Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Molecular Logic Gates based on benzo-18-crown-6 ether of styrylquinoline. A theoretical study

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Table 1S. Selected geometries, distances R in Å, angles φ and dihedral angles δ in degrees of the ground states S_0 (first line) and of first excited state S_1 (second line *in italics*).

	R_{C1C2}	R_{C1H1}	R_{C2H2}	φ_{H1C1C2}	φ_{H2C2C1}	$\delta_{H1C1C2H2}$	$\delta_{C3C1C2C4}$	$\delta_{NC3C1C2}$	$\delta_{C1C2C3C5}$	R_{N-H}	R_{O1-Ca}	R_{O2-Ca}	R_{O3-Ca}	R_{O4-Ca}	R_{O5-Ca}	R_{O6-Ca}	$R_{H...N}$[a]
trans-**1**	1.342	1.087	1.089	121.1	117.2	179.1	179.6	2.2	175.8								
	1.411	*1.086*	*1.086*	*120.1*	*116.1*	*179.4*	*179.6*	*0.6*	*178.9*								
trans-**1**_b	1.342	1.087	1.088	120.9	119.4	178.4	179.8	174.3	176.3								
	1.413	*1.087*	*1.086*	*118.9*	*119.0*	*176.8*	*177.5*	*178.5*	*178.8*								
cis-**1**	1.343	1.087	1.089	117.9	116.7	5.2	6.8	144.9	148.2								
	1.428	*1.090*	*1.090*	*117.5*	*116.8*	*35.9*	*44.7*	*172.5*	*175.1*								
cis-**1**_b	1.343	1.087	1.089	118.0	116.7	5.2	6.9	145.6	146.7								
	1.427	*1.090*	*1.090*	*117.2*	*116.5*	*35.0*	*44.3*	*171.7*	*177.3*								
cis-**1**_c	1.346	1.088	1.090	115.8	114.8	4.0	6.5	24.0	157.2								
	1.416	*1.088*	*1.089*	*117.2*	*166.8*	*25.9*	*31.4*	*7.4*	*116.9*								
cis-**1**_d	1.345	1.088	1.090	116.4	115.5	4.4	5.6	28.0	152.8								
	1.417	*1.089*	*1.089*	*116.6*	*116.4*	*25.6*	*32.5*	*7.2*	*169.5*								
trans-**1H**$^{+}$	1.351	1.086	1.088	120.5	119.1	179.3	179.9	178.3	178.3	1.017							
	1.399	*1.087*	*1.085*	*118.5*	*119.1*	*179.8*	*179.7*	*179.7*	*179.7*	*1.013*							
trans-**1H**$^{+}$_b	1.345	1.085	1.090	120.9	119.9	176.1	179.5	15.5	176.4	1.016							
	1.404	*1.085*	*1.087*	*119.6*	*119.5*	*172.4*	*175.6*	*4.2*	*176.0*	*1.010*							
cis-**1H**$^{+}$	1.348	1.087	1.088	117.9	115.5	5.9	10.6	152.7	150.3	1.017							
	1.406	*1.090*	*1.088*	*116.1*	*115.6*	*22.4*	*30.6*	*166.8*	*168.4*	*1.013*							
cis-**1H**$^{+}$_b	1.343	1.085	1.087	119.9	118.0	5.4	6.1	37.1	127.4	1.018							
	1.378	*1.087*	*1.087*	*119.5*	*119.8*	*6.0*	*7.1*	*32.5*	*134.1*	*1.002*							
trans-**1Ca**$^{++}$	1.341	1.088	1.088	120.9	117.8	179.4	179.3	0.0	176.0		2.593	2.522	2.601	2.578	2.552	2.613	
	1.417	*1.086*	*1.086*	*119.8*	*116.6*	*179.5*	*179.2*	*0.6*	*178.5*		*2.621*	*2.549*	*2.601*	*2.574*	*2.525*	*2.603*	
trans-**1Ca**$^{++}$_b	1.341	1.087	1.088	120.9	119.7	178.1	179.7	174.9	174.3		2.601	2.531	2.600	2.574	2.547	2.612	
	1.416	*1.086*	*1.086*	*119.1*	*119.0*	*175.0*	*177.5*	*177.5*	*177.1*		*2.633*	*2.526*	*2.587*	*2.565*	*2.543*	*2.622*	
cis-**1Ca**$^{++}$	1.345	1.089	1.089	115.4	114.8	1.1	1.3	49.6	150.3		2.597	2.518	2.583	2.593	2.533	2.600	2.115
	1.422	*1.088*	*1.087*	*111.1*	*112.2*	*10.2*	*15.4*	*11.3*	*174.1*		*2.609*	*2.527*	*2.588*	*2.588*	*2.545*	*2.619*	*2.040*
cis-**1Ca**$^{++}$_b	1.345	1.089	1.089	115.0	114.3	1.3	2.1	45.1	155.4		2.574	2.544	2.607	2.589	2.537	2.601	2.089
	1.419	*1.089*	*1.089*	*116.0*	*116.1*	*26.2*	*34.7*	*7.2*	*174.8*		*2.618*	*2.528*	*2.639*	*2.625*	*2.506*	*2.587*	*2.166*
trans-**1H**$^{+}$**Ca**$^{++}$	1.347	1.086	1.087	120.6	119.4	177.9	179.8	174.4	175.2	1.017	2.638	2.531	2.592	2.576	2.534	2.622	
	1.406	*1.087*	*1.085*	*118.5*	*119.1*	*179.4*	*179.6*	*179.1*	*179.0*	*1.013*	*2.702*	*2.533*	*2.572*	*2.550*	*2.526*	*2.647*	
trans-**1H**$^{+}$**Ca**$^{++}$_b	1.343	1.085	1.089	120.9	120.3	176.2	179.9	15.2	175.3	1.016	2.635	2.526	2.571	2.586	2.536	2.619	
	1.408	*1.085*	*1.086*	*119.7*	*119.4*	*171.4*	*175.9*	*4.8*	*174.8*	*1.011*	*2.694*	*2.529*	*2.555*	*2.568*	*2.516*	*2.636*	
cis-**1H**$^{+}$**Ca**$^{++}$	1.344	1.087	1.088	117.8	115.7	5.0	8.2	147.6	33.9	1.018	2.622	2.532	2.587	2.613	2.531	2.603	
	1.416	*1.090*	*1.088*	*116.5*	*116.0*	*28.2*	*36.6*	*168.4*	*11.5*	*1.014*	*2.705*	*2.539*	*2.570*	*2.600*	*2.516*	*2.638*	
cis-**1H**$^{+}$**Ca**$^{++}$_b	1.344	1.087	1.088	117.7	115.5	4.8	8.7	150.1	34.2	1.018	2.675	2.541	2.566	2.598	2.524	2.602	
	1.416	*1.090*	*1.088*	*116.3*	*115.7*	*28.3*	*37.4*	*170.4*	*12.4*	*1.014*	*2.745*	*2.535*	*2.546*	*2.571*	*2.522*	*2.659*	
cis-**1H**$^{+}$**Ca**$^{++}$_c	1.342	1.085	1.088	118.5	116.6	5.1	7.5	34.8	39.7	1.018	2.601	2.530	2.581	2.582	2.518	2.609	

	1.422	*1.087*	*1.088*	*118.0*	*116.9*	*31.4*	*40.9*	*7.8*	*11.9*	*1.014*	*2.694*	*2.550*	*2.558*	*2.570*	*2.514*	*2.617*
cis-**1H^{+}Ca^{++}**_d	1.342	1.085	1.088	118.2	116.4	5.0	7.4	33.9	38.5	1.018	2.611	2.524	2.556	2.607	2.538	2.583

[a] van der Walls distance between N and H atom of phenyl group, see Fig. 2.

Table 2S. Mulliken charges of selected atoms in the ground states S_0 (first line) and in the first excited state S_1 (second line *in italics*).

	q_N	q_{O1}	q_{O2}	q_{O3}	q_{O4}	q_{O5}	q_{O6}	q_{H3}	q_{Ca}
trans-**1**	-0.61	-0.55	-0.53	-0.56	-0.56	-0.53	-0.56		
	-0.62	*-0.54*	*-0.53*	*-0.56*	*-0.56*	*-0.53*	*-0.56*		
cis-**1**	-0.59	-0.55	-0.53	-0.56	-0.56	-0.53	-0.56		
	-0.62	*-0.54*	*-0.53*	*-0.56*	*-0.56*	*-0.53*	*-0.56*		
trans-**1H**$^+$	-0.71	-0.54	-0.53	-0.56	-0.56	-0.53	-0.56	0.36	
	-0.72	*-0.53*	*-0.53*	*-0.56*	*-0.56*	*-0.53*	*-0.55*	*0.35*	
cis-**1H**$^+$	-0.68	-0.55	-0.53	-0.56	-0.56	-0.53	-0.55	0.36	
	-0.71	*-0.53*	*-0.53*	*-0.56*	*-0.56*	*-0.53*	*-0.55*	*0.35*	
trans-**1Ca**$^{++}$	-0.54	-0.63	-0.56	-0.63	-0.63	-0.58	-0.63		1.53
	-0.53	*-0.62*	*-0.58*	*-0.63*	*-0.63*	*-0.58*	*-0.63*		*1.53*
cis-**1Ca**$^{++}$	-0.59	-0.63	-0.58	-0.63	-0.63	-0.58	-0.64		1.53
	-0.58	*-0.62*	*-0.60*	*-0.63*	*-0.63*	*-0.58*	*-0.64*		*1.53*
trans-**1H**$^+$**Ca**$^{++}$	-0.71	-0.62	-0.58	-0.63	-0.63	-0.58	-0.63	0.36	1.53
	-0.72	*-0.60*	*-0.58*	*-0.63*	*-0.64*	*-0.58*	*-0.63*	*0.35*	*1.54*
cis-**1H**$^+$**Ca**$^{++}$	-0.67	-0.62	-0.58	-0.63	-0.63	-0.58	-0.63	0.36	1.53
	-0.71	*-0.60*	*-0.58*	*-0.63*	*-0.63*	*-0.59*	*-0.63*	*0.35*	*1.54*

Table 3S. Dissociation Energies DE (eV) of the calculated minima with respect to *trans*-**1**(*cis*-**1**) + H^+ (DE_1), *trans*-**1**(*cis*-**1**) + Ca^{++} (DE_2), and *trans*-**1**(*cis*-**1**) + H^+ + Ca^{++} (DE_3) of the ground states S_0 and first excited state S_1 in acetonitrile solvent at the M06-2X/6-31G(d,p) level of theory with and without BSSE correction.

	S_0			**S_1**			**S_0**			**S_1**		
	DE_1	**DE_2**	**DE_3**	**DE_1**	**DE_2**	**DE_3**	**DE_1**	**DE_2**	**DE_3**	**DE_1**	**DE_2**	**DE_3**
	BSSE-uncorrected						**BSSE-corrected**					
trans-**1H**$^+$	7.84			8.30			7.81			8.26		
cis-**1H**$^+$	7.83			8.38			7.79			8.34		
trans-**1Ca**$^{++}$		1.54			1.35			1.28			1.09	
cis-**1Ca**$^{++}$		1.55			1.37			1.29			1.11	
trans-**1H**$^+$**Ca**$^{++}$	7.71	1.41	9.25	8.14	1.19	9.49	7.68	1.15	8.95	8.11	0.93	9.19
cis-**1H**$^+$**Ca**$^{++}$	7.69	1.41	9.24	8.22	1.22	9.59	7.66	1.15	8.94	8.19	0.96	9.30

Table 4S. Energy of the ground state, E_0(hartree) and of the excited state E_1(hartree), vertical excitation energies, ΔE_a(eV), for $S_0 \rightarrow S_1$ absorption and ΔE_e(eV) $S_1 \rightarrow S_0$ emission maxima, λ_{max} (nm), and f-Values for absorption and emission, adiabatic excitation energies ΔE_m(eV), energy difference ΔE_i(eV) between the isomers for absorption $\Delta E_i(S_0)$ and emission $\Delta E_i(S_1)$, in acetonitrile solvent at the M06-2X/6-31G(d,p) level of theory.

	$S_0 \rightarrow S_1$				$S_1 \rightarrow S_0$							
	E_0	**λ_{max}**	**ΔE_a**	**f**	**E_0**	**E_1**	**ΔE_e**	**λ_{max}**	**f**	**ΔE_{ad}**	**$\Delta E_i(S_0)$**	**$\Delta E_i(S_1)$**
trans-**1**	-1705.353543	346.38	3.58	1.3978	-1705.340164	-1705.235704	2.84	436.19	1.5315	3.21	0.00	0.00
trans-**1**_b	-1705.352442	333.70	3.72	1.7392	-1705.338091	-1705.230831	2.92	424.79	1.8704	3.31	0.03	0.13
cis-**1**	-1705.346596	311.87	3.98	0.9532	-1705.314539	-1705.227663	2.36	524.47	0.9693	3.24	0.19	0.22
cis-**1**_b	-1705.346588	311.60	3.98	0.9500	-1705.314910	-1705.227571	2.38	521.69	0.9915	3.24	0.19	0.22
cis-**1**_c	-1705.345797	340.50	3.64	0.5765	-1705.320753	-1705.232434	2.40	515.90	0.4886	3.08	0.21	0.09
cis-**1**_d	-1705.345708	337.95	3.67	0.4602	-1705.322171	-1705.232800	2.43	509.82	0.5501	3.07	0.21	0.08
trans-**1H$^+$**	-1705.803637	415.37	2.98	1.6309	-1705.796245	-1705.702644	2.55	486.79	1.8079	2.75	0.00	0.00
trans-**1H$^+$**_b	-1705.797891	381.88	3.25	1.1603	-1705.787001	-1705.690799	2.62	473.61	1.5364	2.91	0.16	0.32
cis-**1H$^+$**	-1705.796321	407.23	3.04	0.7534	-1705.784509	-1705.697469	2.37	523.47	1.0829	2.69	0.20	0.14
cis-**1H$^+$**_b	-1705.792830	347.31	3.57	0.0865	-1705.771512	-1705.671903	2.71	457.43	0.1055	3.29	0.29	0.84
		313.40	3.96	0.4660			3.43	361.23	0.5265			
trans-**1Ca^{++}**	-2382.812566	324.10	3.83	1.8194	-2382.797735	-2382.687744	2.99	414.25	1.8765	3.40	0.00	0.00
trans-**1Ca^{++}**_b	-2382.812297	320.99	3.86	1.7606	-2382.796609	-2382.686045	3.01	412.10	1.8480	3.44	0.01	0.05
cis-**1Ca^{++}**	-2382.806023	296.65	4.18	0.6983	-2382.786975	-2382.680585	2.90	428.27	0.9909	3.41	0.18	0.19
cis-**1Ca^{++}**_b	-2382.805406	303.01	4.09	0.7616	-2382.779426	-2382.687406	2.50	495.14	0.5828	3.21	0.19	0.01
trans-**1H$^+$Ca^{++}**	-2383.257980	379.86	3.26	1.6641	-2383.248261	-2383.148931	2.70	458.70	1.8228	2.97	0.00	0.00
trans-**1H$^+$Ca^{++}**_b	-2383.253846	359.03	3.45	1.1579	-2383.241416	-2383.139587	2.77	447.45	1.5770	3.11	0.11	0.25
cis-**1H$^+$Ca^{++}**	-2383.250656	366.92	3.38	0.7952	-2383.230386	-2383.144753	2.33	532.08	0.9177	2.88	0.20	0.11
cis-**1H$^+$Ca^{++}**_b	-2383.250480	369.21	3.36	0.8195	-2383.230663	-2383.144937	2.33	531.51	0.9437	2.87	0.20	0.11
cis-**1H$^+$Ca^{++}**_c	-2383.248478	334.77	3.70	0.2492	-2383.219978	-2383.136620	2.27	546.60	0.6882	3.04	0.26	0.34
		302.82	4.09	0.6485								
cis-**1H$^+$Ca^{++}**_d	-2383.247887	336.84	3.68	0.2709							0.27	
		304.03	4.08	0.6489								
acetonitrile	-132.703459	110.23	11.25	1.3625	-132.656034	-132.314041	9.31	133.23	1.0299	10.60		

Table 5S. Energy of the ground state, E_0(hartree) and of the excited state E_1(hartree), vertical excitation energies, ΔE_a(eV), for $S_0 \rightarrow S_1$ absorption and ΔE_e(eV) $S_1 \rightarrow S_0$ emission maxima, λ_{max} (nm), and f-Values for absorption and emission, adiabatic excitation energies ΔE_{ad}(eV), energy difference ΔE_i(eV) between the isomers for absorption $\Delta E_i(S_0)$ and emission $\Delta E_i(S_1)$, in acetonitrile solvent at the PBE06-31G(d,p)//M06-2X/6-31G(d,p) level of theory.

	$S_0 \rightarrow S_1$				$S_1 \rightarrow S_0$							
	E_0	**λ_{max}**	**ΔE_a**	**f**	**E_0**	**E_1**	**ΔE_e**	**λ_{max}**	**f**	**ΔE_{ad}**	**$\Delta E_i(S_0)$**	**$\Delta E_i(S_1)$**
trans-**1**	-1704.119298	374.18	3.31	0.9915	-1704.108931	-1704.004537	2.84	436.46	1.3200	3.12	0.00	0.00
cis-**1**	-1704.108796	350.58	3.54	0.4013	-1704.081966	-1703.991387	2.46	503.01	0.7945	3.19	0.29	0.36
trans-**1H**$^+$	-1704.577154	444.99	2.79	1.0207	-1704.572191	-1704.475655	2.63	471.98	1.3633	2.76	0.00	0.00
cis-**1H**$^+$	-1704.566374	477.13	2.60	0.2800	-1704.558218	-1704.467080	2.48	499.94	0.7170	2.70	0.29	0.23
trans-**1Ca**$^{++}$	-2381.393180	335.87	3.69	1.5651	-2381.381327	-2381.269348	3.05	406.90	1.7292	3.37	0.00	0.00
cis-**1Ca**$^{++}$	-2381.383748	325.07	3.81	0.3698	-2381.370865	-2381.264744	2.89	429.35	0.7377	3.24	0.26	0.13
trans-**1H**$^+$**Ca**$^{++}$	-2381.846162	399.56	3.10	1.2435	-2381.839317	-2381.736136	2.81	441.59	1.6073	2.99	0.00	0.00
cis-**1H**$^+$**Ca**$^{++}$	-2381.835978	409.90	3.02	0.4915	-2381.819974	-2381.730045	2.45	506.67	0.7995	2.88	0.28	0.17

Table 6S. Energy of the ground state, E_0(hartree) and of the excited state E_1(hartree), vertical excitation energies, ΔE_a(eV), for $S_0 \rightarrow S_1$ absorption and ΔE_e(eV) $S_1 \rightarrow S_0$ emission maxima, λ_{max} (nm), and f-Values for absorption and emission, adiabatic excitation energies ΔE_m(eV), energy difference ΔE_i(eV) between the isomers for absorption $\Delta E_i(S_0)$ and emission $\Delta E_i(S_1)$, in the gas phase at the M06-2X/6-31G(d,p) level of theory.

	$S_0 \rightarrow S_1$				$S_0 \rightarrow S_1$							
	E_0	**λ_{max}**	**ΔE_a**	**f**	**E_0**	**E_1**	**ΔE_e**	**λ_{max}**	**f**	**ΔE_{ad}**	**$\Delta E_i(S_0)$**	**$\Delta E_i(S_1)$**
trans-**1**	-1705.325657	327.38	3.79	1.0790	-1705.316108	-1705.196243	3.26	380.12	1.1912	3.52	0.00	0.00
trans-**1**_b	-1705.324513	312.97	3.96	1.3315	-1705.314264	-1705.189540	3.39	365.31	1.5166	3.67	0.03	0.18
cis-**1**	-1705.320452	299.91	4.13	0.5440	-1705.290041	-1705.190458	2.71	457.54	0.5637	3.54	0.14	0.16
cis-**1**_b	-1705.320021	300.56	4.13	0.5563	-1705.289438	-1705.190233	2.70	459.29	0.5953	3.53	0.15	0.16
cis-**1**_c	-1705.318292	340.78	3.64	0.2969	-1705.233463	-1705.137448	2.61	474.54	0.0558	4.92	0.20	1.60
cis-**1**_d	-1705.318111	339.82	3.65	0.3390							0.21	
1-tr.state	-1705.264243	457.51	2.71	0.6985	-1705.281722	-1705.137459	3.93	315.84	0.0037	3.45	1.67	1.60
trans-**1H$^+$**	-1705.726478	432.05	2.87	1.2596	-1705.706567	-1705.603173	2.81	440.68	1.1330	3.36	0.00	0.00
trans-**1H$^+$**_b	-1705.716339										0.28	
cis-**1H$^+$**	-1705.719833	459.56	2.70	0.4793	-1705.698908	-1705.603893	2.59	479.54	0.3763	3.15	0.18	-0.02
cis-**1H$^+$**_b	-1705.717750										0.24	
cis-**1H$^+$**_c	-1705.714852										0.32	
trans-**1Ca^{++}**	-2382.566127	344.64	3.60	0.9962	-2382.551722	-2382.430882	3.29	377.06	1.7697	3.68	0.00	0.00
trans-**1Ca^{++}**_b	-2382.563664										0.07	
cis-**1Ca^{++}**	-2382.565287	279.58	4.43	0.2908	-2382.493739	-2382.398694	2.59	479.39	0.0414	4.53	0.02	0.88
		249.15	4.98	0.3125	-2382.493739	-2382.370912	3.34	370.95	0.1484			
cis-**1Ca^{++}**_b	-2382.564770										0.04	
cis-**1Ca^{++}**_c	-2382.559496										0.18	
trans-**1H$^+$Ca^{++}**	-2382.834318	327.87	3.78	0.0780	-2382.821288	-2382.707744	3.09	401.28	0.0219	3.44	0.00	0.00
		319.14	3.89	1.1441	-2382.821288	-2382.691449	3.53	350.92	1.3515			
trans-**1H$^+$Ca^{++}**_c	-2382.832453										0.05	
cis-**1H$^+$Ca^{++}**	-2382.823440	328.52	3.77	0.1972	-2382.810090	-2382.697052	3.08	403.08	0.0272	3.44	0.30	0.29
		320.73	3.87	0.6035	-2382.810090	-2382.681735	3.49	354.98	0.9149			
cis-**1H$^+$Ca^{++}**_b	-2382.822284										0.33	

cis-**1H^{+}Ca^{++}**_c	-2382.819233										0.41
cis-**1H^{+}Ca^{++}**_d	-2382.816324										0.49
acetonitrile	-132.695801	106.33	11.66	0.6919	-132.647115	-132.290047	9.72	127.60	0.6016	11.04	

Table 7S: Geometries of the Calculated Structures in acetonitrile sonvent at the M06-2X/6-31G(d,p) level of theory.

