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

Explore tetra-branched multiple-site SO_2 capture materials

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Supporting Information

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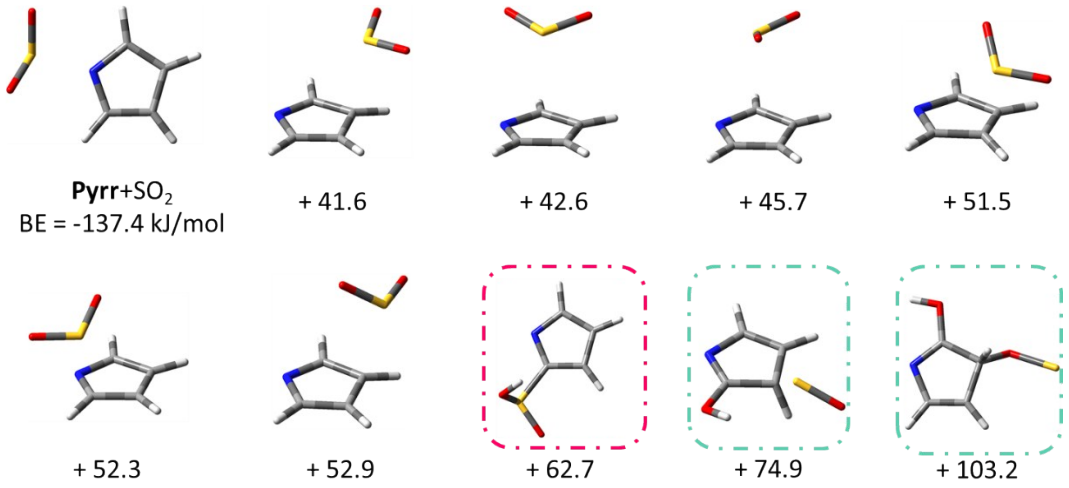

Figure S1. Stable structures of **Pyrr**-SO_2 complexes identified by the configuration search program. The name and the binding energy or the relative binding energy with respect to the most stable one (in kJ/mol) are given below each configuration. Red is oxygen, blue is nitrogen, yellow is sulfur, gray is carbon and white is hydrogen. Structures highlighted in pink and green dotted boxes are the insertion and decomposition products, respectively.

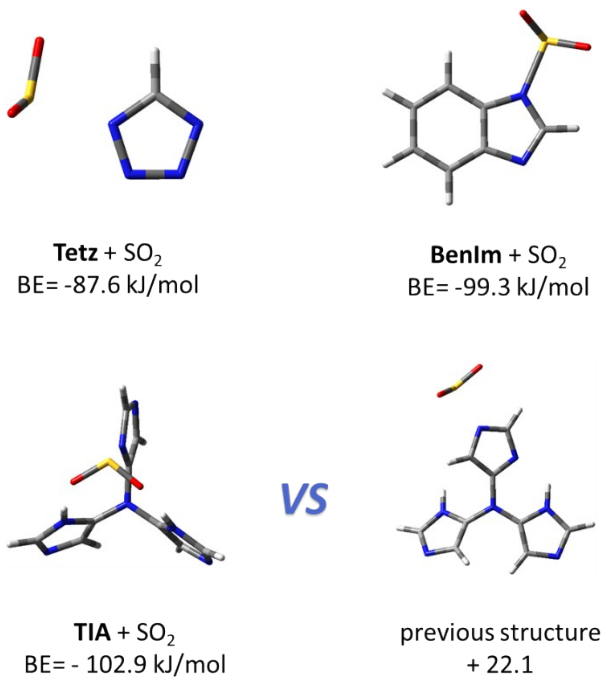

Figure S2. The most stable configurations of the first SO_2 absorptions of three anions. The name and the binding energies and binding energy differences (ΔBE) are given below each configuration.

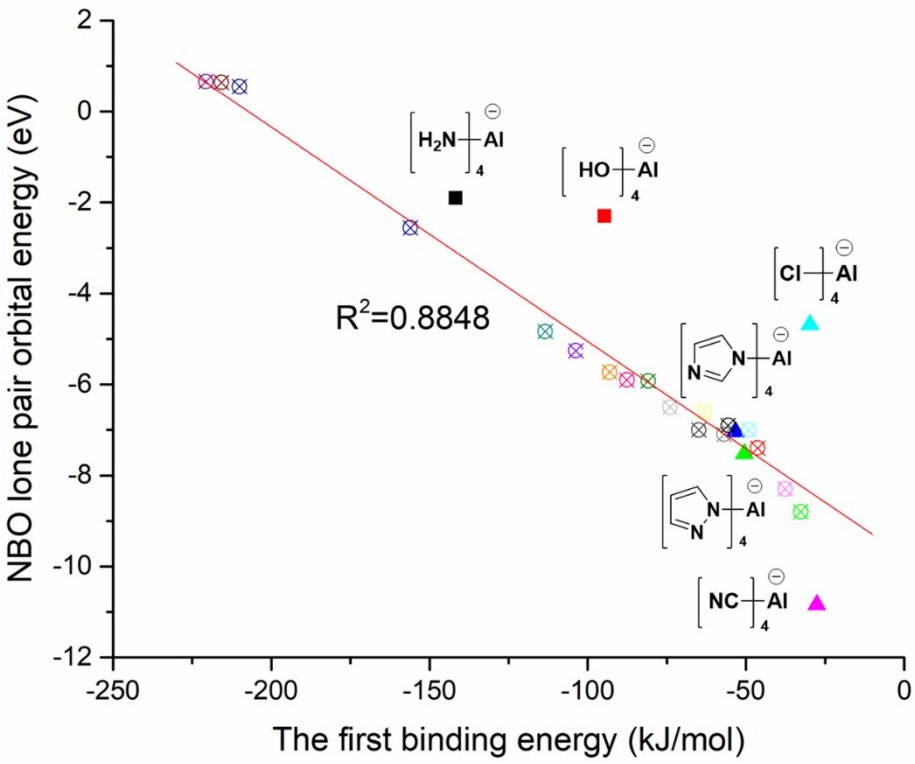

Figure S3. The first binding energy of four tetra-branched anions (solid triangles) and reported anions (half-solid circles) *and* SO_2 versus the NBO orbital energy of the lone pair of the reacting atom. $[\mathbf{Al(NH_2)_4}]^-$ and $[\mathbf{Al(OH)_4}]^-$ (solid squares) are excluded from the linear fitting.

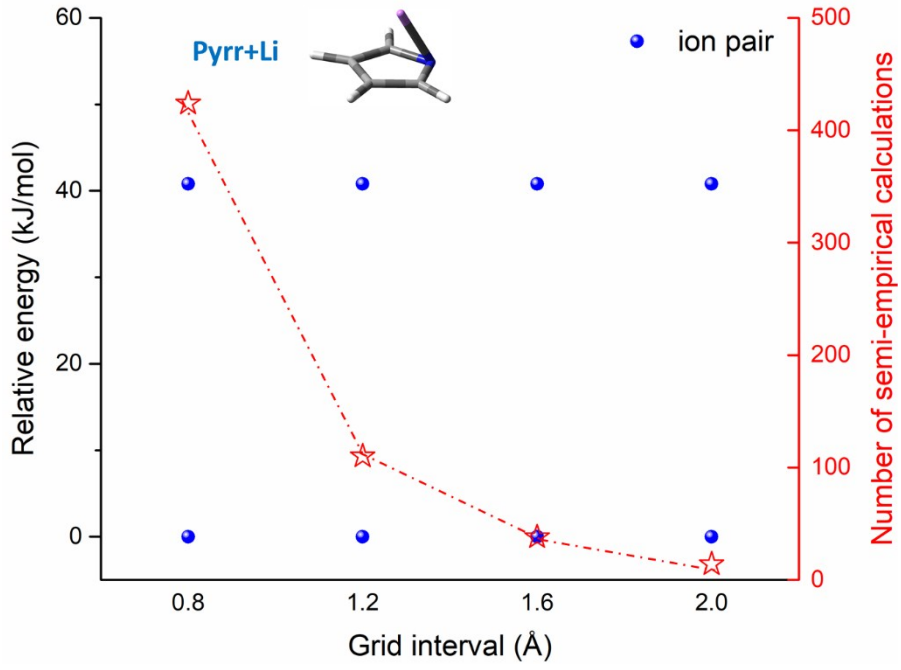

Figure S4. Screening parameters and relative energy of the most stable configurations of **Pyrr** and Li. Insert: the most stable configuration of **Pyrr**-Li Complex.

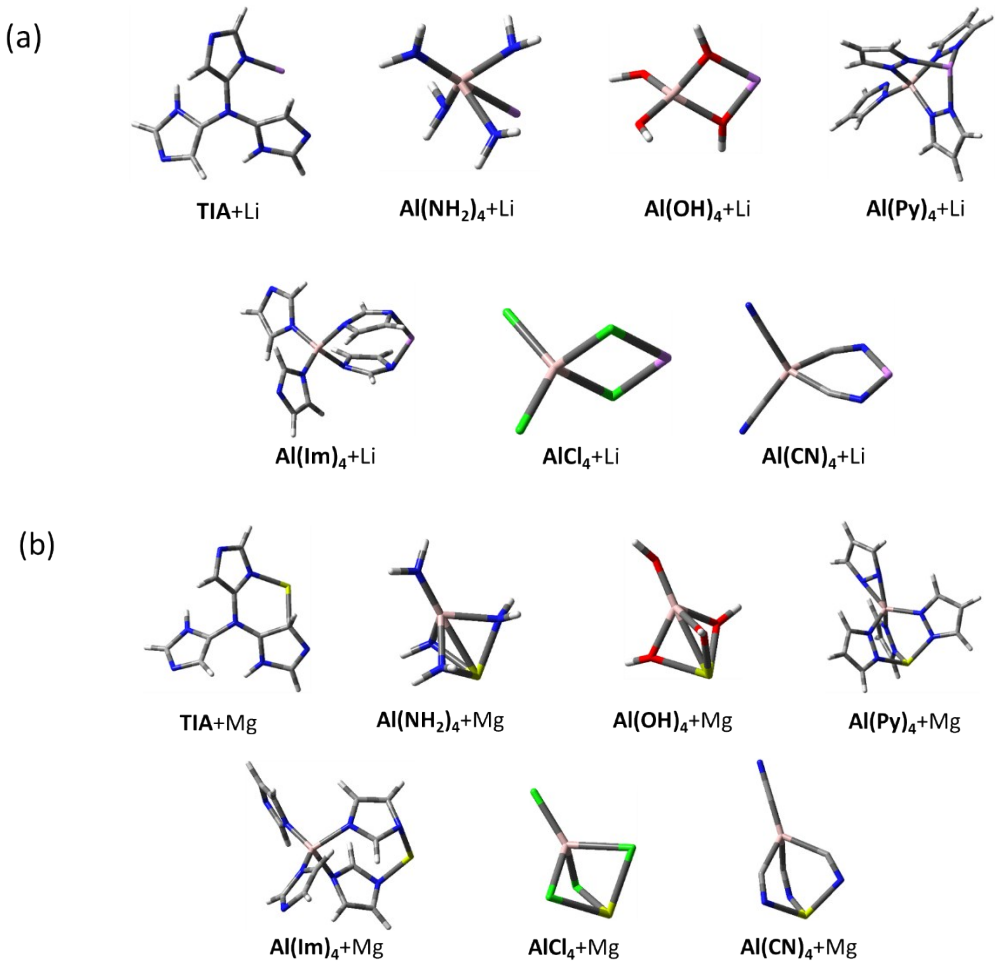

Figure S5. The most stable configurations of ion pairs composed of the studied anions and (a) Li and (b) Mg. Amaranth is lithium and yellow-green is magnesium.

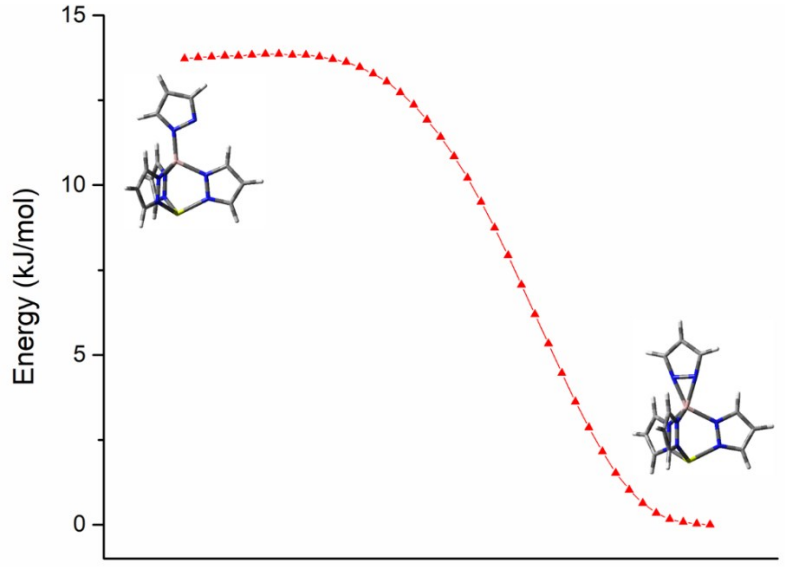

Figure S6. Two stable configurations of the [**Al(Py)$_4$**]$^-$-Mg complex and their interconversion energetics by the IRC method.

