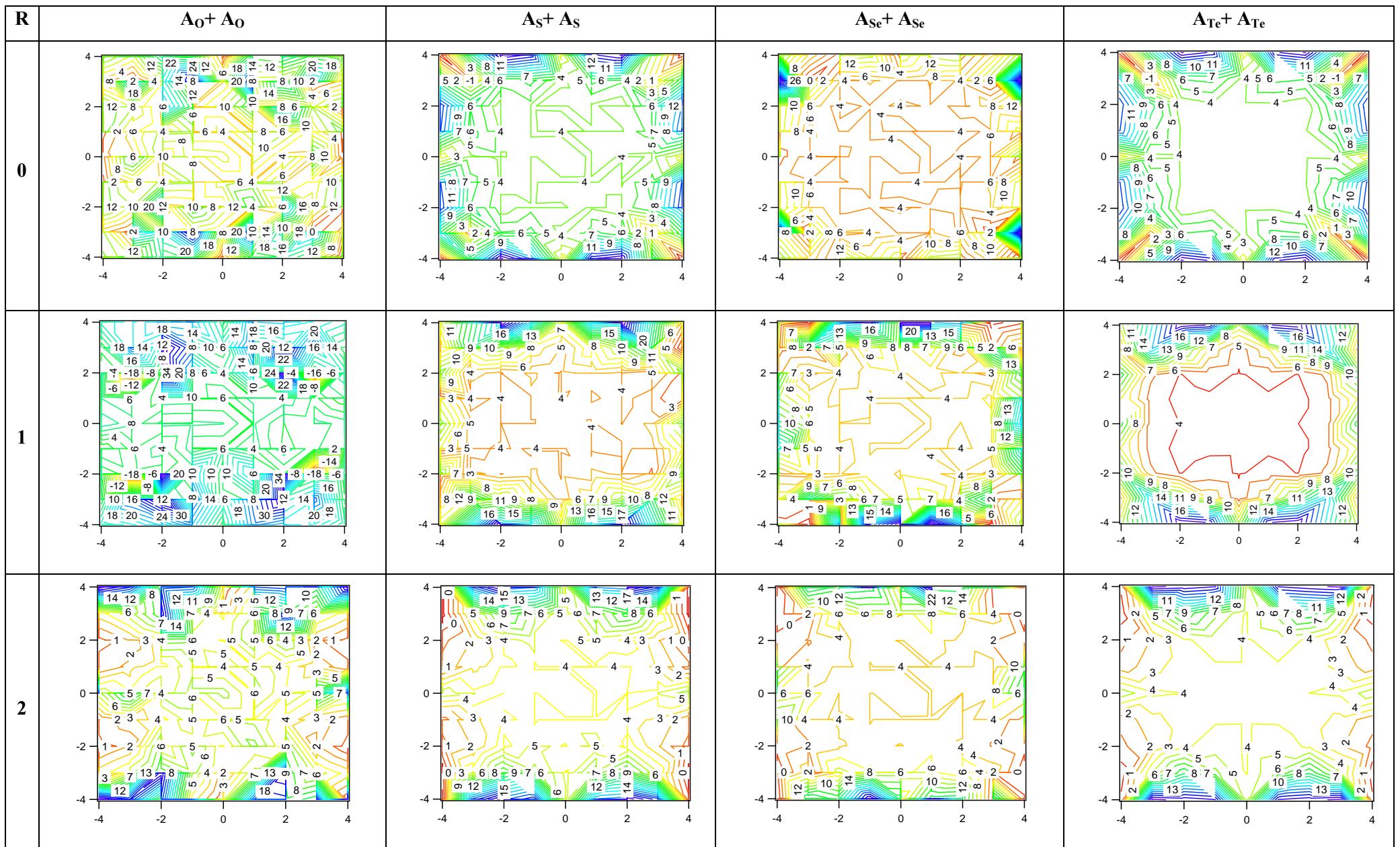
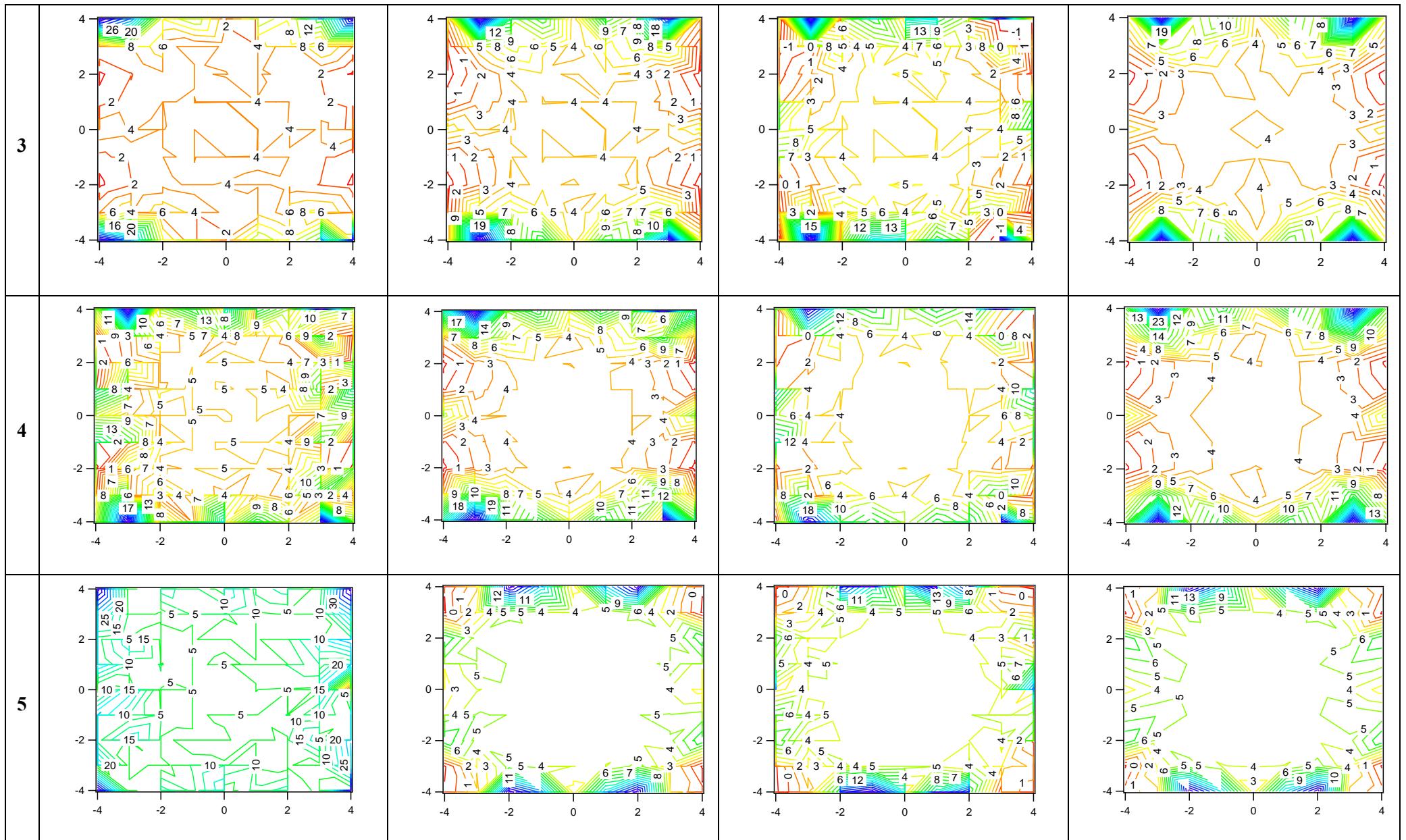


Figure 10S. ¹³C NMR spectra of the capsular complexes at the M06-2X/6-31G(d,p) level of theory. NMR shielding tensors have been computed with the Gauge-Independent Atomic Orbital (GIAO) method. Relative shifts are calculated with respect to the tetramethylsilane (TMS).





