

Fragmentation Energetics of Clusters Relevant to Atmospheric New Particle Formation

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SUPPORTING INFORMATION

Table S1. Thermochemical parameters for all clusters. All values are in hartrees and calculated at gas phase standard state of 1 atm and 298 K. 1 hartree = 27.2116 eV.

Molecular Cluster or Molecule	E _{electronic} (PW91)	E _{electronic} (MP2)	ZPE (PW91)
$[(\text{NH}_4^+)(\text{HSO}_4^-)]$	-756.714796	-755.901875	0.072987
$[(\text{NH}_4^+)_2(\text{HSO}_4^-)]^+$	-813.652698	-812.763187	0.124409
$[(\text{NH}_4^+)_2(\text{HSO}_4^-)(\text{H}_2\text{SO}_4)]^+$	-1513.830516	-1512.21669	0.163448
$[(\text{NH}_4^+)_3(\text{HSO}_4^-)_2]^+$	-1570.416762	-1568.72236	0.202684
$[(\text{NH}_4^+)_3(\text{HSO}_4^-)_2(\text{H}_2\text{SO}_4)]^+$	-2270.593488	-2268.16689	0.242117
$[(\text{NH}_4^+)_4(\text{HSO}_4^-)_3]^+$	-2327.184889	-2324.67346	0.280334
$[(\text{NH}_4^+)_5(\text{HSO}_4^-)_4]^+$	-3083.954882	N/A	0.357987
$[(\text{NH}_4^+)_6(\text{HSO}_4^-)_5]^+$	-3840.716016	N/A	0.436480
H_2SO_4	-700.144548	-699.414695	0.036816
NH_3	-56.538531	-56.456628	0.033692

Cartesian coordinates for optimized free molecules and cluster geometries.

Sulfuric Acid (H_2SO_4)

S	-0.041051	0.116907	-0.005283
O	-0.503645	1.481157	0.236644
O	1.344855	-0.266772	-0.261704
O	-0.521366	-0.844237	1.247885
O	-0.989918	-0.439758	-1.236017
H	-1.358702	-0.472479	1.601060
H	-0.573672	-1.258718	-1.582586

Ammonia (NH_3)

H	0.119902	0.104506	0.322174
N	-0.287899	0.858690	0.878649
H	0.442767	1.556541	1.033208
H	-1.017870	1.297662	0.313669

Ammonium Bisulfate $[(\text{NH}_4^+)(\text{HSO}_4^-)]$

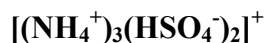
S	-0.6029800	-0.1191970	0.0981450
O	0.4346220	-0.4930190	-1.0481320
O	-1.8056530	-0.9444300	-0.0604340
O	-1.0189560	1.4508290	-0.2749580
O	0.1053790	0.0060310	1.3852330
H	-1.7266280	1.4001600	-0.9515880
H	3.4156910	-0.7236240	-0.1017660
N	2.7349960	0.0385480	-0.0551030
H	3.1910700	0.8976270	-0.3719300
H	1.4482350	-0.2552030	-0.6969420
H	2.4512060	0.1630810	0.9239430



S	0.0926330	0.0291690	0.0436470
O	-0.9441440	-1.0574120	0.1080650
O	0.8853420	0.2423840	1.2849000
O	-0.9229480	1.3493990	-0.1617640
O	0.9636210	-0.0372320	-1.1880160
H	-0.3888750	2.1705310	-0.2065500
H	-3.9393520	-0.5285770	0.8304630
N	-3.4218920	-0.3172620	-0.0310800
H	-3.3680910	0.7020090	-0.1594500
H	-2.3810960	-0.6828090	0.0365080
H	-3.9057380	-0.7401190	-0.8321560
H	2.9339180	-0.0973480	0.8885490
N	3.3401170	-0.2874400	-0.0470150
H	2.4795260	-0.2093360	-0.7035660
H	4.0611810	0.4058940	-0.2770550
H	3.7438540	-1.2311510	-0.0739080



