Supporting Information

The solvent effect on a styryl-bodipy derivative functioning as an AND molecular logic gate.

Demeter Tzeli[a,b] Ioannis D. Petsalakis[a] and Giannoula Theodorakopoulos[a]

[a] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece

[b] Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens 157 71, Greece

Table 1S. Dihedral angles (degrees), N-H^+ bond distances (Å), relative energies ΔE_1(eV) of the S_0 state at PBE0\6-31G(d,p) level of theory

Comp.	State	$C_1NC_2C_3^{(Ca)}$	$C_4NC_5C_6^{(Hg)}$	$C_7NC_8C_9^{(Zn)}$	$N\text{-}H^{(Ca)}$	$N\text{-}H^{(Hg)}$	$N\text{-}H^{(Zn)}$	ΔE_1	Conform.
1	S_0	161.8	169.8	127.7					
	S_1	160.6	172.4	128.5					
	S_2	174.3	168.0	128.4					
1-3W	S_0	160.5	168.6	136.8					
1-3H$^+$_a	S_0	129.3	130.5	130.5	1.032	1.041	1.047	0.00	in-in-in
	S_1	129.3	130.3	130.5	1.032	1.041	1.047		in-in-in
	S_2	129.4	130.2	130.5	1.032	1.041	1.047		in-in-in
1-3H$^+$_b	S_0	130.1	130.7	130.9	1.029	1.041	1.024	0.36	in-in-out
1-3H$^+$_c	S_0	129.5	130.5	140.8	1.031	1.022	1.047	0.51	in-out-in
1-3H$^+$_d	S_0	135.8	140.8	130.6	1.022	1.022	1.047	0.96	out-out-in
	S_1	135.9	141.0	130.6	1.022	1.022	1.047		out-out-in
1-Ca	S_0	127.2	169.3	178.4					
	S_1	127.1	172.1	179.4					
	S_2	127.6	173.4	179.0					
1-Ca-3W	S_0	156.6	168.4	129.9					
1-Ca-3H$^+$_a	S_0	127.0	132.0	130.6	1.026	1.040	1.047	0.00	in-in-in
	S_1	127.1	131.7	130.6	1.026	1.041	1.047		
	S_2	127.5	130.9	130.7	1.025	1.04	1.048		
1-Ca-3H$^+$_b	S_0	139.7	140.7	132.2	1.024	1.022	1.023	0.96	out-out-out
1-Ca-3H$^+$_1W	S_0	129.1	133.4	130.6	1.023	1.034	1.047		in-in-in
	S_1	129.0	133.5	130.6	1.023	1.034	1.047		
	S_2	128.2	133.6	130.6	1.027	1.034	1.047		
1-Ca-3H$^+$-3W	S_0	139.4	139.8	131.5	1.023	1.021	1.024		out-out-out
1-Zn	S_0	161.6	170.0	126.3					
	S_1	161.7	172.5	126.4					
	S_2	163.1	172.1	126.6					
1-Zn-3W	S_0	166.5	155.6	127.9				0.00	
1-Zn-3H$^+$_a	S_0	129.9	131.7	129.6	1.031	1.039	1.024	0.00	in-in-in
	S_1	129.8	131.8	129.3	1.031	1.039	1.024		
	S_2	130.1	130.6	132.2	1.029	1.039	1.025		
1-Zn-3H$^+$_b	S_0	132.6	134.4	140.2	1.024	1.024	1.024	0.77	out-out-out
1-Zn-3H$^+$-W	S_0	128.6	133.1	129.3	1.032	1.033	1.025		in-in-in
	S_1	128.6	133.4	129.6	1.032	1.034	1.025		
	S_2	128.6	133	131.2	1.032	1.035	1.025		
1-Zn-3H$^+$-3W	S_0	131.5	131.3	139.4	1.024	1.025	1.024		out-out-out

1-Hg	S_0	161.4	145.5	179.4					
	S_1	160.6	147.4	177.5					
	S_2	160.5	147.4	177.8					
1-Hg-3W	S_0	173.0	165.7	176.4					
1-Hg-3H$^+$_a	S_0	129.3	133.8	130.4	1.032	1.036	1.047	0.00	in-in-in
	S_1	129.2	133.8	130.5	1.032	1.036	1.047		
	S_2	129.3	133.2	130.6	1.032	1.036	1.049		
1-Hg-3H$^+$_b	S_0	132.4	133.4	130.8	1.023	1.025	1.024	1.03	out-out-out
1-Hg-3H$^+$-W	S_0	129.7	135.1	129.9	1.037	1.036	1.056		in-in-in
	S_1	129.6	134.1	130.0	1.037	1.036	1.056		
	S_2	129.5	133.2	129.9	1.037	1.038	1.057		
1-Hg-3H$^+$-3W_a	S_0	130.5	137.3	139.8	1.024	1.024	1.022	0.00	out-out-out
1-Hg-3H$^+$-3W_b	S_0	130.5	137.3	139.8	1.025	1.022	1.024	0.63	out-out-out
2	S_0	127.1	145.4	127.3					
	S_1	124.0	147.0	128.2					
	S_2	125.1	154.4	127.4					
2-3W	S_0	126.9	143.1	129.0					
2-3H$^+$_a	S_0	128.9	134.5	129.2	1.025	1.035	1.025	0.00	in-in-in
	S_1	129.8	134.0	130.1	1.025	1.033	1.024		
	S_2	130.9	133.8	129.4	1.025	1.033	1.024		
2-3H$^+$_b	S_0	131.4	132.7	140.2	1.038	1.041	1.039	0.26	out-out-out
2-3H$^+$_c	S_0	131.0	132.6	140.1	1.024	1.024	1.023	0.28	out-out-out
2-3H$^+$-3W_a	S_0	130.0	134.3	130.6	1.025	1.037	1.025	0.00	in-in-in
2-3H$^+$-3W_b	S_0	131.0	133.7	139.3	1.025	1.025	1.024	0.18	out-out-out

Table 2S. Van der Waals bond distances between water and **1**, **1-Ca^{2+}**, **1-Zn^{2+}**, **1-Hg^{2+}**, and **2** species at the S_0 state PBE0\6-31G(d,p) level of theory.

	M…OH$_2$	**CH…OH$_2$**	**HOH…C**	**CH…OH$_2$**	**S…HOH**	**HOH…O**	**HOH…C**	**H…N**	**H…N**	**O…HC**
		AC		**DSC**				**DPA**		
1-3W		2.756	2.258	2.504			2.441	1.966	1.955	
1-Ca^{2+}_3W	2.435		2.231	2.447	2.472		2.478	1.962	1.963	
1-Ca^{2+}-3H^{+}_3W	2.432	2.639		2.322,2.455		2.014		1.892		2.454
		HOH…O	**HOH…O**							
1-Zn^{2+}_3W	2.035	2.032	1.955	2.334	2.377		2.573			
1-Zn^{2+}-3H^{+}_3W	1.975	2.016	1.912	2.353,2.244,2.443	2.949	1.911				
		HOH…O	**CH…OH$_2$**							
1-Hg^{2+}_3W	2.572	1.875	2.071					1.868		2.144
1-Hg^{2+}-3H^{+}_3W	2.507	1.917,1.999						1.850		2.301

Table 3S. Vertical and adiabatic excitation energies [corrected values with respect to cLR approach] in eV of the two lowest excited states at the PBE0\6-31G(d,p) level of theory

Comp.	$S_0 \rightarrow S_{em}$ [a]	$S_0 \rightarrow S_{CT}$ [a]	$S_{em} \rightarrow S_0$	$S_{CT} \rightarrow S_0$	$S_0 \rightarrow S_{em}$	$S_0 \rightarrow S_{CT}$
	vert	**vert**	**vert**	**vert**	**adiab**	**adiab**
1	1.80(1.98)[2.06]	2.20(2.20)	1.62[1.91]	1.83[1.26]	1.71[1.99]	2.00[1.43]
1-3H$^+$_a	1.94(2.15)[2.25]	3.17(3.17)	1.74[2.08]	2.87[2.88]	1.84[2.17]	3.02[3.02]
1-Ca^{2+}	1.67(1.85)[1.93]	2.41(2.50)	1.52[1.78]	2.27[2.24]	1.59[1.86][1.95[b]]	2.33[2.30][1.61[b]]
1-Ca^{2+}-3H$^+$	1.93(2.14)[2.24]	3.16(3.17)	1.74[2.08]	2.86[2.87]	1.83[2.17]	3.05[3.06]
1-Ca^{2+}-3H$^+$-1W	1.94(2.15)[2.25]	3.17(3.18)	1.75[2.08]	2.88[2.88]	1.84[2.18]	3.00[3.00]
1-Zn^{2+}	1.79(1.97)[2.04]	2.14(2.14)	1.61[1.87]	1.60[1.21]	1.69[1.96]	1.70[1.31]
1-Zn^{2+}-3H$^+$	1.97(2.17)[2.27]	2.69(2.69)	1.77[2.08]	2.10	1.87[2.18]	2.37
1-Zn^{2+}-3H$^+$-1W	1.94(2.15)[2.25]	2.76(2.76)	1.74[2.07]	2.16	1.83[2.17]	2.49
1-Hg^{2+}	1.74(1.91)[1.99]	2.06(2.06)	1.57[1.85]	1.58[1.24]	1.66[1.93]	1.65[1.55]
1-Hg^{2+}-3H$^+$	1.94(2.15)[2.25]	2.65(2.65)	1.75[2.08]	2.33	1.84[2.18]	2.45
1-Hg^{2+}-3H$^+$-1W	1.97(2.18)[2.28]	2.84(2.84)	1.77[2.10]	2.29	1.87[2.20]	2.43
2	1.88(2.15)[2.24]	2.24(2.43)	1.91[2.00]	1.98[2.10]	1.90[2.16]	2.20[2.40]
2-3H$^+$	2.04	2.69	1.69[1.99]	1.83	1.99	2.30

[a] 20 singlet excited states were calculated (3, 10, 15, and 30 singlet excited states were calculated). [b] In **1-Ca^{2+}**-1W.

Table 4S. Absorption maxima, λ_{max} (nm), vertical excitation energies ΔE_v^a ΔE_v(eV) $S_0 \rightarrow S_x$ absorption maxima, f-Values for absorption, main excitations and their coefficients contributing to the excited state of protonated, un-protonated, complexed with water of **1**, **1-M^{2+}**, and **2** in water solvent (acetonitrile solvent[a]) at the PBE0/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ level of theory.

	State	λ_{max}	ΔE_v^a	f	Excitations	λ_{max}	ΔE_v^a
				Uncorrected data		cLR[f]	
1	S_1	624.2	1.9861	1.1413	0.999|H→L>	601.3	2.0620
	S_2	563.4	2.2005	0.0471	0.992|H-1→L>		
	S_3	449.7	2.7569	0.4599	0.964|H-2→L>		
	S_9	345.5	3.5886	1.0178	0.826|H-6→L+1>+0.357|H→L+1>		
	Expt[b]	692	1.79				
1-w	S_1	624.9	1.9840	1.1518	0.999|H→L>	601.5	2.0612
	S_2	564.8	2.1951	0.0525	0.993|H-1→L>		
	S_3	464.2	2.6710	0.7923	0.989|H-2→L>		
	S_4	382.4	3.2420	1.1959	0.969|H→L+1>		
1-3H$^+$	S_1	577.2	2.1482	1.0801	0.999|H→L>	550.8	2.2511
	S_2	391.6	3.1663	0.0127	0.610|H-2→L> + 0.432|H-2→L> -0.655|H→L+1>		
	S_3	380.7	3.2565	0.0348	0.985|H-4→L>		
	S_4	377.1	3.2880	1.0230	0.783|H-1→L>+0.601|H→L+1>		
	S_5	368.6	3.3634	1.3574	0.777|H-2→L> -0.429|H-1→L> +0.445|H→L+1>		
1-Ca^{2+}	S_1	678.1	1.8285	1.0574	0.999|H→L>	651.7	1.9024
1-Ca^{2+}-1W	S_1[c]	643.2	1.9275	1.1121	0.999|H→L>	618.3	2.0053
1-Ca^{2+}-1W	S_1[d]	631.1	1.9647	1.1461	1.000|H→L>	608.0	2.0393
	S_2	503.6	2.4620	0.7720	0.982|H-1→L>		
	S_4	373.7	3.3174	1.6024	0.937|H→L+1>		
	Expt[b]	672	1.85				
1-Ca^{2+}	S_1	669.7	1.8514	1.0915	0.999|H→L>	643.3	1.9273
	S_2	496.3	2.4980	0.7355	0.980|H-1→L>		
	S_3	402.2	3.0831	0.0710	0.962|H-2→L>		
	S_4	388.7	3.1896	1.5984	0.988|H→L+1>		
1-Ca^{2+}-3H$^+$	S_1	579.3	2.1403	1.0810	1.000|H→L>	552.5	2.2441
	S_2	392.1	3.1624	0.0407	0.737|H-2→L> -0.621|H→L+1>		
	S_3	382.2	3.2444	0.0626	0.901|H-1→L>		
	S_5	373.0	3.3236	2.2965	0.737|H→L+1> +0.655|H-2→L>		
1-Ca^{2+}-3H$^+$-1W	S_1	577.6	2.1467	1.1139	1.000|H→L>	550.7	2.2512
	S_2	390.9	3.1721	0.0162	0.662|H→L+1> -0.452|H-3→L>+0.499|H-2→L>		
	S_3	380.2	3.2608	0.0314	0.990|H-4→L>		
	S_4	372.9	3.3252	2.1391	0.724|H→L+1>-0.520|H-1→L>		
1-Zn^{2+}	S_1	629.4	1.9700	1.1172	0.998|H→L>	607.3	2.0416
	S_3	450.6	2.7516	0.4263	0.991|H-1→L>		
	S_6	382.3	3.2429	0.6807	0.811|H→L+3>+0.474|H-3→L>		
	Expt[b]	668	1.86				
1-Zn^{2+}	S_1	629.2	1.9704	1.1364	0.998|H→L>	606.7	2.0437
	S_2	579.6	2.1393	0.0479	0.993|H-1→L>		
	S_6	393.4	3.1518	1.1761	0.971|H→L+3>		
1-Zn^{2+}-3H$^+$	S_1	570.7	2.1725	0.8668	0.999|H→L>	547.2	2.2657
	S_2	461.2	2.6881	0.0010	0.998|H→L+1>		

	S_6	368.9	3.3611	1.6592	0.712|H→L+3>-0.637|H-1→L>		
1-Zn^{2+}-3$H^+$$_{(out)}$	S_1	558.1	2.2215	1.1199	0.998|H→L>		
	S_2	442.0	2.8049	0.0001	0.995|H→L+1>		
	S_3	405.5	3.0578	0.0335	0.990|H-1→L>		
	S_8	364.4	3.4022	2.1681	0.700|H-3→L>-0.694|H→L+3>		
1-Zn^{2+}-3H^+-1W	S_1	578.0	2.1452	1.1278	1.000|H→L>	551.3	2.2490
	S_2	449.5	2.7583	0.0010	0.997|H→L+1>		
	S_6	373.2	3.3223	1.7084	0.626|H→L+3>-0.614|H-1→L>		
1-Hg^{2+}	S_1	665.5	1.8631	0.0330	0.897|H→L>		
	S_2	643.2	1.9276	1.0263	0.913|H→L+1>	619.3	2.0021
	S_3	559.2	2.2174	0.1017	0.809|H-1→L+1>		
	S_6	468.4	2.6472	0.5346	0.866|H-2→L>		
	S_9	371.9	3.3340	1.7047	0.938|H→L+2>		
	Expt[b]	630	1.97				
1-Hg^{2+}	S_1	646.2	1.9187	1.0549	0.998|H→L>	622.1	1.9930
	S_2	600.8	2.0636	0.0014	0.971|H→L+1>		
	S_3	557.2	2.2251	0.1488	0.985|H-1→L>		
	S_4	486.6	2.5482	0.9547	0.984|H-2→L>		
	S_8	386.8	3.2053	1.5757	0.984|H→L+2>		
1-Hg^{2+}-3H^+	S_1	577.6	2.1465	1.0963	1.000|H→L>	551.1	2.2499
	S_2	467.4	2.6528	0.0001	0.999|H→L+1>		
	S_3	391.0	3.1706	0.0005	0.734|H→L+2>-0.669|H-1→L>		
	S_4	381.3	3.2517	0.0289	0.989|H-3→L>		
	S_5	372.3	3.3306	2.4130	0.671|H→L+2>+0.731|H-1→L>		
1-Hg^{2+}-3H^+-1W	S_1	569.7	2.1762	1.0574	1.000|H→L>	544.4	2.2776
	S_2	437.2	2.8360	0.0001	0.999|H→L+1>		
	S_3	385.9	3.2129	0.0055	0.688|H→L+2>+0.717|H-1→L>		
	S_4	380.8	3.2561	0.0291	0.990|H-3→L>		
	S_5	368.7	3.3629	2.4249	0.717|H→L+2>-0.686|H-1→L>		
2	S_1	577.1	2.1485	1.0118	0.974|H→L>	562.5	2.2042
	S_{10}	359.6	3.4480	0.6065	0.844|H→L+4>-0.297|H-2→L>		
	S_{12}	337.0	3.6796	0.7245	0.866|H-2→L>+0.358|H→L+4>		
	Expt[b]	626	1.98				
2	S_1	575.5	2.1545	1.1161	0.994|H→L>	552.7	2.2434
	S_2	553.8	2.2386	0.0038	0.947|H→L+1>		
	S_3	454.9	2.7258	0.7632	0.986|H-1→L>		
	S_{10}	369.7	3.3537	0.7372	0.825|H→L+4>		
	S_{12}	342.9	3.6154	0.8120	0.913|H-4→L>		
2-3H^+	S_1	608.4	2.0379	1.2927	0.998|H→L>	559.1	2.2180
	S_2	460.7	2.6911	0.0001	0.999|H→L+1>		
	S_7	357.9	3.4647	1.9056	0.845|H→L +4>		
	S_1[e]	645.4	1.9210	1.2770	0.998|H→L>		
	S_9[e]	381.0	3.2544	2.1232	0.632|H-2→L>+0.598|H→L+5>		
2-3H^+-3W[e]	S_1	623.4	1.9890	1.1004	0.999|H→L>	562.5	2.2042

[a] Ref. 35. [b] Reference 12. [c] Global minimum, N atom of AC ligand is tetrahedral. [d] Local minimum, N atom of AC ligand has a quasi planar geometry. [e] B3LYP/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ values. [f] State-specific corrected linear response approach.

Table 5S. Emission maxima, λ_{max} (nm), vertical excitation energies ΔE^{e}_{v} (eV) $S_1 \rightarrow S_0$ and $S_2 \rightarrow S_0$ emission maxima calculated at the S_1 and S_2 potential energy surfaces, f-Values for emission, main excitations and their coefficients contributing to the excited state o of protonated, un-protonated, complexed with water of **1**, **1-M^{2+}**, and **2** in water solvent (acetonitrile solvent[a]) at the PBE0/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ level of theory.

	State	λ_{max}	ΔE^{e}_{v}	f	Excitations	State	λ_{max}	ΔE^{e}_{v}
			Uncorrected data				cLR[a]	
1	S_1	676.4 (758.8[b])	1.8330	1.1513	1.000|H→L>	S_2	649.9	1.9079
	S_2	674.6	1.8379	0.0003	0.993|H-1→L>	S_1	801.4	1.5472
1-w	S_1	763.8	1.6233	1.3438	0.998|H→L>	S_2	650.2	1.9069
	S_2	676.9	1.8316	0.0002	0.993|H-1→L>	S_1	984.1	1.2599
1-3H$^+$	S_1	710.9	1.7442	1.3117	1.000|H→L>	S_1	596.6	2.0782
	S_2	431.3	2.8746	0.0138	0.772|H→L+1> +0.469|H-1→L>	S_2	430.9	2.8770
1-Ca^{2+}	S_1	720.2 (811.1[b])	1.7215	1.0946	1.000|H→L>	S_1	690.8	1.7949
1-Ca^{2+}-1W	S_1	718.6	1.7253	1.1002	1.000|H→L>	S_2	689.3	1.7987
	S_2	521.0	2.3798	0.7907	0.984|H-1→L>	S_2	525.4	2.3598
1-Ca^{2+}-1W	S_2	589.8	2.1023	0.0576	0.988|H-1→L>	S_1	867.6	1.4291
	S_3	424.3	2.9222	0.0871	0.985|H-2→L>	S_3	426.5	2.9073
1-Ca^{2+}	S_1	817.0	1.5175	1.2481	0.998|H→L>	S_1	694.9	1.7841
	S_2	547.0	2.2665	1.2375	0.995|H-1→L>	S_2	554.7	2.2352
1-Ca^{2+}-3H$^+$	S_1	710.9	1.7441	1.3012	1.000|H→L>	S_1	596.1	2.0800
	S_2	434.0	2.8571	0.2138	0.814|H-2→L> -0.502|H→L+1>	S_2	432.2	2.8686
1-Ca^{2+}-3H$^+$-1W	S_1	710.3	1.7454	1.3211	1.000|H→L>	S_1	595.4	2.0824
	S_2	430.6	2.8795	0.0120	0.591|H-1→L> +0.768|H→L+1>	S_2	430.2	2.8819
1-Zn^{2+}	S_1	685.3 (768.8[b])	1.8092	1.1312	1.000|H→L>	S_2	661.1	1.8754
	[S_1][c]	706.5 (793.3[b])	1.7549	1.0904	1.000|H→L>	S_2	682.81	1.8158
	S_2	701.0	1.7688	0.0033	0.992|H-1→L>	S_1	700.9	1.7690
	S_3	563.1	2.2017	0.0001	0.997|H→L+1>	S_3	563.1	2.2018
1-Zn^{2+}	S_1	772.2	1.6055	1.3254	0.998|H→L>	S_1	661.9	1.8731
	S_2	594.5	2.0856	0.1384	0.993|H-1→L>	S_2	1023.2	1.2117
1-Zn^{2+}-3H$^+$	S_1	700.8	1.7691	1.1226	1.000|H→L>	S_1	595.8	2.0808
	S_2	590.5	2.0998	0.0097	0.992|H→L+1>			
1-Zn^{2+}-3H$^+$-out	S_1	688.1	1.8019	1.441	0.999|H→L>			
1-Zn^{2+}-3H$^+$-1W	S_1	712.9	1.7391	1.3293	1.000|H→L>	S_1	597.7	2.0745
	S_2	573.4	2.1622	0.0243	0.993|H→L+1>			
1-Hg^{2+}	S_1	1085.2 (1091.6[b])	1.1425	0.0053	0.983|H→L>	S_1	981.1	1.2637
ACN	[S_1][c]	1913.2 (1930.3[b])	0.6423	0.0037	0.990|H→L>	S_1[c]	[d]	[d]
	S_2	695.3 (781.3[b])	1.7832	1.2739	0.995|H→L>	S_2	665.4	1.8632
	[S_3][c]	711.2[e] (798.9[b])	1.7433	1.1684	0.976|H→L+1>	S_2[c]	805.20	1.5398

	S_3	650.9	1.9048	0.0786	0.990|H-1→L>	S_3	648.0	1.9133
	Expt[f]	653						
1-Hg^{2+}	S_1	787.6	1.5742	1.2945	0.997|H→L>	S_1	671.7	1.8458
	S_2	648.4	1.9121	0.0020	0.983|H→L+1>	S_2	1000	1.2398
1-Hg^{2+}-3H^+	S_1	710.3	1.7456	1.3113	1.000|H→L>	S_1	595.7	2.0812
	S_2	532.3	2.3293	0.0001	0.999|H→L+1>	S_2	[d]	[d]
1-Hg^{2+}-3H^+-1W	S_1	701.4	1.7676	1.2791	1.000|H→L>	S_1	591.0	2.0978
	S_2	532.3 (5.41.1)	2.3293 (2.2913	0.0001 (0.0002	0.999|H→L+1>	S_2	[d]	[d]
2	S_1	648.5 (725.0[b])	1.9118	1.2489	1.000|H→L>	S_1	619.1	2.0027
ACN	S_2	694.5	1.7852	0.0682	0.968|H-1→L>	S_2	596.5	2.0785
	S_3	488.1	2.5400	0.9398	0.987|H-1→L>	S_3	492.9	2.5156
	Expt[g]	656						
2	S_1[g]	650.1	1.9072	1.2518	1.000|H→L>	S_1	1.9978	1.9978
	S_1[g, h]	729.8	1.6989	1.4113	0.998|H→L>	S_1	620.6	1.9978
	S_2[g]	624.9	1.8758	0.0341	0.965|H→L+1>	S_2	597.1	2.0769
2-3H^+	S_1[c]	735.8	1.6851	1.3088	1.000|H→L>	S_1[c]	621.7	1.9944
	S_2[c]	677.0	1.7526	0.0031	0.965|H-1→L>	S_2[c]	589.1	2.1046

[a] Ref. 35. [b] Including 10(3 states) singlet excited states. [c] B3LYP/6-31G $(d,p)_{H,C,\ O,N,S,Ca,Zn}$ $LANL2TZ_{Hg}$ values. [d] No conversion. [e] It is calculated as the forth state. [f] Reference 12. [g] At ACN Emission geometry. [h] Including 3 singlet excited states. [i] State-specific corrected linear response approach.

