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Supporting Information

On the dissolution of Lithium sulfate in water: anion photoelectron spectroscopy and density functional theory calculations

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7) Tables with LC-ωPBE/6-311++G(d,p) optimized geometries

1) Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1. Comparison of the VDEs of $Li_2SO_4(H_2O)^-$ with different functionals and to that of experimental VDEs. All values are given in eV.

		LC-ωPBE		M06-2X		B3LYP		ωB97XD	
Isomers	Exp.VDE	Δ*E*	VDE	Δ*E*	VDE	Δ*E*	VDE	Δ*E*	VDE
1a	1.03	0.00	0.94	0.00	0.98	0.00	1.24	0	0.97
1b		0.003	1.09	0.1	1.02	0.02	1.13	0.06	1。00
1c		0.10	1.22	0.26	1.01	0.23	1.08	0.14	1.02
1d		0.14	0.77	0.28	0.53	0.27	0.72	0.16	0.64
1e	0.32	0.20	0.38	0.36	0.16	0.36	0.40	0.22	0.32

Table S2. Experimental VDEs and ADEs (eV) of $Li_2SO_4(H_2O)_n^-$ (*n* = 0-5) clusters.

Cluster	X'		X	
	VDE	ADE	VDE	ADE
$Li_2SO_4^-$	0.24	0.13	0.75	0.49
$Li_2SO_4(H_2O)^-$	0.32	0.24	1.03	0.84
$Li_2SO_4(H_2O)_2^-$	0.37	0.27	1.07	0.80
$Li_2SO_4(H_2O)_3^-$	0.54	0.28	0.92	0.69
$Li_2SO_4(H_2O)_4^-$	-	-	0.91	0.56
$Li_2SO_4(H_2O)_5^-$	-	-	0.94	0.58

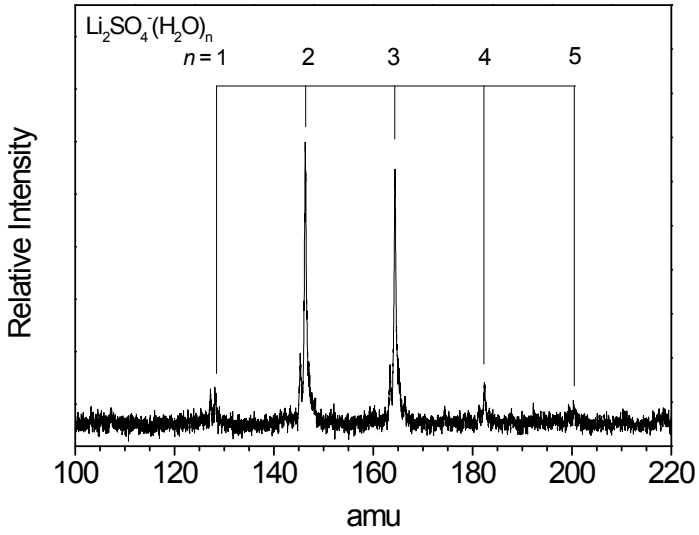


Figure S1 The mass spectrum of $Li_2SO_4(H_2O)_n^-$ (n = 1-5) cluster anions. Although the mass signal $Li_2SO_4^-$ is low as showed in this spectrum, we could increase its intensity by optimizing the experimental condition and take the photoelectron spectrum with confident.

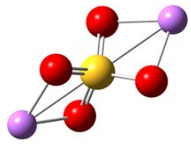
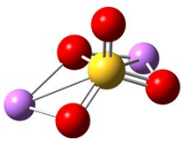
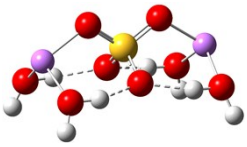
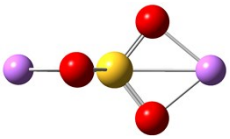
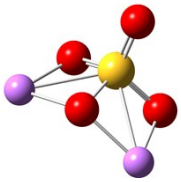
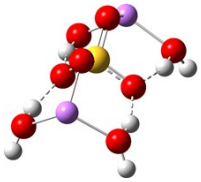
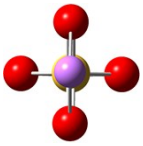
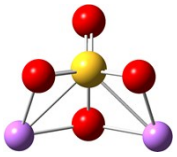
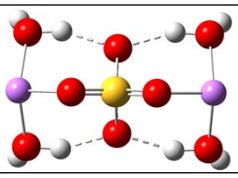
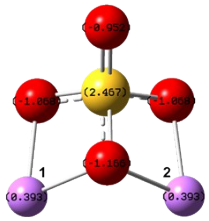
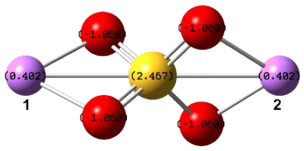
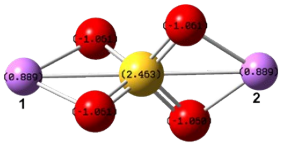
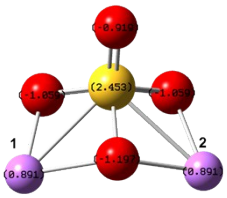
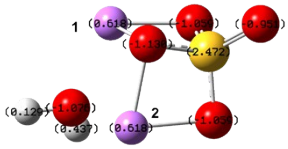
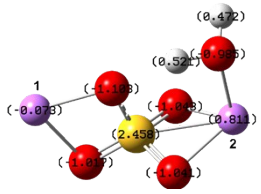
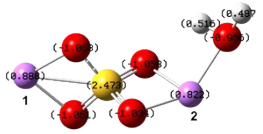
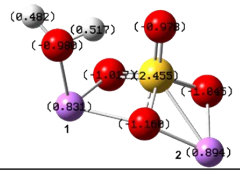
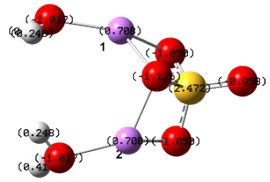
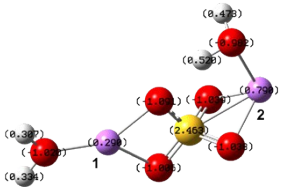
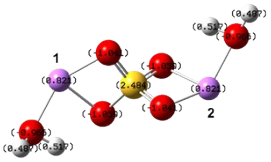
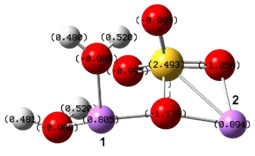
Propeller-shaped	Turtle-shaped	tent-shaped
		
		
		
0a'	0b'	4a'

Figure S2: The propeller-shaped and turtle-shaped Structures of Li_2SO_4 and the tent-shaped structures of $Li_2SO_4(H_2O)_4$ viewed from different angles.

anion		neutral	
Turtle-shaped	Propeller-shaped	Turtle-shaped	Propeller-shaped
			
0a	0b	0a'	0b'
			
1a	1e	1a'	1c'
			
