Supplementary material for the article "Estimating the NH_3:H_2SO_4 ratio of nucleating clusters in atmospheric conditions using quantum chemical methods" by T. Kurtén *et al.* Manuscript number acpd-2007-0032.

Table S1. Cartesian co-ordinates (in Ångström) of the most stable cluster structures found for each stoichiometry. All structures have been optimized at the RI-MP2/aug-cc-pV(D+d)Z level.

$(H_2SO_4)_2$

S	0.114217055	-0.020066518	-2.05082208
O	-0.763179928	-1.165687432	-1.408732301
O	1.142718228	0.409141029	-1.110548125
O	-0.894362183	1.238356631	-2.089018194
O	0.443348174	-0.438611726	-3.385783918
H	-0.915015289	-0.944022311	-0.446245679
H	-1.520578467	1.095989654	-2.822412081
S	-0.114217495	0.020066609	2.050821579
O	0.894363164	-1.238355051	2.089026713
O	-1.142715024	-0.409148741	1.110547536
O	0.763181666	1.165685316	1.408730055
O	-0.443354091	0.438619183	3.385779496
H	1.520589603	-1.095975613	2.822409551
H	0.915018051	0.944017931	0.446244124

$(H_2SO_4)_2$·(NH_3)

S	1.835262133	-0.291802778	-0.038209097
O	2.502071795	0.854852518	-0.707582478
O	1.08894459	0.183345478	1.167288636
O	3.020044861	-1.261866702	0.485796138
O	1.063923998	-1.181085921	-0.912491792
H	1.460187768	2.119788811	-0.370018016
H	3.665536281	-0.705383475	0.955189972
S	-2.088172889	-0.093391479	-0.020505094
O	-1.464521438	-0.361267464	1.411989555
O	-3.514522599	-0.191468167	0.091427912
O	-1.587003925	-1.30745636	-0.897713879
O	-1.488361671	1.140934955	-0.561131798
H	-0.470292296	-0.215429229	1.362018568
H	-0.58832686	-1.268987633	-0.961451418
N	0.640566839	2.697055845	-0.041192086
H	-0.217982959	2.107435992	-0.178719096
H	0.561439644	3.573746285	-0.554310954
H	0.755927014	2.878098497	0.95596464

$(H_2SO_4)_2$·$(NH_3)_2$

S	-2.238411207	0.114422928	-0.181666355
O	-1.508894539	0.006485942	1.168570036

O	-1.307516226	-0.802158247	-1.170462777
O	-3.513153655	-0.575578381	-0.174858871
O	-2.160498273	1.496865052	-0.667535774
H	-0.910465642	-1.488870153	1.206930166
H	-0.238354234	3.003470118	1.661055237
N	-0.011741954	2.237072206	1.030999621
H	-0.594047981	1.378678127	1.241877971
H	0.987711242	1.955268523	1.088288566
H	-0.264825478	2.47628666	0.067426602
O	2.042158104	-1.48049135	0.218536354
O	2.358112721	0.813954222	1.090521544
S	2.137375529	-0.034875109	-0.104183698
O	1.069565574	0.473991472	-0.988337285
O	3.459572268	0.120311391	-1.039065497
H	4.218120616	-0.179257901	-0.508374218
H	-0.434195906	-0.337152247	-1.246895784
H	0.567639002	-2.125492316	0.683109796
N	-0.406053643	-2.396408961	0.9689608
H	-0.889946652	-2.796163941	0.162977121
H	-0.395667712	-3.050381627	1.748775561