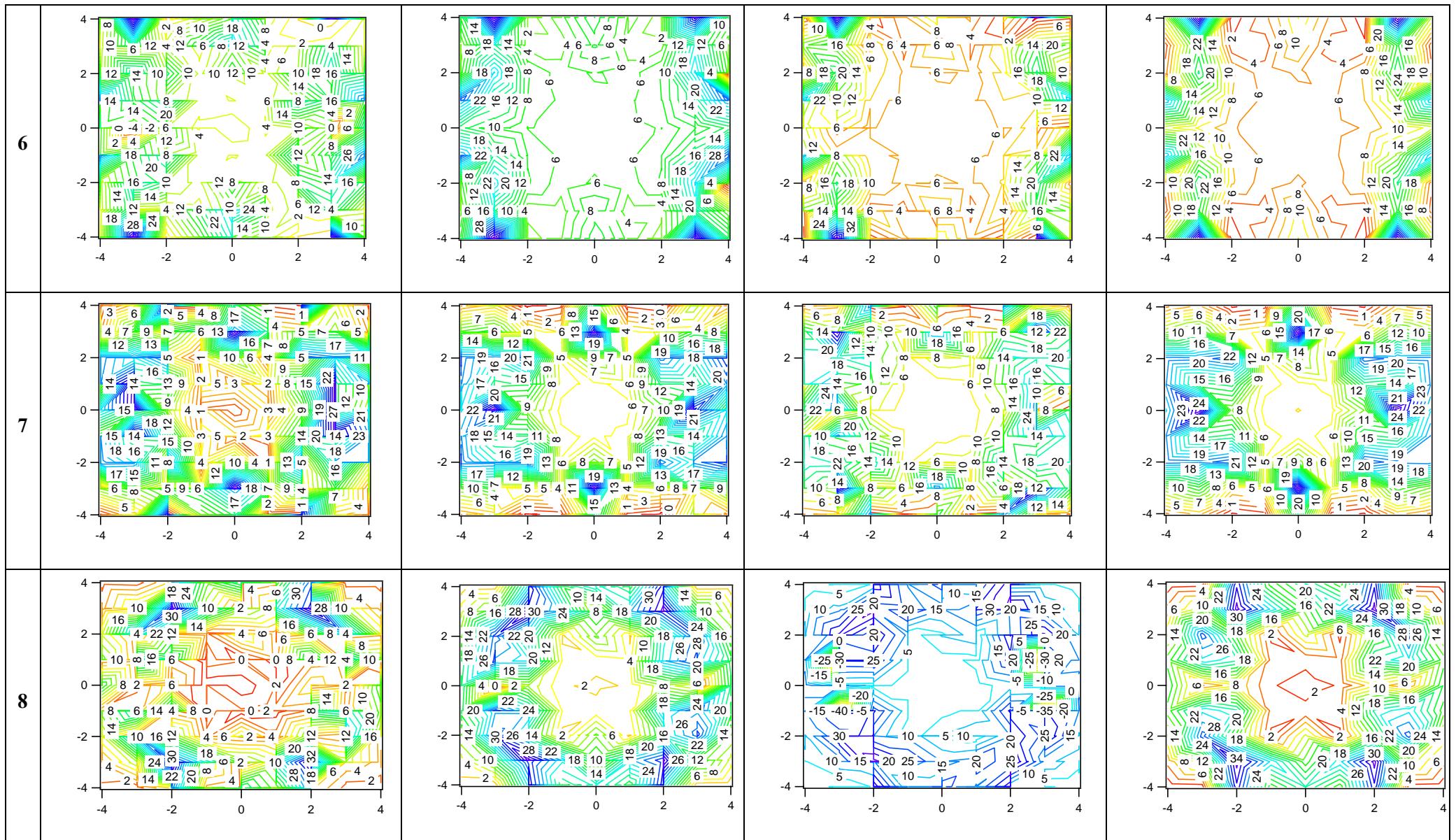
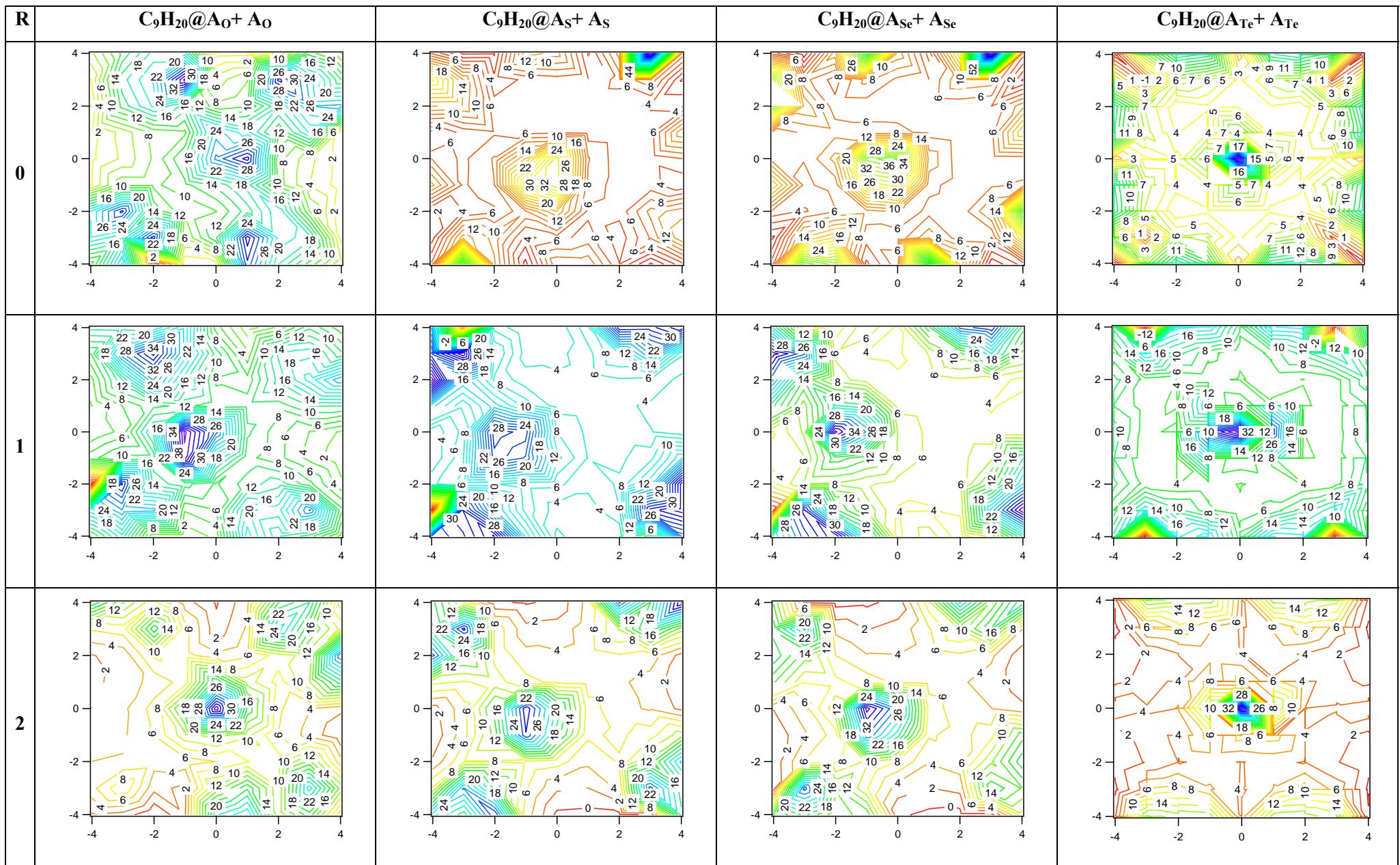
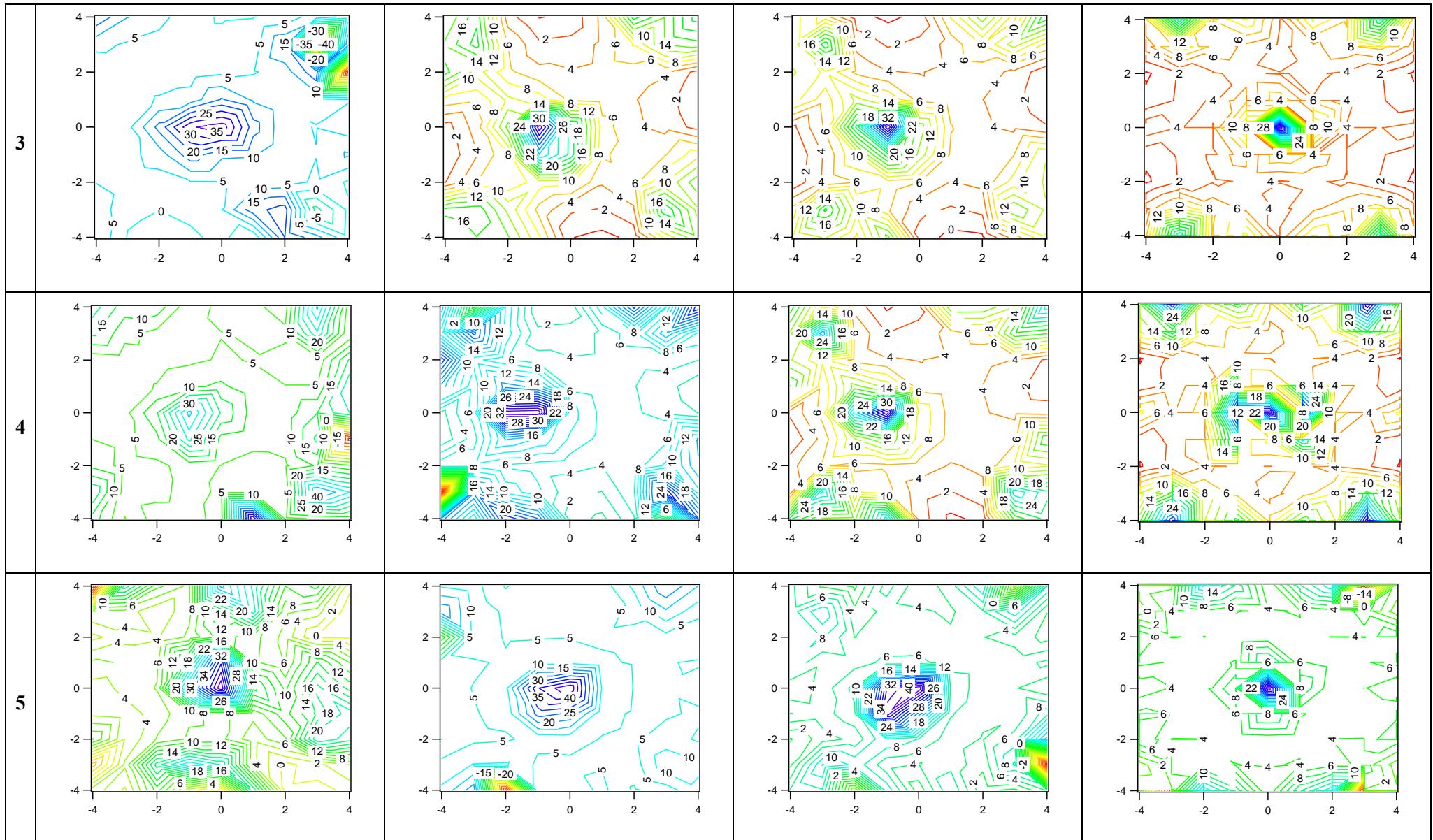


Figure 11S. Magnetic isotropy of $\text{A}_\text{X} + \text{A}_\text{X}$ complexes, where $\text{X} = \text{O}, \text{S}, \text{Se}$ and Te . Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.