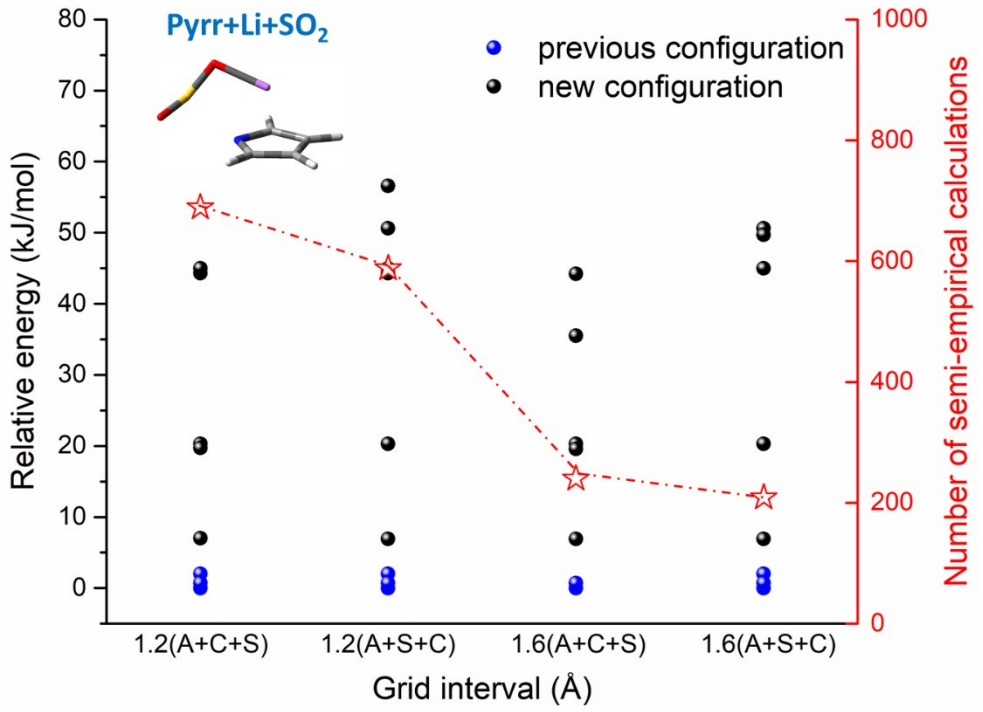

Figure S7. Screening parameters and relative energy of the most stable configurations of **Pyrr**-Li-SO_2. Insert: the most stable configuration of **Pyr**r+Li+SO_2 complex.

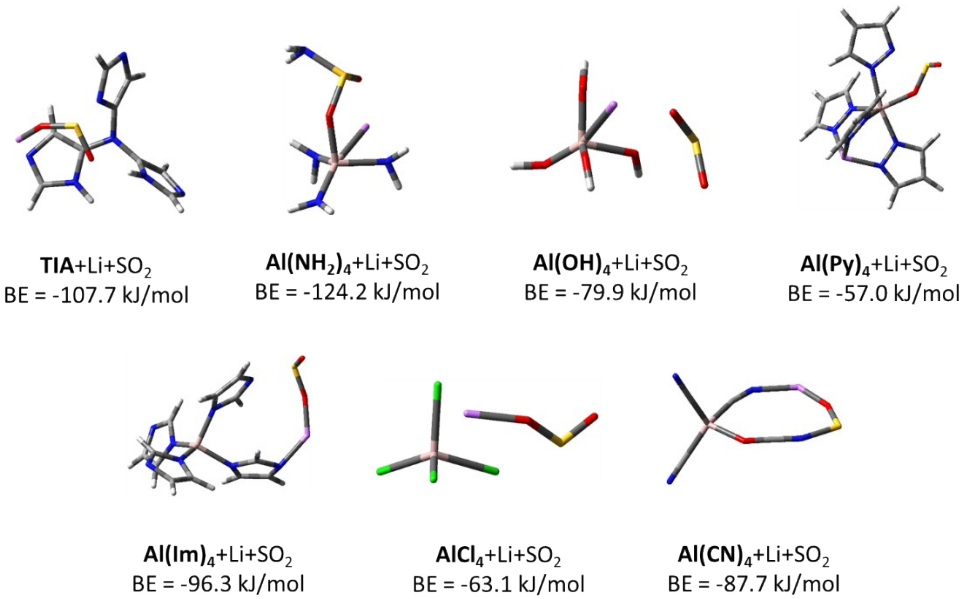

Figure S8. The most stable configurations of the first SO_2 bindings to tetra-branched anions and Li. The name and the binding energies are given below each configuration.

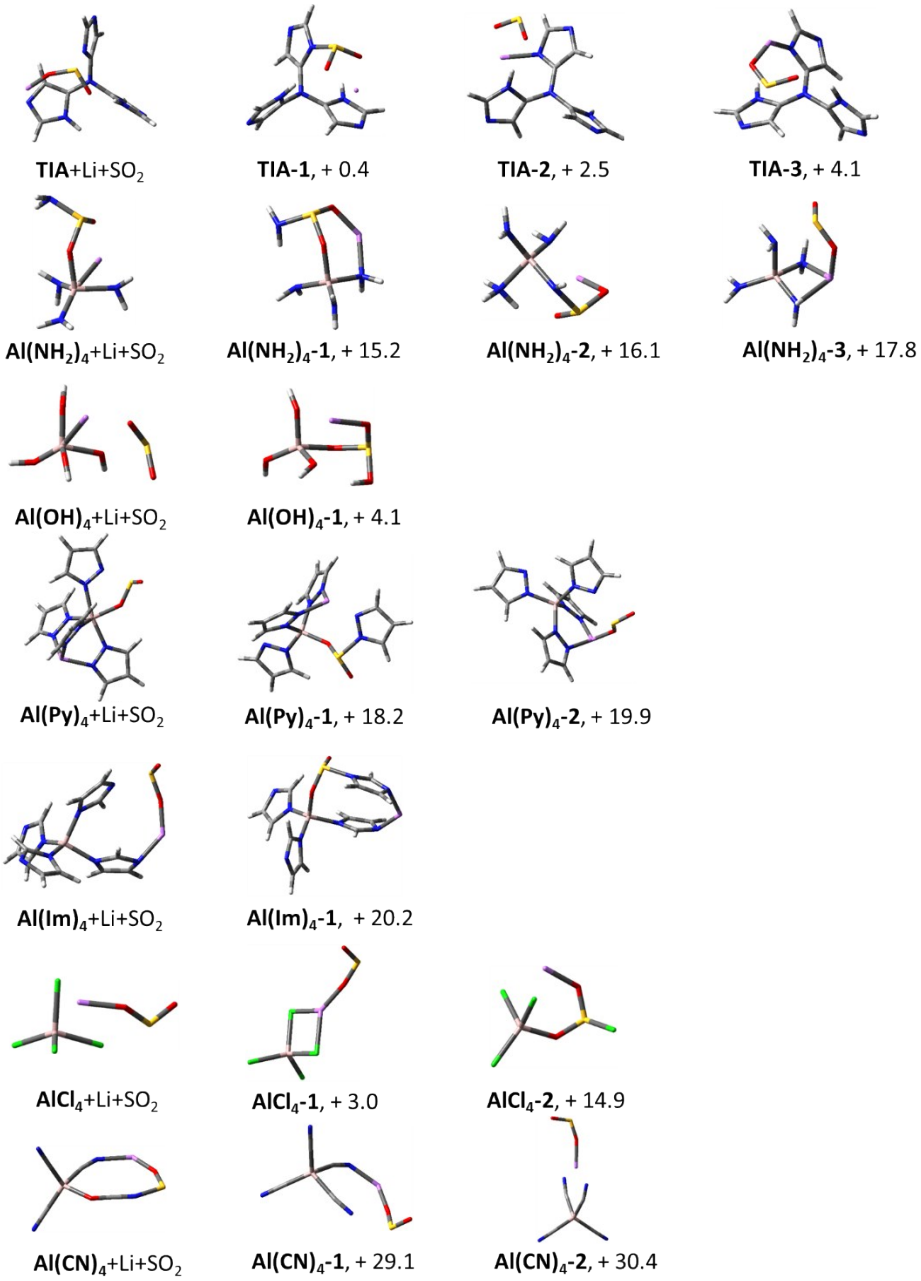

Figure S9. Stable structures of anion-Li complexes identified by the configuration search program. The name and the binding energy or the relative binding energy with respect to the most stable one (in kJ/mol) are given below each configuration.

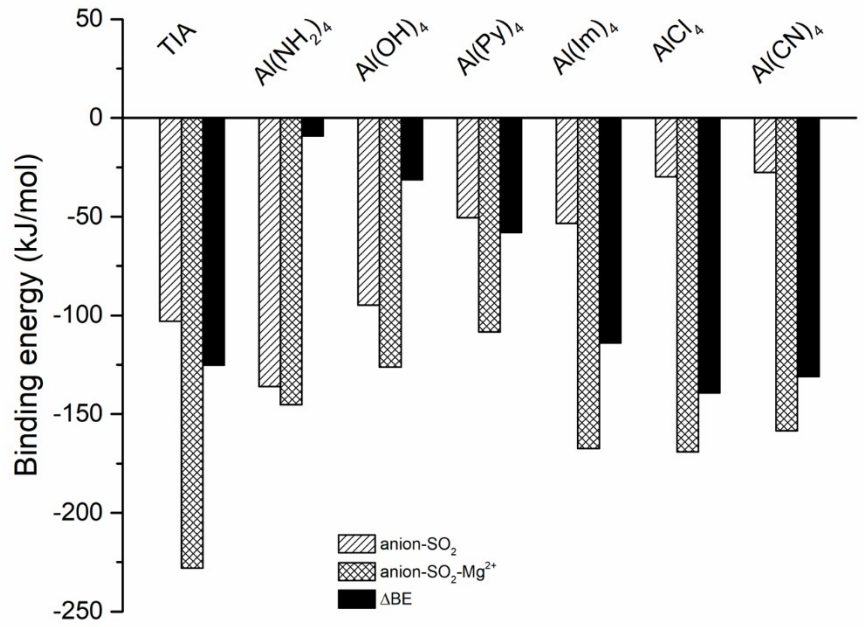

Figure S10. Binding energies between SO_2 and anions alone or with Mg^{2+}. The binding energy differences are represented by filled black bars. Negative ΔBE means that the anion-SO_2 interaction is strengthened by cation. Only the most stable configurations are used.

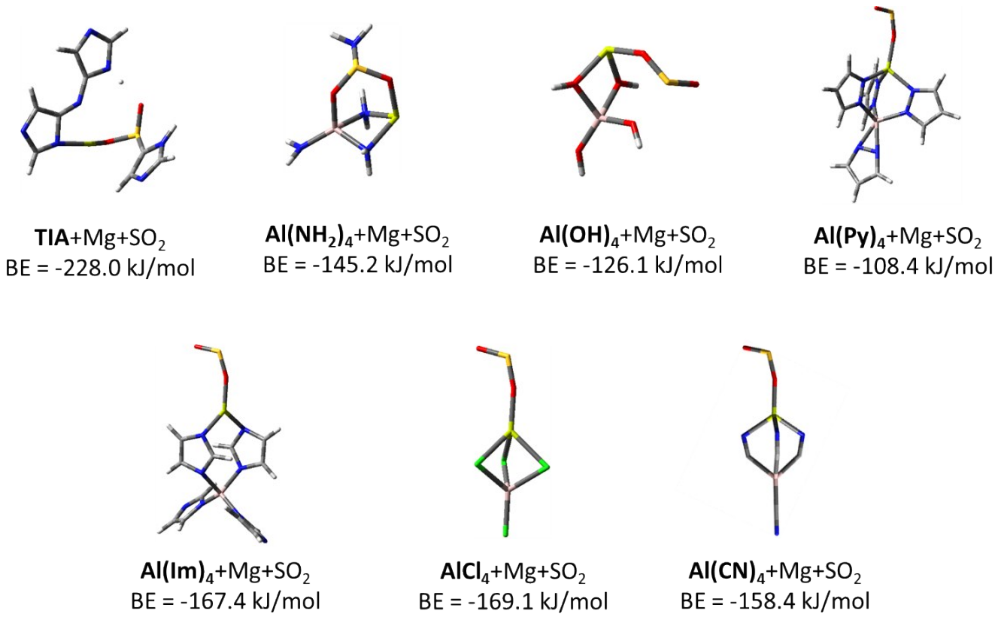

Figure S11. The most stable configurations of the first SO_2 bindings to tetra-branched anions and Mg. The name and the binding energies are given below each configuration.

