Supporting Information

Computational Insight into the Electronic Structure and Absorption Spectra of Lithium Complexes of N-confused Tetraphenylporphyrin

Demeter Tzeli, Ioannis D. Petsalakis and Giannoula Theodorakopoulos*

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

- **TABLE 1S:** Geometry, R(Å) and φ(degrees), Mulliken Charges of **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** Species in the Gas Phase and in Toluene Solvent at the B3LYP, CAM-B3LYP, and M06-2X /6-31G(d,p) Levels of Theory; Crystallographic Data are also included.
- **TABLE 2S:** Excitation Energies, ΔE_e(eV), Absorption Selected Peaks (Q Band and Soret Band), λ(nm), Oscillator Strengths, f, Main Excitations and their Coefficient Contributing to the Excited State of the **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, **1aTHF** Species in the Gas Phase at the B3LYP, CAM-B3LYP, and M06-2X /6-31G(d,p) Levels of Theory.
- **TABLE 3S:** Excitation Energies, ΔE_e(eV), Absorption Selected Peaks (Q band and Soret band), λ(nm), Oscillator Strengths, f, of the **1a**, **1b**, **2**, **1bLi**, **1bLiTHF**, **2LiTHF**, and **1aTHF** Species in Toluene Solvent at the B3LYP, CAM-B3LYP, and M06-2X /6-31G(d,p) Levels of Theory.
- **TABLE 4S:** Relative Energies (eV) of the Four Frontier Orbitals (H-1, H, L, and L+1) of the **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, and **1aTHF** Species at the B3LYP and M06-2X /6-31G(d,p) Levels of Theory in the Gas Phase and in Toluene Solvent.
- **TABLE 5S:** The Coordinates of Optimized Structures of **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** Species in the Gas Phase are given at the M06-2X/6-31G(d,p) Levels of Theory.
- **Figures 1S-6S:** Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in the gas phase and in toluene solvent calculated at the B3LYP, CAM-B3LYP, and M06-2X/6-31G(d,p) level of theory.
- **Figure 7S:** Plots of the M06-2X frontier canonical molecular orbitals of the **1aLi-2**, **1aTHF-1**, and **1aTHF-2** species.

TABLE 1S: Geometry, R(Å) and φ(degrees), Mulliken Charges of **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** Species in the Gas Phase and in Toluene Solvent at the B3LYP, CAM-B3LYP, and M06-2X /6-31G(d,p) Levels of Theory; Crystallographic Data are also included.

Species	Method	R_{Li-N1}	R_{Li-N2}	R_{Li-N3}	R_{Li-O}	R_{Li-C1}	R_{Li-H1}	R_{C1-H1}	φ_{LiH1C1}	q_{Li}	q_{N1}	q_{N2}	q_{N3}	q_{H1}	q_{C1}	q_{O}
1bLi	**B3LYP**	1.924	2.092	2.089		2.422	2.017	1.078	98.4	0.32	-0.66	-0.67	-0.67	0.19	-0.22	
	CAM-B3LYP	1.897	2.080	2.067		2.395	1.996	1.077	97.9	0.29	-0.66	-0.65	-0.66	0.20	-0.22	
	M062X	1.909	2.086	2.059		2.390	1.992	1.078	97.8	0.34	-0.68	-0.67	-0.68	0.22	-0.22	
	M062X[a]	1.916	2.093	2.067		2.394	2.005	1.079	97.3	0.34	-0.68	-0.67	-0.68	0.22	-0.22	
	Cryst. Data[b]	1.916(6)	2.067(6)	2.085(6)		2.363(6)	1.981	1.005	99.4(3)							
1aLi-1	**B3LYP**	1.965	2.624	1.922		2.403	2.084	1.082	93.4	0.34	-0.71	-0.69	-0.67	0.15	-0.25	
	CAM-B3LYP	1.958	2.580	1.921		2.391	2.058	1.081	94.0	0.32	-0.69	-0.69	-0.65	0.16	-0.24	
	M062X	1.979	2.614	1.927		2.398	2.078	1.083	93.3	0.38	-0.72	-0.72	-0.69	0.18	-0.24	
1aLi-2	**B3LYP**	1.964	1.924	2.615		2.391	2.068	1.082	93.4	0.34	-0.71	-0.67	-0.68	0.15	-0.25	
	CAM-B3LYP	1.959	1.922	2.576		2.368	2.043	1.081	93.4	0.32	-0.69	-0.66	-0.69	0.15	-0.24	
	M062X	1.980	1.926	2.616		2.379	2.057	1.083	93.3	038	-0.72	-0.69	-0.72	0.18	-0.23	
1bLiTHF-1	**B3LYP**	1.964	2.167	2.154	2.071	2.483	2.102	1.076	97.5	0.32	-0.63	-0.64	-.065	0.19	-0.22	-0.50
	CAM-B3LYP	1.948	2.150	2.132	2.033	2.446	2.080	1.077	96.4	0.27	-0.62	-0.62	-0.63	0.21	-0.22	-0.50
	M062X	1.942	2.125	2.131	1.987	2.395	2.048	1.079	94.9	0.28	-0.62	-0.63	-0.64	0.24	-0.21	-0.52
	M062X[a]	1.942	2.127	2.134	1.985	2.396	2.044	1.079	95.2	0.28	-0.62	-0.63	-0.64	0.24	-0.21	-0.53
	Cryst. Data[b]	1.938(4)	2.149(4)	2.156(4)	1.983(4)	2.482(4)	2.040	0.957	106.0(2)							
1bLiTHF-2	**B3LYP**	1.972	2.165	2.158	2.044	2.491	2.106	1.078	97.7	0.31	-0.63	-0.65	-0.65	0.19	-0.22	-0.51
	CAM-B3LYP	1.945	2.146	2.127	2.017	2.447	2.069	1.076	97.1	0.26	-0.62	-0.63	-0.63	0.21	-0.22	-0.51
	M062X	1.943	2.116	2.120	1.983	2.398	2.029	1.079	96.2	0.27	-0.63	-0.63	-0.64	0.24	-0.21	-0.53
2LiTHF-1	**B3LYP**	1.966	2.160	2.149	2.064	2.501	2.193	1.078	93.4	0.32	-0.63	-0.64	-0.65	0.18	-0.24	-0.52
	CAM-B3LYP	1.952	2.145	2.124	2.041	2.463	2.176	1.078	92.1	0.28	-0.62	-0.62	-0.63	0.19	-0.23	-0.50

	M062X	1.943	2.125	2.113	2.004	2.406	2.149	1.081	90.1	0.30	-0.62	-0.62	-0.64	0.22	-0.23	-0.52
	M062X[a]	1.946	2.130	2.113	2.002	2.407	2.138	1.080	90.7	0.29	-0.62	-0.62	-0.64	0.22	-0.23	-0.52
2LiTHF-2	**B3LYP**	1.972	2.159	2.154	2.055	2.500	2.196	1.079	93.1	0.32	-0.63	-0.64	-0.65	0.18	-0.24	-0.51
	CAM-B3LYP	1.949	2.140	2.120	2.026	2.464	2.172	1.078	92.3	0.27	-0.62	-0.63	-0.64	0.19	-0.23	-0.51
	M062X	1.949	2.120	2.101	1.992	2.405	2.131	1.081	90.3	0.28	-0.63	-0.63	-0.64	0.22	-0.23	-0.53
	Cryst. Data[b]	1.969(6)	2.172(7)	2.155(7)	2.036(7)	2.416(6)	2.108	0.929								
		$R_{H\text{-}N1}$	**$R_{H2\text{-}O}$**	**$R_{H3\text{-}O}$**	**$R_{H1\text{-}O}$**			**$R_{C1\text{-}H1}$**	**φ_{HH1C1}**	**q_H**	**q_{N1}**	**q_{N2}**	**q_{N3}**	**q_{H1}**	**q_{C1}**	**q_O**
1aTHF-1	**B3LYP**		2.354	2.176				1.079			-0.66	-0.66	-0.66	0.12	-0.18	-0.53
	CAM-B3LYP		2.286	2.050				1.078			-0.65	-0.67	-0.64	0.13	-0.18	-0.53
	M062X		2.063	2.024				1.081			-0.65	-0.69	-0.67	0.15	-0.16	-0.56
1aTHF-2	**B3LYP**				2.390			1.082			-0.70	-0.66	-0.67	0.15	-0.22	-0.48
	CAM-B3LYP				2.286			1.081			-0.69	-0.65	-0.66	0.15	-0.22	-0.49
	M062X				2.184			1.082			-0.69	-0.67	-0.68	0.14	-0.17	-0.51
1a	**B3LYP**							1.079			-0.71	-0.67	-0.66	0.12	-0.21	
	CAM-B3LYP							1.079			-0.70	-0.67	-0.66	0.12	-0.21	
	M062X							1.081			-0.72	-0.70	-0.69	0.14	-0.19	
1b	**B3LYP**	1.015						1.071	142.5	0.32	-0.68	-0.65	-0.65	0.13	-0.09	
	CAM-B3LYP	1.014						1.071	141.8	0.32	-0.68	-0.63	-0.63	0.13	-0.09	
	M062X	1.016						1.073	139.6	0.34	-0.70	-0.64	-0.65	0.16	-0.07	
2	**B3LYP**	1.016						1.073	132.9	0.32	-0.68	-0.64	-0.64	0.12	-0.10	
	CAM-B3LYP	1.015						1.073	130.8	0.32	-0.68	-0.62	-0.62	0.13	-0.10	
	M062X	1.017						1.075	130.0	0.34	-0.71	-0.64	-0.64	0.15	-0.08	

[a] In toluene solvent. [b] Ref. 8.

TABLE 2S: Excitation Energies, ΔE_e(eV), Absorption Selected Peaks (Q Band and Soret Band), λ(nm), Oscillator Strengths, f, Main Excitations and their Coefficient Contributing to the Excited State of the **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, **1aTHF** Species in the Gas Phase at the B3LYP, CAM-B3LYP, and M06-2X /6-31G(d,p) Levels of Theory.

	ΔE_e	λ	f	ΔE_e	λ	f	ΔE_e	λ	f	St.	Excitations
	B3LYP			**CAM-B3LYP**			**M06-2X**				
1a	1.95	636	0.075	1.96	632	0.049	2.01	617	0.060	1st	0.83|H→L⟩+0.49|H-1→L+1⟩
	2.17	571	0.076	2.26	547	0.065	2.31	536	0.088	2nd	0.80|H→L+1⟩-0.54|H-1→L⟩
	2.95	420	0.49	3.23	383	0.94	3.22	385	0.99	3rd	0.72|H-1→L+1⟩+0.42|H-1→L⟩
	3.12	397	1.03	3.32	373	1.33	3.30	375	1.32	4th	0.71|H-1→L⟩+0.47|H→L+1⟩
1b	1.78	696	0.17	2.07	600	0.17	2.06	603	0.19	1st	0.95|H→L⟩
	3.03	410	0.27	3.37	368	1.35	3.32	373	1.35	3rd	0.80|H-1→L⟩+0.58|H→L+1⟩
	3.06	405	0.76	3.58	347	0.34	3.53	352	0.36	4th	0.90|H-1→L+1⟩
2	1.77	700	0.17	2.07	600	0.17	2.05	606	0.19	1st	0.95|H→L⟩
	3.00	413	0.62	3.33	372	1.32	3.28	377	1.37	3rd	0.78|H-1→L⟩-0.61|H→L+1⟩
	3.04	407	0.50	3.58	346	0.32	3.52	352	0.32	4th	0.90|H-1→L+1⟩
1bLi	1.70	729	0.21	1.86	667	0.23	1.87	664	0.25	1st	0.96|H→L⟩
	2.97	417	0.86	3.28	378	1.37	3.24	382	1.42	3rd	0.82|H-1→L⟩-0.57|H→L+1⟩
1aLi-1							2.10	589	0.047	1st	0.83|H→L⟩-0.52|H-1→L+1⟩
							3.20	387	1.24	3rd	0.67|H-1→L⟩-0.58|H→L+1⟩
1aLi-2							2.08	596	0.059	1st	0.85|H→L⟩+0.51|H-1→L+1⟩
							3.24	383	1.22	4th	0.60|H-1→L+1⟩-0.51|H-1→L⟩
1bLiTHF-1	1.65	754	0.19	1.80	688	0.21	1.82	681	0.23	1st	0.97|H→L⟩
	2.93	422	0.70	3.22	385	1.22	3.19	389	1.26	3rd	0.84|H-1→L⟩+0.54|H→L+1⟩
1bLiTHF-1	1.64	754	0.19	1.80	689	0.21	1.83	679	0.23	1st	0.97|H→L⟩
	2.94	422	0.70	3.23	384	1.24	3.20	388	1.28	3rd	0.83|H-1→L⟩-0.54|H→L+1⟩
2LiTHF-1	1.63	761	0.19	1.80	689	0.21	1.81	685	0.23	1st	0.97|H→L⟩
	2.89	429	0.56	3.20	387	1.22	3.16	393	1.23	3rd	0.82|H-1→L⟩-0.56|H→L+1⟩
	2.92	425	0.44	3.63	341	0.29	3.59	346	0.30	5th	0.63|H-2→L⟩-0.64|H-1→L+1⟩
2LiTHF-1	1.63	762	0.19	1.80	690	0.21	1.82	682	0.23	1st	0.97|H→L⟩
	2.89	429	0.57	3.20	387	1.22	3.16	392	1.25	3rd	0.81|H-1→L⟩-0.57|H→L+1⟩

	2.92	425	0.44	3.63	341	0.29	3.59	346	0.27	5th	0.69|H-2→L⟩-0.56|H-1→L+1⟩
1aTHF-1	1.83	678	0.10	1.91	650	0.080	1.90	653	0.088	1st	0.87|H→L⟩+0.43|H-1→L+1⟩
	2.06	602	0.13	2.19	566	0.12	2.21	561	0.14	2nd	0.85|H→L+1⟩-0.48|H-1→L⟩
	2.88	431	0.45	3.18	390	0.83	3.15	394	0.85	3rd	0.71|H-1→L-1⟩+0.50|H-1→L⟩
	3.04	407	0.97	3.25	382	1.13	3.22	385	1.12	4th	0.71|H-1→L⟩-0.52|H-1→L+1⟩
1aTHF-2	1.94	640	0.074	1.96	632	0.048	2.00	620	0.057	1st	0.83|H→L⟩+0.47|H-1→L+1⟩
	2.16	575	0.073	2.26	550	0.063	2.30	539	0.089	2nd	0.80|H→L+1⟩-0.52|H-1→L⟩
	2.92	424	0.45	3.20	367	0.86	3.19	389	0.90	3rd	0.70|H-1→L-1⟩+0.47|H-1→L⟩
	3.10	400	0.98	3.29	377	1.21	3.28	378	1.19	4th	0.69|H-1→L⟩-0.49|H-1→L+1⟩

TABLE 3S: Excitation Energies, ΔE_e(eV), Absorption Selected Peaks (Q band and Soret band), λ(nm), Oscillator Strengths, f, of the **1a**, **1b**, **2**, **1bLi**, **1bLiTHF**, **2LiTHF**, and **1aTHF** Species in Toluene Solvent at the B3LYP, CAM-B3LYP, and M06-2X /6-31G(d,p) Levels of Theory.