Table 6S. Relative energy differences of the molecular orbitals (MO) in eV of protonated, un-protonated, complexed with water of **1**, **1-M^{2+}**, and **2** in water solvent at the PBE0/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ level of theory.

	S_0	S_1	S_2	S_0	S_1	S_2	S_0	S_1	S_2	S_0
	1			**1-3H$^+$**			**1-3H$^+$-3W**			
L+1	3.81	3.59	3.98	3.83	3.60	3.52	3.80			
L	2.36	2.14	2.30	2.52	2.27	2.23	2.34			
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
H-1	-0.49	-0.63	-0.23	-1.01	-1.24	-1.24	-0.61			
H-2	-0.80	-0.93	-0.77	-1.23	-1.36	-1.35	-0.74			
	1-Ca^{2+}			**1Ca^{2+}-3H$^+$**			**1-Ca^{2+}-3H$^+$-1W**			**1-Ca^{2+}-3H$^+$-3W**
L+1	3.76	3.57	3.77	3.85	3.62	3.59	3.85	3.62	3.53	3.84
L	2.22	2.03	2.12	2.50	2.26	2.22	2.51	2.27	2.23	2.51
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H-1	-0.65	-0.75	-0.60	-1.05	-1.18	-1.15	-1.20	-1.30	-1.29	-0.95
H-2	-1.27	-1.41	-1.28	-1.29	-1.33	-1.23	-1.29	-1.38	-1.38	-1.16
H-3							-1.33			
H-4							-1.62			
	1-Zn^{2+}			**1-Zn^{2+}-3H$^+$**			**1-Zn^{2+}-3H$^+$-1W**			**1-Zn^{2+}-3H$^+$-3W**
L+3	3.70			3.89			3.81			3.84
L+1	3.05	2.92	2.92	3.03	2.90	2.46	3.10	2.96	2.52	3.20
L	2.34	2.12	2.12	2.55	2.30	2.36	2.51	2.26	2.33	2.53
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H-1	-0.44	-0.58	-0.57	-1.21	-1.30	-1.35	-1.18	-1.30	-1.33	-1.02
H-2	-0.81	-0.95	-0.95	-1.30	-1.38	-1.43	-1.27	-1.37	-1.42	-1.10
	1-Hg^{2+}			**1-Hg^{2+}-3H$^+$**			**1-Hg^{2+}-3H$^+$-1W**			**1-Hg^{2+}-3H$^+$-3W**
L+2	3.78			3.83			3.88			3.84
L+1	2.51	2.36	2.36	2.98	2.85	2.67	3.20	3.06	2.65	3.14
L	2.30	2.10	2.10	2.51	2.27	2.34	2.55	2.30	2.35	2.54
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H-1	-0.57	-0.71	-0.72	-1.30	-1.34	-1.39	-1.30	-1.33	-1.39	-1.14
H-2	-0.73	-0.84	-0.83	-1.37	-1.50	-1.53	-1.36	-1.49	-1.56	-1.32
H-3										-1.57
	2			**2-3H$^+$**			**2-3H^{+a}**			**2-3H$^+$-3W**
L+5										4.14
L+4	3.83			3.87			3.38			
L+1	2.74	2.76	2.54	3.04			2.31	2.26	2.10	3.10
L	2.42	2.23	2.20	2.57			2.05	2.01	2.09	2.57
H	0.00	0.00	0.00	0.00			0.00	0.00	0.00	0.00
H-1	-0.81	-0.95	-0.94	-1.07			-1.20	-1.29	-1.35	-0.99
H-2	-1.22			-1.33			-1.28			-1.33
H-3	-1.44									
H-4	-1.72									

[a] B3LYP

Table 1S: Geometries of the Calculated Structures at the PBE0/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ level of theory in water solvent.

---

1 (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-3.516779	-0.261311	0.132433
2	6	0	-2.716362	-2.537733	-0.184586
3	6	0	-3.767656	-1.642543	0.033533
4	6	0	-0.593416	-3.151913	-0.501375
5	6	0	-1.387245	-4.326987	-0.501029
6	6	0	-2.705106	-3.967678	-0.310222
7	7	0	-1.408118	-2.085435	-0.308717
8	7	0	-2.231728	0.237869	-0.012576
9	5	0	-1.005185	-0.598551	-0.445483
10	9	0	0.085341	-0.316800	0.386488
11	9	0	-0.663165	-0.309953	-1.766413
12	6	0	-4.391060	0.833168	0.420474
13	6	0	-3.597052	1.966995	0.429478
14	6	0	-2.265598	1.584476	0.157072
15	1	0	-1.017877	-5.337349	-0.614328
16	1	0	-3.935623	2.973514	0.635926
17	6	0	-5.858993	0.824192	0.693114
18	1	0	-6.433903	0.487095	-0.174495
19	1	0	-6.116349	0.152356	1.517064
20	1	0	-6.191488	1.832395	0.952683
21	6	0	-3.847573	-4.925917	-0.250257
22	1	0	-4.301662	-4.955277	0.744779
23	1	0	-4.643795	-4.652735	-0.948429
24	1	0	-3.498542	-5.931785	-0.496465
25	6	0	-5.155897	-2.149644	0.177321
26	6	0	-6.041879	-2.147552	-0.904542
27	6	0	-5.625656	-2.628279	1.401166
28	6	0	-7.341583	-2.613425	-0.776294
29	1	0	-5.711982	-1.761764	-1.865746
30	6	0	-6.924992	-3.097958	1.545795
31	1	0	-4.963383	-2.638564	2.262960
32	6	0	-7.817968	-3.117536	0.453631
33	1	0	-8.017898	-2.546937	-1.621245
34	1	0	-7.229601	-3.466720	2.517950
35	6	0	0.827227	-3.023352	-0.654649
36	6	0	1.641401	-4.062389	-0.967955
37	1	0	1.236410	-2.031924	-0.492927
38	1	0	1.190339	-5.040760	-1.130526
39	6	0	-1.084970	2.404409	0.070060
40	6	0	-1.107311	3.755630	0.096219
41	1	0	-0.143424	1.871479	-0.009967
42	1	0	-2.069111	4.260093	0.176726
43	6	0	3.078721	-4.026776	-1.121431
44	6	0	3.766492	-5.202316	-1.468638
45	6	0	3.862395	-2.871466	-0.937292
46	6	0	5.140522	-5.238110	-1.622883
47	1	0	3.200766	-6.117495	-1.627131
48	6	0	5.234222	-2.889488	-1.085615
49	1	0	3.390570	-1.932979	-0.661159
50	6	0	5.924200	-4.076173	-1.438777
51	1	0	5.600383	-6.176501	-1.907570
52	1	0	5.780015	-1.969846	-0.910710
53	6	0	0.044337	4.644337	0.022715
54	6	0	1.369252	4.188361	-0.108972
55	6	0	-0.167201	6.031239	0.083057
56	6	0	2.426627	5.081763	-0.175976
57	1	0	1.576300	3.123732	-0.162064
58	6	0	0.893790	6.925969	0.016882
59	1	0	-1.181877	6.408205	0.184123
60	6	0	2.202346	6.464163	-0.113702
61	1	0	3.439536	4.700918	-0.278674
62	1	0	0.724290	7.996886	0.065623
63	7	0	-9.108604	-3.600513	0.571506
64	6	0	-9.801800	-4.144464	-0.586837
65	6	0	-9.636647	-3.963921	1.874199
66	6	0	-10.898962	-3.274213	-1.175660
67	1	0	-10.260276	-5.097304	-0.294976
68	1	0	-9.074905	-4.379481	-1.370560
69	6	0	-9.956901	-2.794998	2.789842
70	1	0	-8.959227	-4.649359	2.405897
71	1	0	-10.565878	-4.515068	1.710597
72	8	0	-10.325205	-2.177464	-1.855689
73	1	0	-11.486934	-3.890578	-1.874936
74	1	0	-11.569337	-2.933319	-0.373898
75	8	0	-11.006330	-2.034745	2.238601
76	1	0	-10.246521	-3.203479	3.772154
77	1	0	-9.072739	-2.159181	2.950091
78	6	0	-11.177900	-1.568318	-2.800765
79	6	0	-11.437210	-1.020051	3.118945
80	6	0	-12.421740	-0.935333	-2.210933
81	1	0	-10.574458	-0.797455	-3.289840
82	1	0	-11.491871	-2.295315	-3.567463
83	6	0	-12.427351	-0.129841	2.412625
84	1	0	-11.911705	-1.457990	4.011845
85	1	0	-10.583921	-0.412674	3.459890
86	8	0	-12.035377	0.025524	-1.260911
87	1	0	-13.006831	-0.484075	-3.029609
88	1	0	-13.062816	-1.700157	-1.743766
89	8	0	-11.731936	0.662487	1.476235
90	1	0	-13.189817	-0.758333	1.930427
91	1	0	-12.939507	0.505488	3.152835
92	6	0	-13.118918	0.546969	-0.530223
93	6	0	-12.566576	1.389712	0.601645
94	1	0	-13.745733	-0.271166	-0.140590
95	1	0	-13.767779	1.174622	-1.163393
96	1	0	-13.400576	1.862393	1.142967
97	1	0	-11.943961	2.186208	0.181078
98	7	0	7.290542	-4.087438	-1.600839
99	6	0	7.988674	-5.327412	-1.886885
100	6	0	8.024770	-2.837582	-1.712703
101	6	0	8.085345	-6.320915	-0.725130
102	1	0	8.993189	-5.068287	-2.228080

103	1	0	7.510396	-5.844918	-2.731450
104	6	0	8.515685	-2.284216	-0.375426
105	1	0	7.394177	-2.097964	-2.220389
106	1	0	8.884828	-3.002444	-2.368207
107	1	0	7.092249	-6.549326	-0.328922
108	1	0	8.505466	-7.260648	-1.100185
109	16	0	9.037452	-5.774865	0.718261
110	1	0	7.692476	-2.220135	0.342790
111	1	0	9.277846	-2.943951	0.047908
112	16	0	9.224222	-0.621426	-0.632624
113	6	0	10.733465	-5.856858	0.058566
114	6	0	10.292415	-0.494063	0.834149
115	6	0	11.736668	-5.450881	1.117366
116	1	0	10.945019	-6.879993	-0.267482
117	1	0	10.831977	-5.188281	-0.802257
118	6	0	11.628998	-1.200211	0.627587
119	1	0	10.444818	0.573068	1.018142
120	1	0	9.745898	-0.898607	1.691321
121	8	0	11.482548	-4.116448	1.489750
122	1	0	11.671329	-6.114518	1.994342
123	1	0	12.750760	-5.552489	0.699966
124	8	0	12.420035	-1.213671	1.805434
125	1	0	11.470717	-2.217077	0.255507
126	1	0	12.210994	-0.652391	-0.120089
127	6	0	12.418203	-3.607043	2.418098
128	6	0	12.057951	-2.178192	2.774178
129	1	0	13.437509	-3.642060	2.002499
130	1	0	12.409925	-4.214821	3.337499
131	1	0	12.607157	-1.902848	3.680030
132	1	0	10.985516	-2.135640	3.013189
133	7	0	3.270810	7.421211	-0.180359
134	6	0	4.195947	7.323391	0.949444
135	1	0	4.971957	8.081879	0.795561
136	1	0	4.703118	6.344845	1.001619
137	6	0	3.981549	7.395389	-1.459703
138	1	0	4.465101	6.423787	-1.658745
139	1	0	4.777105	8.146766	-1.400098
140	6	0	3.511566	7.605057	2.264398
141	6	0	3.331899	6.598204	3.213158
142	7	0	3.097118	8.864097	2.462948
143	6	0	2.698550	6.904905	4.413589
144	1	0	3.681422	5.591058	3.007948
145	6	0	2.489216	9.144299	3.616404
146	6	0	2.264365	8.208105	4.623249
147	1	0	2.546283	6.139207	5.168531
148	1	0	2.166235	10.175649	3.749941
149	1	0	1.765624	8.499157	5.541818
150	6	0	3.078224	7.752507	-2.614507
151	6	0	2.715080	6.799343	-3.566336
152	7	0	2.656173	9.023448	-2.670634
153	6	0	1.882803	7.174685	-4.616385
154	1	0	3.078604	5.780089	-3.479083
155	6	0	1.857054	9.369659	-3.680641
156	6	0	1.440372	8.490490	-4.677670
157	1	0	1.585320	6.451807	-5.370287
158	1	0	1.532985	10.409074	-3.700995
159	1	0	0.790870	8.834111	-5.475982

1-3H$^+$ (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	3.529860	0.785128	-0.917353
2	6	0	3.320160	-1.644523	-0.946577
3	6	0	4.111233	-0.487562	-0.974343
4	6	0	1.420332	-2.799264	-0.861556
5	6	0	2.479169	-3.730199	-0.965752
6	6	0	3.670567	-3.033584	-1.016997
7	7	0	1.940895	-1.548629	-0.854732
8	7	0	2.155624	0.925061	-0.802854
9	5	0	1.166493	-0.240785	-0.554014
10	9	0	0.067769	-0.125741	-1.409733
11	9	0	0.733786	-0.232166	0.767567
12	6	0	4.110097	2.095766	-0.986225
13	6	0	3.056995	2.983911	-0.900518
14	6	0	1.856282	2.245285	-0.781389
15	1	0	2.373085	-4.805202	-1.017919
16	1	0	3.134591	4.061762	-0.942344
17	6	0	5.541223	2.489983	-1.138474
18	1	0	6.143781	2.170205	-0.282728
19	1	0	5.994999	2.050230	-2.031327
20	1	0	5.616132	3.576733	-1.217733
21	6	0	5.017093	-3.666016	-1.135623
22	1	0	5.500899	-3.420328	-2.085799
23	1	0	5.693377	-3.342609	-0.339271
24	1	0	4.917669	-4.752239	-1.078861
25	6	0	5.590602	-0.614408	-1.069896
26	6	0	6.370006	-0.597903	0.088567
27	6	0	6.208593	-0.751988	-2.315909
28	6	0	7.753427	-0.724325	0.011029
29	1	0	5.895807	-0.486326	1.058290
30	6	0	7.589573	-0.879717	-2.408534
31	1	0	5.607755	-0.761339	-3.219458
32	6	0	8.339457	-0.871127	-1.239276
33	1	0	8.361221	-0.691046	0.912687
34	1	0	8.059403	-0.989853	-3.380867
35	6	0	0.003348	-3.042435	-0.787868
36	6	0	-0.533993	-4.271383	-0.629123
37	1	0	-0.630954	-2.166431	-0.871952
38	1	0	0.129204	-5.127512	-0.523039
39	6	0	0.505162	2.727448	-0.660100
40	6	0	0.198691	4.027430	-0.458584
41	1	0	-0.275024	1.978179	-0.741045
42	1	0	1.007328	4.750423	-0.372537
43	6	0	-1.955965	-4.582600	-0.563750
44	6	0	-2.342377	-5.902327	-0.272948
45	6	0	-2.965627	-3.629891	-0.777716
46	6	0	-3.678183	-6.265668	-0.187496
47	1	0	-1.579292	-6.656522	-0.106781
48	6	0	-4.304881	-3.979143	-0.694075
49	1	0	-2.713161	-2.603012	-1.018021
50	6	0	-4.649792	-5.294303	-0.399115

51	1	0	-3.942804	-7.292461	0.045157
52	1	0	-5.071653	-3.227687	-0.859993
53	6	0	-1.139305	4.587815	-0.324416
54	6	0	-2.313150	3.817341	-0.409326
55	6	0	-1.268478	5.965950	-0.093760
56	6	0	-3.561349	4.400067	-0.267471
57	1	0	-2.258140	2.748992	-0.587468
58	6	0	-2.514328	6.562513	0.050658
59	1	0	-0.376336	6.581172	-0.024793
60	6	0	-3.650818	5.770801	-0.037255
61	1	0	-4.450872	3.781318	-0.337591
62	1	0	-2.599114	7.628736	0.229883
63	7	0	9.802084	-1.006742	-1.308043
64	6	0	10.263514	-2.268712	-2.006404
65	6	0	10.478115	0.214508	-1.875839
66	6	0	11.387212	-2.893289	-1.214108
67	1	0	10.560481	-2.016678	-3.024670
68	1	0	9.413178	-2.950386	-2.031950
69	6	0	10.120306	1.438629	-1.068614
70	1	0	10.167673	0.317249	-2.916692
71	1	0	11.551008	0.014783	-1.836370
72	8	0	10.831327	-3.173394	0.048115
73	1	0	11.714208	-3.805687	-1.731095
74	1	0	12.254538	-2.220158	-1.142240
75	8	0	10.409040	1.141048	0.273775
76	1	0	10.709873	2.288664	-1.440085
77	1	0	9.057058	1.687540	-1.197485
78	6	0	11.744918	-3.661396	1.020648
79	6	0	9.862876	2.083362	1.180037
80	6	0	12.258314	-2.556302	1.913231
81	1	0	11.190191	-4.384151	1.626901
82	1	0	12.582755	-4.185377	0.544731
83	6	0	10.248480	1.673251	2.575815
84	1	0	10.253436	3.089957	0.974136
85	1	0	8.767674	2.112414	1.078050
86	8	0	11.149516	-1.975936	2.557089
87	1	0	12.966076	-2.986823	2.639867
88	1	0	12.806078	-1.799183	1.328390
89	8	0	9.633991	0.437964	2.874135
90	1	0	11.342908	1.601223	2.630854
91	1	0	9.928285	2.450403	3.286352
92	6	0	11.511131	-0.991851	3.497304
93	6	0	10.257020	-0.263041	3.932883
94	1	0	12.238465	-0.290629	3.059190
95	1	0	11.991888	-1.445553	4.379207
96	1	0	10.496951	0.411473	4.767561
97	1	0	9.524430	-0.993773	4.289475
98	7	0	-6.073911	-5.649998	-0.308432
99	6	0	-6.516919	-6.597460	-1.392753
100	6	0	-6.504657	-6.098193	1.066067
101	6	0	-6.671449	-5.845886	-2.707992
102	1	0	-7.464981	-7.028679	-1.067316
103	1	0	-5.782871	-7.399777	-1.477020
104	6	0	-6.216163	-5.035148	2.114942
105	1	0	-5.991519	-7.035668	1.287559
106	1	0	-7.573966	-6.301645	0.993924
107	1	0	-5.699909	-5.517811	-3.087995
108	1	0	-7.105756	-6.517673	-3.452254
109	16	0	-7.668672	-4.333491	-2.548977
110	1	0	-5.146063	-4.974528	2.323989
111	1	0	-6.544798	-4.044995	1.781862
112	16	0	-7.066753	-5.403582	3.682680
113	6	0	-9.348927	-5.018356	-2.334658
114	6	0	-8.479216	-4.259499	3.586090
115	6	0	-10.286777	-3.981964	-1.751607
116	1	0	-9.719022	-5.343436	-3.310291
117	1	0	-9.315342	-5.882015	-1.665765
118	6	0	-9.500172	-4.620348	2.513381
119	1	0	-8.945382	-4.298499	4.575129
120	1	0	-8.095742	-3.243723	3.443986
121	8	0	-9.899954	-3.700670	-0.428102
122	1	0	-10.288258	-3.063966	-2.360860
123	1	0	-11.307791	-4.393645	-1.779791
124	8	0	-10.552641	-3.674065	2.483592
125	1	0	-9.033104	-4.690859	1.525768
126	1	0	-9.946296	-5.593310	2.744535
127	6	0	-10.772834	-2.791106	0.210722
128	6	0	-10.322475	-2.562312	1.637748
129	1	0	-11.802480	-3.181135	0.209130
130	1	0	-10.779109	-1.825786	-0.321247
131	1	0	-10.902402	-1.729178	2.048464
132	1	0	-9.264212	-2.265422	1.644005
133	7	0	-4.974111	6.398547	0.117813
134	6	0	-5.791300	6.340157	-1.135789
135	1	0	-6.821456	6.584503	-0.861234
136	1	0	-5.772710	5.327560	-1.538337
137	6	0	-5.690594	5.937806	1.349813
138	1	0	-5.637289	4.851416	1.418829
139	1	0	-6.739620	6.227635	1.241331
140	6	0	-5.258276	7.364031	-2.106990
141	6	0	-5.357140	7.190470	-3.483191
142	7	0	-4.737902	8.454259	-1.539572
143	6	0	-4.901479	8.216478	-4.305017
144	1	0	-5.777696	6.280102	-3.897542
145	6	0	-4.294007	9.428418	-2.336009
146	6	0	-4.360620	9.358709	-3.723689
147	1	0	-4.961637	8.120670	-5.384482
148	1	0	-3.868245	10.298316	-1.842346
149	1	0	-3.989504	10.177902	-4.329604
150	6	0	-5.084934	6.628584	2.546789
151	6	0	-5.094518	6.047834	3.810446
152	7	0	-4.594412	7.845220	2.301678
153	6	0	-4.576865	6.784106	4.871258
154	1	0	-5.495172	5.050412	3.958530
155	6	0	-4.090631	8.539883	3.323610
156	6	0	-4.065762	8.054731	4.626872
157	1	0	-4.566647	6.367106	5.873287
158	1	0	-3.691407	9.523086	3.087912
159	1	0	-3.648539	8.657694	5.425792
160	1	0	-4.796570	7.418033	0.276219
161	1	0	10.120999	-1.091926	-0.330375
162	1	0	-6.617118	-4.789632	-0.526872

