New mechanistic pathways for organosulfates formation catalyzed by ammonia and carbinolamine formation catalyzed by sulfuric acid in the atmosphere

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Table S1. The enthalpies of binding of the $H_2SO_4\cdots NH_3$ (M1A and M1B), $HCHO\cdots H_2SO_4$ (C1A and C1B), and $HCHO\cdots NH_3$ (M2A and M2B) complexefor different theoretical methods at 0 K.

Methods	ΔH_0					
	M1A	M1B	C1A	C1B	M2A	M2B
W2X//QCISD/cc-pV(T+d)Z	-14.46	-12.59	-10.66	-9.16	-2.30	-2.10
M08-SO/maug-cc-pVTZ	-14.50	-13.05	-10.50	-9.16	-2.57	-2.45

Table S2.The recrossing effects for the lowest transition state in each reaction between 220 – 320 K

T/K	Γ_{TS1A}	Γ_{TS1B}	Γ_{TS2A}	Γ_{TS4A}	Γ_{TS4B}
220	0.58	0.61	0.16	0.96	0.98
240	0.61	0.64	0.18	0.95	0.98
260	0.64	0.67	0.19	0.94	0.99
280	0.66	0.69	0.2	0.93	0.99
298	0.68	0.71	0.21	0.92	0.1
320	0.70	0.73	0.22	0.91	0.1

Table S3.The tunneling coefficients for the lowest transition state in each reaction between 220 – 320 K[a]

T/K	TS1A	TS1B	TS2A	TS4A	TS4B
220	2.76	3.14	2.17	1.30	1.49
240	2.27	2.48	1.92	1.25	1.40
260	1.97	2.09	1.75	1.21	1.33
280	1.77	1.85	1.62	1.17	1.28
298	1.64	1.70	1.53	1.15	1.24
320	1.52	1.56	1.45	1.13	1.20

[a]The tunneling coefficients calculated by using small-curvature tunneling at the M08-SO/maug-cc-pVTZ

Table S4. Frequencies of optimized structures

Species	Frequencies (cm^{-1}) (QCISD/cc-pV(T+d)Z)	Frequencies (cm^{-1})(M08-SO/maug-cc-pVTZ)
TS1A	803.54i 56.41 171.16 194.15 322.55 379.53 400.52 467.84 547.23 585.95 601.47 732.33 816.32 877.66 1061.90 1173.08 1211.69 1230.87 1272.45 1417.64 1444.99 1475.59 1657.21 1873.12 3124.03 3235.05 3853.95	549.97i 50.59 164.24 176.93 323.03 357.51 394.15 463.31 569.15 587.14 596.68 768.41 795.76 870.19 1050.48 1130.13 1164.29 1196.94 1239.88 1389.40 1433.27 1456.04 1639.36 1984.00 3068.76 3188.19 3813.50
TS1B	849.05i 55.58 173.70 186.95 320.10 361.62 417.93 473.84 541.45 578.21 602.43 734.30 815.60 891.43 1062.46 1176.85 1214.84 1232.66 1272.90 1420.24 1439.98 1474.45 1653.57 1861.02 3130.32 3239.37 3856.98	561.39i 51.10 150.59 167.89 318.46 347.25 400.70 457.49 567.72 586.96 597.34 775.81 798.15 882.99 1050.04 1134.97 1162.71 1196.79 1238.03 1387.19 1430.86 1454.35 1633.20 2000.53 3081.60 3195.79 3817.34
TS1C	916.48i 50.62 184.80 222.26 314.68 384.36 428.13 472.24 529.17 574.37 602.89 728.93 828.51 900.33 1055.75 1185.94 1195.53 1229.14 1266.37 1415.91 1443.62 1473.06 1655.67 1833.78 3124.01 3232.38 3852.58	623.02i 48.36 175.50 199.80 316.65 363.13 418.94 468.48 549.53 590.22 598.13 748.51 797.46 891.29 1043.91 1133.78 1153.82 1195.28 1231.24 1399.82 1430.31 1453.60 1633.93 1919.21 3072.44 3186.82 3815.86
TS1D	912.65i 61.34 162.54 199.94 308.67 371.88 431.91 472.21 547.86 559.02 597.30 729.78 813.25 896.46 1052.86 1179.76 1199.21 1227.97 1265.18 1411.99 1448.01 1473.89 1653.58 1833.47 3124.36 3232.51 3862.22	615.84i 59.56 143.89 171.76 308.45 348.72 421.80 472.61 548.48 583.45 595.58 754.47 781.06 892.65 1041.03 1125.26 1166.44 1191.35 1230.55 1387.44 1431.05 1452.13 1631.24 1935.06 3069.08 3180.54 3828.56
TS2A	884.99i 58.92 89.06 107.85 147.01 168.14 196.45 226.94 281.22 422.03 438.05 487.72 543.88 577.14 585.78 602.08 611.79 631.14 888.78 925.91 1053.02 1185.20 1202.45 1277.44 1301.19 1355.20 1364.32 1468.74 1551.58 1651.12 1660.87 1711.27 1781.12 3113.75 3215.30 3456.74 3559.87 3635.34 3860.30	835.64i 59.30 90.36 119.75 133.89 154.20 186.85 227.10 273.73 408.14 432.89 463.81 527.71 560.83 567.55 589.60 598.83 634.60 878.24 902.62 1041.52 1133.16 1178.97 1245.16 1276.22 1292.27 1334.23 1452.15 1491.40 1599.18 1624.46 1641.46 1693.90 3049.60 3156.33 3404.04 3506.36 3595.47 3820.74