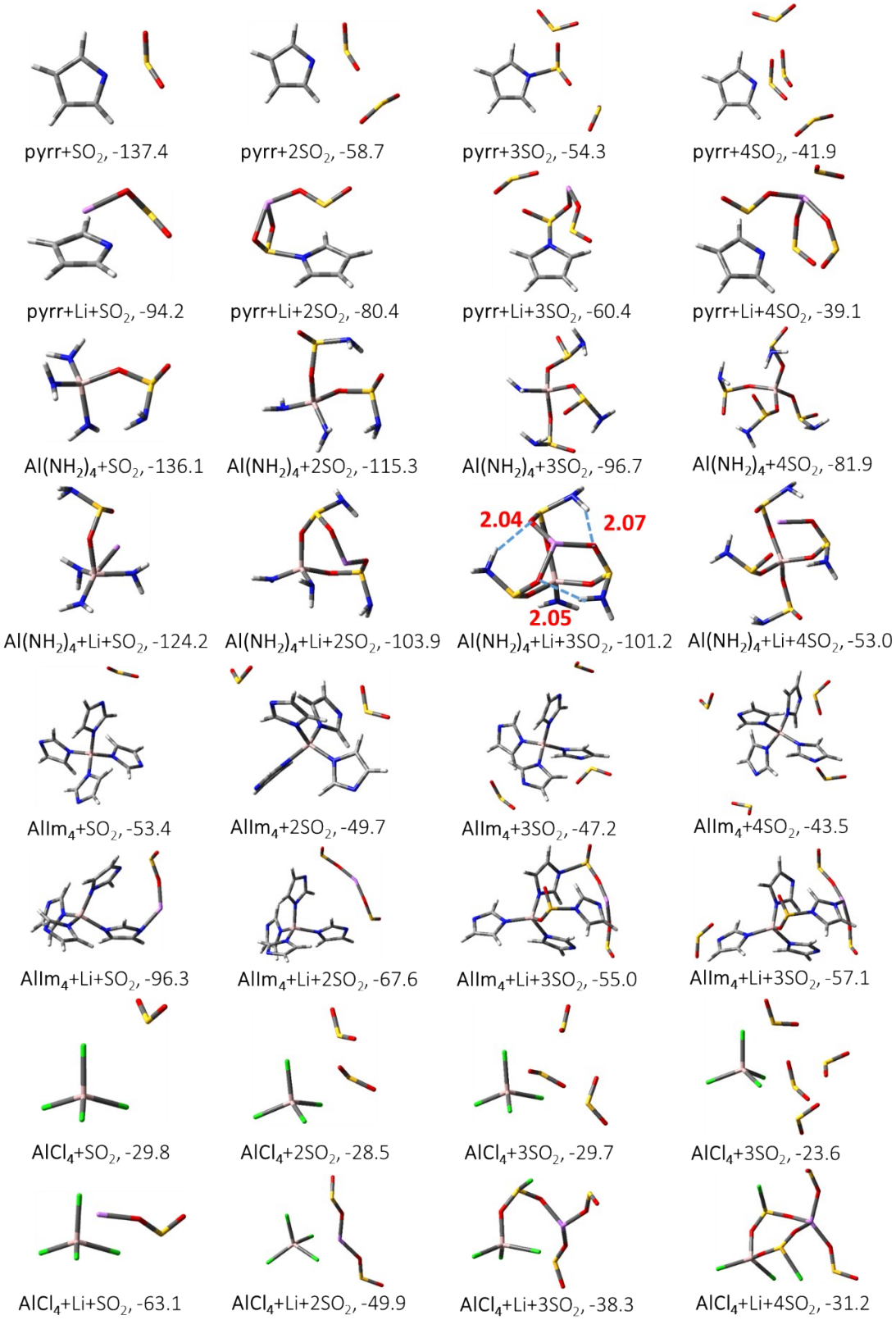

Figure S12. The most stable configurations of the sequential SO_2 absorptions over four representative anions with or without Li. The name and the binding energies (in kJ/mol) are given below each configuration. Dashed lines indicate the key distances of interest (in Å).

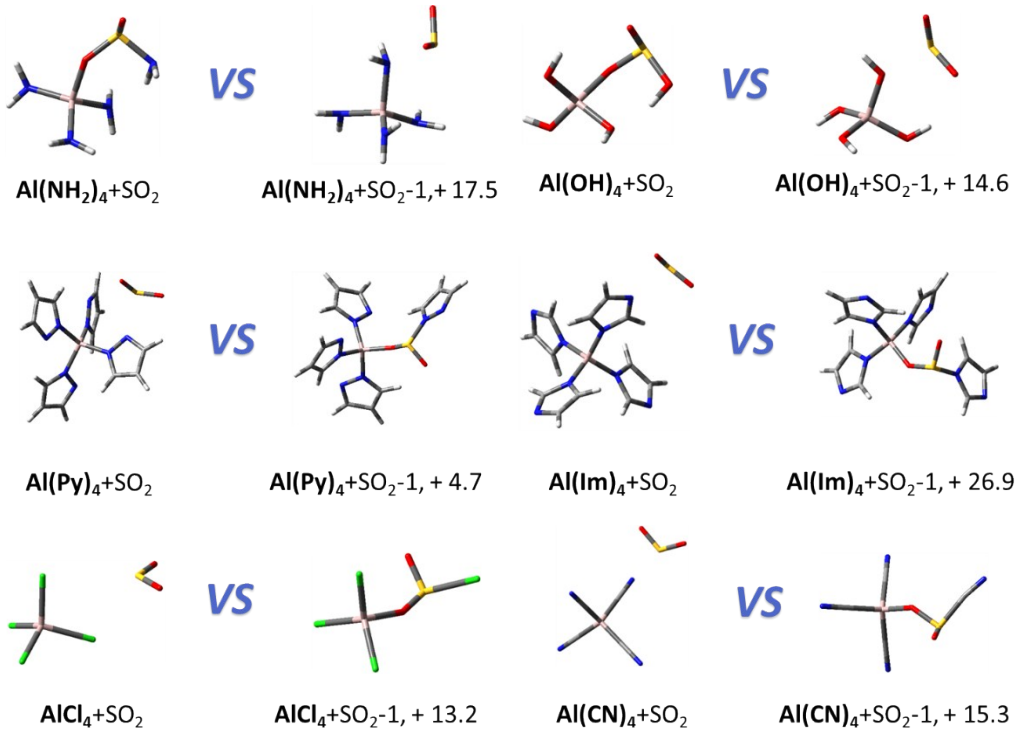

Figure S13. Insertion configurations and absorption configurations of the first SO_2 absorptions over tetra-branched anions. The name and the relative binding energy with respect to the most stable one (in kJ/mol) are given below each configuration.

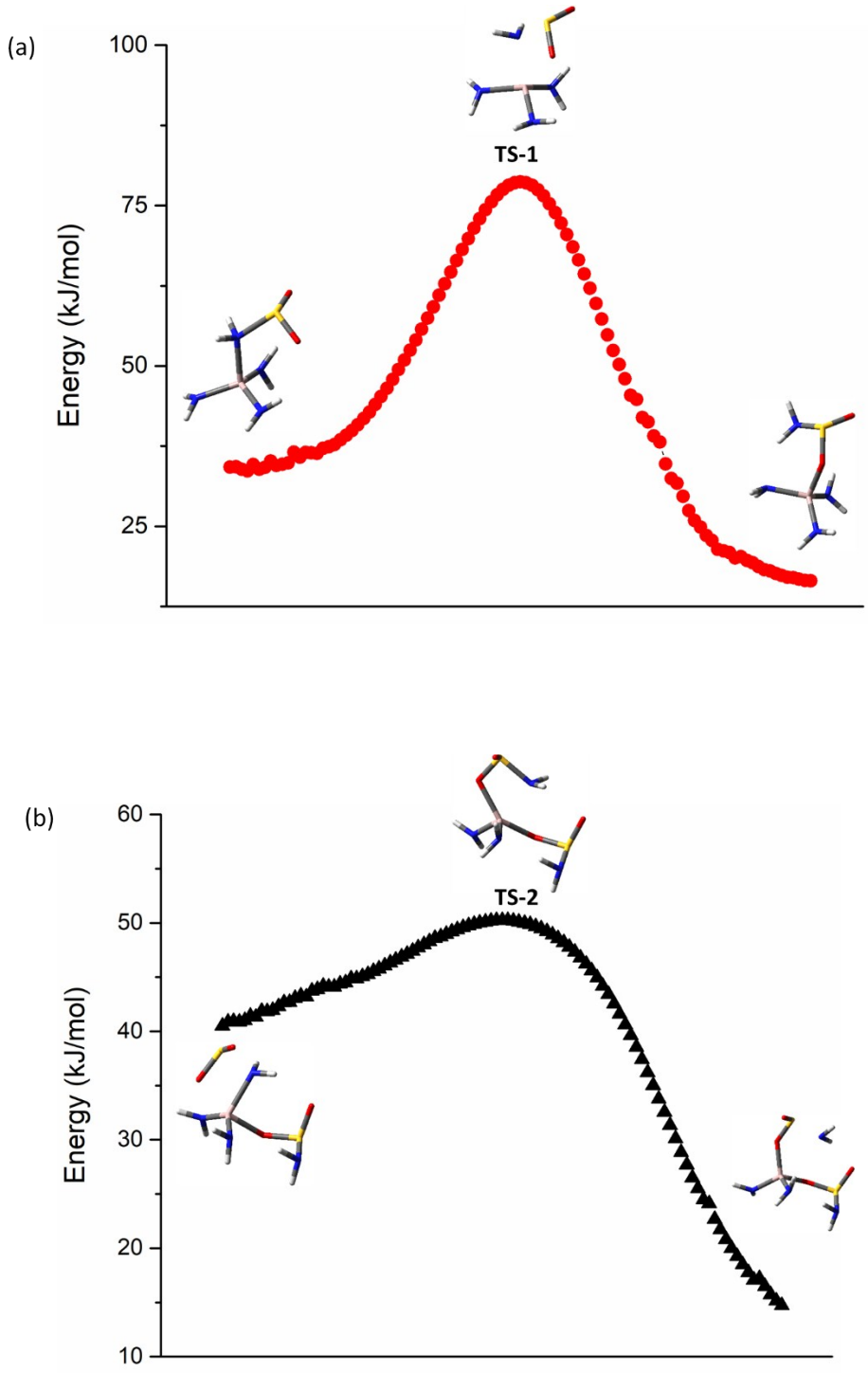

Figure S14. The interconversion energetics of two stable configurations. (a) **Al(NH$_2$)$_4$**-SO$_2$ complex and (b) **Al(NH$_2$)$_4$**-2SO$_2$ complex.

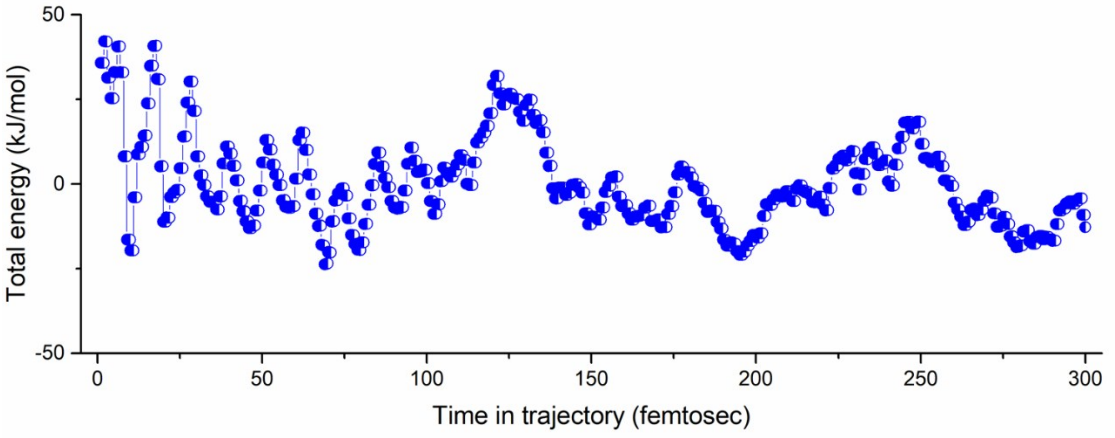

Figure S15. Total energy of $[\mathbf{Al(NH_2)_4}]^-$ observed at 400K during 300 ps ADMP dynamics trajectories.