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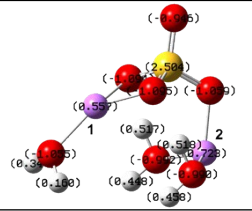	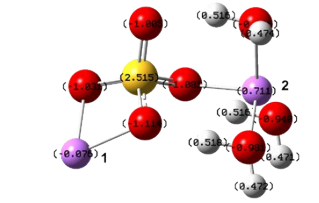	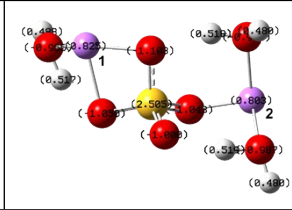	
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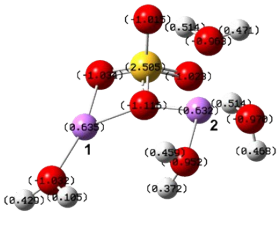
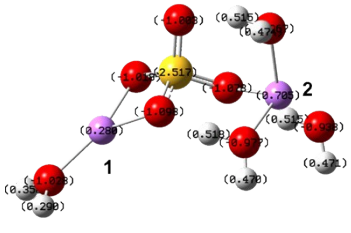
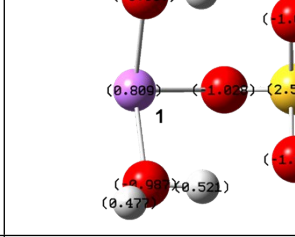
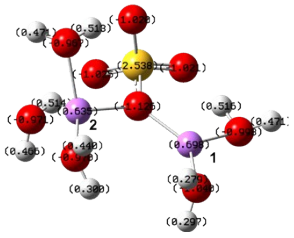
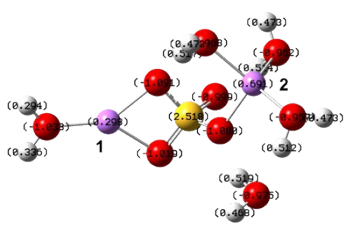
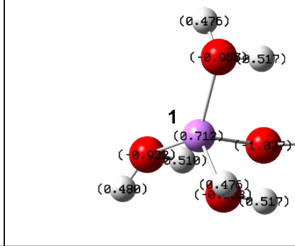
			
4a	4f	4a'	
			
5a	5d	5a'	

Figure S3 Natural bond orbital (NBO) Charge Distributions of the most stable isomers of $Li_2SO_4(H_2O)_n^-$ (n = 0-5) and their corresponding neutrals.

4) Table S3. Cartesian coordinates for stable isomers of $Li_2SO_4(H_2O)_n^-$ (n = 0-5) clusters

$Li_2SO_4^-$

0a

	X	Y	Z
S	0.311115	-0.000065	-0.016388
O	0.037992	1.239767	-0.822600
O	-0.874983	0.000158	0.995982
O	1.604416	0.000207	0.635297
O	0.038113	-1.240237	-0.822040
Li	-1.626791	1.447775	0.052573
Li	-1.627413	-1.447241	0.052566

0b

	X	Y	Z
S	-0.000013	0.000086	-0.000006
O	-0.919912	0.944827	-0.714044
O	-0.919746	-0.944741	0.714060
O	0.919942	0.713894	0.944839
O	0.919743	-0.714298	-0.944612
Li	-2.370395	-0.000057	-0.000024
Li	2.370394	0.000390	-0.000505

$Li_2SO_4(H_2O)^-$

1a

	X	Y	Z
S	-0.760892	0.000012	0.042880
O	-0.293147	1.233805	0.770434
O	0.136425	-0.000127	-1.226071
O	-2.175496	-0.000199	-0.263398
O	-0.292906	-1.233519	0.770721
Li	1.206488	1.331204	-0.370680
Li	1.206582	-1.331197	-0.370548
O	2.678710	0.000004	0.144514
H	2.982334	0.000056	1.068776
H	3.506945	0.000063	-0.382864

1b

	X	Y	Z
S	-0.808495	0.090892	-0.033177
O	-0.882348	-1.140850	-0.888786
O	0.206513	-0.327042	1.070133
O	-2.087404	0.501000	0.513062
O	-0.080144	1.201230	-0.743899
Li	0.481803	-1.980230	0.141901
Li	1.445596	0.878242	0.312374
O	3.196855	0.120546	-0.047142
H	3.257002	-0.747928	0.397219
H	3.364036	-0.096271	-0.973555

1c

	X	Y	Z
S	-0.681581	-0.195502	-0.006206
O	0.338866	-1.143396	0.528577
O	-1.691329	-0.846510	-0.820021
O	0.094539	0.871164	-0.834922
O	-1.261826	0.649885	1.098146
Li	-0.453416	2.195629	0.418178
Li	1.883299	1.185716	-0.819905
O	2.717040	-0.294092	0.047021
H	1.846138	-0.748578	0.284674
H	3.191195	-0.163830	0.869391

1d

	X	Y	Z
S	-0.544236	0.290269	-0.018160
O	-1.842523	-0.167830	-0.593916
O	-0.122257	-0.897249	0.887436
O	-0.611187	1.542889	0.711861
O	0.544327	0.302923	-1.071084
Li	-1.618426	-1.905723	0.220864
Li	1.362629	-1.284560	-0.200037
O	2.905503	-0.016122	0.058417
H	2.938439	0.330103	0.953499
H	2.238719	0.535781	-0.406768

1e

	X	Y	Z
S	-0.469717	0.210992	0.005899
O	0.154065	0.901975	-1.168454
O	0.216848	0.803264	1.199175
O	-0.133925	-1.272899	-0.072392
O	-1.945301	0.271380	0.050948
Li	1.690966	1.088688	-0.034061
Li	-2.024945	-1.718068	-0.015347

O	2.512787	-0.710097	-0.039161
H	1.634865	-1.155271	-0.169303
H	2.823802	-1.055528	0.800387

$Li_2SO_4(H_2O)_2^-$

2a

	X	Y	Z
S	-1.155399	-0.000076	0.031803
O	-0.850340	1.239891	0.825194
O	-0.032747	-0.000105	-1.046997
O	-2.482661	-0.000392	-0.552588
O	-0.849965	-1.239661	0.825652
Li	0.697007	1.547080	-0.221121
Li	0.697433	-1.546898	-0.220539
O	2.570733	-1.945679	0.014247
H	2.943532	-1.908883	0.905454
H	3.188149	-1.398226	-0.507643
O	2.570209	1.945998	0.014495
H	2.942586	1.908293	0.905844
H	3.187921	1.399145	-0.507660

2b

	X	Y	Z
S	0.936066	-0.000013	-0.124377
O	0.082142	-0.000335	-1.355518
O	0.504746	1.189787	0.737275
O	2.353961	-0.000135	-0.412307
O	0.504700	-1.189207	0.738072
Li	-1.727449	-0.000022	-0.996373
Li	-0.084060	0.000584	2.134423
O	-2.033573	1.662846	-0.043262
H	-2.526801	1.648668	0.784895
H	-1.086319	1.748993	0.231879
O	-2.033152	-1.663097	-0.042997
H	-1.085990	-1.748741	0.232462
H	-2.527088	-1.650170	0.784735