Acetonitrile (S_0):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.180888
2	1	0	0.000000	1.027084	-1.548104
3	1	0	-0.889481	-0.513542	-1.548104
4	1	0	0.889481	-0.513542	-1.548104
5	6	0	0.000000	0.000000	0.279958
6	7	0	0.000000	0.000000	1.435699

trans-**1** **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.031335	2.472056	0.106014
2	6	0	-0.711448	2.881985	-0.099703
3	6	0	-2.449226	1.189245	-0.235790
4	6	0	0.212573	2.005157	-0.650361
5	1	0	-0.418914	3.887831	0.174688
6	6	0	-1.506504	0.299363	-0.793095
7	8	0	1.513325	2.291946	-0.895002
8	6	0	-0.196871	0.692209	-1.000748
9	1	0	-1.810796	-0.705649	-1.057565
10	6	0	1.966812	3.597298	-0.570740
11	8	0	0.776339	-0.090188	-1.532180
12	6	0	3.431613	3.674850	-0.921433
13	1	0	1.829906	3.791692	0.500515
14	1	0	1.406917	4.348363	-1.142127
15	6	0	0.418798	-1.407160	-1.918573
16	8	0	4.151012	2.843263	-0.040580
17	1	0	3.580184	3.358047	-1.964563
18	1	0	3.765225	4.719719	-0.831802
19	6	0	1.652100	-2.073268	-2.475722
20	1	0	0.051233	-1.971611	-1.052073
21	1	0	-0.367464	-1.380823	-2.683990
22	6	0	5.535606	2.866880	-0.302998
23	1	0	2.087589	-1.445148	-3.267014
24	1	0	1.365113	-3.036498	-2.924168
25	8	0	2.573237	-2.264919	-1.426993
26	1	0	5.741169	2.538752	-1.332848
27	1	0	5.938013	3.884057	-0.182587
28	6	0	6.229151	1.947315	0.670706
29	6	0	3.756898	-2.889682	-1.867888
30	1	0	7.316676	2.062286	0.576291
31	1	0	5.935660	2.202092	1.697278
32	8	0	5.841683	0.619817	0.361214
33	1	0	3.539077	-3.881394	-2.292558
34	1	0	4.248354	-2.286563	-2.645836
35	6	0	4.684935	-3.054109	-0.690394
36	6	0	6.359930	-0.376661	1.127003
37	1	0	5.546798	-3.667980	-0.981839
38	1	0	4.157046	-3.554677	0.131406
39	8	0	5.108627	-1.762128	-0.290067
40	6	0	7.229125	-0.192648	2.194121
41	6	0	5.956786	-1.684909	0.769487
42	6	0	7.703023	-1.295691	2.915060
43	1	0	7.545124	0.804449	2.475561
44	6	0	6.433193	-2.771737	1.490488
45	6	0	7.307932	-2.574943	2.566238
46	1	0	8.381589	-1.134924	3.745773
47	1	0	6.131726	-3.777755	1.225424
48	1	0	7.670036	-3.434671	3.119631
49	1	0	-2.742405	3.170244	0.536829
50	6	0	-3.846559	0.814855	-0.008538
51	1	0	-4.464464	1.566431	0.480221
52	6	0	-4.437810	-0.341767	-0.346562
53	1	0	-3.882878	-1.129383	-0.850448
54	6	0	-5.855954	-0.635365	-0.087477
55	6	0	-6.386520	-1.880782	-0.540261
56	6	0	-7.903018	-0.014514	0.774443
57	6	0	-7.703712	-2.169991	-0.320888
58	1	0	-5.735442	-2.579615	-1.054935
59	6	0	-8.689821	0.952319	1.456890
60	6	0	-8.518788	-1.226929	0.355344
61	1	0	-8.136091	-3.108741	-0.656438
62	6	0	-9.894042	-1.442325	0.623649
63	6	0	-10.629785	-0.490324	1.283550
64	1	0	-11.682054	-0.658147	1.487203
65	6	0	-10.018764	0.718097	1.703566
66	1	0	-8.204288	1.871154	1.769618
67	1	0	-10.612088	1.462337	2.224976
68	1	0	-10.350807	-2.372428	0.296777
69	7	0	-6.590490	0.260468	0.547877

trans-**1**_b **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.753253	2.990806	0.465776
2	6	0	-0.408500	3.257491	0.194975
3	6	0	-2.331451	1.774694	0.115664
4	6	0	0.378793	2.301263	-0.430401
5	1	0	0.011447	4.214871	0.477542
6	6	0	-1.527098	0.802654	-0.515450
7	8	0	1.687150	2.450849	-0.745271
8	6	0	-0.193758	1.052598	-0.785883
9	1	0	-1.956346	-0.153740	-0.786423

10	6	0	2.297908	3.690325	-0.420345
11	8	0	0.656421	0.180460	-1.384807
12	6	0	3.736512	3.625337	-0.867885
13	1	0	2.251717	3.863743	0.662162
14	1	0	1.786151	4.513839	-0.933825
15	6	0	0.136253	-1.084768	-1.759387
16	8	0	4.418607	2.692179	-0.062389
17	1	0	3.782273	3.332640	-1.927312
18	1	0	4.184884	4.625627	-0.770804
19	6	0	1.255194	-1.875184	-2.390277
20	1	0	-0.243518	-1.616562	-0.877558
21	1	0	-0.682679	-0.963422	-2.479880
22	6	0	5.777161	2.577794	-0.419867
23	1	0	1.713061	-1.289065	-3.200886
24	1	0	0.837948	-2.794591	-2.828264
25	8	0	2.207404	-2.182937	-1.398363
26	1	0	5.877806	2.255677	-1.466990
27	1	0	6.290974	3.544743	-0.309802
28	6	0	6.433487	1.568700	0.488726
29	6	0	3.281389	-2.937698	-1.910905
30	1	0	7.518817	1.576003	0.325031
31	1	0	6.232746	1.826842	1.536447
32	8	0	5.893786	0.294329	0.183116
33	1	0	2.924451	-3.895226	-2.319311
34	1	0	3.790305	-2.391343	-2.718753
35	6	0	4.255408	-3.215168	-0.793089
36	6	0	6.345749	-0.763036	0.908543
37	1	0	5.020331	-3.923341	-1.136875
38	1	0	3.725163	-3.656309	0.060899
39	8	0	4.850884	-1.983933	-0.421666
40	6	0	7.300419	-0.689849	1.914285
41	6	0	5.773017	-2.013629	0.576835
42	6	0	7.693614	-1.846843	2.598363
43	1	0	7.746262	0.261986	2.176019
44	6	0	6.170488	-3.154894	1.260963
45	6	0	7.133063	-3.069453	2.274614
46	1	0	8.439989	-1.771369	3.381720
47	1	0	5.737271	-4.116981	1.015787
48	1	0	7.431580	-3.969824	2.800556
49	1	0	-2.354636	3.750380	0.956009
50	6	0	-3.749202	1.551951	0.416086
51	1	0	-4.224795	2.372120	0.950801
52	6	0	-4.475512	0.472583	0.086200
53	1	0	-4.032510	-0.349070	-0.470933
54	6	0	-5.897816	0.262577	0.389624
55	6	0	-6.648498	1.168699	1.201552
56	6	0	-7.750056	-1.088709	0.094477
57	6	0	-7.968146	0.916012	1.439857
58	1	0	-6.172649	2.041911	1.631351
59	6	0	-8.317091	-2.258339	-0.476517
60	6	0	-8.573935	-0.240987	0.882357
61	1	0	-8.563245	1.584980	2.055483
62	6	0	-9.935350	-0.576635	1.081951
63	6	0	-10.458819	-1.713853	0.517390
64	1	0	-11.501988	-1.968579	0.672013
65	6	0	-9.639830	-2.561019	-0.269024
66	1	0	-7.673658	-2.894106	-1.076040
67	1	0	-10.066286	-3.456894	-0.708565
68	1	0	-10.553773	0.079429	1.688083
69	7	0	-6.433134	-0.826061	-0.136842

***cis*-1 (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.064826	4.139652	-0.930858
2	6	0	0.694529	4.153200	-0.654759
3	6	0	2.887177	3.142432	-0.417882
4	6	0	0.133093	3.171317	0.151188
5	1	0	0.075791	4.936542	-1.074775
6	6	0	2.322245	2.171552	0.431690
7	8	0	-1.179426	3.086283	0.478942
8	6	0	0.965644	2.169086	0.706989
9	1	0	2.967996	1.424657	0.876645
10	6	0	-2.047754	4.077492	-0.047849
11	8	0	0.337949	1.264242	1.501325
12	6	0	-3.449779	3.744504	0.397176
13	1	0	-2.000541	4.080414	-1.144145
14	1	0	-1.762546	5.070563	0.322038
15	6	0	1.128476	0.215610	2.038610
16	8	0	-3.855768	2.561484	-0.251484
17	1	0	-3.474447	3.618098	1.489695
18	1	0	-4.114696	4.581488	0.135430
19	6	0	0.210700	-0.706718	2.800990
20	1	0	1.628365	-0.335905	1.231006
21	1	0	1.892224	0.619846	2.715312
22	6	0	-5.168463	2.185955	0.097567
23	1	0	-0.384792	-0.123999	3.519599
24	1	0	0.817832	-1.428514	3.368007
25	8	0	-0.626364	-1.371263	1.882793
26	1	0	-5.250268	2.019181	1.181917
27	1	0	-5.886137	2.972373	-0.181419
28	6	0	-5.519938	0.918374	-0.640852
29	6	0	-1.526799	-2.245805	2.523579
30	1	0	-6.583756	0.689396	-0.496976
31	1	0	-5.329015	1.048608	-1.713930
32	8	0	-4.713436	-0.123712	-0.119029
33	1	0	-0.984162	-3.008667	3.102268
34	1	0	-2.179632	-1.692877	3.215315
35	6	0	-2.362275	-2.932382	1.472090
36	6	0	-4.868698	-1.362208	-0.657228
37	1	0	-2.962500	-3.726716	1.934187
38	1	0	-1.706330	-3.381080	0.714790
39	8	0	-3.202749	-1.955804	0.881239
40	6	0	-5.758775	-1.684699	-1.673071
41	6	0	-4.040887	-2.368819	-0.106099
42	6	0	-5.837707	-2.999141	-2.149859
43	1	0	-6.397643	-0.922434	-2.102098

44	6	0	-4.128886	-3.669437	-0.584646
45	6	0	-5.029868	-3.983813	-1.609490
46	1	0	-6.537646	-3.233961	-2.944473
47	1	0	-3.500563	-4.447802	-0.169263
48	1	0	-5.085809	-5.004131	-1.973029
49	1	0	2.486321	4.912283	-1.566650
50	6	0	4.327612	3.146518	-0.732181
51	1	0	4.766959	4.136381	-0.844603
52	6	0	5.157457	2.100118	-0.870095
53	1	0	6.217776	2.304644	-0.996884
54	6	0	4.823667	0.657788	-0.878662
55	6	0	3.640267	0.177601	-1.519753
56	6	0	5.467610	-1.488674	-0.328912
57	6	0	3.387756	-1.164184	-1.535664
58	1	0	2.966822	0.884994	-1.989527
59	6	0	6.416445	-2.348906	0.282972
60	6	0	4.305185	-2.054774	-0.917341
61	1	0	2.500488	-1.562514	-2.020352
62	6	0	4.116181	-3.458536	-0.879857
63	6	0	5.047553	-4.267511	-0.277142
64	1	0	4.899153	-5.341826	-0.248217
65	6	0	6.208233	-3.705457	0.308750
66	1	0	7.298783	-1.898360	0.725668
67	1	0	6.936687	-4.357490	0.779834
68	1	0	3.223249	-3.879076	-1.333711
69	7	0	5.713060	-0.146395	-0.328338

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cis-**1**_b **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.919436	3.743892	1.252567
2	6	0	-0.724375	3.759216	0.527082
3	6	0	-2.614805	2.557442	1.458514
4	6	0	-0.203903	2.579634	0.010701
5	1	0	-0.210502	4.699759	0.371802
6	6	0	-2.066335	1.357934	0.964779
7	8	0	0.938100	2.479086	-0.712655
8	6	0	-0.885673	1.359668	0.241995
9	1	0	-2.578091	0.424938	1.166604
10	6	0	1.657687	3.675363	-0.965817
11	8	0	-0.296646	0.254141	-0.281621
12	6	0	2.862095	3.317923	-1.800298
13	1	0	1.978586	4.132917	-0.021312
14	1	0	1.029678	4.391089	-1.511429
15	6	0	-0.982722	-0.978311	-0.129050
16	8	0	3.742303	2.544382	-1.018027
17	1	0	2.541900	2.759079	-2.692134
18	1	0	3.350617	4.245127	-2.136423
19	6	0	-0.181526	-2.040259	-0.839729
20	1	0	-1.075354	-1.233566	0.934448
21	1	0	-1.988643	-0.911594	-0.565250
22	6	0	4.894208	2.165450	-1.736310
23	1	0	0.002046	-1.733557	-1.880222
24	1	0	-0.762747	-2.974653	-0.856691
25	8	0	1.034971	-2.219419	-0.151578
26	1	0	4.622081	1.579196	-2.626443
27	1	0	5.453517	3.052482	-2.070264
28	6	0	5.778904	1.341200	-0.835031
29	6	0	1.849285	-3.197863	-0.755568
30	1	0	6.747039	1.170284	-1.323199
31	1	0	5.949708	1.876801	0.107720
32	8	0	5.123319	0.108560	-0.588694
33	1	0	1.347731	-4.177558	-0.754099
34	1	0	2.070607	-2.929819	-1.799323
35	6	0	3.135632	-3.303623	0.024989
36	6	0	5.753355	-0.776577	0.228835
37	1	0	3.716723	-4.163111	-0.333611
38	1	0	2.912856	-3.448820	1.089925
39	8	0	3.859695	-2.100247	-0.168154
40	6	0	6.990524	-0.568514	0.824929
41	6	0	5.060320	-1.988271	0.459568
42	6	0	7.549362	-1.551422	1.651083
43	1	0	7.530197	0.355037	0.654393
44	6	0	5.624084	-2.956772	1.279732
45	6	0	6.871345	-2.736017	1.877083
46	1	0	8.516080	-1.373358	2.109547
47	1	0	5.102827	-3.888210	1.463642
48	1	0	7.296866	-3.501876	2.516418
49	1	0	-2.313239	4.675651	1.646937
50	6	0	-3.877897	2.567468	2.219779
51	1	0	-3.915909	3.288250	3.035069
52	6	0	-4.959858	1.790983	2.049829
53	1	0	-5.761941	1.867577	2.779792
54	6	0	-5.225770	0.816152	0.968008
55	6	0	-4.829347	1.084038	-0.378782
56	6	0	-6.198279	-1.181807	0.346023
57	6	0	-5.123823	0.175465	-1.354202
58	1	0	-4.309859	2.007974	-0.604841
59	6	0	-6.912824	-2.349499	0.721379
60	6	0	-5.818964	-1.014980	-1.012864
61	1	0	-4.844331	0.353423	-2.389143
62	6	0	-6.156835	-2.013089	-1.959929
63	6	0	-6.844138	-3.135517	-1.568867
64	1	0	-7.099829	-3.899165	-2.295979
65	6	0	-7.225623	-3.302907	-0.215100
66	1	0	-7.195795	-2.458500	1.763297
67	1	0	-7.770740	-4.193901	0.079138
68	1	0	-5.862548	-1.872710	-2.996274
69	7	0	-5.905926	-0.261372	1.310255

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cis-**1**_c **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.143673	3.729861	-1.015978

2	6	0	0.935968	3.748180	-0.312926
3	6	0	2.816073	2.536369	-1.265562
4	6	0	0.371759	2.560486	0.132434
5	1	0	0.445146	4.695010	-0.125223
6	6	0	2.223959	1.332293	-0.838333
7	8	0	-0.788725	2.457452	0.825535
8	6	0	1.028186	1.335399	-0.143665
9	1	0	2.721673	0.398119	-1.054278
10	6	0	-1.477976	3.660748	1.124684
11	8	0	0.399651	0.222335	0.319412
12	6	0	-2.713968	3.299487	1.910068
13	1	0	-1.760861	4.177035	0.198485
14	1	0	-0.842533	4.327153	1.721573
15	6	0	1.045437	-1.021792	0.105473
16	8	0	-3.594222	2.590154	1.069163
17	1	0	-2.433974	2.690475	2.782361
18	1	0	-3.184535	4.224213	2.277266
19	6	0	0.215829	-2.089225	0.773757
20	1	0	1.126483	-1.229344	-0.969525
21	1	0	2.055315	-1.010498	0.537860
22	6	0	-4.784768	2.230717	1.732144
23	1	0	0.047788	-1.821833	1.827694
24	1	0	0.767904	-3.041065	0.747301
25	8	0	-1.010128	-2.202826	0.088375
26	1	0	-4.566231	1.607774	2.612177
27	1	0	-5.325219	3.126261	2.074356
28	6	0	-5.662688	1.465920	0.773545
29	6	0	-1.852762	-3.174404	0.663777
30	1	0	-6.651655	1.310595	1.223433
31	1	0	-5.784139	2.036909	-0.156109
32	8	0	-5.036462	0.222014	0.509164
33	1	0	-1.374867	-4.165689	0.644464
34	1	0	-2.076522	-2.924487	1.711523
35	6	0	-3.133519	-3.233396	-0.130790
36	6	0	-5.673116	-0.627828	-0.339851
37	1	0	-3.738672	-4.085921	0.203795
38	1	0	-2.902453	-3.362160	-1.196080
39	8	0	-3.831242	-2.017296	0.078907
40	6	0	-6.886993	-0.370303	-0.963549
41	6	0	-5.012416	-1.856894	-0.574576
42	6	0	-7.455294	-1.321413	-1.820181
43	1	0	-7.400337	0.567959	-0.792060
44	6	0	-5.585955	-2.793764	-1.424174
45	6	0	-6.809790	-2.523679	-2.048567
46	1	0	-8.403319	-1.104646	-2.300443
47	1	0	-5.090493	-3.738827	-1.609749
48	1	0	-7.242808	-3.265312	-2.711008
49	1	0	2.565455	4.667678	-1.365223
50	6	0	4.071467	2.593913	-2.031937
51	1	0	4.137301	3.476223	-2.667877
52	6	0	5.127785	1.762990	-2.108648
53	1	0	5.888045	2.029531	-2.840220
54	6	0	5.455102	0.544442	-1.343714
55	6	0	6.371064	-0.381550	-1.932182
56	6	0	5.270261	-0.763991	0.547061
57	6	0	6.711241	-1.516477	-1.251908
58	1	0	6.779248	-0.173308	-2.915592
59	6	0	4.696220	-0.959775	1.832624
60	6	0	6.154793	-1.750149	0.031671
61	1	0	7.399822	-2.241680	-1.676564
62	6	0	6.443498	-2.902592	0.804773
63	6	0	5.870235	-3.069588	2.040683
64	1	0	6.092224	-3.953599	2.629024
65	6	0	4.986884	-2.088421	2.557142
66	1	0	4.026689	-0.193030	2.210615
67	1	0	4.541767	-2.233788	3.536111
68	1	0	7.123307	-3.647452	0.400644
69	7	0	4.944047	0.364233	-0.140421

***cis*-1_d (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.636847	3.773724	-1.097107
2	6	0	1.284357	3.954399	-0.789665
3	6	0	3.364186	2.722744	-0.547936
4	6	0	0.645394	3.085622	0.084723
5	1	0	0.742062	4.774511	-1.243629
6	6	0	2.724931	1.877594	0.377822
7	8	0	-0.660624	3.154639	0.442652
8	6	0	1.384875	2.032895	0.678938
9	1	0	3.294885	1.088974	0.847438
10	6	0	-1.435156	4.205139	-0.113021
11	8	0	0.688408	1.230934	1.528326
12	6	0	-2.847062	4.051002	0.394753
13	1	0	-1.427045	4.146318	-1.208743
14	1	0	-1.031904	5.179026	0.192528
15	6	0	1.372315	0.101385	2.048153
16	8	0	-3.409121	2.895867	-0.184979
17	1	0	-2.839308	3.972172	1.492041
18	1	0	-3.426347	4.945728	0.121226
19	6	0	0.367082	-0.765941	2.761924
20	1	0	1.834964	-0.471222	1.233533
21	1	0	2.157392	0.417696	2.747272
22	6	0	-4.725403	2.663099	0.261365
23	1	0	-0.204936	-0.163672	3.483473
24	1	0	0.905215	-1.546466	3.320866
25	8	0	-0.490964	-1.343108	1.803591
26	1	0	-4.743801	2.498119	1.348941
27	1	0	-5.371263	3.525213	0.036088
28	6	0	-5.268757	1.449428	-0.450608
29	6	0	-1.443603	-2.194963	2.397053
30	1	0	-6.337707	1.336130	-0.228025
31	1	0	-5.145086	1.571762	-1.534271
32	8	0	-4.544659	0.318499	0.002587
33	1	0	-0.949180	-3.033035	2.911370
34	1	0	-2.045135	-1.648197	3.138472
35	6	0	-2.345993	-2.745678	1.321325

36	6	0	-4.836574	-0.878418	-0.572472
37	1	0	-2.993290	-3.522701	1.747831
38	1	0	-1.742634	-3.190216	0.518863
39	8	0	-3.124874	-1.674125	0.817665
40	6	0	-5.821283	-1.082373	-1.530491
41	6	0	-4.054101	-1.970862	-0.129248
42	6	0	-6.035480	-2.360819	-2.060366
43	1	0	-6.429828	-0.254095	-1.872477
44	6	0	-4.272877	-3.234051	-0.663205
45	6	0	-5.266137	-3.427728	-1.631507
46	1	0	-6.807365	-2.502819	-2.808884
47	1	0	-3.675223	-4.076247	-0.336341
48	1	0	-5.422923	-4.420278	-2.039783
49	1	0	3.117261	4.458426	-1.789795
50	6	0	4.781701	2.565273	-0.916508
51	1	0	5.269230	3.500635	-1.189452
52	6	0	5.563486	1.471321	-0.958929
53	1	0	6.614642	1.636310	-1.186740
54	6	0	5.210610	0.051270	-0.750377
55	6	0	6.230606	-0.833070	-0.283491
56	6	0	3.672238	-1.665776	-0.799898
57	6	0	5.931022	-2.148652	-0.064220
58	1	0	7.227067	-0.444723	-0.100601
59	6	0	2.338042	-2.086781	-1.051316
60	6	0	4.612789	-2.611612	-0.308523
61	1	0	6.682865	-2.843173	0.300332
62	6	0	4.203206	-3.950157	-0.083970
63	6	0	2.906738	-4.328719	-0.329116
64	1	0	2.595445	-5.352658	-0.150863
65	6	0	1.965274	-3.385865	-0.814246
66	1	0	1.634606	-1.346621	-1.420177
67	1	0	0.942998	-3.699432	-1.000207
68	1	0	4.930616	-4.665189	0.290093
69	7	0	3.988393	-0.361787	-1.025447

