

## Electronic Supplementary Information

### Hydration of the Methanesulfonate–Ammonia/Amine Complex and Its Atmospheric Implications

Shou-Kui Miao,<sup>1,2</sup> Shuai Jiang,<sup>2</sup> Xiu-Qiu Peng,<sup>1,2</sup> Yi-Rong Liu,<sup>2</sup> Ya-Juan Feng,<sup>2</sup>

Yan-Bing Wang,<sup>1,2</sup> Feng Zhao,<sup>1,2</sup> Teng Huang,<sup>1</sup> and Wei Huang<sup>1,2,3\*</sup>

*<sup>1</sup>Laboratory of Atmospheric Physico-Chemistry, Anhui Institute of Optics & Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui 230031, China*

*<sup>2</sup>School of Information Science and Technology, University of Science and Technology of China, Hefei, Anhui 230026, China*

*<sup>3</sup>Center for Excellent in Urban Atmospheric Environment, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen, Fujian 361021, China*

\*E-mail: [huangwei6@ustc.edu.cn](mailto:huangwei6@ustc.edu.cn)

### Table Caption

**Table S1.** PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for  $(\text{MSA}^-)(\text{NH}_3)(\text{H}_2\text{O})_n$  ( $n = 0-3$ ) clusters.

**Table S2.** PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for  $(\text{MSA}^-)(\text{MA})(\text{H}_2\text{O})_n$  ( $n = 0-3$ ) clusters.

**Table S3.** PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for  $(\text{MSA}^-)(\text{DMA})(\text{H}_2\text{O})_n$  ( $n = 0-3$ ) clusters.

**Table S4.** PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for  $(\text{MSA}^-)(\text{TMA})(\text{H}_2\text{O})_n$  ( $n = 0-3$ ) clusters.

**Table S1** $(\text{MSA}^-)(\text{NH}_3)$ 

C	1.325219	1.459959	-0.004956
H	1.955968	1.546690	0.885365
H	1.928955	1.552410	-0.913240
H	0.535270	2.217380	0.009177
O	1.676727	-1.129162	-0.019950
O	-0.242993	-0.208169	1.251361
O	-0.278161	-0.198716	-1.227266
S	0.549146	-0.180643	0.001603
N	-3.115742	0.216403	-0.006272
H	-2.404229	0.120911	-0.743368
H	-3.660930	-0.647506	-0.051747
H	-2.527068	0.114203	0.828635

 $(\text{MSA}^-)(\text{NH}_3)(\text{H}_2\text{O})$ 

C	1.095043	0.821247	1.396268
H	1.694003	1.716865	1.205057
H	0.078429	1.098619	1.692416
H	1.570004	0.197151	2.159448
O	0.287928	0.763244	-1.085460
O	2.390252	-0.418028	-0.514358
O	0.214031	-1.339189	0.219763
S	0.998955	-0.129624	-0.139049
N	-2.714737	-1.234643	0.145425
H	-3.059378	-1.858036	0.875713
H	-3.024506	-1.624303	-0.745146
H	-1.679025	-1.300757	0.152705
O	-2.281725	1.661007	-0.126160
H	-2.618602	0.753131	0.046910
H	-1.395183	1.470061	-0.508179

 $(\text{MSA}^-)(\text{NH}_3)(\text{H}_2\text{O})_2$ 

C	-1.928837	1.404089	-0.168461
H	-1.113969	2.131905	-0.104166
H	-2.417872	1.458755	-1.145624
H	-2.655171	1.560533	0.634544
O	-0.232928	-0.355156	-1.080751
O	-0.602582	-0.246690	1.364454
O	-2.356961	-1.180967	-0.112610
S	-1.232073	-0.249502	0.022745
N	2.545895	-1.449698	-0.609918
H	3.015079	-0.823055	-1.265360

H	2.772610	-2.407231	-0.876454
H	1.537654	-1.305414	-0.770711
O	1.751941	1.756033	-0.905259
H	1.995894	1.472124	0.006192
H	1.037820	1.115563	-1.114580
O	2.147535	0.363177	1.597670
H	2.462179	-0.373394	1.021417
H	1.174665	0.194421	1.622978

(MSA<sup>-</sup>)(NH<sub>3</sub>)(H<sub>2</sub>O)<sub>3</sub>

C	3.085659	0.186917	-0.340119
H	3.607546	0.197869	0.621053
H	3.396482	-0.674255	-0.938485
H	3.261342	1.118974	-0.884941
O	1.167056	-1.231722	0.714329
O	0.977689	1.239381	0.780809
O	0.685290	0.034069	-1.361031
S	1.317685	0.042633	-0.020700
N	-2.263401	1.474041	-1.151683
H	-1.277226	1.644033	-1.366573
H	-2.407293	0.480184	-1.389594
H	-2.824056	2.043480	-1.784486
O	-1.784367	1.215343	1.635763
H	-0.810836	1.284385	1.514700
H	-2.112038	1.410237	0.717342
O	-1.618559	-1.594565	1.346838
H	-0.641706	-1.601640	1.230819
H	-1.793841	-0.638904	1.543526
O	-1.842684	-1.490443	-1.464291
H	-0.936069	-1.130765	-1.564465
H	-1.890818	-1.632024	-0.484539