2c

	X	Y	Z
S	1.045614	-0.057699	0.003675
O	0.848695	1.327658	0.525221
O	2.322755	-0.239707	-0.658357
O	-0.134725	-0.340950	-0.965449
O	0.792141	-1.072721	1.094054
Li	-0.731352	-1.708709	0.238900
Li	-1.788219	0.451771	-0.817553
O	-1.554110	2.089198	0.102495
H	-0.579780	1.921999	0.329827
H	-1.989041	2.382654	0.903088
O	-2.687220	-1.192408	0.052548
H	-3.261548	-1.055852	0.833036
H	-3.254344	-1.731435	-0.542967

2d

	X	Y	Z
S	-0.908270	0.050539	-0.047480
O	-1.205543	-1.358076	-0.466728
O	0.036495	-0.134312	1.162925
O	-2.078498	0.844562	0.269538
O	-0.013932	0.710076	-1.076288
Li	0.192579	-1.996144	0.659433
Li	1.577872	0.262652	0.058830
O	2.067518	-1.710718	-0.169669
H	2.152160	-2.115171	-1.049797
H	2.729573	-2.185861	0.378010
O	1.773780	2.281944	0.074731
H	1.428162	2.589692	0.916500
H	0.976674	2.122090	-0.477362

2e

	X	Y	Z
S	-0.303912	-0.572816	0.008205
O	-1.185655	-0.822257	-1.175181
O	-1.207182	-0.703282	1.194160
O	0.213806	0.859353	-0.067291
O	0.907567	-1.420684	0.064292
Li	-2.609748	-0.186225	-0.053799
Li	2.023089	0.184111	-0.013556
O	-2.357083	1.775362	-0.073897
H	-2.461269	2.256676	0.749663

H	-1.376552	1.699580	-0.188988
O	3.836043	0.736275	-0.004916
H	4.622646	0.175640	0.053777
H	4.177794	1.641367	-0.040998

$Li_2SO_4(H_2O)_3^-$

3a

	X	Y	Z
S	-1.145041	0.316121	0.004377
O	-0.227186	0.807422	1.127710
O	-0.286447	0.564939	-1.241587
O	-2.404193	1.027746	-0.037358
O	-1.302922	-1.163246	0.157410
Li	1.029711	1.439466	-0.167587
Li	0.278931	-2.113343	0.165608
O	1.215175	-1.415463	1.706139
H	2.148510	-1.179364	1.687468
H	0.712902	-0.564647	1.742616
O	2.919382	1.695848	-0.135060
H	3.420174	1.760719	0.693730
H	3.491581	1.143117	-0.700725
O	1.027548	-1.769656	-1.584389
H	0.542677	-0.915572	-1.706428
H	1.959086	-1.575674	-1.728473

3b

	X	Y	Z
S	-0.005456	-0.789986	-0.244184
O	-0.813830	-0.472226	-1.448984
O	-0.777475	-1.610408	0.715372
O	0.334988	0.555418	0.443966
O	1.324142	-1.364829	-0.571874
Li	2.204773	0.186780	0.172865
Li	-1.232964	1.519798	0.694532
O	-1.879162	1.909148	-1.109395
H	-1.555714	1.015866	-1.416147
H	-1.444391	2.548952	-1.676118
O	3.805552	1.151971	0.471052
H	3.842759	2.048676	0.840143
H	4.713666	0.954485	0.202972
O	-2.432198	0.275356	1.573158
H	-1.903755	-0.553077	1.409059
H	-3.293672	0.112660	1.184878

3c

	X	Y	Z
S	0.059925	-0.536256	0.084293
O	-0.785456	-1.050238	-1.024053
O	-0.803746	-0.340429	1.290546
O	0.644632	0.825253	-0.295802
O	1.243288	-1.386211	0.355983
Li	-2.276963	0.679274	0.810117
Li	2.423876	0.094319	-0.075981
O	-3.266200	-0.410796	-0.470212
H	-2.393808	-0.740091	-0.834773
H	-3.759519	-1.198792	-0.237879
O	4.253820	0.573817	-0.189980
H	5.021702	0.005208	-0.035513
H	4.625677	1.425376	-0.462000
O	-1.536587	2.268749	0.004251
H	-1.833339	2.594793	-0.846897
H	-0.612885	1.919952	-0.142030

3d

	X	Y	Z
S	-0.677457	0.868727	0.124800
O	0.367732	1.755990	0.724308
O	0.095117	0.089584	-0.968172
O	-1.819980	1.579942	-0.426935
O	-1.096164	-0.210401	1.092408
Li	1.698105	0.955747	-0.387581
Li	-0.223748	-1.593241	-0.074648
O	1.365792	-2.574974	0.501406
H	1.723277	-2.336909	1.365769
H	2.151486	-2.607716	-0.071223
O	3.544243	0.435331	-0.400648
H	4.027462	0.365783	0.435894
H	3.752632	-0.409453	-0.845198
O	-2.190653	-2.034868	-0.549154
H	-2.290407	-1.365003	0.155960
H	-2.359684	-1.541806	-1.357381

3e

	X	Y	Z
S	1.025411	-0.034329	-0.253614
O	-0.216415	0.598173	-0.813986

O	1.062673	-1.448497	-0.673517
O	0.931507	0.070490	1.270724
O	2.247048	0.734565	-0.593804
Li	-1.865368	-0.087715	-0.057571
Li	2.469648	1.249975	1.288464
O	-2.607546	1.611702	-0.936979
H	-1.658822	1.695078	-1.150535
H	-2.834190	2.392309	-0.429039
O	-1.559390	-2.028154	-0.351929
H	-0.602123	-1.990115	-0.600949
H	-1.577864	-2.512598	0.476470
O	-1.599629	0.001499	1.900718
H	-0.601543	0.007709	1.827726
H	-1.819261	0.709605	2.507696

$Li_2SO_4(H_2O)_4^-$

4a

	X	Y	Z
S	-0.191040	-1.231849	-0.011690
O	0.576198	-1.538482	1.221216
O	0.530662	-1.680872	-1.222741
O	-0.358210	0.298057	-0.092323
O	-1.597489	-1.730562	0.047841
Li	-2.233015	0.093472	-0.027219
Li	1.222701	1.333507	-0.049941
O	2.062899	0.626690	1.646079
H	1.583084	-0.244201	1.617743
H	1.805219	1.037062	2.473030
O	-3.437075	1.560801	0.006209
H	-4.377120	1.709736	0.156382
H	-3.035890	2.452749	0.009236
O	2.315435	0.337510	-1.406490
H	3.113408	-0.019683	-1.011372
H	1.720466	-0.444278	-1.527805
O	0.662134	3.240855	-0.200389
H	0.461424	3.544547	-1.092291
H	-0.152092	3.429129	0.292568