TS2B	877.99i 36.30 83.69 108.46 140.68 182.36 198.17 225.72 294.29 412.47 458.09 490.19 539.84 573.70 587.07 601.42 616.28 630.69 890.49 931.17 1047.57 1187.19 1198.70 1279.15 1303.94 1355.36 1368.02 1468.75 1554.30 1649.99 1651.82 1714.94 1782.42 3109.41 3210.43 3469.14 3556.95 3635.43 3859.16	825.88i 55.44 84.81 111.38 133.11 165.54 188.43 225.79 285.98 402.92 449.63 468.74 522.01 560.65 568.80 589.87 603.05 629.90 880.42 909.02 1036.47 1134.95 1174.40 1246.71 1277.24 1293.67 1340.70 1451.90 1494.66 1588.49 1624.97 1645.74 1695.28 3044.44 3151.05 3415.14 3499.55 3595.64 3820.58
TS2C	808.36i 28.06 55.07 123.30 154.03 181.58 231.93 244.26 315.88 402.43 458.88 477.35 494.96 581.97 593.40 616.19 624.68 656.37 860.22 932.65 1056.35 1172.62 1225.16 1271.58 1312.45 1363.84 1394.58 1469.02 1599.32 1635.50 1659.08 1734.50 1806.95 3094.01 3201.88 3271.89 3563.12 3635.80 3859.69	686.57i 22.85 43.35 105.08 139.65 161.81 209.30 235.49 324.58 398.69 443.47 465.62 480.18 569.86 584.13 595.73 608.57 624.24 846.91 895.12 1045.75 1132.70 1187.63 1240.25 1282.08 1307.26 1366.40 1454.92 1537.99 1573.62 1644.72 1663.71 1722.85 3028.47 3146.75 3263.01 3527.86 3600.31 3823.21
TS3	1567.01i 245.90 3514.49 718.38 1391.04 3627.95 801.38 1489.30 821.76 1567.99 1039.68 1590.59 1200.82 2217.91 1232.98 2953.61 1253.36 2974.88	-1484.24i 1248.37 3479.08 251.79 1347.82 3591.93 714.12 1444.06 784.42 1518.64 804.85 1546.77 1022.45 2178.93 1168.48 2909.90 1200.14 2928.74
TS4A	318.79i 29.54 53.71 119.26 169.92 174.72 192.89 260.75 301.35 352.88 413.08 451.28 533.09 578.34 587.72 606.81 675.33 859.35 973.68 1033.12 1189.24 1194.83 1204.20 1235.19 1270.07 1290.72 1446.20 1470.94 1575.38 1595.46 1661.73 1704.32 1920.87 3053.49 3124.97 3450.23 3585.77 3631.75 3852.64	297.12i 35.71 48.26 116.10 164.77 169.22 176.81 249.71 278.64 339.72 401.58 440.45 520.77 558.90 570.15 577.77 611.49 851.69 877.02 1015.99 1125.16 1140.54 1153.45 1189.61 1224.24 1254.48 1411.77 1468.54 1516.13 1583.56 1611.48 1647.12 1910.40 2996.25 3077.14 3422.18 3562.06 3612.38 3813.22
TS4B	377.93i 29.93 44.78 122.34 165.18 174.00 185.96 205.74 292.38 364.64 407.62 436.77 539.34 561.13 588.37 603.40 660.56 900.56 959.81 1029.71 1152.33 1190.31 1210.69 1230.42 1267.77 1297.62 1414.11 1450.84 1507.12 1603.85 1665.49 1704.38 1757.17 3068.80 3148.40 3436.97	342.57i 21.18 48.14 116.30 143.54 159.33 172.21 192.28 286.26 359.76 413.13 428.57 517.11 544.63 551.35 584.94 610.68 874.78 897.15 1012.97 1125.75 1136.48 1173.69 1181.83 1213.83 1271.62 1379.46 1436.54 1470.23 1546.67 1616.00 1644.95 1749.20 3010.06 3099.42 3400.72