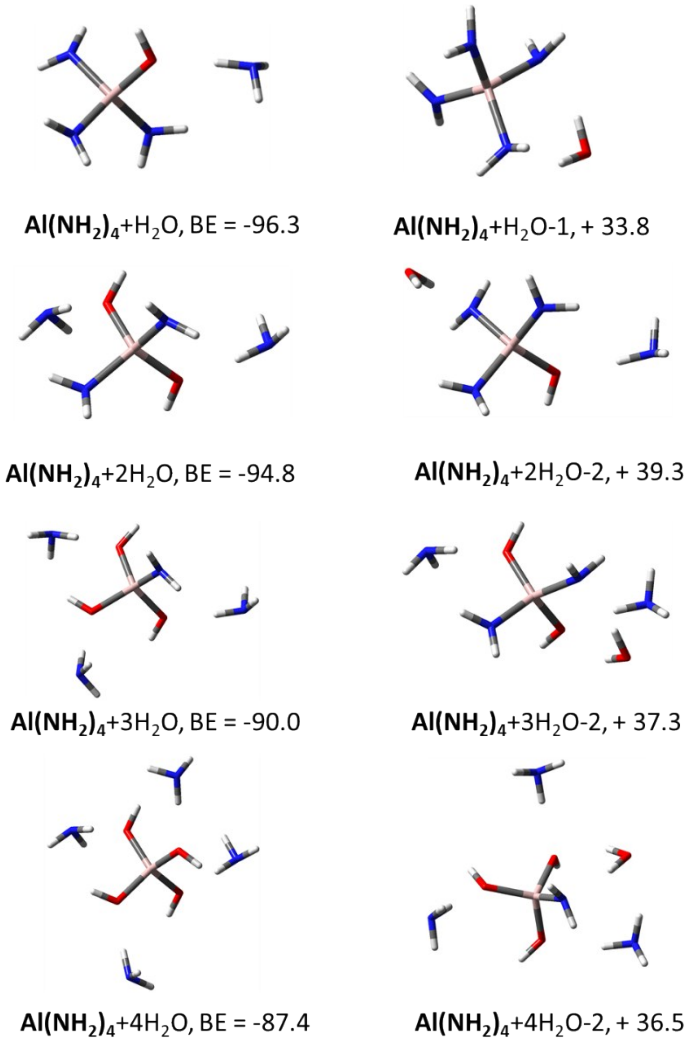

Figure S16. The stable configurations of the sequential H_2O absorptions over $[\mathbf{Al(NH_2)_4}]^-$. The name and the binding energy or the relative binding energy with respect to the most stable one (in kJ/mol) are given below each configuration.

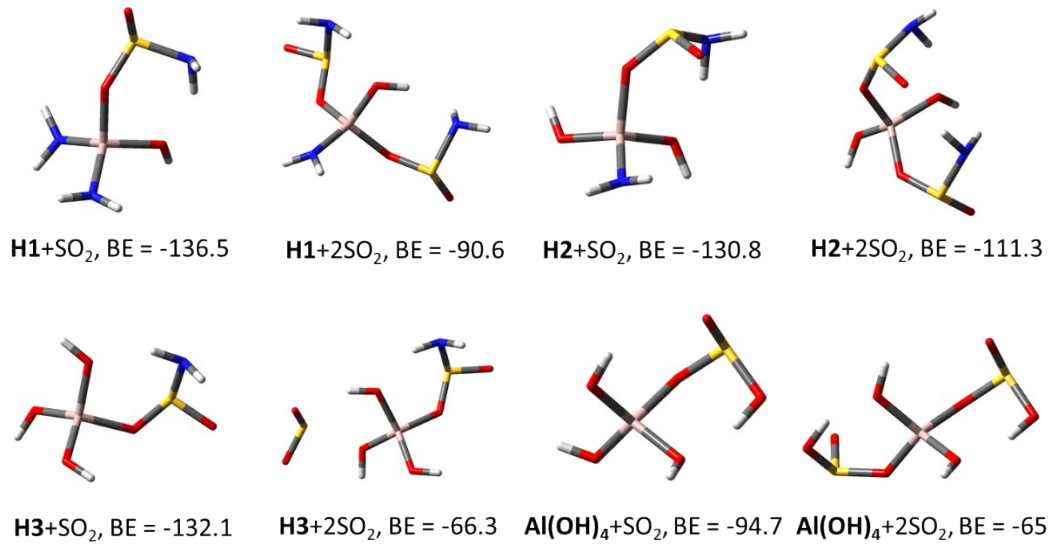

Figure S17. The most stable configurations of the sequential SO_2 absorptions over three tetra-branched heteroleptic anions and $[\mathbf{Al(OH)_4}]^-$. The name and the binding energies (in kJ/mol) are given below each configuration.

Cartesian coordinates of the key molecules:

TIA+SO_2

-1 1

N	-0.01446023	-0.26601077	-0.21719585
C	1.17254959	-0.43273848	0.52494405
C	-1.14971054	0.31754108	0.39219635
C	-0.06182807	-0.63879552	-1.57593376
N	1.92954710	0.64110080	0.94803683
C	2.99165349	0.13386014	1.62467178
N	2.98156954	-1.18644309	1.65114406
C	1.84120511	-1.54909180	0.97232621
H	1.68003755	1.62464436	0.77860591
H	3.73750384	0.76379993	2.08627570
H	1.56552784	-2.58276635	0.83078387
H	-2.33227089	-1.32881520	1.25464960
C	-2.19392324	-0.27386739	1.06680331
C	-2.58682356	1.82132508	1.08552628
N	-3.09192288	0.66870974	1.49956873
N	-1.41778848	1.68337641	0.41122891
H	-3.03809277	2.78925920	1.25373607
C	-0.03971689	-1.86136434	-2.20700219
C	-0.16031709	-0.39315101	-3.75976651
N	-0.09259712	-1.69870806	-3.57200995

N	-0.13375602	0.29492824	-2.58989136
H	0.02199618	-2.83710303	-1.75020626
H	-0.23793006	0.09850555	-4.71813711
H	-0.18256759	1.31069135	-2.43405327
S	-0.48812049	3.26207636	-0.28324318
O	-0.39393895	2.94569368	-1.74824187
O	0.84384473	3.16120363	0.40284302

TIA+Li+SO_2

0 1

N	-0.17016691	-0.54914775	-0.08067842
C	0.85840268	-0.80600808	0.80770782
C	-1.48856471	-0.72280159	0.40575465
C	0.06857828	0.28201327	-1.19935378
N	2.08512566	-0.18953568	0.74248007
C	2.79072997	-0.53572302	1.86158963
N	2.09390395	-1.35652637	2.62319815
C	0.88913519	-1.56592557	1.95805869
H	2.36984711	0.45041628	0.01431110
H	3.78911900	-0.17775553	2.05653181
H	0.12386674	-2.22286513	2.33831107
H	-2.41116594	-2.33079489	-0.77862056
C	-2.47009969	-1.59390852	0.00847802
C	-3.30921816	-0.44972896	1.60454754
N	-3.60604157	-1.41400591	0.75648406
N	-2.03876276	0.02346159	1.45455565
H	-3.98124663	-0.05256278	2.35185718
C	0.46690509	0.00323805	-2.48440472
C	0.22452520	2.13033333	-2.37746342
N	0.56437763	1.16448944	-3.20936948
N	-0.08004992	1.65631931	-1.14159123
H	0.67545945	-0.96327393	-2.91675591
H	0.18119870	3.18088942	-2.62226437
H	-0.33451125	2.15747762	-0.28786102
S	-1.41831947	1.47783811	2.52040811
O	-0.53085063	2.20619667	1.56186612
O	-0.57601451	0.77625027	3.57836555
Li	0.87901716	-0.23141065	3.81769370

TIA+Mg+SO_2

1 1

N	-0.89696448	-0.35765086	-0.40912913
C	2.86523632	0.01925875	1.14339315
C	-1.86504323	-0.54445339	0.46949387

C	-0.94627756	0.10136913	-1.65383852
N	3.03300748	1.36873853	0.98885677
C	2.65033532	1.96369453	2.16056134
N	2.24916399	1.08402845	3.04752742
C	2.38518361	-0.14327384	2.43912552
H	3.32919869	1.82385550	0.13405775
H	2.67580849	3.03422034	2.30149536
H	2.29361048	-1.06559615	3.00210459
H	-3.98704207	0.05700314	-0.10581836
C	-3.29030428	-0.35912059	0.60823843
C	-2.51067195	-1.22783344	2.41112541
N	-3.66402265	-0.77556604	1.79388642
N	-1.42247662	-1.11336500	1.68235585
H	-2.52678868	-1.63849380	3.41076893
C	-1.97499576	0.55149647	-2.53729637
C	-0.12836236	0.65487649	-3.60708586
N	-1.46069803	0.88230787	-3.71200633
N	0.22267780	0.19459054	-2.41100165
H	-3.03388965	0.62636879	-2.33582773
H	0.57881219	0.82453477	-4.40574869
H	1.18027841	-0.05217699	-2.07245395
Mg	0.53496816	-1.23524671	1.06669011
S	3.15578072	-1.20319936	-0.19504718
O	2.68150595	-0.38881757	-1.38909704
O	2.01159703	-2.18760849	0.28343107

$Al(NH_2)_4+SO_2$

-1 1

Al	0.31367202	0.45245303	0.02192700
N	1.05201908	-1.21654309	-0.43351703
N	-0.41792203	0.20217402	1.70448613
N	-0.87254707	1.27484210	-1.12593408
N	3.73994528	-0.04218300	0.49731004
H	1.22376609	-1.39175111	-1.41917711
H	0.55048404	-2.02492415	-0.07964901
H	-0.90985807	0.96781808	2.14876916
H	0.09065301	-0.29854402	2.42360418
H	-1.87512914	1.16375809	-1.06129908
H	-0.65917505	2.17855716	-1.52555912
H	2.99257623	-0.72329205	0.28889202
H	3.72310828	0.17603201	1.49448811
S	3.34454426	1.43682111	-0.33075203
O	4.04235931	2.47848819	0.48851604
O	1.77542114	1.58347112	-0.08670901

$Al(NH_2)_4+2SO_2$

-1 1

Al	-0.84554546	0.69462404	-0.50956914
N	-0.52495750	0.73158739	1.31744241
H	-0.53663100	1.64255182	1.76226167
H	-1.05274801	0.09284937	1.90144663
N	2.27923415	-0.40658330	0.62588729
H	1.49864496	0.04728182	1.13086349
H	2.10925782	-1.41123527	0.64585012
N	-2.17404293	-0.44500973	-1.04974791
H	-2.03238734	-1.00335827	-1.88189060
H	-3.14975702	-0.18126263	-1.00389100
N	0.95611914	3.93331872	-1.82448318
H	0.82949100	4.54793797	-1.02037534
H	1.57864513	3.15892802	-1.56449445
S	-0.58940833	3.32200392	-2.26038119
O	-1.46456696	4.53269730	-2.22710821
O	-0.97966628	2.43733761	-0.96706336
S	2.20102033	0.08942349	-1.03129346
O	0.63780030	0.00791949	-1.35757086
O	2.59315541	1.53765872	-0.98548763

$Al(NH_2)_4+3SO_2$

-1 1

Al	0.59439850	1.20409452	0.08483780
N	-0.11165942	2.04671223	1.54302952
H	-0.99081282	1.70115982	1.90933480
H	0.49206494	2.28174444	2.32060865
N	2.58385122	-1.80062972	0.03989716
H	2.78784302	-1.93499311	1.03057012
H	1.57126427	-1.74312666	-0.08816303
N	-1.82350703	-0.65444837	-2.36006158
H	-1.13864805	-1.26215502	-2.80222905
H	-1.69503874	0.31909507	-2.67854323
N	-1.85912248	3.29018362	-0.91284774
H	-2.35450515	2.40040957	-0.78606459
H	-1.39908978	3.51082799	-0.02658123
S	-0.65872102	3.08645784	-2.12873981
O	-1.33248724	2.17421127	-3.11503040
O	0.49136757	2.24395875	-1.38405791
S	3.29170443	-0.28636650	-0.42615128
O	2.31494906	0.77385316	0.30838860
O	4.58044346	-0.27153206	0.31801135