$(H_2SO_4)_2 \cdot (NH_3)_3$

S	-1.961289107	-0.582727372	-0.393640427
O	-1.405792935	0.010882885	0.889280309
O	-0.828483162	-1.674680632	-0.833010441
O	-3.15949644	-1.379060096	-0.202094739
O	-1.98631143	0.454822494	-1.448785443
H	-0.643162868	-1.178268841	1.620406689
H	0.006146511	3.113727996	-1.260492874
N	-0.275278249	2.417557474	-0.573430452
H	-0.92939058	2.821911519	0.137583622
H	0.567059656	2.024901992	-0.105792236
H	-0.805219937	1.643659545	-1.037201063
O	2.352712238	-1.136566607	0.849765405
O	1.967518876	1.301339139	0.696662763
S	2.235932759	0.045870024	-0.042186328
O	1.366428677	-0.14650577	-1.218077768
O	3.703802808	0.213070686	-0.730825288
H	4.337944147	0.347304224	-0.005396391
H	-2.284207216	1.825247307	1.417181614
H	-0.013603014	-1.159431496	-1.075804713
N	-2.31833227	2.849019041	1.356931862
H	-3.249147819	3.090103176	1.017608975
H	-2.253056615	3.210230192	2.307322558
H	0.960796284	-1.71633732	1.53513538
N	0.001374843	-1.994637086	1.866686664

H	-0.317966587	-2.798455021	1.323857977
H	-0.001685258	-2.205999071	2.862085369

$(H_2SO_4)_2 \cdot (NH_3)_4$

S	2.07635174	-0.304736764	0.043059533
O	1.291660512	0.034357179	1.300398301
O	1.699990464	0.907640659	-0.978633195
O	3.512167838	-0.23596779	0.205811997
O	1.520387987	-1.537897831	-0.569351579
H	0.687179137	1.650344359	1.419843935
H	-0.975348966	-2.723738199	-2.467450621
N	-0.962667721	-2.309805153	-1.537717672
H	-0.877408919	-3.043143484	-0.780715593
H	-1.809116434	-1.730740132	-1.371453178
H	-0.108779175	-1.733689437	-1.405386218
O	-2.408534646	1.319657034	0.989194307
O	-1.150906163	-0.83951445	0.933733129
S	-1.942185926	0.274591488	0.056286524
O	-0.932189549	0.810612715	-0.914114572
O	-2.987049002	-0.523626996	-0.600839801
H	0.600420298	-3.230110754	0.760060986
H	0.706460234	0.872370647	-1.035727686
N	-0.289914566	-3.736074055	0.753832812
H	-0.101764723	-4.690740976	1.054176171
H	-0.865806429	-3.296971454	1.473155948
H	-0.907400719	2.194085347	1.412569415
N	0.087617037	2.508710113	1.417810892
H	0.257734196	3.050463509	0.526442382
H	0.283252564	3.079018638	2.238007865
H	-0.358983253	3.069967859	-1.5847808
N	0.387384332	3.62428762	-1.158834474
H	0.299162219	4.57463489	-1.514308207
H	1.263995001	3.243978328	-1.519571008
H	-0.215346428	-0.509785502	1.116361864

Table S2. The electronic and Gibbs free energies (at three different temperatures) of ammonia addition reactions, in kcal mol^{-1}, used in the sensitivity analysis. All values correspond to reactant pressures of 1 atm.

Reaction	ΔE_0	ΔG (298 K)	ΔG (273K)	ΔG (248 K)
$(H_2SO_4)_2 + NH_3 \leftrightarrow (H_2SO_4)_2 \cdot (NH_3)$	-33.85	-19.71	-20.79	-21.80
$(H_2SO_4)_2 \cdot (NH_3) + NH_3 \leftrightarrow (H_2SO_4)_2 \cdot (NH_3)_2$	-26.20	-11.53	-12.47	-13.36
$(H_2SO_4)_2 \cdot (NH_3)_2 + NH_3 \leftrightarrow (H_2SO_4)_2 \cdot (NH_3)_3$	-21.71	-7.05	-7.88	-8.66
$(H_2SO_4)_2 \cdot (NH_3)_3 + NH_3 \leftrightarrow (H_2SO_4)_2 \cdot (NH_3)_4$	-26.50	-7.42	-8.45	-9.42