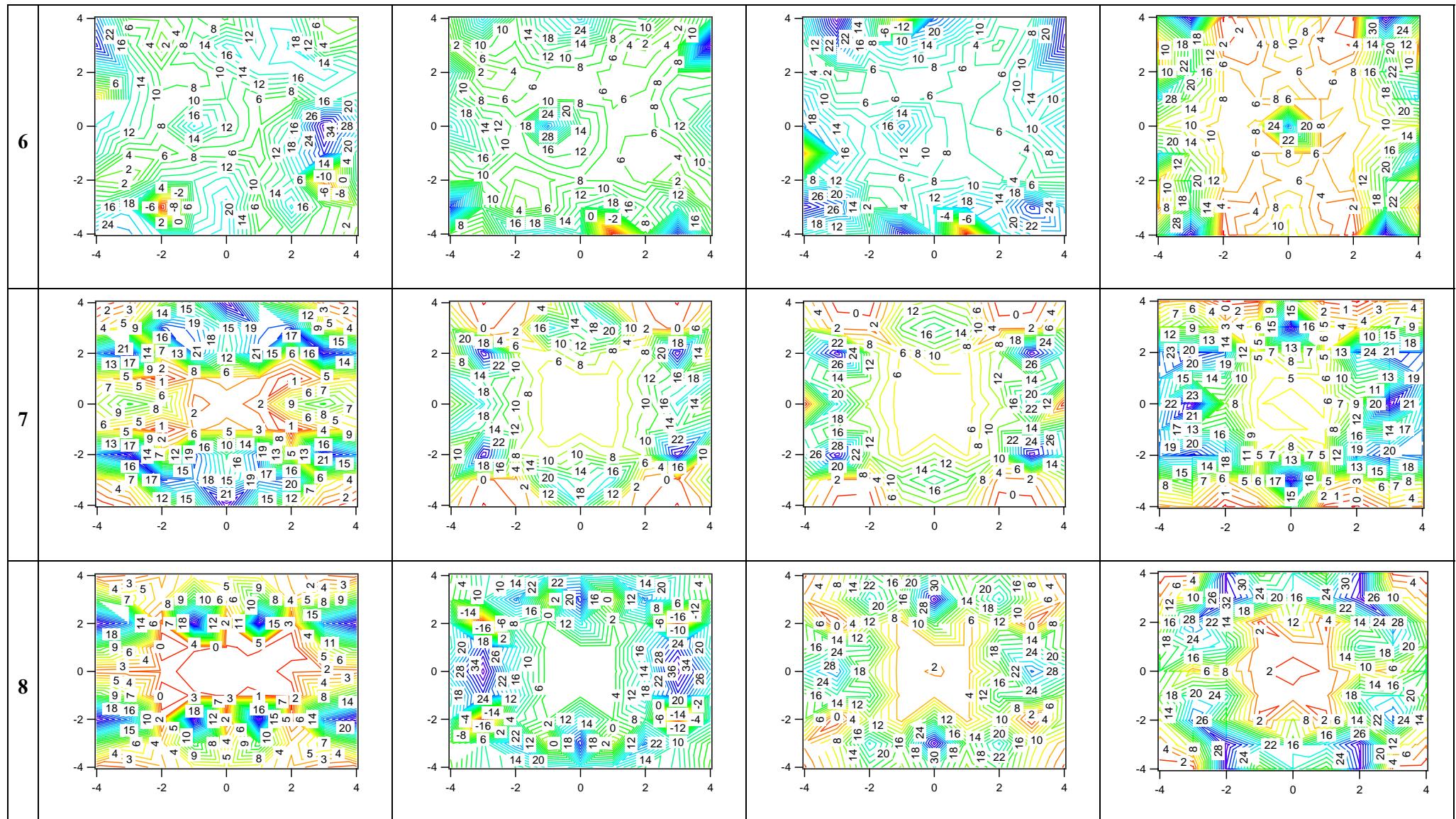
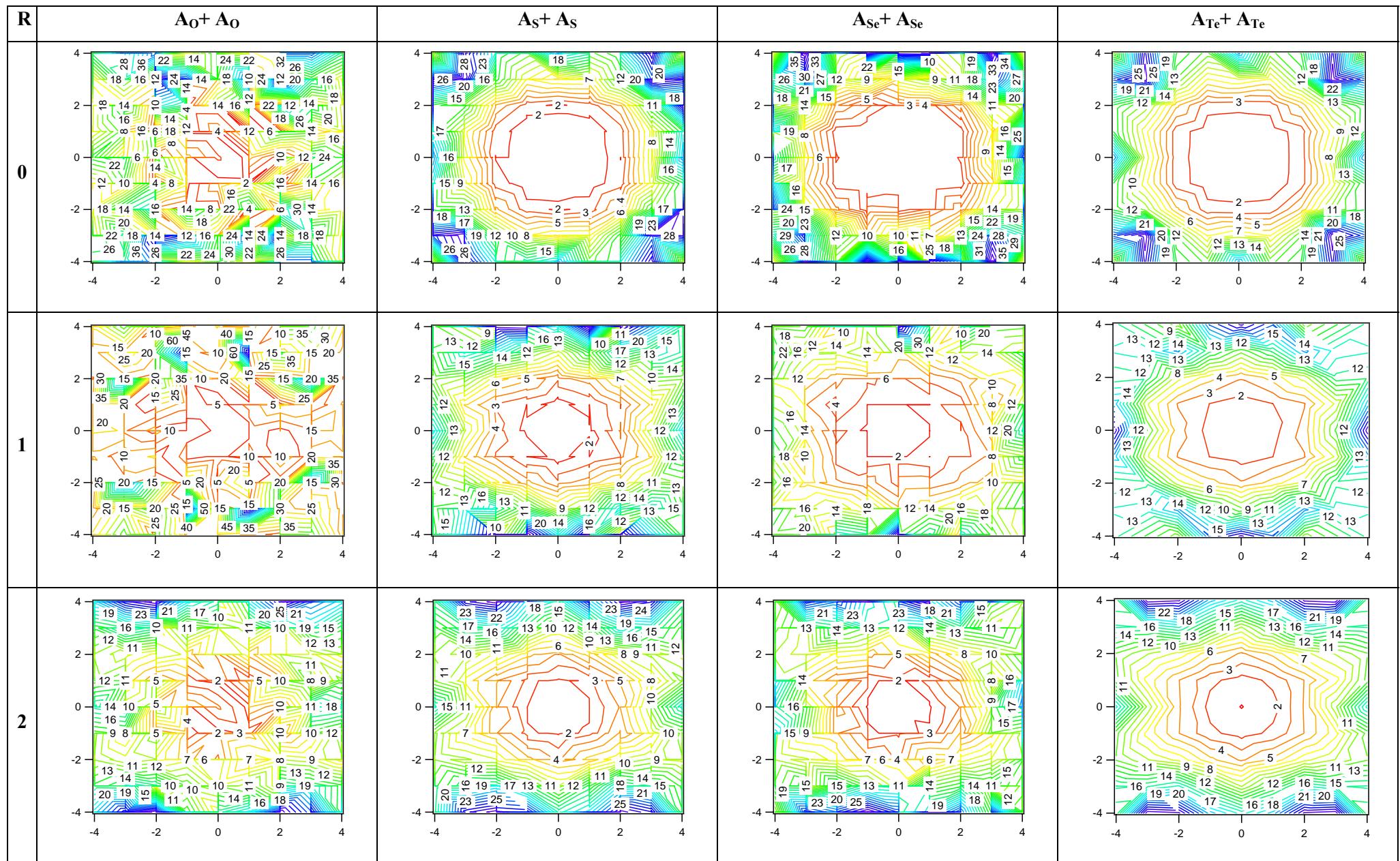
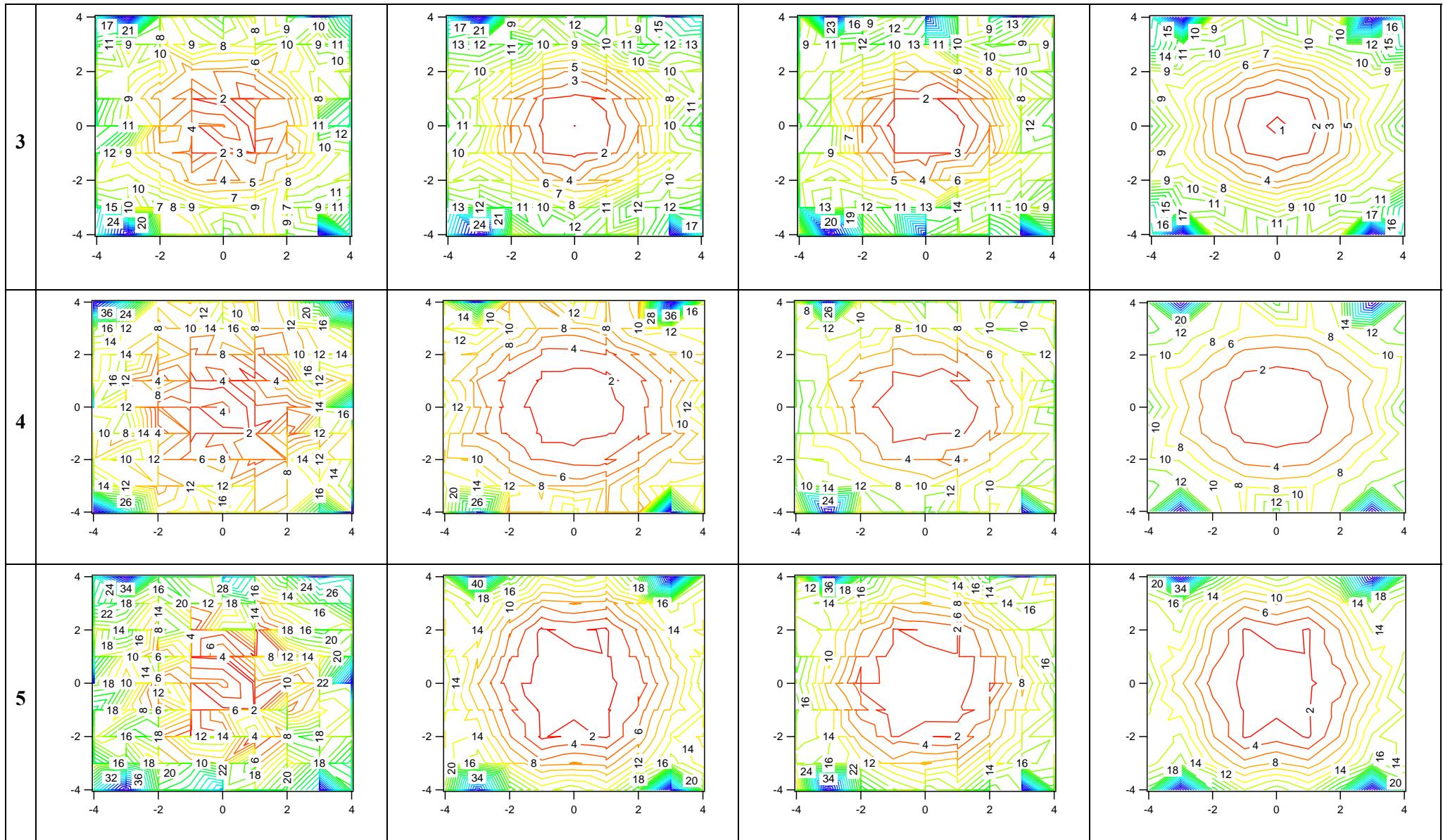


Figure 12S. Magnetic isotropy of $\text{C}_9\text{H}_{20}@\text{Ax} + \text{Ax}$ complexes, where X = O, S, Se and Te. Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.





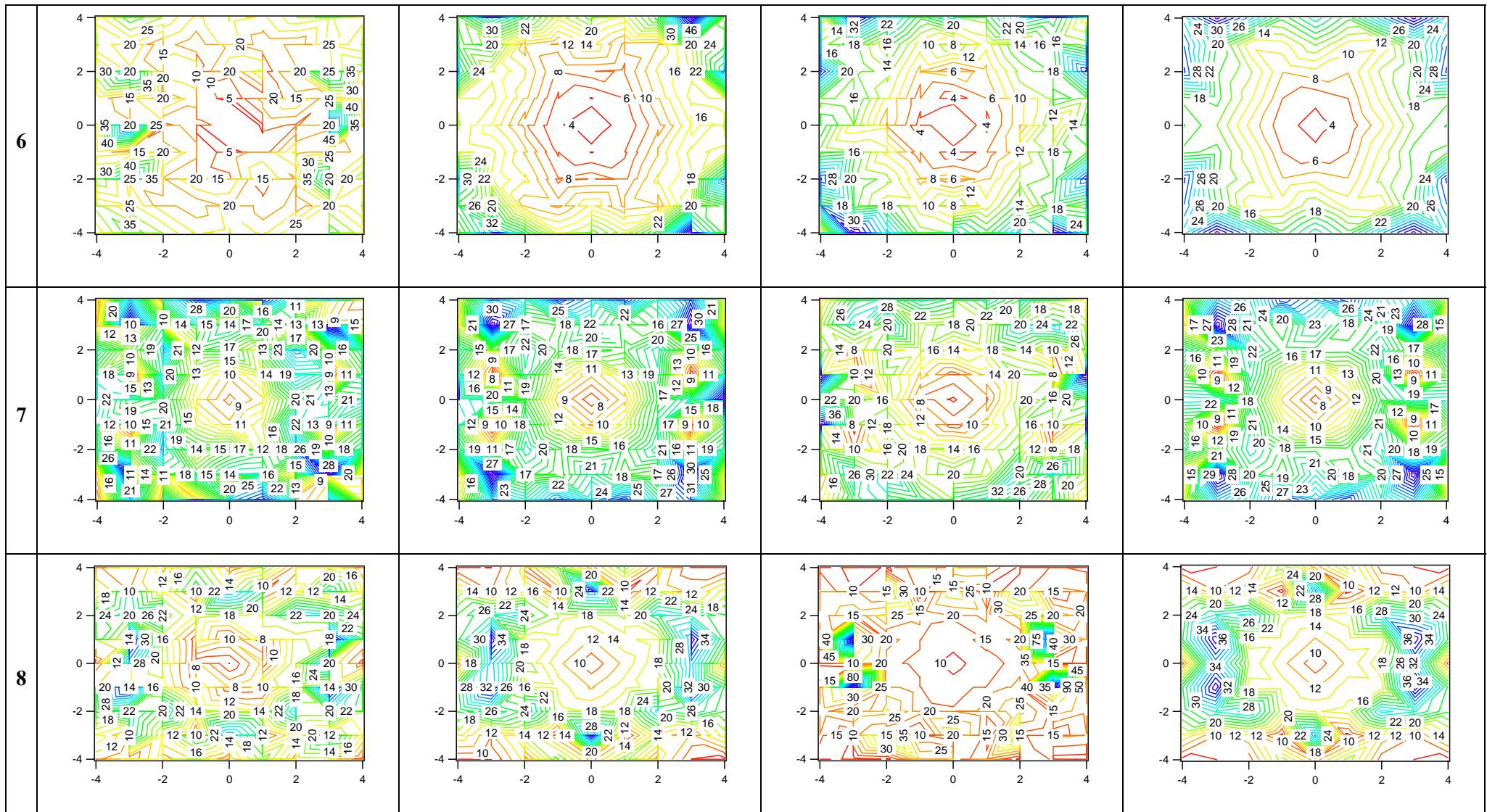
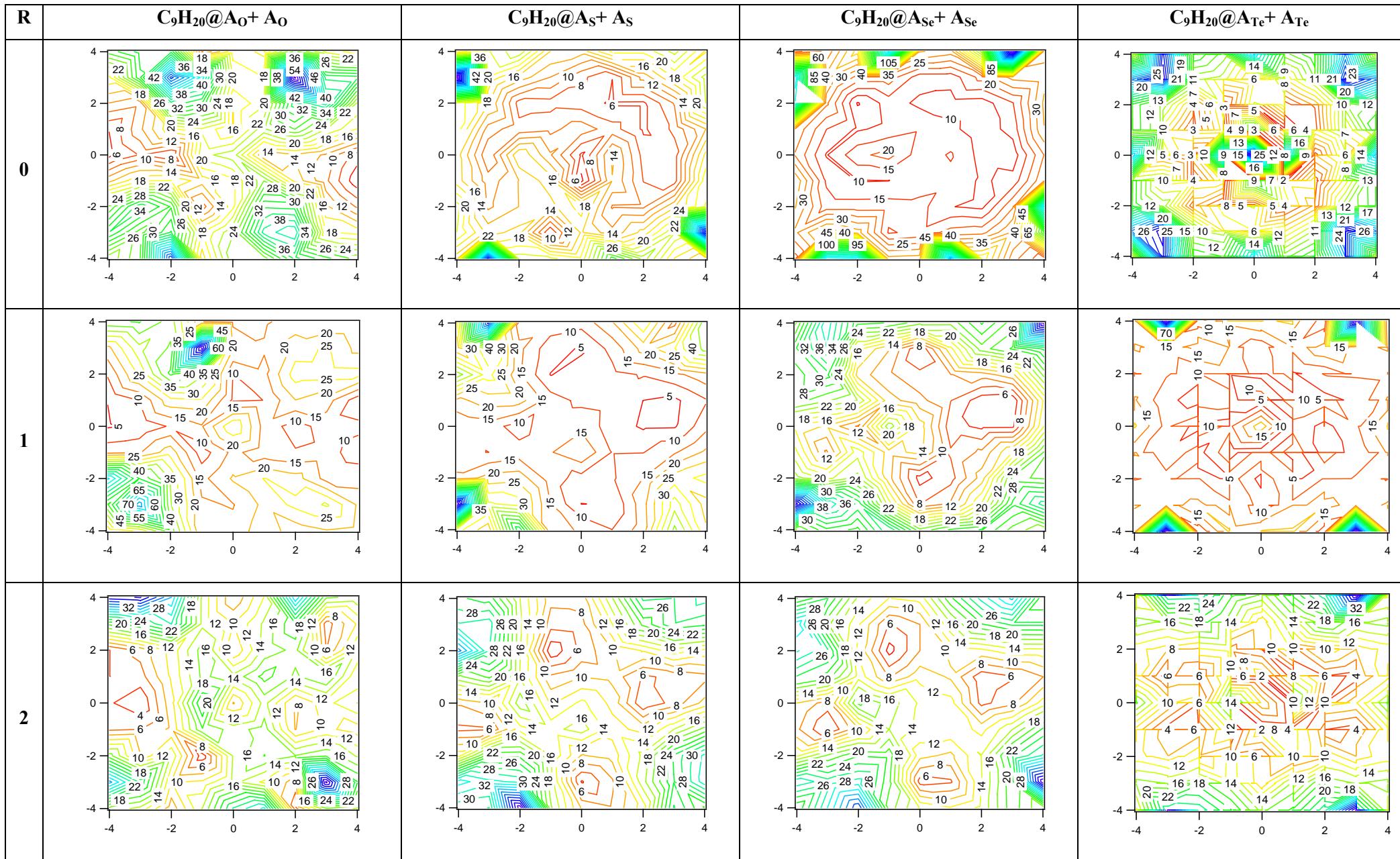