S	-1.71413667	-0.78861680	-0.66573196
O	-0.17616692	-0.40163031	-0.32734753
O	-2.56752510	0.34608752	-0.17371544

$Al(NH_2)_4+4SO_2$

-1 1

Al	1.33507033	1.27627689	0.14851307
N	-0.64660747	2.48071688	3.30068766
H	-1.18288670	1.91953802	2.63222606
H	-0.28375018	1.88930233	4.04766553
N	2.78486402	-1.99769680	-0.28855491
H	3.37192113	-2.05754666	0.54381456
H	1.81797945	-1.82423214	-0.01076140
N	-2.01622552	-0.48096037	-1.11372230
H	-1.70894695	-1.33908641	-1.56446232
H	-1.77623029	0.33794352	-1.69593712
N	-1.57538086	3.56777570	-0.70005363
H	-1.88032948	2.75886752	-0.14673470
H	-1.15907678	4.26352929	-0.08442412
S	-0.42962268	3.07635671	-1.87557335
O	-1.10098946	1.89953232	-2.52160764
O	0.80444305	2.52852227	-1.00436059
S	3.34323697	-0.65729898	-1.23118006
O	2.90625740	0.60409159	-0.30103862
O	4.82091254	-0.76233051	-1.13852487
S	-1.31699603	-0.36403294	0.42302269
O	0.26320693	-0.18840702	0.12422922
O	-1.80191461	0.97595275	0.92400637
S	0.68008283	3.23093056	2.51451084
O	1.38820922	1.96462289	1.77428911
O	1.57429936	3.62645613	3.63296070

$Al(NH_2)_4+Li+SO_2$

0 1

Al	0.87406991	0.27910465	0.67858013
N	0.82009263	-1.00311927	1.94529382
H	1.35855826	-0.97681521	2.79988931
H	0.05452984	-1.65290246	2.05708239
N	2.54092622	0.98896379	0.14200172
H	3.28758679	0.30934024	0.02447705
H	2.94288835	1.74598722	0.68647695
N	0.23306547	-0.13328857	-1.05309516
H	0.50159129	-1.04664816	-1.41026848

H	-0.76371381	-0.05412316	-1.22792269
N	-1.80591579	3.44189224	0.00011284
H	-2.12650673	2.72764546	-0.65171186
H	-2.35511491	3.41793367	0.85557831
S	-0.14378699	3.24714978	0.34243617
O	0.42843247	3.06904956	-1.05372436
O	-0.06010744	1.83862852	1.07147149
Li	1.40133201	1.51406206	-1.50116835

$Al(NH_2)_4$+Li+2SO_2

0 1

Al	0.10316758	1.47769797	1.20471029
N	-0.14170227	2.46419392	2.68715097
H	-0.30678948	2.08457205	3.60822005
H	0.22210953	3.40269961	2.77365983
N	3.10619627	-0.40010877	-0.67682723
H	2.59698569	0.13944809	-1.37861908
H	3.86576313	0.13730740	-0.26821281
N	-1.28433114	0.40667195	0.51074819
H	-1.43931057	-0.44702866	1.04422533
H	-2.18581365	0.87685165	0.49424050
N	-0.93682596	3.09298986	-2.28022623
H	-1.69806176	2.54042098	-1.88930190
H	-1.07985581	4.08091553	-2.08612059
S	0.58199988	2.57699951	-1.69737973
O	0.55399740	1.09102353	-2.02512108
O	0.47829905	2.69690636	-0.12387031
S	2.04856433	-0.99612422	0.51796203
O	1.49970046	0.30259657	1.26296823
O	0.91593972	-1.53870640	-0.33393738
Li	-0.30323271	-0.33644107	-1.10283262

$Al(NH_2)_4$+Li+3SO_2

0 1

Al	-0.06268758	1.46148682	1.15778669
N	-0.14977717	2.35479495	2.69856293
H	-0.46296983	1.97968403	3.58052629
H	0.19233704	3.29572855	2.81871899
N	3.02466557	-0.39311220	-0.65947483
H	2.68016004	0.37264234	-1.24594894
H	3.81106077	-0.10707819	-0.08329363
N	-2.10032650	-1.71677493	0.06721470
H	-1.12318937	-1.94655358	-0.13882217
H	-2.74102053	-2.34092655	-0.41470229

N	-0.81509839	2.91909746	-2.48915498
H	-1.43753951	2.12948568	-2.28964905
H	-1.24880582	3.81238650	-2.27459487
S	0.67175869	2.75712363	-1.70156741
O	1.10317711	1.36151078	-2.14870289
O	0.32678119	2.64481281	-0.15811165
S	1.78829867	-1.05314223	0.28859346
O	1.20036779	0.16015739	1.11868988
O	0.74272788	-1.40081489	-0.77207742
S	-2.45402235	-0.10871526	-0.34153467
O	-1.62444003	0.63460992	0.76338657
O	-1.75446070	0.19453588	-1.67610591
Li	0.05255118	-0.20434947	-2.06105444

$Al(NH_2)_4$+Li+4SO_2

0 1

Al	0.28529029	1.34551959	0.84718695
N	-1.11039375	2.45421662	4.33897710
H	-0.48026448	1.92094905	4.93227465
H	-1.80417295	1.84567602	3.90686852
N	2.93981641	-0.43305928	-1.50573148
H	2.46111232	0.30658625	-2.02801462
H	3.83725636	-0.13261849	-1.13710586
N	-2.03340205	-1.84464353	0.04432652
H	-2.31312212	-2.22075197	0.94527155
H	-1.05604351	-2.05231218	-0.17967315
N	-1.21117927	2.84034201	-2.52191308
H	-1.79127017	2.06195394	-2.19658840
H	-1.56559128	3.73779559	-2.20208192
S	0.40577937	2.64247611	-2.09298330
O	0.71423818	1.24788899	-2.63546043
O	0.41289582	2.49911955	-0.50997043
S	1.96540085	-1.10144971	-0.30332018
O	1.57258574	0.10493292	0.65765018
O	0.70137889	-1.44519144	-1.08884381
S	-2.36687367	-0.19413458	-0.06534383
O	-1.30323184	0.50899785	0.89087823
O	-1.92217472	0.12127726	-1.48964866
Li	-0.26186299	-0.32767608	-2.28061038
S	-0.25700201	3.32940848	3.14018549
O	-1.32755488	3.76966750	2.20671528
O	0.57877308	2.13847528	2.38482822

$Al(NH_2)_4$+Mg+SO_2

1 1

Al	0.31117132	-0.22636516	0.23117172
N	1.51237344	-0.19852912	1.76452612
H	2.13887357	-1.00168623	1.79622551
H	1.06998503	-0.17151812	2.68137213
N	1.56263372	0.81468309	-0.82867207
H	2.18406650	0.25310201	-1.40808738
H	1.14150281	1.50388091	-1.45034459
N	-0.35267095	-1.75034381	-0.37107517
H	-0.70464997	-2.49662075	0.21270653
H	-0.63653608	-1.91646714	-1.32671444
N	-0.64105814	3.27270626	-0.51186507
H	-0.44074768	4.27325250	-0.50697711
H	-1.56425527	3.13199009	-0.92376981
S	-0.63462244	2.68166429	1.11092105
O	0.85384328	2.94289035	1.45564509
O	-0.79787563	1.16032530	0.79631916
Mg	2.18589703	1.59989360	0.98412960

$Al(OH)_4+SO_2$

-1 1

Al	0.68227738	-0.06288496	-0.52337680
O	0.68647915	0.75485326	1.07750811
H	0.81543407	0.21433985	1.85791847
O	2.28192225	-0.16529558	-1.24652697
H	2.41787225	-0.90731582	-1.83725734
O	-0.07623079	-1.65668368	-0.50861907
H	-1.03425540	-1.62290123	-0.43457587
O	-1.24959825	2.52545584	0.49472043
H	-0.55615896	1.94877717	0.92177282
S	-1.75028727	1.76890099	-0.91491112
O	-2.63940336	0.64003598	-0.50936156
O	-0.37080515	1.15681952	-1.41499533

$Al(OH)_4+Li+SO_2$

0 1

Al	-0.24038993	-0.46351805	0.31496613
O	1.05887014	0.76919770	0.39807799
H	1.03614426	1.51993689	0.99059976
O	0.57840371	-1.18563922	-1.10942624
H	0.18076831	-1.86057683	-1.65943136
O	-0.76631459	-1.39665815	1.66731160
H	-0.23614576	-2.00182993	2.18370088
O	-1.68422996	0.41551471	-0.33378523

H	-2.57396293	0.17374255	-0.06085286
Li	1.31078759	0.52726691	-1.47442962
S	-1.55675066	1.47061994	-2.36321379
O	-0.07181852	1.53656715	-2.38513527
O	-2.13564906	0.45221533	-3.23395755

$Al(OH)_4$+Mg+SO_2

1 1

Al	0.93771615	0.36195704	-0.14840780
O	1.65894406	0.45925493	1.54326777
H	2.59764040	0.42952006	1.73953990
O	1.67462067	-0.70213226	-1.21674604
H	1.69728420	-0.93036655	-2.14299422
O	-0.64115829	0.03824567	0.74611856
H	-1.48605742	-0.14813314	0.33007385
O	0.68066714	2.10020162	-0.55391306
H	0.98417875	2.50320051	-1.37469759
Mg	-0.03025406	0.92345730	2.36664251
S	-0.48610411	3.60871217	0.72642263
O	-0.33244286	2.81118796	2.01199251
O	-1.80380423	3.48921983	0.14623631

$Al(Py)_4$+SO_2

-1 1

Al	0.85055977	0.32298653	1.23327529
N	0.98239060	0.19438199	3.10773794
C	2.02986541	-0.16469661	3.89858092
C	1.60225423	-0.15844555	5.21385699
H	2.98851383	-0.39076461	3.45666332
C	0.24649915	0.22328722	5.13340324
H	2.18008743	-0.39137504	6.09444219
H	-0.46854638	0.35379091	5.93427056
N	2.54834243	0.69320233	0.48977693
C	2.94798253	1.55554500	-0.48358399
C	4.67452621	0.40845944	0.26665029
C	4.31211714	1.40734161	-0.66157931
H	2.22308920	2.18976066	-0.97061735
H	5.65187650	-0.01224914	0.46098520
H	4.94621153	1.93796762	-1.35442793
N	-0.35161796	1.68769655	0.76268010
C	-1.35765425	2.30632189	1.43709085
C	-1.95549118	3.21567513	0.58444591
H	-1.56684984	2.03718380	2.46069439
C	-1.23763548	3.08220788	-0.62234093

H	-2.78873644	3.86620472	0.79832551
H	-1.37968044	3.61003321	-1.55579403
N	0.35573192	-1.35845659	0.48539766
C	0.94962294	-2.00996996	-0.54716031
C	-0.72458267	-3.22289950	0.21220811
C	0.29009154	-3.20862381	-0.76088578
H	1.80422534	-1.57998837	-1.04612481
H	-1.47458781	-3.97182344	0.42324534
H	0.51294495	-3.95974700	-1.50163037
N	-0.12613800	0.43412770	3.87441527
N	3.62087593	-0.02106381	0.95568558
N	-0.67761535	-2.11653820	0.94799843
N	-0.27780496	2.16744472	-0.52037321
S	-2.46083521	-1.95756547	2.72528225
O	-3.44322089	-1.03995515	2.13529583
O	-2.79977398	-3.38931444	2.61742740

$Al(Py)_4$+Li+SO_2

0 1

Al	0.42468193	-0.21970330	1.32509114
N	1.03103792	0.58590775	3.16588114
C	1.84428664	1.58377577	3.53348638
C	1.80950200	1.74558230	4.92424678
H	2.40749694	2.12383515	2.78869939
C	0.91740817	0.77988326	5.37399626
H	2.35399135	2.46032868	5.51898416
H	0.57194865	0.53738404	6.36645570
N	2.28790871	-0.39984282	0.84271982
C	3.33311665	-0.92272634	1.52962702
C	4.01861033	-0.30484372	-0.46430839
C	4.46492553	-0.88577799	0.73294245
H	3.21129752	-1.28349707	2.53954075
H	4.58075943	-0.08224744	-1.35993993
H	5.45725722	-1.22590277	0.97945766
N	-0.17520667	1.51410321	0.74646797
C	-0.97376389	2.42521249	1.35360560
C	-1.15034800	3.50689517	0.50726000
H	-1.37094497	2.24704351	2.34167757
C	-0.40373483	3.17327990	-0.63333630
H	-1.73246250	4.39585252	0.68609119
H	-0.26342572	3.74222414	-1.54131857
N	-0.31721812	-1.27288110	-0.14408387
C	-1.16742337	-2.32852900	-0.13113963
C	-0.67418383	-1.83362043	-2.21436524