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trans-**1H$^+$ (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.733518	3.008695	-0.463936
2	6	0	0.384687	3.280330	-0.240605
3	6	0	2.301865	1.804603	-0.050271
4	6	0	-0.414444	2.343663	0.404130
5	1	0	-0.031703	4.222798	-0.572427
6	6	0	1.488992	0.853536	0.606829
7	8	0	-1.722640	2.499116	0.677074
8	6	0	0.151523	1.110096	0.832921
9	1	0	1.915112	-0.083938	0.940650
10	6	0	-2.338207	3.723918	0.294488
11	8	0	-0.711001	0.270899	1.452374
12	6	0	-3.786519	3.656025	0.708186
13	1	0	-2.265542	3.857639	-0.791448
14	1	0	-1.844946	4.566066	0.794208
15	6	0	-0.197011	-0.970240	1.913054
16	8	0	-4.436076	2.690938	-0.085642
17	1	0	-3.855910	3.395826	1.774796
18	1	0	-4.241576	4.648125	0.569099
19	6	0	-1.331335	-1.731909	2.551374
20	1	0	0.210801	-1.546314	1.072667
21	1	0	0.598576	-0.802274	2.649768
22	6	0	-5.803969	2.573920	0.235332
23	1	0	-1.816033	-1.106486	3.315680
24	1	0	-0.922257	-2.623750	3.049979
25	8	0	-2.249553	-2.096842	1.547732
26	1	0	-5.932443	2.289953	1.290363
27	1	0	-6.324406	3.529810	0.073151
28	6	0	-6.419656	1.522550	-0.653488
29	6	0	-3.331955	-2.838368	2.062787
30	1	0	-7.509649	1.520916	-0.524561
31	1	0	-6.188987	1.743104	-1.703642
32	8	0	-5.874023	0.268612	-0.281228
33	1	0	-2.978349	-3.770993	2.527781
34	1	0	-3.871634	-2.259397	2.826786
35	6	0	-4.266627	-3.179476	0.929188
36	6	0	-6.303474	-0.825266	-0.964855
37	1	0	-5.036699	-3.877048	1.282923
38	1	0	-3.706355	-3.656638	0.114712
39	8	0	-4.858341	-1.972634	0.479923
40	6	0	-7.222766	-0.805762	-2.005349
41	6	0	-5.744885	-2.056309	-0.547167
42	6	0	-7.593957	-1.997804	-2.639673
43	1	0	-7.656495	0.131032	-2.333679
44	6	0	-6.119993	-3.232495	-1.182726
45	6	0	-7.047040	-3.201406	-2.231884
46	1	0	-8.312129	-1.965087	-3.451837
47	1	0	-5.698473	-4.180236	-0.870477
48	1	0	-7.329632	-4.128604	-2.718553
49	1	0	2.347401	3.747504	-0.969450
50	6	0	3.711605	1.582888	-0.317437
51	1	0	4.209642	2.414472	-0.810711
52	6	0	4.422926	0.473176	-0.021826
53	1	0	3.946357	-0.375319	0.460656
54	6	0	5.827696	0.319479	-0.318780
55	6	0	6.657587	1.301849	-0.919233
56	6	0	7.713512	-1.181328	-0.205739
57	6	0	7.977408	1.036763	-1.151295
58	1	0	6.236358	2.260501	-1.187702
59	6	0	8.205193	-2.444164	0.166839
60	6	0	8.552131	-0.216263	-0.802369
61	1	0	8.609088	1.791378	-1.609871
62	6	0	9.909808	-0.540450	-1.021633
63	6	0	10.390256	-1.775743	-0.656871
64	1	0	11.431413	-2.025755	-0.825168
65	6	0	9.532905	-2.727278	-0.061493
66	1	0	7.542825	-3.172243	0.622946
67	1	0	9.925858	-3.697592	0.221341
68	1	0	10.557427	0.200051	-1.479381
69	7	0	6.394444	-0.852840	0.002389

70	1	0	5.805682	-1.561713	0.431830

trans-**1H$^+$**_b **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.762694	2.904398	-0.501186
2	6	0	0.412807	3.207635	-0.315671
3	6	0	2.304430	1.715617	-0.020129
4	6	0	-0.413566	2.317382	0.356678
5	1	0	0.019816	4.140723	-0.699117
6	6	0	1.464848	0.812791	0.666535
7	8	0	-1.727614	2.506572	0.599613
8	6	0	0.125793	1.099712	0.852883
9	1	0	1.870718	-0.111580	1.057778
10	6	0	-2.312815	3.719878	0.146298
11	8	0	-0.759603	0.301771	1.497134
12	6	0	-3.771996	3.694480	0.526144
13	1	0	-2.212884	3.804055	-0.942777
14	1	0	-1.818787	4.578140	0.617991
15	6	0	-0.272883	-0.921551	2.027435
16	8	0	-4.418901	2.705316	-0.240040
17	1	0	-3.871779	3.482884	1.601115
18	1	0	-4.207499	4.686325	0.332475
19	6	0	-1.431832	-1.635755	2.676780
20	1	0	0.144321	-1.543716	1.225318
21	1	0	0.509863	-0.730086	2.772321
22	6	0	-5.794211	2.618384	0.056846
23	1	0	-1.922271	-0.967247	3.399814
24	1	0	-1.048371	-2.509165	3.225833
25	8	0	-2.334909	-2.033720	1.671709
26	1	0	-5.947865	2.381671	1.120132
27	1	0	-6.299902	3.572111	-0.157080
28	6	0	-6.404276	1.535874	-0.797796
29	6	0	-3.443410	-2.727200	2.197830
30	1	0	-7.496670	1.551327	-0.691961
31	1	0	-6.149664	1.707292	-1.851678
32	8	0	-5.880382	0.294310	-0.358690
33	1	0	-3.119562	-3.639822	2.720722
34	1	0	-3.990273	-2.098396	2.916082
35	6	0	-4.357276	-3.111276	1.060926
36	6	0	-6.311432	-0.825787	-0.997159
37	1	0	-5.148277	-3.776078	1.431335
38	1	0	-3.786924	-3.639803	0.286195
39	8	0	-4.916232	-1.919700	0.535001
40	6	0	-7.207616	-0.844769	-2.057600
41	6	0	-5.780776	-2.042311	-0.506691
42	6	0	-7.583558	-2.061421	-2.640188
43	1	0	-7.619317	0.080898	-2.441136
44	6	0	-6.160130	-3.243146	-1.091413
45	6	0	-7.064033	-3.250996	-2.161025
46	1	0	-8.283205	-2.059408	-3.468943
47	1	0	-5.760505	-4.180223	-0.723184
48	1	0	-7.350866	-4.197238	-2.606932
49	1	0	2.396350	3.609561	-1.030198
50	6	0	3.723661	1.454097	-0.244886
51	1	0	4.238660	2.267315	-0.755978
52	6	0	4.395815	0.337507	0.087499
53	1	0	3.884645	-0.505953	0.539928
54	6	0	5.814795	0.109688	-0.140493
55	6	0	7.777755	-1.312895	-0.321062
56	6	0	7.935226	1.072985	-0.688069
57	1	0	6.228822	2.104188	-0.448579
58	6	0	8.407097	-2.581636	-0.265044
59	6	0	8.569630	-0.172594	-0.648369
60	1	0	8.464663	1.993149	-0.906640
61	6	0	9.959106	-0.308013	-0.909382
62	6	0	10.534260	-1.548292	-0.847970
63	1	0	11.593056	-1.669396	-1.045764
64	6	0	9.750349	-2.687822	-0.523295
65	1	0	7.814662	-3.455669	-0.017025
66	1	0	10.228864	-3.660446	-0.478790
67	1	0	10.542017	0.573279	-1.154940
68	1	0	5.779233	-1.989545	0.173193
69	6	0	6.399090	-1.133786	-0.070247
70	7	0	6.636396	1.173914	-0.440916

cis-**1H$^+$ (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.962125	4.152686	-0.912785
2	6	0	0.584871	4.144508	-0.690017
3	6	0	2.777282	3.164841	-0.366523
4	6	0	0.011634	3.161246	0.108269
5	1	0	-0.030244	4.914348	-1.138340
6	6	0	2.201030	2.188097	0.472118
7	8	0	-1.302571	3.064964	0.395633
8	6	0	0.838387	2.174396	0.707133
9	1	0	2.841677	1.461510	0.956958
10	6	0	-2.171820	4.039448	-0.167767
11	8	0	0.194991	1.283164	1.498126
12	6	0	-3.578011	3.701637	0.258672
13	1	0	-2.101078	4.018939	-1.262102
14	1	0	-1.901433	5.040359	0.190142
15	6	0	0.978567	0.264450	2.101638
16	8	0	-3.959747	2.499769	-0.368736
17	1	0	-3.622262	3.601870	1.353231
18	1	0	-4.244587	4.526206	-0.035951
19	6	0	0.046652	-0.634843	2.874309
20	1	0	1.503978	-0.315109	1.330981
21	1	0	1.718523	0.704728	2.781838
22	6	0	-5.278049	2.123983	-0.039623
23	1	0	-0.572672	-0.029367	3.552459
24	1	0	0.644424	-1.327587	3.485595
25	8	0	-0.758506	-1.341385	1.959677

26	1	0	-5.383935	1.988642	1.046899
27	1	0	-5.994114	2.896246	-0.358825
28	6	0	-5.602927	0.832246	-0.747465
29	6	0	-1.665919	-2.203316	2.608801
30	1	0	-6.668291	0.599813	-0.621872
31	1	0	-5.387430	0.931233	-1.819270
32	8	0	-4.801868	-0.187084	-0.174806
33	1	0	-1.129023	-2.942363	3.222547
34	1	0	-2.337218	-1.634178	3.268733
35	6	0	-2.473793	-2.928917	1.562060
36	6	0	-4.939117	-1.444005	-0.673660
37	1	0	-3.077110	-3.713581	2.036400
38	1	0	-1.799455	-3.395324	0.832133
39	8	0	-3.309013	-1.977579	0.924688
40	6	0	-5.803458	-1.804923	-1.698797
41	6	0	-4.121098	-2.427327	-0.068729
42	6	0	-5.866099	-3.135123	-2.132281
43	1	0	-6.434335	-1.060053	-2.168497
44	6	0	-4.192636	-3.743754	-0.504815
45	6	0	-5.067574	-4.096948	-1.539459
46	1	0	-6.545437	-3.400514	-2.935041
47	1	0	-3.572435	-4.505213	-0.047902
48	1	0	-5.110712	-5.129406	-1.868936
49	1	0	2.396865	4.928535	-1.534972
50	6	0	4.215078	3.202215	-0.638922
51	1	0	4.630676	4.199706	-0.768377
52	6	0	5.101458	2.189496	-0.720066
53	1	0	6.154890	2.442277	-0.807427
54	6	0	4.812916	0.760764	-0.763768
55	6	0	3.668994	0.185596	-1.366609
56	6	0	5.687565	-1.439431	-0.326507
57	6	0	3.543358	-1.175937	-1.434262
58	1	0	2.920922	0.844268	-1.786732
59	6	0	6.728282	-2.222231	0.204451
60	6	0	4.545821	-2.033306	-0.908347
61	1	0	2.672861	-1.617649	-1.909634
62	6	0	4.465697	-3.444687	-0.953657
63	6	0	5.483100	-4.208006	-0.435003
64	1	0	5.423119	-5.289698	-0.468579
65	6	0	6.615135	-3.591971	0.145699
66	1	0	7.595018	-1.746177	0.650707
67	1	0	7.408790	-4.209364	0.551511
68	1	0	3.591849	-3.904381	-1.403101
69	7	0	5.753865	-0.066867	-0.293608
70	1	0	6.580129	0.349251	0.129507

***cis*-1H$^+$_b (S$_0$):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.641711	0.709852	-1.152777
2	6	0	3.990935	1.908705	-0.843011
3	6	0	4.334719	-0.450869	-0.452564
4	6	0	3.023998	1.950994	0.154490
5	1	0	4.232145	2.803305	-1.403915
6	6	0	3.437644	-0.384173	0.630170
7	8	0	2.274282	3.031771	0.465690
8	6	0	2.773594	0.792383	0.933213
9	1	0	3.248588	-1.285299	1.201060
10	6	0	2.219237	4.109239	-0.463409
11	8	0	1.849690	0.927314	1.914567
12	6	0	0.848921	4.735065	-0.362877
13	1	0	2.348717	3.737917	-1.485103
14	1	0	3.006194	4.838897	-0.242686
15	6	0	1.626814	-0.195512	2.757463
16	8	0	-0.075155	3.802015	-0.876685
17	1	0	0.613262	4.988531	0.680752
18	1	0	0.837856	5.663365	-0.953358
19	6	0	0.410028	0.088233	3.603373
20	1	0	1.418351	-1.091475	2.159457
21	1	0	2.511347	-0.377816	3.379932
22	6	0	-1.376676	4.327423	-1.003235
23	1	0	0.466416	1.101475	4.027045
24	1	0	0.374106	-0.630808	4.435391
25	8	0	-0.717588	-0.057356	2.771859
26	1	0	-1.763938	4.660567	-0.029301
27	1	0	-1.381695	5.189506	-1.686937
28	6	0	-2.268506	3.247778	-1.566065
29	6	0	-1.940674	0.123508	3.447248
30	1	0	-3.232603	3.673484	-1.872295
31	1	0	-1.784480	2.800649	-2.443788
32	8	0	-2.463503	2.273936	-0.552711
33	1	0	-2.004628	-0.533162	4.327628
34	1	0	-2.053069	1.164048	3.785421
35	6	0	-3.039956	-0.238037	2.478248
36	6	0	-3.287127	1.231802	-0.836982
37	1	0	-4.016841	-0.237193	2.977799
38	1	0	-2.844647	-1.240186	2.075751
39	8	0	-3.007869	0.720502	1.432447
40	6	0	-3.819551	0.953305	-2.090183
41	6	0	-3.599112	0.389826	0.256753
42	6	0	-4.667369	-0.147025	-2.267803
43	1	0	-3.581710	1.585596	-2.936994
44	6	0	-4.463449	-0.682325	0.075839
45	6	0	-4.994361	-0.954574	-1.191290
46	1	0	-5.072190	-0.351142	-3.253042
47	1	0	-4.731581	-1.310068	0.917843
48	1	0	-5.665629	-1.797511	-1.317445
49	1	0	5.354257	0.682235	-1.970869
50	6	0	4.834330	-1.771937	-0.889117
51	1	0	5.902138	-1.884422	-1.061624
52	6	0	4.048206	-2.842979	-1.086493
53	1	0	4.493241	-3.804326	-1.322744
54	6	0	2.575864	-2.839394	-1.025927
55	6	0	0.402850	-3.784169	-0.492529
56	6	0	0.590498	-1.589454	-1.495876
57	1	0	2.468581	-0.979699	-1.894246
58	6	0	-0.409012	-4.819835	0.028716

59	6	0	-0.228413	-2.599557	-0.973610
60	1	0	0.193838	-0.665376	-1.901167
61	6	0	-1.640372	-2.459299	-0.928136
62	6	0	-2.394389	-3.480446	-0.412207
63	1	0	-3.473854	-3.386122	-0.369227
64	6	0	-1.772960	-4.663299	0.065190
65	1	0	0.058881	-5.726266	0.397665
66	1	0	-2.392618	-5.458081	0.466712
67	1	0	-2.104703	-1.549113	-1.299707
68	1	0	2.316996	-4.759793	-0.166879
69	6	0	1.817515	-3.872839	-0.541193
70	7	0	1.904403	-1.737357	-1.513570

trans-**1Ca**$^{++}$ **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.941409	2.821847	0.673082
2	6	0	-0.587365	3.099121	0.469123
3	6	0	-2.509533	1.618007	0.258871
4	6	0	0.208341	2.158424	-0.161525
5	1	0	-0.175106	4.043500	0.803037
6	6	0	-1.682348	0.662241	-0.363165
7	8	0	1.542651	2.301811	-0.444765
8	6	0	-0.344684	0.933588	-0.569252
9	1	0	-2.095123	-0.287136	-0.679116
10	6	0	2.116721	3.596297	-0.250272
11	8	0	0.547216	0.078457	-1.166910
12	6	0	3.463398	3.564994	-0.922004
13	1	0	2.217656	3.793837	0.822070
14	1	0	1.483417	4.360121	-0.710647
15	6	0	0.009037	-1.116550	-1.737396
16	8	0	4.173510	2.461271	-0.369103
17	1	0	3.360390	3.440715	-2.006767
18	1	0	3.995432	4.499512	-0.715147
19	6	0	1.140330	-1.793804	-2.462027
20	1	0	-0.374452	-1.761290	-0.939462
21	1	0	-0.796927	-0.868877	-2.434710
22	6	0	5.568940	2.469818	-0.659540
23	1	0	1.489569	-1.191137	-3.309391
24	1	0	0.804119	-2.768816	-2.829406
25	8	0	2.189306	-1.957235	-1.513186
26	1	0	5.741339	2.116325	-1.683262
27	1	0	5.972700	3.481893	-0.556151
28	6	0	6.223505	1.565796	0.350313
29	6	0	3.185858	-2.888314	-1.921319
30	1	0	7.288608	1.449488	0.128215
31	1	0	6.095735	1.966031	1.361580
32	8	0	5.560431	0.305057	0.247552
33	1	0	2.718630	-3.807515	-2.290032
34	1	0	3.803861	-2.454718	-2.717200
35	6	0	4.011428	-3.196307	-0.701662
36	6	0	6.061818	-0.727965	1.001389
37	1	0	4.861159	-3.831529	-0.967969
38	1	0	3.403830	-3.688462	0.064856
39	8	0	4.477879	-1.938180	-0.209456
40	6	0	7.073607	-0.617001	1.941320
41	6	0	5.458916	-1.968705	0.752267
42	6	0	7.484031	-1.758312	2.638324
43	1	0	7.547018	0.337034	2.137829
44	6	0	5.863092	-3.097314	1.445997
45	6	0	6.885046	-2.984139	2.394486
46	1	0	8.275937	-1.671468	3.373434
47	1	0	5.397787	-4.058066	1.261952
48	1	0	7.202061	-3.867046	2.937699
49	1	0	-2.563144	3.565140	1.161561
50	6	0	-3.942870	1.389484	0.476245
51	1	0	-4.474685	2.174201	1.009344
52	6	0	-4.646303	0.322808	0.068527
53	1	0	-4.167978	-0.487042	-0.477589
54	6	0	-6.084527	0.147898	0.298703
55	6	0	-8.116165	-1.146851	0.057348
56	6	0	-8.025823	1.002733	1.183493
57	6	0	-8.850479	-2.278394	-0.383751
58	6	0	-8.795437	-0.117042	0.755802
59	1	0	-8.530563	1.805192	1.722175
60	6	0	-10.184918	-0.225398	1.002847
61	6	0	-10.873509	-1.329602	0.564796
62	1	0	-11.938481	-1.419270	0.750309
63	6	0	-10.197722	-2.362158	-0.132913
64	1	0	-8.332929	-3.069678	-0.917729
65	1	0	-10.757484	-3.228605	-0.470272
66	1	0	-10.691413	0.572575	1.538356
67	20	0	3.060983	0.200362	-0.464723
68	7	0	-6.743254	1.143211	0.975442
69	6	0	-6.726854	-0.981282	-0.161511
70	1	0	-6.170540	-1.747591	-0.693849

trans-**1Ca**$^{++}$_b **(S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.884896	2.938821	0.698742
2	6	0	-0.532305	3.189219	0.455712
3	6	0	-2.484187	1.741858	0.310987
4	6	0	0.228984	2.227097	-0.184750
5	1	0	-0.093617	4.128560	0.769503
6	6	0	-1.693875	0.765240	-0.325939
7	8	0	1.558954	2.340024	-0.495573
8	6	0	-0.357145	1.009257	-0.568514
9	1	0	-2.133413	-0.179399	-0.619192
10	6	0	2.167210	3.620176	-0.310832
11	8	0	0.504716	0.131857	-1.177124
12	6	0	3.511609	3.547034	-0.983329
13	1	0	2.275609	3.822163	0.759999
14	1	0	1.553639	4.397294	-0.775642

15	6	0	-0.066155	-1.061564	-1.719663
16	8	0	4.193021	2.431234	-0.419127
17	1	0	3.404370	3.414502	-2.066711
18	1	0	4.067548	4.469633	-0.786170
19	6	0	1.043982	-1.777543	-2.440472
20	1	0	-0.454715	-1.683000	-0.905877
21	1	0	-0.873850	-0.808344	-2.413018
22	6	0	5.587284	2.401811	-0.712824
23	1	0	1.404593	-1.195803	-3.297515
24	1	0	0.681101	-2.748393	-2.792912
25	8	0	2.092688	-1.955083	-1.493283
26	1	0	5.748581	2.035732	-1.733793
27	1	0	6.017298	3.403966	-0.618362
28	6	0	6.220668	1.490547	0.303240
29	6	0	3.055847	-2.929216	-1.881554
30	1	0	7.281861	1.345377	0.079808
31	1	0	6.105482	1.903026	1.311037
32	8	0	5.526424	0.245444	0.214836
33	1	0	2.556284	-3.840896	-2.225598
34	1	0	3.685054	-2.536171	-2.689606
35	6	0	3.874374	-3.234321	-0.656016
36	6	0	6.004316	-0.788571	0.983569
37	1	0	4.705684	-3.898275	-0.910228
38	1	0	3.254901	-3.693639	0.121188
39	8	0	4.376408	-1.979664	-0.189873
40	6	0	7.026781	-0.688677	1.913476
41	6	0	5.365671	-2.017075	0.763265
42	6	0	7.412147	-1.827556	2.628448
43	1	0	7.527807	0.255146	2.089348
44	6	0	5.744810	-3.143051	1.475527
45	6	0	6.777703	-3.040792	2.413044
46	1	0	8.212693	-1.748661	3.355056
47	1	0	5.251755	-4.093790	1.313337
48	1	0	7.075253	-3.921778	2.970132
49	1	0	-2.478016	3.697653	1.198791
50	6	0	-3.913629	1.537478	0.579700
51	1	0	-4.382299	2.336267	1.150600
52	6	0	-4.647844	0.491578	0.172659
53	1	0	-4.206219	-0.302338	-0.424384
54	6	0	-6.079827	0.280184	0.431224
55	6	0	-6.843551	1.150427	1.267457
56	6	0	-7.929774	-1.040487	0.017461
57	6	0	-8.171379	0.896112	1.456660
58	1	0	-6.372931	1.997543	1.751977
59	6	0	-8.488204	-2.175632	-0.627056
60	6	0	-8.768863	-0.225935	0.824601
61	1	0	-8.779081	1.538136	2.088229
62	6	0	-10.138103	-0.559296	0.968654
63	6	0	-10.652815	-1.662253	0.333146
64	1	0	-11.701853	-1.915419	0.444427
65	6	0	-9.818105	-2.476779	-0.471494
66	1	0	-7.833030	-2.786700	-1.239259
67	1	0	-10.239294	-3.345622	-0.966843
68	1	0	-10.768780	0.071316	1.588774
69	7	0	-6.605684	-0.776527	-0.164173
70	20	0	3.021266	0.188929	-0.479376

***cis*-1Ca^{++} (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.138072	3.751696	1.177261
2	6	0	-0.912042	3.770368	0.512339
3	6	0	-2.862581	2.568378	1.341287
4	6	0	-0.395088	2.584536	0.014292
5	1	0	-0.379109	4.705420	0.391565
6	6	0	-2.307353	1.366968	0.866375
7	8	0	0.787484	2.455912	-0.666857
8	6	0	-1.093923	1.386151	0.204953
9	1	0	-2.843679	0.442596	1.034589
10	6	0	1.437770	3.660351	-1.079194
11	8	0	-0.472131	0.274457	-0.311195
12	6	0	2.541322	3.243487	-2.015103
13	1	0	1.847518	4.172928	-0.202665
14	1	0	0.726622	4.313103	-1.594027
15	6	0	-1.212702	-0.945300	-0.268034
16	8	0	3.327459	2.287774	-1.310026
17	1	0	2.138133	2.797296	-2.931958
18	1	0	3.147590	4.116678	-2.276340
19	6	0	-0.428844	-1.950942	-1.067005
20	1	0	-1.311230	-1.272416	0.773369
21	1	0	-2.207123	-0.798672	-0.702767
22	6	0	4.621225	2.068057	-1.863089
23	1	0	-0.385176	-1.671718	-2.126690
24	1	0	-0.900003	-2.935561	-0.973963
25	8	0	0.882088	-1.974445	-0.511002
26	1	0	4.548511	1.431707	-2.752991
27	1	0	5.083071	3.021402	-2.139475
28	6	0	5.439259	1.410407	-0.783232
29	6	0	1.655902	-3.105393	-0.899669
30	1	0	6.415088	1.106539	-1.173808
31	1	0	5.572941	2.089862	0.065085
32	8	0	4.701127	0.261085	-0.362613
33	1	0	1.054545	-4.017848	-0.833922
34	1	0	2.011327	-2.982199	-1.930094
35	6	0	2.806540	-3.191616	0.066857
36	6	0	5.335410	-0.609915	0.489586
37	1	0	3.499456	-3.982777	-0.235242
38	1	0	2.443851	-3.382360	1.082408
39	8	0	3.462835	-1.923371	0.024623
40	6	0	6.549038	-0.372663	1.114542
41	6	0	4.651419	-1.814595	0.704981
42	6	0	7.084097	-1.349358	1.960717
43	1	0	7.083371	0.555695	0.955154
44	6	0	5.180626	-2.779376	1.547105
45	6	0	6.406907	-2.539111	2.175414
46	1	0	8.034487	-1.163921	2.447979
47	1	0	4.658114	-3.711636	1.722041