S	-2.2314750	0.1540040	-0.2718010
O	-1.0479090	-0.7284470	-0.7468510
O	-1.8161680	1.5890980	-0.2136630
O	-2.2946770	-0.4054980	1.3140320
O	-3.5120580	-0.1470650	-0.9083110
H	-3.2034770	-0.2323750	1.6440790
H	0.5949410	-2.6608990	0.7058870
N	-0.4052390	-2.9441810	0.6180900
H	-0.8532130	-2.9634530	1.5419630
H	-0.8547030	-2.1768200	0.0248750
H	-0.4844300	-3.8642250	0.1696800
H	-0.5775560	2.4598110	0.3367810
N	0.2766190	3.0213610	0.6492920
H	0.0635370	3.5520650	1.5019620
H	1.0503640	2.3361640	0.8335760
H	0.5537650	3.6728850	-0.0946530
S	2.1587110	-0.1381950	-0.0197900
O	2.0060130	0.8621990	1.0571010
O	2.0466220	-1.5721330	0.3366820
O	1.2167650	0.2102310	-1.2504030
O	3.6135200	0.1627740	-0.6499130
H	0.2263780	-0.1526690	-1.0765210
H	3.8521100	-0.5329650	-1.3032480



S	-2.4826990	0.0739780	0.0176770
O	-1.7496580	-1.0566230	0.7458420

O	-3.9447670	-0.0068130	0.0044940
O	-1.9598740	-0.1947820	-1.5765980
O	-1.8627400	1.3908430	0.4037110
H	-2.7634130	-0.1179730	-2.1351870
H	-0.7290200	2.2213250	-0.4600420
N	0.1820730	2.6416940	-0.8172740
H	0.3228590	2.3880940	-1.8017000
H	0.1862260	3.6619460	-0.7123530
H	0.9479000	2.1842100	-0.2447070
S	2.4826480	-0.0739490	0.0175860
O	3.9447270	0.0065860	0.0039220
O	1.8625460	-1.3906600	0.4039340
O	1.9593930	0.1946570	-1.5765880
O	1.7500320	1.0568450	0.7458670
H	2.7628130	0.1179010	-2.1353560
H	-0.7289310	-0.4468360	1.9530310
N	0.0003230	-0.0002560	2.5847650
H	-0.4457610	0.7093860	3.1768280
H	0.4468150	-0.7106310	3.1756410
H	0.7292190	0.4469980	1.9531190
H	-0.1863120	-3.6617860	-0.7128630
N	-0.1820230	-2.6415110	-0.8175390
H	-0.9477830	-2.1840460	-0.2448630
H	0.7291000	-2.2213250	-0.4602080
H	-0.3227900	-2.3876480	-1.8019010



S	-0.7028230	1.9887040	0.2344850
O	0.1929780	1.6086720	-0.9184290
O	-2.1645640	1.7344370	-0.0433970
O	-0.4919200	3.6195820	0.2482780
O	-0.2634920	1.4726100	1.5642850
H	-1.0414350	4.0078420	0.9645080
H	0.0169140	-0.2348300	2.0656990
N	0.0988870	-1.2786440	2.0691250
H	0.1757560	-1.6467430	3.0229670
H	-0.7489610	-1.6447510	1.5915800
H	0.9399060	-1.5409340	1.4826600
S	3.3431810	-1.1305540	-0.0147270
O	4.4844470	-2.0292190	0.1686330
O	3.3402400	-0.2364680	-1.2307210
O	3.3560530	-0.0378910	1.2779550
O	1.9602490	-1.7682830	0.1255560
H	4.1614680	-0.2489080	1.7979070
H	-0.6691810	-1.4978470	-1.4967350
N	0.2294090	-1.1376390	-1.8806950
H	0.3817290	-1.4451100	-2.8468290
H	0.2010840	-0.1003570	-1.8092910
H	1.0072320	-1.4708820	-1.2368290

H	1.8307000	2.3018730	-0.9218280
N	2.8805040	2.3570440	-0.9382390
H	3.2180650	1.3416300	-1.0567940
H	3.2030730	2.9531080	-1.7084630
H	3.2215870	2.7315310	-0.0457370
S	-3.2835990	-1.1899720	-0.1494460
O	-1.8233820	-1.5330740	-0.0080740
O	-4.2580690	-2.2545040	-0.2506030
O	-3.6736460	-0.2263140	1.0889580
O	-3.4087680	-0.2278790	-1.4505990
H	-3.1437090	0.6196780	0.9899010
H	-2.9249790	0.6251560	-1.2437680