	ΔE_e	λ	f	ΔE_e	λ	f	ΔE_e	λ	f
	B3LYP			**CAM-B3LYP**			**M06-2X**		
1a	1.93	644	0.13	1.94	639	0.085	1.99	624	0.11
	2.16	574	0.12	2.25	551	0.094	2.29	540	0.13
	2.88	430	0.88	3.12	398	1.35	3.10	400	1.39
	2.97	417	1.45	3.14	394	1.63	3.13	396	1.59
1b	1.76	703	0.24	2.05	606	0.23	2.03	609	0.26
	2.90	427	1.46	3.20	388	1.72	3.15	393	1.75
	2.98	416	0.15	3.49	359	0.68	3.44	360	0.69
2	1.75	707	0.24	2.05	606	0.23	2.03	612	0.26
	2.87	432	1.49	3.17	391	1.68	3.12	397	1.72
	2.97	417	0.09	3.50	354	0.65	3.44	360	0.65
1bLi	1.67	744	0.29	1.82	681	0.31	1.83	679	0.34
	2.83	438	1.56	3.11	399	1.73	3.04	404	1.75
	2.97	418	0.13	3.56	3.48	0.64	349	355	0.60
1bLiTHF-1	1.62	765	0.27	1.77	699	0.28	1.79	692	0.31
	2.81	442	1.43	3.08	402	1.57	3.05	407	1.59
				3.53	351	0.59	3.48	356	0.54
1bLiTHF-2	1.62	767	0.27	1.77	701	0.29	1.80	690	0.31
	2.81	442	1.43	3.08	402	1.59	3.05	406	1.62
				3.53	351	0.60	3.47	358	0.56
2LiTHF-1	1.60	773	0.26	1.77	700	0.28	1.78	696	0.31
	2.78	445	1.42	3.06	405	1.56	3.02	410	1.56
	3.32	373	0.36	3.53	351	0.26	3.50	354	0.51
				3.57	347	0.31			
2LiTHF-2	1.60	774	0.26	1.77	702	0.29	1.78	695	0.31
	2.78	445	1.42	3.06	405	1.57	3.02	410	1.59
	3.32	373	0.36	3.53	351	0.26	3.50	354	0.51
				3.57	347	0.31			
1aTHF-1	1.80	689	0.17	1.87	662	0.13	1.87	663	0.14

	2.03	610	0.21	2.16	573	0.18	2.18	568	0.22
	2.82	440	0.77	3.08	403	1.18	3.05	407	1.19
	2.92	425	1.29	3.10	400	1.42	3.03	403	1.38
1aTHF-2	1.91	648	0.13	1.94	640	0.082	1.99	624	0.10
	2.15	578	0.11	2.24	553	0.090	2.29	542	0.13
	2.87	433	0.79	3.10	400	1.25	3.09	402	1.28
	2.96	418	1.36	3.14	395	1.52	3.13	397	1.47

TABLE 4S: Relative Energies (eV) of the Four Frontier Orbitals of the **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1bLiTHF**, **2LiTHF**, and **1aTHF** Species at the B3LYP and M06-2X /6-31G(d,p) Levels of Theory in the Gas Phase and in Toluene Solvent.

	H-1	**H**	**L**	**L+1**	**H-1**	**H**	**L**	**L+1**
	B3LYP				**M06-2X**			
1a	0	0.54	2.96	3.06	0	0.57	4.45	4.53
1b	0	0.77	2.85	3.43	0	0.80	4.51	5.13
1b[a]	0	0.76	2.86	3.42	0	0.79	4.51	5.10
2	0	0.75	2.83	3.43	0	0.78	4.49	5.15
2[a]	0	0.74	2.84	3.42	0	0.76	4.49	5.12
1bLi	0	0.83	2.79	3.43	0	0.97	4.41	5.15
1bLi[a]	0	0.82	2.80	3.42	0	0.96	4.42	5.13
1aLi-1					0	0.37	4.31	4.47
1aLi-2					0	0.42	4.33	4.49
1bLiTHF-1	0	0.86	2.78	3.41	0	1.00	4.41	5.14
1bLiTHF-1[a]	0	0.86	2.79	3.41	0	0.99	4.42	5.12
1bLiTHF-2	0	0.87	2.78	3.42	0	1.00	4.41	5.12
2LiTHF-1	0	0.86	2.77	3.44	0	1.00	4.42	5.19
2LiTHF-1[a]	0	0.86	2.78	3.43	0	0.99	4.42	5.17
2LiTHF-2	0	0.87	2.77	3.44	0	1.00	4.41	5.18
1aTHF-1	0	0.70	2.95	3.05	0	0.75	4.44	4.53
1aTHF-2	0	0.55	2.95	3.06	0	0.58	4.45	4.52

[a] In toluene solvent.

TABLE 5S: The Coordinates of Optimized Structures of 1a, 1b, 2, 1bLi, 1aLi, 1bLiTHF, 2LiTHF, 1aTHF, and 1bTHF Species in the Gas Phase are given at the M06-2X/6-31G(d,p) Levels of Theory.

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.139406	-2.959180	-0.195025
2	6	0	-0.675168	-4.314142	-0.284838
3	6	0	0.683061	-4.315584	-0.153490
4	6	0	1.115910	-2.953499	-0.013559
5	6	0	1.131158	2.910250	-0.168468
6	6	0	0.703839	4.255721	-0.360551
7	6	0	-0.668237	4.271648	-0.305913
8	6	0	-1.122321	2.942010	-0.074517
9	6	0	-2.452713	2.489734	0.053563
10	6	0	-2.789518	1.129511	0.010412
11	6	0	-4.050348	-0.587740	0.355893
12	1	0	-4.894163	-1.191869	0.674171
13	6	0	-1.994515	0.021146	-0.366193
14	6	0	-2.774856	-1.115029	-0.138739
15	6	0	-2.452893	-2.492571	-0.198486
16	6	0	-3.510011	3.505267	0.273364
17	6	0	-3.568155	-3.472903	-0.219695
18	6	0	-3.634757	-4.546281	0.678045
19	6	0	-4.700120	-5.439734	0.633570
20	6	0	-5.717014	-5.272828	-0.303497
21	6	0	-5.667553	-4.202356	-1.192759
22	6	0	-4.604171	-3.308154	-1.148643
23	1	0	-1.319255	-5.166247	-0.442919
24	1	0	1.343873	-5.169113	-0.160021
25	1	0	1.366386	5.092336	-0.522668
26	1	0	-1.322254	5.119996	-0.441587
27	1	0	-1.049392	0.060662	-0.889232
28	1	0	-2.856998	-4.660682	1.427178
29	1	0	-4.742461	-6.261603	1.341173
30	1	0	-6.547720	-5.970320	-0.335809
31	1	0	-6.456549	-4.064528	-1.924953
32	1	0	-4.557694	-2.476284	-1.845220
33	7	0	-0.008175	-2.181418	-0.055003
34	7	0	0.005542	2.156621	-0.012455
35	7	0	-4.062313	0.704779	0.447590
36	6	0	-3.334846	4.528191	1.214082
37	1	0	-2.426532	4.553279	1.808228
38	6	0	-4.705692	3.455902	-0.454311
39	6	0	-4.323178	5.486794	1.411550
40	1	0	-4.176514	6.266356	2.152192
41	6	0	-5.499686	5.438018	0.669629
42	1	0	-6.270438	6.187083	0.820861
43	6	0	-5.688066	4.418909	-0.261888
44	1	0	-6.605548	4.373626	-0.839699
45	1	0	-4.851794	2.656122	-1.171603
46	6	0	2.448195	2.409307	-0.116084
47	6	0	2.803200	1.063440	0.022278
48	6	0	3.531172	3.430560	-0.249072
49	6	0	4.371513	3.731960	0.826871
50	6	0	3.711865	4.109550	-1.458324
51	6	0	5.373437	4.689222	0.694796
52	1	0	4.231014	3.209389	1.768643
53	6	0	4.711168	5.069051	-1.589506
54	1	0	3.064894	3.872402	-2.298146
55	6	0	5.544654	5.360958	-0.512832
56	1	0	6.017436	4.914636	1.538901
57	1	0	4.842602	5.583571	-2.536105
58	1	0	6.324478	6.108632	-0.615370
59	6	0	4.201262	0.639615	0.023714
60	6	0	4.191949	-0.703169	0.112652
61	6	0	2.785753	-1.104909	0.148583
62	7	0	1.965067	-0.021570	0.103082
63	1	0	5.053897	1.297033	-0.060491
64	1	0	5.035332	-1.377501	0.112990
65	6	0	2.420855	-2.469528	0.126438
66	6	0	3.504410	-3.492507	0.226039
67	6	0	3.793489	-4.346167	-0.843622
68	6	0	4.253929	-3.609221	1.401407
69	6	0	4.804608	-5.297310	-0.738220
70	1	0	3.225441	-4.250455	-1.764807
71	6	0	5.268206	-4.555711	1.505469
72	1	0	4.032313	-2.947657	2.233938
73	6	0	5.544506	-5.404289	0.436275
74	1	0	5.020649	-5.949142	-1.578843
75	1	0	5.839968	-4.633264	2.424839
76	1	0	6.334395	-6.143973	0.517900
77	1	0	0.035238	-1.185224	0.115764
78	1	0	0.059050	1.180147	0.249823

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.468604	2.788803	-0.034654
2	6	0	1.218126	4.228989	-0.048626
3	6	0	-0.121674	4.381390	-0.010130
4	6	0	-0.682732	3.025129	0.002569
5	6	0	-1.457535	-2.756825	-0.083414
6	6	0	-1.257899	-4.209762	-0.139896
7	6	0	0.077724	-4.400348	-0.166947
8	6	0	0.681704	-3.069285	-0.109540
9	6	0	2.037346	-2.809500	-0.095009
10	6	0	2.554465	-1.472494	-0.110623
11	6	0	4.085791	0.118447	0.294034
12	1	0	5.033686	0.536892	0.600133
13	6	0	1.950204	-0.250864	-0.346031
14	6	0	2.897225	0.766769	-0.079025
15	6	0	2.713103	2.196643	-0.046481
16	6	0	3.016353	-3.922814	0.005434
17	6	0	3.939589	3.033304	0.014026
18	6	0	4.125868	3.985192	1.024508
19	6	0	5.284698	4.754271	1.068271
20	6	0	6.276664	4.583287	0.105832
21	6	0	6.107378	3.632462	-0.897949
22	6	0	4.952219	2.859450	-0.939498
23	1	0	1.972628	5.000778	-0.099784
24	1	0	-0.686928	5.301810	0.007317
25	1	0	-2.038686	-4.956482	-0.151580
26	1	0	0.614312	-5.335879	-0.236867
27	1	0	0.938127	-0.111005	-0.672936
28	1	0	3.357696	4.105052	1.782266
29	1	0	5.415513	5.484954	1.860083
30	1	0	7.178697	5.185748	0.139420
31	1	0	6.874362	3.495987	-1.653708
32	1	0	4.813487	2.123136	-1.725648
33	7	0	0.265214	2.098301	-0.011708
34	7	0	-0.303468	-2.100338	-0.070289
35	7	0	3.872164	-1.204436	0.266373
36	1	0	4.537964	-1.916768	0.527623
37	6	0	2.911978	-4.879274	1.024041
38	1	0	2.101042	-4.795754	1.740914
39	6	0	4.086873	-4.015417	-0.896142
40	6	0	3.840317	-5.909910	1.126255
41	1	0	3.745419	-6.641589	1.922133
42	6	0	4.893464	-5.997495	0.219269
43	1	0	5.618483	-6.800670	0.301573
44	6	0	5.014787	-5.047070	-0.791783
45	1	0	5.829203	-5.113076	-1.506218
46	1	0	4.170557	-3.282256	-1.693909
47	6	0	-2.744701	-2.130043	-0.029669
48	6	0	-2.952924	-0.764138	0.018234
49	6	0	-3.950118	-3.009909	-0.033862
50	6	0	-4.816531	-3.032594	1.064466
51	6	0	-4.238792	-3.830347	-1.130755
52	6	0	-5.945155	-3.847318	1.065612
53	1	0	-4.591800	-2.405291	1.922411
54	6	0	-5.362790	-4.650851	-1.127960
55	1	0	-3.575339	-3.813740	-1.990906
56	6	0	-6.220481	-4.660160	-0.030415
57	1	0	-6.605050	-3.852070	1.927437
58	1	0	-5.574708	-5.277326	-1.988806
59	1	0	-7.098693	-5.297760	-0.030062
60	6	0	-4.255250	-0.124589	-0.056715
61	6	0	-4.076109	1.212314	-0.046163
62	6	0	-2.652175	1.486239	0.041221
63	7	0	-2.025678	0.255326	0.076343
64	1	0	-5.185773	-0.664610	-0.145983
65	1	0	-4.831741	1.979163	-0.126094
66	6	0	-2.092398	2.747849	0.027961
67	6	0	-3.024571	3.913365	-0.001605
68	6	0	-3.039336	4.776410	-1.103821
69	6	0	-3.898619	4.169455	1.060144
70	6	0	-3.903509	5.865535	-1.143129
71	1	0	-2.366802	4.580246	-1.934175
72	6	0	-4.769263	5.255325	1.018976
73	1	0	-3.886187	3.509356	1.922854
74	6	0	-4.772461	6.107604	-0.081638
75	1	0	-3.903926	6.521512	-2.007927
76	1	0	-5.440495	5.439691	1.851979
77	1	0	-5.447970	6.956446	-0.112329
78	1	0	-1.021450	0.118179	0.149523