**Table S2**

(MSA<sup>-</sup>)(MA)

C	2.176636	-1.185291	-0.000026
H	2.795031	-1.103707	-0.899382
H	2.794930	-1.103832	0.899411
H	1.621789	-2.128637	-0.000122
O	1.815127	1.401611	0.000128
O	0.199102	-0.013096	-1.239133
O	0.198975	-0.013262	1.239030
S	0.986039	0.183912	0.000001
C	-3.472615	0.367843	-0.000013

H	-2.982550	1.360605	-0.000088
H	-4.126940	0.321941	-0.883287
H	-4.126884	0.322045	0.883307
N	-2.553387	-0.769260	0.000028
H	-1.903993	-0.661705	0.786859
H	-1.904065	-0.661814	-0.786873

(MSA<sup>-</sup>)(MA)(H<sub>2</sub>O)

C	-1.886739	1.053871	0.945270
H	-1.032404	1.657653	1.267524
H	-2.582079	1.659509	0.356085
H	-2.398066	0.607680	1.803732
O	-0.544001	0.411559	-1.199536
O	-0.372910	-1.068065	0.777095
O	-2.461293	-1.018937	-0.551585
S	-1.270824	-0.280965	-0.107190
C	3.081400	-1.020362	-0.406191
H	2.546517	-0.718150	-1.314002
H	4.130108	-0.709665	-0.518333
H	3.054397	-2.124823	-0.356520
N	2.470704	-0.341476	0.737738
H	1.472614	-0.607954	0.801910
H	2.915796	-0.632352	1.607748
O	1.504881	2.218394	-0.257258
H	1.988051	1.483966	0.190553
H	0.761951	1.725248	-0.672030

(MSA<sup>-</sup>)(MA)(H<sub>2</sub>O)<sub>2</sub>

C	2.547815	0.695153	0.152634
H	3.145535	0.458705	1.037909
H	3.160198	0.635864	-0.752086
H	2.085984	1.683731	0.240780
O	1.899399	-1.828258	-0.151933
O	0.463536	-0.412141	1.284055
O	0.444422	-0.101187	-1.170078
S	1.233911	-0.532424	0.021224
C	-2.719699	-1.714613	-0.045249
H	-3.109112	-0.229848	-1.426359
H	-1.532357	-0.298446	-0.937637
H	-1.996056	-1.859256	0.765152
N	-2.508496	-0.382465	-0.617216
H	-3.728762	-1.785620	0.384344
H	-2.590321	-2.547504	-0.759689
O	-0.263265	2.722544	-0.849908

H	0.026519	1.829363	-1.131287
H	-0.788013	2.502556	-0.044974
O	-1.644559	1.500165	1.357908
H	-2.165592	0.952644	0.715935
H	-0.856092	0.921625	1.484174

(MSA<sup>-</sup>)(MA)(H<sub>2</sub>O)<sub>3</sub>

C	3.083345	-1.271462	-0.226957
H	2.867122	-2.334942	-0.090346
H	3.450639	-1.079179	-1.239060
H	3.805947	-0.926249	0.518011
O	0.630481	-0.871604	-1.034909
O	1.120652	-0.663331	1.382066
O	1.927278	1.067383	-0.199625
S	1.552533	-0.348355	0.002016
C	-3.584984	-1.664459	-0.081963
H	-3.591373	-2.385312	0.747081
H	-4.498067	-1.060770	0.007736
H	-3.658225	-2.238566	-1.025099
N	-2.413832	-0.800180	0.018438
H	-2.369683	-0.122305	-0.755741
H	-1.546194	-1.334727	-0.074104
O	-1.288935	0.795168	2.061030
H	-0.418182	0.341977	2.005156
H	-1.839676	0.241455	1.439650
O	-1.323633	1.115772	-2.035139
H	-0.600467	0.466226	-1.908943
H	-1.107155	1.786910	-1.338475
O	-0.447410	2.683589	0.139959
H	0.444782	2.287344	0.023570
H	-0.820795	2.132790	0.875718

**Table S3**

(MSA<sup>-</sup>)(DMA)