C	-1.42489015	-2.72416594	-1.43383260
H	-1.53474458	-2.72449222	0.80065258
H	-0.58569853	-1.78169443	-3.29036255
H	-2.05876788	-3.53026905	-1.76523923
N	0.48393599	0.10098905	4.29469076
N	2.71770909	-0.01890626	-0.39966460
N	-0.01338845	-0.96821467	-1.44365565
N	0.17611699	1.98038148	-0.49258352
Li	1.18179326	0.59176931	-1.51856796
S	-0.87392098	-1.22438593	4.03201903
O	-0.53292240	-1.30506338	2.51527367
O	-2.12522448	-0.50160325	4.27466037

$Al(Py)_4$+Mg+SO_2

1 1

Al	0.60335341	0.42416634	1.09805653
N	0.60247340	0.56415180	3.01605934
C	0.10072174	1.52340826	3.82072947
C	0.34424709	1.19114217	5.14586843
H	-0.39714164	2.38524907	3.40374780
C	1.02523214	-0.02389415	5.07969078
H	0.06903610	1.74803076	6.02561528
H	1.40502115	-0.63266101	5.88727586
N	2.46713453	0.08139110	0.71158664
C	3.30008346	0.71646426	-0.13908013
C	4.42223177	-0.88915225	0.85813412
C	4.55675774	0.13038932	-0.08344037
H	2.94854233	1.54662145	-0.73129152
H	5.16435022	-1.59150384	1.20835242
H	5.43624994	0.40387108	-0.64161477
N	-0.71414300	1.43733595	0.17811406
C	-1.62371946	2.18277085	-0.46758715
C	-1.11339890	3.46782606	-0.64376803
H	-2.57816012	1.77506077	-0.76337209
C	0.15888957	3.45015081	-0.06445647
H	-1.59977391	4.30139638	-1.12315799
H	0.88791067	4.24190554	0.01800895
N	-0.07879273	-1.38625979	0.87811407
C	-1.11208381	-1.80382995	0.11682759
C	-0.26295574	-3.55174013	1.14269510
C	-1.26746924	-3.17621326	0.25195903
H	-1.67359661	-1.10195762	-0.47859844
H	-0.02612738	-4.53419170	1.52393168
H	-1.99900260	-3.80650520	-0.22496654

N	1.18232599	-0.40528257	3.80279512
N	3.16951409	-0.92360049	1.33631113
N	0.45218844	-2.48150716	1.51902385
N	0.40053656	2.23125352	0.43077721
S	3.46516123	-4.14435593	5.00360808
O	2.98987678	-3.42248505	3.79567365
O	3.09024580	-3.57011193	6.27412174
Mg	2.03087473	-1.94585289	2.71702717

$Al(Im)_4+SO_2$

-1 1

Al	0.34170999	-2.33033028	-1.74717895
N	2.11453723	-2.46271484	-2.34573279
C	2.55019536	-2.55288321	-3.66173864
C	3.27130160	-2.44268505	-1.60591864
C	3.92087631	-2.57992969	-3.63224545
H	1.85718319	-2.61058189	-4.48658746
H	3.25402362	-2.38486738	-0.52693091
H	4.60647080	-2.64898608	-4.46383515
N	0.20248518	-2.68345129	0.08995880
C	0.61720633	-1.87997756	1.14407990
C	-0.28640967	-3.81436224	0.69707174
C	0.35640362	-2.56640550	2.30210666
H	1.04155737	-0.90131553	0.98215715
H	-0.69452682	-4.63423729	0.12339501
H	0.54070991	-2.25512875	3.31971548
N	-0.71867152	-3.51771851	-2.74256144
C	-1.97158148	-3.31765966	-3.26755188
C	-0.42272684	-4.83787511	-3.05550204
H	-2.47649421	-2.36553754	-3.18748453
C	-1.49925448	-5.34256070	-3.73872476
H	0.51852511	-5.28895160	-2.78267711
H	-1.62820330	-6.33496527	-4.14481245
N	-0.28280056	-0.55560231	-2.01979828
C	0.21842069	0.38723846	-2.86143985
C	-1.40376866	0.03064633	-1.44615312
H	1.11094829	0.23745453	-3.44982670
C	-1.52854120	1.29017530	-1.96736356
H	-1.99851494	-0.48667966	-0.71064660
H	-2.25825538	2.05866932	-1.76618776
N	4.36870188	-2.51143451	-2.33210360
N	-0.49983044	1.49877163	-2.85369805
N	-2.47249310	-4.37738592	-3.86985263
N	-0.21434127	-3.78557656	2.01256467

S	-0.29447160	3.52509647	-4.06944428
O	-1.32031080	4.25967966	-3.30798453
O	1.10247657	3.88429034	-3.78157852

$Al(Im)_4+2SO_2$

-1 1

Al	0.08827104	-2.06294866	-1.66070682
N	1.93139422	-1.75203417	-1.96699582
C	2.50199210	-0.88516866	-2.89095136
C	2.98351819	-2.39508209	-1.38893241
C	3.85948179	-1.04570637	-2.82854399
H	1.90171182	-0.22605953	-3.49706336
H	2.86803092	-3.12937017	-0.60609727
H	4.64324676	-0.54464825	-3.37435855
N	-0.10669620	-2.52786693	0.14074059
C	0.47875931	-1.92244409	1.24705724
C	-0.93177059	-3.48781041	0.67685080
C	-0.02188383	-2.54653918	2.36010252
H	1.20246627	-1.12854906	1.14722983
H	-1.52565411	-4.13914521	0.05158399
H	0.20971112	-2.35108881	3.39652042
N	-0.54435284	-3.39316074	-2.81585235
C	-1.84836515	-3.70687881	-3.11859163
C	0.20318029	-4.34852392	-3.49330400
H	-2.67828904	-3.12989604	-2.73496481
C	-0.68193818	-5.16139928	-4.15218333
H	1.28084414	-4.35776325	-3.45460097
H	-0.46724803	-6.00944670	-4.78510029
N	-0.87751344	-0.47993016	-2.04990100
C	-1.32835525	-0.05915862	-3.26389829
C	-1.21360495	0.53901679	-1.16734296
H	-1.22348086	-0.64076529	-4.16732979
C	-1.84662243	1.51791688	-1.88425799
H	-0.98513716	0.47349189	-0.11586229
H	-2.25136613	2.46385146	-1.56070609
N	4.14511554	-1.99730349	-1.87901986
N	-1.90935113	1.12662019	-3.19990735
N	-1.97400071	-4.75063648	-3.91101458
N	-0.91012693	-3.53215557	1.99259814
S	-2.91362573	2.46003409	-4.91300846
O	-3.00509622	3.69610845	-4.11836484
O	-1.84901640	2.41852646	-5.92646377
S	6.37959031	-2.68480535	-1.36559328
O	7.04974725	-1.57668939	-2.06586650

O	6.35095854	-2.60136039	0.10200891

$Al(Im)_4+3SO_2$

-1 1

Al	0.05446400	-1.54954312	-1.76649414
N	1.89886814	-1.43448811	-2.14985217
C	2.69680320	-0.29510302	-2.17183417
C	2.75093421	-2.46626519	-2.40985618
C	3.97807930	-0.69204805	-2.44144319
H	2.28794818	0.69001505	-2.01327315
H	2.42996218	-3.49575127	-2.46185219
H	4.87774037	-0.10481701	-2.53639519
N	-0.23732902	-1.32838210	0.08626301
C	0.53797404	-0.61672905	0.99408807
C	-1.30177410	-1.77920513	0.80854806
C	-0.08936801	-0.67260105	2.20873017
H	1.46418611	-0.14786501	0.70378706
H	-2.09241316	-2.37893318	0.38319303
H	0.19554701	-0.24178802	3.15554424
N	-0.63308005	-3.21033524	-2.26689817
C	-1.39634911	-3.51246227	-3.37099326
C	-0.41831903	-4.43988434	-1.65246213
H	-1.73358213	-2.74735521	-4.05559731
C	-1.05515908	-5.38619041	-2.41189818
H	0.14931601	-4.53100035	-0.73944106
H	-1.10975808	-6.45134050	-2.24410917
N	-0.78992106	-0.15111601	-2.71181721
C	-0.46407704	0.34593803	-3.93889230
C	-1.93086515	0.54738404	-2.33217818
H	0.39600403	0.01572100	-4.50185534
C	-2.23451717	1.42265611	-3.33861525
H	-2.41525318	0.37343703	-1.38486110
H	-3.03396623	2.14323216	-3.40681026
N	3.99451430	-2.05840216	-2.58705720
N	-1.30226610	1.28448510	-4.33958333
N	-1.66992213	-4.79356537	-3.49198927
N	-1.24420709	-1.40537611	2.07416916
S	-1.25295110	2.53798919	-6.40436850
O	-1.98785715	3.71948429	-5.92821847
O	0.20298302	2.68756720	-6.54142948
S	5.98773344	-3.33739226	-3.08011724
O	6.95333254	-2.30513618	-2.67279720
O	5.79949245	-4.45705534	-2.14682916
S	-2.78129121	-1.81867114	3.88605430

O	-2.24887317	-0.78495606	4.78745336
O	-4.04822231	-1.50307212	3.21087825

$Al(Im)_4+4SO_2$

-1 1

Al	0.39254305	-1.26532834	-1.61436072
N	2.19264664	-0.72412583	-1.52912416
C	2.85591917	0.12932942	-2.40546256
C	3.14561769	-1.12090725	-0.63549693
C	4.16047985	0.20334773	-2.00135157
H	2.34575686	0.61439417	-3.22193735
H	2.93915234	-1.78383300	0.19142557
H	4.97960617	0.77190251	-2.41257374
N	-0.21658022	-1.51276847	0.14908673
C	0.02250966	-0.69158307	1.24746708
C	-1.06181064	-2.47939350	0.61037517
C	-0.68237698	-1.19998814	2.30391620
H	0.67742014	0.16288285	1.18698521
H	-1.43823814	-3.27803202	-0.01103762
H	-0.75612952	-0.84469877	3.31966481
N	0.23622682	-2.85998132	-2.60110069
C	1.22523059	-3.74711948	-2.91233311
C	-0.92649571	-3.42358804	-3.11869418
H	2.25917449	-3.59519456	-2.64148284
C	-0.58313718	-4.60850681	-3.70969979
H	-1.88365943	-2.93467547	-3.03179929
H	-1.20325185	-5.33408746	-4.21204536
N	-0.65357894	0.03915974	-2.48261958
C	-0.78098413	0.24902958	-3.82433298
C	-1.40199504	1.04905786	-1.88771703
H	-0.31531908	-0.37437676	-4.57340299
C	-1.93814729	1.81034050	-2.88982960
H	-1.49301910	1.13122196	-0.81670056
H	-2.56964552	2.68195863	-2.82465577
N	4.32522271	-0.58656735	-0.88863882
N	-1.53729263	1.29472320	-4.09999187
N	0.77137350	-4.79619361	-3.57149364
N	-1.35785886	-2.32168655	1.88657458
S	-1.96260255	2.03606770	-6.37163228
O	-1.86218061	3.48828831	-6.17409893
O	-0.79396397	1.37573309	-6.97267613
S	1.94905594	-6.75817297	-4.43441668
O	0.75545495	-7.60095167	-4.59624212
O	2.80822669	-7.05585819	-3.28119192

S	-2.85336965	-3.59094664	3.34201997
O	-2.94282752	-2.56820673	4.39462770
O	-4.01571159	-3.71433715	2.45244019
S	6.45404623	-0.74693139	0.30110951
O	7.08265229	0.40195803	-0.36731939
O	5.98922107	-0.52653269	1.67686593