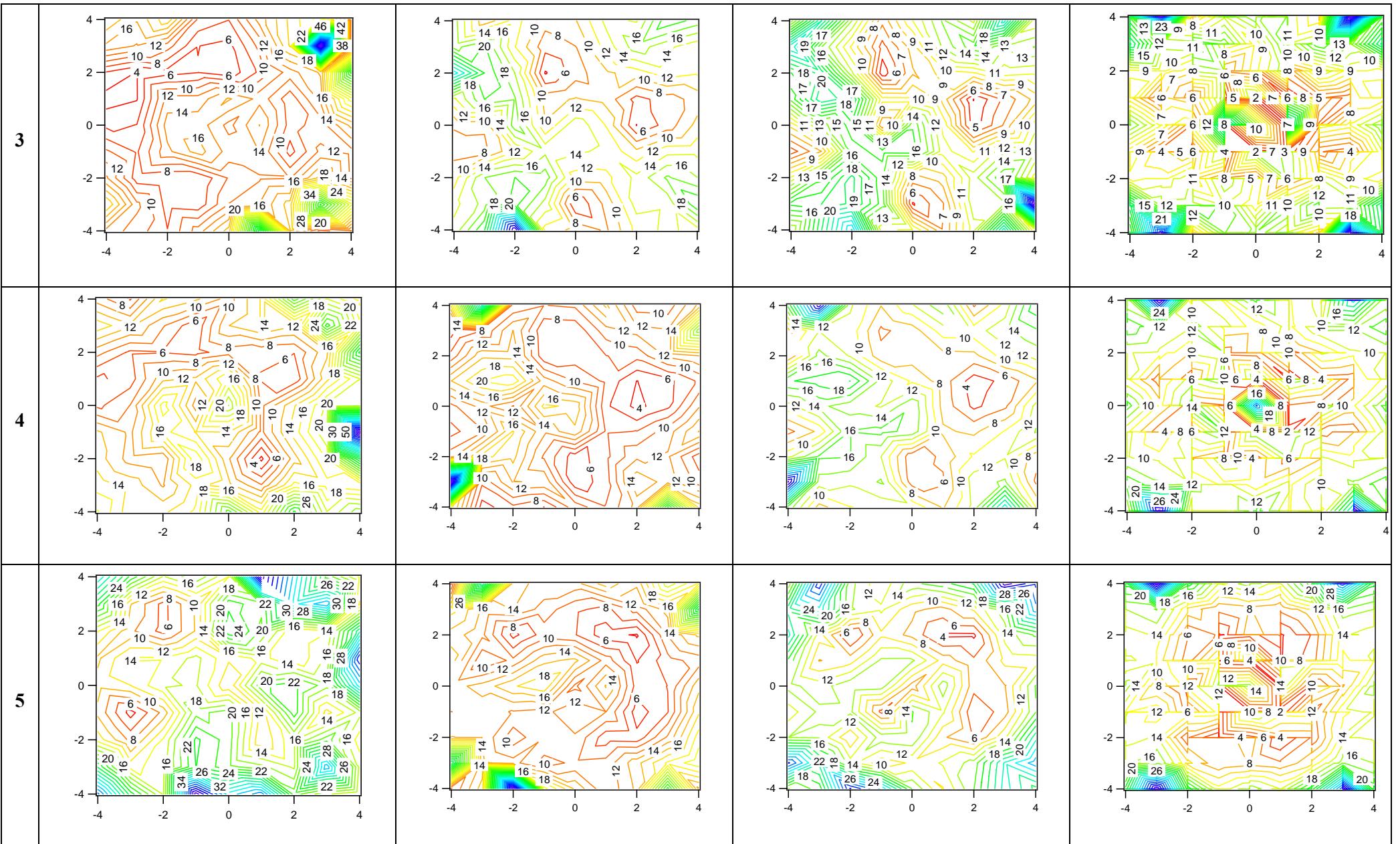


Figure 13S. Magnetic anisotropy of $\text{Ax} + \text{Ax}$ complexes, where $\text{X} = \text{O}, \text{S}, \text{Se}$ and Te . Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.