C	-2.134483	1.433284	0.019887
H	-2.717200	1.530643	-0.901423
H	-2.789669	1.483325	0.895225
H	-1.365706	2.210740	0.071918
O	-2.416760	-1.162128	-0.058735
O	-0.462007	-0.156023	-1.201407
O	-0.542930	-0.219702	1.270974

S	-1.316034	-0.186205	0.013782
C	2.625670	1.263696	0.177279
N	2.467615	0.041022	-0.595000
C	2.808493	-1.134585	0.193304
H	2.275169	2.119894	-0.414010
H	3.691029	1.429716	0.409043
H	2.064139	1.256490	1.134107
H	1.475878	-0.037159	-0.866528
H	2.597799	-2.040102	-0.389674
H	2.242277	-1.204174	1.143718
H	3.885016	-1.128794	0.432620

(MSA<sup>-</sup>)(DMA)(H<sub>2</sub>O)

C	-2.153155	0.634133	-1.318107
H	-2.991925	1.261870	-1.002281
H	-1.326491	1.254041	-1.679010
H	-2.473115	-0.077161	-2.085570
O	-1.107575	0.734595	1.072726
O	-2.741045	-1.065233	0.586890
O	-0.474156	-1.147086	-0.404405
S	-1.577916	-0.299858	0.118986
C	3.116375	-0.730707	-1.123990
N	2.244330	-0.161101	-0.114451
C	2.676438	-0.456173	1.242139
H	2.695562	-0.548345	-2.120470
H	3.269177	-1.826260	-1.012456
H	4.109475	-0.255833	-1.083140
H	1.279201	-0.512326	-0.242135
H	1.923512	-0.084846	1.946103
H	3.630718	0.050021	1.456538
H	2.821838	-1.541251	1.429589
O	0.951534	2.456145	0.018702
H	1.553412	1.688121	-0.126741
H	0.176963	2.006522	0.425394

(MSA<sup>-</sup>)(DMA)(H<sub>2</sub>O)<sub>2</sub>

C	-2.861793	0.804005	-0.322306
H	-3.235525	0.712925	-1.346491
H	-3.670740	0.648069	0.397481
H	-2.386248	1.778098	-0.170960
O	-2.297455	-1.756573	-0.319338
O	-0.548942	-0.160444	-1.044168
O	-1.177382	-0.304901	1.344752
S	-1.623910	-0.480517	-0.057805

C	3.184299	0.104802	-1.022544
N	2.257723	-0.457096	-0.052322
C	2.592705	-1.812244	0.353186
H	2.821007	1.091258	-1.334242
H	3.310421	-0.527301	-1.926627
H	4.177951	0.229379	-0.565412
H	1.301418	-0.439056	-0.436296
H	1.804662	-2.199915	1.009037
H	3.540100	-1.815696	0.913628
H	2.706867	-2.511408	-0.501436
O	0.410897	2.569184	-0.699142
H	0.042079	1.705369	-0.981740
H	0.673761	2.364243	0.228664
O	1.076457	1.359534	1.826131
H	0.227055	0.859646	1.789303
H	1.665822	0.758535	1.300327

(MSA<sup>-</sup>)(DMA)(H<sub>2</sub>O)<sub>3</sub>

C	-2.967955	-1.479041	-0.653249
H	-3.348010	-1.069907	-1.593628
H	-2.574740	-2.488712	-0.802252
H	-3.749294	-1.477750	0.112064
O	-0.609975	-0.482681	-1.169572
O	-2.228478	0.911227	0.086524
O	-1.156655	-1.040688	1.177891
S	-1.623484	-0.424345	-0.084049
C	2.494294	-2.115276	0.279280
N	2.225035	-0.723646	-0.045004
C	3.253903	-0.103646	-0.868960
H	1.640396	-2.531820	0.826147
H	3.383443	-2.186265	0.923657
H	2.679345	-2.745555	-0.615671
H	1.311878	-0.650960	-0.511096
H	2.896087	0.878709	-1.199618
H	3.508018	-0.703955	-1.767670
H	4.177953	0.023926	-0.284678
O	-0.126522	2.768059	0.859077
H	-0.944005	2.276203	0.625885
H	0.368060	2.098799	1.395879
O	1.045678	0.559748	2.192389
H	0.218319	0.045006	2.068126
H	1.608883	0.183515	1.459387
O	0.790558	2.111245	-1.757577
H	0.259071	1.291167	-1.757877



H	0.566791	2.485127	-0.871137
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**Table S4**

(MSA<sup>-</sup>)(TMA)