1-Ca^{2+} (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-3.320281	0.331801	-0.064523
2	6	0	-2.820213	-2.048545	0.067993
3	6	0	-3.741771	-0.992958	0.111386
4	6	0	-0.803702	-2.982969	-0.145640
5	6	0	-1.728592	-4.014659	0.145512
6	6	0	-2.984111	-3.455442	0.283396
7	7	0	-1.476803	-1.804476	-0.180856
8	7	0	-1.979463	0.625325	-0.275646
9	5	0	-0.889559	-0.429724	-0.575857
10	9	0	0.259138	-0.164157	0.179507
11	9	0	-0.561929	-0.413047	-1.932238
12	6	0	-4.048097	1.566854	-0.050032
13	6	0	-3.115331	2.565770	-0.244672
14	6	0	-1.837219	1.971233	-0.383652
15	1	0	-1.487857	-5.062586	0.264339
16	1	0	-3.323914	3.626916	-0.269676
17	6	0	-5.511031	1.802048	0.136100
18	1	0	-6.112453	1.197626	-0.549037
19	1	0	-5.839478	1.552668	1.149788
20	1	0	-5.738782	2.855632	-0.043570
21	6	0	-4.222105	-4.221019	0.616825
22	1	0	-4.717933	-3.828469	1.509401
23	1	0	-4.956454	-4.184123	-0.193597
24	1	0	-3.969409	-5.268642	0.797663
25	6	0	-5.177494	-1.275287	0.374134
26	6	0	-6.037096	-1.669158	-0.655857
27	6	0	-5.704119	-1.139704	1.656774
28	6	0	-7.383427	-1.895960	-0.409017
29	1	0	-5.652224	-1.785127	-1.664732
30	6	0	-7.052452	-1.377906	1.911785
31	1	0	-5.054816	-0.845025	2.476032
32	6	0	-7.919831	-1.746887	0.878703
33	1	0	-8.026263	-2.188219	-1.234661
34	1	0	-7.402476	-1.267471	2.930807
35	6	0	0.611566	-3.072824	-0.368579
36	6	0	1.282911	-4.246753	-0.469884
37	1	0	1.141262	-2.129903	-0.450429
38	1	0	0.718143	-5.174815	-0.385979
39	6	0	-0.565056	2.604643	-0.579887
40	6	0	-0.418743	3.938719	-0.782004
41	1	0	0.302890	1.955463	-0.537912
42	1	0	-1.316403	4.555344	-0.819612
43	6	0	2.702273	-4.419302	-0.693396
44	6	0	3.236847	-5.715665	-0.784444
45	6	0	3.612789	-3.354414	-0.831751
46	6	0	4.583669	-5.948676	-0.999445
47	1	0	2.569896	-6.569288	-0.688335
48	6	0	4.959383	-3.568491	-1.046205
49	1	0	3.263382	-2.328222	-0.764316
50	6	0	5.493612	-4.877222	-1.145338
51	1	0	4.920678	-6.975393	-1.073403
52	1	0	5.608102	-2.704283	-1.126977
53	6	0	0.818066	4.665568	-0.956268
54	6	0	2.094942	4.072152	-0.931830
55	6	0	0.780464	6.057868	-1.148460
56	6	0	3.247571	4.813892	-1.088505
57	1	0	2.193357	3.000637	-0.783119
58	6	0	1.925087	6.816541	-1.307312
59	1	0	-0.183272	6.561654	-1.164966
60	6	0	3.205317	6.217042	-1.291505
61	1	0	4.199546	4.298506	-1.049174
62	1	0	1.811733	7.886016	-1.434919
63	7	0	-9.329932	-1.966230	1.073593
64	6	0	-9.708598	-3.368424	0.777137
65	6	0	-9.839200	-1.559915	2.390852
66	6	0	-11.164425	-3.552032	0.407698
67	1	0	-9.483103	-4.016837	1.636643
68	1	0	-9.100793	-3.716492	-0.059086
69	6	0	-9.918314	-0.058768	2.564549
70	1	0	-9.263326	-2.005981	3.213028
71	1	0	-10.856330	-1.947247	2.486920
72	8	0	-11.438802	-2.788782	-0.766176
73	1	0	-11.329979	-4.615688	0.199109
74	1	0	-11.843853	-3.262887	1.219307
75	8	0	-10.891526	0.432069	1.647859
76	1	0	-10.236003	0.165143	3.590132
77	1	0	-8.956622	0.437181	2.385091
78	6	0	-12.709277	-3.051271	-1.365938
79	6	0	-11.182106	1.819126	1.792747
80	6	0	-13.775809	-2.126360	-0.827866
81	1	0	-12.579372	-2.878628	-2.438026
82	1	0	-12.996645	-4.096734	-1.213670
83	6	0	-12.491233	2.073296	1.094551
84	1	0	-11.282621	2.079523	2.852628
85	1	0	-10.371536	2.419627	1.358918
86	8	0	-13.319888	-0.796795	-1.048850
87	1	0	-14.716683	-2.301989	-1.364398
88	1	0	-13.954118	-2.285132	0.244293
89	8	0	-12.361109	1.641623	-0.258822
90	1	0	-13.288237	1.513257	1.597868
91	1	0	-12.736188	3.141521	1.125517
92	6	0	-14.262962	0.207187	-0.694970
93	6	0	-13.603793	1.542699	-0.955509
94	1	0	-14.548628	0.091836	0.359146
95	1	0	-15.168471	0.114394	-1.307533
96	1	0	-14.271426	2.363879	-0.674232
97	1	0	-13.363135	1.639444	-2.017682
98	7	0	6.833708	-5.086542	-1.382306
99	6	0	7.373805	-6.433014	-1.415464
100	6	0	7.675512	-3.990599	-1.833581
101	6	0	7.484167	-7.139574	-0.061085
102	1	0	8.360667	-6.380894	-1.880063
103	1	0	6.765989	-7.068494	-2.076240
104	6	0	8.331163	-3.203831	-0.699212
105	1	0	7.080377	-3.319965	-2.465097
106	1	0	8.456510	-4.400963	-2.480297
107	1	0	6.517085	-7.148033	0.449044
108	1	0	7.767444	-8.184200	-0.230713
109	16	0	8.625362	-6.398058	1.137536

110	1	0	7.583653	-2.886134	0.034160
111	1	0	9.062461	-3.830254	-0.181482
112	16	0	9.167505	-1.733494	-1.386240
113	6	0	10.230246	-6.820800	0.386393
114	6	0	10.382405	-1.406940	-0.072332
115	6	0	11.369924	-6.308771	1.241545
116	1	0	10.308935	-7.908246	0.290982
117	1	0	10.304601	-6.376219	-0.610915
118	6	0	11.619825	-2.288836	-0.209817
119	1	0	10.651863	-0.350046	-0.151281
120	1	0	9.887752	-1.546702	0.893527
121	8	0	11.284308	-4.904532	1.310416
122	1	0	11.329978	-6.746970	2.251571
123	1	0	12.322073	-6.619084	0.783208
124	8	0	12.518477	-2.130752	0.876764
125	1	0	11.330597	-3.338035	-0.324071
126	1	0	12.173996	-1.990314	-1.105169
127	6	0	12.351626	-4.313069	2.022928
128	6	0	12.164875	-2.809261	2.066062
129	1	0	13.316683	-4.555735	1.550980
130	1	0	12.377332	-4.697242	3.055636
131	1	0	12.824472	-2.404925	2.840278
132	1	0	11.130049	-2.592717	2.368239
133	7	0	4.362875	6.928815	-1.478295
134	6	0	5.652238	6.290404	-1.343906
135	1	0	6.403389	7.025882	-1.648658
136	1	0	5.742696	5.448824	-2.044482
137	6	0	4.380687	8.351814	-1.781615
138	1	0	3.413190	8.650575	-2.185186
139	1	0	5.119737	8.521649	-2.571567
140	6	0	6.020351	5.816520	0.051909
141	6	0	7.022988	4.853625	0.200327
142	7	0	5.393381	6.368880	1.091333
143	6	0	7.394835	4.463397	1.480079
144	1	0	7.499105	4.420768	-0.674955
145	6	0	5.756142	5.980015	2.317417
146	6	0	6.747697	5.039083	2.570013
147	1	0	8.171829	3.718573	1.624881
148	1	0	5.222578	6.447316	3.143528
149	1	0	6.998853	4.763791	3.588908
150	6	0	4.762764	9.217461	-0.600613
151	6	0	3.809674	9.691829	0.303262
152	7	0	6.069125	9.481167	-0.474243
153	6	0	4.230726	10.456497	1.384201
154	1	0	2.757821	9.464573	0.161791
155	6	0	6.461708	10.212129	0.572396
156	6	0	5.589197	10.721791	1.528041
157	1	0	3.511089	10.841555	2.100626
158	1	0	7.530109	10.407049	0.647246
159	1	0	5.965825	11.314748	2.354876
160	20	0	-10.868389	-0.346718	-0.711800

1-Ca^{2+}-$3H^{+}$ (S_0):

Atom	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	9.093600	-0.872263	-0.596140
2	6	0	9.539956	-2.317901	-0.600039
3	6	0	9.719222	-0.029392	-1.703751
4	6	0	7.618125	-0.788222	-0.570498
5	6	0	11.001166	-2.456416	-0.240436
6	1	0	9.334529	-2.724639	-1.591796
7	1	0	8.914843	-2.829389	0.133859
8	6	0	10.686442	1.026139	-1.207055
9	1	0	8.897672	0.477767	-2.208873
10	1	0	10.193065	-0.708896	-2.413601
11	8	0	11.224131	-1.929505	1.066344
12	1	0	11.244202	-3.522188	-0.281495
13	1	0	11.646150	-1.935987	-0.952072
14	8	0	11.933601	0.485638	-0.776652
15	1	0	10.845134	1.729747	-2.029230
16	1	0	10.249976	1.595616	-0.379616
17	6	0	11.746777	-2.871896	2.010540
18	6	0	13.036531	0.787608	-1.647611
19	6	0	13.222907	-3.103125	1.771099
20	1	0	11.566696	-2.440924	2.998809
21	1	0	11.201505	-3.820162	1.955228
22	6	0	14.224467	-0.029347	-1.212619
23	1	0	12.784181	0.529099	-2.681306
24	1	0	13.255553	1.859866	-1.587370
25	8	0	13.864598	-1.836003	1.692903
26	1	0	13.643983	-3.707960	2.583440
27	1	0	13.380086	-3.644117	0.828624
28	8	0	14.495087	0.284587	0.149827
29	1	0	14.012827	-1.098699	-1.331080
30	1	0	15.087698	0.225560	-1.838563
31	6	0	15.133072	-1.884406	1.048401
32	6	0	15.555748	-0.460781	0.749168
33	1	0	15.047144	-2.477355	0.128957
34	1	0	15.881980	-2.364272	1.690091
35	1	0	16.443450	-0.456321	0.107290
36	1	0	15.795179	0.072660	1.673162
37	6	0	2.802037	0.781098	-0.497116
38	6	0	2.575803	-1.643872	-0.351476
39	6	0	3.375399	-0.496165	-0.440720
40	6	0	0.663571	-2.779030	-0.272471
41	6	0	1.718182	-3.720500	-0.247492
42	6	0	2.916712	-3.035827	-0.290653
43	7	0	1.194497	-1.534013	-0.332019
44	7	0	1.427563	0.936975	-0.413983
45	5	0	0.420204	-0.205717	-0.136722
46	9	0	-0.642919	-0.129569	-1.040153
47	9	0	-0.063579	-0.120842	1.164163
48	6	0	3.390788	2.079444	-0.665320
49	6	0	2.342256	2.977065	-0.657597
50	6	0	1.136174	2.256517	-0.493495
51	1	0	1.605657	-4.795655	-0.217511
52	1	0	2.426147	4.047732	-0.784860
53	6	0	4.823380	2.456197	-0.848246
54	1	0	5.409252	2.284399	0.059912
55	1	0	5.299534	1.885068	-1.650095
56	1	0	4.893264	3.517520	-1.096851

57	6	0	4.262094	-3.681914	-0.277596
58	1	0	4.770703	-3.585138	-1.241755
59	1	0	4.920192	-3.244698	0.478319
60	1	0	4.153897	-4.747263	-0.062126
61	6	0	4.856263	-0.626205	-0.482379
62	6	0	5.610729	-0.391113	0.668311
63	6	0	5.505157	-0.962553	-1.673717
64	6	0	6.998439	-0.473281	0.629663
65	1	0	5.115801	-0.133347	1.598795
66	6	0	6.891311	-1.049116	-1.725734
67	1	0	4.925028	-1.150503	-2.571181
68	1	0	7.578025	-0.284859	1.528805
69	1	0	7.378886	-1.307710	-2.660312
70	6	0	-0.757752	-3.005383	-0.270697
71	6	0	-1.322630	-4.221544	-0.108680
72	1	0	-1.372834	-2.127347	-0.435916
73	1	0	-0.681395	-5.085822	0.052006
74	6	0	-0.211692	2.756123	-0.412113
75	6	0	-0.504605	4.067558	-0.275030
76	1	0	-0.999363	2.011665	-0.457163
77	1	0	0.312353	4.783713	-0.213947
78	6	0	-2.750251	-4.512134	-0.141636
79	6	0	-3.167844	-5.848346	-0.013014
80	6	0	-3.735013	-3.524252	-0.305764
81	6	0	-4.509337	-6.196866	-0.061579
82	1	0	-2.424512	-6.628228	0.121596
83	6	0	-5.079942	-3.858468	-0.353819
84	1	0	-3.459109	-2.479676	-0.397976
85	6	0	-5.454634	-5.192640	-0.236687
86	1	0	-4.803183	-7.237570	0.038063
87	1	0	-5.827326	-3.080186	-0.480173
88	6	0	-1.836349	4.648426	-0.169324
89	6	0	-3.019437	3.893574	-0.264206
90	6	0	-1.949113	6.030233	0.047370
91	6	0	-4.261001	4.494101	-0.139201
92	1	0	-2.976750	2.824067	-0.438960
93	6	0	-3.188147	6.644366	0.175745
94	1	0	-1.049482	6.633874	0.121317
95	6	0	-4.334201	5.867094	0.083175
96	1	0	-5.158123	3.887404	-0.216566
97	1	0	-3.260364	7.712792	0.347154
98	7	0	-6.881504	-5.539586	-0.313422
99	6	0	-7.218355	-6.333333	-1.551666
100	6	0	-7.452042	-6.134419	0.964691
101	6	0	-7.226572	-5.415921	-2.764841
102	1	0	-8.203175	-6.772267	-1.386098
103	1	0	-6.489818	-7.138710	-1.655011
104	6	0	-8.422663	-5.141494	1.579369
105	1	0	-6.617562	-6.358751	1.628511
106	1	0	-7.950423	-7.068403	0.701397
107	1	0	-6.227037	-5.024181	-2.973026
108	1	0	-7.545072	-5.985896	-3.641107
109	16	0	-8.298388	-3.965033	-2.527079
110	1	0	-7.888379	-4.264017	1.957531
111	1	0	-9.140371	-4.808673	0.820277
112	16	0	-9.356933	-5.915316	2.936414
113	6	0	-9.950910	-4.726229	-2.699905
114	6	0	-10.705220	-4.697627	3.031775
115	6	0	-11.047099	-3.775075	-2.269894
116	1	0	-10.093352	-4.993457	-3.750279
117	1	0	-10.011195	-5.634641	-2.094772
118	6	0	-11.721078	-4.850798	1.899203
119	1	0	-11.180298	-4.844485	4.005081
120	1	0	-10.260806	-3.697535	3.037006
121	8	0	-11.003628	-3.602049	-0.872151
122	1	0	-10.951297	-2.805382	-2.783677
123	1	0	-12.011370	-4.210811	-2.574117
124	8	0	-12.558766	-3.713230	1.794190
125	1	0	-11.223408	-5.048372	0.944135
126	1	0	-12.376765	-5.700256	2.112249
127	6	0	-12.034527	-2.745234	-0.413780
128	6	0	-11.994449	-2.619821	1.095904
129	1	0	-13.018981	-3.128429	-0.723339
130	1	0	-11.911640	-1.743003	-0.854909
131	1	0	-12.593000	-1.747568	1.376704
132	1	0	-10.959599	-2.423012	1.411439
133	7	0	-5.650242	6.512775	0.225487
134	6	0	-6.458078	6.462372	-1.034425
135	1	0	-7.488465	6.714394	-0.767806
136	1	0	-6.444415	5.450278	-1.438519
137	6	0	-6.382369	6.064528	1.452908
138	1	0	-6.348709	4.977336	1.521893
139	1	0	-7.425426	6.372745	1.337642
140	6	0	-5.909382	7.483850	-1.999579
141	6	0	-6.005076	7.316912	-3.376818
142	7	0	-5.378925	8.565898	-1.425968
143	6	0	-5.534715	8.340972	-4.192736
144	1	0	-6.434538	6.413108	-3.796367
145	6	0	-4.921054	9.538266	-2.216711
146	6	0	-4.983178	9.474750	-3.604843
147	1	0	-5.591965	8.250208	-5.272790
148	1	0	-4.487493	10.401328	-1.717885
149	1	0	-4.600634	10.292098	-4.206116
150	6	0	-5.772675	6.744594	2.653903
151	6	0	-5.797465	6.162428	3.916713
152	7	0	-5.262771	7.954102	2.412956
153	6	0	-5.274449	6.889515	4.981249
154	1	0	-6.213683	5.170910	4.061430
155	6	0	-4.754043	8.639768	3.438477
156	6	0	-4.743206	8.152665	4.741238
157	1	0	-5.275740	6.471148	5.982762
158	1	0	-4.338983	9.617242	3.206281
159	1	0	-4.321297	8.748374	5.543140
160	20	0	12.520370	0.337750	1.675372
161	1	0	9.407719	-0.501109	0.306798
162	1	0	-7.397995	-4.653196	-0.484597
163	1	0	-5.460421	7.530387	0.382151

1-Ca^{2+}-$3H^{+}$-1W (S_0):

Atom	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.766981	0.435580	-0.270377
2	6	0	2.249897	-1.943198	-0.116350
3	6	0	3.178216	-0.903346	-0.256748
4	6	0	0.225296	-2.834493	0.117200
5	6	0	1.159835	-3.895984	0.119082
6	6	0	2.425752	-3.363665	-0.025559
7	7	0	0.896419	-1.665558	-0.015336
8	7	0	1.423321	0.757473	-0.158090
9	5	0	0.262942	-0.267064	-0.224319
10	9	0	-0.364467	-0.202988	-1.463534
11	9	0	-0.664393	-0.005587	0.787300
12	6	0	3.514399	1.657045	-0.366584
13	6	0	2.586621	2.676987	-0.308113
14	6	0	1.298457	2.105527	-0.184736
15	1	0	0.924486	-4.944810	0.238215
16	1	0	2.809443	3.734811	-0.334158
17	6	0	4.987506	1.861333	-0.492245
18	1	0	5.527338	1.494995	0.386140
19	1	0	5.399417	1.341936	-1.362460
20	1	0	5.201276	2.926989	-0.599670
21	6	0	3.686421	-4.161832	-0.051126
22	1	0	4.228907	-4.039280	-0.993308
23	1	0	4.370313	-3.871421	0.751852
24	1	0	3.452092	-5.221739	0.069412
25	6	0	4.624993	-1.219514	-0.402518
26	6	0	5.462853	-1.252327	0.713193
27	6	0	5.156914	-1.463703	-1.671952
28	6	0	6.822513	-1.506891	0.564410
29	1	0	5.057274	-1.067215	1.702371
30	6	0	6.512543	-1.721271	-1.833036
31	1	0	4.509714	-1.442584	-2.542433
32	6	0	7.327954	-1.732203	-0.708100
33	1	0	7.473219	-1.515570	1.433967
34	1	0	6.910393	-1.896254	-2.827269
35	6	0	-1.208367	-2.886402	0.235839
36	6	0	-1.920358	-4.032767	0.180451
37	1	0	-1.705590	-1.931812	0.370980
38	1	0	-1.396172	-4.972920	0.021095
39	6	0	0.022539	2.765310	-0.089104
40	6	0	-0.133913	4.096716	-0.256121
41	1	0	-0.826169	2.128393	0.136154
42	1	0	0.740397	4.703143	-0.483906
43	6	0	-3.369213	-4.144921	0.288457
44	6	0	-3.963767	-5.402312	0.094178
45	6	0	-4.208400	-3.055053	0.575327
46	6	0	-5.338949	-5.576119	0.168029
47	1	0	-3.336125	-6.261008	-0.123583
48	6	0	-5.582575	-3.214824	0.650242
49	1	0	-3.791679	-2.069189	0.749234
50	6	0	-6.139494	-4.473903	0.444097
51	1	0	-5.760869	-6.562949	0.011700
52	1	0	-6.214923	-2.358847	0.870333
53	6	0	-1.384036	4.839247	-0.169326
54	6	0	-2.625360	4.238050	0.107160
55	6	0	-1.352624	6.227194	-0.374072
56	6	0	-3.784443	4.992823	0.176963
57	1	0	-2.694267	3.167993	0.269292
58	6	0	-2.507423	6.995455	-0.305841
59	1	0	-0.406075	6.713197	-0.591052
60	6	0	-3.714425	6.368510	-0.029652
61	1	0	-4.729488	4.502206	0.389833
62	1	0	-2.468350	8.067421	-0.465547
63	7	0	8.777455	-1.958743	-0.860157
64	6	0	9.078025	-3.365765	-1.327433
65	6	0	9.452293	-0.877748	-1.662131
66	6	0	10.525906	-3.617620	-1.679884
67	1	0	8.463006	-3.558254	-2.207190
68	1	0	8.746379	-4.018128	-0.518096
69	6	0	9.317617	0.458695	-0.973937
70	1	0	9.023356	-0.865046	-2.664636
71	1	0	10.505287	-1.147253	-1.715127
72	8	0	11.367025	-3.322964	-0.580628
73	1	0	10.593045	-4.682498	-1.940653
74	1	0	10.819895	-3.050250	-2.572326
75	8	0	9.814198	0.311537	0.344728
76	1	0	9.903532	1.178951	-1.556980
77	1	0	8.277435	0.807794	-0.948955
78	6	0	12.744669	-3.575985	-0.855921
79	6	0	10.220881	1.536695	0.946087
80	6	0	13.459894	-2.330073	-1.319899
81	1	0	13.192772	-3.945857	0.070668
82	1	0	12.854397	-4.362316	-1.611148
83	6	0	11.644046	1.881447	0.574668
84	1	0	9.553331	2.356455	0.656537
85	1	0	10.133759	1.395056	2.027152
86	8	0	13.396767	-1.350468	-0.287145
87	1	0	14.506798	-2.568311	-1.546874
88	1	0	12.998006	-1.929871	-2.232388
89	8	0	12.512192	0.861262	1.068894
90	1	0	11.749238	1.963762	-0.514066
91	1	0	11.921321	2.845479	1.018096
92	6	0	13.851355	-0.068633	-0.716145
93	6	0	13.812675	0.859422	0.474737
94	1	0	13.206265	0.293215	-1.527570
95	1	0	14.878466	-0.135944	-1.095665
96	1	0	14.107264	1.871559	0.180530
97	1	0	14.508517	0.516258	1.246104
98	7	0	-7.604094	-4.598745	0.492474
99	6	0	-8.264443	-4.657478	-0.874738
100	6	0	-8.102888	-5.640638	1.457505
101	6	0	-8.189415	-5.997675	-1.577941
102	1	0	-7.789354	-3.876096	-1.470606
103	1	0	-9.310536	-4.388207	-0.709215
104	6	0	-8.050275	-5.096849	2.875747
105	1	0	-7.489009	-6.536007	1.357825
106	1	0	-9.124952	-5.886205	1.165757
107	1	0	-7.180682	-6.215739	-1.937374
108	1	0	-8.509552	-6.827443	-0.941700
109	16	0	-9.233019	-5.979398	-3.067896
110	1	0	-8.393587	-5.870050	3.567522
111	1	0	-7.022170	-4.845390	3.154053
112	16	0	-9.024440	-3.577683	3.115669
113	6	0	-10.917125	-6.265010	-2.416602
114	6	0	-10.721258	-4.237163	3.314746