48	1	0	6.820703	-3.294540	2.833548
49	1	0	-2.541585	4.684348	1.558387
50	6	0	-4.177182	2.665451	1.998722
51	1	0	-4.269473	3.549156	2.628312
52	6	0	-5.303111	1.940633	1.876807
53	1	0	-6.170963	2.333506	2.404186
54	6	0	-5.622347	0.756120	1.046644
55	6	0	-5.169519	-1.364451	0.251412
56	6	0	-7.192498	-0.249317	-0.486936
57	6	0	-4.317329	-2.499973	0.247871
58	6	0	-6.344325	-1.385466	-0.545787
59	1	0	-8.106253	-0.232750	-1.074190
60	6	0	-6.625397	-2.520541	-1.346553
61	6	0	-5.772718	-3.596154	-1.348722
62	1	0	-5.989952	-4.462352	-1.964481
63	6	0	-4.610307	-3.586185	-0.539013
64	1	0	-3.442242	-2.485130	0.890575
65	1	0	-3.952454	-4.449167	-0.538253
66	1	0	-7.524871	-2.521899	-1.955366
67	20	0	2.121134	0.234213	-0.493207
68	7	0	-4.825628	-0.294357	1.027267
69	6	0	-6.847414	0.802188	0.312358
70	1	0	-7.475972	1.683041	0.385735

***cis*-1Ca^{++}_b (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.179208	4.016583	0.969999
2	6	0	-0.810497	4.010677	0.702280
3	6	0	-3.008953	2.967034	0.565392
4	6	0	-0.264987	2.944660	0.005861
5	1	0	-0.188597	4.831239	1.039047
6	6	0	-2.445026	1.904844	-0.164590
7	8	0	1.057771	2.805778	-0.324282
8	6	0	-1.088647	1.897846	-0.428907
9	1	0	-3.096402	1.117907	-0.521212
10	6	0	1.900411	3.951654	-0.181598
11	8	0	-0.435547	0.908734	-1.127186
12	6	0	3.174492	3.621869	-0.914246
13	1	0	2.095585	4.133259	0.880167
14	1	0	1.418989	4.826947	-0.627369
15	6	0	-1.252046	-0.132267	-1.661586
16	8	0	3.648687	2.395258	-0.367591
17	1	0	2.993453	3.509687	-1.990219
18	1	0	3.908880	4.417815	-0.753340
19	6	0	-0.337929	-1.045077	-2.432763
20	1	0	-1.741484	-0.672810	-0.842855
21	1	0	-2.011999	0.294167	-2.324760
22	6	0	5.000098	2.095628	-0.703056
23	1	0	0.092284	-0.537058	-3.304363
24	1	0	-0.904248	-1.919944	-2.770524
25	8	0	0.697072	-1.442922	-1.539414
26	1	0	5.061200	1.738913	-1.738398
27	1	0	5.625843	2.987283	-0.592871
28	6	0	5.456738	1.040019	0.268230
29	6	0	1.433534	-2.572874	-1.995799
30	1	0	6.460218	0.688566	0.009467
31	1	0	5.452314	1.433141	1.290309
32	8	0	4.520602	-0.034304	0.165342
33	1	0	0.750305	-3.352550	-2.348369
34	1	0	2.099660	-2.280267	-2.816574
35	6	0	2.215029	-3.086473	-0.817366
36	6	0	4.807251	-1.178036	0.869319
37	1	0	2.886754	-3.891564	-1.130066
38	1	0	1.542936	-3.447551	-0.031876
39	8	0	2.972671	-1.979237	-0.327752
40	6	0	5.839675	-1.320062	1.782554
41	6	0	3.948754	-2.252757	0.599142
42	6	0	6.012684	-2.547466	2.431054
43	1	0	6.509037	-0.496158	1.996942
44	6	0	4.118484	-3.466326	1.245072
45	6	0	5.161378	-3.608497	2.166035
46	1	0	6.820111	-2.658537	3.145711
47	1	0	3.455578	-4.298988	1.044359
48	1	0	5.295526	-4.558752	2.670071
49	1	0	-2.601797	4.850775	1.520884
50	6	0	-4.426176	3.046072	0.954934
51	1	0	-4.722160	4.055674	1.235796
52	6	0	-5.383989	2.118405	1.134138
53	1	0	-6.315190	2.494218	1.554790
54	6	0	-5.391258	0.647896	0.967457
55	6	0	-6.046183	-0.106153	1.990185
56	6	0	-4.911219	-1.280002	-0.210577
57	6	0	-6.084732	-1.468119	1.903005
58	1	0	-6.490876	0.416016	2.830481
59	6	0	-4.358037	-1.882667	-1.370813
60	6	0	-5.503752	-2.109451	0.778202
61	1	0	-6.558706	-2.067058	2.675672
62	6	0	-5.504055	-3.515563	0.601372
63	6	0	-4.943927	-4.073880	-0.520775
64	1	0	-4.945101	-5.150508	-0.652890
65	6	0	-4.370671	-3.247435	-1.518176
66	1	0	-3.946138	-1.233308	-2.137230
67	1	0	-3.945648	-3.699905	-2.408201
68	1	0	-5.956427	-4.139111	1.367214
69	7	0	-4.858528	0.079432	-0.096541
70	20	0	2.036616	0.430273	-0.475541

***trans*-1H^{+}Ca^{++} (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.878279	2.926502	0.618058
2	6	0	-0.530037	3.189306	0.376398
3	6	0	-2.457087	1.714727	0.243065

4	6	0	0.245299	2.225594	-0.247470
5	1	0	-0.105149	4.138364	0.677649
6	6	0	-1.656474	0.735064	-0.379532
7	8	0	1.568507	2.354385	-0.550321
8	6	0	-0.323182	0.991595	-0.620224
9	1	0	-2.081239	-0.219844	-0.660981
10	6	0	2.170094	3.634899	-0.330596
11	8	0	0.550125	0.121394	-1.216262
12	6	0	3.543482	3.565472	-0.940305
13	1	0	2.231030	3.827440	0.745313
14	1	0	1.578062	4.414486	-0.818136
15	6	0	-0.004002	-1.083162	-1.755797
16	8	0	4.204128	2.456365	-0.339622
17	1	0	3.488525	3.429502	-2.027167
18	1	0	4.082917	4.492667	-0.720669
19	6	0	1.109094	-1.777766	-2.493126
20	1	0	-0.371319	-1.711933	-0.937882
21	1	0	-0.823123	-0.843035	-2.440188
22	6	0	5.614374	2.450358	-0.544006
23	1	0	1.448237	-1.186725	-3.352396
24	1	0	0.756355	-2.752823	-2.844309
25	8	0	2.172852	-1.942857	-1.561101
26	1	0	5.843942	2.113215	-1.562382
27	1	0	6.024187	3.454680	-0.397393
28	6	0	6.195962	1.518476	0.484325
29	6	0	3.158321	-2.886203	-1.972894
30	1	0	7.270274	1.392200	0.320277
31	1	0	6.015886	1.900616	1.494560
32	8	0	5.524913	0.268246	0.320052
33	1	0	2.679196	-3.796331	-2.348151
34	1	0	3.784284	-2.456104	-2.764142
35	6	0	3.973415	-3.213426	-0.750546
36	6	0	5.988319	-0.789367	1.065292
37	1	0	4.818048	-3.855165	-1.017445
38	1	0	3.354538	-3.706830	0.006134
39	8	0	4.449609	-1.966084	-0.239420
40	6	0	6.959033	-0.706960	2.050662
41	6	0	5.395202	-2.021454	0.756989
42	6	0	7.339897	-1.867184	2.732417
43	1	0	7.423993	0.239940	2.295520
44	6	0	5.771023	-3.169360	1.435829
45	6	0	6.752267	-3.084838	2.428824
46	1	0	8.100389	-1.800991	3.502099
47	1	0	5.314273	-4.124348	1.207004
48	1	0	7.046460	-3.983157	2.959370
49	1	0	-2.483772	3.683711	1.105091
50	6	0	-3.876650	1.510824	0.512304
51	1	0	-4.352869	2.323583	1.055149
52	6	0	-4.611443	0.446468	0.137454
53	1	0	-4.163818	-0.361097	-0.434494
54	6	0	-6.023507	0.299044	0.430891
55	6	0	-6.791316	1.172396	1.238498
56	6	0	-7.975966	-1.062947	0.056240
57	6	0	-8.122188	0.926132	1.438088
58	1	0	-6.315684	2.025346	1.702054
59	6	0	-8.534467	-2.200486	-0.553887
60	6	0	-8.759803	-0.199316	0.852102
61	1	0	-8.709947	1.594955	2.059188
62	6	0	-10.130291	-0.497533	1.029769
63	6	0	-10.674853	-1.608693	0.432796
64	1	0	-11.725340	-1.838998	0.567605
65	6	0	-9.871850	-2.459606	-0.360214
66	1	0	-7.916816	-2.853012	-1.161850
67	1	0	-10.316834	-3.332718	-0.824307
68	1	0	-10.734479	0.163616	1.641891
69	7	0	-6.645731	-0.759070	-0.106526
70	1	0	-6.095520	-1.387634	-0.686332
71	20	0	3.086402	0.196349	-0.556502

***trans*-1H^{+}Ca^{++}_b (S$_0$):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.913357	2.880996	-0.621382
2	6	0	0.556154	3.174621	-0.480647
3	6	0	2.458259	1.705265	-0.108893
4	6	0	-0.262498	2.279027	0.185984
5	1	0	0.161341	4.095326	-0.891092
6	6	0	1.617436	0.802244	0.571332
7	8	0	-1.603374	2.435186	0.398001
8	6	0	0.275666	1.090595	0.713481
9	1	0	2.019529	-0.113003	0.986912
10	6	0	-2.182410	3.684886	0.011390
11	8	0	-0.636167	0.296656	1.357591
12	6	0	-3.610327	3.653064	0.485199
13	1	0	-2.138395	3.784643	-1.077881
14	1	0	-1.641544	4.509592	0.484521
15	6	0	-0.126901	-0.827085	2.079923
16	8	0	-4.199643	2.481512	-0.072267
17	1	0	-3.666250	3.618172	1.579710
18	1	0	-4.130886	4.547208	0.127410
19	6	0	-1.284889	-1.390480	2.857981
20	1	0	0.263257	-1.568674	1.375128
21	1	0	0.666842	-0.504691	2.760528
22	6	0	-5.624263	2.492395	-0.062816
23	1	0	-1.642829	-0.676513	3.609386
24	1	0	-0.970267	-2.311573	3.359437
25	8	0	-2.314352	-1.669239	1.915585
26	1	0	-5.996269	2.303909	0.951289
27	1	0	-5.998204	3.461549	-0.408189
28	6	0	-6.072128	1.416828	-1.016093
29	6	0	-3.335687	-2.531849	2.409177
30	1	0	-7.159693	1.305007	-0.976175
31	1	0	-5.759772	1.650590	-2.039318
32	8	0	-5.439393	0.208959	-0.587826
33	1	0	-2.892615	-3.370825	2.955298
34	1	0	-4.004661	-1.978331	3.079075
35	6	0	-4.072797	-3.051498	1.203874

36	6	0	-5.848612	-0.958487	-1.187456
37	1	0	-4.939452	-3.644364	1.510814
38	1	0	-3.409331	-3.658940	0.579635
39	8	0	-4.501168	-1.903649	0.468618
40	6	0	-6.699891	-1.039250	-2.277415
41	6	0	-5.329918	-2.124008	-0.605314
42	6	0	-7.039213	-2.296732	-2.786844
43	1	0	-7.102028	-0.143659	-2.734540
44	6	0	-5.664044	-3.368782	-1.113413
45	6	0	-6.527071	-3.448585	-2.211185
46	1	0	-7.706824	-2.358959	-3.638559
47	1	0	-5.267543	-4.274194	-0.670676
48	1	0	-6.790058	-4.422895	-2.607027
49	1	0	2.552191	3.584806	-1.144782
50	6	0	3.888565	1.454979	-0.301676
51	1	0	4.408017	2.271222	-0.802000
52	6	0	4.554262	0.341829	0.046451
53	1	0	4.035622	-0.502025	0.489969
54	6	0	5.979827	0.112047	-0.152038
55	6	0	7.941180	-1.315710	-0.293871
56	6	0	8.109370	1.069683	-0.665853
57	1	0	6.402728	2.105751	-0.460572
58	6	0	8.565156	-2.585199	-0.223270
59	6	0	8.740212	-0.178330	-0.612184
60	1	0	8.644908	1.987988	-0.877425
61	6	0	10.132506	-0.317456	-0.851256
62	6	0	10.703505	-1.559616	-0.776923
63	1	0	11.764835	-1.683857	-0.958440
64	6	0	9.912623	-2.695601	-0.460403
65	1	0	7.966767	-3.456909	0.018417
66	1	0	10.387874	-3.669212	-0.405025
67	1	0	10.721534	0.561215	-1.091295
68	1	0	5.932334	-1.985152	0.171206
69	20	0	-3.108033	0.274601	0.493171
70	7	0	6.807325	1.174376	-0.442137
71	6	0	6.557739	-1.131667	-0.066165

***cis*-1H^{+}Ca^{++} (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.802578	-0.019180	0.796198
2	6	0	-1.814746	0.838589	0.314052
3	6	0	-2.641156	-1.402648	0.735423
4	6	0	-0.652147	0.306397	-0.223058
5	1	0	-1.961540	1.909435	0.374314
6	6	0	-1.440475	-1.933318	0.227899
7	8	0	0.385881	1.034314	-0.733485
8	6	0	-0.462532	-1.084873	-0.254575
9	1	0	-1.297590	-3.007575	0.214542
10	6	0	0.196868	2.449668	-0.837891
11	8	0	0.737358	-1.481671	-0.780298
12	6	0	1.407865	2.989385	-1.548870
13	1	0	0.116417	2.880841	0.165048
14	1	0	-0.710346	2.663347	-1.410589
15	6	0	0.912506	-2.877717	-1.040981
16	8	0	2.542816	2.566383	-0.799598
17	1	0	1.470411	2.607931	-2.575229
18	1	0	1.354917	4.082566	-1.574510
19	6	0	2.171891	-2.999226	-1.856690
20	1	0	1.009439	-3.416069	-0.092585
21	1	0	0.056955	-3.262401	-1.603930
22	6	0	3.733488	3.284130	-1.113234
23	1	0	2.057161	-2.521099	-2.836507
24	1	0	2.409243	-4.058485	-1.999811
25	8	0	3.204884	-2.357715	-1.115446
26	1	0	4.123013	2.958014	-2.084978
27	1	0	3.528014	4.358867	-1.149760
28	6	0	4.716131	2.998338	-0.009880
29	6	0	4.519839	-2.699543	-1.545455
30	1	0	5.688385	3.441998	-0.244426
31	1	0	4.350366	3.388784	0.945368
32	8	0	4.832703	1.576269	0.066768
33	1	0	4.593592	-3.777910	-1.718820
34	1	0	4.762124	-2.167965	-2.473173
35	6	0	5.452133	-2.307748	-0.430850
36	6	0	5.837404	1.074450	0.858799
37	1	0	6.492820	-2.451118	-0.736861
38	1	0	5.245131	-2.896350	0.469241
39	8	0	5.204570	-0.926634	-0.164848
40	6	0	6.612737	1.819393	1.732546
41	6	0	6.041926	-0.306946	0.731027
42	6	0	7.604943	1.178383	2.481480
43	1	0	6.457266	2.885691	1.840803
44	6	0	7.022557	-0.940873	1.476713
45	6	0	7.807610	-0.186518	2.354906
46	1	0	8.212890	1.762728	3.162630
47	1	0	7.186703	-2.007468	1.386533
48	1	0	8.576702	-0.683205	2.935298
49	1	0	-3.692191	0.407891	1.246001
50	6	0	-3.647673	-2.341631	1.249478
51	1	0	-3.243465	-3.243916	1.703685
52	6	0	-4.986907	-2.228840	1.266660
53	1	0	-5.553539	-2.989960	1.797046
54	6	0	-5.799520	-1.196841	0.621337
55	6	0	-7.846099	0.057573	0.756307
56	6	0	-6.397488	0.288424	-1.177209
57	1	0	-4.626583	-0.922120	-1.161430
58	6	0	-9.003819	0.370116	1.491513
59	6	0	-7.581542	0.663382	-0.491952
60	1	0	-6.195783	0.726287	-2.149990
61	6	0	-8.512475	1.600723	-0.999692
62	6	0	-9.641051	1.906570	-0.279708
63	1	0	-10.354249	2.625370	-0.666170
64	6	0	-9.884089	1.288249	0.968997
65	1	0	-9.184209	-0.106592	2.448959
66	1	0	-10.779792	1.542339	1.524511
67	1	0	-8.315674	2.066451	-1.959590

68	1	0	-7.133567	-1.275533	2.139940
69	20	0	2.811254	0.066054	-0.503024
70	7	0	-6.933583	-0.849023	1.237874
71	6	0	-5.523389	-0.618912	-0.637446

***cis*-1H^{+}Ca^{++}_b (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.978884	0.935182	1.180478
2	6	0	-1.887711	0.298554	1.772005
3	6	0	-2.793581	1.976331	0.271952
4	6	0	-0.602031	0.719327	1.464777
5	1	0	-2.056270	-0.502913	2.479883
6	6	0	-1.487091	2.412557	-0.015511
7	8	0	0.547121	0.198151	1.982965
8	6	0	-0.405460	1.784976	0.571177
9	1	0	-1.343178	3.237229	-0.703922
10	6	0	0.418363	-0.823284	2.975671
11	8	0	0.905157	2.129066	0.372501
12	6	0	1.807871	-1.099908	3.482886
13	1	0	-0.016205	-1.719545	2.520674
14	1	0	-0.218556	-0.474186	3.793684
15	6	0	1.152881	3.361776	-0.312215
16	8	0	2.607729	-1.427393	2.350157
17	1	0	2.224088	-0.224604	3.996388
18	1	0	1.775737	-1.943203	4.180459
19	6	0	2.612433	3.669912	-0.121525
20	1	0	0.914758	3.242834	-1.374235
21	1	0	0.540788	4.157831	0.121179
22	6	0	3.839871	-2.057779	2.690547
23	1	0	2.844026	3.849162	0.935728
24	1	0	2.875216	4.559174	-0.703505
25	8	0	3.336993	2.539103	-0.595115
26	1	0	4.535867	-1.320272	3.107796
27	1	0	3.669032	-2.848868	3.427735
28	6	0	4.382344	-2.662226	1.423645
29	6	0	4.729453	2.791538	-0.767009
30	1	0	5.376992	-3.082038	1.599251
31	1	0	3.710687	-3.441180	1.048222
32	8	0	4.461331	-1.599538	0.470893
33	1	0	4.879273	3.744159	-1.285528
34	1	0	5.228219	2.833064	0.209034
35	6	0	5.271803	1.670491	-1.612139
36	6	0	5.164442	-1.847736	-0.683971
37	1	0	6.358910	1.753447	-1.703825
38	1	0	4.813160	1.681242	-2.606591
39	8	0	4.926863	0.458746	-0.939550
40	6	0	5.604402	-3.094867	-1.096680
41	6	0	5.424353	-0.710221	-1.460808
42	6	0	6.315989	-3.204246	-2.295854
43	1	0	5.400597	-3.978921	-0.504917
44	6	0	6.128495	-0.820286	-2.649001
45	6	0	6.576034	-2.079389	-3.062326
46	1	0	6.661333	-4.179536	-2.619122
47	1	0	6.337393	0.053213	-3.254098
48	1	0	7.128159	-2.164726	-3.991292
49	1	0	-3.980231	0.627957	1.461645
50	6	0	-3.908633	2.706876	-0.346243
51	1	0	-3.724917	3.768397	-0.499432
52	6	0	-5.124970	2.270426	-0.716653
53	1	0	-5.844500	3.010417	-1.057167
54	6	0	-5.605833	0.890428	-0.757353
55	6	0	-4.818905	-0.231579	-1.099247
56	6	0	-7.555540	-0.509929	-0.618563
57	6	0	-5.400092	-1.469434	-1.189361
58	1	0	-3.767410	-0.082048	-1.305068
59	6	0	-8.936832	-0.605364	-0.371669
60	6	0	-6.785387	-1.649162	-0.943013
61	1	0	-4.801569	-2.331647	-1.466235
62	6	0	-7.434179	-2.904272	-1.019767
63	6	0	-8.782790	-2.996100	-0.777806
64	1	0	-9.281552	-3.956675	-0.836116
65	6	0	-9.533026	-1.841968	-0.452267
66	1	0	-9.506724	0.282803	-0.120710
67	1	0	-10.596867	-1.933208	-0.263712
68	1	0	-6.847899	-3.781491	-1.271887
69	7	0	-6.913469	0.702252	-0.550675
70	1	0	-7.478364	1.516221	-0.318318
71	20	0	2.798799	0.353167	0.546949

***cis*-1H^{+}Ca^{++}_c (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.808042	-0.156155	1.190361
2	6	0	-1.844249	0.743003	0.733423
3	6	0	-2.651197	-1.529200	1.005195
4	6	0	-0.714704	0.261502	0.091900
5	1	0	-1.982355	1.804853	0.893575
6	6	0	-1.486083	-2.011184	0.380822
7	8	0	0.294825	1.035347	-0.408075
8	6	0	-0.533553	-1.120802	-0.080174
9	1	0	-1.352824	-3.079729	0.258742
10	6	0	0.065821	2.447260	-0.479007
11	8	0	0.624257	-1.466350	-0.725208
12	6	0	1.203163	3.017479	-1.284451
13	1	0	0.062084	2.866606	0.532169
14	1	0	-0.891412	2.644537	-0.970263
15	6	0	0.799268	-2.844336	-1.069596
16	8	0	2.399380	2.588710	-0.643505
17	1	0	1.178443	2.659020	-2.320280
18	1	0	1.138439	4.110257	-1.280064
19	6	0	2.009481	-2.910475	-1.963749
20	1	0	0.956580	-3.430163	-0.157937
21	1	0	-0.083042	-3.211516	-1.602075

22	6	0	3.556573	3.343937	-0.990232
23	1	0	1.831690	-2.387384	-2.910741
24	1	0	2.247017	-3.958743	-2.172379
25	8	0	3.079561	-2.294222	-1.255325
26	1	0	3.893901	3.076588	-1.998624
27	1	0	3.333927	4.415351	-0.957356
28	6	0	4.603480	3.015944	0.041500
29	6	0	4.370699	-2.567643	-1.794634
30	1	0	5.559318	3.476215	-0.226156
31	1	0	4.289553	3.359537	1.032654
32	8	0	4.730174	1.592286	0.046973
33	1	0	4.454157	-3.625841	-2.062180
34	1	0	4.543187	-1.955317	-2.687858
35	6	0	5.361122	-2.243295	-0.707679
36	6	0	5.773875	1.059553	0.764183
37	1	0	6.385116	-2.328427	-1.083332
38	1	0	5.222473	-2.910261	0.149680
39	8	0	5.093865	-0.896175	-0.313960
40	6	0	6.589090	1.767163	1.632439
41	6	0	5.976118	-0.313269	0.563212
42	6	0	7.618954	1.096943	2.301072
43	1	0	6.436339	2.826562	1.797606
44	6	0	6.995897	-0.976173	1.226822
45	6	0	7.820620	-0.259403	2.099885
46	1	0	8.257150	1.652068	2.979026
47	1	0	7.158232	-2.036423	1.075814
48	1	0	8.619234	-0.777737	2.618111
49	1	0	-3.677046	0.224951	1.717485
50	6	0	-3.650023	-2.497803	1.498963
51	1	0	-3.244223	-3.400950	1.949190
52	6	0	-4.986988	-2.383205	1.482164
53	1	0	-5.578230	-3.142353	1.984381
54	6	0	-5.785614	-1.335360	0.833294
55	6	0	-7.723428	0.113798	0.637449
56	6	0	-5.979825	0.132395	-1.042444
57	6	0	-8.957125	0.613128	1.119355
58	6	0	-7.197817	0.645079	-0.575889
59	1	0	-5.520714	0.464141	-1.966547
60	6	0	-7.898816	1.654293	-1.285945
61	6	0	-9.088622	2.117488	-0.790417
62	1	0	-9.634796	2.890170	-1.319022
63	6	0	-9.616377	1.591939	0.417428
64	1	0	-9.365594	0.215720	2.042091
65	1	0	-10.560345	1.974750	0.790125
66	1	0	-7.482202	2.044129	-2.208690
67	1	0	-7.369601	-1.306229	2.241508
68	20	0	2.712304	0.082111	-0.507029
69	7	0	-5.340663	-0.802380	-0.357314
70	6	0	-6.988328	-0.889321	1.315882
71	1	0	-4.462608	-1.156365	-0.730861