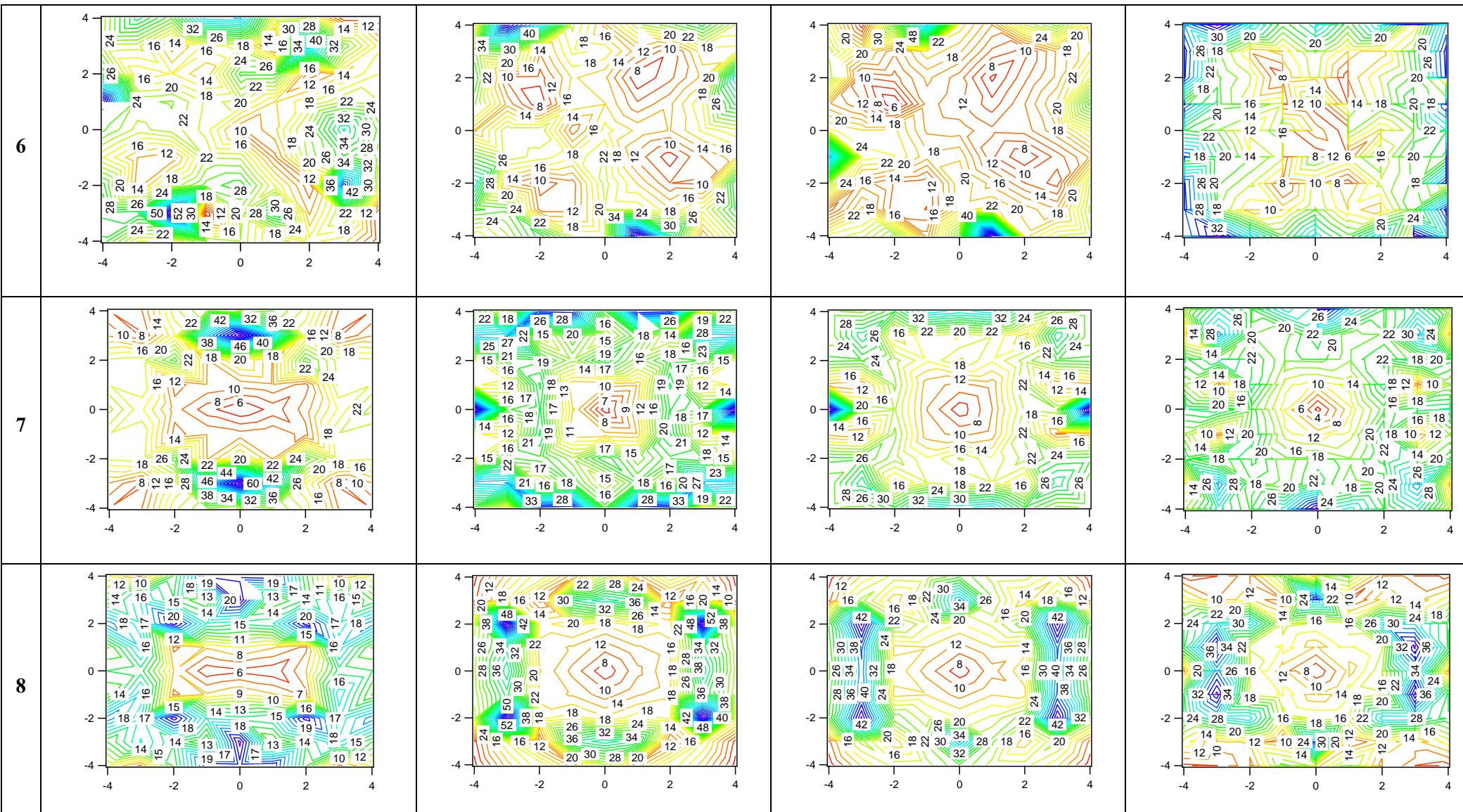
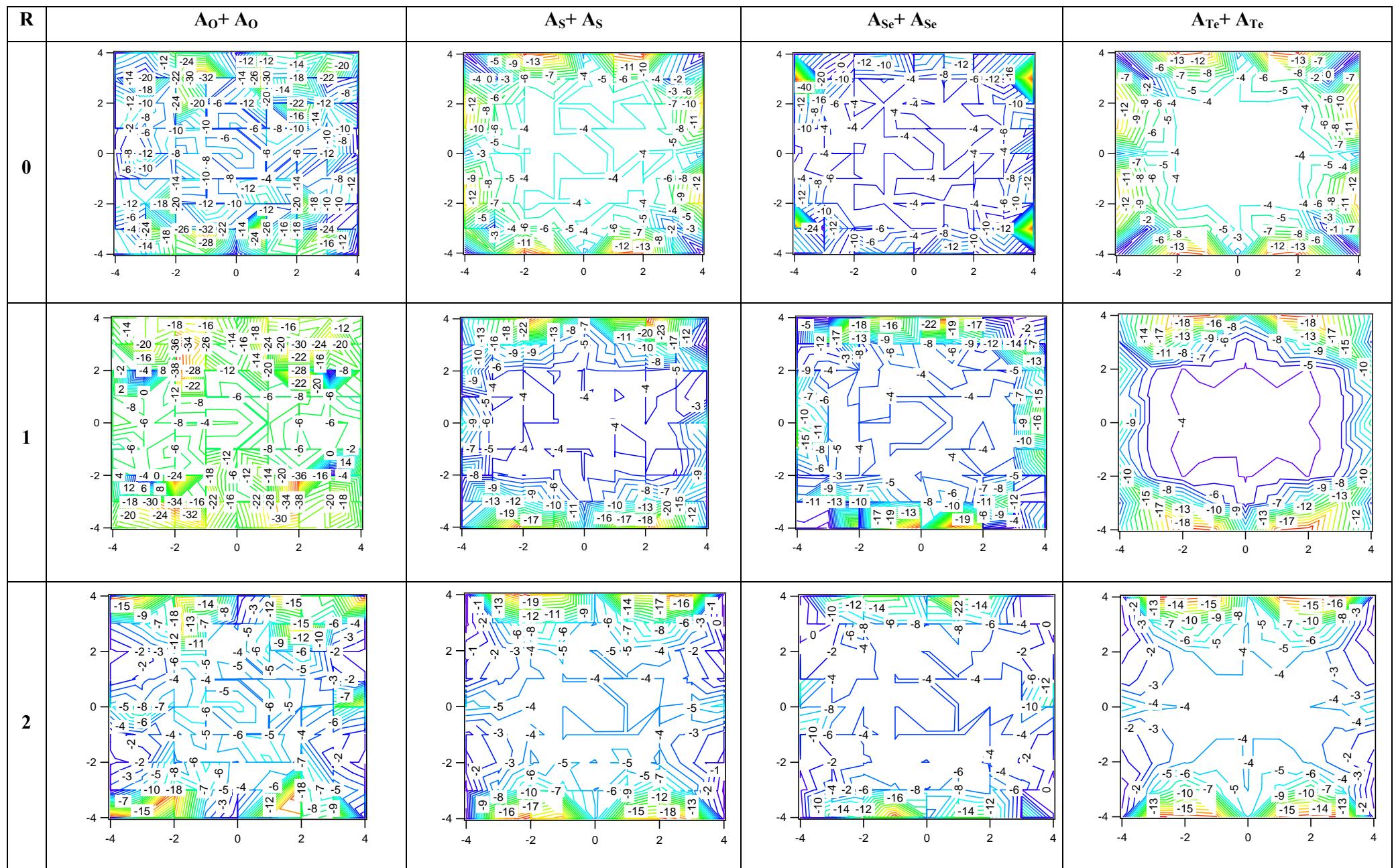
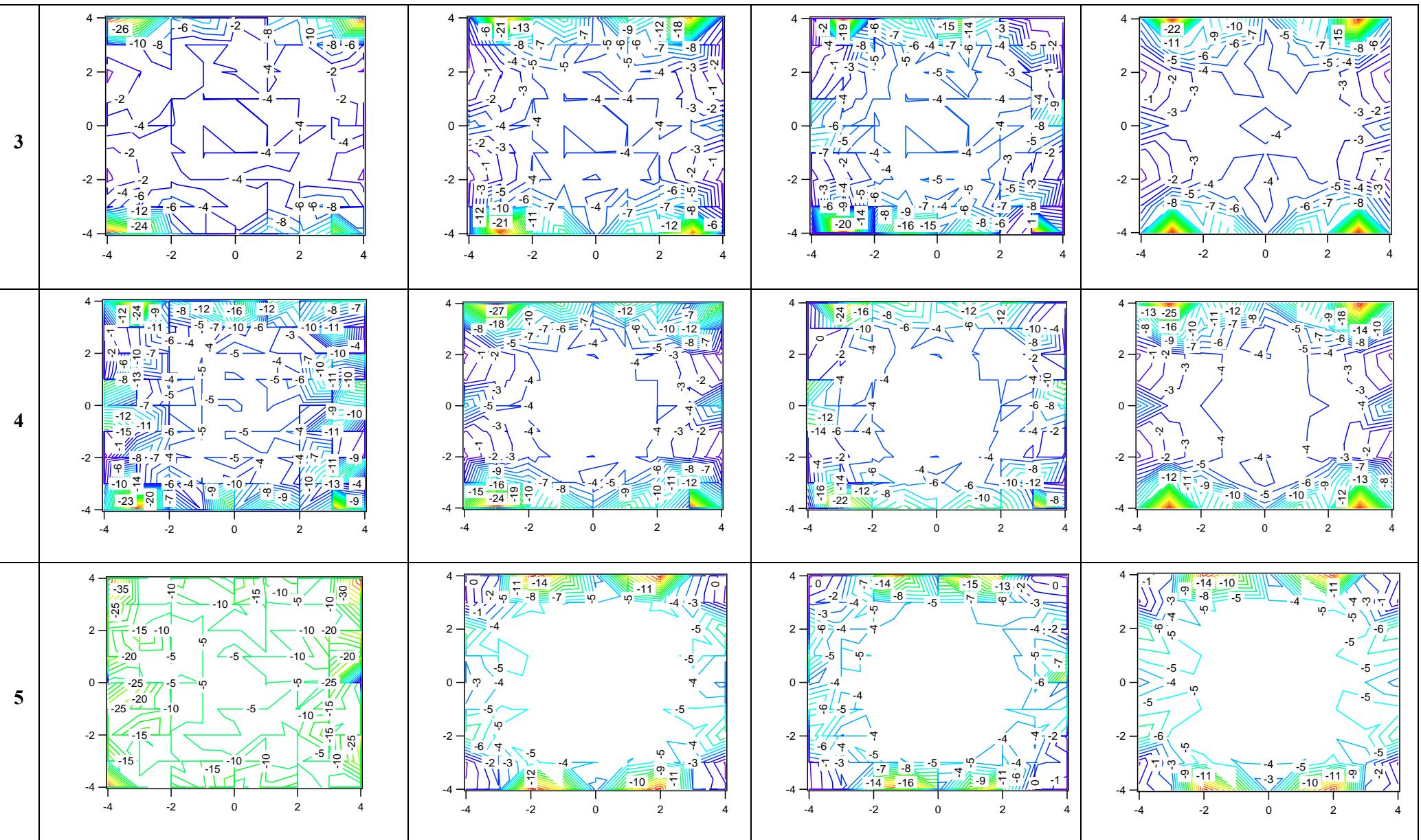


Figure 14S. Magnetic anisotropy of $\text{C}_9\text{H}_{20}@\text{Ax} + \text{Ax}$ complexes, where $\text{X} = \text{O}, \text{S}, \text{Se}$ and Te . Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.