115	6	0	-11.772694	-5.037752	-2.171028
116	1	0	-11.408399	-6.876591	-3.178839
117	1	0	-10.847932	-6.874228	-1.509670
118	6	0	-11.610059	-4.296517	2.082404
119	1	0	-10.633594	-5.230881	3.765813
120	1	0	-11.191843	-3.584414	4.055519
121	8	0	-11.350105	-4.372234	-1.000160
122	1	0	-11.724654	-4.360020	-3.036257
123	1	0	-12.819580	-5.360968	-2.058898
124	8	0	-12.053763	-3.011024	1.688097
125	1	0	-11.136180	-4.823199	1.250346
126	1	0	-12.500913	-4.875688	2.360359
127	6	0	-12.028346	-3.146764	-0.782093
128	6	0	-11.525519	-2.487112	0.487776
129	1	0	-13.112819	-3.315822	-0.706868
130	1	0	-11.850189	-2.466828	-1.629682
131	1	0	-11.843819	-1.440036	0.466964
132	1	0	-10.426671	-2.492171	0.496135
133	7	0	-4.940644	7.181022	0.043847
134	6	0	-5.917021	6.853847	-1.043315
135	1	0	-6.877145	7.293154	-0.757997
136	1	0	-6.038451	5.773006	-1.112187
137	6	0	-5.531823	7.213098	1.419351
138	1	0	-5.583473	6.200085	1.818161
139	1	0	-6.550324	7.599765	1.323478
140	6	0	-5.428683	7.469540	-2.331210
141	6	0	-5.730928	6.914724	-3.570063
142	7	0	-4.736284	8.600754	-2.182413
143	6	0	-5.298320	7.586200	-4.709162
144	1	0	-6.287405	5.985871	-3.639978
145	6	0	-4.316655	9.232296	-3.280411
146	6	0	-4.578750	8.768049	-4.565140
147	1	0	-5.514410	7.186720	-5.694959
148	1	0	-3.748184	10.145520	-3.123787
149	1	0	-4.219307	9.317911	-5.427917
150	6	0	-4.706442	8.138438	2.278860
151	6	0	-4.605152	7.965004	3.655034
152	7	0	-4.134532	9.149768	1.622202
153	6	0	-3.880419	8.905599	4.379957
154	1	0	-5.079567	7.120156	4.143386
155	6	0	-3.432897	10.041288	2.324665
156	6	0	-3.282957	9.965485	3.705396
157	1	0	-3.778429	8.806915	5.456015
158	1	0	-2.973212	10.847240	1.758294
159	1	0	-2.705387	10.716080	4.233558
160	20	0	12.046407	-1.460828	1.837604
161	1	0	-4.647558	8.167878	-0.146317
162	1	0	-7.962946	-3.716846	0.896775
163	1	0	9.172276	-1.873783	0.079705
164	8	0	11.745327	-2.782677	3.845768
165	1	0	12.208085	-3.614750	3.991027
166	1	0	11.647028	-2.382710	4.716407

1-Zn^{2+} (S_0):

Atom	Atomic Type		X	Y	Z
1	6	0	-3.855418	-0.332458	0.396229
2	6	0	-3.350359	-2.689574	0.059332
3	6	0	-4.277714	-1.674556	0.299175
4	6	0	-1.324449	-3.561755	-0.287335
5	6	0	-2.251270	-4.635142	-0.218532
6	6	0	-3.509476	-4.116933	-0.003833
7	7	0	-2.001503	-2.401082	-0.113238
8	7	0	-2.520405	0.000054	0.241766
9	5	0	-1.421286	-0.974299	-0.244078
10	9	0	-0.278525	-0.844337	0.553980
11	9	0	-1.089141	-0.703830	-1.571180
12	6	0	-4.589416	0.866831	0.650799
13	6	0	-3.660172	1.894680	0.643570
14	6	0	-2.387924	1.345015	0.383919
15	1	0	-2.006060	-5.685549	-0.298353
16	1	0	-3.873737	2.940831	0.817708
17	6	0	-6.052456	1.048899	0.887602
18	1	0	-6.653931	0.592367	0.096612
19	1	0	-6.374291	0.591596	1.828184
20	1	0	-6.288069	2.115247	0.930287
21	6	0	-4.750109	-4.930728	0.152056
22	1	0	-5.255321	-4.721163	1.099308
23	1	0	-5.475087	-4.721529	-0.640088
24	1	0	-4.500796	-5.994084	0.118790
25	6	0	-5.715082	-2.010119	0.459087
26	6	0	-6.543725	-2.169309	-0.656018
27	6	0	-6.287277	-2.169713	1.721992
28	6	0	-7.888570	-2.477789	-0.520218
29	1	0	-6.132265	-2.030355	-1.652470
30	6	0	-7.628948	-2.496003	1.873966
31	1	0	-5.671191	-2.050137	2.609395
32	6	0	-8.467964	-2.671543	0.752905
33	1	0	-8.515265	-2.529246	-1.403365
34	1	0	-8.011274	-2.628466	2.878951
35	6	0	0.094423	-3.609197	-0.486171
36	6	0	0.772982	-4.754083	-0.753011
37	1	0	0.621323	-2.665359	-0.399137
38	1	0	0.209519	-5.683638	-0.826593
39	6	0	-1.113434	2.004840	0.269157
40	6	0	-0.947691	3.345472	0.296947
41	1	0	-0.254551	1.350077	0.166103
42	1	0	-1.821031	3.983980	0.418152
43	6	0	2.196477	-4.892107	-0.959692
44	6	0	2.739598	-6.165100	-1.206267
45	6	0	3.104742	-3.816222	-0.928759
46	6	0	4.093107	-6.366426	-1.405085
47	1	0	2.073863	-7.024031	-1.245723
48	6	0	4.457832	-3.998683	-1.126479
49	1	0	2.747136	-2.808198	-0.740295
50	6	0	5.001858	-5.283617	-1.377123
51	1	0	4.438376	-7.373664	-1.603181
52	1	0	5.104461	-3.130860	-1.074069
53	6	0	0.320696	4.051603	0.175032
54	6	0	1.543965	3.407932	-0.088106
55	6	0	0.341700	5.445947	0.312623

56	6	0	2.716439	4.131170	-0.205657
57	1	0	1.582900	2.330959	-0.213907
58	6	0	1.520184	6.177853	0.197611
59	1	0	-0.585825	5.973849	0.515987
60	6	0	2.720655	5.525575	-0.065984
61	1	0	3.641203	3.600208	-0.415381
62	1	0	1.462256	7.252715	0.320417
63	7	0	-9.801392	-3.014006	0.882032
64	6	0	-10.492035	-3.709473	-0.194060
65	6	0	-10.417639	-3.070514	2.195536
66	6	0	-11.458202	-2.875415	-1.018451
67	1	0	-11.065839	-4.533735	0.246277
68	1	0	-9.757559	-4.168700	-0.863275
69	6	0	-10.684135	-1.722687	2.843351
70	1	0	-9.822638	-3.680972	2.891533
71	1	0	-11.379566	-3.577277	2.086774
72	8	0	-10.737514	-2.001032	-1.861210
73	1	0	-12.074409	-3.562712	-1.620591
74	1	0	-12.125780	-2.315057	-0.348824
75	8	0	-11.636232	-1.013333	2.086322
76	1	0	-11.056234	-1.905620	3.864984
77	1	0	-9.758646	-1.133681	2.935127
78	6	0	-11.473648	-1.515323	-2.962651
79	6	0	-12.025719	0.184749	2.721452
80	6	0	-12.677475	-0.672575	-2.593753
81	1	0	-10.770585	-0.911297	-3.544333
82	1	0	-11.818042	-2.347346	-3.598289
83	6	0	-12.879501	0.996353	1.781099
84	1	0	-12.595553	-0.031348	3.639392
85	1	0	-11.143005	0.777214	3.009508
86	8	0	-12.250351	0.411405	-1.807713
87	1	0	-13.164541	-0.332915	-3.523026
88	1	0	-13.420104	-1.274242	-2.045356
89	8	0	-12.051335	1.537406	0.776157
90	1	0	-13.661469	0.347471	1.361262
91	1	0	-13.380466	1.799943	2.344236
92	6	0	-13.317000	1.161266	-1.278406
93	6	0	-12.752234	2.153317	-0.281843
94	1	0	-14.049893	0.494584	-0.796320
95	1	0	-13.854740	1.711171	-2.068531
96	1	0	-13.565661	2.793036	0.093952
97	1	0	-12.026789	2.795935	-0.791479
98	7	0	6.348714	-5.459499	-1.592438
99	6	0	6.898338	-6.790524	-1.775716
100	6	0	7.203146	-4.313604	-1.858997
101	6	0	6.961629	-7.662990	-0.518571
102	1	0	7.901548	-6.677758	-2.191873
103	1	0	6.319775	-7.336857	-2.534874
104	6	0	7.806629	-3.682249	-0.604701
105	1	0	6.630825	-3.566222	-2.421541
106	1	0	8.012089	-4.636053	-2.520730
107	1	0	5.975372	-7.740441	-0.052913
108	1	0	7.260638	-8.676366	-0.808260
109	16	0	8.048026	-7.075353	0.809172
110	1	0	7.028230	-3.467834	0.133968
111	1	0	8.523514	-4.367981	-0.145141
112	16	0	8.653314	-2.129696	-1.058405
113	6	0	9.685361	-7.396612	0.077882
114	6	0	9.811051	-1.971640	0.335575
115	6	0	10.784868	-6.995985	1.038528
116	1	0	9.775694	-8.463005	-0.151178
117	1	0	9.797918	-6.828919	-0.851021
118	6	0	11.062926	-2.820337	0.134223
119	1	0	10.071353	-0.911954	0.407363
120	1	0	9.279814	-2.240532	1.253513
121	8	0	10.685103	-5.612762	1.285317
122	1	0	10.707418	-7.561499	1.980794
123	1	0	11.757414	-7.241448	0.583748
124	8	0	11.914827	-2.802920	1.268661
125	1	0	10.790321	-3.846631	-0.130333
126	1	0	11.649673	-2.402282	-0.689674
127	6	0	11.718043	-5.116911	2.112374
128	6	0	11.518677	-3.632044	2.343643
129	1	0	12.703289	-5.294022	1.653206
130	1	0	11.704601	-5.632587	3.086419
131	1	0	12.143745	-3.331172	3.190226
132	1	0	10.471069	-3.458915	2.629278
133	7	0	3.985875	6.242765	-0.215511
134	6	0	4.953479	5.848345	0.835773
135	1	0	5.965498	6.023827	0.453240
136	1	0	4.883608	4.787476	1.087248
137	6	0	4.512096	6.107028	-1.594962
138	1	0	4.306478	5.122633	-2.021724
139	1	0	5.601216	6.224338	-1.560465
140	6	0	4.786075	6.691805	2.076441
141	6	0	4.944874	6.183244	3.356751
142	7	0	4.547988	8.000530	1.875238
143	6	0	4.862138	7.050955	4.441307
144	1	0	5.129935	5.124248	3.497446
145	6	0	4.463874	8.842281	2.915304
146	6	0	4.621304	8.402900	4.219343
147	1	0	4.980334	6.672274	5.451207
148	1	0	4.266553	9.882633	2.683311
149	1	0	4.548496	9.108082	5.038612
150	6	0	3.968699	7.190580	-2.494698
151	6	0	3.657348	6.968941	-3.827847
152	7	0	3.870308	8.418967	-1.954228
153	6	0	3.245131	8.042274	-4.611250
154	1	0	3.736652	5.969651	-4.241184
155	6	0	3.470106	9.457348	-2.702599
156	6	0	3.152536	9.308243	-4.042345
157	1	0	2.993722	7.889320	-5.655607
158	1	0	3.407758	10.418392	-2.205056
159	1	0	2.833184	10.167531	-4.619716
160	30	0	4.168623	8.423019	-0.008004

1-Zn^{2+}-$3H^{+}$ (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-3.926581	-1.027029	-1.028906
2	6	0	-4.310618	1.380441	-0.899621

3	6	0	-4.799997	0.071247	-1.009407
4	6	0	-2.740392	2.942820	-0.678996
5	6	0	-3.987918	3.604960	-0.736406
6	6	0	-4.979461	2.651835	-0.873855
7	7	0	-2.950876	1.609856	-0.787139
8	7	0	-2.558662	-0.831937	-0.949383
9	5	0	-1.864740	0.516891	-0.659713
10	9	0	-0.848377	0.743971	-1.594558
11	9	0	-1.324866	0.516675	0.622078
12	6	0	-4.169689	-2.437796	-1.128465
13	6	0	-2.927074	-3.044758	-1.093643
14	6	0	-1.943603	-2.037181	-0.981881
15	1	0	-4.136057	4.675470	-0.692440
16	1	0	-2.734717	-4.106326	-1.171659
17	6	0	-5.466734	-3.163431	-1.261151
18	1	0	-6.127879	-2.974317	-0.409954
19	1	0	-6.011747	-2.864297	-2.161426
20	1	0	-5.283022	-4.238625	-1.316262
21	6	0	-6.437233	2.950607	-0.981656
22	1	0	-6.856365	2.596603	-1.928264
23	1	0	-7.011582	2.475533	-0.180949
24	1	0	-6.596995	4.029320	-0.921549
25	6	0	-6.267740	-0.155232	-1.099508
26	6	0	-7.021932	-0.329020	0.062715
27	6	0	-6.900017	-0.190038	-2.345353
28	6	0	-8.396752	-0.529499	-0.010696
29	1	0	-6.535022	-0.307759	1.032359
30	6	0	-8.273156	-0.387826	-2.434143
31	1	0	-6.317915	-0.057984	-3.251558
32	6	0	-9.000105	-0.547373	-1.261328
33	1	0	-8.981016	-0.684734	0.894446
34	1	0	-8.755065	-0.408196	-3.406638
35	6	0	-1.407574	3.457582	-0.523829
36	6	0	-1.063486	4.732247	-0.242983
37	1	0	-0.625572	2.713652	-0.619227
38	1	0	-1.827710	5.492425	-0.094535
39	6	0	-0.507639	-2.141292	-0.930056
40	6	0	0.181191	-3.268820	-0.656757
41	1	0	0.028048	-1.213798	-1.104199
42	1	0	-0.350535	-4.184553	-0.405972
43	6	0	0.322625	5.148675	-0.047196
44	6	0	0.608254	6.362591	0.599547
45	6	0	1.402397	4.346871	-0.451116
46	6	0	1.913507	6.735664	0.896027
47	1	0	-0.207225	7.012889	0.901035
48	6	0	2.707103	4.706767	-0.160935
49	1	0	1.232159	3.429796	-1.003720
50	6	0	2.953671	5.888617	0.529065
51	1	0	2.098603	7.668090	1.420216
52	1	0	3.526348	4.074029	-0.485893
53	6	0	1.639149	-3.332439	-0.602554
54	6	0	2.454656	-2.383287	-1.245649
55	6	0	2.261571	-4.358436	0.122669
56	6	0	3.834119	-2.430628	-1.138487
57	1	0	2.008944	-1.605309	-1.855641
58	6	0	3.644786	-4.415317	0.247505
59	1	0	1.656003	-5.112554	0.615391
60	6	0	4.410923	-3.442598	-0.377187
61	1	0	4.439519	-1.689610	-1.652017
62	1	0	4.103480	-5.210770	0.828002
63	7	0	-10.455207	-0.756332	-1.320465
64	6	0	-11.206776	0.350401	-2.035904
65	6	0	-10.838139	-2.113855	-1.851573
66	6	0	-12.317848	0.851129	-1.145286
67	1	0	-11.579180	-0.036708	-2.984590
68	1	0	-10.496243	1.154872	-2.224809
69	6	0	-10.200863	-3.202709	-1.023395
70	1	0	-10.524963	-2.169343	-2.895209
71	1	0	-11.927849	-2.162995	-1.797587
72	8	0	-11.675585	1.315214	0.017659
73	1	0	-12.853066	1.655463	-1.668347
74	1	0	-13.043542	0.053597	-0.926467
75	8	0	-10.528719	-2.938322	0.316934
76	1	0	-10.590238	-4.173531	-1.361419
77	1	0	-9.110728	-3.210569	-1.168281
78	6	0	-12.542537	1.717873	1.067703
79	6	0	-9.797505	-3.733398	1.233736
80	6	0	-12.842537	0.586132	2.022731
81	1	0	-12.016445	2.511576	1.606529
82	1	0	-13.475776	2.134565	0.668413
83	6	0	-10.193464	-3.330932	2.628654
84	1	0	-10.018669	-4.799260	1.081789
85	1	0	-8.717676	-3.581759	1.086834
86	8	0	-11.620449	0.144906	2.564451
87	1	0	-13.519473	0.956876	2.809156
88	1	0	-13.359396	-0.241099	1.508947
89	8	0	-9.756900	-2.008495	2.859963
90	1	0	-11.284103	-3.417757	2.724561
91	1	0	-9.737648	-4.023838	3.352096
92	6	0	-11.785707	-0.843608	3.553977
93	6	0	-10.418958	-1.371941	3.935141
94	1	0	-12.431158	-1.655177	3.182858
95	1	0	-12.274338	-0.427191	4.449833
96	1	0	-10.515326	-2.048037	4.796958
97	1	0	-9.782230	-0.533158	4.233256
98	7	0	4.342720	6.202356	0.904099
99	6	0	4.876828	7.481368	0.320428
100	6	0	4.568130	6.083399	2.391598
101	6	0	4.885015	7.434883	-1.201579
102	1	0	5.887937	7.590368	0.717526
103	1	0	4.270808	8.311562	0.687369
104	6	0	4.790350	4.633908	2.785307
105	1	0	3.697465	6.505212	2.895355
106	1	0	5.440934	6.690700	2.639159
107	1	0	3.870588	7.533002	-1.597621
108	1	0	5.463284	8.287028	-1.568201
109	16	0	5.498983	5.879272	-1.910738
110	1	0	4.816529	4.575734	3.875443
111	1	0	3.973460	3.993467	2.440459
112	16	0	6.378742	4.039184	2.105437
113	6	0	7.282166	5.898107	-1.524288
114	6	0	5.937031	2.509479	1.215690
115	6	0	7.900678	4.628778	-2.080570
116	1	0	7.751272	6.771953	-1.984305

117	1	0	7.433622	5.933481	-0.441667
118	6	0	7.245096	1.794711	0.875907
119	1	0	5.296522	1.884740	1.842957
120	1	0	5.407593	2.767980	0.296763
121	8	0	7.234619	3.527815	-1.506350
122	1	0	7.809500	4.602370	-3.177590
123	1	0	8.973042	4.618175	-1.833078
124	8	0	7.084057	0.773080	-0.090053
125	1	0	7.988309	2.526546	0.537652
126	1	0	7.640888	1.300387	1.767463
127	6	0	7.664845	2.273631	-1.993940
128	6	0	6.776796	1.189966	-1.413655
129	1	0	8.719618	2.087595	-1.736820
130	1	0	7.578586	2.242815	-3.091091
131	1	0	6.882287	0.288130	-2.023845
132	1	0	5.732291	1.522933	-1.493906
133	7	0	5.885529	-3.512164	-0.258740
134	6	0	6.551864	-3.972793	-1.561926
135	1	0	7.412674	-3.325078	-1.740552
136	1	0	5.835890	-3.815226	-2.365499
137	6	0	6.507369	-2.234587	0.311295
138	1	0	5.784100	-1.429636	0.214035
139	1	0	7.365919	-1.970031	-0.307215
140	6	0	6.974787	-5.408685	-1.489000
141	6	0	6.411868	-6.354915	-2.329158
142	7	0	7.928213	-5.740698	-0.586245
143	6	0	6.840215	-7.678114	-2.252608
144	1	0	5.645571	-6.056175	-3.034800
145	6	0	8.325300	-7.022981	-0.501725
146	6	0	7.809524	-8.015736	-1.320775
147	1	0	6.412626	-8.429235	-2.907714
148	1	0	9.078586	-7.259199	0.241175
149	1	0	8.170343	-9.031879	-1.217403
150	6	0	6.922705	-2.400113	1.740151
151	6	0	6.317164	-1.656570	2.740023
152	7	0	7.925027	-3.267190	2.013601
153	6	0	6.756860	-1.790200	4.054717
154	1	0	5.509029	-0.980141	2.487844
155	6	0	8.338871	-3.403194	3.285402
156	6	0	7.786190	-2.677494	4.329182
157	1	0	6.295204	-1.211130	4.847024
158	1	0	9.139555	-4.110695	3.469109
159	1	0	8.163852	-2.818388	5.334638
160	30	0	8.806274	-4.471347	0.685445
161	1	0	6.053705	-4.249108	0.432518
162	1	0	4.937492	5.476440	0.458498
163	1	0	-10.767433	-0.731357	-0.338477