C	2.510264	-0.001571	1.577602
H	3.110735	0.897695	1.747513
H	1.628962	-0.002421	2.226795
H	3.111058	-0.900980	1.745603
O	1.152592	1.237877	-0.277794
O	3.196724	0.001243	-0.942546
O	1.153040	-1.237551	-0.280446
S	1.953631	0.000168	-0.150573
N	-2.800672	-0.000120	0.345420
C	-4.244512	-0.000210	0.251365
C	-2.227200	1.202621	-0.245992
C	-2.227008	-1.202364	-0.246812
H	-4.608306	0.000129	-0.805113
H	-4.655911	-0.891399	0.745638
H	-4.656063	0.890562	0.746262
H	-2.502367	1.309005	-1.320719
H	-2.602300	2.088569	0.285863
H	-1.131694	1.179915	-0.176650
H	-1.131506	-1.179528	-0.177500
H	-2.601950	-2.088735	0.284450
H	-2.502167	-1.308071	-1.321607

(MSA<sup>-</sup>)(TMA)(H<sub>2</sub>O)

C	2.328396	0.695504	1.392301
H	2.690772	-0.008207	2.148046
H	3.089051	1.451748	1.175673
H	1.397911	1.173557	1.714852
O	3.299469	-0.769635	-0.549320
O	1.004260	-1.251713	0.253942
O	1.450507	0.794169	-1.064104
S	1.999560	-0.224103	-0.131143
N	-2.526633	-0.112151	0.040337
C	-3.948814	0.164443	-0.020415
C	-2.051996	-0.801521	-1.156919
C	-2.163171	-0.845133	1.248030
H	-4.562655	-0.764309	-0.069660
H	-4.258739	0.729691	0.868557
H	-4.173343	0.768626	-0.908923
H	-2.561230	-1.780471	-1.298041

H	-2.245834	-0.178193	-2.038875
H	-0.972110	-0.970442	-1.070419
H	-1.080528	-1.021204	1.245518
H	-2.435675	-0.254788	2.133158
H	-2.685241	-1.825895	1.310551
O	-0.769583	2.278222	-0.102606
H	0.031638	1.829338	-0.465332
H	-1.404264	1.533145	-0.010461

(MSA<sup>-</sup>)(TMA)(H<sub>2</sub>O)<sub>2</sub>

C	-3.652316	-0.647392	0.019300
H	-3.842264	-1.412095	0.778246
H	-4.167380	0.283833	0.272394
H	-3.959253	-1.001117	-0.969425
O	-1.558393	0.155911	1.343201
O	-1.250510	-1.610019	-0.366827
O	-1.710751	0.718221	-1.067269
S	-1.877500	-0.318382	-0.025303
N	2.438080	-0.468171	-0.041807
C	1.955801	-0.193232	-1.394930
C	2.122887	-1.832027	0.369216
C	3.853629	-0.173320	0.092160
H	2.068501	0.874256	-1.617921
H	2.510951	-0.787396	-2.153509
H	0.891394	-0.442016	-1.460781
H	2.422301	-1.978742	1.415326
H	1.041870	-1.994167	0.280872
H	2.653204	-2.585637	-0.253917
H	4.170896	-0.330822	1.131290
H	4.484016	-0.814568	-0.564525
H	4.039895	0.875012	-0.172520
O	0.972517	1.364120	1.671853
H	0.065885	0.973271	1.647815
H	1.493220	0.727692	1.120903
O	0.216752	2.904308	-0.655011
H	-0.483437	2.255386	-0.878058
H	0.546712	2.543923	0.199254

(MSA<sup>-</sup>)(TMA)(H<sub>2</sub>O)<sub>3</sub>

C	3.142063	-1.356226	0.306083
H	3.634538	-0.392821	0.472630
H	3.225828	-1.998479	1.187579
H	3.553920	-1.855516	-0.575833
O	0.908241	-0.375043	1.245174

O	1.380918	-0.134064	-1.175177
O	0.767768	-2.343587	-0.241456
S	1.395761	-1.038496	0.010316
N	-2.806834	-0.033817	-0.026809
C	-2.494398	-0.078290	1.400115
C	-4.143865	0.483161	-0.267358
C	-2.615406	-1.339891	-0.652952
H	-3.180763	-0.757801	1.950071
H	-1.461216	-0.416900	1.538386
H	-2.584103	0.928219	1.827132
H	-4.933762	-0.164240	0.174446
H	-4.239776	1.485607	0.168590
H	-4.325856	0.557297	-1.347076
H	-2.781263	-1.254206	-1.734318
H	-1.590595	-1.692363	-0.485376
H	-3.322850	-2.096404	-0.249729
O	3.059790	2.202610	-0.492743
H	2.630990	1.431948	-0.915918
H	2.343287	2.494395	0.116458
O	0.662279	2.468687	1.099404
H	0.075643	2.413706	0.307280
H	0.794439	1.513399	1.298077
O	-0.813795	1.705193	-1.219728
H	-1.516490	1.132042	-0.821020
H	-0.058267	1.081895	-1.327890