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.394325	3.117721	0.138122
2	6	0	0.288186	4.401422	0.276735
3	6	0	1.610300	4.129474	0.271219
4	6	0	1.721696	2.672166	0.149608
5	6	0	0.642474	-3.045837	-0.046200
6	6	0	0.004679	-4.359715	0.115318
7	6	0	-1.320237	-4.122357	0.189672
8	6	0	-1.487034	-2.676355	0.029271
9	6	0	-2.699231	-2.019446	0.010970
10	6	0	-2.779787	-0.585172	-0.085923
11	6	0	-3.633844	1.413866	-0.605830
12	1	0	-4.331769	2.121345	-1.032353
13	6	0	-1.849354	0.370521	0.278985
14	6	0	-2.372624	1.643440	-0.042188
15	6	0	-1.757593	2.943596	0.041732
16	6	0	-3.961799	-2.784833	0.184855
17	6	0	-2.662124	4.119036	-0.036289
18	6	0	-2.452734	5.138613	-0.973964
19	6	0	-3.324058	6.220624	-1.050167
20	6	0	-4.417735	6.301746	-0.192106
21	6	0	-4.641087	5.290061	0.739106
22	6	0	-3.775742	4.204121	0.810821
23	1	0	-0.192879	5.363733	0.378965
24	1	0	2.433516	4.825935	0.337872
25	1	0	0.514565	-5.310750	0.167537
26	1	0	-2.114225	-4.838292	0.345121
27	1	0	-0.902580	0.164840	0.744858
28	1	0	-1.610382	5.062204	-1.654541
29	1	0	-3.152904	6.997808	-1.788188
30	1	0	-5.095813	7.147016	-0.251652
31	1	0	-5.490012	5.347837	1.412991
32	1	0	-3.944283	3.416358	1.538898
33	7	0	0.533685	2.087868	0.083850
34	7	0	-0.250743	-2.066684	-0.102441
35	7	0	-3.883749	0.094393	-0.634253
36	6	0	-4.319652	-3.843642	-0.657263
37	1	0	-3.653308	-4.119339	-1.469598
38	6	0	-4.836688	-2.416491	1.215324
39	6	0	-5.524112	-4.516832	-0.472354
40	1	0	-5.793371	-5.330773	-1.138003
41	6	0	-6.385429	-4.143680	0.556371
42	1	0	-7.325007	-4.667925	0.697658
43	6	0	-6.036245	-3.093249	1.403210
44	1	0	-6.698880	-2.802312	2.212170
45	1	0	-4.560809	-1.592801	1.868225
46	6	0	2.060423	-2.854226	-0.119303
47	6	0	2.685956	-1.622386	-0.137575
48	6	0	2.931421	-4.067443	-0.113353
49	6	0	3.711024	-4.397026	-1.227019
50	6	0	2.987985	-4.897164	1.012515
51	6	0	4.528000	-5.524630	-1.215518
52	1	0	3.668992	-3.758854	-2.105137
53	6	0	3.797193	-6.028985	1.022479
54	1	0	2.392753	-4.641600	1.884760
55	6	0	4.570709	-6.345467	-0.092042
56	1	0	5.126027	-5.765993	-2.088736
57	1	0	3.829777	-6.659808	1.905283
58	1	0	5.203800	-7.226910	-0.084154
59	6	0	4.125133	-1.430681	-0.068030
60	6	0	4.376920	-0.107559	-0.003995
61	6	0	3.110238	0.604639	-0.034673
62	7	0	2.126599	-0.362323	-0.127044

63	1	0	4.837233	-2.241439	-0.033792
64	1	0	5.336717	0.376838	0.094675
65	6	0	2.975361	1.971837	0.080678
66	6	0	4.226564	2.783631	0.141365
67	6	0	4.551703	3.514318	1.290296
68	6	0	5.099600	2.829635	-0.950539
69	6	0	5.719875	4.268375	1.345218
70	1	0	3.881105	3.480229	2.144437
71	6	0	6.271713	3.578618	-0.894655
72	1	0	4.846907	2.271544	-1.847575
73	6	0	6.584382	4.301145	0.253447
74	1	0	5.959622	4.825476	2.245492
75	1	0	6.937053	3.602389	-1.751986
76	1	0	7.496313	4.887939	0.297200
77	1	0	1.129488	-0.169288	-0.182061
78	6	0	-5.027831	-0.471024	-1.339025
79	1	0	-4.699122	-1.287222	-1.983237
80	1	0	-5.779066	-0.852843	-0.645815
81	1	0	-5.463627	0.315451	-1.955918

59	1	0	-5.223155	-5.673763	-1.824498
60	1	0	-6.621650	-5.844350	0.219100
61	6	0	-4.306123	-0.462421	0.036037
62	6	0	-4.239995	0.881645	0.015667
63	6	0	-2.813635	1.232052	0.068219
64	7	0	-2.063132	0.096716	0.131066
65	1	0	-5.184778	-1.088561	-0.022979
66	1	0	-5.053215	1.588347	-0.065941
67	6	0	-2.320779	2.528571	-0.018298
68	6	0	-3.314805	3.641796	-0.067768
69	6	0	-3.429513	4.445098	-1.208560
70	6	0	-4.163626	3.895323	1.015060
71	6	0	-4.361421	5.476094	-1.263513
72	1	0	-2.780396	4.247912	-2.057283
73	6	0	-5.100488	4.923973	0.959938
74	1	0	-4.079497	3.277283	1.904626
75	6	0	-5.200634	5.718715	-0.178389
76	1	0	-4.437262	6.086137	-2.158257
77	1	0	-5.749292	5.108113	1.810676
78	1	0	-5.929025	6.522237	-0.221225

58	1	0	5.191548	7.089920	-0.351869
59	6	0	4.011881	1.377786	-0.150868
60	6	0	4.261812	0.047043	-0.124259
61	6	0	2.981360	-0.611068	0.034917
62	7	0	1.976951	0.302388	0.102005
63	1	0	4.720827	2.180983	-0.287524
64	1	0	5.211524	-0.453497	-0.241525
65	6	0	2.847005	-2.026564	0.064126
66	6	0	4.082846	-2.857169	0.132536
67	6	0	4.347049	-3.811098	-0.857606
68	6	0	4.998744	-2.708609	1.180796
69	6	0	5.491254	-4.599959	-0.799955
70	1	0	3.646676	-3.922811	-1.680301
71	6	0	6.145349	-3.494863	1.237124
72	1	0	4.800732	-1.972187	1.954466
73	6	0	6.394097	-4.443982	0.248297
74	1	0	5.680772	-5.331618	-1.578920
75	1	0	6.843702	-3.370160	2.058556
76	1	0	7.288321	-5.057177	0.293449
77	1	0	0.357948	-1.300346	-0.778814
78	3	0	0.078056	0.326651	0.659331

1bLi

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.248334	2.846113	-0.166343
2	6	0	0.857418	4.248663	-0.209958
3	6	0	-0.490087	4.273475	-0.158982
4	6	0	-0.934520	2.880405	-0.099340
5	6	0	-1.238867	-2.786885	-0.110789
6	6	0	-0.928404	-4.216649	-0.223222
7	6	0	0.410833	-4.317171	-0.324531
8	6	0	0.936019	-2.956815	-0.249688
9	6	0	2.281561	-2.638149	-0.246522
10	6	0	2.721888	-1.271020	-0.247986
11	6	0	4.011268	0.438157	0.436659
12	1	0	4.834185	0.928864	0.935433
13	6	0	2.105000	-0.097260	-0.643406
14	6	0	2.886042	0.994858	-0.181887
15	6	0	2.554338	2.396679	-0.141393
16	6	0	3.323037	-3.684488	-0.108383
17	6	0	3.675750	3.349005	0.047993
18	6	0	3.639119	4.311259	1.067167
19	6	0	4.705141	5.182803	1.259947
20	6	0	5.829687	5.105303	0.442175
21	6	0	5.885575	4.144351	-0.564707
22	6	0	4.822197	3.268324	-0.755215
23	1	0	1.535436	5.085931	-0.290471
24	1	0	-1.136803	5.138129	-0.156461
25	1	0	-1.653612	-5.016931	-0.218828
26	1	0	1.001756	-5.212084	-0.456572
27	1	0	1.244573	-0.038899	-1.291529
28	1	0	2.772521	4.353006	1.719549
29	1	0	4.661076	5.916927	2.058214
30	1	0	6.660769	5.786798	0.592637
31	1	0	6.758590	4.079927	-1.206482
32	1	0	4.861898	2.521635	-1.542932
33	3	0	-0.157414	-0.011938	0.123695
34	7	0	0.114468	2.042688	-0.115993
35	7	0	-0.107937	-2.053785	-0.139895
36	7	0	3.904120	-0.901664	0.382726
37	1	0	4.540370	-1.564965	0.801241
38	6	0	3.220820	-4.682385	0.872171
39	1	0	2.359281	-4.683110	1.532439
40	6	0	4.468503	-3.661116	-0.919700
41	6	0	4.214142	-5.645171	1.013616
42	1	0	4.116215	-6.408846	1.778536
43	6	0	5.336979	-5.620807	0.189854
44	1	0	6.112826	-6.370949	0.303134
45	6	0	5.462855	-4.623238	-0.774408
46	1	0	6.334503	-4.598598	-1.420708
47	1	0	4.559803	-2.891016	-1.680931
48	6	0	-2.566885	-2.303046	0.022817
49	6	0	-2.920214	-0.949901	0.093875
50	6	0	-3.678299	-3.299192	0.068420
51	6	0	-4.478289	-3.403520	1.211876
52	6	0	-3.964137	-4.128851	-1.022405
53	6	0	-5.532153	-4.310793	1.266711
54	1	0	-4.261692	-2.762326	2.061718
55	6	0	-5.013362	-5.041495	-0.967271
56	1	0	-3.358055	-4.045760	-1.920463
57	6	0	-5.801192	-5.135062	0.177498
58	1	0	-6.140230	-4.376324	2.163653

1aLi-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.599564	-3.110084	-0.227934
2	6	0	0.073946	-4.355796	-0.012443
3	6	0	1.407560	-4.115396	0.153362
4	6	0	1.638043	-2.709488	0.006914
5	6	0	0.563060	3.052439	-0.078296
6	6	0	-0.051660	4.345795	-0.277717
7	6	0	-1.398109	4.138666	-0.265604
8	6	0	-1.595031	2.726069	-0.046280
9	6	0	-2.842652	2.054822	0.018612
10	6	0	-2.937212	0.655381	-0.058757
11	6	0	-3.863604	-1.271678	0.240901
12	1	0	-4.587162	-2.020819	0.547038
13	6	0	-1.953318	-0.291366	-0.455086
14	6	0	-2.520964	-1.558117	-0.258049
15	6	0	-1.964307	-2.864942	-0.276292
16	6	0	-4.077704	2.853210	0.192266
17	6	0	-2.903787	-4.018332	-0.194969
18	6	0	-2.861026	-4.917739	0.876929
19	6	0	-3.763708	-5.973264	0.953594
20	6	0	-4.728542	-6.141212	-0.036402
21	6	0	-4.792259	-5.241842	-1.097611
22	6	0	-3.889875	-4.185672	-1.174100
23	1	0	-0.424156	-5.312096	0.047575
24	1	0	2.179011	-4.834836	0.384386
25	1	0	0.470607	5.280673	-0.417616
26	1	0	-2.182037	4.864828	-0.424048
27	1	0	-1.076378	-0.026330	-1.032308
28	1	0	-2.128331	-4.768986	1.664688
29	1	0	-3.721859	-6.657220	1.795227
30	1	0	-5.434042	-6.963503	0.024378
31	1	0	-5.547070	-5.362111	-1.868041
32	1	0	-3.939122	-3.479720	-1.998022
33	7	0	0.394086	-2.124013	-0.194609
34	7	0	-0.390924	2.101168	0.071457
35	7	0	-4.106775	0.000121	0.357463
36	6	0	-4.131732	3.908075	1.113051
37	1	0	-3.262248	4.120221	1.727688
38	6	0	-5.219237	2.565847	-0.568339
39	6	0	-5.291333	4.661437	1.261166
40	1	0	-5.320118	5.469154	1.985627
41	6	0	-6.413513	4.374873	0.488810
42	1	0	-7.318248	4.963984	0.601881
43	6	0	-6.373472	3.323957	-0.425096
44	1	0	-7.246170	3.092801	-1.027412
45	1	0	-5.186246	1.743866	-1.274501
46	6	0	1.957267	2.797423	-0.061652
47	6	0	2.578834	1.542273	-0.009001
48	6	0	2.854002	3.990911	-0.149678
49	6	0	3.656200	4.349066	0.938127
50	6	0	2.909012	4.764437	-1.313470
51	6	0	4.493060	5.458601	0.866277
52	1	0	3.617551	3.748089	1.842030
53	6	0	3.746404	5.873723	-1.385622
54	1	0	2.293255	4.485401	-2.163669
55	6	0	4.539533	6.224216	-0.295766
56	1	0	5.106771	5.726616	1.720423
57	1	0	3.782151	6.462421	-2.296768