$Al(Im)_4$+Li+SO_2

0 1

Al	-0.00131520	-2.27656945	-1.75403889
N	1.85252518	-1.80751957	-1.91128745
C	2.74659289	-2.27435362	-2.86386210
C	2.32586067	-0.58700789	-1.55797497
C	3.70148308	-1.31105683	-3.04387692
H	2.62167109	-3.23643323	-3.33382140
H	1.82837689	0.04184117	-0.83269598
H	4.56055610	-1.32430078	-3.69597322
N	-0.46827601	-2.68283598	-0.01005391
C	0.24667631	-2.43282918	1.15891037
C	-1.67370718	-3.18709838	0.43115765
C	-0.55753994	-2.79478648	2.20630620
H	1.25394998	-2.04788713	1.14116816
H	-2.44979428	-3.49418080	-0.25626634
H	-0.33916649	-2.75232929	3.26251201
N	-0.45248370	-3.56057013	-3.00839807
C	-1.02575183	-3.38722186	-4.24998432
C	-0.15522358	-4.92037355	-2.95575825
H	-1.38306493	-2.42376903	-4.58485538
C	-0.55987728	-5.46576232	-4.14516178
H	0.28898507	-5.37361695	-2.08316134
H	-0.50038111	-6.49563708	-4.46255997
N	-0.74876977	-0.56289765	-2.24047230
C	-0.21279269	0.21247797	-3.20665789
C	-1.42825233	0.31003463	-1.39819735
H	0.40769891	-0.15902308	-4.00787943
C	-1.26799317	1.57996538	-1.87900002
H	-1.95366944	-0.04206581	-0.52549300
H	-1.61862215	2.52701557	-1.50280723
N	3.42352202	-0.23170959	-2.21998906
N	-0.49537609	1.49595687	-3.01631101
N	-1.10648067	-4.49329416	-4.95249845
N	-1.76360176	-3.26695928	1.73880137
Li	3.27422943	1.60846490	-2.84820540
S	0.57629659	3.13340790	-3.85109872

O	0.21208453	4.14807481	-2.85938765
O	1.95769671	2.56047767	-3.63206851

$Al(Im)_4+Li+2SO_2$

0 1

Al	0.10691942	-2.20618830	-1.76464265
N	1.97829046	-1.85156958	-2.01819984
C	2.87860692	-2.57363520	-2.79251628
C	2.63469584	-0.73463732	-1.64085051
C	4.04494959	-1.86423869	-2.86185156
H	2.60764045	-3.51536067	-3.24133502
H	2.20800271	0.05253134	-1.03942823
H	4.96536780	-2.07063542	-3.38267696
N	-0.28461727	-2.66804343	-0.01645060
C	0.38694626	-2.30995339	1.15008441
C	-1.40089252	-3.34569134	0.43020941
C	-0.35075959	-2.78526225	2.20086528
H	1.32305569	-1.77453663	1.13175186
H	-2.12433673	-3.76498635	-0.25499860
H	-0.13872851	-2.70670183	3.25627274
N	-0.45130001	-3.46025704	-3.00499070
C	-1.00173500	-3.25190558	-4.25195511
C	-0.26948722	-4.84065561	-2.93818605
H	-1.27178157	-2.26495937	-4.60022091
C	-0.71358996	-5.36110979	-4.12454062
H	0.13134241	-5.32121459	-2.05928171
H	-0.73944595	-6.39531454	-4.43217513
N	-0.61359587	-0.46932403	-2.15158708
C	-0.16967566	0.37903402	-3.10295698
C	-1.55295344	0.24582554	-1.41814744
H	0.58104624	0.13479143	-3.83782009
C	-1.63757896	1.50337185	-1.94690746
H	-2.06562728	-0.19191640	-0.57727713
H	-2.22599761	2.35490426	-1.64754350
N	3.86732668	-0.70940003	-2.13438324
N	-0.75578394	1.56595078	-3.00214501
N	-1.17247558	-4.35400459	-4.94378175
N	-1.47326712	-3.43440943	1.73799297
Li	2.89184462	2.85539923	-3.26916157
S	-0.20339223	3.29622377	-4.07243570
O	-0.60362467	4.30818644	-3.09084432
O	1.28049020	3.01088759	-4.06596730
S	5.18196064	0.93497045	-2.06354172
O	5.95892625	0.65544925	-3.27443737

O	4.11867054	1.98963556	-2.26499680

$Al(Im)_4+Li+3SO_2$

0 1

Al	1.11334994	-2.25652678	-2.73895057
N	2.33276350	-3.02985649	-3.87994620
C	2.11387180	-3.50019696	-5.17252117
C	3.64927317	-3.35315925	-3.61832056
C	3.28676605	-4.06297161	-5.59733743
H	1.16199445	-3.38703476	-5.66691201
H	4.12084126	-3.10575160	-2.67773215
H	3.49965883	-4.52576325	-6.54881474
N	1.97023717	-1.36642431	-1.29193661
C	2.78617413	-0.24072549	-1.32046294
C	1.65064130	-1.54629396	0.01491151
C	2.91762138	0.21702572	-0.03971380
H	3.17121118	0.15925214	-2.24339538
H	1.02333547	-2.34489055	0.37775549
H	3.44583642	1.07490565	0.34320829
N	-0.02244193	-3.49192369	-1.85051537
C	-1.21395563	-3.16410682	-1.29179674
C	0.36975599	-4.66661419	-1.21980520
H	-1.79060568	-2.29479308	-1.56710475
C	-0.59122291	-4.98865526	-0.30064993
H	1.28477399	-5.17314585	-1.48171609
H	-0.64524716	-5.82885676	0.37256402
N	-1.44237975	0.47666913	-2.17875530
C	-0.98109354	0.53299044	-0.90008144
C	-2.78258399	0.13175466	-2.11884320
H	0.03871794	0.79104472	-0.66112691
C	-3.07467273	0.00262834	-0.79083460
H	-3.38815529	0.02008332	-3.00288433
H	-4.01198421	-0.27399345	-0.33669060
N	4.24586213	-3.96583844	-4.61289142
N	-1.93992008	0.24344357	-0.03428053
N	-1.58045097	-4.03223513	-0.36160932
N	2.19355309	-0.61659032	0.78383910
S	-0.41228172	0.38666329	-3.70555630
O	0.75050468	1.22476654	-3.38267106
O	-0.01807377	-1.14740312	-3.58793320
Li	-1.53963606	-0.67073683	1.73667087
S	1.53633584	-0.14717943	2.84707371
O	1.84401287	1.28424296	2.83650397
O	0.09407420	-0.46798350	2.61469012

S	-3.14941282	-3.47968610	1.18574470
O	-4.21494127	-2.98577036	0.30892393
O	-2.37117013	-2.39090594	1.84898163

$Al(Im)_4$+Li+4SO_2

0 1

Al	1.18888371	-1.61979624	-2.55781684
N	2.67426200	-1.97150599	-3.60829250
C	2.70718916	-2.39283277	-4.93577835
C	3.97639334	-2.02685296	-3.18843801
C	4.00959794	-2.67520576	-5.24050534
H	1.81401093	-2.44965671	-5.53662328
H	4.29568371	-1.76493878	-2.18966662
H	4.42863183	-3.02754145	-6.16945688
N	1.60836747	-0.44444901	-1.12951472
C	1.98093719	0.89494855	-1.18175313
C	1.28914971	-0.67845655	0.17017990
C	1.86228480	1.41376048	0.07636308
H	2.26189856	1.37197356	-2.10561227
H	0.95973607	-1.63397761	0.54620724
H	2.03458871	2.41514335	0.43578544
N	0.51358988	-3.14825873	-1.66460197
C	-0.75393994	-3.24989421	-1.19026608
C	1.25347535	-4.07657359	-0.93979576
H	-1.58228817	-2.65974901	-1.55068013
C	0.40679445	-4.68497812	-0.05419218
H	2.30531662	-4.23321496	-1.11862492
H	0.60890833	-5.46031449	0.66693868
N	-2.16026168	0.04773392	-2.29325464
C	-1.82989283	0.31127696	-0.99929249
C	-3.29692190	-0.74462653	-2.27636355
H	-0.98229315	0.92173664	-0.72962795
C	-3.60832294	-0.91866000	-0.95813288
H	-3.76876589	-1.09436249	-3.17955918
H	-4.41661567	-1.49078155	-0.53314623
N	4.79255797	-2.44008905	-4.13288075
N	-2.67961415	-0.26558125	-0.16475572
N	-0.85163879	-4.15250585	-0.22739119
N	1.42334696	0.40876898	0.91012052
S	-1.08179586	0.28827829	-3.76175146
O	-0.31651924	1.49770004	-3.43101171
O	-0.16630250	-0.99767184	-3.55221809
Li	-2.11546228	-0.92016357	1.67750779
S	0.49804209	0.69314216	2.91489982

O	0.28274901	2.13847586	2.83206109
O	-0.71866935	-0.12712627	2.62663429
S	-2.62720071	-4.13120081	1.19836465
O	-3.72877796	-4.07840604	0.23342290
O	-2.32821184	-2.81319350	1.83355197
S	7.12796812	-2.93680849	-3.31354837
O	6.77855318	-2.56348879	-1.93508596
O	7.20143814	-4.37060515	-3.60413110

$Al(Im)_4$+Mg+SO_2

1 1

Al	-0.22874232	-2.03626482	-2.40522261
N	1.41590469	-1.82132935	-3.44985942
C	2.04384081	-2.89509613	-4.06734032
C	2.41126945	-1.10583917	-2.88915648
C	3.38499474	-2.80319991	-3.82067177
H	1.48909801	-3.63335475	-4.62402007
H	2.23791947	-0.20286356	-2.32041825
H	4.18869048	-3.43236560	-4.17029008
N	0.68097921	-2.24595785	-0.68257553
C	0.92246157	-1.16951606	0.16091552
C	1.82422582	-2.96006579	-0.67921572
C	2.21135097	-1.25880920	0.60651953
H	0.16534544	-0.43065379	0.36978124
H	1.95345572	-3.86311423	-1.25947779
H	2.73859158	-0.62562857	1.30310516
N	-1.05208273	-3.61131835	-2.88574950
C	-1.66132710	-3.89547391	-4.09762154
C	-1.11714406	-4.80949127	-2.18344774
H	-1.78480037	-3.14663973	-4.86819555
C	-1.74501985	-5.72177711	-3.00185763
H	-0.75230842	-4.90576883	-1.17313568
H	-1.98285188	-6.75296772	-2.79043725
N	-1.17327021	-0.45678798	-2.41254086
C	-0.85794950	0.73399595	-3.04479398
C	-2.32069194	-0.16189404	-1.68451708
H	-0.01724656	0.82113192	-3.71831939
C	-2.61390325	1.16418870	-1.91567997
H	-2.83564497	-0.90399636	-1.09398161
H	-3.43799546	1.74122605	-1.52543125
N	3.62001064	-1.66776056	-3.04237575
N	-1.69016090	1.71024502	-2.76693915
N	-2.07609002	-5.13657746	-4.19552944
N	2.80047244	-2.39494066	0.04735008

Mg	4.41939773	-2.02944768	-1.17702811
S	7.60632837	-1.65205656	-0.01604242
O	6.30385959	-2.05593799	-0.68607228
O	7.49931926	-0.44899234	0.79283391

$AlCl_4$+SO_2

-1 1

Al	-1.09848950	0.56213621	0.32986643
Cl	0.44832353	-0.25060450	-0.99364048
Cl	-0.23277600	2.24017623	1.40486672
Cl	-2.77480250	1.22623685	-0.86491321
Cl	-1.72289152	-0.97329882	1.71875873
S	3.07783484	1.60838910	-0.45552508
O	3.40364845	2.19688633	-1.75686562
O	4.07920309	0.70856815	0.12155448

$AlCl_4$+2SO_2

-1 1

Al	-1.04692688	-0.07852841	0.35800189
Cl	0.12797028	1.69133836	0.90612690
Cl	-1.90605534	0.29274284	-1.59583817
Cl	0.30304668	-1.77680434	0.25841070
Cl	-2.58034055	-0.41371262	1.83391750
S	3.09095419	-0.31534613	-1.29391403
O	4.24428929	-0.33449333	-0.39196212
O	3.26386419	-0.97530564	-2.58827412
S	0.69317163	3.16288606	-1.88088742
O	0.79915177	4.59238681	-1.58230128
O	1.93880241	2.47210603	-2.22432747

$AlCl_4$+3SO_2

-1 1

Al	-0.87118734	0.43670541	0.90220929
Cl	-1.51849149	2.50613032	1.11336524
Cl	0.51645080	0.32575515	-0.77321762
Cl	0.19892538	-0.13107263	2.71278157
Cl	-2.55733686	-0.85753046	0.57983887
S	1.08634459	4.45853012	0.14915313
O	0.74672416	5.61823591	-0.67701113
O	1.50360966	4.73848928	1.52412757
S	3.59985830	1.11724184	0.42004109
O	4.70988413	0.28540680	-0.04773551
O	3.55020180	2.48631739	-0.09592336
S	1.77680113	2.64896902	3.86565254