4b

	X	Y	Z
S	-0.727002	0.124888	-0.368098
O	-0.317050	1.597275	-0.446737
O	0.045431	-0.513453	-1.515996
O	-2.166467	-0.019360	-0.555774
O	-0.223729	-0.437882	0.915654
Li	0.379815	1.222588	-2.339419
Li	1.625992	-0.270978	1.094654
O	1.969849	1.625411	0.998541
H	1.136815	1.854476	0.519486
H	2.692661	1.942924	0.444499
O	2.351523	-1.339504	-0.341923
H	3.105472	-1.016621	-0.848999
H	1.563293	-1.232123	-0.926071
O	-1.525380	1.837207	-2.904221
H	-2.039116	1.027750	-2.786841
H	-1.553533	2.219199	-2.012552
O	2.090398	1.812582	-2.999931
H	2.914053	1.403268	-2.669792
H	2.351729	2.717873	-3.212384

4c

	X	Y	Z
S	-0.291217	-0.913613	-0.479983
O	0.925623	-1.729145	-0.760715
O	0.112332	-0.084598	0.776269
O	-1.485673	-1.709996	-0.195524
O	-0.528936	0.119639	-1.533621
Li	1.888355	-0.808415	0.619006
Li	-0.150600	1.594747	-0.238396

4d

	X	Y	Z
S	-0.719793	-0.915986	-0.009519
O	-1.352139	-0.364142	-1.235102
O	-1.710668	-1.605346	0.849262
O	-0.191606	0.294842	0.793261
O	0.439729	-1.783448	-0.328959
Li	1.564479	0.839648	0.978092
Li	-1.557713	1.568591	1.171286

O	1.526508	2.564431	-0.533449	O	-2.220997	2.059919	-0.611472
H	2.054074	2.247642	-1.276656	H	-1.952475	1.196324	-1.025659
H	2.177278	2.694514	0.176891	H	-1.733957	2.750942	-1.066077
O	3.640497	-0.192884	1.070012	O	2.637656	-0.574856	0.265120
H	4.313421	-0.124472	0.375280	H	3.282014	-0.580475	-0.441884
H	3.693977	0.678048	1.511375	H	1.874415	-1.164451	-0.014876
O	-2.119310	1.995435	-0.110115	O	-2.969995	0.455031	1.939493
H	-2.238233	1.416527	-0.874976	H	-2.604323	-0.426291	1.657074
H	-2.424597	1.446894	0.642603	H	-3.809729	0.542753	1.484471
O	-2.470577	0.034456	1.846142	O	1.902641	2.647012	1.571552
H	-1.499620	0.043290	1.899762	H	1.623069	2.945888	2.452348
H	-2.594320	-0.721673	1.251250	H	1.610658	3.375457	0.993669

4e

	X	Y	Z
S	0.966458	-0.039510	-0.094381
O	0.133914	-0.156431	-1.336100
O	0.503877	1.216496	0.651296
O	2.388152	-0.034096	-0.362148
O	0.541061	-1.156592	0.854458
Li	-1.775128	-0.146134	-1.170861
Li	0.018105	0.145036	2.163677
O	-1.967870	1.659446	-0.285901
H	-2.563117	1.825605	0.452193
H	-1.048477	1.693162	0.084546
O	-2.030092	-1.638896	0.058565
H	-1.101827	-1.702458	0.384652
H	-2.588357	-1.590706	0.841061
O	-1.240110	0.174994	3.591028
H	-1.992613	0.796578	3.559756
H	-1.627811	-0.628469	3.973584
O	-1.743856	0.789975	-3.012586
H	-0.791573	0.645837	-2.884244
H	-1.911615	1.634400	-2.578457

4f

	X	Y	Z
S	0.974338	-0.086306	-0.289823
O	-0.255116	0.612087	-0.789742
O	0.946326	-1.488587	-0.747601
O	0.935446	-0.022497	1.240256
O	2.218284	0.637525	-0.654078
Li	-1.922499	-0.089268	-0.064939
Li	2.579554	0.987413	1.217701
O	-2.666997	1.583058	-0.963423
H	-1.722914	1.694163	-1.178695
H	-2.938234	2.382412	-0.509971
O	-1.674223	-2.009175	-0.435890
H	-0.714716	-1.990011	-0.680374
H	-1.720058	-2.559907	0.348467
O	-1.608442	-0.040407	1.892153
H	-0.613104	-0.051774	1.814295
H	-1.818713	0.638048	2.534625
O	3.688865	1.908642	2.445746
H	3.554863	1.962201	3.404202
H	4.416309	2.519750	2.261493

$Li_2SO_4(H_2O)_5^-$

5a

	X	Y	Z
S	0.187153	1.372546	-0.046965
O	1.159369	1.595536	1.053771
O	-0.284280	-0.092952	0.064465
O	0.831410	1.521341	-1.374587
O	-1.002913	2.247854	0.088107
Li	1.189225	-1.369094	0.048761
Li	-2.035371	-0.699425	0.060508
O	0.726068	-3.280190	0.000925
H	-0.001149	-3.672079	0.510705

5b

	X	Y	Z
S	-0.218072	0.973470	-0.255490
O	0.967715	1.852686	-0.075353
O	0.076163	-0.039886	-1.345901
O	-1.448884	1.718494	-0.527904
O	-0.380346	0.111801	1.000924
Li	2.546307	0.933678	0.301832
Li	-0.407453	-1.555383	-0.120747
O	2.822443	-0.181175	-1.250728
H	3.104971	-1.095258	-1.120654

H	0.664427	-3.710867	-0.860340	H	1.882807	-0.218348	-1.537958
O	-3.153765	0.846669	0.204963	O	2.185269	0.043842	1.973602
H	-3.856144	1.154153	-0.366808	H	1.207521	0.002455	1.874013
H	-2.413612	1.524098	0.176788	H	2.487997	-0.864400	2.100679
O	2.261218	-0.711514	-1.491139	O	0.723010	-3.067897	0.219758
H	1.786551	0.150385	-1.629635	H	0.564201	-4.007346	0.071909
H	3.141372	-0.467564	-1.197363	H	1.668736	-3.014267	0.468311
O	-2.718475	-2.500563	-0.118121	O	-2.294025	-1.660120	-0.777863
H	-2.393451	-3.109076	-0.803628	H	-2.808814	-1.116195	-0.143885
H	-2.847012	-3.086244	0.646673	H	-2.112872	-1.061249	-1.512092
O	2.296895	-0.706932	1.588330	O	-3.195958	0.200308	1.076435
H	2.083141	-0.999593	2.475101	H	-2.329434	0.088714	1.500657
H	1.955631	0.226720	1.512459	H	-2.993335	0.950745	0.493874