1aLi-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495979	2.802025	0.003072
2	6	0	1.247649	4.216997	-0.133185
3	6	0	-0.105055	4.375197	-0.125731
4	6	0	-0.672659	3.049602	0.000573
5	6	0	-1.539415	-2.759937	-0.027261
6	6	0	-1.261680	-4.154964	0.118705
7	6	0	0.084583	-4.344519	-0.021270
8	6	0	0.715854	-3.075177	-0.219561
9	6	0	2.076800	-2.786292	-0.235779
10	6	0	2.590497	-1.462663	-0.218102
11	6	0	4.078471	0.015796	0.319371
12	1	0	4.996810	0.444056	0.707590
13	6	0	1.956114	-0.227476	-0.433702
14	6	0	2.897298	0.771724	-0.079701
15	6	0	2.758234	2.166321	0.010758
16	6	0	3.045475	-3.911594	-0.123490
17	6	0	3.983041	2.994257	0.127681
18	6	0	4.097361	3.997519	1.099958
19	6	0	5.257782	4.756997	1.199147
20	6	0	6.321308	4.529447	0.328491
21	6	0	6.220665	3.534026	-0.639858
22	6	0	5.062425	2.771362	-0.738076
23	1	0	2.003579	4.979482	-0.254078
24	1	0	-0.661801	5.297159	-0.205875
25	1	0	-2.009245	-4.904134	0.332659
26	1	0	0.616249	-5.281773	0.045239
27	1	0	1.065745	-0.020104	-1.013959
28	1	0	3.275057	4.161790	1.789823
29	1	0	5.336134	5.523314	1.963720
30	1	0	7.225727	5.124386	0.405676
31	1	0	7.043136	3.353873	-1.324563
32	1	0	4.974015	2.003996	-1.501225
33	7	0	0.314434	2.127937	0.094397
34	7	0	-0.315826	-2.130382	-0.205882
35	7	0	3.905873	-1.270500	0.244020
36	6	0	2.989986	-4.812703	0.944277
37	1	0	2.241970	-4.672670	1.719163
38	6	0	4.051495	-4.064826	-1.082717
39	6	0	3.900890	-5.860589	1.036104
40	1	0	3.849446	-6.546828	1.875448
41	6	0	4.882974	-6.018341	0.062823
42	1	0	5.594055	-6.835223	0.133341
43	6	0	4.958347	-5.114090	-0.994232
44	1	0	5.729426	-5.224442	-1.749993
45	1	0	4.116195	-3.349655	-1.896703
46	6	0	-2.772534	-2.115231	0.012715
47	6	0	-2.952452	-0.706621	-0.004974
48	6	0	-3.981321	-2.985307	0.066179
49	6	0	-4.913202	-2.858525	1.103381
50	6	0	-4.203681	-3.954743	-0.919193
51	6	0	-6.034842	-3.679959	1.153767
52	1	0	-4.746331	-2.111275	1.873912
53	6	0	-5.323080	-4.779127	-0.867197
54	1	0	-3.491056	-4.051174	-1.733259
55	6	0	-6.242192	-4.643963	0.169830
56	1	0	-6.745573	-3.571277	1.966788

57	1	0	-5.480892	-5.522525	-1.642052
58	1	0	-7.116911	-5.284954	0.210101
59	6	0	-4.252553	-0.091898	-0.189176
60	6	0	-4.051875	1.246299	-0.188199
61	6	0	-2.629145	1.461640	-0.003536
62	7	0	-1.984276	0.243561	0.101530
63	1	0	-5.179467	-0.624738	-0.340963
64	1	0	-4.786133	2.024716	-0.333614
65	6	0	-2.057843	2.741506	-0.009474
66	6	0	-2.997411	3.901431	-0.089581
67	6	0	-3.026245	4.719803	-1.223872
68	6	0	-3.868110	4.183762	0.967635
69	6	0	-3.903227	5.797580	-1.296997
70	1	0	-2.358432	4.498729	-2.051537
71	6	0	-4.745296	5.261852	0.894792
72	1	0	-3.850584	3.549333	1.849125
73	6	0	-4.764136	6.072225	-0.237341
74	1	0	-3.917597	6.420120	-2.185955
75	1	0	-5.412540	5.470552	1.725064
76	1	0	-5.447863	6.913034	-0.294368
77	1	0	-0.301595	-1.297730	-0.776859
78	3	0	-0.084869	0.328901	0.655527

1bLiTHF-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.501006	2.827768	-0.417575
2	6	0	1.205002	4.252848	-0.495293
3	6	0	-0.139043	4.366104	-0.467044
4	6	0	-0.672060	3.003072	-0.394072
5	6	0	-1.341633	-2.664099	-0.548589
6	6	0	-1.123786	-4.108699	-0.697846
7	6	0	0.210447	-4.298739	-0.722379
8	6	0	0.816938	-2.978828	-0.570926
9	6	0	2.175107	-2.734606	-0.491865
10	6	0	2.683627	-1.390981	-0.448914
11	6	0	4.058320	0.231331	0.275507
12	1	0	4.898807	0.670187	0.793124
13	6	0	2.152334	-0.180846	-0.858982
14	6	0	2.989708	0.856918	-0.376851
15	6	0	2.768005	2.281925	-0.365628
16	6	0	3.155363	-3.837764	-0.354487
17	6	0	3.965451	3.144128	-0.220573
18	6	0	4.027506	4.162681	0.740957
19	6	0	5.169737	4.945228	0.872508
20	6	0	6.272056	4.721848	0.051132
21	6	0	6.228812	3.704133	-0.898795
22	6	0	5.089671	2.918238	-1.028332
23	1	0	1.936686	5.042717	-0.584973
24	1	0	-0.728066	5.270967	-0.491879
25	1	0	-1.900129	-4.856318	-0.769455
26	1	0	0.748873	-5.226531	-0.854223
27	1	0	1.291563	-0.064967	-1.499402
28	1	0	3.177818	4.318429	1.398527
29	1	0	5.203264	5.725076	1.626869
30	1	0	7.162580	5.333609	0.154551
31	1	0	7.083080	3.524051	-1.543820
32	1	0	5.050656	2.129519	-1.773858
33	3	0	-0.056784	0.051830	0.037219
34	7	0	0.317903	2.102434	-0.374895
35	7	0	-0.167871	-2.011856	-0.481895
36	7	0	3.867202	-1.098105	0.220398
37	1	0	4.452373	-1.799970	0.649585
38	6	0	2.967099	-4.869613	0.576730
39	1	0	2.081112	-4.856274	1.204261
40	6	0	4.329569	-3.839600	-1.124115
41	6	0	3.907613	-5.885209	0.712334
42	1	0	3.745755	-6.673546	1.440510
43	6	0	5.061012	-5.882447	-0.068558
44	1	0	5.796171	-6.672965	0.041267
45	6	0	5.270050	-4.854663	-0.985424
46	1	0	6.164671	-4.847141	-1.599966
47	1	0	4.484343	-3.046300	-1.850274
48	6	0	-2.636541	-2.086783	-0.443359
49	6	0	-2.890904	-0.713652	-0.332504
50	6	0	-3.815354	-3.002446	-0.450009
51	6	0	-4.640500	-3.087524	0.677408
52	6	0	-4.136887	-3.778128	-1.570246
53	6	0	-5.754233	-3.922117	0.687729
54	1	0	-4.396304	-2.486778	1.549927
55	6	0	-5.245582	-4.619518	-1.559415
56	1	0	-3.511010	-3.708752	-2.455750
57	6	0	-6.058520	-4.693377	-0.430838
58	1	0	-6.381684	-3.972748	1.572210
59	1	0	-5.482062	-5.210446	-2.438883
60	1	0	-6.925868	-5.345688	-0.424813
61	6	0	-4.242426	-0.133569	-0.389372
62	6	0	-4.088266	1.202688	-0.356683
63	6	0	-2.642128	1.455685	-0.278040
64	7	0	-1.965955	0.271593	-0.242784
65	1	0	-5.159630	-0.696300	-0.487853
66	1	0	-4.852069	1.963935	-0.425660
67	6	0	-2.077039	2.726219	-0.324495
68	6	0	-3.007714	3.893644	-0.351584
69	6	0	-3.085359	4.720361	-1.478744
70	6	0	-3.834607	4.176459	0.740870
71	6	0	-3.958942	5.802399	-1.510135
72	1	0	-2.454967	4.500253	-2.335878
73	6	0	-4.714232	5.255382	0.709175
74	1	0	-3.780457	3.537985	1.618645
75	6	0	-4.776667	6.073449	-0.415370
76	1	0	-4.006731	6.430108	-2.394534
77	1	0	-5.347184	5.460679	1.566993
78	1	0	-5.459265	6.916847	-0.439733
79	1	0	-0.137634	1.290483	3.560643
80	6	0	-0.619994	0.859593	2.672359
81	8	0	0.331751	0.044634	1.985846
82	6	0	-1.773015	-0.082669	3.068940
83	1	0	-0.912696	1.664043	1.994782
84	6	0	0.316800	-1.213952	2.650414
85	6	0	-1.165900	-1.496329	2.901100
86	1	0	-2.096943	0.107504	4.095092
87	1	0	-2.631703	0.052546	2.406361
88	1	0	0.809774	-1.938454	1.998116
89	1	0	0.873151	-1.127677	3.596031
90	1	0	-1.323851	-2.135154	3.773019
91	1	0	-1.594440	-1.989617	2.025533

1bLiTHF-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.431724	2.806031	-0.437712
2	6	0	1.120795	4.229695	-0.453284
3	6	0	-0.223844	4.327779	-0.404804
4	6	0	-0.744247	2.958474	-0.383149
5	6	0	-1.363747	-2.712044	-0.519418
6	6	0	-1.130789	-4.159730	-0.593112
7	6	0	0.204360	-4.334457	-0.653069
8	6	0	0.797238	-3.000549	-0.593273
9	6	0	2.154995	-2.741877	-0.560944
10	6	0	2.659545	-1.397494	-0.564455
11	6	0	4.042798	0.233867	0.121887
12	1	0	4.895037	0.678315	0.614872
13	6	0	2.105151	-0.190824	-0.954069
14	6	0	2.945809	0.852726	-0.490140
15	6	0	2.706044	2.273584	-0.437878
16	6	0	3.146618	-3.834614	-0.411549
17	6	0	3.898798	3.145866	-0.310272
18	6	0	3.992524	4.132276	0.681487
19	6	0	5.131969	4.922635	0.790604
20	6	0	6.200259	4.738700	-0.083906
21	6	0	6.126119	3.752384	-1.064505
22	6	0	4.989827	2.958980	-1.171601
23	1	0	1.842534	5.030942	-0.519286
24	1	0	-0.821267	5.227266	-0.386884
25	1	0	-1.898104	-4.919985	-0.591325
26	1	0	0.749495	-5.262688	-0.748275
27	1	0	1.224581	-0.080171	-1.567306
28	1	0	3.170047	4.258117	1.378959
29	1	0	5.190471	5.677481	1.568461
30	1	0	7.088248	5.356812	0.001622
31	1	0	6.953233	3.603377	-1.751379
32	1	0	4.926116	2.194236	-1.939983
33	3	0	-0.099722	0.014767	-0.032924
34	7	0	0.256335	2.067211	-0.403550
35	7	0	-0.197879	-2.043114	-0.530779
36	7	0	3.863589	-1.095833	0.064359
37	1	0	4.464208	-1.793746	0.478412
38	6	0	3.001417	-4.823743	0.572210
39	1	0	2.139941	-4.785938	1.231834
40	6	0	4.291392	-3.864618	-1.223556
41	6	0	3.953106	-5.827619	0.717244
42	1	0	3.823511	-6.583782	1.484934
43	6	0	5.075925	-5.854510	-0.106505
44	1	0	5.819782	-6.635835	0.010399
45	6	0	5.243731	-4.867426	-1.075186
46	1	0	6.115525	-4.881768	-1.721564
47	1	0	4.414714	-3.101871	-1.987521
48	6	0	-2.665026	-2.146962	-0.418883
49	6	0	-2.935390	-0.774521	-0.342567
50	6	0	-3.834490	-3.073442	-0.415306
51	6	0	-4.699890	-3.105100	0.684745
52	6	0	-4.110562	-3.913253	-1.501415
53	6	0	-5.806433	-3.948761	0.702049
54	1	0	-4.492233	-2.456361	1.531431
55	6	0	-5.212149	-4.763556	-1.483235
56	1	0	-3.455116	-3.886247	-2.367519
57	6	0	-6.064625	-4.783445	-0.381761
58	1	0	-6.463720	-3.957842	1.565991
59	1	0	-5.412204	-5.404137	-2.336645
60	1	0	-6.926181	-5.443311	-0.370086
61	6	0	-4.286456	-0.207253	-0.469955
62	6	0	-4.144194	1.130321	-0.454233
63	6	0	-2.705478	1.396898	-0.310926
64	7	0	-2.022193	0.220312	-0.230437
65	1	0	-5.193047	-0.779663	-0.604263
66	1	0	-4.909499	1.883506	-0.573877
67	6	0	-2.147231	2.672210	-0.341578
68	6	0	-3.086335	3.831077	-0.398726
69	6	0	-3.104363	4.682397	-1.510717
70	6	0	-3.986044	4.079560	0.643758
71	6	0	-3.990342	5.752500	-1.575810
72	1	0	-2.416947	4.490097	-2.329817
73	6	0	-4.878402	5.146282	0.577769
74	1	0	-3.978537	3.424610	1.510667
75	6	0	-4.881351	5.987860	-0.531104
76	1	0	-3.991859	6.397845	-2.448688
77	1	0	-5.568984	5.322886	1.396587
78	1	0	-5.575084	6.820919	-0.582553
79	1	0	0.558932	1.826539	2.442232
80	6	0	-0.195026	1.047930	2.571764
81	8	0	0.285103	-0.124123	1.907787
82	6	0	-0.440424	0.627773	4.035556
83	1	0	-1.125611	1.374983	2.087293
84	6	0	-0.414811	-1.220703	2.492901
85	6	0	-0.389916	-0.916612	3.990697
86	1	0	0.324696	1.028050	4.703646
87	1	0	-1.408412	0.993233	4.384926
88	1	0	-1.441919	-1.249663	2.097674
89	1	0	0.101213	-2.137972	2.202578
90	1	0	0.543649	-1.280895	4.426624
91	1	0	-1.219300	-1.386832	4.522751