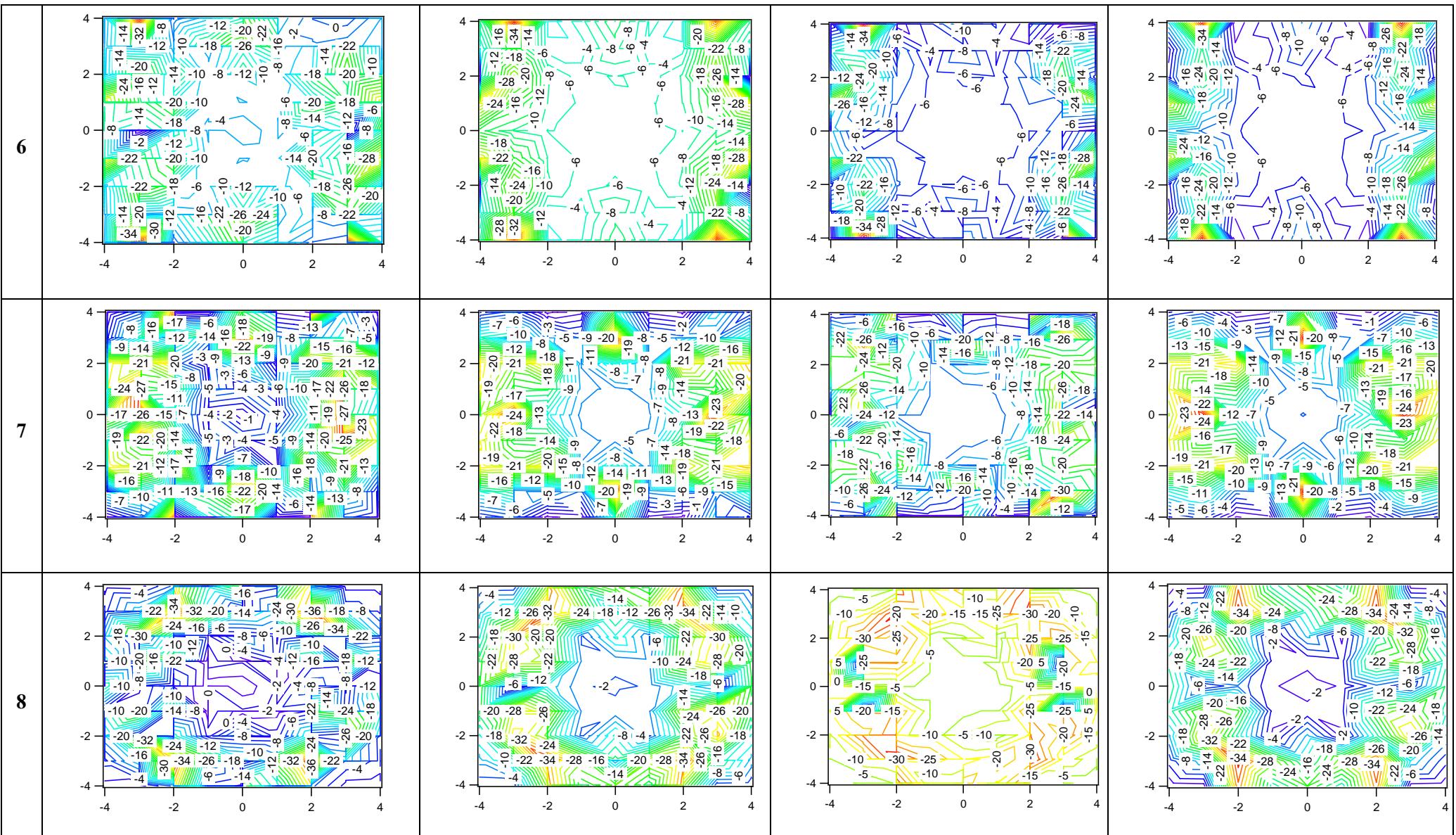
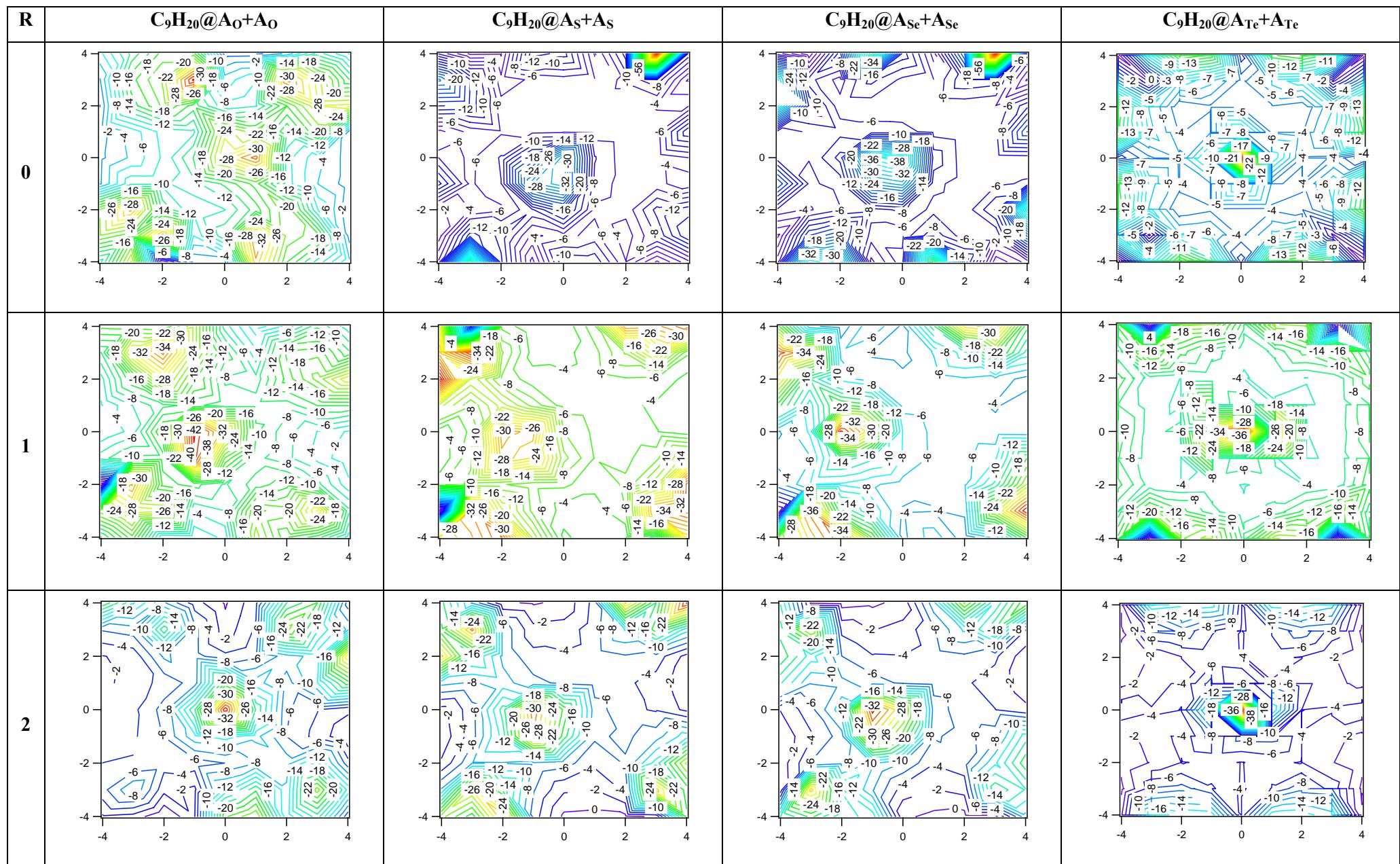
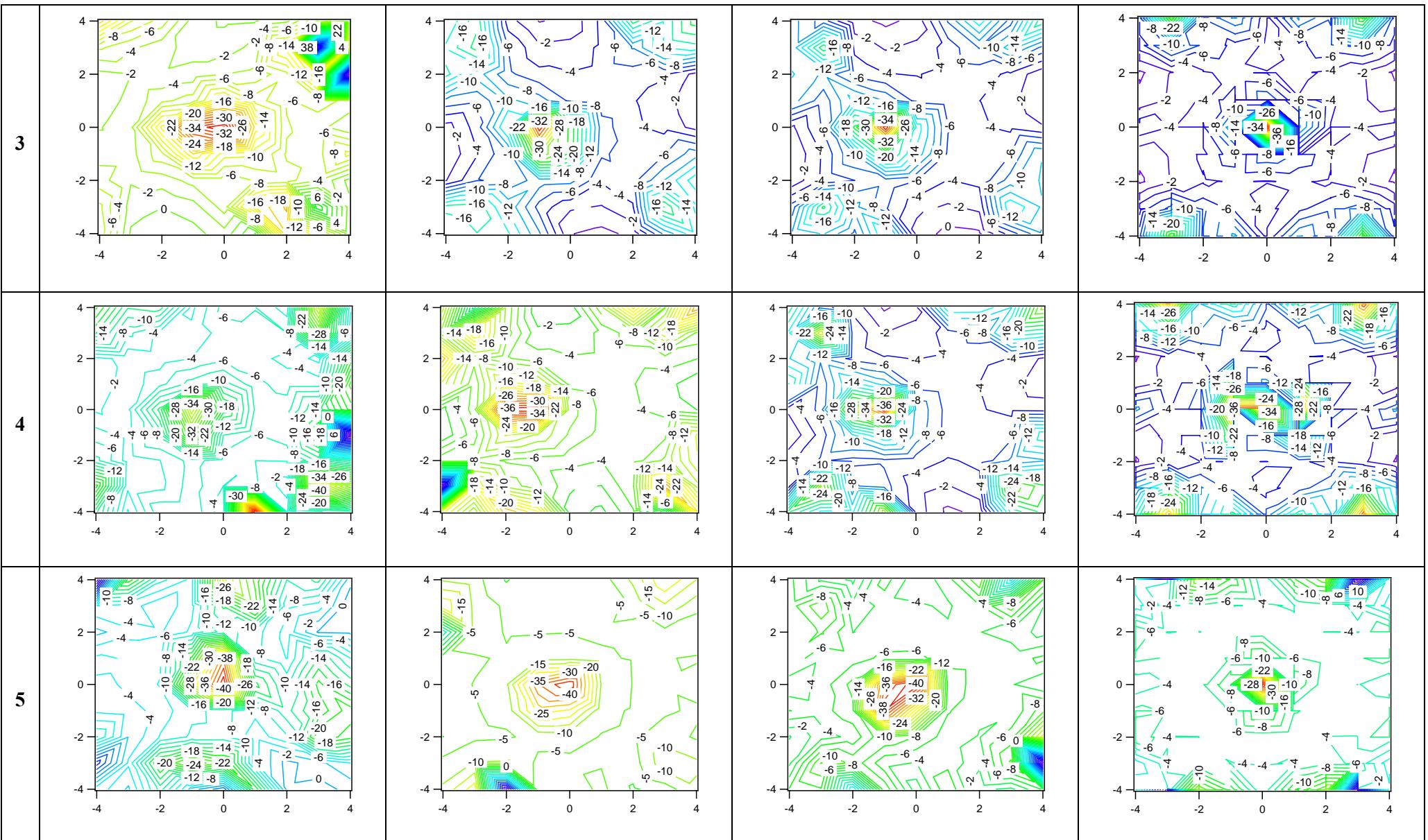


Figure 15S. NICS aromaticity indexes of $\mathbf{A}_X + \mathbf{A}_X$ complexes, where $X = \text{O}, \text{S}, \text{Se}$ and Te . Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.