O	3.07585546	2.25236058	3.31941212
O	1.72114461	2.87955350	5.31019961

$AlCl_4$+4SO_2

-1 1

Al	-1.37763911	0.14058401	1.17685609
Cl	-1.99893315	2.04813215	2.00522815
Cl	-1.71518413	0.14372201	-0.97931308
Cl	0.77026106	-0.07926701	1.48712412
Cl	-2.44750119	-1.48033212	2.09675516
S	2.33428818	2.81520122	-0.78464206
O	2.55306520	3.86169230	-1.77946313
O	1.27938810	4.07312931	1.69048613
S	4.17392232	1.05275508	2.40134718
O	5.62556644	0.87868207	2.38811218
O	3.53141827	2.32296318	-0.09402401
S	0.84986907	3.53593227	2.98435623
O	3.64644028	2.14555116	3.21833824
O	0.51068904	4.51700734	4.01454331
S	1.07043508	-0.91031707	-2.21171517
O	0.67821805	-1.60988212	-3.43465426
O	1.79076814	0.35470803	-2.38274618

$AlCl_4$+Li+SO_2

0 1

Al	-0.13305096	0.51208772	0.46926969
Cl	0.63189788	-0.75588492	1.96289658
Cl	1.25738534	0.85659380	-1.22230471
Cl	-2.01754259	-0.09548518	-0.40410321
Cl	-0.39011632	2.61735824	1.09939871
Li	0.21297887	2.94471889	-1.12071050
S	-2.44001275	2.08044711	-2.70053472
O	-3.76579937	2.65719987	-2.58735609
O	-1.32567971	2.94268052	-2.24830228

$AlCl_4$+Li+2SO_2

0 1

Al	-1.01239912	-0.33594339	-0.74596582
Cl	-0.78733643	-2.37214600	-1.25027107
Cl	0.86157000	0.82041336	-0.88073447
Cl	-2.49886837	0.74256400	-1.88778748
Cl	-1.47605771	-0.01157777	1.38900986
Li	-0.05660262	1.91898985	1.04777023
S	-2.44539451	3.57768035	-0.42591322

O	-1.23406911	3.28981957	0.36883749
O	-2.31094826	4.61754679	-1.42949017
S	2.31194593	1.01176148	3.07325912
O	1.30618447	1.88841867	2.45455436
O	3.05959539	1.56497435	4.18572662

$AlCl_4$+Li+3SO_2

0 1

Al	-1.59098770	-0.03716018	0.57140900
Cl	-0.21405692	1.35989265	1.52504238
Cl	-1.93525477	-1.67461691	1.93650017
Cl	-3.31957938	0.84020554	-0.24226502
Cl	1.61355835	0.79591807	-2.06221508
Li	1.78118393	-0.03599938	1.72487798
S	3.86348431	1.90991349	0.10889518
O	3.80833905	3.35850328	0.17547300
O	3.23236617	1.17454115	1.21703746
S	0.86699935	-1.13226698	-1.11127058
O	1.63786157	-1.18866990	0.15846066
O	-0.59541784	-0.76426304	-0.80714704
S	0.44476364	-1.87681292	4.11120994
O	1.39041778	-1.08450879	3.30518008
O	0.03432102	-1.29565481	5.37650160

$AlCl_4$+Li+4SO_2

0 1

Al	-2.05579796	-0.07027701	0.32638002
Cl	-1.17755905	1.44923796	4.09934498
Cl	-2.06500176	-1.65620090	1.74552170
Cl	-3.81340166	0.31478802	-0.75809669
Cl	1.60468060	1.17969407	-1.78797750
Li	1.93782054	-0.08536120	1.79861132
S	-0.48855349	2.14818608	2.06332597
O	0.82167675	1.47645021	1.89916762
O	-1.52936964	1.47116207	1.14881067
S	4.23309816	1.64921595	0.21762542
O	4.10074393	3.05199395	0.56971761
O	3.67132724	0.66531866	1.15393368
S	0.74884355	-0.82737272	-1.10562679
O	1.42883621	-1.05430408	0.19008244
O	-0.71840237	-0.43386426	-0.87412816
S	0.55157308	-1.42698452	4.46610325
O	1.54234898	-1.04817022	3.44441811
O	1.05906466	-1.56620265	5.81993621

$AlCl_4$+Mg+SO_2

1 1

Al	-0.21967413	-0.20882926	1.09885895
Cl	-0.49807905	-1.29601571	2.81758810
Cl	1.72270193	-0.20081690	-0.03640452
Cl	-1.46432360	-0.52400130	-0.75129260
Cl	-0.43177354	2.03232617	1.03123762
Mg	0.14631284	1.24947361	-1.20218947
S	0.24981117	3.16803551	-4.06920553
O	-1.00435670	3.86781614	-4.14320877
O	0.41474300	2.27393453	-2.87912939

$Al(CN)_4$+SO_2

-1 1

Al	0.55740680	1.28474132	-0.05244328
C	1.91695837	0.36027621	-1.14094806
N	2.71805877	-0.18270607	-1.77762923
C	-0.48504291	2.52853012	-1.17076034
N	-1.09420184	3.26163398	-1.82905182
C	-0.66815037	-0.07520076	0.72309392
N	-1.37100224	-0.86960410	1.18671028
C	1.42314977	2.25690077	1.42907527
N	1.93332213	2.82350590	2.30124217
S	-2.67041733	-2.86475949	2.69908817
O	-3.80291613	-2.12724999	3.25814536
O	-2.97221638	-3.87361271	1.68399011

$Al(CN)_4$+Li+SO_2

0 1

Al	-0.84190180	0.05494374	0.64793548
C	1.91097314	-0.59007723	0.13506188
N	2.98232411	-0.37590234	-0.27416675
C	-0.23010585	1.70166315	-0.30328252
N	0.36371688	2.52114867	-0.86126063
C	-2.10234342	-0.96709726	-0.39785324
N	-2.85191220	-1.56616534	-1.04452391
C	-1.22822304	0.39131833	2.50945490
N	-1.44721837	0.61441816	3.62354600
Li	2.13415768	2.96536748	-1.58567544
S	4.25500467	0.60225719	-1.09886563
O	0.79701365	-0.85083705	0.57800334
O	3.51969812	1.91927399	-1.50233545

$Al(CN)_4$+Mg+SO_2

1 1

Al	-0.47393567	-0.25918917	-0.16866410
C	1.44235512	0.33288394	-0.51975877
N	2.17066615	1.21112846	-0.30727057
C	-1.02286578	1.64623816	-0.63031074
N	-0.71371484	2.74801546	-0.43687971
C	-1.30393472	-1.86469899	-0.72017809
N	-1.81179780	-2.84753890	-1.05769459
C	-0.20425482	0.40868842	1.73615633
N	0.24574880	1.30258161	2.32380073
Mg	1.02975334	2.64578294	0.83120339
S	2.51716862	5.51458702	2.05692878
O	2.49364324	5.41719549	3.49222320
O	1.91747085	4.35985313	1.32214874

H1+SO_2

-1 1

Al	0.08381200	0.38959300	0.81787000
N	-1.20762300	-2.30042700	-1.14259200
N	-0.20479300	0.74828800	2.60113600
N	1.02029100	1.78152000	0.05338800
H	-0.28457600	-2.19073400	-0.70239000
H	-1.18093300	-1.88848500	-2.07625000
H	-1.07219400	0.53980600	3.07604000
H	0.25267800	1.52241900	3.06253500
H	0.63049700	2.71589000	0.03501200
H	1.50967300	1.62803100	-0.81977400
O	0.93562200	-1.16196300	0.48543600
H	1.58637300	-1.43723000	1.13218600
S	-2.33026400	-1.34632100	-0.22071400
O	-3.42597700	-1.06653700	-1.20131300
O	-1.52853000	0.02001300	0.00782900

H1+2SO_2

-1 1

Al	0.56048364	0.69792051	0.13620264
N	-0.48266665	-2.21231279	-1.39750518
N	3.84999721	-0.27924076	1.02003692
N	-0.22270072	2.28607895	-0.26090272
H	0.33439750	-1.62599177	-1.60715532
H	-1.28944232	-1.86027892	-1.91375226
H	3.46991297	-1.09868334	1.49849398

H	4.85723598	-0.27030401	1.17289188
H	-1.16058681	2.49767483	0.04875626
H	0.27566490	3.14406118	-0.44728508
O	1.58412547	-0.02964175	-1.11540307
H	2.47894623	-0.24795472	-0.83149345
S	-0.85277541	-2.05566766	0.28841629
O	-2.29395372	-2.43225373	0.36264397
O	-0.76856186	-0.45933449	0.51493604
S	3.16575260	1.14666221	1.82469315
O	1.65519209	0.73171478	1.62544117
O	3.49510629	1.04614947	3.27461727

H2+SO_2

-1 1

Al	-0.43173968	0.15252051	0.56294967
N	-1.23318079	-0.22485046	2.17124882
N	1.22937093	3.12854752	-0.30745508
H	-2.10167572	-0.74495779	2.16792894
H	-1.29877928	0.50065714	2.87465543
H	1.64293490	3.89426295	0.22074114
H	1.52766350	2.23732034	0.11787368
O	1.32606055	0.42743631	0.79020501
H	1.72365102	-0.04258615	1.52474749
O	-0.90436096	-1.10177327	-0.59346553
H	-0.85010029	-0.86681355	-1.52045589
S	-0.50702422	3.27019243	-0.10250730
O	-0.74684661	3.71651727	1.31238242
O	-0.87401349	1.73963097	-0.28320110

H2+2SO_2

-1 1

Al	-0.83799073	0.67324566	0.22480489
N	-1.07554107	1.96026537	3.40223469
N	1.95451188	2.76532782	0.30409269
H	-0.27964403	1.33020904	3.28895765
H	-0.90454036	2.78403229	2.81401565
H	2.46485179	3.33079776	0.97899982
H	1.78021223	1.83461932	0.70672199
O	0.63019775	0.25758609	1.13083202
H	0.75449714	-0.64694645	1.42162356
O	-1.29941573	-0.43932039	-1.04358731
H	-2.21783960	-0.71008402	-1.06769248
S	0.42284213	3.55326697	0.02809851
O	-0.10793534	3.98871459	1.36920065

O	-0.37894543	2.28621080	-0.48414135
S	-2.48674078	1.12373201	2.89252812
O	-2.25670112	0.91772820	1.30539218
O	-2.35469151	-0.21077267	3.55655888

H3+SO_2

-1 1

Al	0.47909847	-0.10066222	0.16799211
N	-2.91266307	0.08626323	-0.85565089
H	-2.88280691	-0.33433069	-1.78516016
H	-2.20012295	0.82528065	-0.79989113
O	-0.33860595	1.40997755	-0.32294879
H	-0.02021662	2.21654183	0.08449431
O	1.11125311	0.15004927	1.80024706
H	1.85837684	-0.39716765	2.04632729
O	1.77031704	-0.73149439	-0.86275400
H	1.49583829	-1.32571602	-1.56262390
S	-2.46193009	-1.16401496	0.26196164
O	-3.11576144	-2.38219827	-0.30784340
O	-0.88280094	-1.30700065	0.00110010

H3+2SO_2

-1 1

Al	0.52259058	-0.51632807	0.24372338
N	-2.91175695	-0.37487740	-0.46280648
H	-2.90589265	-0.16609895	-1.46149451
H	-2.32698876	0.30941711	0.03244228
O	-0.50605257	0.81593126	0.77129068
H	-0.24244476	1.30754932	1.55409281
O	1.28163565	-1.15995918	1.76164963
H	2.15862140	-1.54939905	1.69136902
O	1.86073923	-0.29217827	-0.87053642
H	1.70379468	-0.50031487	-1.79227157
S	-2.20592484	-1.94132996	-0.26880022
O	-2.71813672	-2.70052558	-1.44679509
O	-0.63700958	-1.65486308	-0.54229517
S	0.99993616	-0.45983765	3.89715453
O	2.33513856	-0.81675112	4.40570102
O	0.77947535	0.97552182	3.65175395

$Al(OH)_4$+2SO_2

-1 1

Al	0.54785608	0.85712048	-0.52443952
O	0.36007527	1.33790280	1.17316395

H	0.89194796	0.94224305	1.86392540
O	3.21963498	-0.66489813	-1.80943656
H	2.31804269	-0.99939024	-1.56371130
O	0.71181021	-0.87716870	-0.83512185
H	-0.07909317	-1.41920014	-0.86308092
O	-2.14861696	2.33215154	0.86348966
H	-1.28487198	2.01183450	1.23240303
S	-2.41327996	1.57039591	-0.60329794
O	-2.72815043	0.14579732	-0.30794502
O	-0.93608691	1.61754230	-1.21667832
S	3.09378207	0.92528091	-2.32705742
O	2.07040317	1.49703506	-1.22758290
O	2.41024942	0.91305811	-3.64112602