2LiTHF-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.485700	3.139003	-0.557017
2	6	0	-0.213388	4.406333	-0.719135
3	6	0	-1.532233	4.122185	-0.679008
4	6	0	-1.641979	2.669528	-0.519712
5	6	0	-0.616169	-2.934229	-0.481232
6	6	0	0.012656	-4.244616	-0.703251
7	6	0	1.341292	-4.032960	-0.755111
8	6	0	1.540637	-2.601905	-0.526926
9	6	0	2.769837	-1.981763	-0.428560
10	6	0	2.857763	-0.545508	-0.303781
11	6	0	3.571182	1.421747	0.485204
12	1	0	4.154662	2.100595	1.091824
13	6	0	2.045416	0.439533	-0.837158
14	6	0	2.470456	1.690080	-0.329220
15	6	0	1.850920	2.989429	-0.429380
16	6	0	4.030073	-2.761089	-0.475006
17	6	0	2.746448	4.163343	-0.301760
18	6	0	2.458175	5.224292	0.568648
19	6	0	3.330161	6.301809	0.685619
20	6	0	4.506109	6.337668	-0.059667
21	6	0	4.811643	5.283114	-0.916950
22	6	0	3.945269	4.202205	-1.029239
23	1	0	0.255298	5.369740	-0.859794
24	1	0	-2.359671	4.812965	-0.745579
25	1	0	-0.512163	-5.182974	-0.806813
26	1	0	2.122947	-4.754953	-0.942082

27	1	0	1.268417	0.272261	-1.569415
28	1	0	1.555266	5.182647	1.169654
29	1	0	3.095585	7.110855	1.370133
30	1	0	5.184868	7.179488	0.032499
31	1	0	5.726052	5.303212	-1.501336
32	1	0	4.179704	3.380260	-1.698738
33	3	0	-0.173014	0.046590	0.008211
34	7	0	-0.433737	2.100705	-0.470352
35	7	0	0.315928	-1.971534	-0.383753
36	7	0	3.802413	0.093960	0.505484
37	6	0	4.239762	-3.880261	0.341521
38	1	0	3.451098	-4.191167	1.020836
39	6	0	5.070577	-2.341487	-1.316243
40	6	0	5.449948	-4.565801	0.309736
41	1	0	5.598089	-5.425897	0.955227
42	6	0	6.474072	-4.141409	-0.533155
43	1	0	7.419449	-4.673829	-0.553422
44	6	0	6.279677	-3.027145	-1.347569
45	1	0	7.071558	-2.693531	-2.010898
46	1	0	4.915108	-1.470834	-1.948016
47	6	0	-2.020699	-2.765658	-0.358427
48	6	0	-2.665638	-1.525805	-0.253241
49	6	0	-2.878574	-3.987739	-0.384350
50	6	0	-3.616127	-4.358813	0.745706
51	6	0	-2.981148	-4.777726	-1.535201
52	6	0	-4.431219	-5.487337	0.727790
53	1	0	-3.543628	-3.747642	1.641888
54	6	0	-3.787658	-5.911766	-1.552662
55	1	0	-2.423362	-4.488896	-2.421857
56	6	0	-4.516216	-6.269678	-0.420672
57	1	0	-4.996190	-5.758924	1.614157
58	1	0	-3.854320	-6.511142	-2.455405
59	1	0	-5.148061	-7.151984	-0.434546
60	6	0	-4.129537	-1.371783	-0.277330
61	6	0	-4.376119	-0.049414	-0.281359
62	6	0	-3.066660	0.621444	-0.264288
63	7	0	-2.069980	-0.311327	-0.216289
64	1	0	-4.841451	-2.182967	-0.329907
65	1	0	-5.332590	0.449684	-0.341288
66	6	0	-2.903641	1.996019	-0.385172
67	6	0	-4.137132	2.837203	-0.391839
68	6	0	-4.511287	3.568958	-1.525279
69	6	0	-4.958667	2.893997	0.739474
70	6	0	-5.670256	4.338920	-1.524593
71	1	0	-3.885720	3.522486	-2.412430
72	6	0	-6.122174	3.658347	0.739976
73	1	0	-4.673718	2.327210	1.621845
74	6	0	-6.479929	4.385597	-0.391888
75	1	0	-5.946641	4.897027	-2.413735
76	1	0	-6.746533	3.688726	1.627522
77	1	0	-7.384991	4.984505	-0.392692
78	1	0	-0.551403	1.379595	3.499324
79	6	0	-0.886001	0.787173	2.636516
80	8	0	0.263946	0.290227	1.948848
81	6	0	-1.677115	-0.455060	3.089166
82	1	0	-1.427771	1.433352	1.943056
83	6	0	0.654690	-0.886604	2.647763
84	6	0	-0.660655	-1.611789	2.940574
85	1	0	-2.025839	-0.341888	4.118573
86	1	0	-2.545993	-0.618721	2.447085
87	1	0	1.338847	-1.444538	2.003574
88	1	0	1.169962	-0.598962	3.577364
89	1	0	-0.598400	-2.243047	3.829862
90	1	0	-0.925542	-2.236841	2.084574
91	6	0	4.759777	-0.535617	1.404823
92	1	0	4.275288	-1.347473	1.950052
93	1	0	5.614530	-0.939933	0.859285
94	1	0	5.100252	0.217534	2.115754

2LiTHF-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.391396	-3.079870	-0.632246
2	6	0	0.337103	-4.333912	-0.763986
3	6	0	1.648650	-4.020426	-0.708706
4	6	0	1.726366	-2.563771	-0.569574
5	6	0	0.582226	3.012908	-0.399448
6	6	0	-0.072951	4.319473	-0.559429
7	6	0	-1.394930	4.081188	-0.650126
8	6	0	-1.565039	2.635649	-0.501368
9	6	0	-2.783143	1.988320	-0.457069
10	6	0	-2.851236	0.548420	-0.379929
11	6	0	-3.538826	-1.445328	0.362114
12	1	0	-4.120853	-2.146203	0.944613
13	6	0	-2.008119	-0.409792	-0.913388
14	6	0	-2.414239	-1.677287	-0.431295
15	6	0	-1.761903	-2.960769	-0.523356
16	6	0	-4.058836	2.742567	-0.513538
17	6	0	-2.632229	-4.155167	-0.403838
18	6	0	-2.341614	-5.201135	0.483555
19	6	0	-3.192985	-6.296012	0.592461
20	6	0	-4.351011	-6.364394	-0.178085
21	6	0	-4.659500	-5.324842	-1.052415
22	6	0	-3.813577	-4.227077	-1.156843
23	1	0	-0.108280	-5.309448	-0.896241
24	1	0	2.491620	-4.694084	-0.751805
25	1	0	0.431393	5.273772	-0.599579
26	1	0	-2.188513	4.795699	-0.813388
27	1	0	-1.220086	-0.213890	-1.626266
28	1	0	-1.452607	-5.135796	1.103295
29	1	0	-2.956593	-7.093176	1.290215
30	1	0	-5.013550	-7.219712	-0.092369
31	1	0	-5.560562	-5.369312	-1.655929
32	1	0	-4.050535	-3.416366	-1.839019
33	3	0	0.195419	0.017640	-0.050456
34	7	0	0.504185	-2.020340	-0.546266
35	7	0	-0.328321	2.026634	-0.372508
36	7	0	-3.801562	-0.124671	0.395174
37	6	0	-4.325475	3.825217	0.334994
38	1	0	-3.568661	4.131182	1.051662
39	6	0	-5.060529	2.326955	-1.402617
40	6	0	-5.552478	4.479299	0.287500
41	1	0	-5.744836	5.311021	0.957985
42	6	0	-6.537287	4.059450	-0.603329
43	1	0	-7.495866	4.567166	-0.635924
44	6	0	-6.286338	2.980966	-1.449782
45	1	0	-7.047199	2.649787	-2.149685
46	1	0	-4.861526	1.483368	-2.058230
47	6	0	1.991741	2.871308	-0.284927
48	6	0	2.666471	1.645311	-0.225551
49	6	0	2.823645	4.111346	-0.301712
50	6	0	3.594300	4.466751	0.811083
51	6	0	2.872819	4.933653	-1.434090
52	6	0	4.388050	5.610419	0.795628
53	1	0	3.564794	3.831984	1.692540
54	6	0	3.658350	6.082138	-1.449107
55	1	0	2.290902	4.657350	-2.309093
56	6	0	4.419409	6.424189	-0.333577
57	1	0	4.978249	5.869294	1.669276
58	1	0	3.683953	6.705251	-2.337734
59	1	0	5.035292	7.317739	-0.345736
60	6	0	4.131152	1.523660	-0.305958
61	6	0	4.404820	0.207758	-0.346881
62	6	0	3.111281	-0.491395	-0.295551
63	7	0	2.097880	0.416663	-0.193772
64	1	0	4.823117	2.351209	-0.368585
65	1	0	5.368386	-0.269271	-0.453970
66	6	0	2.973838	-1.867791	-0.438276
67	6	0	4.224338	-2.681897	-0.480052
68	6	0	4.582105	-3.406887	-1.623469
69	6	0	5.079912	-2.719963	0.626684
70	6	0	5.757476	-4.150766	-1.656252
71	1	0	3.930540	-3.374889	-2.492342
72	6	0	6.259516	-3.458348	0.593886
73	1	0	4.808273	-2.159546	1.517037
74	6	0	6.600687	-4.178407	-0.547626
75	1	0	6.020414	-4.703246	-2.552963
76	1	0	6.909337	-3.474617	1.463347
77	1	0	7.518407	-4.757158	-0.574244
78	1	0	0.100363	-2.172444	2.158967
79	6	0	0.527010	-1.218620	2.475337
80	8	0	-0.248182	-0.178572	1.882036
81	6	0	0.437241	-0.938265	3.976036
82	1	0	1.563284	-1.153581	2.109052
83	6	0	0.114622	1.019863	2.571400
84	6	0	0.331358	0.603551	4.040347
85	1	0	-0.463052	-1.400638	4.388254
86	1	0	1.298526	-1.329022	4.521551
87	1	0	1.035567	1.422125	2.126777
88	1	0	-0.689314	1.741775	2.416605
89	1	0	-0.503280	0.913410	4.672516
90	1	0	1.238166	1.059743	4.443090
91	6	0	-4.791228	0.466363	1.285946
92	1	0	-4.334809	1.274125	1.860016
93	1	0	-5.641523	0.865974	0.730065
94	1	0	-5.132719	-0.309529	1.971462