5c

	X	Y	Z
S	0.468605	-1.035386	-0.075485
O	-0.527092	-2.017707	-0.556674
O	0.515495	-1.027013	1.431890
O	-0.004544	0.363928	-0.477321
O	1.818369	-1.249776	-0.638089
Li	1.278463	1.753761	-0.180687
Li	-1.855340	0.749399	-0.085122
O	-2.771401	-0.717970	-1.110755
H	-2.001479	-1.333949	-1.005965
H	-2.876835	-0.582070	-2.053740
O	2.809209	1.140683	-1.275707
H	2.580488	0.183512	-1.167280
H	2.747341	1.335584	-2.213084
O	-2.004582	-0.058776	1.751247
H	-2.594973	-0.814742	1.715824
H	-1.101463	-0.442156	1.853673
O	-2.153821	2.656186	-0.454493
H	-2.106524	3.317839	0.247588
H	-1.620676	3.044091	-1.169847
O	1.927744	1.269826	1.630805
H	2.865200	1.065235	1.616267
H	1.466844	0.408307	1.774542

5d

	X	Y	Z
S	0.625947	-0.167446	-0.712797
O	-0.609658	0.575773	-0.272425
O	0.237303	-1.192475	-1.697248
O	1.224118	-0.810983	0.534820
O	1.676450	0.764444	-1.195692
Li	-1.953663	-0.485695	0.634108
Li	2.831503	0.244889	0.276254
O	-1.985255	2.815239	-0.228805
H	-1.304116	2.126141	-0.409467
H	-1.526807	3.532337	0.211838
O	-2.100503	-2.019142	-0.629492
H	-1.318996	-1.814069	-1.198515
H	-1.889225	-2.856871	-0.211728
O	-0.871560	-1.312210	2.092257
H	0.007155	-1.213711	1.641043
H	-0.769455	-0.926198	2.963340
O	4.476906	0.629087	1.125159
H	4.807586	0.250001	1.953835
H	5.123360	1.310494	0.888981
O	-3.424211	0.816615	0.871289
H	-3.025915	1.659735	0.552581
H	-4.227527	0.693398	0.362983

5e

	X	Y	Z
S	0.234359	1.080724	0.320516
O	-0.993158	1.891768	0.076377
O	-0.039280	0.099383	1.438562
O	1.424249	1.889626	0.561292
O	0.444921	0.171882	-0.903812
Li	-2.458979	0.860273	-0.436495

5f

	X	Y	Z
S	-0.532448	-1.085762	-0.059188
O	-0.426208	-0.921624	1.440578
O	0.306447	-2.206742	-0.520916
O	0.017060	0.217729	-0.644900
O	-1.950639	-1.211494	-0.459487
Li	-1.086985	1.760265	-0.326424

Li	0.373270	-1.460619	0.311899	Li	1.886065	0.604623	-0.330046
O	3.200586	0.069867	-0.819892	O	1.873663	0.490104	1.707269
H	2.319333	0.120050	-1.235440	H	1.073179	-0.084345	1.781871
H	3.122064	0.789708	-0.176517	H	1.649753	1.303331	2.166096
O	-1.947493	0.081577	-2.126461	O	-1.542894	1.494386	1.594679
H	-0.984346	0.077218	-1.902407	H	-2.490099	1.491057	1.746676
H	-2.159193	-0.807602	-2.428835	H	-1.231609	0.563924	1.729032
O	-2.711903	-0.379507	1.029176	O	2.748160	-1.139994	-0.727398
H	-2.613473	-1.305071	0.764223	H	3.232628	-1.459819	0.036277
H	-1.854856	-0.183567	1.467574	H	1.921838	-1.682902	-0.757147
O	-1.146493	-2.745771	0.137471	O	2.229907	2.417470	-1.026212
H	-1.171094	-3.565338	0.656603	H	1.814294	2.623174	-1.877458
H	-1.389218	-3.047194	-0.763123	H	2.008278	3.193105	-0.485945
O	2.190310	-2.198781	0.270913	O	-2.798620	1.207685	-1.155392
H	2.380072	-2.957341	-0.284481	H	-2.639712	0.244077	-0.982236
H	2.742373	-1.451732	-0.059724	H	-2.871640	1.305770	-2.106527

Table S4. Cartesian coordinates for stable isomers of $Li_2SO_4(H_2O)_n$ (n = 0-5) clusters

Li_2SO_4

	0a'				**0b'**		
	X	Y	Z		X	Y	Z
S	-0.000013	-0.280700	0.022145	S	0.000010	0.000190	-0.000118
O	-1.246121	-0.143776	0.844099	O	-0.921047	0.757703	-0.908271
O	0.000072	1.083052	-0.781971	O	-0.920453	-0.757798	0.908157
O	-0.000373	-1.419372	-0.861256	O	0.920863	0.908052	0.757968
O	1.246377	-0.144202	0.843727	O	0.920631	-0.908637	-0.757317
Li	-1.718503	1.351303	-0.101289	Li	-2.349765	0.000007	0.000346
Li	1.718664	1.351115	-0.101301	Li	2.349737	0.000677	-0.001031

$Li_2SO_4(H_2O)$

	1a'				**1b'**		
	X	Y	Z		X	Y	Z
S	-0.516251	0.074849	0.005318	S	0.613009	0.000172	0.000066
O	0.055194	1.174401	-0.828122	O	-0.294850	1.188063	0.001796
O	0.613501	-0.382291	0.876016	O	-0.297266	-1.185870	-0.001692
O	-1.058152	-1.047975	-0.834576	O	1.540460	-0.002493	1.183507
O	-1.696977	0.530360	0.810691	O	1.540245	0.000994	-1.183565
Li	1.745240	0.940423	-0.037145	Li	-1.765416	0.002645	-0.000335
Li	-2.711540	-0.755933	-0.050110	Li	2.958009	-0.002106	-0.000191
O	3.148517	-0.386870	0.015956	O	-3.699279	-0.000925	-0.000012
H	2.496260	-1.016779	0.363916	H	-4.269850	0.771305	0.000385
H	3.752118	-0.858573	-0.559465	H	-4.264890	-0.776816	0.000641

	1c'				**1d'**		
	X	Y	Z		X	Y	Z

S	0.497826	-0.228167	0.075793	S	-0.618618	0.277236	-0.009114
O	-0.192391	-1.209267	-0.764966	O	-1.666189	-0.342227	-0.878240
O	-0.091847	-0.146847	1.437811	O	-0.256207	-0.874157	0.967993
O	0.254548	1.204077	-0.502247	O	-1.043170	1.480553	0.676660
O	1.984854	-0.354332	0.055901	O	0.667577	0.467196	-0.782212
Li	2.089669	1.305041	-0.758523	Li	-1.391320	-2.047634	-0.044920
Li	-1.297651	1.208299	0.701079	Li	1.464913	-1.063925	0.250801
O	-2.593834	0.133058	-0.284285	O	3.114511	0.046537	0.010142
H	-1.944542	-0.492843	-0.673584	H	3.743718	-0.104110	-0.697003
H	-3.287377	-0.410031	0.095503	H	2.410111	0.624475	-0.357319