1-Zn^{2+}-$3H^{+}$-1W (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	3.962812	0.540758	-0.658772
2	6	0	3.897688	-1.881971	-0.384820
3	6	0	4.617262	-0.696169	-0.574806
4	6	0	2.073398	-3.121028	-0.092753
5	6	0	3.189445	-3.988952	-0.043439
6	6	0	4.334368	-3.239664	-0.223998
7	7	0	2.514988	-1.856849	-0.293179
8	7	0	2.582249	0.610883	-0.570134
9	5	0	1.634681	-0.615310	-0.583625
10	9	0	1.024958	-0.737850	-1.827233
11	9	0	0.659694	-0.477658	0.407378
12	6	0	4.473470	1.874156	-0.795485
13	6	0	3.371847	2.706595	-0.784441
14	6	0	2.210872	1.911428	-0.646910
15	1	0	3.153010	-5.055746	0.129834
16	1	0	3.395400	3.785657	-0.851739
17	6	0	5.886415	2.340053	-0.913944
18	1	0	6.477864	2.079770	-0.031003
19	1	0	6.391480	1.899041	-1.778329
20	1	0	5.905649	3.426295	-1.026403
21	6	0	5.720062	-3.793094	-0.222438
22	1	0	6.248410	-3.575288	-1.155130
23	1	0	6.323543	-3.379109	0.590823
24	1	0	5.681606	-4.877490	-0.098144
25	6	0	6.101257	-0.746548	-0.668717
26	6	0	6.882075	-0.640450	0.483798
27	6	0	6.722048	-0.898674	-1.911199
28	6	0	8.269400	-0.684403	0.400403
29	1	0	6.406394	-0.520283	1.451709
30	6	0	8.108102	-0.946066	-2.006568
31	1	0	6.120392	-0.981367	-2.810336
32	6	0	8.862397	-0.838613	-0.844677
33	1	0	8.876747	-0.588810	1.294483
34	1	0	8.575905	-1.065535	-2.978482
35	6	0	0.675716	-3.434627	0.049530
36	6	0	0.196945	-4.697198	0.082902
37	1	0	0.006488	-2.584935	0.131925
38	1	0	0.891340	-5.528190	-0.023064
39	6	0	0.833903	2.324106	-0.569229
40	6	0	0.430319	3.604819	-0.715159
41	1	0	0.116570	1.540079	-0.351335
42	1	0	1.174007	4.376424	-0.902613
43	6	0	-1.201406	-5.079430	0.228950
44	6	0	-1.540605	-6.438605	0.132251
45	6	0	-2.234532	-4.156090	0.462345
46	6	0	-2.854617	-6.871188	0.248235
47	1	0	-0.759148	-7.171791	-0.042340
48	6	0	-3.549698	-4.574794	0.580188
49	1	0	-2.017404	-3.098249	0.560684
50	6	0	-3.852303	-5.929455	0.470766
51	1	0	-3.074873	-7.929820	0.164395
52	1	0	-4.334977	-3.845673	0.759467
53	6	0	-0.941970	4.083029	-0.612008
54	6	0	-2.053500	3.222632	-0.536464
55	6	0	-1.171584	5.466655	-0.578218
56	6	0	-3.337328	3.721654	-0.402707
57	1	0	-1.920315	2.147935	-0.589579
58	6	0	-2.453604	5.983999	-0.440185
59	1	0	-0.331773	6.150853	-0.647565
60	6	0	-3.517854	5.101503	-0.345589

61	1	0	-4.179603	3.038073	-0.345935
62	1	0	-2.605860	7.058924	-0.402835
63	7	0	10.329757	-0.895646	-0.923070
64	6	0	10.810254	-2.228031	-1.437061
65	6	0	10.922999	0.280299	-1.649402
66	6	0	12.271068	-2.438293	-1.107400
67	1	0	10.627560	-2.275288	-2.511029
68	1	0	10.198601	-2.977234	-0.932175
69	6	0	10.530174	1.563658	-0.949433
70	1	0	10.584710	0.258844	-2.686276
71	1	0	12.004642	0.148845	-1.617875
72	8	0	12.407370	-2.196335	0.271787
73	1	0	12.524624	-3.476512	-1.364449
74	1	0	12.922197	-1.787407	-1.706841
75	8	0	10.747063	1.351945	0.424988
76	1	0	11.154700	2.371520	-1.353489
77	1	0	9.478290	1.817454	-1.143124
78	6	0	13.737543	-2.342748	0.755317
79	6	0	10.692176	2.533495	1.216379
80	6	0	14.561999	-1.082760	0.610720
81	1	0	13.650120	-2.592156	1.816671
82	1	0	14.234702	-3.178338	0.246041
83	6	0	12.081667	3.037165	1.533366
84	1	0	10.107679	3.310894	0.709871
85	1	0	10.178952	2.274242	2.147726
86	8	0	14.068465	-0.126446	1.515926
87	1	0	15.618752	-1.317487	0.818765
88	1	0	14.515564	-0.706052	-0.424056
89	8	0	12.671275	2.134458	2.443703
90	1	0	12.662591	3.114766	0.603258
91	1	0	12.021796	4.045977	1.971360
92	6	0	14.592575	1.162978	1.300181
93	6	0	14.080522	2.075031	2.396250
94	1	0	14.296911	1.532999	0.304756
95	1	0	15.694377	1.157749	1.330948
96	1	0	14.525027	3.073894	2.277795
97	1	0	14.401354	1.678287	3.365054
98	7	0	-5.266375	-6.327922	0.549818
99	6	0	-5.915129	-6.541874	-0.807996
100	6	0	-5.554846	-7.423931	1.541275
101	6	0	-5.573630	-7.852241	-1.487106
102	1	0	-5.610220	-5.692173	-1.421364
103	1	0	-6.992620	-6.486389	-0.635073
104	6	0	-5.613750	-6.850215	2.947345
105	1	0	-4.780008	-8.186218	1.460351
106	1	0	-6.508748	-7.869751	1.256849
107	1	0	-4.537855	-7.874412	-1.835023
108	1	0	-5.732013	-8.716957	-0.836658
109	16	0	-6.585475	-8.063647	-2.983532
110	1	0	-5.781469	-7.663638	3.657723
111	1	0	-4.661807	-6.380004	3.212440
112	16	0	-6.890043	-5.570422	3.162438
113	6	0	-8.177858	-8.689059	-2.341167
114	6	0	-8.402936	-6.578165	3.386060
115	6	0	-9.267805	-7.663878	-2.098966
116	1	0	-8.529520	-9.386280	-3.107149
117	1	0	-7.988551	-9.274107	-1.435733
118	6	0	-9.260692	-6.858382	2.161893
119	1	0	-8.100708	-7.518739	3.858067
120	1	0	-9.003502	-6.026861	4.115230
121	8	0	-8.993512	-6.921048	-0.930322
122	1	0	-9.359124	-6.993540	-2.966516
123	1	0	-10.225832	-8.195540	-1.986861
124	8	0	-9.973698	-5.710199	1.740479
125	1	0	-8.687456	-7.292315	1.338597
126	1	0	-10.005410	-7.607974	2.461165
127	6	0	-9.905760	-5.855572	-0.726306
128	6	0	-9.554019	-5.097568	0.539167
129	1	0	-10.934517	-6.238657	-0.653400
130	1	0	-9.863703	-5.161095	-1.579834
131	1	0	-10.077354	-4.136665	0.507511
132	1	0	-8.476854	-4.881187	0.553682
133	7	0	-4.883299	5.643430	-0.176486
134	6	0	-5.778686	5.372609	-1.390678
135	1	0	-6.714925	4.945877	-1.026574
136	1	0	-5.279589	4.622262	-1.999554
137	6	0	-5.512040	5.232804	1.160671
138	1	0	-4.910199	4.424225	1.568114
139	1	0	-6.509401	4.841529	0.957254
140	6	0	-6.017158	6.622520	-2.183178
141	6	0	-5.498048	6.743759	-3.462704
142	7	0	-6.746819	7.613825	-1.618894
143	6	0	-5.733865	7.906068	-4.192600
144	1	0	-4.914799	5.932153	-3.881975
145	6	0	-6.959058	8.738633	-2.322954
146	6	0	-6.475184	8.921431	-3.609307
147	1	0	-5.337160	8.011140	-5.196474
148	1	0	-7.544083	9.512809	-1.840883
149	1	0	-6.684224	9.847071	-4.131770
150	6	0	-5.555848	6.388523	2.114140
151	6	0	-4.771879	6.358414	3.257449
152	7	0	-6.363633	7.437848	1.826442
153	6	0	-4.809747	7.428600	4.146282
154	1	0	-4.135891	5.501435	3.446385
155	6	0	-6.381402	8.473859	2.685310
156	6	0	-5.628375	8.505979	3.849543
157	1	0	-4.204333	7.416618	5.045979
158	1	0	-7.030399	9.309167	2.445722
159	1	0	-5.694550	9.368408	4.501735
160	30	0	-7.600383	7.647113	0.199700
161	1	0	-4.767538	6.660501	-0.131770
162	1	0	-5.780722	-5.519585	0.937079
163	1	0	10.700993	-0.817841	0.036754
164	8	0	-9.481137	7.370854	0.798038
165	1	0	-9.827130	7.988250	1.456377
166	1	0	-10.147339	7.300886	0.101613

1-Hg^{2+} (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.530118	0.005594	-0.475269

2	6	0	3.772077	-2.191138	0.248789
3	6	0	4.806289	-1.329418	-0.159797
4	6	0	1.671878	-2.764761	0.739487
5	6	0	2.470733	-3.924011	0.856956
6	6	0	3.779157	-3.589037	0.552865
7	7	0	2.469504	-1.730571	0.366303
8	7	0	3.235457	0.503958	-0.394620
9	5	0	2.041127	-0.252122	0.229412
10	9	0	0.919371	-0.150789	-0.605746
11	9	0	1.728442	0.281937	1.480373
12	6	0	5.389293	1.072114	-0.904479
13	6	0	4.578688	2.176555	-1.072132
14	6	0	3.246889	1.813436	-0.749134
15	1	0	2.114303	-4.912772	1.113935
16	1	0	4.903002	3.152972	-1.406663
17	6	0	6.863303	1.058242	-1.139517
18	1	0	7.407923	0.653088	-0.282042
19	1	0	7.133094	0.439312	-2.000699
20	1	0	7.215937	2.075595	-1.327122
21	6	0	4.919986	-4.552401	0.535878
22	1	0	5.447616	-4.542076	-0.422283
23	1	0	5.663873	-4.318084	1.303429
24	1	0	4.550353	-5.564967	0.717027
25	6	0	6.193657	-1.845088	-0.270616
26	6	0	7.018761	-1.953287	0.853705
27	6	0	6.723854	-2.226170	-1.504592
28	6	0	8.321560	-2.417902	0.753357
29	1	0	6.641403	-1.645713	1.825708
30	6	0	8.020796	-2.710963	-1.618607
31	1	0	6.108294	-2.154065	-2.397612
32	6	0	8.856536	-2.827991	-0.487631
33	1	0	8.955397	-2.424666	1.633169
34	1	0	8.369889	-3.011525	-2.599425
35	6	0	0.255288	-2.610290	0.934387
36	6	0	-0.553792	-3.573845	1.433827
37	1	0	-0.156278	-1.650677	0.640245
38	1	0	-0.114361	-4.525300	1.731322
39	6	0	2.059495	2.617936	-0.772577
40	6	0	2.065499	3.955967	-1.001476
41	1	0	1.125473	2.093654	-0.600846
42	1	0	3.024850	4.447236	-1.162139
43	6	0	-1.990270	-3.472506	1.626560
44	6	0	-2.694292	-4.549837	2.186246
45	6	0	-2.743294	-2.334924	1.279799
46	6	0	-4.067753	-4.510235	2.389005
47	1	0	-2.147092	-5.440230	2.486611
48	6	0	-4.111432	-2.289846	1.468155
49	1	0	-2.255536	-1.469003	0.842468
50	6	0	-4.816395	-3.378886	2.022418
51	1	0	-4.542490	-5.359559	2.866964
52	1	0	-4.649312	-1.398445	1.165457
53	6	0	0.919836	4.835559	-1.052331
54	6	0	-0.410967	4.409267	-0.876341
55	6	0	1.110116	6.210199	-1.280149
56	6	0	-1.472509	5.289072	-0.928762
57	1	0	-0.625303	3.360330	-0.692022
58	6	0	0.058143	7.105869	-1.335383
59	1	0	2.121620	6.587836	-1.411485
60	6	0	-1.277939	6.673178	-1.171269
61	1	0	-2.471473	4.898692	-0.776525
62	1	0	0.288983	8.151339	-1.499266
63	7	0	10.147703	-3.315429	-0.578125
64	6	0	10.773437	-3.962092	0.565825
65	6	0	10.741802	-3.574496	-1.877227
66	6	0	11.839827	-3.155213	1.287594
67	1	0	11.244168	-4.890122	0.218693
68	1	0	10.002935	-4.257184	1.285161
69	6	0	11.112726	-2.336065	-2.675610
70	1	0	10.091392	-4.209271	-2.498246
71	1	0	11.659829	-4.143672	-1.711595
72	8	0	11.234161	-2.117284	2.028012
73	1	0	12.386633	-3.835143	1.961113
74	1	0	12.554308	-2.751960	0.555777
75	8	0	12.131708	-1.630491	-2.008687
76	1	0	11.453737	-2.664493	-3.671544
77	1	0	10.239048	-1.684192	-2.830063
78	6	0	12.038998	-1.591476	3.060297
79	6	0	12.610388	-0.547957	-2.774964
80	6	0	13.311718	-0.918676	2.587004
81	1	0	11.412613	-0.859826	3.579989
82	1	0	12.313842	-2.379827	3.780006
83	6	0	13.564902	0.270500	-1.943145
84	1	0	13.129699	-0.911046	-3.676544
85	1	0	11.778069	0.093286	-3.106021
86	8	0	12.975834	0.118057	1.700420
87	1	0	13.854866	-0.538698	3.468533
88	1	0	13.975399	-1.646266	2.092392
89	8	0	12.822433	0.988172	-0.983899
90	1	0	14.295308	-0.404467	-1.474064
91	1	0	14.121423	0.960110	-2.597985
92	6	0	14.097456	0.694272	1.077277
93	6	0	13.608757	1.633448	-0.007285
94	1	0	14.744255	-0.090882	0.653525
95	1	0	14.711320	1.262264	1.796086
96	1	0	14.472066	2.145332	-0.460042
97	1	0	12.965202	2.395228	0.445151
98	7	0	-6.203344	-3.286580	2.193673
99	6	0	-6.948036	-4.485422	2.551065
100	6	0	-6.704324	-2.043072	2.795604
101	6	0	-6.917365	-5.636861	1.545068
102	1	0	-7.986289	-4.185229	2.709509
103	1	0	-6.605483	-4.905161	3.512355
104	6	0	-7.243092	-0.976158	1.838405
105	1	0	-5.912340	-1.579773	3.395922
106	1	0	-7.505423	-2.311073	3.490668
107	1	0	-5.895814	-5.951805	1.321082
108	1	0	-7.421499	-6.494467	2.001984
109	16	0	-7.650028	-5.401367	-0.101146
110	1	0	-7.802098	-0.241135	2.426927
111	1	0	-6.448946	-0.445165	1.309790
112	16	0	-8.380477	-1.732368	0.642784
113	6	0	-9.421960	-5.182590	0.268215
114	6	0	-9.262466	-0.271121	-0.008701
115	6	0	-10.200730	-4.790824	-0.972973

116	1	0	-9.794614	-6.136535	0.651965
117	1	0	-9.548897	-4.411535	1.031281
118	6	0	-10.625441	-0.618397	-0.632152
119	1	0	-9.418763	0.383528	0.853495
120	1	0	-8.642158	0.266291	-0.730375
121	8	0	-9.846532	-3.474694	-1.320988
122	1	0	-9.997372	-5.483522	-1.804576
123	1	0	-11.274949	-4.858069	-0.742548
124	8	0	-10.666572	-0.574429	-2.041566
125	1	0	-10.988186	-1.579188	-0.247870
126	1	0	-11.336439	0.151404	-0.318934
127	6	0	-10.443183	-2.998147	-2.508483
128	6	0	-9.973308	-1.576595	-2.754583
129	1	0	-11.541570	-3.021690	-2.435224
130	1	0	-10.148830	-3.629566	-3.361299
131	1	0	-10.136095	-1.334347	-3.809058
132	1	0	-8.888543	-1.520188	-2.569880
133	7	0	-2.351664	7.522491	-1.253730
134	6	0	-2.229356	8.929376	-1.604367
135	1	0	-3.008067	9.167745	-2.336837
136	1	0	-1.271063	9.101466	-2.094369
137	6	0	-3.689303	7.051858	-0.976036
138	1	0	-3.956140	6.222977	-1.646405
139	1	0	-4.371010	7.873823	-1.216972
140	6	0	-2.405000	9.862352	-0.425957
141	6	0	-1.329330	10.234014	0.383708
142	7	0	-3.654068	10.290305	-0.205471
143	6	0	-1.562102	11.071516	1.467893
144	1	0	-0.328990	9.872239	0.167070
145	6	0	-3.866199	11.089691	0.843482
146	6	0	-2.861319	11.509124	1.709028
147	1	0	-0.743793	11.380054	2.111898
148	1	0	-4.892826	11.418455	0.996091
149	1	0	-3.092405	12.164633	2.542218
150	6	0	-3.966675	6.638095	0.459390
151	6	0	-5.065645	5.816536	0.728852
152	7	0	-3.167138	7.107570	1.417874
153	6	0	-5.348491	5.484737	2.047554
154	1	0	-5.684015	5.446892	-0.084457
155	6	0	-3.446046	6.775819	2.682067
156	6	0	-4.520027	5.974933	3.053770
157	1	0	-6.197068	4.850191	2.286231
158	1	0	-2.771940	7.172709	3.439579
159	1	0	-4.696283	5.740097	4.098278
160	80	0	-6.528540	-2.916280	-1.215382

1-Hg^{2+}-3H^{+} (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.628271	0.606833	-0.693152
2	6	0	3.910692	-1.698112	-0.347433
3	6	0	4.915714	-0.762233	-0.629867
4	6	0	1.842090	-2.374178	0.115313
5	6	0	2.655248	-3.527389	0.024105
6	6	0	3.946716	-3.129584	-0.262958
7	7	0	2.610231	-1.282145	-0.114947
8	7	0	3.338522	1.064571	-0.473793
9	5	0	2.163585	0.193198	0.033997
10	9	0	1.023548	0.428115	-0.741022
11	9	0	1.888181	0.482268	1.366318
12	6	0	5.461076	1.737437	-0.990450
13	6	0	4.636597	2.843407	-0.935966
14	6	0	3.328338	2.411373	-0.613642
15	1	0	2.319427	-4.548856	0.140730
16	1	0	4.935633	3.864530	-1.129645
17	6	0	6.917743	1.780927	-1.311622
18	1	0	7.525972	1.372637	-0.498670
19	1	0	7.156318	1.204391	-2.210343
20	1	0	7.225602	2.815347	-1.479791
21	6	0	5.100466	-4.058128	-0.447181
22	1	0	5.532074	-3.980208	-1.449581
23	1	0	5.906183	-3.853816	0.264044
24	1	0	4.769590	-5.088517	-0.299144
25	6	0	6.304034	-1.231695	-0.886365
26	6	0	7.212727	-1.356835	0.166532
27	6	0	6.706109	-1.548028	-2.187373
28	6	0	8.512713	-1.793576	-0.070732
29	1	0	6.906541	-1.110548	1.178201
30	6	0	8.001415	-1.985383	-2.439264
31	1	0	6.003356	-1.452654	-3.008850
32	6	0	8.883462	-2.104491	-1.372672
33	1	0	9.226270	-1.871486	0.747109
34	1	0	8.303734	-2.231051	-3.452564
35	6	0	0.431848	-2.273441	0.384957
36	6	0	-0.341739	-3.322139	0.741418
37	1	0	0.001365	-1.284374	0.270438
38	1	0	0.112672	-4.305597	0.843451
39	6	0	2.127617	3.191016	-0.463334
40	6	0	2.115040	4.542071	-0.452699
41	1	0	1.206144	2.626479	-0.368348
42	1	0	3.058487	5.077864	-0.537853
43	6	0	-1.773185	-3.271302	1.010284
44	6	0	-2.448108	-4.466014	1.310952
45	6	0	-2.519297	-2.080270	0.986852
46	6	0	-3.812219	-4.487140	1.571909
47	1	0	-1.893618	-5.399157	1.339304
48	6	0	-3.880319	-2.087491	1.243663
49	1	0	-2.039150	-1.131736	0.773088
50	6	0	-4.518186	-3.290503	1.535321
51	1	0	-4.295074	-5.431259	1.800451
52	1	0	-4.439151	-1.155890	1.219268
53	6	0	0.936634	5.390389	-0.331633
54	6	0	-0.373454	4.884885	-0.244210
55	6	0	1.110542	6.782843	-0.307197
56	6	0	-1.461696	5.735083	-0.139300
57	1	0	-0.552418	3.815316	-0.261657
58	6	0	0.027534	7.646435	-0.201077
59	1	0	2.112268	7.196801	-0.373741
60	6	0	-1.251062	7.112093	-0.119418
61	1	0	-2.461686	5.316406	-0.077625
62	1	0	0.176798	8.720600	-0.184528