1aTHF-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.567184	-3.081412	-0.526765
2	6	0	0.126863	-4.302836	-0.816905
3	6	0	1.467257	-4.052156	-0.775109
4	6	0	1.650578	-2.663789	-0.451748
5	6	0	0.638359	3.046940	-0.499715
6	6	0	0.016804	4.261066	-0.913929
7	6	0	-1.339315	4.049039	-0.948254
8	6	0	-1.584664	2.701315	-0.561295
9	6	0	-2.829631	2.040988	-0.461342
10	6	0	-2.928706	0.640989	-0.432523
11	6	0	-3.856497	-1.249779	0.042089
12	1	0	-4.572908	-1.974608	0.416781
13	6	0	-1.954224	-0.325038	-0.761414
14	6	0	-2.513070	-1.566078	-0.453349
15	6	0	-1.945334	-2.865492	-0.483076
16	6	0	-4.052574	2.869691	-0.368541
17	6	0	-2.847319	-4.041116	-0.444188
18	6	0	-2.603607	-5.117263	0.420625
19	6	0	-3.466304	-6.206896	0.459373
20	6	0	-4.590588	-6.238952	-0.362148
21	6	0	-4.848297	-5.173091	-1.220940
22	6	0	-3.985938	-4.083304	-1.261351
23	1	0	-0.361776	-5.231049	-1.074386
24	1	0	2.273537	-4.740187	-0.980761
25	1	0	0.551367	5.160286	-1.181127
26	1	0	-2.107374	4.741523	-1.259545
27	1	0	-0.999099	-0.139507	-1.233167
28	1	0	-1.741146	-5.080128	1.079357
29	1	0	-3.266677	-7.027305	1.141386
30	1	0	-5.264550	-7.088885	-0.330355
31	1	0	-5.721259	-5.192110	-1.865397
32	1	0	-4.177747	-3.257126	-1.939575
33	7	0	0.404408	-2.121462	-0.333224
34	7	0	-0.355515	2.132473	-0.317639
35	7	0	-4.104245	0.023439	0.055987
36	6	0	-4.087436	4.019087	0.432859
37	1	0	-3.212392	4.284099	1.018074
38	6	0	-5.203884	2.515301	-1.085469
39	6	0	-5.236006	4.799914	0.505065
40	1	0	-5.248332	5.682066	1.137187
41	6	0	-6.367861	4.444872	-0.223271
42	1	0	-7.264163	5.054794	-0.170203
43	6	0	-6.347889	3.299039	-1.016393
44	1	0	-7.228077	3.015890	-1.584565
45	1	0	-5.186218	1.620638	-1.697331
46	6	0	2.022356	2.814200	-0.315667
47	6	0	2.619804	1.555756	-0.178415
48	6	0	2.889085	4.026061	-0.316658
49	6	0	2.661477	5.065154	0.594012
50	6	0	3.939260	4.156845	-1.233435
51	6	0	3.469133	6.197712	0.597147
52	1	0	1.849534	4.970384	1.309186
53	6	0	4.746141	5.290387	-1.231932
54	1	0	4.110130	3.362143	-1.953528
55	6	0	4.514724	6.313033	-0.315550
56	1	0	3.285251	6.988608	1.317404
57	1	0	5.552329	5.378105	-1.953309
58	1	0	5.144273	7.197007	-0.314238
59	6	0	4.040768	1.389274	0.134164
60	6	0	4.275435	0.062528	0.129208
61	6	0	2.995172	-0.578283	-0.182773
62	7	0	2.011017	0.340373	-0.329627
63	1	0	4.734986	2.188979	0.347492
64	1	0	5.202131	-0.452468	0.336886
65	6	0	2.866065	-1.980828	-0.300648
66	6	0	4.099860	-2.816266	-0.300760
67	6	0	5.109136	-2.605010	-1.248286
68	6	0	4.269668	-3.839988	0.639227
69	6	0	6.255261	-3.393711	-1.253994
70	1	0	4.979463	-1.819930	-1.987446
71	6	0	5.414563	-4.630719	0.633065
72	1	0	3.495221	-4.004515	1.383075
73	6	0	6.411089	-4.409710	-0.314026
74	1	0	7.024457	-3.220168	-1.999897

75	1	0	5.531657	-5.415508	1.373695
76	1	0	7.304534	-5.025704	-0.319717
77	1	0	0.245293	-1.184939	0.036443
78	1	0	-0.200443	1.225618	0.123533
79	1	0	1.666035	-0.738127	2.211092
80	6	0	0.932505	-0.001722	2.554915
81	8	0	-0.218245	-0.049663	1.695018
82	6	0	0.418853	-0.283063	3.970983
83	1	0	1.381321	0.994099	2.462615
84	6	0	-1.392075	-0.342540	2.460995
85	6	0	-1.055008	0.118035	3.872212
86	1	0	0.499906	-1.350356	4.199780
87	1	0	0.973592	0.269844	4.731448
88	1	0	-2.238351	0.178407	2.007489
89	1	0	-1.589717	-1.424196	2.429253
90	1	0	-1.686061	-0.346124	4.632619
91	1	0	-1.163254	1.204887	3.944708

1aTHF-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.844483	-2.958063	-0.159819
2	6	0	0.247931	-4.259313	-0.070696
3	6	0	-1.105541	-4.125653	-0.190151
4	6	0	-1.401380	-2.728273	-0.332639
5	6	0	-0.820657	3.076051	-0.101798
6	6	0	-0.265755	4.375999	0.092121
7	6	0	1.100065	4.253389	0.070229
8	6	0	1.423254	2.880878	-0.145834
9	6	0	2.707429	2.310075	-0.278277
10	6	0	2.919153	0.923776	-0.280604
11	6	0	4.005352	-0.895367	-0.697651
12	1	0	4.787237	-1.566549	-1.039353
13	6	0	2.016566	-0.111114	0.050264
14	6	0	2.680657	-1.310305	-0.222645
15	6	0	2.204158	-2.642129	-0.193552
16	6	0	3.853952	3.229668	-0.479099
17	6	0	3.187372	-3.751919	-0.280818
18	6	0	3.054413	-4.761536	-1.242751
19	6	0	3.993149	-5.782790	-1.334033
20	6	0	5.083811	-5.809716	-0.468246
21	6	0	5.233127	-4.806062	0.485622
22	6	0	4.294384	-3.783258	0.577798
23	1	0	0.805605	-5.172932	0.072742
24	1	0	-1.846255	-4.910800	-0.186638
25	1	0	-0.844735	5.277397	0.223523
26	1	0	1.833008	5.034213	0.206865
27	1	0	1.075679	-0.004347	0.574027
28	1	0	2.218960	-4.723418	-1.935370
29	1	0	3.879102	-6.551821	-2.091471
30	1	0	5.817148	-6.606163	-0.541725
31	1	0	6.081671	-4.820427	1.162132
32	1	0	4.403834	-3.000847	1.323692
33	7	0	-0.205859	-2.068359	-0.277370
34	7	0	0.224472	2.214789	-0.227547
35	7	0	4.148167	0.392380	-0.733278
36	6	0	3.778023	4.264604	-1.419076
37	1	0	2.879863	4.370686	-2.019658
38	6	0	5.035096	3.073322	0.257379
39	6	0	4.848300	5.132841	-1.606967
40	1	0	4.775700	5.923013	-2.347276
41	6	0	6.009714	4.980053	-0.855414
42	1	0	6.844444	5.658757	-0.999109
43	6	0	6.099935	3.946783	0.075182
44	1	0	7.005466	3.820140	0.659822
45	1	0	5.105221	2.261981	0.973443
46	6	0	-2.180251	2.717265	-0.209165
47	6	0	-2.673687	1.421165	-0.395811
48	6	0	-3.153944	3.845074	-0.104065
49	6	0	-3.926222	4.227788	-1.205209
50	6	0	-3.298011	4.545026	1.098011
51	6	0	-4.825799	5.285039	-1.105372
52	1	0	-3.812263	3.689577	-2.141760
53	6	0	-4.195651	5.603617	1.197259
54	1	0	-2.704517	4.244787	1.956864
55	6	0	-4.961930	5.976253	0.095645
56	1	0	-5.416043	5.573083	-1.969522
57	1	0	-4.300642	6.133839	2.138505
58	1	0	-5.662684	6.801274	0.173756
59	6	0	-4.108902	1.147368	-0.433557
60	6	0	-4.239990	-0.188027	-0.545416
61	6	0	-2.882616	-0.732980	-0.562614
62	7	0	-1.954757	0.256370	-0.490310
63	1	0	-4.889088	1.889350	-0.348568
64	1	0	-5.149201	-0.770368	-0.569509
65	6	0	-2.652396	-2.125584	-0.508966
66	6	0	-3.827996	-3.041641	-0.591233
67	6	0	-4.201758	-3.826292	0.504396
68	6	0	-4.580801	-3.126023	-1.767370
69	6	0	-5.297341	-4.680771	0.424821
70	1	0	-3.629287	-3.752014	1.425474
71	6	0	-5.679448	-3.976246	-1.846107
72	1	0	-4.294241	-2.517824	-2.620566
73	6	0	-6.038849	-4.758165	-0.751185
74	1	0	-5.577105	-5.279745	1.285754
75	1	0	-6.252247	-4.031827	-2.766442
76	1	0	-6.894228	-5.423299	-0.813195
77	1	0	-0.153698	-1.069923	-0.437648
78	1	0	0.067831	1.232568	-0.413606
79	1	0	1.621471	0.797730	2.678318
80	6	0	0.777981	0.254448	3.113529
81	8	0	-0.316824	0.352420	2.218557
82	6	0	1.013847	-1.250775	3.264578
83	1	0	0.515636	0.713841	4.079683
84	6	0	-1.249704	-0.627743	2.653512
85	6	0	-0.411189	-1.835861	3.127170
86	1	0	1.654228	-1.605830	2.451253
87	1	0	1.492103	-1.507193	4.212381
88	1	0	-1.842272	-0.220805	3.486344
89	1	0	-1.917556	-0.843872	1.819180
90	1	0	-0.435622	-2.654432	2.402408
91	1	0	-0.786096	-2.222685	4.078069

1bTHF-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.028591	2.902874	-0.538151
2	6	0	0.686071	4.322985	-0.516532
3	6	0	-0.654617	4.388769	-0.371263
4	6	0	-1.125362	3.001941	-0.329974
5	6	0	-1.538098	-2.822275	-0.423212
6	6	0	-1.244237	-4.256850	-0.476015
7	6	0	0.100704	-4.359216	-0.543156
8	6	0	0.617134	-2.993204	-0.522162
9	6	0	1.956299	-2.644685	-0.554625
10	6	0	2.384712	-1.282286	-0.628003
11	6	0	3.826280	0.408034	-0.340748
12	1	0	4.749900	0.892917	-0.059568
13	6	0	1.688260	-0.106786	-0.856653
14	6	0	2.579393	0.974923	-0.664046
15	6	0	2.307074	2.387881	-0.623175
16	6	0	2.999656	-3.695603	-0.428603
17	6	0	3.481459	3.298136	-0.618418
18	6	0	3.659866	4.256944	0.387289
19	6	0	4.776950	5.087096	0.384408
20	6	0	5.733450	4.971171	-0.620874
21	6	0	5.571225	4.015532	-1.621351
22	6	0	4.458511	3.181880	-1.616581
23	1	0	1.383771	5.142254	-0.615163
24	1	0	-1.274553	5.270604	-0.299245
25	1	0	-1.972759	-5.054414	-0.455023
26	1	0	0.695158	-5.258353	-0.620842
27	1	0	0.655001	-0.042610	-1.138504
28	1	0	2.919501	4.334065	1.178250
29	1	0	4.903784	5.820897	1.173909
30	1	0	6.604120	5.618900	-0.622074
31	1	0	6.311941	3.920685	-2.408984
32	1	0	4.325874	2.440078	-2.398509
33	7	0	-0.122765	2.137156	-0.437834
34	7	0	-0.426781	-2.091164	-0.461881
35	7	0	3.704853	-0.920235	-0.347549
36	1	0	4.402481	-1.564130	-0.003913
37	6	0	2.953073	-4.616201	0.627700
38	1	0	2.140218	-4.550716	1.344992
39	6	0	4.066752	-3.768412	-1.335435
40	6	0	3.936154	-5.590240	0.765062
41	1	0	3.885592	-6.292114	1.591202
42	6	0	4.986140	-5.657974	-0.146879
43	1	0	5.754065	-6.416888	-0.038256
44	6	0	5.048884	-4.744619	-1.196704
45	1	0	5.861186	-4.796447	-1.914673
46	1	0	4.106762	-3.064866	-2.162466
47	6	0	-2.856052	-2.278081	-0.305956
48	6	0	-3.145605	-0.927687	-0.223690
49	6	0	-4.001982	-3.233149	-0.262830
50	6	0	-4.816108	-3.320433	0.871632
51	6	0	-4.282981	-4.064410	-1.353503
52	6	0	-5.888326	-4.206797	0.913176
53	1	0	-4.595785	-2.685832	1.725375
54	6	0	-5.350426	-4.955991	-1.310688
55	1	0	-3.657929	-4.000502	-2.239870
56	6	0	-6.157857	-5.028188	-0.177969
57	1	0	-6.509104	-4.259568	1.802099
58	1	0	-5.557837	-5.589591	-2.167399
59	1	0	-6.992532	-5.721098	-0.146384
60	6	0	-4.484999	-0.369757	-0.188598
61	6	0	-4.387130	0.975513	-0.144512
62	6	0	-2.980857	1.335747	-0.158798
63	7	0	-2.280157	0.146650	-0.207103
64	1	0	-5.385214	-0.964344	-0.225854
65	1	0	-5.192084	1.694916	-0.139589
66	6	0	-2.503404	2.632129	-0.183009
67	6	0	-3.507381	3.728797	-0.046937
68	6	0	-3.732304	4.636235	-1.088654
69	6	0	-4.247028	3.866604	1.132510
70	6	0	-4.672848	5.652830	-0.953102
71	1	0	-3.166298	4.532934	-2.010325
72	6	0	-5.191999	4.879363	1.267225
73	1	0	-4.070326	3.168725	1.945953
74	6	0	-5.406467	5.776434	0.224513
75	1	0	-4.838783	6.345839	-1.771931
76	1	0	-5.756241	4.970504	2.190108
77	1	0	-6.141973	6.567638	0.328693
78	1	0	2.809572	1.150745	3.887475
79	6	0	2.594553	0.943924	2.826815
80	8	0	3.244391	-0.251484	2.429687
81	6	0	1.093251	0.703356	2.606166
82	1	0	3.000666	1.759988	2.220253
83	6	0	2.408495	-1.316181	2.848669
84	6	0	0.963336	-0.837882	2.633582
85	1	0	0.494887	1.189307	3.380531
86	1	0	0.773118	1.092869	1.637250
87	1	0	2.672968	-2.198406	2.256363
88	1	0	2.594392	-1.540855	3.911325
89	1	0	0.307337	-1.189365	3.433611
90	1	0	0.563818	-1.203216	1.684088
91	1	0	-1.267123	0.071329	-0.217480