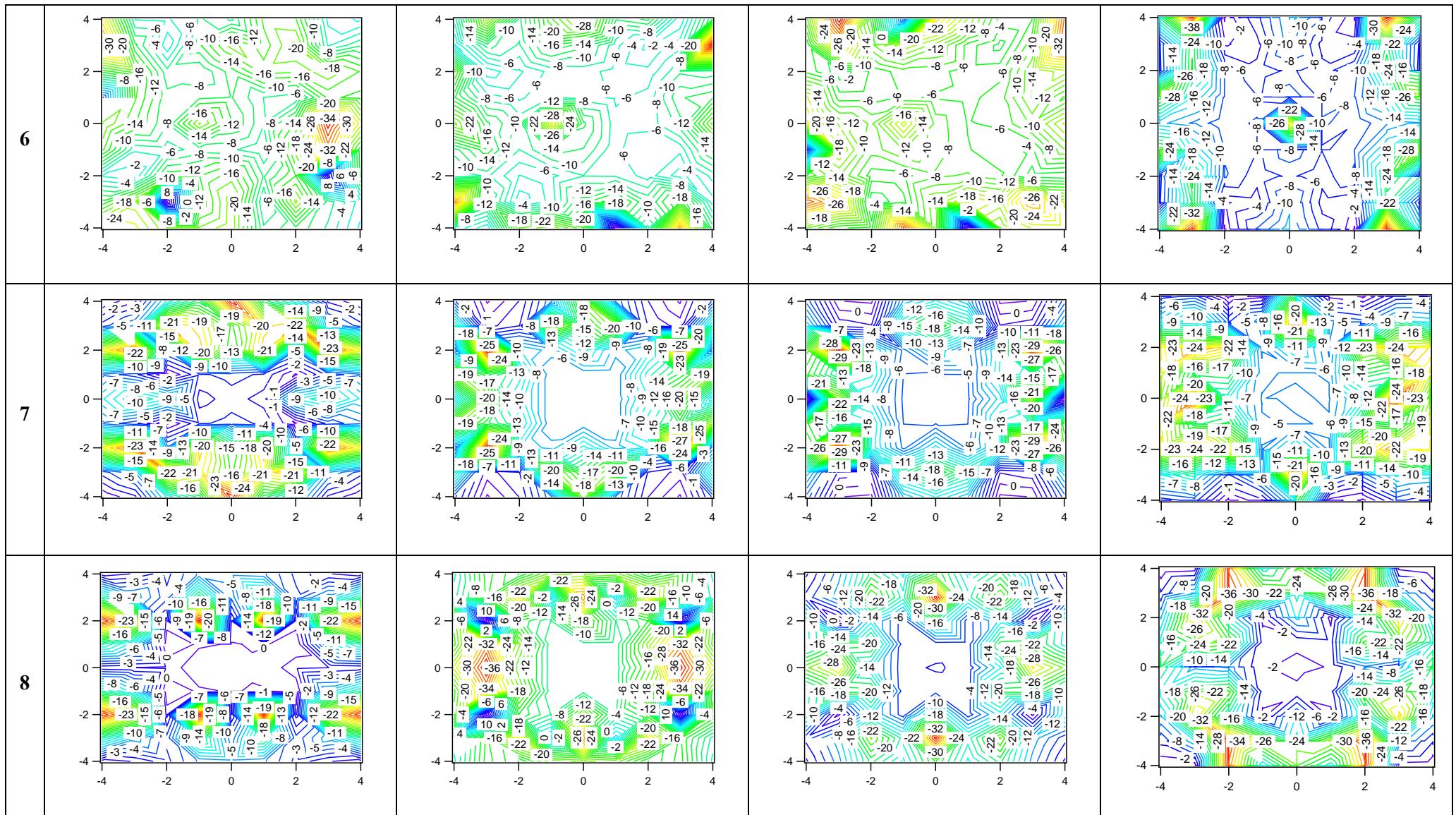


Figure 16S. NICS aromaticity indexes of $\text{C}_9\text{H}_{20}@\text{Ax} + \text{Ax}$ complexes, where $\text{X} = \text{O}, \text{S}, \text{Se}$ and Te . Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.