1e' **1f'**

	X	Y	Z		X	Y	Z
S	-0.568650	0.266930	0.014190	S	-0.693550	-0.000037	0.071823
O	-1.952938	-0.278833	-0.161721	O	-0.102759	1.224129	0.730477
O	0.268653	-1.049395	0.268329	O	0.031895	0.000135	-1.313877
O	-0.426345	1.177489	1.129206	O	-2.124662	-0.001002	-0.037539
O	0.010830	0.779119	-1.262480	O	-0.101231	-1.223364	0.730859
Li	-1.359021	-1.955079	0.275268	Li	1.067343	1.440308	-0.697265
Li	1.498710	-0.336893	-1.123257	Li	1.067893	-1.439669	-0.697781
O	2.836990	-0.169436	0.274818	O	2.424148	-0.000049	0.255926
H	3.217487	0.646101	0.609024	H	1.801945	-0.001226	1.008082
H	2.150085	-0.442277	0.905751	H	3.313810	0.000344	0.618813

$Li_2SO_4(H_2O)_2$

2a' **2b'**

	X	Y	Z		X	Y	Z
S	-0.156874	-0.349766	-0.004387	S	0.776948	0.110970	-0.236558
O	-1.171055	-0.033586	1.074611	O	0.541636	1.563195	-0.403446
O	-0.967569	-1.036466	-1.068125	O	0.076017	-0.663372	-1.295059
O	0.950608	-1.199027	0.504857	O	0.169209	-0.319807	1.119571
O	0.478753	0.901225	-0.514326	O	2.210586	-0.248554	-0.103129
Li	-2.530731	-0.713242	-0.120372	Li	1.876779	-1.003744	1.676037
Li	2.213275	0.192165	-0.004761	Li	-1.673921	-0.212235	1.042171
O	-3.349597	1.079147	0.062447	O	-2.014621	1.567749	0.327889
H	-2.541701	1.181416	0.607929	H	-1.080240	1.781531	0.055984
H	-3.273740	1.722598	-0.645627	H	-2.532150	1.627296	-0.477317
O	4.060306	0.628836	-0.000073	O	-2.180809	-1.562353	-0.283715
H	4.473186	1.440018	-0.328425	H	-1.372566	-1.324086	-0.820183
H	4.793041	0.094416	0.336569	H	-2.062192	-2.486241	-0.053076

2c' **2d'**

	X	Y	Z		X	Y	Z
S	-0.816765	-0.543155	-0.008344	S	0.821509	-0.051272	-0.007969
O	-1.403765	0.567939	-0.810389	O	-0.456261	0.646982	0.354638
O	-1.793568	-1.229095	0.818917	O	0.514368	-1.445673	-0.388196

O	0.303594	0.084833	0.873356	O	1.795913	0.016924	1.136210
O	-0.026311	-1.478154	-0.887160	O	1.514868	0.696546	-1.116620
Li	1.569896	-0.994677	-0.042973	Li	-2.163477	-0.072168	0.355327
Li	0.870802	1.822289	0.921487	Li	2.953179	0.920110	0.021983
O	-0.337351	2.822624	-0.166921	O	-2.802939	1.731059	-0.026006
H	-0.859265	2.025230	-0.493674	H	-1.874829	2.001203	-0.117878
H	-0.035714	3.302714	-0.938763	H	-3.331227	2.235530	-0.645405
O	3.416722	-0.400618	-0.085006	O	-2.012476	-1.886583	-0.043751
H	3.527045	0.323967	0.565067	H	-1.027488	-1.919000	-0.214166
H	3.759319	-0.015334	-0.901746	H	-2.367974	-2.773343	-0.067620

2e' **2f'**

	X	Y	Z		X	Y	Z
S	0.823404	-0.225615	-0.022930	S	0.036623	0.591465	-0.091329
O	0.075166	-0.582741	-1.256206	O	-1.205512	1.397326	-0.096642
O	0.252586	-1.056083	1.066822	O	-0.032953	-0.246584	1.205583
O	0.642641	1.263772	0.283720	O	1.286965	1.340724	-0.164159
O	2.306188	-0.359295	-0.156515	O	-0.014253	-0.502358	-1.145619
Li	-1.186729	-1.557388	-0.142248	Li	-1.954220	0.080735	1.120030
Li	2.488446	1.439928	0.231424	Li	0.932050	-1.611375	0.200154
O	-2.886432	-0.743932	0.093639	O	-2.487993	-1.290201	-0.200752
H	-2.672707	0.224458	0.051327	H	-1.717563	-1.136299	-0.794845
H	-3.525168	-0.858185	0.798648	H	-3.267999	-1.293027	-0.759074
O	-2.019095	1.776915	-0.030936	O	2.765814	-0.982536	0.132064
H	-1.055290	1.709062	0.157073	H	3.434008	-1.151525	-0.534678
H	-2.077734	2.160167	-0.908750	H	2.552854	-0.025691	0.072973

$Li_2SO_4(H_2O)_3$

3a' **3b'**

	X	Y	Z		X	Y	Z
S	0.192850	-0.414525	-0.088977	S	-0.216669	-0.278662	0.220547
O	-0.731397	-1.229953	-0.898011	O	0.815599	-0.172390	1.284424
O	-0.411308	-0.127806	1.243226	O	0.213334	-1.242499	-0.811121
O	0.460427	0.929229	-0.780281	O	-0.398780	1.117721	-0.395045
O	1.550775	-1.024803	0.032689	O	-1.569451	-0.596104	0.770295
Li	-2.136922	0.561376	1.047444	Li	-2.233315	1.069411	0.020513
Li	2.304330	0.568751	-0.797271	Li	2.499435	0.267911	0.618832
O	-3.154802	-0.803412	0.120505	O	2.871601	-1.224147	-0.538845
H	-2.365241	-1.126807	-0.383783	H	1.929026	-1.443215	-0.749502
H	-3.621357	-1.579015	0.434421	H	3.397302	-1.425508	-1.312777
O	3.791525	0.378838	0.416421	O	-3.821074	0.088137	-0.484075
H	3.310045	-0.334996	0.864814	H	-3.372775	-0.721835	-0.189411
H	4.340163	0.831194	1.058160	H	-4.375500	-0.126483	-1.235284
O	-1.856390	2.089184	-0.107164	O	2.128966	1.968936	-0.238194
H	-2.415890	2.265468	-0.865738	H	2.478458	2.348474	-1.045136
H	-0.957743	1.873940	-0.461381	H	1.152404	1.856754	-0.367663

3c' **3d'**

	X	Y	Z
S	0.124683	-0.420283	0.048740
O	-0.688355	-1.010824	-1.034755
O	-0.708857	-0.262800	1.274085
O	0.617715	0.975338	-0.364995
O	1.383365	-1.174980	0.309956
Li	-2.299384	0.625501	0.876810
Li	2.383820	0.350035	-0.155383
O	-3.216639	-0.488582	-0.421046
H	-2.361723	-0.809045	-0.811997
H	-3.770278	-1.260964	-0.299623
O	4.307520	0.485682	-0.187595
H	4.831919	-0.281974	0.055879
H	4.916341	1.187501	-0.426855
O	-1.688988	2.257189	0.031718
H	-2.071910	2.558054	-0.794357
H	-0.754811	1.994079	-0.170512