***cis*-1H^{+}Ca^{++}_d (S_0):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.041111	-1.312885	1.141494
2	6	0	1.965336	-0.710391	1.794846
3	6	0	2.832967	-2.240636	0.121359
4	6	0	0.671949	-1.051700	1.431983
5	1	0	2.152015	0.005819	2.585066
6	6	0	1.516440	-2.600648	-0.221912
7	8	0	-0.465434	-0.537533	1.987318
8	6	0	0.449911	-2.007647	0.427073
9	1	0	1.350954	-3.338089	-0.998951
10	6	0	-0.308291	0.317702	3.123544
11	8	0	-0.870781	-2.274424	0.181032
12	6	0	-1.697209	0.617250	3.619570
13	1	0	0.198309	1.238524	2.816989
14	1	0	0.274200	-0.191128	3.896881
15	6	0	-1.173181	-3.427645	-0.611271
16	8	0	-2.418799	1.137309	2.506990
17	1	0	-2.190131	-0.285584	3.999993
18	1	0	-1.643204	1.361874	4.420266
19	6	0	-2.646620	-3.681562	-0.434444
20	1	0	-0.934167	-3.222269	-1.659653
21	1	0	-0.595173	-4.285987	-0.257052
22	6	0	-3.603598	1.841317	2.866988
23	1	0	-2.878334	-3.957102	0.601358
24	1	0	-2.960139	-4.491648	-1.101151
25	8	0	-3.312641	-2.471479	-0.780548
26	1	0	-4.377049	1.133485	3.189553
27	1	0	-3.395181	2.543122	3.681003
28	6	0	-4.041209	2.602640	1.643980
29	6	0	-4.715749	-2.624340	-0.977443
30	1	0	-5.011102	3.076426	1.819940
31	1	0	-3.300631	3.360900	1.369477
32	8	0	-4.152173	1.639833	0.592619
33	1	0	-4.919587	-3.518076	-1.576074
34	1	0	-5.223893	-2.716737	-0.009879
35	6	0	-5.180859	-1.404377	-1.726367
36	6	0	-4.835657	2.019118	-0.537529
37	1	0	-6.270236	-1.411608	-1.828575
38	1	0	-4.715541	-1.360142	-2.716842
39	8	0	-4.766971	-0.275802	-0.954814
40	6	0	-5.184311	3.320791	-0.857228
41	6	0	-5.176353	0.960781	-1.391467
42	6	0	-5.887376	3.566580	-2.040839
43	1	0	-4.917073	4.142362	-0.203561
44	6	0	-5.871049	1.206349	-2.565130
45	6	0	-6.227537	2.520739	-2.884518
46	1	0	-6.162120	4.584799	-2.291462
47	1	0	-6.141357	0.396084	-3.230798
48	1	0	-6.772320	2.712189	-3.801927
49	1	0	4.050906	-1.067671	1.454894
50	6	0	3.953180	-2.911296	-0.566787
51	1	0	3.797681	-3.965130	-0.786350
52	6	0	5.139024	-2.396058	-0.927024
53	1	0	5.888975	-3.067909	-1.332268

54	6	0	5.570647	-0.994664	-0.861061
55	6	0	7.237557	0.754029	-0.617854
56	6	0	4.920174	1.295826	-1.062038
57	1	0	3.685432	-0.282519	-1.272397
58	6	0	8.567228	1.181376	-0.389623
59	6	0	6.227093	1.738796	-0.819930
60	1	0	4.098096	1.975612	-1.253016
61	6	0	6.549735	3.120559	-0.792438
62	6	0	7.846347	3.500234	-0.567874
63	1	0	8.109754	4.551410	-0.543619
64	6	0	8.856126	2.523519	-0.366517
65	1	0	9.342707	0.439164	-0.234935
66	1	0	9.875852	2.849364	-0.191097
67	1	0	5.766165	3.854229	-0.949582
68	1	0	7.623716	-1.378716	-0.497632
69	20	0	-2.620899	-0.404971	0.519635
70	6	0	6.870741	-0.613678	-0.651250
71	7	0	4.643635	0.001524	-1.079121

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acetonitrile (S_1):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.218976
2	1	0	0.000000	1.023729	-1.618398
3	1	0	-0.886576	-0.511865	-1.618398
4	1	0	0.886576	-0.511865	-1.618398
5	6	0	0.000000	0.000000	0.224616
6	7	0	0.000000	0.000000	1.545907

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trans-**1** **(S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.039316	2.500310	0.143433
2	6	0	-0.738839	2.902182	-0.056504
3	6	0	-2.483690	1.188557	-0.213505
4	6	0	0.193552	2.014806	-0.623050
5	1	0	-0.437648	3.903621	0.223973
6	6	0	-1.520798	0.296350	-0.789322
7	8	0	1.474914	2.303460	-0.862956
8	6	0	-0.220112	0.693751	-0.989480
9	1	0	-1.825424	-0.703095	-1.068739
10	6	0	1.947932	3.612982	-0.548926
11	8	0	0.756786	-0.066890	-1.527938
12	6	0	3.408679	3.671042	-0.916195
13	1	0	1.822228	3.805364	0.522768
14	1	0	1.384287	4.358671	-1.121154
15	6	0	0.408627	-1.380606	-1.944497
16	8	0	4.126221	2.841578	-0.033634
17	1	0	3.543579	3.344726	-1.958049
18	1	0	3.749043	4.714532	-0.838918
19	6	0	1.648485	-2.029173	-2.506382
20	1	0	0.038882	-1.960358	-1.089783
21	1	0	-0.373379	-1.337425	-2.712691
22	6	0	5.512129	2.865929	-0.294772
23	1	0	2.088718	-1.382377	-3.279678
24	1	0	1.365866	-2.981922	-2.979101
25	8	0	2.560014	-2.243089	-1.454136
26	1	0	5.718054	2.539740	-1.324937
27	1	0	5.912806	3.883216	-0.171646
28	6	0	6.204275	1.944162	0.677604
29	6	0	3.742999	-2.869301	-1.896236
30	1	0	7.291817	2.060291	0.585065
31	1	0	5.909028	2.195523	1.704508
32	8	0	5.817690	0.618074	0.362336
33	1	0	3.522175	-3.856215	-2.330150
34	1	0	4.239698	-2.261221	-2.666843
35	6	0	4.665821	-3.046406	-0.716563
36	6	0	6.337112	-0.382039	1.122690
37	1	0	5.527897	-3.658950	-1.010078
38	1	0	4.134168	-3.553012	0.099076
39	8	0	5.088948	-1.758086	-0.304624
40	6	0	7.205335	-0.203570	2.191357
41	6	0	5.935796	-1.688248	0.756294
42	6	0	7.680078	-1.310948	2.905133
43	1	0	7.519997	0.792128	2.479302
44	6	0	6.412606	-2.779393	1.470274
45	6	0	7.286600	-2.588387	2.547717
46	1	0	8.358150	-1.155040	3.737164
47	1	0	6.112177	-3.783934	1.198368
48	1	0	7.649559	-3.451180	3.095745
49	1	0	-2.753973	3.190748	0.579961
50	6	0	-3.826036	0.839077	0.008866
51	1	0	-4.476697	1.584527	0.456116
52	6	0	-4.418745	-0.401425	-0.307046
53	1	0	-3.825332	-1.187258	-0.765926
54	6	0	-5.771690	-0.686068	-0.065573
55	6	0	-6.306405	-1.970196	-0.431212
56	6	0	-7.844549	-0.000812	0.733121
57	6	0	-7.617418	-2.255183	-0.211267
58	1	0	-5.641512	-2.700036	-0.884346
59	6	0	-8.674226	0.995925	1.338817
60	6	0	-8.457882	-1.261057	0.391219
61	1	0	-8.041027	-3.218309	-0.481252
62	6	0	-9.819907	-1.468164	0.653082
63	6	0	-10.593352	-0.479078	1.239965
64	1	0	-11.645780	-0.653706	1.437181
65	6	0	-10.006329	0.758307	1.582065
66	1	0	-8.209669	1.942943	1.595517
67	1	0	-10.616213	1.529986	2.042391
68	1	0	-10.261779	-2.425171	0.386678
69	7	0	-6.554384	0.280407	0.514350

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trans-**1**_b **(S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.707443	3.114840	0.509176
2	6	0	-0.376679	3.352264	0.262416
3	6	0	-2.342930	1.893528	0.108806
4	6	0	0.403073	2.383196	-0.397003
5	1	0	0.069853	4.287207	0.577172
6	6	0	-1.532841	0.916524	-0.560584
7	8	0	1.698023	2.516017	-0.689542
8	6	0	-0.200556	1.150014	-0.805429
9	1	0	-1.978436	-0.018261	-0.871141
10	6	0	2.351949	3.736637	-0.342355
11	8	0	0.641665	0.296292	-1.425016
12	6	0	3.789616	3.626379	-0.781001
13	1	0	2.301105	3.887841	0.741935
14	1	0	1.864010	4.576150	-0.850422
15	6	0	0.105314	-0.944464	-1.865763
16	8	0	4.430472	2.664744	0.022853
17	1	0	3.835061	3.344006	-1.843005
18	1	0	4.265474	4.612225	-0.669460
19	6	0	1.221248	-1.728925	-2.507996
20	1	0	-0.299807	-1.502318	-1.012416
21	1	0	-0.697460	-0.771144	-2.592882
22	6	0	5.794686	2.523060	-0.306259
23	1	0	1.706769	-1.119978	-3.284975
24	1	0	0.792969	-2.620089	-2.991349
25	8	0	2.144659	-2.095827	-1.509914
26	1	0	5.910979	2.222783	-1.358028
27	1	0	6.329337	3.473625	-0.160686
28	6	0	6.400888	1.475037	0.592974
29	6	0	3.207750	-2.864063	-2.026112
30	1	0	7.489952	1.456437	0.457474
31	1	0	6.179765	1.712638	1.641433
32	8	0	5.835262	0.224493	0.240427
33	1	0	2.832000	-3.795596	-2.475538
34	1	0	3.750605	-2.305004	-2.802518
35	6	0	4.146283	-3.207854	-0.896524
36	6	0	6.246089	-0.865183	0.941827
37	1	0	4.900573	-3.923991	-1.247197
38	1	0	3.584119	-3.663640	-0.071148
39	8	0	4.763457	-2.005929	-0.468875
40	6	0	7.173693	-0.846304	1.974843
41	6	0	5.657143	-2.090964	0.551732
42	6	0	7.524007	-2.034378	2.628321
43	1	0	7.630600	0.086639	2.282050
44	6	0	6.012228	-3.263363	1.205548
45	6	0	6.948124	-3.233096	2.246871
46	1	0	8.249020	-2.002335	3.434439
47	1	0	5.567176	-4.207114	0.914544
48	1	0	7.214272	-4.157028	2.748726
49	1	0	-2.300547	3.867424	1.019149
50	6	0	-3.706088	1.708083	0.388537
51	1	0	-4.199538	2.519391	0.916007
52	6	0	-4.458018	0.566601	0.030066
53	1	0	-3.976680	-0.220666	-0.543553
54	6	0	-5.805725	0.313008	0.327017
55	6	0	-6.614161	1.220620	1.108100
56	6	0	-7.606632	-1.147428	0.103696
57	6	0	-7.911527	0.921295	1.375974
58	1	0	-6.180114	2.139411	1.486979
59	6	0	-8.159548	-2.369021	-0.404392
60	6	0	-8.475945	-0.295870	0.877048
61	1	0	-8.531309	1.590371	1.966712
62	6	0	-9.806274	-0.676116	1.110241
63	6	0	-10.305905	-1.864164	0.605549
64	1	0	-11.335954	-2.148368	0.792788
65	6	0	-9.466060	-2.709309	-0.157591
66	1	0	-7.506098	-3.009124	-0.988838
67	1	0	-9.863554	-3.639910	-0.551734
68	1	0	-10.441023	-0.018038	1.698529
69	7	0	-6.329429	-0.859338	-0.158417

***cis*-1 (S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.842314	4.189434	-0.976396
2	6	0	0.498506	4.174483	-0.680990
3	6	0	2.718524	3.161172	-0.508207
4	6	0	-0.043176	3.146827	0.113314
5	1	0	-0.143645	4.956548	-1.066613
6	6	0	2.155782	2.143209	0.333902
7	8	0	-1.335891	3.035614	0.439791
8	6	0	0.813988	2.130977	0.632079
9	1	0	2.819388	1.398561	0.752609
10	6	0	-2.242041	4.032770	-0.027690
11	8	0	0.197684	1.210192	1.409150
12	6	0	-3.621875	3.654935	0.447100
13	1	0	-2.221891	4.069738	-1.123160
14	1	0	-1.958627	5.012807	0.373384
15	6	0	1.007344	0.171287	1.943385
16	8	0	-4.021588	2.485315	-0.227016
17	1	0	-3.612549	3.496203	1.535491
18	1	0	-4.307651	4.487603	0.229693
19	6	0	0.110439	-0.757107	2.722250
20	1	0	1.504082	-0.374354	1.130693
21	1	0	1.772769	0.592089	2.607549
22	6	0	-5.325219	2.084681	0.132131
23	1	0	-0.481567	-0.177499	3.446231
24	1	0	0.734918	-1.467644	3.284564
25	8	0	-0.730711	-1.436119	1.819196
26	1	0	-5.390513	1.900642	1.214656
27	1	0	-6.056453	2.865282	-0.126408
28	6	0	-5.667994	0.822420	-0.619171
29	6	0	-1.612538	-2.317524	2.476705
30	1	0	-6.727828	0.580160	-0.467880

31	1	0	-5.488784	0.966954	-1.692441
32	8	0	-4.845116	-0.215818	-0.116118
33	1	0	-1.053495	-3.074090	3.047845
34	1	0	-2.258655	-1.768617	3.177835
35	6	0	-2.459229	-3.012007	1.439593
36	6	0	-5.000371	-1.453492	-0.656451
37	1	0	-3.047615	-3.809052	1.912117
38	1	0	-1.812057	-3.458051	0.673240
39	8	0	-3.313485	-2.040610	0.860374
40	6	0	-5.900002	-1.778023	-1.663024
41	6	0	-4.161123	-2.456930	-0.117166
42	6	0	-5.977967	-3.092126	-2.141092
43	1	0	-6.547061	-1.018022	-2.083744
44	6	0	-4.248457	-3.757249	-0.596379
45	6	0	-5.159752	-4.074064	-1.611325
46	1	0	-6.685657	-3.328916	-2.928226
47	1	0	-3.611746	-4.533108	-0.189099
48	1	0	-5.215427	-5.094084	-1.975729
49	1	0	2.249075	4.981211	-1.597738
50	6	0	4.079608	3.200057	-0.845062
51	1	0	4.427919	4.122188	-1.311330
52	6	0	5.070077	2.215112	-0.549173
53	1	0	6.049572	2.566882	-0.225006
54	6	0	4.959847	0.822830	-0.685498
55	6	0	3.826243	0.209440	-1.346628
56	6	0	5.885034	-1.268303	-0.266084
57	6	0	3.735371	-1.145235	-1.421510
58	1	0	3.074816	0.845550	-1.800523
59	6	0	6.945027	-2.069090	0.271403
60	6	0	4.766946	-1.954400	-0.859767
61	1	0	2.898654	-1.623390	-1.924135
62	6	0	4.743678	-3.361579	-0.895348
63	6	0	5.781312	-4.099815	-0.366257
64	1	0	5.755052	-5.183792	-0.398197
65	6	0	6.889355	-3.437470	0.220128
66	1	0	7.786921	-1.550648	0.719315
67	1	0	7.702884	-4.026060	0.633571
68	1	0	3.890666	-3.856532	-1.352737
69	7	0	5.984207	0.063074	-0.193065

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cis-**1**_b (**S_1**):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.765536	3.932501	1.087132
2	6	0	-0.539682	3.923614	0.462622
3	6	0	-2.559070	2.746899	1.189191
4	6	0	-0.029862	2.731235	-0.084773
5	1	0	0.030366	4.841582	0.390461
6	6	0	-2.008223	1.533520	0.654734
7	8	0	1.141133	2.622848	-0.722354
8	6	0	-0.787441	1.526705	0.022854
9	1	0	-2.563684	0.614197	0.780863
10	6	0	1.952575	3.787218	-0.858147
11	8	0	-0.207101	0.438744	-0.533876
12	6	0	3.206325	3.385910	-1.592903
13	1	0	2.207191	4.180254	0.133011
14	1	0	1.413598	4.555318	-1.424827
15	6	0	-0.951475	-0.772272	-0.513803
16	8	0	3.960191	2.533366	-0.763701
17	1	0	2.940887	2.881439	-2.533787
18	1	0	3.773922	4.295101	-1.841660
19	6	0	-0.164551	-1.808620	-1.275257
20	1	0	-1.103428	-1.105021	0.520841
21	1	0	-1.931535	-0.620457	-0.984304
22	6	0	5.175356	2.149139	-1.367526
23	1	0	0.089516	-1.422050	-2.273391
24	1	0	-0.789093	-2.705400	-1.405311
25	8	0	1.001451	-2.112589	-0.545481
26	1	0	4.988380	1.635584	-2.322169
27	1	0	5.802884	3.029884	-1.570680
28	6	0	5.912800	1.224025	-0.431907
29	6	0	1.805071	-3.068027	-1.199285
30	1	0	6.921419	1.035136	-0.821765
31	1	0	5.999062	1.685713	0.560148
32	8	0	5.176579	0.015938	-0.353860
33	1	0	1.252268	-4.008077	-1.347409
34	1	0	2.122333	-2.699480	-2.186080
35	6	0	3.016087	-3.341184	-0.343055
36	6	0	5.690021	-0.982811	0.412511
37	1	0	3.585135	-4.182252	-0.759854
38	1	0	2.698232	-3.599868	0.675163
39	8	0	3.806267	-2.164598	-0.328708
40	6	0	6.861515	-0.898780	1.152985
41	6	0	4.938387	-2.181827	0.423084
42	6	0	7.299522	-1.996384	1.904656
43	1	0	7.442230	0.015573	1.154271
44	6	0	5.383663	-3.265135	1.168932
45	6	0	6.567418	-3.170542	1.910980
46	1	0	8.216712	-1.915541	2.477962
47	1	0	4.818548	-4.189129	1.181215
48	1	0	6.900474	-4.025475	2.489414
49	1	0	-2.154274	4.859096	1.497824
50	6	0	-3.801815	2.798587	1.837793
51	1	0	-4.020957	3.725850	2.367586
52	6	0	-4.746989	1.739531	1.987831
53	1	0	-5.238086	1.642903	2.956280
54	6	0	-5.175326	0.818591	1.019752
55	6	0	-4.829501	0.962994	-0.379302
56	6	0	-6.336751	-1.142634	0.561550
57	6	0	-5.220245	0.018350	-1.276273
58	1	0	-4.279273	1.842208	-0.695711
59	6	0	-7.135390	-2.243522	1.013393
60	6	0	-5.984161	-1.103031	-0.834123
61	1	0	-4.979169	0.114918	-2.331816
62	6	0	-6.420237	-2.125362	-1.698263
63	6	0	-7.184318	-3.172352	-1.226731

64	1	0	-7.515531	-3.956037	-1.899732
65	6	0	-7.541671	-3.222133	0.144327
66	1	0	-7.401357	-2.270084	2.065408
67	1	0	-8.145454	-4.048887	0.506375
68	1	0	-6.144055	-2.073107	-2.748516
69	7	0	-5.960624	-0.215540	1.448025

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cis-**1**_c (**S_1**):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.385312	3.687605	-1.116924
2	6	0	1.219965	3.714039	-0.390674
3	6	0	3.035416	2.453983	-1.429644
4	6	0	0.624511	2.508404	0.043680
5	1	0	0.763006	4.663720	-0.142398
6	6	0	2.373497	1.237691	-1.048225
7	8	0	-0.497833	2.437479	0.769193
8	6	0	1.212986	1.265050	-0.306980
9	1	0	2.782658	0.299982	-1.391585
10	6	0	-1.145951	3.651100	1.143817
11	8	0	0.542129	0.168220	0.128417
12	6	0	-2.361894	3.288017	1.957908
13	1	0	-1.445577	4.205254	0.246913
14	1	0	-0.467459	4.269716	1.742392
15	6	0	1.134020	-1.094209	-0.143447
16	8	0	-3.288928	2.638253	1.120787
17	1	0	-2.068739	2.638534	2.795911
18	1	0	-2.790309	4.211241	2.376454
19	6	0	0.309565	-2.148311	0.549919
20	1	0	1.148717	-1.281231	-1.224914
21	1	0	2.163477	-1.120851	0.237755
22	6	0	-4.476182	2.305262	1.805835
23	1	0	0.210615	-1.898293	1.616969
24	1	0	0.830725	-3.114963	0.473668
25	8	0	-0.955069	-2.211269	-0.067733
26	1	0	-4.259150	1.648168	2.660925
27	1	0	-4.969810	3.211286	2.188376
28	6	0	-5.408941	1.603857	0.850516
29	6	0	-1.793391	-3.173223	0.529688
30	1	0	-6.393430	1.481498	1.320005
31	1	0	-5.525561	2.202289	-0.062329
32	8	0	-4.845051	0.340230	0.544350
33	1	0	-1.344181	-4.175835	0.464935
34	1	0	-1.957512	-2.940960	1.592426
35	6	0	-3.111729	-3.180045	-0.202694
36	6	0	-5.542638	-0.466704	-0.298817
37	1	0	-3.727921	-4.018689	0.146541
38	1	0	-2.934336	-3.297541	-1.279476
39	8	0	-3.758654	-1.945765	0.057753
40	6	0	-6.756546	-0.143588	-0.890457
41	6	0	-4.947561	-1.723255	-0.562371
42	6	0	-7.390340	-1.056682	-1.742407
43	1	0	-7.219277	0.816688	-0.698259
44	6	0	-5.586636	-2.622681	-1.405492
45	6	0	-6.810453	-2.286802	-1.997053
46	1	0	-8.337343	-0.788228	-2.198043
47	1	0	-5.142503	-3.589080	-1.610598
48	1	0	-7.295216	-2.999936	-2.654969
49	1	0	2.848895	4.618544	-1.428239
50	6	0	4.259448	2.465149	-2.119811
51	1	0	4.535440	3.405114	-2.596186
52	6	0	5.154342	1.380417	-2.281820
53	1	0	5.789329	1.386783	-3.165832
54	6	0	5.368923	0.329269	-1.371109
55	6	0	6.179189	-0.794854	-1.776287
56	6	0	4.862570	-0.724117	0.645864
57	6	0	6.279870	-1.888352	-0.977725
58	1	0	6.667044	-0.758953	-2.746229
59	6	0	4.197341	-0.711493	1.908744
60	6	0	5.582614	-1.911058	0.277131
61	1	0	6.869311	-2.751470	-1.273606
62	6	0	5.605093	-3.010336	1.148946
63	6	0	4.933674	-2.974056	2.360083
64	1	0	4.953490	-3.834281	3.020677
65	6	0	4.226224	-1.812794	2.734587
66	1	0	3.650602	0.187690	2.177647
67	1	0	3.700505	-1.788034	3.684298
68	1	0	6.162254	-3.896800	0.856275
69	7	0	4.793673	0.369682	-0.131475