63	7	0	10.262330	-2.555009	-1.612711
64	6	0	10.353108	-3.875807	-2.346390
65	6	0	11.114789	-1.501063	-2.272582
66	6	0	11.423034	-4.729201	-1.706636
67	1	0	10.549495	-3.678912	-3.400619
68	1	0	9.386150	-4.368208	-2.240621
69	6	0	11.135588	-0.238277	-1.445698
70	1	0	10.709536	-1.317308	-3.268840
71	1	0	12.115217	-1.929837	-2.361739
72	8	0	11.002256	-4.901687	-0.375404
73	1	0	11.477333	-5.683640	-2.248072
74	1	0	12.413280	-4.253329	-1.767101
75	8	0	11.515834	-0.605756	-0.144679
76	1	0	11.846471	0.465834	-1.901211
77	1	0	10.145544	0.240336	-1.446930
78	6	0	11.921714	-5.574663	0.472533
79	6	0	11.304343	0.424343	0.804355
80	6	0	12.749482	-4.604613	1.282497
81	1	0	11.321685	-6.188914	1.151246
82	1	0	12.574757	-6.240482	-0.104738
83	6	0	11.757378	-0.074723	2.150437
84	1	0	11.878250	1.322602	0.535756
85	1	0	10.238046	0.694990	0.834504
86	8	0	11.867115	-3.832148	2.059862
87	1	0	13.448372	-5.176233	1.914491
88	1	0	13.353340	-3.957507	0.624964
89	8	0	10.934670	-1.154398	2.536250
90	1	0	12.810192	-0.378093	2.076111
91	1	0	11.696732	0.744506	2.883032
92	6	0	12.532831	-2.955902	2.937820
93	6	0	11.518399	-1.990660	3.515754
94	1	0	13.329825	-2.412282	2.406722
95	1	0	13.014461	-3.510530	3.759642
96	1	0	11.991309	-1.397560	4.312051
97	1	0	10.696704	-2.559756	3.961701
98	7	0	-5.973095	-3.256937	1.757392
99	6	0	-6.783272	-3.631584	0.532921
100	6	0	-6.432618	-3.919709	3.029272
101	6	0	-6.869100	-5.119089	0.250900
102	1	0	-6.318665	-3.104187	-0.303623
103	1	0	-7.785904	-3.229217	0.697365
104	6	0	-6.164530	-3.002150	4.211513
105	1	0	-5.912575	-4.870952	3.143926
106	1	0	-7.499995	-4.115656	2.918816
107	1	0	-5.931051	-5.522661	-0.137826
108	1	0	-7.151296	-5.703958	1.130500
109	16	0	-8.100443	-5.496746	-1.036260
110	1	0	-6.485873	-3.501548	5.129016
111	1	0	-5.093392	-2.800639	4.308594
112	16	0	-6.977460	-1.379541	4.073417
113	6	0	-9.716947	-5.375695	-0.189559
114	6	0	-8.684037	-1.765100	4.612019
115	6	0	-10.450394	-4.052457	-0.239092
116	1	0	-10.328849	-6.131542	-0.689302
117	1	0	-9.569181	-5.704058	0.843837
118	6	0	-9.707765	-2.102431	3.539207
119	1	0	-8.618730	-2.577947	5.342549
120	1	0	-9.019051	-0.872380	5.147863
121	8	0	-9.827276	-3.113141	0.604710
122	1	0	-10.497285	-3.679314	-1.273843
123	1	0	-11.485037	-4.231021	0.092341
124	8	0	-10.104681	-0.954977	2.811972
125	1	0	-9.365127	-2.896690	2.870926
126	1	0	-10.598471	-2.484195	4.055994
127	6	0	-10.398280	-1.816825	0.513207
128	6	0	-9.693898	-0.869086	1.465469
129	1	0	-11.471264	-1.853164	0.750698
130	1	0	-10.288541	-1.437498	-0.514700
131	1	0	-9.933516	0.152846	1.155242
132	1	0	-8.605832	-0.991441	1.367094
133	7	0	-2.403023	8.024133	-0.018565
134	6	0	-3.282743	7.973539	-1.229399
135	1	0	-4.226544	8.458890	-0.964520
136	1	0	-3.488514	6.935290	-1.488349
137	6	0	-3.130188	7.897189	1.284101
138	1	0	-3.313581	6.844613	1.499383
139	1	0	-4.094542	8.399617	1.166084
140	6	0	-2.608642	8.730868	-2.346668
141	6	0	-2.815792	8.405740	-3.683068
142	7	0	-1.849281	9.753821	-1.948967
143	6	0	-2.209037	9.201440	-4.650158
144	1	0	-3.432656	7.556168	-3.957641
145	6	0	-1.263135	10.505085	-2.883016
146	6	0	-1.418725	10.272886	-4.245930
147	1	0	-2.346301	8.982102	-5.704362
148	1	0	-0.644751	11.324485	-2.525107
149	1	0	-0.924598	10.913114	-4.968479
150	6	0	-2.318465	8.580406	2.356781
151	6	0	-2.370585	8.175025	3.686283
152	7	0	-1.597326	9.620811	1.934053
153	6	0	-1.642457	8.905345	4.620522
154	1	0	-2.962630	7.314402	3.980330
155	6	0	-0.894168	10.309045	2.835403
156	6	0	-0.890365	9.994185	4.190548
157	1	0	-1.657178	8.622345	5.668368
158	1	0	-0.311145	11.144822	2.456615
159	1	0	-0.305163	10.585139	4.886568
160	80	0	-7.931961	-3.291207	-2.943140
161	1	0	-2.008927	8.993941	-0.012419
162	1	0	-6.221931	-2.265056	1.920854
163	1	0	10.668765	-2.723196	-0.679443

1-Hg^{2+}-$3H^{+}$-1W (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.795090	1.017774	-0.665557
2	6	0	4.587732	-1.411387	-0.610887
3	6	0	5.370782	-0.256075	-0.746684
4	6	0	2.713176	-2.561057	-0.277559
5	6	0	3.761372	-3.496032	-0.429707
6	6	0	4.939170	-2.801248	-0.634095

7	7	0	3.224491	-1.311593	-0.385190
8	7	0	3.431983	1.161293	-0.459318
9	5	0	2.406586	0.001193	-0.448038
10	9	0	1.629994	0.031128	-1.601944
11	9	0	1.579380	0.108126	0.674756
12	6	0	5.375294	2.327749	-0.756109
13	6	0	4.331120	3.218481	-0.606135
14	6	0	3.136378	2.481863	-0.427571
15	1	0	3.661944	-4.570810	-0.358452
16	1	0	4.415353	4.296701	-0.604665
17	6	0	6.801275	2.719819	-0.956385
18	1	0	7.433078	2.396522	-0.123180
19	1	0	7.222779	2.280917	-1.865366
20	1	0	6.875017	3.806777	-1.035613
21	6	0	6.279233	-3.433248	-0.813339
22	1	0	6.715331	-3.194706	-1.788061
23	1	0	6.993132	-3.099676	-0.054402
24	1	0	6.186253	-4.519139	-0.740111
25	6	0	6.837262	-0.382505	-0.961309
26	6	0	7.706084	-0.365399	0.131538
27	6	0	7.355400	-0.508477	-2.253618
28	6	0	9.081275	-0.470453	-0.054633
29	1	0	7.308525	-0.262951	1.136431
30	6	0	8.726958	-0.614796	-2.455309
31	1	0	6.685209	-0.521599	-3.107064
32	6	0	9.567560	-0.595573	-1.348444
33	1	0	9.760167	-0.425990	0.795109
34	1	0	9.118201	-0.712285	-3.463008
35	6	0	1.318113	-2.797441	-0.005719
36	6	0	0.709658	-3.992471	-0.163852
37	1	0	0.752501	-1.936858	0.338044
38	1	0	1.266771	-4.827433	-0.584422
39	6	0	1.793730	2.964643	-0.234288
40	6	0	1.444280	4.261235	-0.382564
41	1	0	1.055963	2.218108	0.040450
42	1	0	2.206810	4.980299	-0.675760
43	6	0	-0.691256	-4.254729	0.149221
44	6	0	-1.339776	-5.350816	-0.441179
45	6	0	-1.425181	-3.448218	1.034899
46	6	0	-2.681155	-5.619695	-0.195836
47	1	0	-0.788976	-5.996797	-1.118119
48	6	0	-2.759922	-3.711292	1.296248
49	1	0	-0.944767	-2.621430	1.547097
50	6	0	-3.379803	-4.792611	0.675576
51	1	0	-3.150938	-6.466166	-0.685045
52	1	0	-3.310750	-3.077907	1.986789
53	6	0	0.109352	4.818886	-0.209006
54	6	0	-0.995802	4.059784	0.217864
55	6	0	-0.090110	6.180587	-0.484724
56	6	0	-2.247667	4.635919	0.357060
57	1	0	-0.882005	3.006110	0.448679
58	6	0	-1.341345	6.769664	-0.352796
59	1	0	0.748704	6.787893	-0.811345
60	6	0	-2.409301	5.989540	0.068659
61	1	0	-3.085014	4.030117	0.689943
62	1	0	-1.476596	7.824748	-0.570489
63	7	0	11.021589	-0.703034	-1.534604
64	6	0	11.430268	-1.974846	-2.227726
65	6	0	11.619528	0.530817	-2.154950
66	6	0	12.845361	-2.344749	-1.797645
67	1	0	11.354163	-1.837149	-3.307775
68	1	0	10.710855	-2.734831	-1.918867
69	6	0	11.397488	1.715169	-1.238936
70	1	0	11.162734	0.682870	-3.133602
71	1	0	12.685590	0.335766	-2.279843
72	8	0	12.987348	-2.201101	-0.404209
73	1	0	13.055261	-3.367163	-2.135574
74	1	0	13.586316	-1.685423	-2.258213
75	8	0	11.820118	1.310613	0.038670
76	1	0	11.977393	2.567290	-1.620220
77	1	0	10.337102	2.006630	-1.226528
78	6	0	12.546127	-3.316880	0.359596
79	6	0	11.520706	2.237615	1.067235
80	6	0	12.663018	-2.950573	1.815507
81	1	0	11.503537	-3.574435	0.127133
82	1	0	13.174047	-4.191131	0.142341
83	6	0	11.708705	1.546891	2.393678
84	1	0	12.183454	3.111632	1.001351
85	1	0	10.481054	2.584348	0.974790
86	8	0	11.700784	-1.965792	2.114277
87	1	0	12.514914	-3.849971	2.432813
88	1	0	13.678750	-2.573301	2.009877
89	8	0	10.675088	0.597767	2.543090
90	1	0	12.700344	1.075414	2.410103
91	1	0	11.674276	2.290346	3.204233
92	6	0	11.939819	-1.339928	3.353604
93	6	0	10.849053	-0.316917	3.603749
94	1	0	12.937582	-0.873601	3.354873
95	1	0	11.926367	-2.068055	4.180518
96	1	0	11.059076	0.203726	4.550360
97	1	0	9.888149	-0.830421	3.705156
98	7	0	-4.816398	-4.986586	0.938406
99	6	0	-5.702647	-4.296154	-0.077858
100	6	0	-5.226559	-6.393072	1.276280
101	6	0	-5.909573	-5.051935	-1.375546
102	1	0	-5.227393	-3.329667	-0.261058
103	1	0	-6.666009	-4.135001	0.412494
104	6	0	-4.860743	-6.696183	2.721083
105	1	0	-4.739778	-7.086283	0.590272
106	1	0	-6.305145	-6.456584	1.123440
107	1	0	-5.009683	-5.067639	-1.995762
108	1	0	-6.230817	-6.085097	-1.217968
109	16	0	-7.177216	-4.266629	-2.424656
110	1	0	-5.152261	-7.722910	2.955789
111	1	0	-3.779238	-6.622175	2.869531
112	16	0	-5.615422	-5.548605	3.916082
113	6	0	-8.776844	-4.702198	-1.653051
114	6	0	-7.316982	-6.211825	4.051916
115	6	0	-9.367390	-3.756902	-0.627855
116	1	0	-9.460072	-4.764744	-2.504334
117	1	0	-8.674704	-5.709960	-1.239144
118	6	0	-8.394592	-5.581513	3.182921
119	1	0	-7.262092	-7.289041	3.864224
120	1	0	-7.591020	-6.078437	5.102265

121	8	0	-8.679407	-3.870634	0.595062
122	1	0	-9.344920	-2.719951	-0.999490
123	1	0	-10.424335	-4.034487	-0.493110
124	8	0	-8.774865	-4.303144	3.655971
125	1	0	-8.110336	-5.547578	2.127955
126	1	0	-9.279452	-6.228039	3.252581
127	6	0	-9.170700	-2.994253	1.597132
128	6	0	-8.392552	-3.184888	2.885371
129	1	0	-10.238971	-3.182266	1.778073
130	1	0	-9.060382	-1.950652	1.264186
131	1	0	-8.587343	-2.315542	3.521239
132	1	0	-7.315080	-3.192697	2.669334
133	7	0	-3.733725	6.609594	0.188876
134	6	0	-4.720613	6.030017	-0.799084
135	1	0	-4.966708	5.022959	-0.459517
136	1	0	-4.190581	5.973406	-1.750470
137	6	0	-4.241727	6.668890	1.601481
138	1	0	-3.735609	5.911382	2.200748
139	1	0	-5.314830	6.452027	1.583044
140	6	0	-5.964247	6.869166	-0.913900
141	6	0	-6.087294	7.827577	-1.918406
142	7	0	-6.922920	6.630789	-0.008828
143	6	0	-7.260635	8.573586	-1.984707
144	1	0	-5.285369	7.981574	-2.633616
145	6	0	-8.039154	7.356712	-0.079094
146	6	0	-8.257911	8.334820	-1.047010
147	1	0	-7.391701	9.324762	-2.757172
148	1	0	-8.798920	7.143338	0.669376
149	1	0	-9.189896	8.889620	-1.061131
150	6	0	-3.989637	8.068215	2.118545
151	6	0	-4.150155	8.403670	3.459656
152	7	0	-3.636696	8.953501	1.187637
153	6	0	-3.935708	9.726173	3.828865
154	1	0	-4.434202	7.652268	4.189026
155	6	0	-3.428743	10.224005	1.546159
156	6	0	-3.569603	10.656443	2.857581
157	1	0	-4.050183	10.028544	4.865057
158	1	0	-3.139644	10.908861	0.753942
159	1	0	-3.392337	11.695539	3.111521
160	80	0	-6.754407	-1.457089	-2.111169
161	8	0	-4.314864	-1.010855	-2.496508
162	1	0	-3.930683	-0.687840	-1.673051
163	1	0	-3.880230	-1.856671	-2.656761
164	1	0	-3.613373	7.639354	-0.013465
165	1	0	11.451396	-0.762681	-0.592652
166	1	0	-5.020424	-4.481850	1.820091

---

2 (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.039240	-0.073851	-0.087666
2	6	0	3.187887	-2.280863	0.483011
3	6	0	4.247785	-1.440090	0.142591
4	6	0	1.066489	-2.799261	0.898381
5	6	0	1.825384	-3.991709	1.010104
6	6	0	3.147737	-3.687566	0.754002
7	7	0	1.893103	-1.783166	0.583253
8	7	0	2.771876	0.477588	0.038324
9	5	0	1.501673	-0.280537	0.512950
10	9	0	0.466421	-0.094192	-0.404180
11	9	0	1.104022	0.174764	1.762918
12	6	0	4.943198	0.965109	-0.472012
13	6	0	4.187014	2.120229	-0.557316
14	6	0	2.848427	1.797066	-0.231673
15	1	0	1.427835	-4.973942	1.225044
16	1	0	4.550650	3.096677	-0.845412
17	6	0	6.412639	0.877518	-0.752257
18	1	0	6.971212	0.554561	0.130697
19	1	0	6.630067	0.160968	-1.549116
20	1	0	6.784506	1.857697	-1.056461
21	6	0	4.275364	-4.673076	0.751818
22	1	0	4.729061	-4.762917	-0.239072
23	1	0	5.069615	-4.379445	1.443139
24	1	0	3.902325	-5.654542	1.049982
25	6	0	5.619433	-1.998500	0.000955
26	6	0	6.501011	-2.007259	1.083287
27	6	0	6.045690	-2.507128	-1.223005
28	6	0	7.790666	-2.498663	0.932103
29	1	0	6.179155	-1.619940	2.045160
30	6	0	7.337104	-3.006283	-1.374375
31	1	0	5.366448	-2.514248	-2.070129
32	6	0	8.232873	-2.991857	-0.301908
33	1	0	8.455374	-2.499283	1.790608
34	1	0	7.625383	-3.396915	-2.342358
35	6	0	-0.364842	-2.618300	1.033038
36	6	0	-1.166530	-3.552442	1.578622
37	1	0	-0.767147	-1.683833	0.654460
38	1	0	-0.716486	-4.451461	1.997171
39	6	0	1.687954	2.665088	-0.169302
40	6	0	1.789636	4.005047	-0.229119
41	1	0	0.725334	2.174019	-0.064914
42	1	0	2.779409	4.450503	-0.311572
43	6	0	-2.624430	-3.480996	1.673696
44	6	0	-3.306980	-4.388962	2.489757
45	6	0	-3.389635	-2.551017	0.948471
46	6	0	-4.694997	-4.378203	2.596539
47	1	0	-2.740109	-5.113811	3.067186
48	6	0	-4.769752	-2.551188	1.032082
49	1	0	-2.903735	-1.843950	0.283660
50	6	0	-5.450265	-3.468898	1.849978
51	1	0	-5.170098	-5.078894	3.273375
52	1	0	-5.350147	-1.850415	0.437712
53	6	0	0.685061	4.965659	-0.178960
54	6	0	-0.667396	4.589506	-0.153336
55	6	0	0.985143	6.332235	-0.165972
56	6	0	-1.669898	5.544583	-0.103933
57	1	0	-0.945952	3.541621	-0.184780
58	6	0	-0.017891	7.294855	-0.112407
59	1	0	2.022670	6.650944	-0.196857
60	6	0	-1.354974	6.908613	-0.066975
61	1	0	-2.704573	5.216668	-0.112909

62	1	0	0.268541	8.340819	-0.123148
63	7	0	9.587732	-3.492746	-0.400540
64	6	0	9.687645	-4.769111	0.356059
65	6	0	10.077975	-3.650531	-1.783167
66	6	0	11.101483	-5.321471	0.419524
67	1	0	9.032385	-5.532948	-0.086101
68	1	0	9.334759	-4.574537	1.370585
69	6	0	10.243549	-2.313371	-2.481028
70	1	0	9.451901	-4.328109	-2.376954
71	1	0	11.073185	-4.099169	-1.729784
72	8	0	11.996036	-4.250484	0.701436
73	1	0	11.144875	-6.070438	1.217582
74	1	0	11.403173	-5.804771	-0.517157
75	8	0	11.256980	-1.606341	-1.773704
76	1	0	10.563750	-2.476027	-3.516254
77	1	0	9.320148	-1.722239	-2.486141
78	6	0	13.320401	-4.657006	1.054930
79	6	0	11.506604	-0.291087	-2.261062
80	6	0	14.292254	-3.749156	0.341526
81	1	0	13.432434	-4.586394	2.141629
82	1	0	13.497687	-5.690649	0.743941
83	6	0	12.881881	0.094745	-1.771506
84	1	0	11.490809	-0.279851	-3.356181
85	1	0	10.736751	0.394697	-1.885155
86	8	0	13.932419	-2.402934	0.638658
87	1	0	15.315075	-3.952593	0.678919
88	1	0	14.233402	-3.905698	-0.743856
89	8	0	12.902009	-0.084471	-0.355386
90	1	0	13.626908	-0.555223	-2.243327
91	1	0	13.105242	1.137615	-2.019876
92	6	0	14.837472	-1.464093	0.062953
93	6	0	14.216045	-0.089962	0.205270
94	1	0	15.000630	-1.721390	-0.991462
95	1	0	15.802699	-1.501305	0.580678
96	1	0	14.842779	0.669796	-0.272221
97	1	0	14.099494	0.165091	1.261582
98	7	0	-6.874049	-3.407902	1.874635
99	6	0	-7.575639	-4.538700	2.488438
100	6	0	-7.394798	-2.107407	2.367073
101	6	0	-7.360020	-5.910350	1.846315
102	1	0	-8.641938	-4.297416	2.471405
103	1	0	-7.306236	-4.640092	3.551872
104	6	0	-8.179191	-1.285800	1.344728
105	1	0	-6.556978	-1.495478	2.710843
106	1	0	-8.028354	-2.293008	3.242213
107	1	0	-6.301662	-6.163758	1.768764
108	1	0	-7.829162	-6.661604	2.486802
109	16	0	-7.994117	-6.190078	0.160255
110	1	0	-8.558977	-0.383803	1.831621
111	1	0	-7.537739	-0.992232	0.508348
112	16	0	-9.566378	-2.270037	0.698648
113	6	0	-9.796872	-6.020446	0.397495
114	6	0	-10.237087	-1.198177	-0.614451
115	6	0	-10.506054	-5.849468	-0.934143
116	1	0	-10.152311	-6.925427	0.894447
117	1	0	-10.005309	-5.152991	1.027425
118	6	0	-11.515186	-1.844975	-1.192589
119	1	0	-10.449074	-0.215561	-0.188690
120	1	0	-9.489199	-1.075837	-1.402501
121	8	0	-10.202746	-4.571085	-1.457152
122	1	0	-10.213794	-6.635460	-1.645866
123	1	0	-11.587730	-5.934866	-0.762291
124	8	0	-11.494412	-1.943481	-2.602610
125	1	0	-11.687982	-2.830194	-0.741980
126	1	0	-12.378128	-1.218878	-0.959024
127	6	0	-10.843022	-4.327459	-2.702834
128	6	0	-10.603893	-2.894397	-3.148532
129	1	0	-11.924726	-4.501592	-2.608639
130	1	0	-10.449486	-5.018840	-3.460594
131	1	0	-10.756378	-2.839132	-4.229144
132	1	0	-9.553678	-2.620417	-2.957385
133	7	0	-2.422020	7.906692	-0.062125
134	6	0	-2.969597	8.075503	-1.426101
135	1	0	-3.939547	8.578885	-1.346958
136	1	0	-3.126435	7.115458	-1.927581
137	6	0	-3.444515	7.650652	0.972525
138	1	0	-3.770253	6.608599	1.010918
139	1	0	-4.323555	8.256554	0.727757
140	6	0	-2.044070	8.952228	-2.241647
141	6	0	-1.804426	8.721167	-3.588863
142	7	0	-1.495208	10.001813	-1.603806
143	6	0	-0.986059	9.602124	-4.289377
144	1	0	-2.253982	7.862771	-4.074367
145	6	0	-0.705140	10.852589	-2.275251
146	6	0	-0.426652	10.687796	-3.624136
147	1	0	-0.784233	9.437990	-5.342144
148	1	0	-0.290357	11.678092	-1.707713
149	1	0	0.218116	11.394282	-4.131482
150	6	0	-2.932006	8.085874	2.327304
151	6	0	-3.152932	7.345894	3.480052
152	7	0	-2.287328	9.264787	2.366134
153	6	0	-2.704114	7.847778	4.698627
154	1	0	-3.667159	6.393716	3.417822
155	6	0	-1.851418	9.751582	3.536344
156	6	0	-2.045123	9.071737	4.730453
157	1	0	-2.864710	7.285968	5.612279
158	1	0	-1.335855	10.704752	3.503385
159	1	0	-1.678233	9.494512	5.657281
160	20	0	11.484490	-1.874065	0.650986
161	80	0	-7.419514	-3.713737	-1.117985
162	30	0	-1.880347	10.085408	0.461819

2-3H$^+$ (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.263383	0.659808	0.193390
2	6	0	4.044731	-1.769201	0.170234
3	6	0	4.840253	-0.616604	0.153919
4	6	0	2.140094	-2.914356	0.227178
5	6	0	3.196432	-3.852145	0.182433
6	6	0	4.392456	-3.161060	0.151670