	3576.52 3629.61 3856.16	3548.70 3610.07 3816.39
TS4C	389.76i 30.44 51.39 125.79 162.11 174.02 185.48 235.76 294.96 365.10 411.56 439.94 543.76 557.21 581.80 599.93 663.45 901.11 958.46 1024.21 1138.77 1193.55 1228.30 1230.40 1266.38 1305.94 1408.25 1448.45 1499.24 1602.24 1666.01 1703.96 1745.90 3071.04 3152.02 3433.78 3575.17 3630.07 3853.36	366.41i 47.85 69.03 97.78 112.32 147.36 163.35 209.57 315.33 369.42 424.30 426.11 506.38 544.58 547.96 585.08 601.27 867.90 897.53 1000.86 1110.61 1138.33 1164.75 1206.31 1217.86 1289.29 1372.61 1405.37 1464.65 1542.31 1602.61 1637.29 1731.68 3012.67 3104.67 3430.61 3547.06 3603.65 3813.25

Table S5. The tunneling coefficients calculated by one-dimensional Wigner correction.

	TS1A		TS1B	
T/K	QCISD/cc-pV(T+d)Z	M08-SO/maug-cc-pVTZ	QCISD/cc-pV(T+d)Z	M08-SO/maug-cc-pVTZ
220	2.15	1.54	2.28	1.56
240	1.97	1.45	1.97	1.47
260	1.82	1.39	1.82	1.40
280	1.71	1.33	1.71	1.35
298	1.63	1.29	1.63	1.31
320	1.54	1.25	1.54	1.27

Table S6. The rate ratio ($\frac{V_1}{V_2}$) under the conditions of different [NH_3] and temperatures.

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	2.06E-04	2.06E-05	2.06E-06	2.06E-07	2.06E-08
230	2.05E-03	2.05E-04	2.05E-05	2.05E-06	2.05E-07
240	1.67E-02	1.67E-03	1.67E-04	1.67E-05	1.67E-06
250	1.13E-01	1.13E-02	1.13E-03	1.13E-04	1.13E-05
260	6.55E-01	6.55E-02	6.55E-03	6.55E-04	6.55E-05
270	3.29E+00	3.29E-01	3.29E-02	3.29E-03	3.29E-04
280	1.46E+01	1.46E+00	1.46E-01	1.46E-02	1.46E-03
290	5.79E+01	5.79E+00	5.79E-01	5.79E-02	5.79E-03
298	2.08E+02	2.08E+01	2.08E+00	2.08E-01	2.08E-02
300	6.82E+02	6.82E+01	6.82E+00	6.82E-01	6.82E-02
320	2.06E+03	2.06E+02	2.06E+01	2.06E+00	2.06E-01

Table S7. The rate ratio ($\frac{V_1^{'}}{V_3}$) under the conditions of different [H_2SO_4] and temperatures.