	X	Y	Z
S	0.180105	0.003743	-0.602082
O	1.662287	0.003545	-0.777314
O	0.011457	-0.004715	0.947758
O	-0.453912	-1.220898	-1.122817
O	-0.452113	1.235048	-1.109301
Li	1.889166	-0.007615	1.123405
Li	-1.823491	-0.007342	1.361101
O	-2.424883	1.660573	0.614119
H	-3.251308	1.963214	0.236693
H	-1.738524	1.715698	-0.100675
O	3.788960	-0.005869	0.880707
H	3.729276	0.001076	-0.084768
H	4.710532	0.004143	1.139354
O	-2.423631	-1.668842	0.599138
H	-3.250921	-1.964943	0.218372
H	-1.738245	-1.715436	-0.117069

3e'

	X	Y	Z
S	-0.202066	-0.433531	-0.452170
O	-1.642462	-0.832271	-0.442480
O	0.708493	-1.587998	-0.522730
O	-0.012734	0.233738	0.942424
O	0.086931	0.590880	-1.474784
Li	1.777892	0.791920	1.115546
Li	-1.854334	-0.010523	1.287391
O	-3.540693	0.683407	0.656419
H	-3.318669	0.344047	-0.226203
H	-4.074527	1.472446	0.556507
O	1.944459	2.083305	-0.303674
H	2.673446	2.354787	-0.862395
H	1.251209	1.692652	-0.896815
O	2.751952	-0.861827	1.011862
H	2.091229	-1.347113	0.454086
H	3.622916	-1.111045	0.701462

3f'

	X	Y	Z
S	0.340640	-0.016358	0.569624
O	-0.909610	-0.031076	1.359999
O	0.342311	-1.191084	-0.407919
O	1.563949	-0.012141	1.370319
O	0.332265	1.180269	-0.382047
Li	-2.448418	0.003751	0.292188
Li	1.290459	0.033596	-1.627640
O	3.107137	0.065154	-0.933532
H	2.851166	0.122581	0.013805
H	3.771381	-0.624384	-0.987038
O	-2.266926	1.688533	-0.648343
H	-1.276841	1.724103	-0.620792
H	-2.591230	2.571793	-0.469037
O	-2.270622	-1.655019	-0.704140
H	-2.607260	-2.539482	-0.556250
H	-1.281648	-1.704085	-0.668611

$Li_2SO_4(H_2O)_4$

4a'

	X	Y	Z
S	0.000008	-0.000111	-0.501052
O	0.000150	1.229561	0.378668
O	-0.000323	-1.229830	0.378556
O	1.235485	-0.000291	-1.318197
O	-1.235346	0.000161	-1.318515
Li	2.812422	-0.000153	-0.327442
Li	-2.811704	0.000444	-0.327034

4b'

	X	Y	Z
S	0.023141	0.200586	0.592595
O	1.196573	0.463237	1.440110
O	0.338708	0.664185	-0.829943
O	-1.200508	0.899738	1.048069
O	-0.261781	-1.279273	0.505785
Li	2.043574	0.009206	-1.286089
Li	-2.730916	0.578780	0.043453

O	-2.622507	1.650149	0.657004	O	3.341476	0.767831	-0.079094
H	-2.911415	1.977235	1.508907	H	2.692816	0.751586	0.669017
H	-1.632682	1.701456	0.636141	H	3.799162	1.608300	-0.039406
O	2.622579	-1.649749	0.657336	O	1.835038	-1.895414	-1.039224
H	2.911211	-1.977248	1.509192	H	1.025448	-1.904518	-0.468991
H	1.632856	-1.701382	0.636164	H	2.491281	-2.433873	-0.592929
O	-2.623180	-1.649755	0.656644	O	-2.149167	1.257469	-1.673997
H	-1.633395	-1.701503	0.635598	H	-1.174331	1.159688	-1.535744
H	-2.911973	-1.976213	1.508833	H	-2.338041	0.994333	-2.575140
O	2.622838	1.649690	0.656630	O	-2.921486	-1.320588	0.259247
H	1.633093	1.701256	0.635671	H	-3.318225	-2.078346	-0.169697
H	2.911863	1.978930	1.507672	H	-1.965801	-1.526020	0.421219

4c'

	X	Y	Z
S	0.105370	-0.179226	0.629467
O	0.113171	1.148323	-0.073567
O	1.400131	-0.356973	1.328085
O	-0.064735	-1.285719	-0.402882
O	-1.081424	-0.299790	1.511198
Li	2.867077	-0.149525	0.185009
Li	-1.881648	-1.520073	0.244990
O	2.703975	1.669342	-0.465721
H	1.716201	1.687581	-0.395966
H	3.025214	2.505884	-0.126958
O	-3.358793	-0.766720	-0.675878
H	-3.135303	0.202034	-0.699915
H	-3.787305	-0.979265	-1.505607
O	-2.486817	1.745565	-0.640872
H	-1.517774	1.634408	-0.505613
H	-2.788059	2.243828	0.122245
O	2.489810	-1.428540	-1.210902
H	1.523966	-1.574965	-1.059294
H	2.598299	-1.246999	-2.146044

4d'

	X	Y	Z
S	-0.064506	-0.356379	-0.391556
O	-0.869863	0.165398	-1.515019
O	-0.885177	-1.275159	0.447751
O	0.385392	0.809834	0.499856
O	1.202587	-0.998251	-0.837776
Li	-2.499028	-0.490177	0.958808
Li	2.305763	0.305490	0.196349
O	-1.879034	1.072227	1.913231
H	-2.263879	1.946804	1.836486
H	-0.961320	1.128848	1.546643
O	3.165151	-1.290560	0.954200
H	2.509479	-1.821360	0.472672
H	3.286773	-1.681363	1.820550
O	2.478556	2.116798	-0.569900
H	2.669789	2.352367	-1.479773
H	1.514500	2.165018	-0.453660
O	-3.396870	-0.037706	-0.696554
H	-3.994970	-0.521207	-1.267575
H	-2.554487	0.093751	-1.202657

4e'

	X	Y	Z
S	-0.099565	-0.223717	0.161641
O	-0.661855	-1.511636	-0.309665
O	1.431285	-0.409719	0.121158
O	-0.434961	-0.016609	1.610414
O	-0.459636	0.937497	-0.663188
Li	1.216527	-2.350368	0.337195
Li	2.266742	1.230695	0.522020
O	0.882465	-3.463767	-1.235367
H	0.112248	-2.886257	-1.388905
H	1.312707	-3.614620	-2.077964

4f'

	X	Y	Z
S	0.707515	0.339389	-1.009428
O	1.456908	-0.518748	-1.935321
O	1.695104	0.961564	0.001453
O	-0.284859	-0.448963	-0.206781
O	0.051685	1.510475	-1.642624
Li	2.711448	-0.396629	0.819892
Li	0.801723	2.668749	-0.313926
O	-2.185480	1.305241	0.677318
H	-2.829387	1.373711	-0.031403
H	-1.573319	0.587937	0.394494