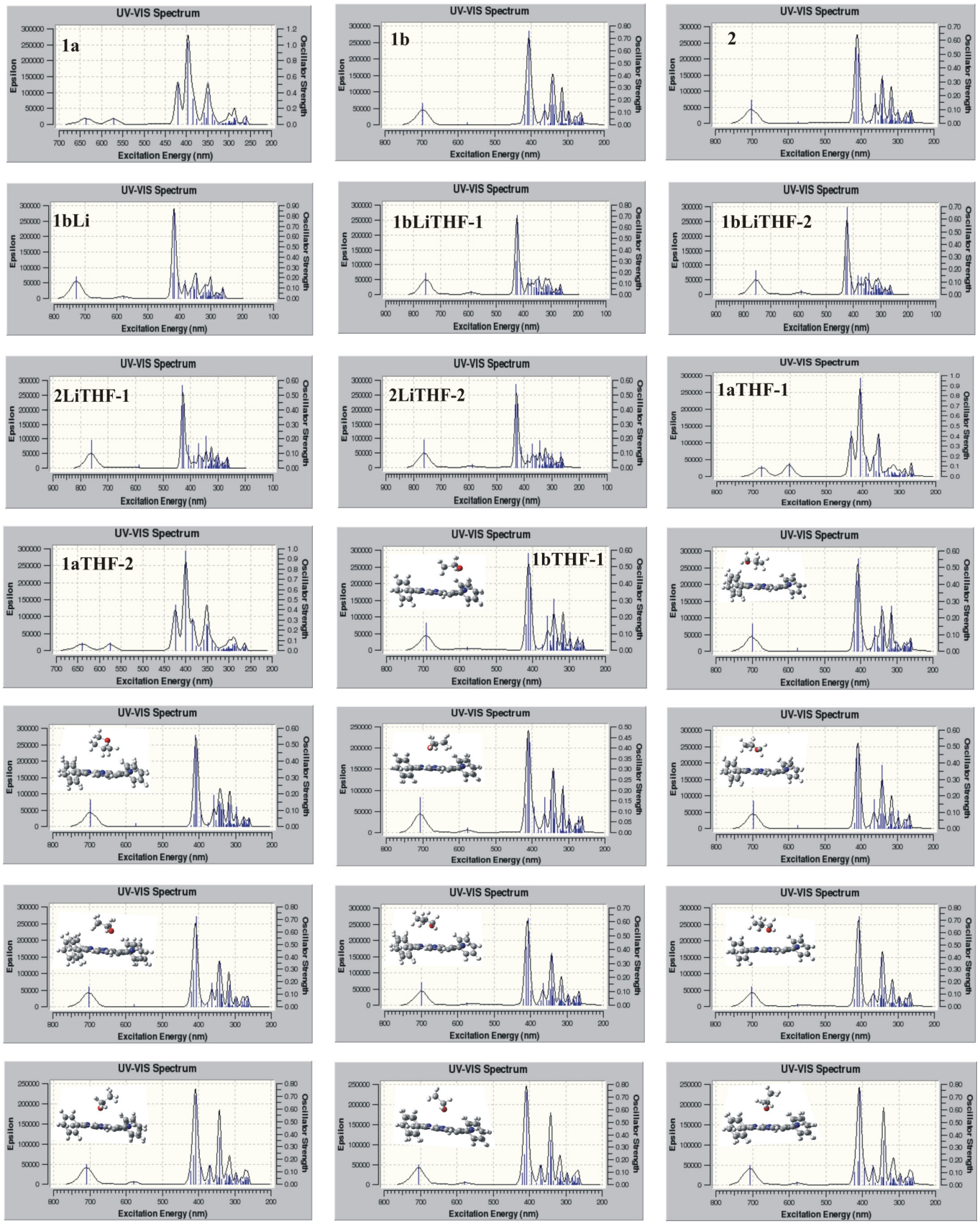

Figure 1S: Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1LiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in the gas phase calculated at the B3LYP/6-31G(d,p) level of theory.

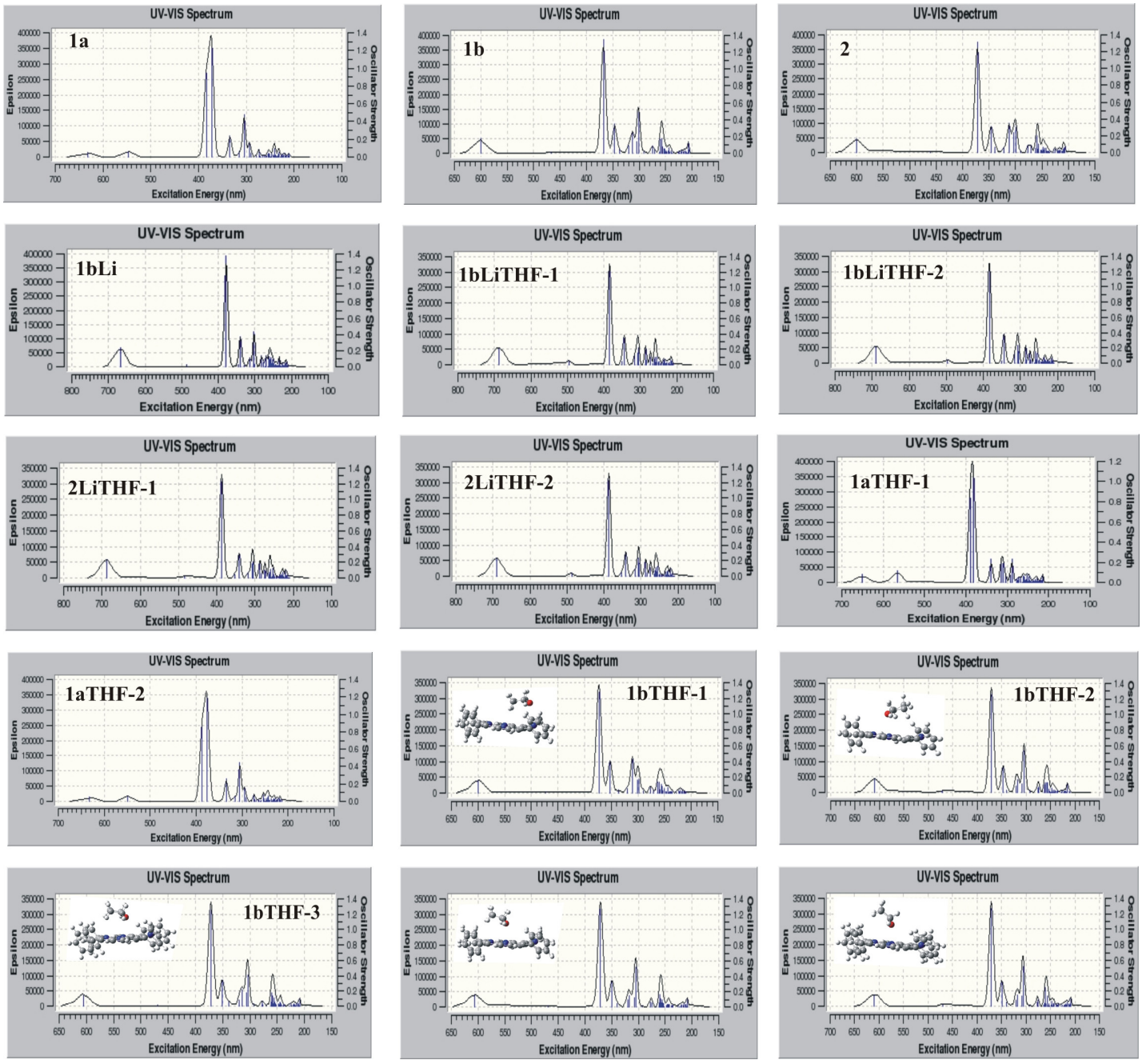

Figure 2S: Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1LiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in the gas phase calculated at the CAM-B3LYP/6-31G(d,p) level of theory.

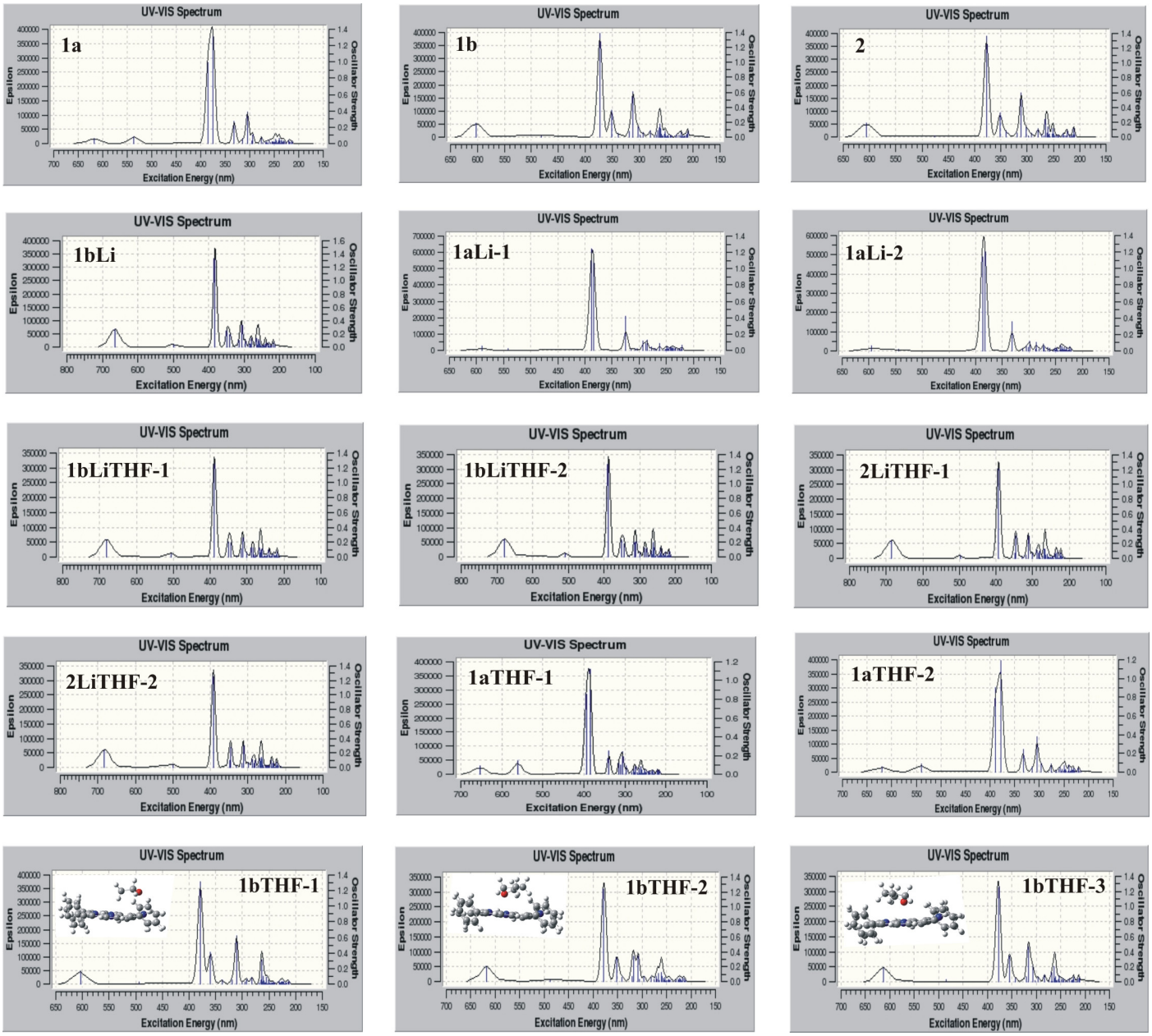

Figure 3S: Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1aLi**, **1LiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in the gas phase calculated at the M06-2X/6-31G(d,p) level of theory.