7	7	0	2.663224	-1.666625	0.227587
8	7	0	2.886303	0.806513	0.224286
9	5	0	1.863464	-0.349295	0.081146
10	9	0	1.247672	-0.294909	-1.164907
11	9	0	0.896161	-0.258293	1.085598
12	6	0	4.855581	1.966491	0.199499
13	6	0	3.804111	2.861301	0.227391
14	6	0	2.594186	2.128838	0.234092
15	1	0	3.083664	-4.927451	0.214191
16	1	0	3.892032	3.938980	0.249991
17	6	0	6.297781	2.350497	0.190030
18	1	0	6.816320	2.007170	1.090417
19	1	0	6.829254	1.926939	-0.667253
20	1	0	6.387462	3.438074	0.142874
21	6	0	5.740908	-3.800064	0.136002
22	1	0	6.301156	-3.550597	-0.770152
23	1	0	6.351913	-3.485346	0.987063
24	1	0	5.632279	-4.886046	0.178147
25	6	0	6.318446	-0.754166	0.056465
26	6	0	7.118357	-0.772351	1.199474
27	6	0	6.912598	-0.878356	-1.203366
28	6	0	8.499480	-0.916851	1.090203
29	1	0	6.666393	-0.677691	2.181424
30	6	0	8.287443	-1.026343	-1.324709
31	1	0	6.295557	-0.864751	-2.095726
32	6	0	9.063523	-1.043211	-0.170755
33	1	0	9.116351	-0.932275	1.984112
34	1	0	8.728063	-1.133703	-2.310884
35	6	0	0.722197	-3.166092	0.305447
36	6	0	0.164891	-4.343220	-0.050020
37	1	0	0.106429	-2.344507	0.659667
38	1	0	0.793298	-5.115371	-0.490043
39	6	0	1.238470	2.613306	0.235226
40	6	0	0.912784	3.919736	0.123408
41	1	0	0.465794	1.859068	0.342032
42	1	0	1.706926	4.659638	0.048472
43	6	0	-1.251954	-4.672644	0.066587
44	6	0	-1.794133	-5.679038	-0.747642
45	6	0	-2.098271	-4.033510	0.986931
46	6	0	-3.137096	-6.026946	-0.673654
47	1	0	-1.155968	-6.191963	-1.460731
48	6	0	-3.436188	-4.383469	1.082894
49	1	0	-1.701529	-3.280505	1.659738
50	6	0	-3.945543	-5.378349	0.252490
51	1	0	-3.522536	-6.797349	-1.332559
52	1	0	-4.074111	-3.892085	1.813013
53	6	0	-0.440216	4.460308	0.101572
54	6	0	-1.586127	3.650858	-0.011898
55	6	0	-0.615987	5.849924	0.186559
56	6	0	-2.855001	4.203163	-0.017403
57	1	0	-1.490623	2.575167	-0.109599
58	6	0	-1.883473	6.420578	0.187169
59	1	0	0.252868	6.496131	0.263038
60	6	0	-2.985830	5.585728	0.090329
61	1	0	-3.722710	3.556772	-0.109916
62	1	0	-1.995817	7.498607	0.261825
63	7	0	10.524725	-1.224570	-0.288993
64	6	0	10.858562	-2.649303	-0.729870
65	6	0	11.181367	-0.116728	-1.077131
66	6	0	12.113578	-2.838030	-1.545698
67	1	0	10.022002	-2.993029	-1.338464
68	1	0	10.883456	-3.242684	0.185622
69	6	0	11.275220	1.130223	-0.232499
70	1	0	10.617503	0.055503	-1.992862
71	1	0	12.187128	-0.450646	-1.323889
72	8	0	13.290423	-2.527588	-0.817654
73	1	0	12.118733	-3.899623	-1.825625
74	1	0	12.066628	-2.260757	-2.477995
75	8	0	12.010601	0.792992	0.935162
76	1	0	11.786811	1.889880	-0.834261
77	1	0	10.288217	1.520807	0.047083
78	6	0	14.479976	-2.673012	-1.604286
79	6	0	12.522507	1.921181	1.644739
80	6	0	15.007902	-1.317460	-2.003285
81	1	0	15.213426	-3.203256	-0.988478
82	1	0	14.287681	-3.278366	-2.495330
83	6	0	13.838995	2.374408	1.055787
84	1	0	11.802228	2.746845	1.637624
85	1	0	12.660257	1.595481	2.680028
86	8	0	15.248126	-0.576485	-0.812552
87	1	0	15.938241	-1.431486	-2.573635
88	1	0	14.282520	-0.781136	-2.631049
89	8	0	14.760859	1.287998	1.129069
90	1	0	13.712801	2.688467	0.012687
91	1	0	14.225413	3.228894	1.624180
92	6	0	15.641614	0.770328	-1.060039
93	6	0	15.902376	1.419186	0.279043
94	1	0	14.845241	1.287148	-1.611757
95	1	0	16.555331	0.795291	-1.666602
96	1	0	16.173146	2.471778	0.151167
97	1	0	16.727548	0.912944	0.788609
98	7	0	-5.380400	-5.688313	0.369358
99	6	0	-6.252081	-4.889231	-0.581330
100	6	0	-5.714895	-7.153818	0.422872
101	6	0	-6.296366	-5.394010	-2.008984
102	1	0	-5.866198	-3.868203	-0.544569
103	1	0	-7.256561	-4.908099	-0.152499
104	6	0	-5.417964	-7.700827	1.809374
105	1	0	-5.142647	-7.680477	-0.340310
106	1	0	-6.775142	-7.245337	0.182734
107	1	0	-5.359162	-5.213984	-2.542018
108	1	0	-6.525754	-6.461156	-2.074368
109	16	0	-7.569896	-4.498941	-2.953717
110	1	0	-5.630824	-8.772611	1.823232
111	1	0	-4.358449	-7.577238	2.053677
112	16	0	-6.346762	-6.869239	3.135575
113	6	0	-9.136731	-5.279872	-2.428331
114	6	0	-7.976391	-7.699100	3.033414
115	6	0	-9.902321	-4.624904	-1.295632
116	1	0	-9.762184	-5.252038	-3.325013
117	1	0	-8.936395	-6.332247	-2.204118
118	6	0	-9.068230	-7.040820	2.202406
119	1	0	-7.797843	-8.719818	2.680019
120	1	0	-8.322142	-7.770172	4.068700

121	8	0	-9.283543	-4.891387	-0.057253
122	1	0	-9.975489	-3.539180	-1.465232
123	1	0	-10.925519	-5.031673	-1.297296
124	8	0	-9.623604	-5.910896	2.848166
125	1	0	-8.734064	-6.793573	1.191215
126	1	0	-9.875809	-7.777626	2.100548
127	6	0	-9.942562	-4.267276	1.033077
128	6	0	-9.272164	-4.641859	2.340991
129	1	0	-11.000215	-4.567762	1.061684
130	1	0	-9.904859	-3.172856	0.913118
131	1	0	-9.602674	-3.924766	3.099293
132	1	0	-8.183254	-4.534210	2.244583
133	7	0	-4.339201	6.183766	0.105131
134	6	0	-5.074535	6.018882	-1.232679
135	1	0	-6.062121	5.607677	-1.016129
136	1	0	-4.520664	5.291200	-1.820864
137	6	0	-5.159056	5.724501	1.320980
138	1	0	-4.690472	4.822350	1.706382
139	1	0	-6.159353	5.463689	0.972226
140	6	0	-5.193925	7.316864	-1.976680
141	6	0	-4.569003	7.471190	-3.204374
142	7	0	-5.946410	8.308094	-1.441392
143	6	0	-4.730326	8.659241	-3.913971
144	1	0	-3.963718	6.664595	-3.601638
145	6	0	-6.091680	9.456769	-2.125019
146	6	0	-5.508322	9.666970	-3.365189
147	1	0	-4.250303	8.788785	-4.877950
148	1	0	-6.703246	10.223114	-1.663638
149	1	0	-5.666475	10.608466	-3.877233
150	6	0	-5.223355	6.783734	2.377496
151	6	0	-4.590134	6.597605	3.595989
152	7	0	-5.925711	7.909296	2.106185
153	6	0	-4.682832	7.585457	4.573669
154	1	0	-4.031270	5.686308	3.775212
155	6	0	-5.998659	8.866910	3.046850
156	6	0	-5.398114	8.738548	4.290851
157	1	0	-4.197181	7.452286	5.534272
158	1	0	-6.558810	9.762272	2.805156
159	1	0	-5.497755	9.538590	5.014522
160	20	0	14.221194	-1.121998	1.414921
161	80	0	-7.636514	-1.552033	-1.449881
162	30	0	-6.833829	8.340675	0.354296
163	1	0	-4.182038	7.189969	0.221180
164	1	0	-5.673631	-5.354771	1.303877
165	1	0	10.897223	-1.115963	0.659767

2-3H$^+$-3W (S_0):

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.278482	0.288396	0.059695
2	6	0	3.984823	-2.121580	-0.170639
3	6	0	4.814246	-0.995204	-0.112389
4	6	0	2.052451	-3.219099	-0.111273
5	6	0	3.079286	-4.176984	-0.276093
6	6	0	4.291502	-3.515608	-0.311086
7	7	0	2.610464	-1.987605	-0.046388
8	7	0	2.907635	0.470797	0.146170
9	5	0	1.846622	-0.639889	-0.059775
10	9	0	1.198230	-0.466271	-1.278025
11	9	0	0.912044	-0.600915	0.978015
12	6	0	4.910801	1.572416	0.163967
13	6	0	3.888613	2.489024	0.305639
14	6	0	2.656608	1.794191	0.283223
15	1	0	2.938752	-5.248482	-0.320070
16	1	0	4.012813	3.557028	0.421009
17	6	0	6.361232	1.924466	0.139324
18	1	0	6.894261	1.518036	1.004291
19	1	0	6.862132	1.543025	-0.755106
20	1	0	6.473355	3.010918	0.155139
21	6	0	5.620838	-4.180754	-0.442424
22	1	0	6.137014	-3.881775	-1.359763
23	1	0	6.284753	-3.937452	0.392248
24	1	0	5.488224	-5.264638	-0.467474
25	6	0	6.288075	-1.151404	-0.241622
26	6	0	7.094252	-1.235549	0.894385
27	6	0	6.876249	-1.187157	-1.509921
28	6	0	8.477616	-1.327469	0.769784
29	1	0	6.645361	-1.216239	1.882058
30	6	0	8.255159	-1.282173	-1.646698
31	1	0	6.253678	-1.129335	-2.396689
32	6	0	9.037979	-1.338566	-0.499177
33	1	0	9.101081	-1.380707	1.657832
34	1	0	8.696952	-1.304381	-2.638029
35	6	0	0.635636	-3.440009	0.034171
36	6	0	0.029595	-4.596872	-0.309689
37	1	0	0.063677	-2.614493	0.447150
38	1	0	0.612665	-5.376006	-0.797186
39	6	0	1.320718	2.328521	0.354193
40	6	0	1.069877	3.656288	0.348051
41	1	0	0.513544	1.604915	0.405234
42	1	0	1.911542	4.344392	0.311300
43	6	0	-1.380944	-4.905836	-0.103906
44	6	0	-1.968675	-5.950403	-0.834597
45	6	0	-2.175770	-4.218816	0.828352
46	6	0	-3.302672	-6.297245	-0.660991
47	1	0	-1.371457	-6.499475	-1.556136
48	6	0	-3.504272	-4.563412	1.020559
49	1	0	-1.746018	-3.430346	1.436861
50	6	0	-4.057107	-5.603284	0.277641
51	1	0	-3.722911	-7.104208	-1.251208
52	1	0	-4.098903	-4.032050	1.758715
53	6	0	-0.234997	4.301961	0.360055
54	6	0	-1.452819	3.600421	0.281463
55	6	0	-0.279947	5.703229	0.421526
56	6	0	-2.665202	4.269787	0.251853
57	1	0	-1.459169	2.517501	0.225040
58	6	0	-1.486808	6.389348	0.395428
59	1	0	0.645719	6.266892	0.484810
60	6	0	-2.663990	5.662159	0.305960
61	1	0	-3.589097	3.703543	0.176297
62	1	0	-1.496380	7.474858	0.437988

63	7	0	10.507869	-1.391686	-0.623689
64	6	0	10.979597	-2.731862	-1.174943
65	6	0	11.064959	-0.164896	-1.302070
66	6	0	12.284368	-2.731290	-1.936978
67	1	0	10.205102	-3.082820	-1.857797
68	1	0	11.015154	-3.408147	-0.318557
69	6	0	11.014674	0.998322	-0.342499
70	1	0	10.504419	0.029012	-2.215681
71	1	0	12.103414	-0.378455	-1.544840
72	8	0	13.393851	-2.368917	-1.128350
73	1	0	12.409317	-3.759653	-2.300380
74	1	0	12.220252	-2.083404	-2.820334
75	8	0	11.726421	0.600533	0.822382
76	1	0	11.481228	1.856569	-0.837898
77	1	0	9.986284	1.273009	-0.074438
78	6	0	14.617973	-2.285338	-1.870214
79	6	0	12.046786	1.681089	1.699081
80	6	0	14.993690	-0.843579	-2.113663
81	1	0	15.390797	-2.787559	-1.279587
82	1	0	14.531083	-2.813768	-2.824476
83	6	0	13.321721	2.363362	1.260927
84	1	0	11.224462	2.403532	1.743728
85	1	0	12.169963	1.241333	2.693053
86	8	0	15.107409	-0.198915	-0.850137
87	1	0	15.949109	-0.795779	-2.650950
88	1	0	14.233333	-0.333894	-2.721452
89	8	0	14.369631	1.395557	1.260127
90	1	0	13.208675	2.792987	0.258429
91	1	0	13.566137	3.177387	1.953941
92	6	0	15.338189	1.204125	-0.950411
93	6	0	15.496462	1.744217	0.452700
94	1	0	14.495962	1.675885	-1.474058
95	1	0	16.253021	1.398912	-1.523903
96	1	0	15.637893	2.829269	0.430596
97	1	0	16.371709	1.296357	0.932053
98	7	0	-5.476495	-5.921211	0.507489
99	6	0	-6.423434	-5.192844	-0.424061
100	6	0	-5.778877	-7.384569	0.679418
101	6	0	-6.549262	-5.780239	-1.815613
102	1	0	-6.058971	-4.164425	-0.469384
103	1	0	-7.398492	-5.205077	0.069514
104	6	0	-5.369123	-7.825619	2.075939
105	1	0	-5.253900	-7.954847	-0.086396
106	1	0	-6.852076	-7.507130	0.525819
107	1	0	-5.655422	-5.607183	-2.420509
108	1	0	-6.749126	-6.855327	-1.804989
109	16	0	-7.907506	-4.984115	-2.732006
110	1	0	-5.588407	-8.889329	2.195101
111	1	0	-4.292243	-7.695802	2.220245
112	16	0	-6.174366	-6.874443	3.402792
113	6	0	-9.417680	-5.774691	-2.070880
114	6	0	-7.813467	-7.682684	3.513568
115	6	0	-10.141586	-5.070077	-0.942161
116	1	0	-10.088908	-5.829385	-2.932312
117	1	0	-9.164607	-6.800874	-1.787407
118	6	0	-8.961226	-7.068367	2.727975
119	1	0	-7.679908	-8.732122	3.231604
120	1	0	-8.065852	-7.661077	4.577587
121	8	0	-9.436844	-5.228877	0.267666
122	1	0	-10.269794	-4.002388	-1.177968
123	1	0	-11.146039	-5.512344	-0.853955
124	8	0	-9.407011	-5.857666	3.309995
125	1	0	-8.718798	-6.933439	1.670905
126	1	0	-9.796688	-7.779785	2.774026
127	6	0	-9.993076	-4.482738	1.338141
128	6	0	-9.160091	-4.668693	2.592785
129	1	0	-11.029371	-4.797646	1.528970
130	1	0	-10.007741	-3.413643	1.074918
131	1	0	-9.412377	-3.858190	3.283550
132	1	0	-8.094475	-4.563416	2.343024
133	7	0	-3.940674	6.402057	0.220541
134	6	0	-4.582618	6.295164	-1.167921
135	1	0	-5.642245	6.074618	-1.030699
136	1	0	-4.117901	5.459960	-1.686244
137	6	0	-4.898591	6.111340	1.379139
138	1	0	-4.586500	5.176927	1.840241
139	1	0	-5.896144	5.967076	0.963315
140	6	0	-4.395555	7.579100	-1.919228
141	6	0	-3.619026	7.614071	-3.066952
142	7	0	-4.995867	8.691871	-1.433891
143	6	0	-3.457444	8.817455	-3.749843
144	1	0	-3.144308	6.705834	-3.420203
145	6	0	-4.826143	9.851305	-2.091775
146	6	0	-4.070432	9.955949	-3.250080
147	1	0	-2.855982	8.857889	-4.651546
148	1	0	-5.320622	10.720725	-1.676972
149	1	0	-3.973817	10.917276	-3.740215
150	6	0	-4.875498	7.234435	2.372058
151	6	0	-4.333870	7.042785	3.634079
152	7	0	-5.378766	8.430335	1.986110
153	6	0	-4.310156	8.102512	4.537417
154	1	0	-3.932914	6.072252	3.903146
155	6	0	-5.336329	9.453244	2.858403
156	6	0	-4.817291	9.329548	4.138721
157	1	0	-3.893841	7.967035	5.529762
158	1	0	-5.737802	10.401573	2.518420
159	1	0	-4.816731	10.188205	4.799346
160	20	0	14.095829	-1.102676	1.249943
161	80	0	-7.938882	-2.026996	-1.616420
162	30	0	-6.255707	8.902073	0.180258
163	1	0	-3.682065	7.388297	0.324251
164	1	0	-5.714067	-5.539730	1.441627
165	1	0	10.859814	-1.318801	0.335777
166	8	0	-9.476177	0.220718	-1.259714
167	1	0	-9.043549	0.877329	-1.817122
168	1	0	-10.293713	0.013617	-1.726595
169	8	0	13.776924	-2.420067	3.258807
170	1	0	13.950515	-3.366301	3.295601
171	1	0	13.948266	-2.086225	4.145443
172	8	0	-8.236210	9.036281	0.204830
173	1	0	-8.626921	9.606514	0.879915
174	1	0	-8.669573	9.248153	-0.632131

Absorption

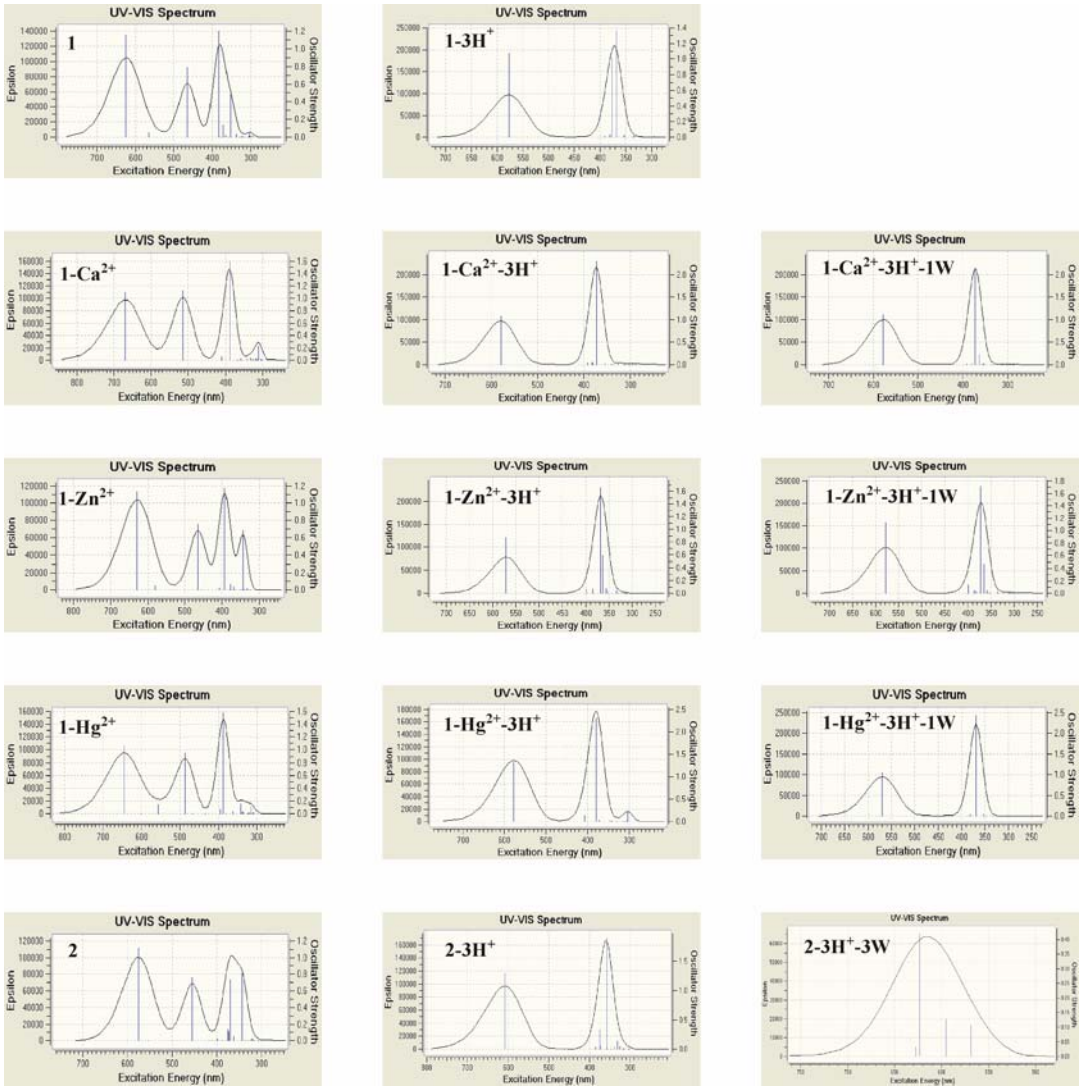

Figure 1S. Absorption spectra (S_0) of the lowest in energy of **1**, **2**, **1-Ca^{2+}**, **1-Zn^{2+}**, and **1-Hg^{2+}**, their protonated species and their protonated, and complexed with water species in water solvent at the PBE0/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ level of theory.