T/K	[H_2SO_4] = 10^6 molecules cm^{-3}	[H_2SO_4] = 10^7 molecules cm^{-3}	[H_2SO_4] = 10^8 molecules cm^{-3}
220	5.75E-21	5.75E-22	5.75E-23
230	3.72E-20	3.72E-21	3.72E-22
240	2.04E-19	2.04E-20	2.04E-21
250	9.80E-19	9.80E-20	9.80E-21
260	4.29E-18	4.29E-19	4.29E-20
270	1.92E-17	1.92E-18	1.92E-19
280	1.17E-16	1.17E-17	1.17E-18
290	1.18E-15	1.18E-16	1.18E-17
298	1.44E-14	1.44E-15	1.44E-16
300	1.68E-13	1.68E-14	1.68E-15
320	1.72E-12	1.72E-13	1.72E-14

Table S8. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-04	3.32E-03	3.32E-02	3.32E-01	3.32E+00
230	7.48E-05	7.48E-04	7.48E-03	7.48E-02	7.48E-01
240	1.92E-05	1.92E-04	1.92E-03	1.92E-02	1.92E-01
250	5.50E-06	5.50E-05	5.50E-04	5.50E-03	5.50E-02
260	1.74E-06	1.74E-05	1.74E-04	1.74E-03	1.74E-02
270	6.04E-07	6.04E-06	6.04E-05	6.04E-04	6.04E-03
280	2.27E-07	2.27E-06	2.27E-05	2.27E-04	2.27E-03
290	9.11E-08	9.11E-07	9.11E-06	9.11E-05	9.11E-04
298	4.61E-08	4.61E-07	4.61E-06	4.61E-05	4.61E-04
300	3.91E-08	3.91E-07	3.91E-06	3.91E-05	3.91E-04
320	8.49E-09	8.49E-08	8.49E-07	8.49E-06	8.49E-05

[a]The concentrations of [OH] = 10^4 molecules cm^{-3} and [H_2SO_4] = 10^6 molecules cm^{-3}.

Table S9. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-05	3.32E-04	3.32E-03	3.32E-02	3.32E-01
230	7.48E-06	7.48E-05	7.48E-04	7.48E-03	7.48E-02
240	1.92E-06	1.92E-05	1.92E-04	1.92E-03	1.92E-02
250	5.50E-07	5.50E-06	5.50E-05	5.50E-04	5.50E-03
260	1.74E-07	1.74E-06	1.74E-05	1.74E-04	1.74E-03
270	6.04E-08	6.04E-07	6.04E-06	6.04E-05	6.04E-04
280	2.27E-08	2.27E-07	2.27E-06	2.27E-05	2.27E-04
290	9.11E-09	9.11E-08	9.11E-07	9.11E-06	9.11E-05
298	4.61E-09	4.61E-08	4.61E-07	4.61E-06	4.61E-05
300	3.91E-09	3.91E-08	3.91E-07	3.91E-06	3.91E-05
320	8.49E-10	8.49E-09	8.49E-08	8.49E-07	8.49E-06

[a]The concentrations of [OH] = 10^5 molecules cm^{-3} and [H_2SO_4] = 10^6 molecules cm^{-3}.

Table S10. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-06	3.32E-05	3.32E-04	3.32E-03	3.32E-02
230	7.48E-07	7.48E-06	7.48E-05	7.48E-04	7.48E-03
240	1.92E-07	1.92E-06	1.92E-05	1.92E-04	1.92E-03
250	5.50E-08	5.50E-07	5.50E-06	5.50E-05	5.50E-04
260	1.74E-08	1.74E-07	1.74E-06	1.74E-05	1.74E-04
270	6.04E-09	6.04E-08	6.04E-07	6.04E-06	6.04E-05
280	2.27E-09	2.27E-08	2.27E-07	2.27E-06	2.27E-05
290	9.11E-10	9.11E-09	9.11E-08	9.11E-07	9.11E-06
298	4.61E-10	4.61E-09	4.61E-08	4.61E-07	4.61E-06
300	3.91E-10	3.91E-09	3.91E-08	3.91E-07	3.91E-06
320	8.49E-11	8.49E-10	8.49E-09	8.49E-08	8.49E-07

[a]The concentrations of [OH] = 10^6 molecules cm^{-3} and [H_2SO_4] = 10^6 molecules cm^{-3}.