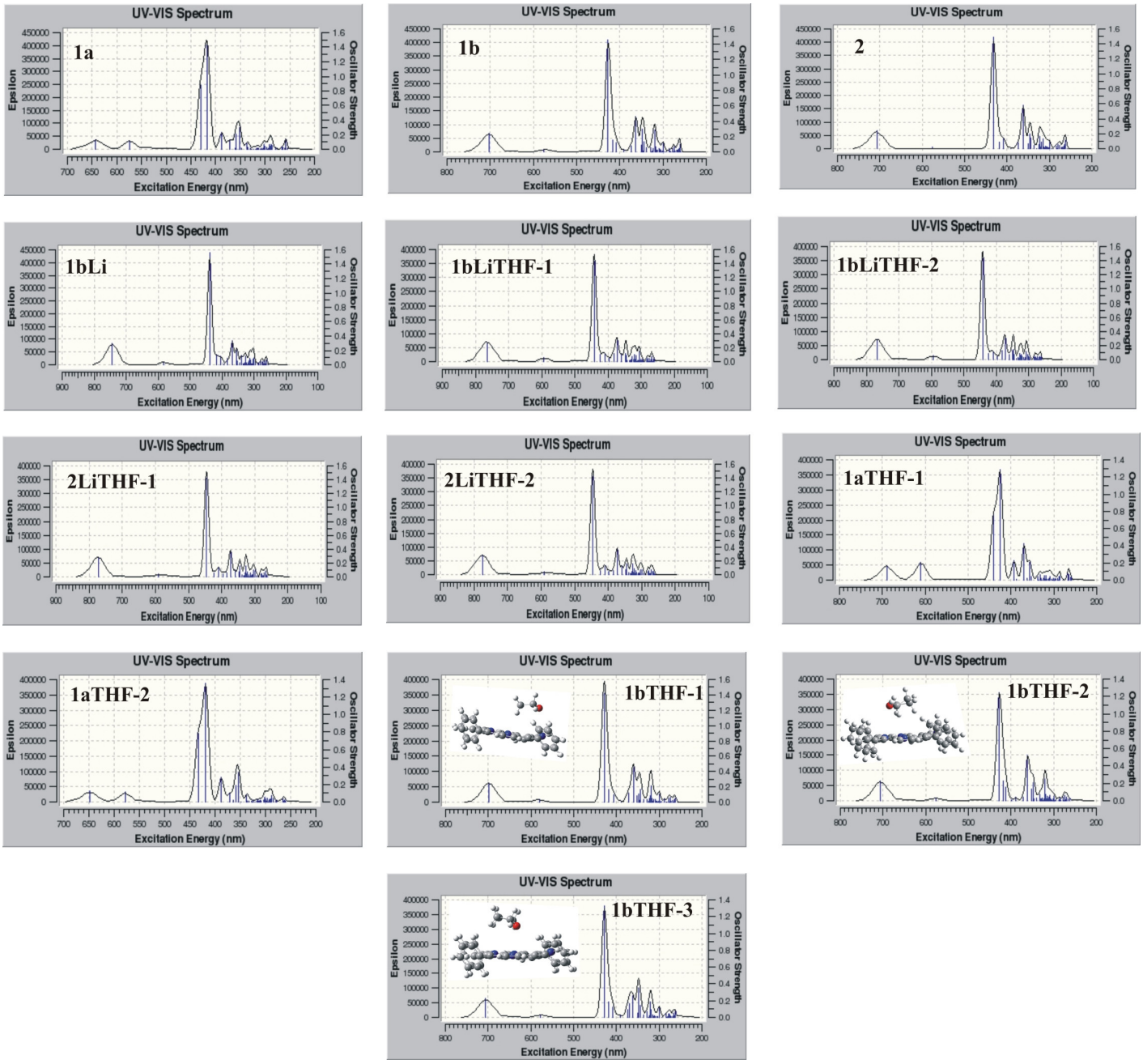

Figure 4S: Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1LiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in toluene solvent calculated at the B3LYP/6-31G(d,p) level of theory.

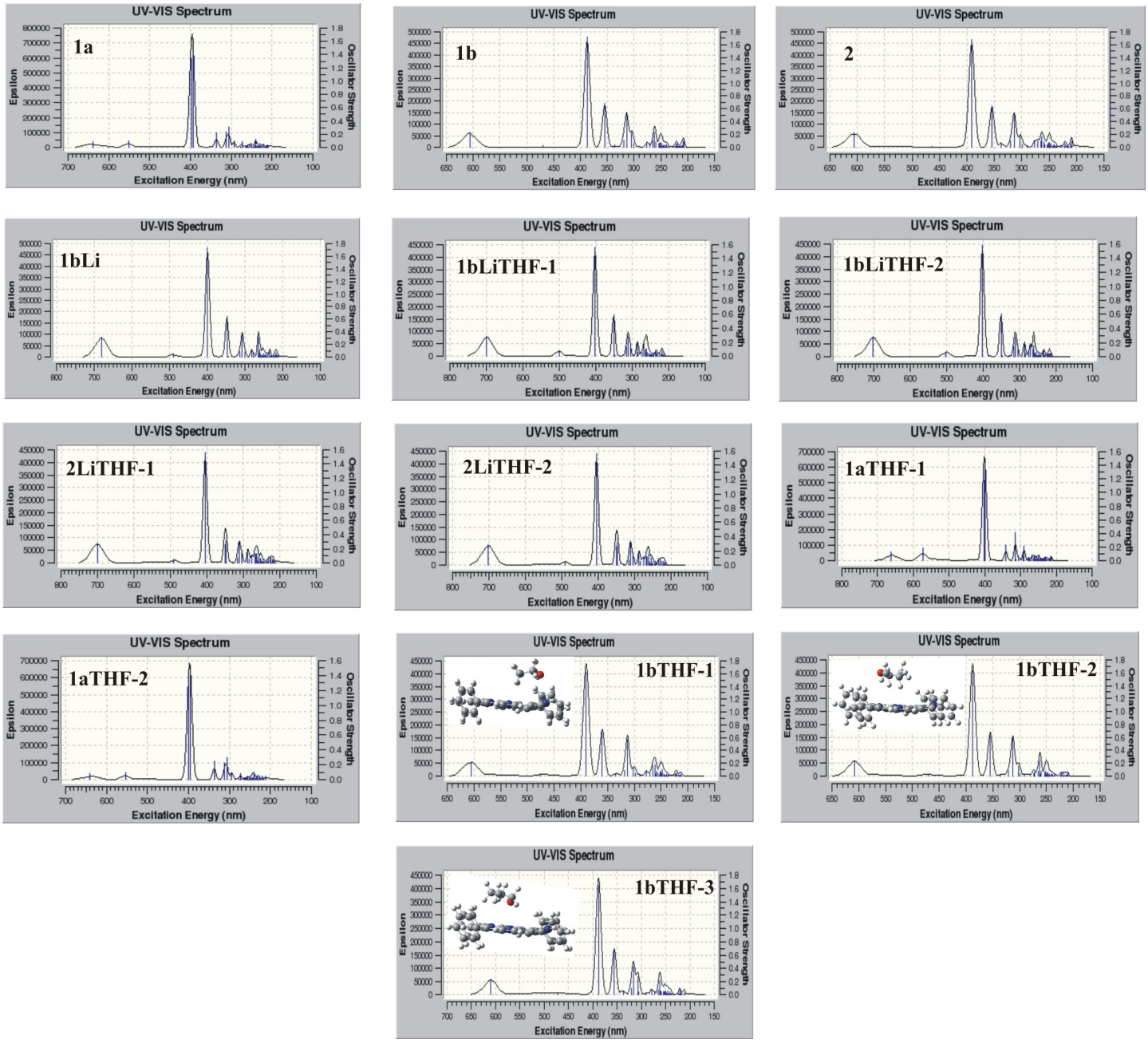

Figure 5S: Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1LiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in toluene solvent calculated at the CAM-B3LYP/6-31G(d,p) level of theory.

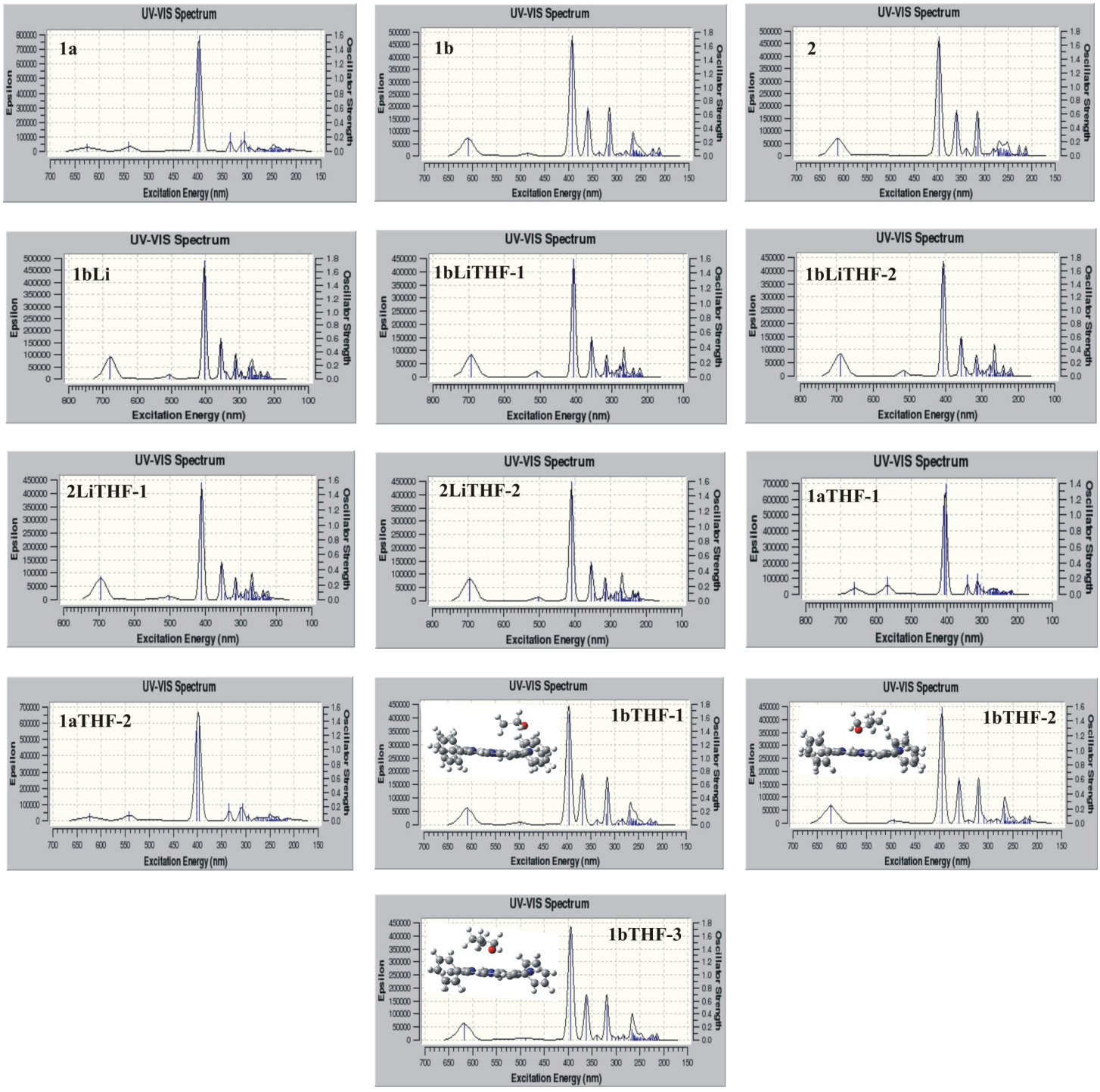

Figure 6S: Absorption spectrum of **1a**, **1b**, **2**, **1bLi**, **1LiTHF**, **2LiTHF**, **1aTHF**, and **1bTHF** species in toluene solvent calculated at the M06-2X/6-31G(d,p) level of theory.

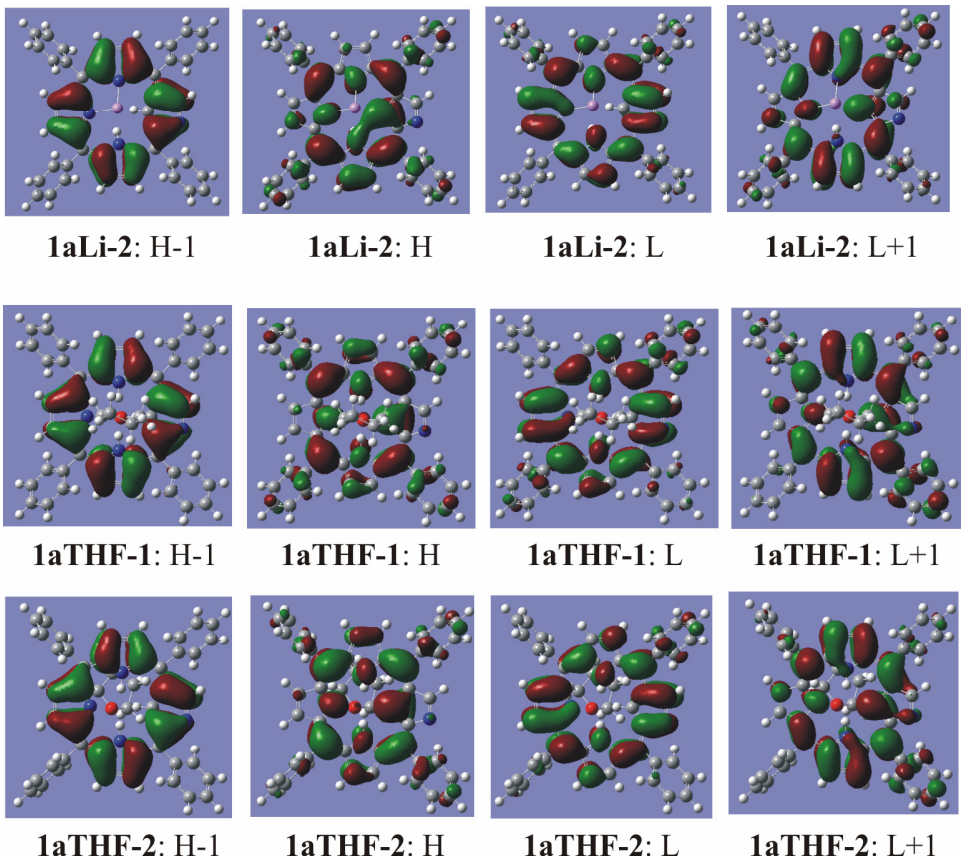

Figure 7S: Plots of the M06-2X frontier canonical molecular orbitals of the **1aLi-2**, **1aTHF-1**, and **1aTHF-2** species.