Emission

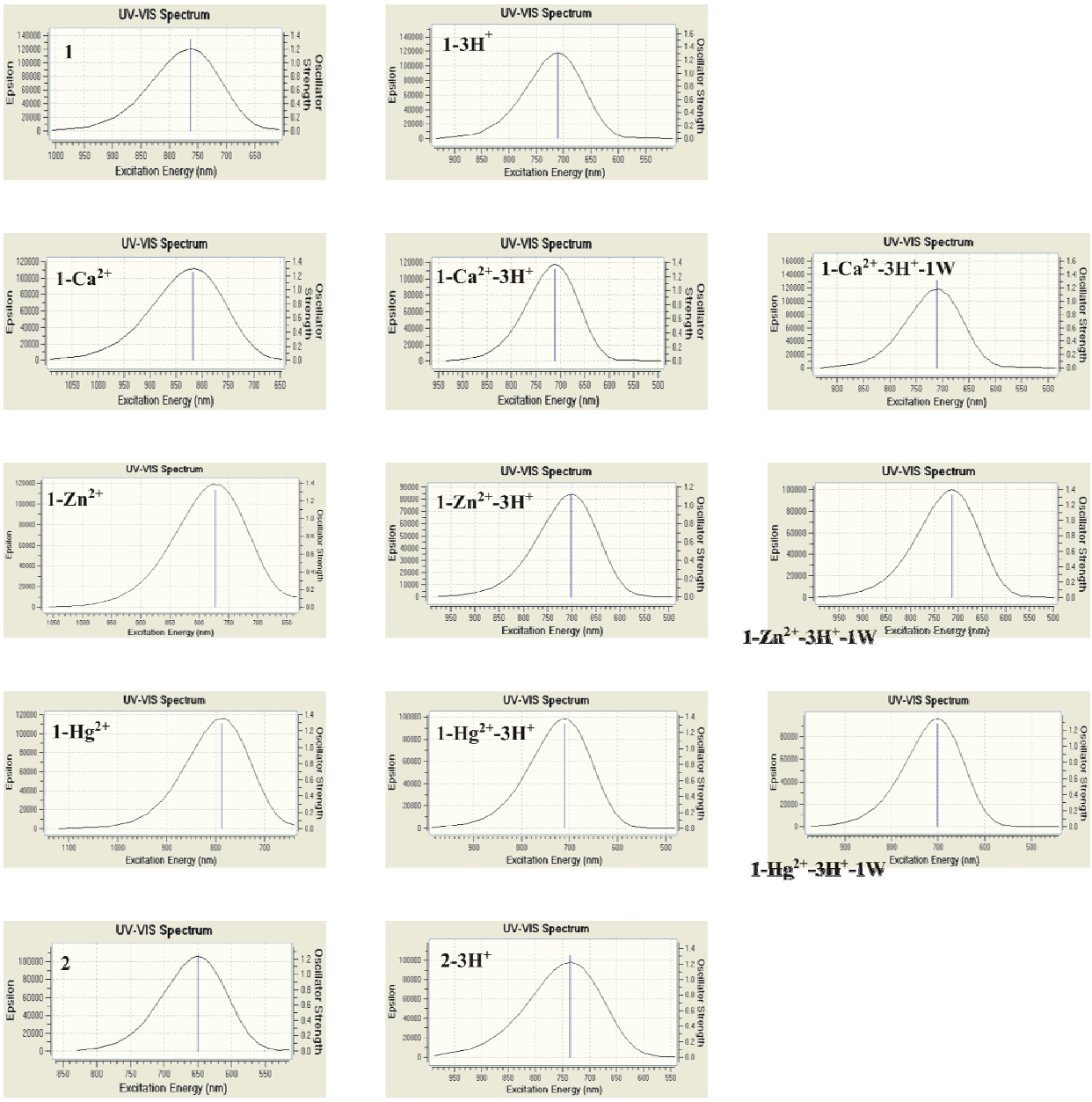

Figure 2S. Emission spectra of the lowest in energy of un-protonated, protonated, and complexed with water of **1**, **2**, **1-Ca^{2+}**, **1-Zn^{2+}**, and **1-Hg^{2+}** in water solvent at the PBE0/6-31G(d,p)$_{H,C,O,N,S,Ca,Zn}$ LANL2TZ$_{Hg}$ level of theory.

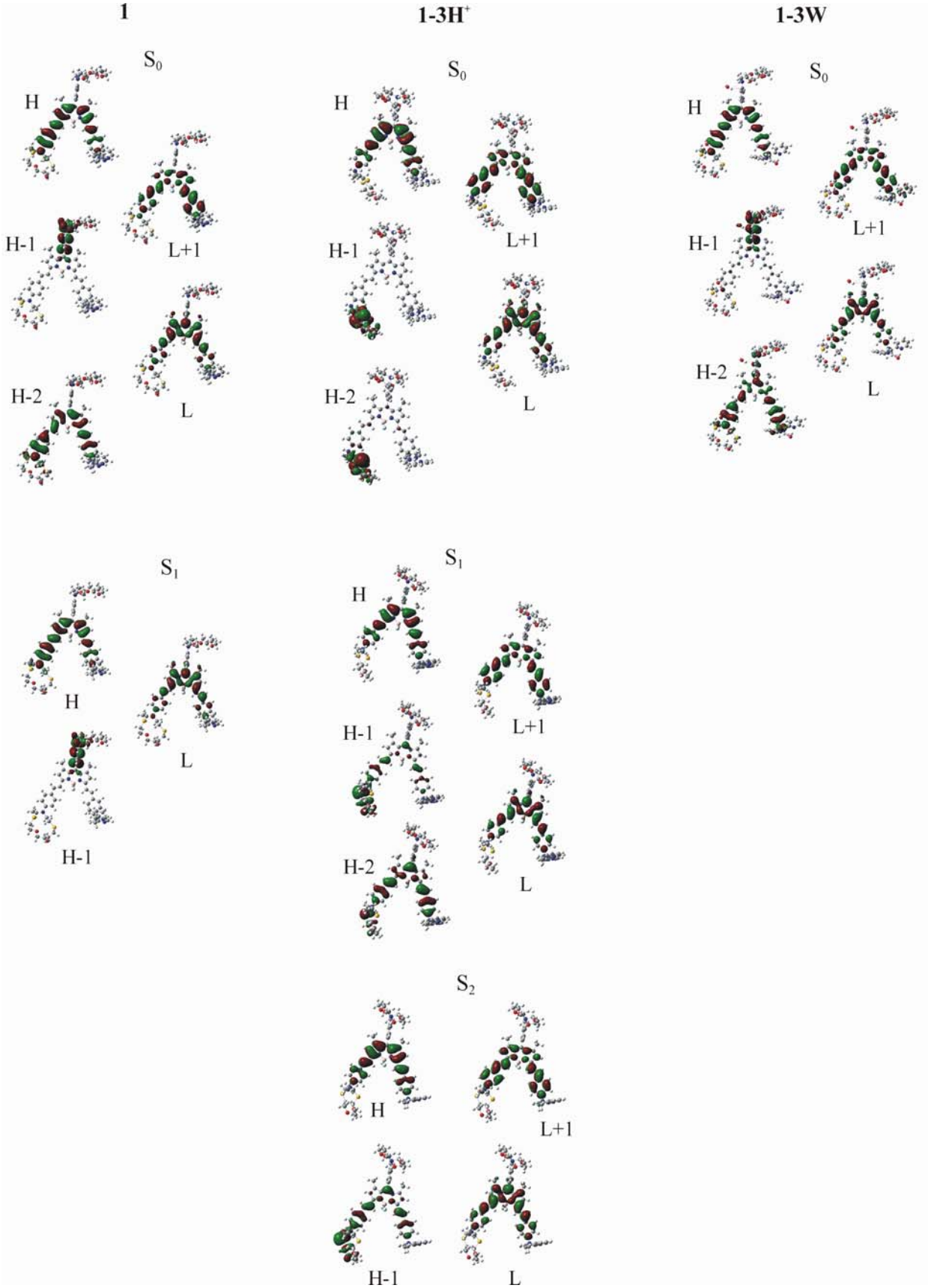

Figure 3S. Electron density plots of the MO involved in the major peaks excitations of the S_0, S_1,and S_2 potential surfaces of un-protonated, protonated, complexed and/or attached with water molecules **1** via PBE0.

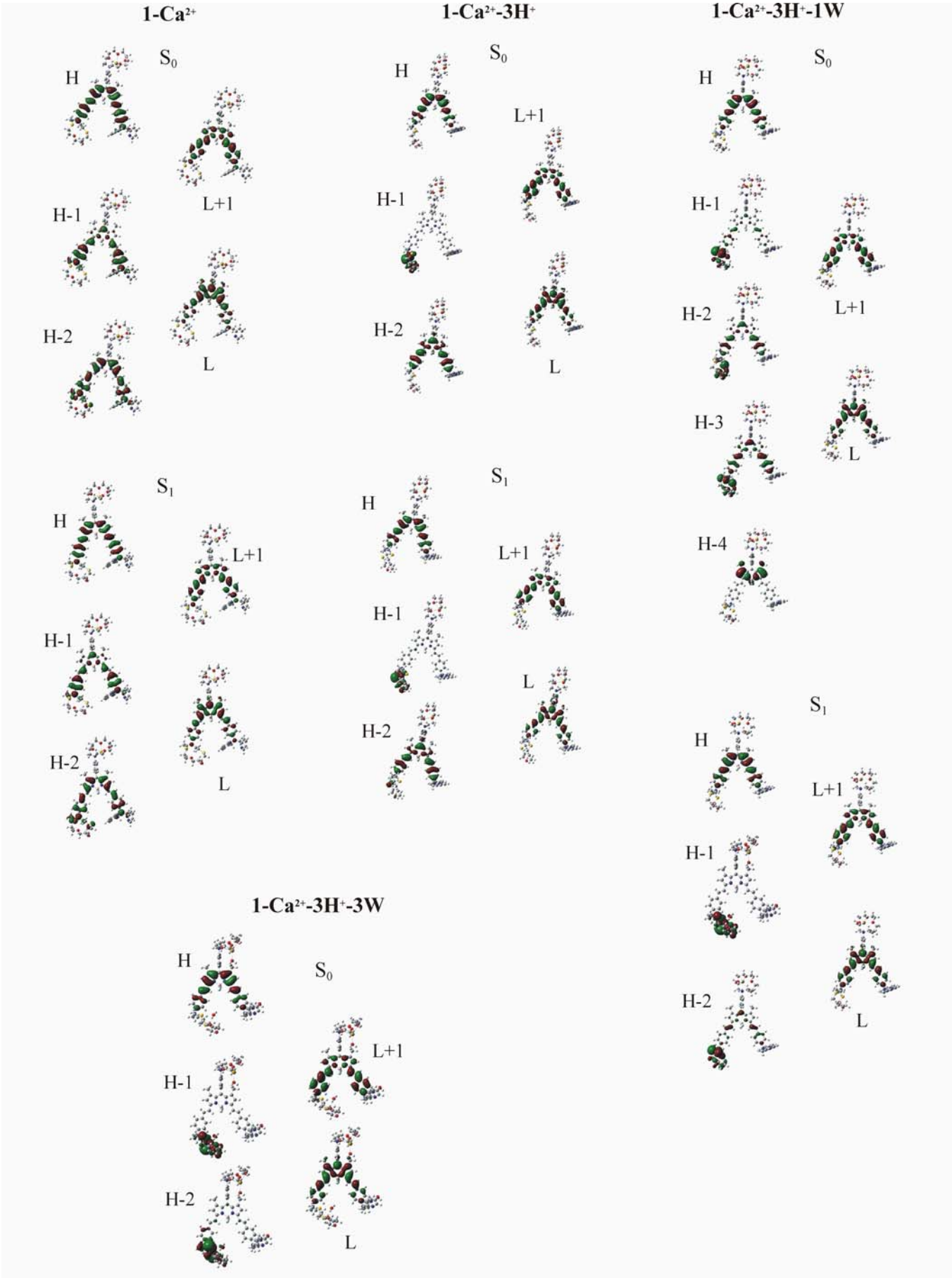

Figure 4S. Electron density plots of the MO involved in the major peaks excitations of the S_0, S_1,and S_2 potential surfaces of un-protonated, protonated, complexed and/or attached with water molecules **1-Ca^{2+}** via PBE0.

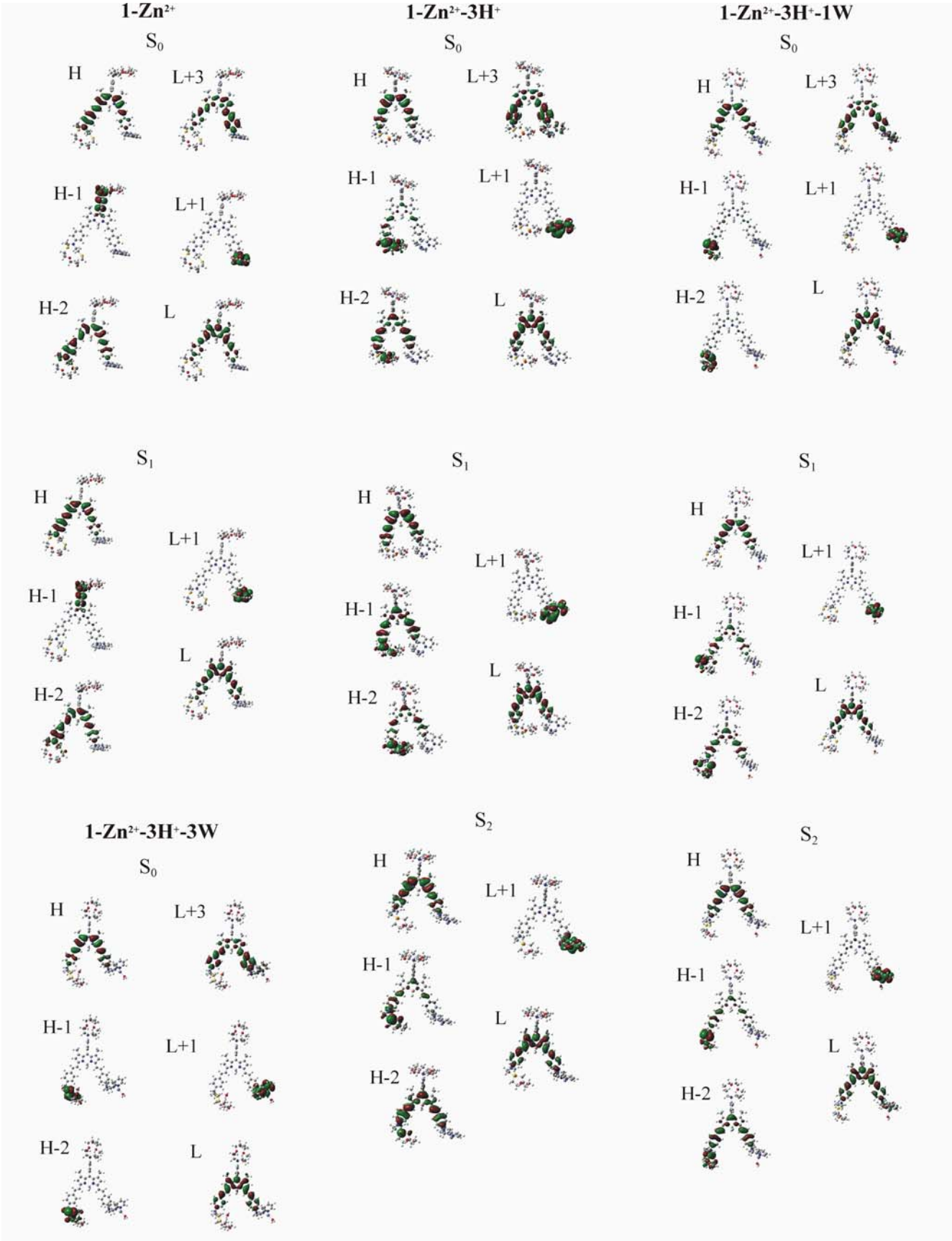

Figure 5S. Electron density plots of the MO involved in the major peaks excitations of the S_0, S_1,and S_2 potential surfaces of un-protonated, protonated, complexed and/or attached with water molecules **1-Zn^{2+}** via PBE0.

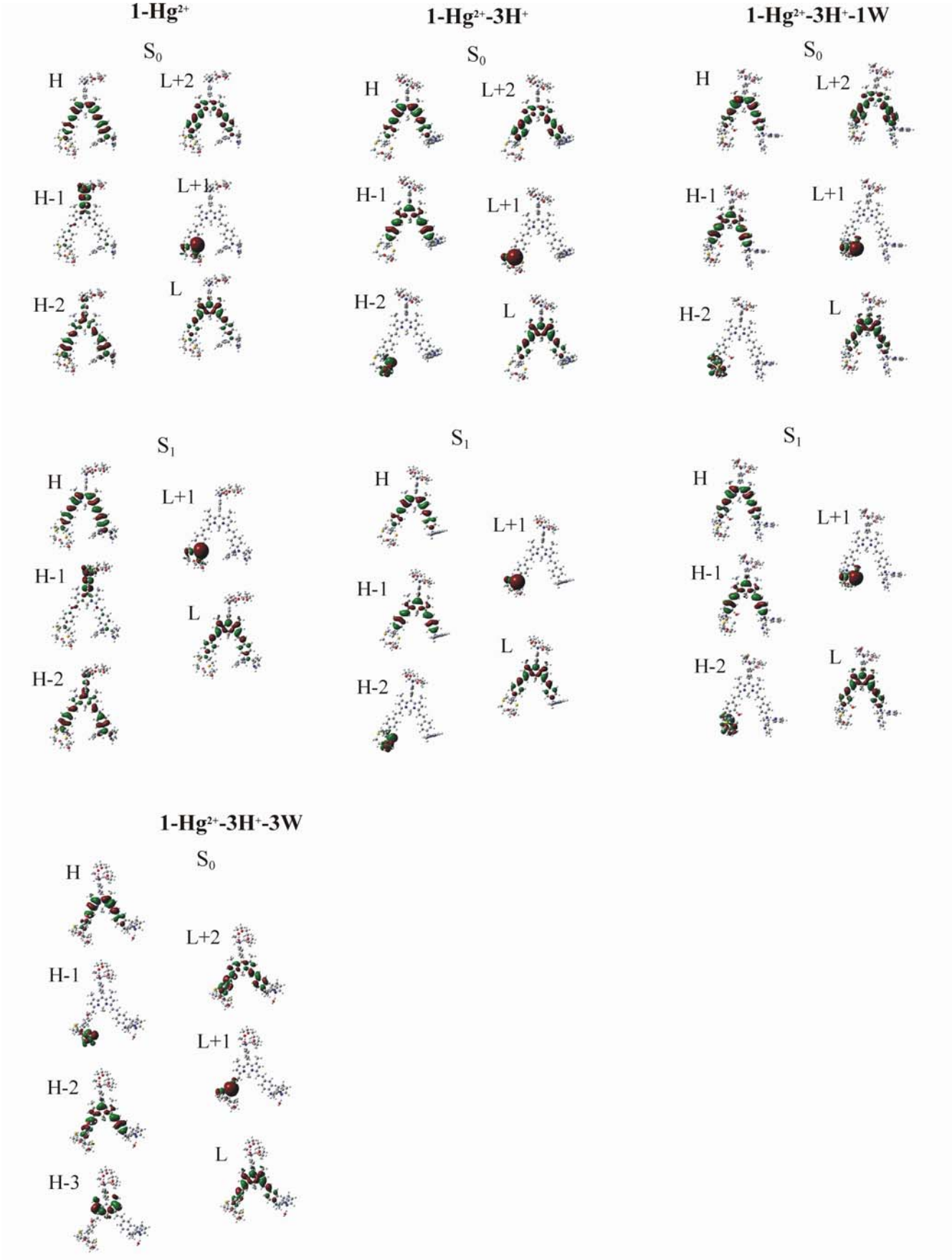

Figure 6S. Electron density plots of the MO involved in the major peaks excitations of the S_0, S_1,and S_2 potential surfaces of un-protonated, protonated, complexed and/or attached with water molecules **1-Hg^{2+}** via PBE0.

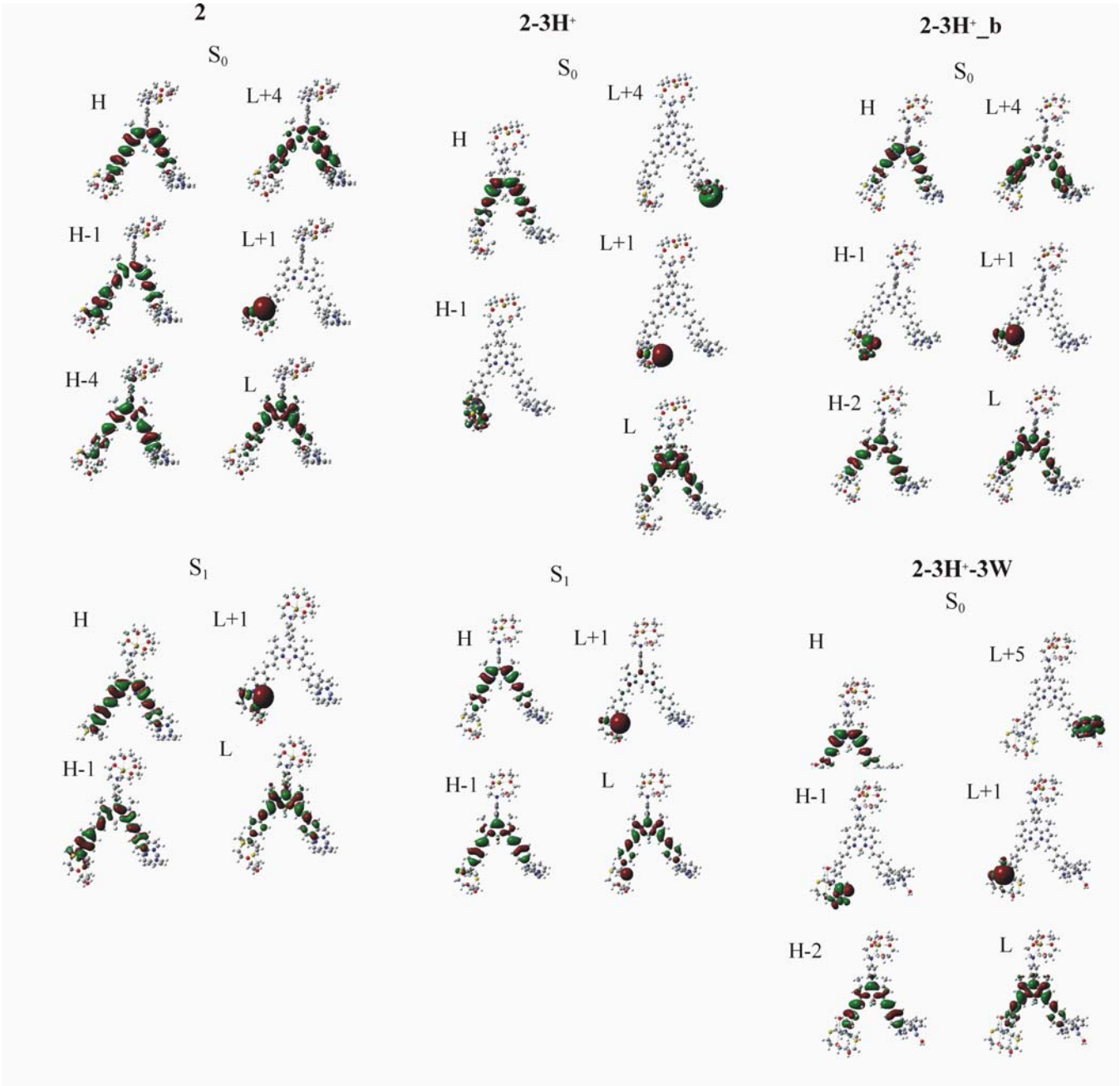

Figure 7S. Electron density plots of the MO involved in the major peaks excitations of the S_0, S_1,and S_2 potential surfaces of un-protonated, protonated, complexed and/or attached with water molecules **2** via PBE0.