Table S11. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-03	3.32E-02	3.32E-01	3.32E+00	3.32E+01
230	7.48E-04	7.48E-03	7.48E-02	7.48E-01	7.48E+00
240	1.92E-04	1.92E-03	1.92E-02	1.92E-01	1.92E+00
250	5.50E-05	5.50E-04	5.50E-03	5.50E-02	5.50E-01
260	1.74E-05	1.74E-04	1.74E-03	1.74E-02	1.74E-01
270	6.04E-06	6.04E-05	6.04E-04	6.04E-03	6.04E-02
280	2.27E-06	2.27E-05	2.27E-04	2.27E-03	2.27E-02
290	9.11E-07	9.11E-06	9.11E-05	9.11E-04	9.11E-03
298	4.61E-07	4.61E-06	4.61E-05	4.61E-04	4.61E-03
300	3.91E-07	3.91E-06	3.91E-05	3.91E-04	3.91E-03
320	8.49E-08	8.49E-07	8.49E-06	8.49E-05	8.49E-04

[a]The concentrations of [OH] = 10^4 molecules cm^{-3} and [H_2SO_4] = 10^7 molecules cm^{-3}.

Table S12. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-04	3.32E-03	3.32E-02	3.32E-01	3.32E+00
230	7.48E-05	7.48E-04	7.48E-03	7.48E-02	7.48E-01
240	1.92E-05	1.92E-04	1.92E-03	1.92E-02	1.92E-01
250	5.50E-06	5.50E-05	5.50E-04	5.50E-03	5.50E-02
260	1.74E-06	1.74E-05	1.74E-04	1.74E-03	1.74E-02
270	6.04E-07	6.04E-06	6.04E-05	6.04E-04	6.04E-03
280	2.27E-07	2.27E-06	2.27E-05	2.27E-04	2.27E-03
290	9.11E-08	9.11E-07	9.11E-06	9.11E-05	9.11E-04
298	4.61E-08	4.61E-07	4.61E-06	4.61E-05	4.61E-04
300	3.91E-08	3.91E-07	3.91E-06	3.91E-05	3.91E-04
320	8.49E-09	8.49E-08	8.49E-07	8.49E-06	8.49E-05

[a]The concentrations of [OH] = 10^5 molecules cm^{-3} and [H_2SO_4] = 10^7 molecules cm^{-3}.

Table S13. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-05	3.32E-04	3.32E-03	3.32E-02	3.32E-01
230	7.48E-06	7.48E-05	7.48E-04	7.48E-03	7.48E-02
240	1.92E-06	1.92E-05	1.92E-04	1.92E-03	1.92E-02
250	5.50E-07	5.50E-06	5.50E-05	5.50E-04	5.50E-03
260	1.74E-07	1.74E-06	1.74E-05	1.74E-04	1.74E-03
270	6.04E-08	6.04E-07	6.04E-06	6.04E-05	6.04E-04
280	2.27E-08	2.27E-07	2.27E-06	2.27E-05	2.27E-04
290	9.11E-09	9.11E-08	9.11E-07	9.11E-06	9.11E-05
298	4.61E-09	4.61E-08	4.61E-07	4.61E-06	4.61E-05
300	3.91E-09	3.91E-08	3.91E-07	3.91E-06	3.91E-05
320	8.49E-10	8.49E-09	8.49E-08	8.49E-07	8.49E-06

[a]The concentrations of [OH] = 10^6 molecules cm^{-3} and [H_2SO_4] = 10^7 molecules cm^{-3}.