S	-3.3548230	-1.3176200	0.0846780
O	-2.5948060	-0.5656220	-1.0168330
O	-4.3460770	-2.2946580	-0.3785280
O	-4.2133970	-0.0027340	0.7325280
O	-2.4220490	-1.7738890	1.1630240
H	-4.9943010	-0.3805020	1.1903240
H	0.6728830	-1.3423610	1.4068180
N	-0.0103660	-0.8953680	2.0766740
H	0.0971910	0.1355080	2.0355480
H	-0.9879100	-1.1657960	1.7717830
H	0.1670830	-1.2324920	3.0284380
S	0.3091740	2.4747550	0.0124680
O	-0.8947420	3.3130770	-0.2878570
O	0.3450920	1.1391400	-0.6390540
O	0.1271940	2.0080890	1.6448780
O	1.5888530	3.2513850	-0.0298740
H	0.0846170	2.8183570	2.1956490
H	0.5053070	-1.7209370	-1.1911320
N	-0.1096730	-1.2855910	-1.9354230
H	-0.1182640	-1.8630740	-2.7819620
H	-1.0930580	-1.1333640	-1.5701960
H	0.2906430	-0.3552560	-2.1238050
H	-3.9193110	2.1172490	-0.2769980
N	-3.2194230	2.0830820	-1.0290770
H	-3.6086430	2.4920160	-1.8848210
H	-2.3362690	2.5971730	-0.7373400
H	-2.9898240	1.0523080	-1.1606000
H	4.6540180	2.3339010	0.4933880
N	3.9360180	1.8593340	-0.0646170
H	3.7285350	0.8882950	0.3384810
H	3.0349920	2.4256760	-0.0625530
H	4.2717660	1.7521270	-1.0279880
S	2.9931080	-1.7082720	0.0483410
O	3.2418890	-0.5234700	0.9428870
O	3.9472300	-2.8212980	0.1064500

O	3.1326160	-1.0434950	-1.5148090
O	1.5200930	-2.0978090	0.1128580
H	3.7501090	-1.6405560	-1.9890970

$[(\text{NH}_4^+)_5(\text{HSO}_4^-)_4]^+$

S	2.5363800	2.9880820	0.0537040
O	3.1837120	2.4136410	1.2769330
O	3.4220130	3.3499260	-1.0629470
O	1.7182960	4.3585570	0.5715310
O	1.3145710	2.1571420	-0.3702810
H	2.3874170	5.0274720	0.8306780
H	-1.0913670	3.7468180	1.0024900
N	-1.0552900	2.7528950	0.7546780
H	-1.2394360	2.1447450	1.5826040
H	-1.7766970	2.5060680	0.0443610
H	-0.0902850	2.5325540	0.3528420
S	-1.4178330	-0.6594530	2.4836180
O	-0.0256840	-0.8515680	1.9943350
O	-1.9351650	0.7409600	2.5228970
O	-1.4741260	-1.0895610	4.0717480
O	-2.3918290	-1.5919890	1.7587710
H	-1.1391510	-2.0083510	4.1592220
H	1.4040590	1.1969090	-1.7838470
N	1.3124330	0.3802230	-2.4477140
H	1.7278400	0.5999500	-3.3583680
H	1.8092680	-0.4339750	-1.9880460
H	0.2990460	0.1654540	-2.5408420
H	2.9778880	0.7563830	1.6238140
N	2.7774040	-0.2770020	1.7104160
H	3.4578990	-0.7393370	2.3215930
H	1.8163600	-0.4261010	2.0704610
H	2.8135640	-0.7191720	0.7531460
H	-5.3118690	-0.3991110	0.6556130
N	-4.4755320	0.0411100	1.0535510
H	-4.7319020	0.6307980	1.8532030
H	-3.7709390	-0.6873110	1.3801740
H	-3.9881090	0.6240240	0.3110190
S	-2.7124960	0.6301370	-2.0998500
O	-2.9853840	1.3881770	-0.8104430
O	-2.8382370	1.3997450	-3.3445050
O	-3.9610480	-0.5087800	-2.0603170
O	-1.4662110	-0.2170910	-1.9703650
H	-4.3784850	-0.4925970	-2.9480020
S	2.3565790	-2.9071470	-0.6140830
O	1.0886370	-3.3914190	-1.2701230
O	2.5666960	-1.4119090	-0.8198910
O	3.5863340	-3.5116170	-1.5338720
O	2.5441330	-3.3224160	0.7935980
H	3.5733920	-4.4896760	-1.4522280