O	1.763073	2.379427	-0.940009	O	3.694219	-1.164886	-0.639724
H	1.666043	3.322561	-1.073733	H	3.001667	-0.996661	-1.325015
H	0.870125	1.970358	-1.052408	H	4.098392	-2.009606	-0.839304
O	0.716460	-2.465277	2.240160	O	-0.523968	3.366992	0.841495
H	0.230854	-1.613383	2.297255	H	-0.537850	3.772152	1.708857
H	0.110068	-3.136774	2.559100	H	-1.228269	2.663584	0.829210
O	1.549612	1.636268	2.264632	O	1.336964	-1.454534	1.664357
H	0.731724	1.076426	2.228487	H	1.256974	-2.392234	1.843062
H	1.307765	2.464934	2.679883	H	0.574900	-1.201297	1.084911

$Li_2SO_4(H_2O)_5$

	5a'				**5b'**		
	X	Y	Z		X	Y	Z
S	0.280756	-0.055660	-0.380583	S	0.295819	0.084828	0.423761
O	0.400721	1.264131	0.342846	O	1.464907	-0.007025	1.333271
O	0.459515	-1.175148	0.614118	O	0.228404	-1.179008	-0.392733
O	1.356739	-0.143728	-1.397789	O	0.503172	1.263511	-0.500068
O	-1.075928	-0.149896	-0.972345	O	-0.978304	0.266248	1.156407
Li	3.076256	-0.052247	-0.682899	Li	3.097444	-0.216009	0.461525
Li	-2.567190	0.059771	0.289914	Li	-2.523064	1.016181	0.468143
O	-2.133623	1.838620	1.031951	O	3.167609	1.391613	-0.603351
H	-2.448295	2.654404	0.638976	H	2.189604	1.541892	-0.659904
H	-1.161125	1.803236	0.858457	H	3.544153	1.622840	-1.452579
O	3.087879	-1.612678	0.452137	O	-3.775073	-0.309909	-0.072054
H	3.524834	-1.870092	1.264013	H	-3.249233	-1.137233	-0.241126
H	2.110498	-1.654317	0.612429	H	-4.527932	-0.324441	-0.663062
O	-2.030867	-1.264088	1.636241	O	-2.176181	-2.360949	-0.562431
H	-1.090805	-1.416131	1.375890	H	-1.276774	-1.951148	-0.563927
H	-2.018330	-1.039558	2.568299	H	-2.134843	-3.058636	0.094629
O	3.032975	1.678239	0.172615	O	2.805770	-1.868997	-0.495871
H	2.051795	1.737036	0.302469	H	3.112028	-2.227785	-1.328970
H	3.447825	2.051196	0.950717	H	1.817451	-1.810379	-0.542998
O	-3.709301	-0.367471	-1.283290	O	-1.860233	2.435270	-0.642360
H	-2.899112	-0.490202	-1.800246	H	-0.910042	2.152979	-0.695474
H	-4.256721	-1.141076	-1.428324	H	-2.108769	2.790624	-1.495544

	5c'				**5d'**		
	X	Y	Z		X	Y	Z
S	-0.295699	-0.356219	-0.399686	S	0.283685	0.385611	0.375067
O	-0.703259	-0.184472	1.059442	O	1.269379	1.286902	0.995553
O	1.077969	-0.914874	-0.439315	O	0.702811	0.120405	-1.066538
O	-0.277146	1.024748	-1.003763	O	-1.090145	0.945190	0.368107
O	-1.286906	-1.216550	-1.067913	O	0.259681	-0.954369	1.065623
Li	-2.534189	0.247067	1.119689	Li	2.530375	-0.322134	-1.093679
Li	2.510788	0.176528	0.306123	Li	-2.517343	-0.206435	-0.301301
O	1.720049	0.516586	2.079638	O	3.524147	1.170391	-0.385942
H	0.789071	0.239975	1.914636	H	2.792549	1.405750	0.239477

H	1.677701	1.415736	2.410677	H	3.847533	1.988348	-0.765017
O	-3.519587	-1.226454	0.358110	O	2.575709	-1.865028	0.067758
H	-3.810475	-2.069702	0.707024	H	1.721816	-1.738388	0.552338
H	-2.796025	-1.412877	-0.292117	H	3.249947	-2.019734	0.731705
O	3.683226	-1.360488	-0.167711	O	-1.707620	-0.702239	-2.027266
H	2.897142	-1.829152	-0.485412	H	-0.780762	-0.399873	-1.886606
H	4.167576	-1.966463	0.395385	H	-1.653457	-1.629237	-2.267385
O	-2.606580	1.842716	0.038263	O	-2.291195	-1.772724	0.871283
H	-3.283747	2.019283	-0.617192	H	-2.734519	-1.883958	1.713762
H	-1.750457	1.757745	-0.451643	H	-1.335415	-1.623833	1.073257
O	2.271788	1.836749	-0.727284	O	-3.691105	1.365930	0.029015
H	2.716580	2.028917	-1.554260	H	-2.907997	1.860915	0.312266
H	1.317590	1.701586	-0.945281	H	-4.174555	1.922845	-0.583307

5e'

	X	Y	Z
S	-0.300720	-0.232913	-0.591515
O	-0.302336	-1.508648	0.218707
O	-0.578512	0.900718	0.385636
O	-1.371574	-0.246693	-1.601419
O	1.044102	-0.039574	-1.180846
Li	-2.319979	0.773617	1.084771
Li	2.658202	-0.589511	-0.468285
O	2.223260	-2.299599	0.271171
H	1.236672	-2.200283	0.304445
H	2.491035	-2.855173	1.002642
O	3.535045	0.889792	0.341862
H	2.839257	1.583478	0.492485
H	4.208634	1.007405	1.011684
O	-2.282361	-0.971665	1.912645
H	-1.530436	-1.355011	1.390426
H	-2.960806	-1.645934	1.964215
O	1.515315	2.571167	0.721978
H	1.404453	3.240193	0.043205
H	0.725855	1.984773	0.639222
O	-3.415488	1.017763	-0.472098
H	-4.293845	0.770529	-0.761436
H	-2.767078	0.605550	-1.098358

5f'

	X	Y	Z
S	-0.236184	-0.111766	-0.486807
O	1.033822	-0.266584	-1.239516
O	-0.603042	1.335974	-0.357667
O	0.029752	-0.690913	0.891867
O	-1.375564	-0.841711	-1.099358
Li	-2.972109	-0.670415	-0.148852
Li	1.971479	-0.818951	0.541924
O	2.484432	-2.423334	-0.515188
H	1.970471	-2.021277	-1.235885
H	2.195366	-3.333904	-0.436440
O	-3.274684	1.228262	-0.246391
H	-2.327194	1.496851	-0.342102
H	-3.714899	1.900121	0.274379
O	1.669837	2.746026	0.124469
H	1.985076	3.005946	-0.743922
H	0.786924	2.341487	-0.034687
O	3.006402	0.674294	1.163334
H	2.585673	1.498189	0.808245
H	3.387986	0.895587	2.013010
O	-2.457003	-1.399776	1.570538
H	-1.479823	-1.246508	1.506107
H	-2.720359	-1.178043	2.464289