Table S14. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-02	3.32E-01	3.32E+00	3.32E+01	3.32E+02
230	7.48E-03	7.48E-02	7.48E-01	7.48E+00	7.48E+01
240	1.92E-03	1.92E-02	1.92E-01	1.92E+00	1.92E+01
250	5.50E-04	5.50E-03	5.50E-02	5.50E-01	5.50E+00
260	1.74E-04	1.74E-03	1.74E-02	1.74E-01	1.74E+00
270	6.04E-05	6.04E-04	6.04E-03	6.04E-02	6.04E-01
280	2.27E-05	2.27E-04	2.27E-03	2.27E-02	2.27E-01
290	9.11E-06	9.11E-05	9.11E-04	9.11E-03	9.11E-02
298	4.61E-06	4.61E-05	4.61E-04	4.61E-03	4.61E-02
300	3.91E-06	3.91E-05	3.91E-04	3.91E-03	3.91E-02
320	8.49E-07	8.49E-06	8.49E-05	8.49E-04	8.49E-03

[a]The concentrations of [OH] = 10^4 molecules cm^{-3} and [H_2SO_4] = 10^8 molecules cm^{-3}.

Table S15. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-03	3.32E-02	3.32E-01	3.32E+00	3.32E+01
230	7.48E-04	7.48E-03	7.48E-02	7.48E-01	7.48E+00
240	1.92E-04	1.92E-03	1.92E-02	1.92E-01	1.92E+00
250	5.50E-05	5.50E-04	5.50E-03	5.50E-02	5.50E-01
260	1.74E-05	1.74E-04	1.74E-03	1.74E-02	1.74E-01
270	6.04E-06	6.04E-05	6.04E-04	6.04E-03	6.04E-02
280	2.27E-06	2.27E-05	2.27E-04	2.27E-03	2.27E-02
290	9.11E-07	9.11E-06	9.11E-05	9.11E-04	9.11E-03
298	4.61E-07	4.61E-06	4.61E-05	4.61E-04	4.61E-03
300	3.91E-07	3.91E-06	3.91E-05	3.91E-04	3.91E-03
320	8.49E-08	8.49E-07	8.49E-06	8.49E-05	8.49E-04

[a]The concentrations of [OH] = 10^5 molecules cm^{-3} and [H_2SO_4] = 10^8 molecules cm^{-3}.

Table S16. The rate ratio ($\frac{V_2}{V_{HCHO+OH}}$) under the conditions of different [NH_3] and temperatures.[a]

T/K	[NH_3] = 10^9 molecules cm^{-3}	[NH_3] = 10^{10} molecules cm^{-3}	[NH_3] = 10^{11} molecules cm^{-3}	[NH_3] = 10^{12} molecules cm^{-3}	[NH_3] = 10^{13} molecules cm^{-3}
220	3.32E-04	3.32E-03	3.32E-02	3.32E-01	3.32E+00
230	7.48E-05	7.48E-04	7.48E-03	7.48E-02	7.48E-01
240	1.92E-05	1.92E-04	1.92E-03	1.92E-02	1.92E-01
250	5.50E-06	5.50E-05	5.50E-04	5.50E-03	5.50E-02
260	1.74E-06	1.74E-05	1.74E-04	1.74E-03	1.74E-02
270	6.04E-07	6.04E-06	6.04E-05	6.04E-04	6.04E-03
280	2.27E-07	2.27E-06	2.27E-05	2.27E-04	2.27E-03
290	9.11E-08	9.11E-07	9.11E-06	9.11E-05	9.11E-04
298	4.61E-08	4.61E-07	4.61E-06	4.61E-05	4.61E-04
300	3.91E-08	3.91E-07	3.91E-06	3.91E-05	3.91E-04
320	8.49E-09	8.49E-08	8.49E-07	8.49E-06	8.49E-05

[a]The concentrations of [OH] = 10^6 molecules cm^{-3} and [H_2SO_4] = 10^8 molecules cm^{-3}.