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cis-**1**_d (**S_1**):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.700069	3.766112	-1.108810
2	6	0	1.374760	3.939757	-0.793651
3	6	0	3.446887	2.659524	-0.596770
4	6	0	0.723721	3.028368	0.066351
5	1	0	0.827543	4.773698	-1.214877
6	6	0	2.788007	1.786222	0.332640
7	8	0	-0.563296	3.111218	0.422209
8	6	0	1.453773	1.948152	0.631802
9	1	0	3.367431	1.015235	0.816170
10	6	0	-1.335548	4.208782	-0.060764
11	8	0	0.744318	1.150830	1.469363
12	6	0	-2.734443	4.054497	0.479543
13	1	0	-1.355824	4.197715	-1.156542
14	1	0	-0.899368	5.152952	0.285071
15	6	0	1.412443	0.006327	1.982099
16	8	0	-3.329766	2.936361	-0.135209
17	1	0	-2.700244	3.930069	1.571895
18	1	0	-3.300158	4.971958	0.257925
19	6	0	0.397671	-0.835551	2.712979
20	1	0	1.852596	-0.572935	1.159510
21	1	0	2.211261	0.308660	2.671466

22	6	0	-4.653438	2.729494	0.304955
23	1	0	-0.136287	-0.222181	3.454208
24	1	0	0.926146	-1.636538	3.251781
25	8	0	-0.502400	-1.377114	1.773317
26	1	0	-4.678415	2.549899	1.389873
27	1	0	-5.276274	3.610519	0.089355
28	6	0	-5.222103	1.537992	-0.424020
29	6	0	-1.465957	-2.205355	2.382487
30	1	0	-6.294485	1.447715	-0.207563
31	1	0	-5.090341	1.669186	-1.505722
32	8	0	-4.526219	0.386633	0.021048
33	1	0	-0.984109	-3.055512	2.888786
34	1	0	-2.042207	-1.644272	3.133280
35	6	0	-2.397389	-2.733559	1.320174
36	6	0	-4.845029	-0.799257	-0.562505
37	1	0	-3.058608	-3.493848	1.755389
38	1	0	-1.816583	-3.193420	0.509970
39	8	0	-3.155377	-1.642541	0.826437
40	6	0	-5.830899	-0.973578	-1.525043
41	6	0	-4.090070	-1.912420	-0.123068
42	6	0	-6.074293	-2.243573	-2.062529
43	1	0	-6.417723	-0.128693	-1.864484
44	6	0	-4.338853	-3.167196	-0.663533
45	6	0	-5.333241	-3.331279	-1.636134
46	1	0	-6.846567	-2.363184	-2.814560
47	1	0	-3.764092	-4.026037	-0.338968
48	1	0	-5.513038	-4.317693	-2.049799
49	1	0	3.188080	4.458304	-1.787901
50	6	0	4.788931	2.495758	-0.977187
51	1	0	5.251528	3.348077	-1.473298
52	6	0	5.621548	1.373152	-0.746723
53	1	0	6.690204	1.566099	-0.668605
54	6	0	5.239068	0.020619	-0.688085
55	6	0	6.216590	-0.955483	-0.268277
56	6	0	3.594786	-1.626468	-0.792554
57	6	0	5.854129	-2.249966	-0.078372
58	1	0	7.232079	-0.621946	-0.074654
59	6	0	2.245631	-2.008334	-1.066360
60	6	0	4.492970	-2.639885	-0.311112
61	1	0	6.571892	-2.994904	0.253468
62	6	0	4.029073	-3.950407	-0.121796
63	6	0	2.710909	-4.285219	-0.383732
64	1	0	2.363802	-5.301324	-0.228716
65	6	0	1.819319	-3.300308	-0.858009
66	1	0	1.569447	-1.237253	-1.424081
67	1	0	0.786568	-3.565691	-1.063539
68	1	0	4.726735	-4.703309	0.236321
69	7	0	3.962403	-0.352280	-1.007493

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trans-1H$^+$ (S_1):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.682844	3.077138	-0.515861
2	6	0	0.356801	3.329838	-0.273900
3	6	0	2.301807	1.846186	-0.116383
4	6	0	-0.430592	2.362422	0.383044
5	1	0	-0.081147	4.269025	-0.586499
6	6	0	1.495752	0.874133	0.544400
7	8	0	-1.709792	2.503533	0.675553
8	6	0	0.164194	1.114157	0.790212
9	1	0	1.933527	-0.062734	0.859855
10	6	0	-2.367816	3.735826	0.346369
11	8	0	-0.682456	0.276173	1.404374
12	6	0	-3.800764	3.621617	0.796409
13	1	0	-2.322232	3.891332	-0.736442
14	1	0	-1.867991	4.562069	0.862017
15	6	0	-0.161908	-0.969450	1.864115
16	8	0	-4.448005	2.672525	-0.015349
17	1	0	-3.838693	3.327849	1.855433
18	1	0	-4.271552	4.611341	0.699860
19	6	0	-1.290612	-1.731591	2.509878
20	1	0	0.238547	-1.538426	1.016622
21	1	0	0.638160	-0.791238	2.592050
22	6	0	-5.814758	2.540306	0.311314
23	1	0	-1.772474	-1.107218	3.276612
24	1	0	-0.872565	-2.619914	3.006947
25	8	0	-2.210794	-2.100766	1.510836
26	1	0	-5.934284	2.235630	1.361265
27	1	0	-6.340351	3.496164	0.169394
28	6	0	-6.427439	1.501173	-0.593513
29	6	0	-3.279529	-2.861555	2.028716
30	1	0	-7.516681	1.490603	-0.459075
31	1	0	-6.203380	1.741301	-1.640783
32	8	0	-5.871272	0.245678	-0.244467
33	1	0	-2.909113	-3.794270	2.479662
34	1	0	-3.818258	-2.297051	2.803845
35	6	0	-4.220527	-3.200416	0.899844
36	6	0	-6.295587	-0.840455	-0.943565
37	1	0	-4.979890	-3.910208	1.252337
38	1	0	-3.662456	-3.661933	0.074874
39	8	0	-4.827955	-1.994194	0.471271
40	6	0	-7.222441	-0.812935	-1.976936
41	6	0	-5.721681	-2.072074	-0.549939
42	6	0	-7.586505	-1.998615	-2.627278
43	1	0	-7.667886	0.124634	-2.286988
44	6	0	-6.089970	-3.241971	-1.200687
45	6	0	-7.025088	-3.203144	-2.242461
46	1	0	-8.310981	-1.960164	-3.433571
47	1	0	-5.656535	-4.190155	-0.906447
48	1	0	-7.302375	-4.125131	-2.741852
49	1	0	2.286849	3.822815	-1.022470
50	6	0	3.677138	1.669624	-0.399542
51	1	0	4.169144	2.496719	-0.901555
52	6	0	4.420492	0.528409	-0.080106
53	1	0	3.917290	-0.296066	0.419009
54	6	0	5.788481	0.337958	-0.348839
55	6	0	6.637930	1.278205	-0.996981

56	6	0	7.681541	-1.182646	-0.156204
57	6	0	7.957648	1.006526	-1.217910
58	1	0	6.219186	2.223526	-1.318711
59	6	0	8.191292	-2.422655	0.267434
60	6	0	8.529766	-0.240531	-0.803868
61	1	0	8.592218	1.733981	-1.713176
62	6	0	9.878769	-0.574930	-1.007712
63	6	0	10.374751	-1.795908	-0.588521
64	1	0	11.417188	-2.045649	-0.750456
65	6	0	9.523934	-2.716639	0.049636
66	1	0	7.534182	-3.133575	0.757790
67	1	0	9.916292	-3.673347	0.377752
68	1	0	10.523315	0.145648	-1.501640
69	7	0	6.370386	-0.856898	0.042773
70	1	0	5.784883	-1.538881	0.510222

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trans-**1H$^+$**_b **(S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.740679	2.953990	-0.511086
2	6	0	0.414904	3.238503	-0.291816
3	6	0	2.321380	1.716268	-0.091828
4	6	0	-0.402255	2.299439	0.364916
5	1	0	0.003553	4.182809	-0.624255
6	6	0	1.483321	0.772365	0.576218
7	8	0	-1.686505	2.474076	0.636669
8	6	0	0.155682	1.047827	0.799940
9	1	0	1.901089	-0.162374	0.924671
10	6	0	-2.305979	3.715595	0.278816
11	8	0	-0.719181	0.239243	1.421941
12	6	0	-3.745699	3.649278	0.717744
13	1	0	-2.247143	3.852350	-0.806129
14	1	0	-1.791142	4.539528	0.783743
15	6	0	-0.230572	-1.007049	1.908788
16	8	0	-4.412941	2.702914	-0.081387
17	1	0	-3.799343	3.375260	1.781512
18	1	0	-4.190423	4.648671	0.600216
19	6	0	-1.382312	-1.733684	2.555324
20	1	0	0.168140	-1.600972	1.077401
21	1	0	0.564903	-0.835123	2.643620
22	6	0	-5.782930	2.607374	0.243277
23	1	0	-1.857253	-1.085936	3.306884
24	1	0	-0.990238	-2.623310	3.070942
25	8	0	-2.301901	-2.098283	1.553691
26	1	0	-5.912266	2.322651	1.297748
27	1	0	-6.286571	3.572446	0.084648
28	6	0	-6.417368	1.567773	-0.645848
29	6	0	-3.392782	-2.824633	2.074047
30	1	0	-7.506911	1.584835	-0.514681
31	1	0	-6.185004	1.785040	-1.696326
32	8	0	-5.891404	0.305800	-0.274016
33	1	0	-3.049160	-3.758832	2.542983
34	1	0	-3.924164	-2.235159	2.835725
35	6	0	-4.333183	-3.158930	0.943303
36	6	0	-6.340562	-0.782661	-0.953684
37	1	0	-5.111866	-3.844502	1.301553
38	1	0	-3.780785	-3.647098	0.130052
39	8	0	-4.908878	-1.945924	0.490378
40	6	0	-7.262789	-0.751726	-1.991086
41	6	0	-5.799780	-2.020634	-0.533556
42	6	0	-7.654614	-1.940164	-2.619843
43	1	0	-7.682857	0.190757	-2.321032
44	6	0	-6.194957	-3.193071	-1.163582
45	6	0	-7.125076	-3.150793	-2.209709
46	1	0	-8.375149	-1.899128	-3.429519
47	1	0	-5.787080	-4.146099	-0.849229
48	1	0	-7.424079	-4.075106	-2.692062
49	1	0	2.368090	3.679436	-1.018883
50	6	0	3.689736	1.498095	-0.352685
51	1	0	4.204854	2.326428	-0.831313
52	6	0	4.390691	0.313165	-0.079185
53	1	0	3.852038	-0.556033	0.283582
54	6	0	5.764073	0.125542	-0.255916
55	6	0	7.764632	-1.287628	-0.248578
56	6	0	7.911994	1.063173	-0.857755
57	1	0	6.184148	2.115296	-0.751057
58	6	0	8.422157	-2.537769	-0.051691
59	6	0	8.552402	-0.149469	-0.674667
60	1	0	8.442626	1.958603	-1.160881
61	6	0	9.954340	-0.306939	-0.883959
62	6	0	10.543165	-1.524609	-0.681877
63	1	0	11.609456	-1.643664	-0.840391
64	6	0	9.769530	-2.652529	-0.262524
65	1	0	7.833435	-3.393175	0.265573
66	1	0	10.262622	-3.606523	-0.112097
67	1	0	10.540296	0.550021	-1.202043
68	1	0	5.783798	-1.949701	0.266243
69	6	0	6.398474	-1.112436	-0.050084
70	7	0	6.587292	1.193432	-0.661986

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cis-**1H$^+$ (S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.790295	4.192481	-0.959852
2	6	0	0.446051	4.184237	-0.682558
3	6	0	2.657951	3.157811	-0.483250
4	6	0	-0.101821	3.154173	0.109843
5	1	0	-0.191429	4.966480	-1.073982
6	6	0	2.098430	2.143942	0.352032
7	8	0	-1.380646	3.042069	0.421097
8	6	0	0.756781	2.132371	0.645884
9	1	0	2.757013	1.400910	0.781707
10	6	0	-2.304037	4.032932	-0.052139
11	8	0	0.133333	1.230882	1.421346

12	6	0	-3.678585	3.634537	0.418226
13	1	0	-2.274098	4.062892	-1.146393
14	1	0	-2.027071	5.011189	0.354139
15	6	0	0.933242	0.202170	2.000383
16	8	0	-4.057740	2.462154	-0.260696
17	1	0	-3.672058	3.476006	1.506464
18	1	0	-4.370879	4.460837	0.198130
19	6	0	0.018973	-0.705686	2.782490
20	1	0	1.440429	-0.363318	1.209263
21	1	0	1.683786	0.645492	2.665599
22	6	0	-5.367523	2.055577	0.072788
23	1	0	-0.592147	-0.108516	3.475215
24	1	0	0.633243	-1.396836	3.378767
25	8	0	-0.794506	-1.410501	1.875317
26	1	0	-5.454675	1.877618	1.154546
27	1	0	-6.096231	2.830906	-0.206840
28	6	0	-5.685890	0.786913	-0.678218
29	6	0	-1.680925	-2.290736	2.530146
30	1	0	-6.747517	0.539645	-0.549456
31	1	0	-5.483207	0.925746	-1.748093
32	8	0	-4.868517	-0.242404	-0.149192
33	1	0	-1.124903	-3.033017	3.122178
34	1	0	-2.344574	-1.737036	3.210510
35	6	0	-2.501638	-3.006078	1.486429
36	6	0	-5.004539	-1.485689	-0.681895
37	1	0	-3.092069	-3.802452	1.957397
38	1	0	-1.836403	-3.455438	0.737716
39	8	0	-3.352042	-2.047986	0.880606
40	6	0	-5.878250	-1.824439	-1.706373
41	6	0	-4.172880	-2.479023	-0.113365
42	6	0	-5.936726	-3.143279	-2.174179
43	1	0	-6.519590	-1.071887	-2.148933
44	6	0	-4.240702	-3.784049	-0.582482
45	6	0	-5.125480	-4.115315	-1.616096
46	1	0	-6.623622	-3.391942	-2.975877
47	1	0	-3.610112	-4.552638	-0.152415
48	1	0	-5.166369	-5.138881	-1.972400
49	1	0	2.208899	4.983554	-1.573444
50	6	0	4.038341	3.240231	-0.792018
51	1	0	4.382769	4.210553	-1.143478
52	6	0	5.036592	2.261583	-0.637494
53	1	0	6.054097	2.630286	-0.507986
54	6	0	4.891694	0.861926	-0.713939
55	6	0	3.780015	0.189652	-1.300721
56	6	0	5.922940	-1.299394	-0.282490
57	6	0	3.728370	-1.172948	-1.360044
58	1	0	2.991614	0.791473	-1.735496
59	6	0	7.004659	-2.035531	0.233579
60	6	0	4.798070	-1.970406	-0.838434
61	1	0	2.884161	-1.669278	-1.827528
62	6	0	4.794943	-3.375635	-0.867706
63	6	0	5.861090	-4.093427	-0.360680
64	1	0	5.851017	-5.177093	-0.385458
65	6	0	6.965136	-3.415234	0.189181
66	1	0	7.856974	-1.513759	0.656927
67	1	0	7.801069	-3.982550	0.584650
68	1	0	3.937110	-3.883524	-1.297601
69	7	0	5.929552	0.066335	-0.261877
70	1	0	6.731387	0.524515	0.155206

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trans-1Ca^{++} (S_1):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.909382	2.942192	-0.618185
2	6	0	0.567730	3.206540	-0.446408
3	6	0	2.511060	1.731558	-0.146883
4	6	0	-0.238795	2.271135	0.213550
5	1	0	0.147239	4.130874	-0.823467
6	6	0	1.659283	0.790609	0.530222
7	8	0	-1.575263	2.407106	0.447997
8	6	0	0.325716	1.069305	0.696778
9	1	0	2.071826	-0.135155	0.907656
10	6	0	-2.179000	3.667637	0.141375
11	8	0	-0.575761	0.250258	1.327761
12	6	0	-3.580754	3.606661	0.686701
13	1	0	-2.189240	3.811134	-0.944090
14	1	0	-1.618795	4.475926	0.620337
15	6	0	-0.051134	-0.884530	2.020669
16	8	0	-4.199721	2.463549	0.104492
17	1	0	-3.576938	3.518455	1.779884
18	1	0	-4.119731	4.516186	0.401431
19	6	0	-1.206450	-1.495896	2.767621
20	1	0	0.358823	-1.597145	1.297610
21	1	0	0.731896	-0.566636	2.715611
22	6	0	-5.618418	2.447494	0.244673
23	1	0	-1.585244	-0.817730	3.541379
24	1	0	-0.881714	-2.430459	3.236281
25	8	0	-2.221275	-1.754092	1.802709
26	1	0	-5.891531	2.178884	1.272192
27	1	0	-6.033779	3.432592	0.008190
28	6	0	-6.136057	1.435710	-0.742049
29	6	0	-3.205502	-2.693763	2.222702
30	1	0	-7.217291	1.310253	-0.630504
31	1	0	-5.900736	1.743376	-1.766428
32	8	0	-5.467593	0.208970	-0.445371
33	1	0	-2.728009	-3.558201	2.695401
34	1	0	-3.893037	-2.225945	2.937320
35	6	0	-3.930843	-3.138377	0.980195
36	6	0	-5.872081	-0.907076	-1.136885
37	1	0	-4.776723	-3.780310	1.242831
38	1	0	-3.252951	-3.672669	0.306217
39	8	0	-4.399851	-1.948543	0.342762
40	6	0	-6.781695	-0.916753	-2.181810
41	6	0	-5.280333	-2.101317	-0.701597
42	6	0	-7.103126	-2.132627	-2.794141
43	1	0	-7.243408	0.000808	-2.525421
44	6	0	-5.597869	-3.304315	-1.310112

45	6	0	-6.518104	-3.312826	-2.363495
46	1	0	-7.815077	-2.140587	-3.611598
47	1	0	-5.143725	-4.230570	-0.979645
48	1	0	-6.767449	-4.253928	-2.840176
49	1	0	2.533961	3.665706	-1.132239
50	6	0	3.875512	1.506457	-0.367519
51	1	0	4.436769	2.277885	-0.886024
52	6	0	4.593847	0.346727	0.015325
53	1	0	4.080598	-0.460178	0.530025
54	6	0	5.953584	0.157432	-0.240493
55	6	0	7.965573	-1.230308	-0.112959
56	6	0	7.911333	0.991307	-1.144030
57	6	0	8.696684	-2.408409	0.245567
58	6	0	8.666106	-0.179338	-0.792559
59	1	0	8.435321	1.798201	-1.659614
60	6	0	10.027345	-0.315005	-1.090578
61	6	0	10.709281	-1.466279	-0.733160
62	1	0	11.763492	-1.571575	-0.964852
63	6	0	10.029593	-2.513044	-0.061388
64	1	0	8.178675	-3.212540	0.760014
65	1	0	10.576527	-3.409693	0.212562
66	1	0	10.540442	0.492712	-1.605963
67	20	0	-3.030523	0.227249	0.463522
68	7	0	6.649806	1.172246	-0.899535
69	6	0	6.616197	-1.044534	0.155525
70	1	0	6.048937	-1.816575	0.668676

***trans*-1Ca^{++}_b (S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.864237	3.035988	0.725332
2	6	0	-0.524443	3.257011	0.495460
3	6	0	-2.514978	1.830542	0.307165
4	6	0	0.231816	2.277914	-0.162314
5	1	0	-0.064377	4.181296	0.823238
6	6	0	-1.709776	0.834254	-0.344877
7	8	0	1.550652	2.382169	-0.469751
8	6	0	-0.375621	1.064650	-0.564725
9	1	0	-2.158378	-0.099857	-0.652558
10	6	0	2.191191	3.647028	-0.262425
11	8	0	0.482526	0.190116	-1.175917
12	6	0	3.533965	3.550948	-0.934739
13	1	0	2.302057	3.823883	0.812281
14	1	0	1.595757	4.444620	-0.715091
15	6	0	-0.097637	-0.983916	-1.753539
16	8	0	4.193518	2.418132	-0.378806
17	1	0	3.425540	3.430952	-2.019300
18	1	0	4.105459	4.461783	-0.728025
19	6	0	1.009548	-1.696521	-2.481606
20	1	0	-0.501935	-1.618185	-0.957766
21	1	0	-0.895214	-0.701055	-2.447003
22	6	0	5.591398	2.373994	-0.658416
23	1	0	1.386791	-1.098877	-3.320302
24	1	0	0.635522	-2.652428	-2.861878
25	8	0	2.046131	-1.913742	-1.529186
26	1	0	5.757988	2.018374	-1.682160
27	1	0	6.032328	3.369512	-0.547106
28	6	0	6.203343	1.442272	0.352815
29	6	0	2.994639	-2.898495	-1.927902
30	1	0	7.264608	1.287004	0.136927
31	1	0	6.083675	1.843203	1.364700
32	8	0	5.494998	0.206838	0.241529
33	1	0	2.480946	-3.796804	-2.285848
34	1	0	3.632904	-2.504589	-2.728342
35	6	0	3.804630	-3.234488	-0.704441
36	6	0	5.958421	-0.847179	0.991938
37	1	0	4.624823	-3.908916	-0.966900
38	1	0	3.175737	-3.694199	0.064882
39	8	0	4.327647	-1.995764	-0.218345
40	6	0	6.975504	-0.776635	1.930084
41	6	0	5.310257	-2.064344	0.740426
42	6	0	7.345895	-1.934621	2.621869
43	1	0	7.484107	0.158272	2.130308
44	6	0	5.674270	-3.209298	1.429804
45	6	0	6.702174	-3.137018	2.375550
46	1	0	8.142801	-1.879173	3.354681
47	1	0	5.173479	-4.151535	1.243743
48	1	0	6.988680	-4.032625	2.914799
49	1	0	-2.450175	3.795079	1.233297
50	6	0	-3.886426	1.664549	0.545114
51	1	0	-4.383699	2.473141	1.072849
52	6	0	-4.648059	0.545912	0.127456
53	1	0	-4.170777	-0.224120	-0.471537
54	6	0	-6.004057	0.310224	0.381527
55	6	0	-6.814371	1.197596	1.186307
56	6	0	-7.826283	-1.093002	0.026937
57	6	0	-8.126322	0.917494	1.395424
58	1	0	-6.369334	2.082285	1.627526
59	6	0	-8.387746	-2.275582	-0.562864
60	6	0	-8.701501	-0.255761	0.812853
61	1	0	-8.749865	1.569145	2.000886
62	6	0	-10.048254	-0.611196	0.976159
63	6	0	-10.554801	-1.758599	0.391433
64	1	0	-11.598313	-2.023554	0.524286
65	6	0	-9.709339	-2.590900	-0.382696
66	1	0	-7.727421	-2.902111	-1.153772
67	1	0	-10.117605	-3.488762	-0.836294
68	1	0	-10.690039	0.031627	1.572737
69	7	0	-6.536985	-0.825867	-0.176338
70	20	0	3.008994	0.189437	-0.473187