H	-1.5566090	-1.8634610	-1.2575070
N	-1.4244410	-2.7269160	-0.6807990
H	-0.4036700	-3.0323710	-0.7830650
H	-1.6646570	-2.4787420	0.3048250
H	-2.0413520	-3.4734410	-1.0158310



S	-3.7779657	-0.1927335	-2.6099879
O	-3.8345137	1.2479515	-2.2015539
O	-4.4478737	-0.5449685	-3.8684249
O	-4.5445357	-1.0640385	-1.3764459
O	-2.3599557	-0.7448905	-2.4356219
H	-5.4786367	-1.1691685	-1.6560759
H	-2.6421307	-3.6008495	-0.9096909
N	-2.0549277	-2.7895175	-0.6933489
H	-2.3324277	-2.3860735	0.2288561
H	-1.0519667	-3.0673795	-0.6192489
H	-2.1908827	-2.0451795	-1.4437379
S	-2.0719687	-0.6354495	2.7735211
O	-2.6814577	0.6471705	2.3429831
O	-2.3008087	-1.8478445	1.9345101
O	-2.8172117	-1.0676465	4.1875961
O	-0.5883157	-0.5060775	3.1290751
H	-2.9721297	-0.2510655	4.7087891
H	-1.0314000	0.2093460	-2.4108860
N	-0.1182660	0.6676480	-2.1530350
H	0.1949510	1.3091670	-2.8875150
H	-0.2451360	1.2016130	-1.2393960
H	0.5789100	-0.0870060	-1.9933490
H	-3.6325497	1.9461905	-0.6991709
N	-3.4733677	2.4660395	0.2099681
H	-4.3520827	2.8898325	0.5242041
H	-3.1277097	1.8017655	0.9310021
H	-2.7473277	3.2140435	0.0552121
H	-0.2485350	-3.7851240	3.2221350
N	0.4213120	-3.1269300	2.8088670
H	0.0660870	-2.1311480	2.9588510
H	1.3409620	-3.2475180	3.2460420
H	0.5101890	-3.2989830	1.7654880
S	1.7986953	-2.4673465	-0.4523419
O	0.6559813	-3.3074115	0.0841111
O	3.0224843	-3.2763595	-0.7875769
O	2.1685153	-1.5694345	0.8684831
O	1.3977283	-1.5558295	-1.5642559
S	-0.1819987	3.4768835	0.3089421
O	0.3414993	3.8755215	1.6600031
O	-0.4175577	1.9720085	0.2543341
O	1.0078403	3.7708355	-0.7923619
O	-1.3426187	4.2599875	-0.1929039

H	1.8561890	1.2312630	1.7732980
N	1.2743400	1.4574290	2.6036600
H	0.8512680	2.4169260	2.3857090
H	0.5142050	0.7488890	2.7223070
H	1.8594580	1.5020720	3.4435300
S	4.1105220	1.1044580	-0.2589590
O	5.2741320	1.9895530	-0.1192460
O	4.2682150	-0.3108820	0.2532070
O	3.9894830	0.7793300	-1.9534500
O	2.7676070	1.6685310	0.1141100
H	4.4106410	1.5401480	-2.4077340
H	5.7063070	-1.9440710	-1.4178930
N	4.8974950	-1.9648810	-2.0505530
H	4.5628720	-0.9800470	-2.1666290
H	5.1678690	-2.3698210	-2.9533830
H	4.1172810	-2.5513640	-1.5883880
H	1.2531199	4.7386065	-0.7361720
H	2.7265822	-2.0976119	1.4911317