Table S17. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E-01	6.02E+00	6.02E+01
230	1.24E-01	1.24E+00	1.24E+01
240	2.92E-02	2.92E-01	2.92E+00
250	7.75E-03	7.75E-02	7.75E-01
260	2.29E-03	2.29E-02	2.29E-01
270	7.41E-04	7.41E-03	7.41E-02
280	2.61E-04	2.61E-03	2.61E-02
290	9.92E-05	9.92E-04	9.92E-03
298	4.79E-05	4.79E-04	4.79E-03
300	4.02E-05	4.02E-04	4.02E-03
320	7.92E-06	7.92E-05	7.92E-04

[a]The concentrations of [OH] = 10^4 molecules cm^{-3} and [H_2SO_4] = 10^6 molecules cm^{-3}.

Table S18. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E-02	6.02E-01	6.02E+00
230	1.24E-02	1.24E-01	1.24E+00
240	2.92E-03	2.92E-02	2.92E-01
250	7.75E-04	7.75E-03	7.75E-02
260	2.29E-04	2.29E-03	2.29E-02
270	7.41E-05	7.41E-04	7.41E-03
280	2.61E-05	2.61E-04	2.61E-03
290	9.92E-06	9.92E-05	9.92E-04
298	4.79E-06	4.79E-05	4.79E-04
300	4.02E-06	4.02E-05	4.02E-04
320	7.92E-07	7.92E-06	7.92E-05

[a]The concentrations of [OH] = 10^5 molecules cm^{-3} and [H_2SO_4] = 10^6 molecules cm^{-3}.

Table S19. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E-03	6.02E-02	6.02E-01
230	1.24E-03	1.24E-02	1.24E-01
240	2.92E-04	2.92E-03	2.92E-02
250	7.75E-05	7.75E-04	7.75E-03
260	2.29E-05	2.29E-04	2.29E-03
270	7.41E-06	7.41E-05	7.41E-04
280	2.61E-06	2.61E-05	2.61E-04
290	9.92E-07	9.92E-06	9.92E-05
298	4.79E-07	4.79E-06	4.79E-05
300	4.02E-07	4.02E-06	4.02E-05
320	7.92E-08	7.92E-07	7.92E-06

[a]The concentrations of [OH] = 10^6 molecules cm^{-3} and [H_2SO_4] = 10^6 molecules cm^{-3}.

Table S20. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E+00	6.02E+01	6.02E+02
230	1.24E+00	1.24E+01	1.24E+02
240	2.92E-01	2.92E+00	2.92E+01
250	7.75E-02	7.75E-01	7.75E+00
260	2.29E-02	2.29E-01	2.29E+00
270	7.41E-03	7.41E-02	7.41E-01
280	2.61E-03	2.61E-02	2.61E-01
290	9.92E-04	9.92E-03	9.92E-02
298	4.79E-04	4.79E-03	4.79E-02
300	4.02E-04	4.02E-03	4.02E-02
320	7.92E-05	7.92E-04	7.92E-03

[a]The concentrations of [OH] = 10^4 molecules cm^{-3} and [H_2SO_4] = 10^7 molecules cm^{-3}.

Table S21. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E-01	6.02E+00	6.02E+01
230	1.24E-01	1.24E+00	1.24E+01
240	2.92E-02	2.92E-01	2.92E+00
250	7.75E-03	7.75E-02	7.75E-01
260	2.29E-03	2.29E-02	2.29E-01
270	7.41E-04	7.41E-03	7.41E-02
280	2.61E-04	2.61E-03	2.61E-02
290	9.92E-05	9.92E-04	9.92E-03
298	4.79E-05	4.79E-04	4.79E-03
300	4.02E-05	4.02E-04	4.02E-03
320	7.92E-06	7.92E-05	7.92E-04

[a]The concentrations of [OH] = 10^5 molecules cm^{-3} and [H_2SO_4] = 10^7 molecules cm^{-3}.

Table S22. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E-02	6.02E-01	6.02E+00
230	1.24E-02	1.24E-01	1.24E+00
240	2.92E-03	2.92E-02	2.92E-01
250	7.75E-04	7.75E-03	7.75E-02
260	2.29E-04	2.29E-03	2.29E-02
270	7.41E-05	7.41E-04	7.41E-03
280	2.61E-05	2.61E-04	2.61E-03
290	9.92E-06	9.92E-05	9.92E-04
298	4.79E-06	4.79E-05	4.79E-04
300	4.02E-06	4.02E-05	4.02E-04
320	7.92E-07	7.92E-06	7.92E-05

[a]The concentrations of [OH] = 10^6 molecules cm^{-3} and [H_2SO_4] = 10^7 molecules cm^{-3}.