***trans*-1H^{+}Ca^{++} (S_1):**

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

1	6	0	-1.860791	3.026864	0.652279
2	6	0	-0.526493	3.265790	0.428411
3	6	0	-2.483785	1.798567	0.256948
4	6	0	0.248085	2.281409	-0.203876
5	1	0	-0.082709	4.202754	0.739822
6	6	0	-1.670517	0.802454	-0.371723
7	8	0	1.549300	2.402146	-0.496931
8	6	0	-0.339790	1.042549	-0.592616
9	1	0	-2.106761	-0.139479	-0.673576
10	6	0	2.192836	3.669849	-0.263651
11	8	0	0.527912	0.181442	-1.190566
12	6	0	3.558064	3.569248	-0.886666
13	1	0	2.263798	3.835427	0.815218
14	1	0	1.614361	4.467023	-0.736679
15	6	0	-0.033574	-1.013903	-1.754854
16	8	0	4.203372	2.448536	-0.292456
17	1	0	3.490575	3.438626	-1.973166
18	1	0	4.112625	4.487799	-0.668654
19	6	0	1.070666	-1.699549	-2.512818
20	1	0	-0.400500	-1.653191	-0.945459
21	1	0	-0.853165	-0.751865	-2.429996
22	6	0	5.617347	2.433926	-0.484668
23	1	0	1.411909	-1.090647	-3.358583
24	1	0	0.703397	-2.660466	-2.887131
25	8	0	2.135925	-1.901779	-1.590546
26	1	0	5.851670	2.112963	-1.506921
27	1	0	6.032430	3.432574	-0.316680
28	6	0	6.184694	1.479564	0.531107
29	6	0	3.114992	-2.838923	-2.034248
30	1	0	7.260089	1.354115	0.374168
31	1	0	5.995675	1.840273	1.547533
32	8	0	5.512386	0.234720	0.333281
33	1	0	2.628387	-3.734817	-2.433088
34	1	0	3.739310	-2.389049	-2.815571
35	6	0	3.933389	-3.205948	-0.824897
36	6	0	5.968881	-0.844357	1.052842
37	1	0	4.772938	-3.844950	-1.113091
38	1	0	3.314420	-3.716207	-0.079684
39	8	0	4.420296	-1.976436	-0.280183
40	6	0	6.938567	-0.792734	2.040951
41	6	0	5.367522	-2.064101	0.713322
42	6	0	7.311837	-1.972868	2.691969
43	1	0	7.407927	0.144965	2.311854
44	6	0	5.736494	-3.231796	1.360856
45	6	0	6.717893	-3.178916	2.355740
46	1	0	8.071604	-1.931664	3.464166
47	1	0	5.274341	-4.177517	1.105950
48	1	0	7.007335	-4.092489	2.862291
49	1	0	-2.464902	3.784083	1.140545
50	6	0	-3.860871	1.637072	0.504630
51	1	0	-4.359442	2.468629	0.991943
52	6	0	-4.610855	0.499433	0.157037
53	1	0	-4.104487	-0.324335	-0.338873
54	6	0	-5.982662	0.326523	0.388907
55	6	0	-6.834331	1.274487	1.029322
56	6	0	-7.894749	-1.154235	0.115865
57	6	0	-8.164584	1.023749	1.206405
58	1	0	-6.408538	2.206249	1.379548
59	6	0	-8.416113	-2.376789	-0.346667
60	6	0	-8.745866	-0.203492	0.753009
61	1	0	-8.800214	1.754884	1.694634
62	6	0	-10.107780	-0.512604	0.906913
63	6	0	-10.613252	-1.714395	0.449128
64	1	0	-11.665381	-1.945383	0.570745
65	6	0	-9.759759	-2.644018	-0.177896
66	1	0	-7.758657	-3.093650	-0.827413
67	1	0	-10.162285	-3.585743	-0.535425
68	1	0	-10.753542	0.212610	1.391849
69	7	0	-6.573663	-0.853515	-0.035197
70	1	0	-5.986965	-1.539483	-0.495825
71	20	0	3.092195	0.184821	-0.535762

***trans*-1H^{+}Ca^{++}_b (S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.901539	2.950218	-0.585577
2	6	0	0.565281	3.232420	-0.411173
3	6	0	2.474932	1.722040	-0.137071
4	6	0	-0.251638	2.295414	0.232591
5	1	0	0.158839	4.168448	-0.772028
6	6	0	1.624394	0.782794	0.527838
7	8	0	-1.568287	2.449449	0.465466
8	6	0	0.295848	1.072454	0.706013
9	1	0	2.032293	-0.146324	0.902670
10	6	0	-2.174108	3.707347	0.122297
11	8	0	-0.608892	0.271555	1.337787
12	6	0	-3.596827	3.634431	0.606263
13	1	0	-2.138329	3.834544	-0.963632
14	1	0	-1.639360	4.521103	0.619029
15	6	0	-0.097832	-0.878267	2.024245
16	8	0	-4.176653	2.480310	0.004877
17	1	0	-3.643173	3.555553	1.698753
18	1	0	-4.127944	4.537585	0.289233
19	6	0	-1.246854	-1.451696	2.809078
20	1	0	0.271472	-1.603119	1.291759
21	1	0	0.711134	-0.577442	2.696388
22	6	0	-5.602966	2.492311	0.000638
23	1	0	-1.590100	-0.752170	3.580347
24	1	0	-0.926171	-2.383617	3.285755
25	8	0	-2.291708	-1.708515	1.876909
26	1	0	-5.983681	2.284045	1.007498
27	1	0	-5.971296	3.469141	-0.328321
28	6	0	-6.046013	1.438017	-0.977557
29	6	0	-3.299050	-2.597262	2.355126
30	1	0	-7.134651	1.334068	-0.950424
31	1	0	-5.721175	1.688112	-1.992935
32	8	0	-5.426864	0.217270	-0.565487

33	1	0	-2.840446	-3.449170	2.866975
34	1	0	-3.963502	-2.072423	3.051789
35	6	0	-4.048441	-3.085486	1.143579
36	6	0	-5.841406	-0.936694	-1.188188
37	1	0	-4.906900	-3.692729	1.445040
38	1	0	-3.389580	-3.669816	0.492912
39	8	0	-4.494547	-1.919897	0.446970
40	6	0	-6.693088	-0.991460	-2.279314
41	6	0	-5.327014	-2.115796	-0.629941
42	6	0	-7.037545	-2.236861	-2.814051
43	1	0	-7.090944	-0.085286	-2.718952
44	6	0	-5.666337	-3.348549	-1.162959
45	6	0	-6.530090	-3.402197	-2.261829
46	1	0	-7.704586	-2.279064	-3.667391
47	1	0	-5.273092	-4.264625	-0.739717
48	1	0	-6.796775	-4.367090	-2.677727
49	1	0	2.538499	3.671685	-1.086475
50	6	0	3.844551	1.497222	-0.371577
51	1	0	4.369896	2.319663	-0.848723
52	6	0	4.538299	0.305778	-0.088244
53	1	0	3.991242	-0.564806	0.257384
54	6	0	5.909951	0.119149	-0.248504
55	6	0	7.902346	-1.307391	-0.248849
56	6	0	8.064668	1.053122	-0.821093
57	1	0	6.345348	2.113133	-0.708959
58	6	0	8.551447	-2.565284	-0.069773
59	6	0	8.698205	-0.168064	-0.654367
60	1	0	8.602238	1.950119	-1.106892
61	6	0	10.096573	-0.328195	-0.862312
62	6	0	10.678981	-1.555108	-0.678539
63	1	0	11.744873	-1.676790	-0.836904
64	6	0	9.899628	-2.683588	-0.279995
65	1	0	7.957227	-3.422115	0.232207
66	1	0	10.386839	-3.642689	-0.144281
67	1	0	10.688856	0.529646	-1.165324
68	1	0	5.916801	-1.967317	0.246362
69	20	0	-3.114500	0.243987	0.520317
70	7	0	6.742474	1.187097	-0.630147
71	6	0	6.538306	-1.129326	-0.053902

***cis*-1H^{+}Ca^{++} (S_1):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.864952	-0.033439	0.581320
2	6	0	-1.863492	0.814072	0.159014
3	6	0	-2.691301	-1.457017	0.561921
4	6	0	-0.654844	0.281417	-0.301612
5	1	0	-2.016598	1.885044	0.196627
6	6	0	-1.428532	-1.974886	0.133338
7	8	0	0.378286	1.002261	-0.765185
8	6	0	-0.443850	-1.128277	-0.300160
9	1	0	-1.280653	-3.047850	0.141273
10	6	0	0.206380	2.425608	-0.895514
11	8	0	0.774990	-1.507143	-0.770495
12	6	0	1.433041	2.938370	-1.597096
13	1	0	0.114475	2.863938	0.102396
14	1	0	-0.688658	2.633390	-1.487266
15	6	0	0.981867	-2.910536	-0.990143
16	8	0	2.556091	2.534820	-0.819783
17	1	0	1.509576	2.531431	-2.612395
18	1	0	1.379840	4.030376	-1.652064
19	6	0	2.255846	-3.040075	-1.779900
20	1	0	1.065988	-3.415972	-0.022991
21	1	0	0.142925	-3.321596	-1.558608
22	6	0	3.745226	3.258616	-1.136862
23	1	0	2.156598	-2.582377	-2.770992
24	1	0	2.495273	-4.102069	-1.896944
25	8	0	3.276977	-2.383493	-1.035648
26	1	0	4.143170	2.918392	-2.100177
27	1	0	3.528088	4.329983	-1.194207
28	6	0	4.725852	3.005254	-0.024510
29	6	0	4.597539	-2.736573	-1.443511
30	1	0	5.690537	3.462874	-0.263099
31	1	0	4.350156	3.402838	0.923780
32	8	0	4.867980	1.586748	0.072933
33	1	0	4.672826	-3.820017	-1.579554
34	1	0	4.843665	-2.236070	-2.387391
35	6	0	5.525512	-2.306641	-0.339454
36	6	0	5.887118	1.112538	0.864628
37	1	0	6.565836	-2.465607	-0.638564
38	1	0	5.315104	-2.859879	0.582111
39	8	0	5.282722	-0.915359	-0.125466
40	6	0	6.655253	1.885260	1.720260
41	6	0	6.114479	-0.266892	0.756642
42	6	0	7.663970	1.274294	2.471865
43	1	0	6.481062	2.950140	1.812812
44	6	0	7.110396	-0.871274	1.506562
45	6	0	7.888507	-0.088973	2.366383
46	1	0	8.266791	1.880056	3.138670
47	1	0	7.292162	-1.936206	1.434321
48	1	0	8.669344	-0.563099	2.949945
49	1	0	-3.779690	0.388466	0.979156
50	6	0	-3.670925	-2.359069	1.022439
51	1	0	-3.333996	-3.375442	1.217163
52	6	0	-5.019576	-2.079179	1.352395
53	1	0	-5.455129	-2.669533	2.158461
54	6	0	-5.870248	-1.174219	0.707989
55	6	0	-7.966160	0.050049	0.810188
56	6	0	-6.481565	0.317199	-1.115974
57	1	0	-4.725994	-0.892758	-1.109138
58	6	0	-9.144886	0.362055	1.514188
59	6	0	-7.686973	0.676888	-0.437785
60	1	0	-6.280808	0.751101	-2.090355
61	6	0	-8.614113	1.601445	-0.955294
62	6	0	-9.767766	1.900693	-0.261110
63	1	0	-10.477545	2.614820	-0.662399
64	6	0	-10.026973	1.274983	0.976587

65	1	0	-9.344302	-0.118432	2.466324
66	1	0	-10.936375	1.515027	1.516918
67	1	0	-8.400868	2.072526	-1.909732
68	1	0	-7.280816	-1.268938	2.208307
69	20	0	2.891043	0.040934	-0.482797
70	7	0	-7.072595	-0.850218	1.308594
71	6	0	-5.610005	-0.579088	-0.568037

***cis*-1H^{+}Ca^{++}_b (S$_1$):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.957796	0.811293	1.073875
2	6	0	-1.882503	0.201750	1.685003
3	6	0	-2.775627	1.928327	0.192761
4	6	0	-0.588489	0.673769	1.440067
5	1	0	-2.046462	-0.631438	2.356661
6	6	0	-1.445550	2.409692	-0.019551
7	8	0	0.534280	0.166400	1.968493
8	6	0	-0.381064	1.788948	0.576083
9	1	0	-1.301941	3.257730	-0.677983
10	6	0	0.426949	-0.893243	2.935185
11	8	0	0.923359	2.147395	0.433976
12	6	0	1.819734	-1.135258	3.451615
13	1	0	0.030365	-1.785388	2.441190
14	1	0	-0.233666	-0.583045	3.749116
15	6	0	1.183432	3.373817	-0.264271
16	8	0	2.639352	-1.439811	2.326834
17	1	0	2.207413	-0.253155	3.975072
18	1	0	1.796692	-1.982386	4.144719
19	6	0	2.645857	3.672291	-0.083655
20	1	0	0.939553	3.243044	-1.323318
21	1	0	0.577974	4.176857	0.165222
22	6	0	3.870436	-2.073166	2.675128
23	1	0	2.888133	3.841502	0.972756
24	1	0	2.902489	4.567414	-0.659260
25	8	0	3.365422	2.546398	-0.576686
26	1	0	4.558809	-1.338900	3.109447
27	1	0	3.690456	-2.872668	3.400677
28	6	0	4.431818	-2.664618	1.409535
29	6	0	4.757437	2.803589	-0.755517
30	1	0	5.423546	-3.085492	1.598373
31	1	0	3.766967	-3.440234	1.015693
32	8	0	4.526508	-1.593594	0.467021
33	1	0	4.900527	3.760029	-1.268692
34	1	0	5.260597	2.840795	0.218328
35	6	0	5.301660	1.690744	-1.610603
36	6	0	5.241739	-1.831261	-0.683733
37	1	0	6.387691	1.782211	-1.705389
38	1	0	4.839216	1.703815	-2.603154
39	8	0	4.968462	0.471736	-0.944056
40	6	0	5.703076	-3.071414	-1.093741
41	6	0	5.488096	-0.690547	-1.460342
42	6	0	6.422730	-3.169707	-2.289142
43	1	0	5.509430	-3.958779	-0.503598
44	6	0	6.199841	-0.789465	-2.644652
45	6	0	6.669375	-2.041372	-3.054895
46	1	0	6.784408	-4.139641	-2.610580
47	1	0	6.396634	0.087216	-3.249253
48	1	0	7.227491	-2.118356	-3.980976
49	1	0	-3.960163	0.468106	1.300942
50	6	0	-3.845410	2.623509	-0.404952
51	1	0	-3.610773	3.606526	-0.809015
52	6	0	-5.208910	2.244836	-0.466127
53	1	0	-5.937236	3.055363	-0.441488
54	6	0	-5.716202	0.952486	-0.639213
55	6	0	-4.937358	-0.182431	-1.032366
56	6	0	-7.690447	-0.463335	-0.592782
57	6	0	-5.510611	-1.413246	-1.170457
58	1	0	-3.890418	-0.030640	-1.263504
59	6	0	-9.075208	-0.591670	-0.373986
60	6	0	-6.909335	-1.601298	-0.944764
61	1	0	-4.912454	-2.263349	-1.482282
62	6	0	-7.549079	-2.847917	-1.078109
63	6	0	-8.906773	-2.965869	-0.865320
64	1	0	-9.394305	-3.928377	-0.969082
65	6	0	-9.665675	-1.829818	-0.512933
66	1	0	-9.659621	0.281119	-0.102079
67	1	0	-10.733272	-1.929782	-0.348588
68	1	0	-6.951641	-3.711773	-1.351786
69	7	0	-7.072833	0.745464	-0.472920
70	1	0	-7.643016	1.541255	-0.209468
71	20	0	2.867025	0.335874	0.531412

***cis*-1H^{+}Ca^{++}_c (S$_1$):**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.852240	-0.099595	0.893982
2	6	0	-1.890657	0.766325	0.410906
3	6	0	-2.663728	-1.517938	0.844858
4	6	0	-0.709975	0.254445	-0.128628
5	1	0	-2.055304	1.834521	0.468439
6	6	0	-1.418479	-2.016782	0.339240
7	8	0	0.285881	0.996308	-0.649856
8	6	0	-0.478529	-1.151154	-0.148919
9	1	0	-1.255595	-3.087802	0.326240
10	6	0	0.083807	2.417356	-0.737740
11	8	0	0.717522	-1.504450	-0.699694
12	6	0	1.292601	2.976787	-1.434925
13	1	0	-0.002127	2.827590	0.272675
14	1	0	-0.824543	2.623892	-1.310232
15	6	0	0.925056	-2.895021	-0.985543
16	8	0	2.427206	2.569836	-0.677308
17	1	0	1.369432	2.603735	-2.463164
18	1	0	1.218185	4.068842	-1.454539

19	6	0	2.135362	-2.970841	-1.877432
20	1	0	1.093200	-3.435454	-0.048708
21	1	0	0.049911	-3.299994	-1.501648
22	6	0	3.598109	3.336581	-0.952281
23	1	0	1.949328	-2.478035	-2.839035
24	1	0	2.386777	-4.021752	-2.054788
25	8	0	3.197437	-2.319189	-1.188809
26	1	0	3.990884	3.077951	-1.942983
27	1	0	3.362177	4.405371	-0.925828
28	6	0	4.597128	3.017072	0.127188
29	6	0	4.486998	-2.559447	-1.750111
30	1	0	5.551796	3.504880	-0.090390
31	1	0	4.229909	3.339100	1.107192
32	8	0	4.760692	1.597061	0.119558
33	1	0	4.591741	-3.614477	-2.021998
34	1	0	4.627923	-1.940732	-2.644570
35	6	0	5.486681	-2.213843	-0.678607
36	6	0	5.817745	1.081917	0.832305
37	1	0	6.506280	-2.271532	-1.070970
38	1	0	5.378513	-2.886885	0.178286
39	8	0	5.191416	-0.875216	-0.275367
40	6	0	6.609738	1.798269	1.714353
41	6	0	6.059528	-0.280609	0.608270
42	6	0	7.660972	1.148233	2.369438
43	1	0	6.422311	2.848588	1.900676
44	6	0	7.101293	-0.923286	1.257323
45	6	0	7.905150	-0.196978	2.141809
46	1	0	8.282094	1.709916	3.057690
47	1	0	7.296762	-1.974803	1.086464
48	1	0	8.720790	-0.699656	2.648772
49	1	0	-3.736548	0.305796	1.371673
50	6	0	-3.636749	-2.416160	1.315293
51	1	0	-3.321790	-3.443251	1.490207
52	6	0	-4.976472	-2.085432	1.659182
53	1	0	-5.435175	-2.613266	2.491601
54	6	0	-5.814629	-1.215713	0.963574
55	6	0	-7.878392	0.082733	0.741821
56	6	0	-6.171131	0.161761	-0.989738
57	6	0	-9.153421	0.517604	1.217994
58	6	0	-7.399705	0.604416	-0.517450
59	1	0	-5.767123	0.483119	-1.943083
60	6	0	-8.195705	1.529816	-1.247497
61	6	0	-9.409783	1.922002	-0.752785
62	1	0	-10.018051	2.628746	-1.306228
63	6	0	-9.891060	1.410633	0.491613
64	1	0	-9.518592	0.129554	2.163598
65	1	0	-10.855644	1.742111	0.860086
66	1	0	-7.825966	1.914696	-2.192716
67	1	0	-7.416085	-1.217783	2.391004
68	20	0	2.804294	0.057145	-0.467071
69	7	0	-5.423496	-0.693778	-0.283392
70	6	0	-7.082863	-0.816924	1.438862
71	1	0	-4.577993	-1.061598	-0.704904

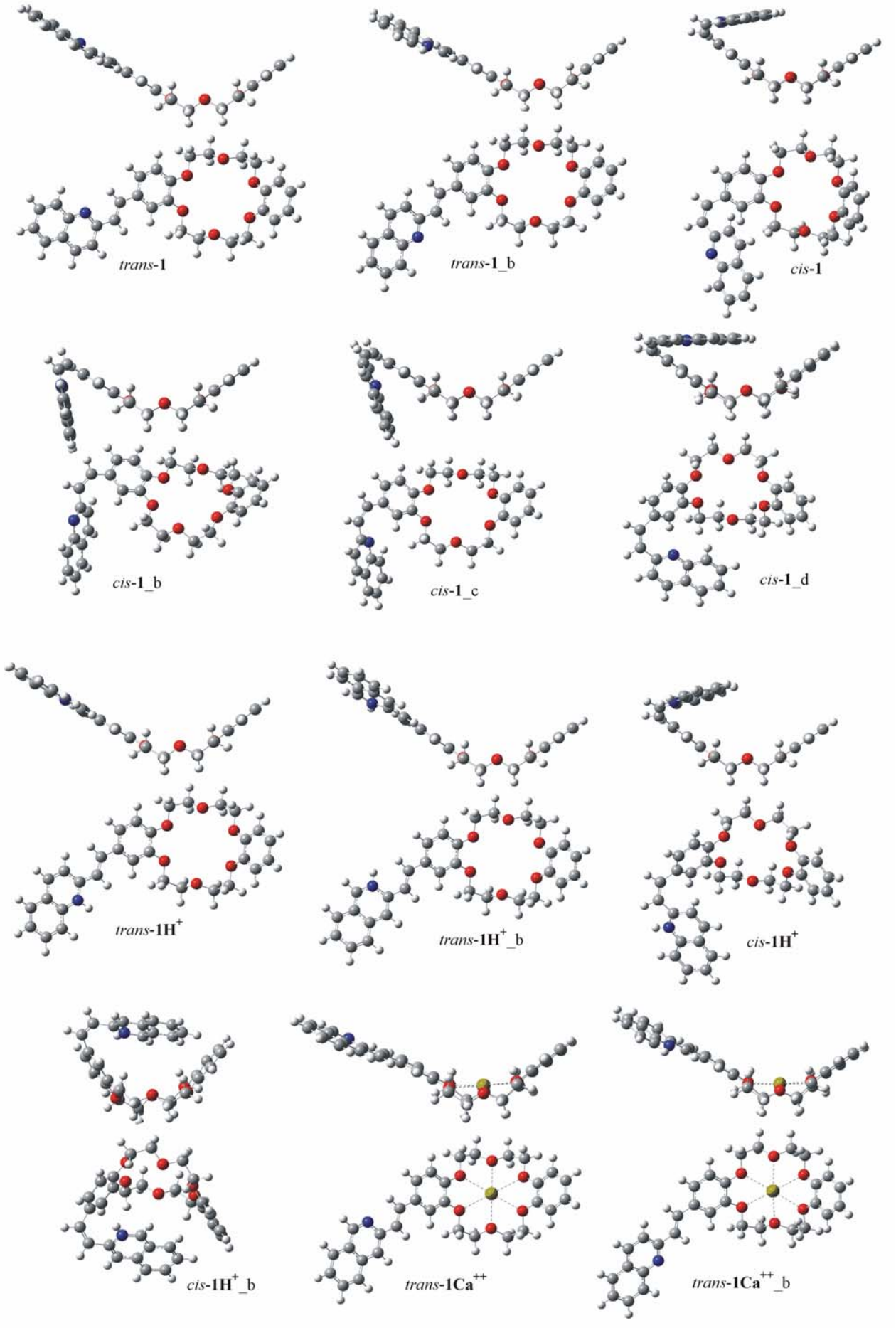

Figure 1S (continues)

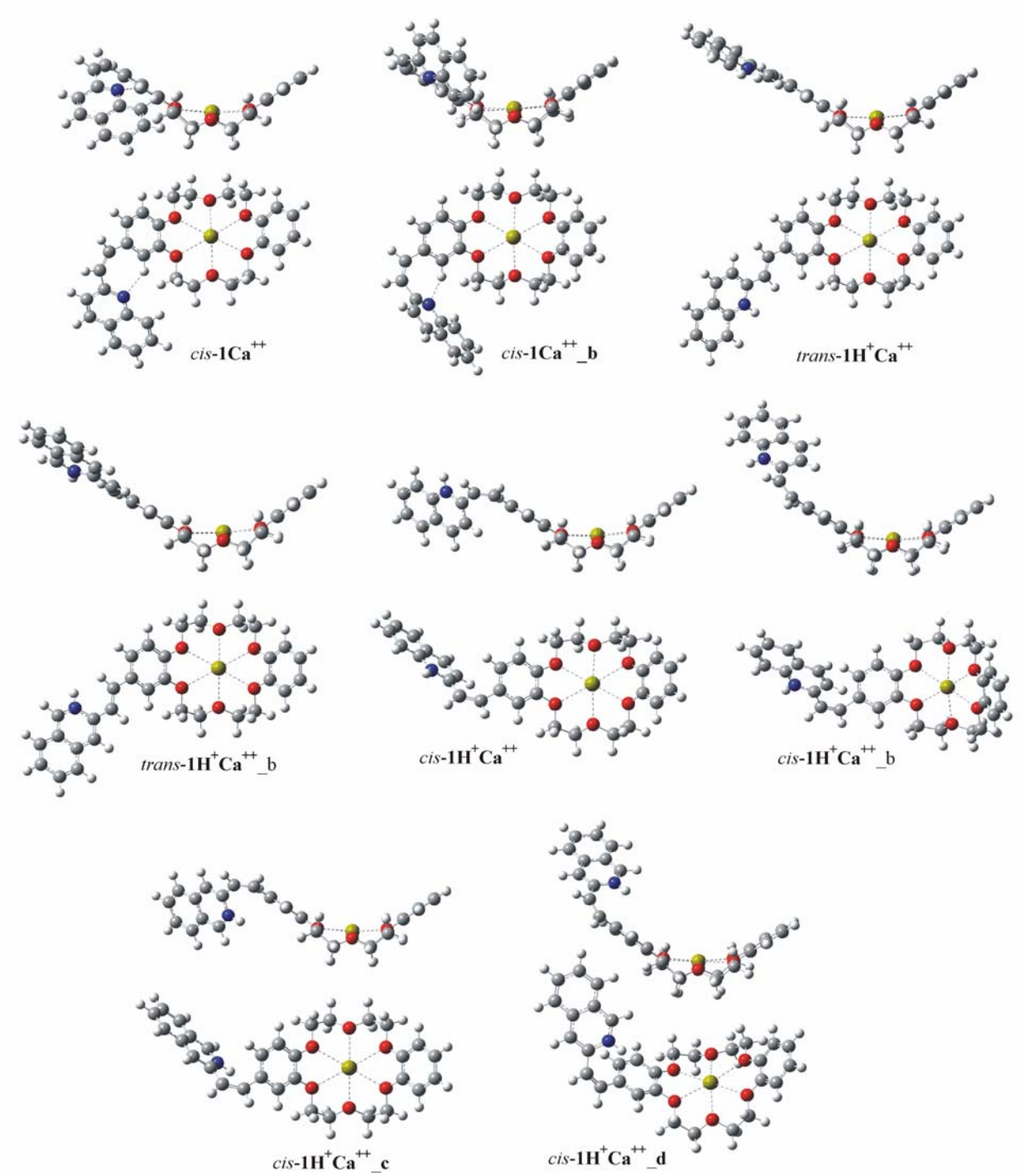

Figure 1S. Calculated minima structures of the **1**, **1H**$^{+}$, **1Ca**$^{++}$, and **1H**$^{+}$**Ca**$^{++}$ trans and cis isomers in acetonitrile solvent at the M06-2X level of theory viewed in two different angles. (H atoms = white, C = grey, O = red, N = blue and Ca = yellow spheres).

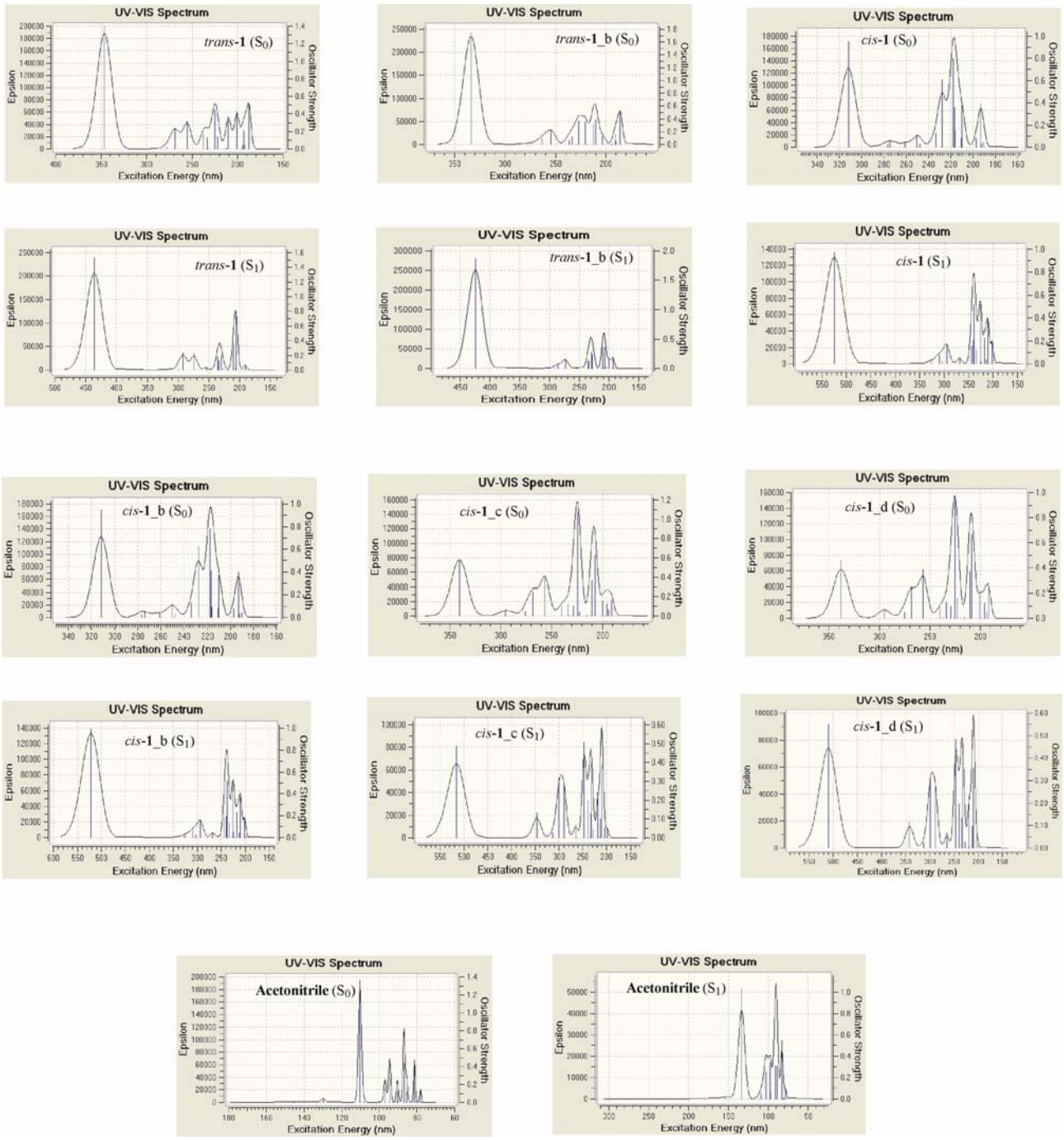

Figure 2S. Absorption (under S_0) and emission (under S_1) spectra of the **1** trans and cis isomers and acetonitrile in acetonitrile solvent at the M06-2X levels of theory.

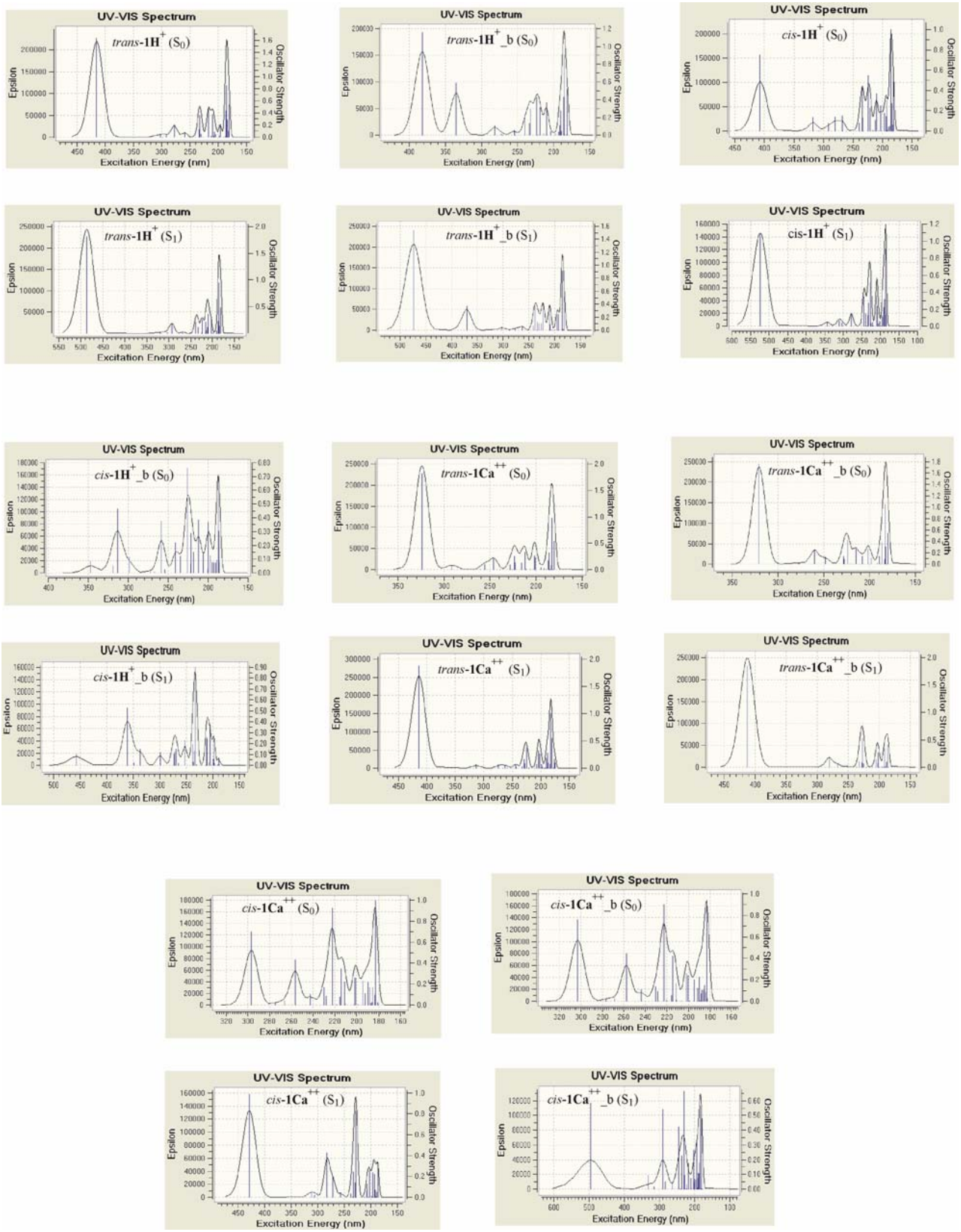

Figure 3S. Absorption (under S_0) and emission (under S_1) spectra of the **1H**$^+$ and **1Ca**$^{++}$ trans and cis isomers in acetonitrile solvent at the M06-2X levels of theory.

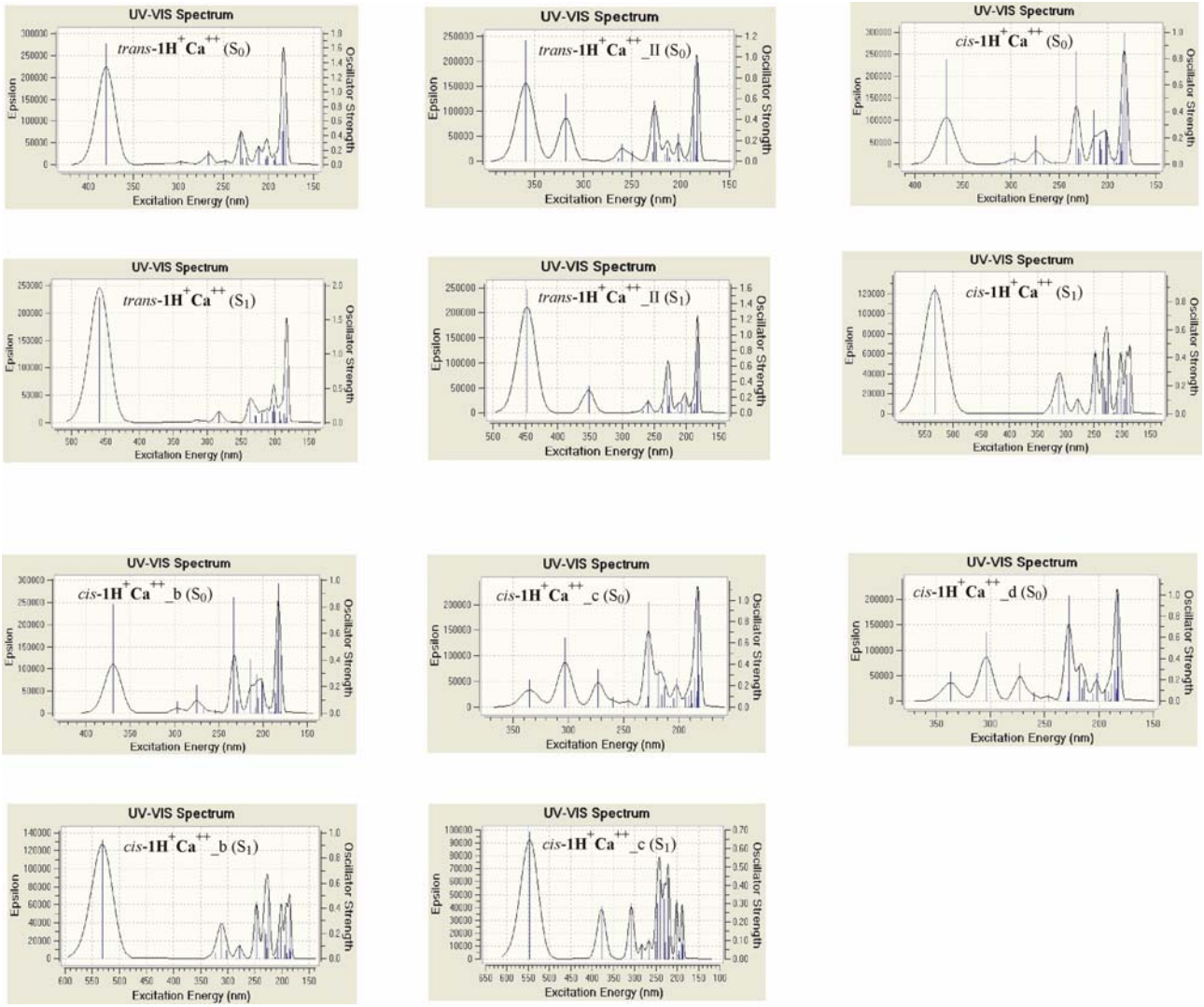

Figure 4S. Absorption (under S_0) and emission (under S_1) spectra of the **1H$^+$Ca^{++}** trans and cis isomers in acetonitrile solvent at the M06-2X levels of theory.

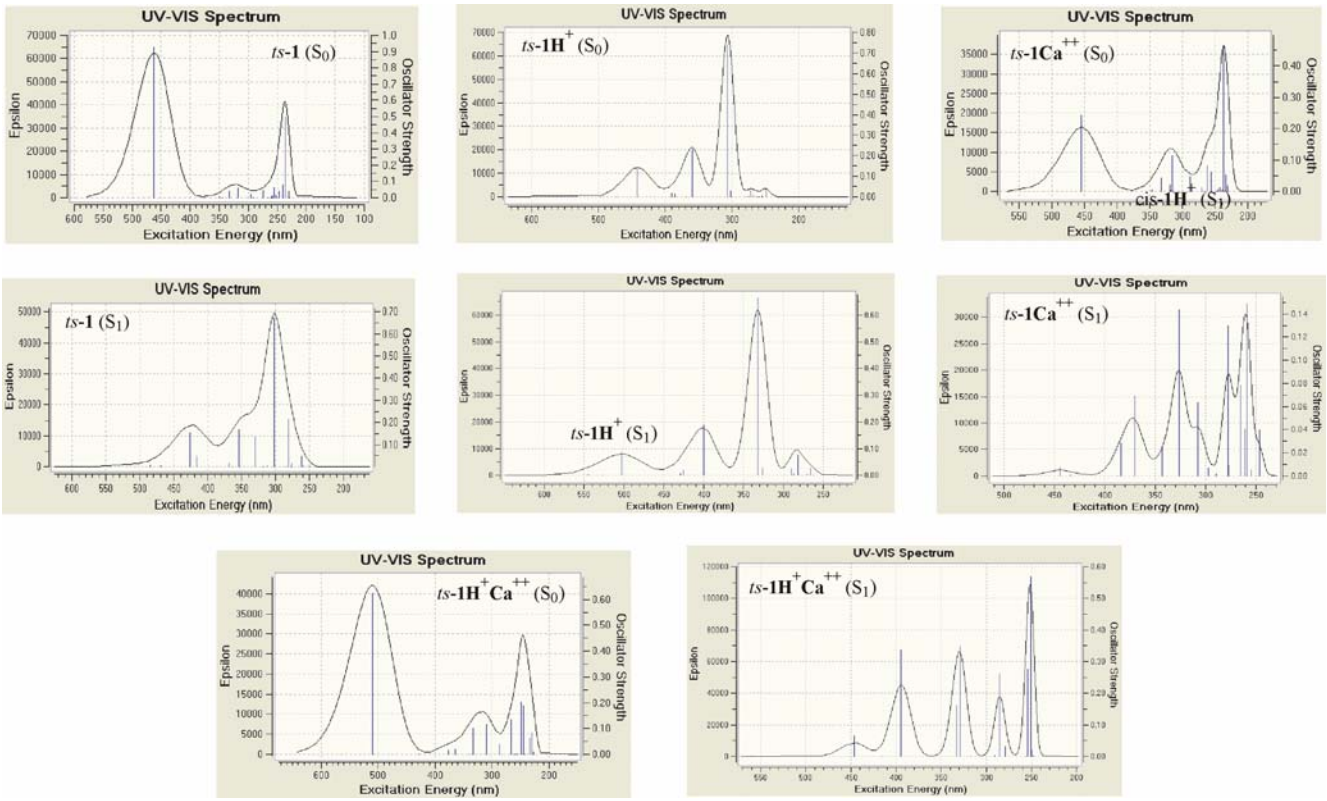

Figure 5S. Spectra of the *ts*-**1** *ts*-**1H**$^{+}$, *ts*-**1Ca**$^{++}$ and *ts*-**1H**$^{+}$**Ca**$^{++}$ structures in acetonitrile solvent at the S_0 and S_1 potential energy curves at the PBE0 level of theory at the vis-UV area.

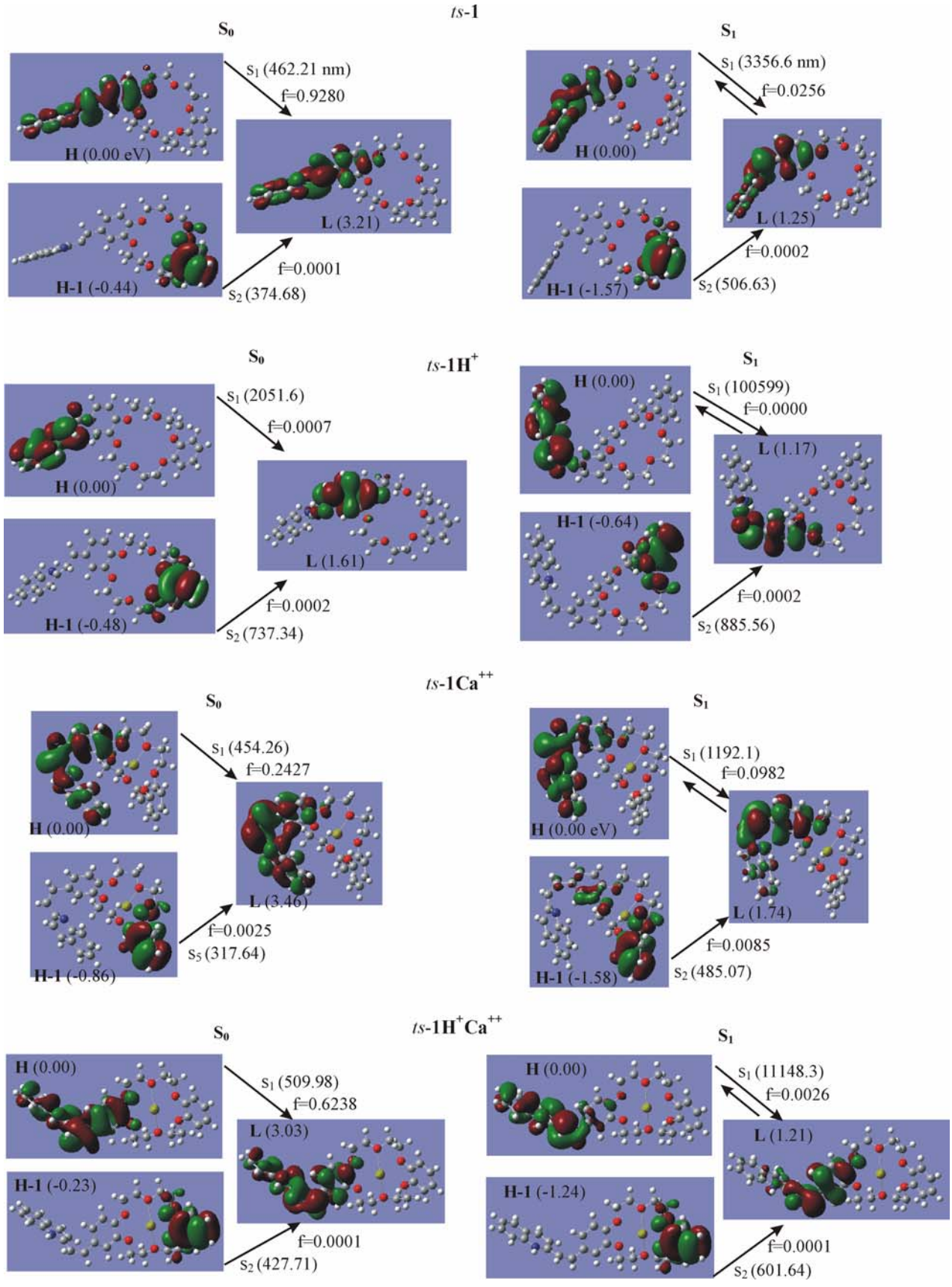

Figure 6S. Electron density plots of the HOMO (H), HOMO-1 (H-1) and LUMO (L) molecular orbitals involved in the s_1 or s_2 excitations of the S_0 and S_1 potential energy curves of *ts*-**1** *ts*-**1H**$^+$, *ts*-**1Ca**$^{++}$ and *ts*-**1H**$^+$**Ca**$^{++}$ structures. The relative energies of MO are given in parentheses; f-values and λ_{max} in nm of the s_1 or s_2 excitations are also given.