Table S23. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E+01	6.02E+02	6.02E+03
230	1.24E+01	1.24E+02	1.24E+03
240	2.92E+00	2.92E+01	2.92E+02
250	7.75E-01	7.75E+00	7.75E+01
260	2.29E-01	2.29E+00	2.29E+01
270	7.41E-02	7.41E-01	7.41E+00
280	2.61E-02	2.61E-01	2.61E+00
290	9.92E-03	9.92E-02	9.92E-01
298	4.79E-03	4.79E-02	4.79E-01
300	4.02E-03	4.02E-02	4.02E-01
320	7.92E-04	7.92E-03	7.92E-02

[a]The concentrations of [OH] = 10^4 molecules cm^{-3} and [H_2SO_4] = 10^8 molecules cm^{-3}.

Table S24. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E+00	6.02E+01	6.02E+02
230	1.24E+00	1.24E+01	1.24E+02
240	2.92E-01	2.92E+00	2.92E+01
250	7.75E-02	7.75E-01	7.75E+00
260	2.29E-02	2.29E-01	2.29E+00
270	7.41E-03	7.41E-02	7.41E-01
280	2.61E-03	2.61E-02	2.61E-01
290	9.92E-04	9.92E-03	9.92E-02
298	4.79E-04	4.79E-03	4.79E-02
300	4.02E-04	4.02E-03	4.02E-02
320	7.92E-05	7.92E-04	7.92E-03

[a]The concentrations of at [OH] = 10^5 molecules cm^{-3} and [H_2SO_4] = 10^8 molecules cm^{-3}.

Table S25. The rate ratio ($\frac{V_3}{V_{NH_3+OH}}$) under the conditions of different [HCHO] and temperatures.[a]

T/K	[HCHO] = 10^{10} molecules cm^{-3}	[HCHO] = 10^{11} molecules cm^{-3}	[HCHO] = 10^{12} molecules cm^{-3}
220	6.02E-01	6.02E+00	6.02E+01
230	1.24E-01	1.24E+00	1.24E+01
240	2.92E-02	2.92E-01	2.92E+00
250	7.75E-03	7.75E-02	7.75E-01
260	2.29E-03	2.29E-02	2.29E-01
270	7.41E-04	7.41E-03	7.41E-02
280	2.61E-04	2.61E-03	2.61E-02
290	9.92E-05	9.92E-04	9.92E-03
298	4.79E-05	4.79E-04	4.79E-03
300	4.02E-05	4.02E-04	4.02E-03
320	7.92E-06	7.92E-05	7.92E-04

[a]The concentrations of at [OH] = 10^6 molecules cm^{-3} and [H_2SO_4] = 10^8 molecules cm^{-3}.

Table S26. Cartesian coordinates (Å) of optimized structures by M08-SO/maug-cc-pVTZ

Species	Cartesian coordinates			
H_2SO_4	S	0.00000000	0.00000000	0.15402900
	O	0.00000000	1.24989400	0.82244200
	O	1.22717200	0.03307300	-0.84073700
	H	1.47444600	-0.87208300	-1.08587600
	O	0.00000000	-1.24989400	0.82244200
	O	-1.22717200	-0.03307300	-0.84073700
	H	-1.47444600	0.87208300	-1.08587600
HCHO	C	0.00000000	0.00000000	-0.52602400
	H	0.00000000	-0.94356100	-1.11014300
	H	0.00000000	0.94356100	-1.11014300
	O	0.00000000	0.00000000	0.67205400
C1A	O	-2.50448600	-0.65105900	0.06772000
	O	0.04131200	1.20985400	-0.30289900
	O	0.11689300	-1.21635200	-0.33541100
	H	-0.85208800	-1.06127200	-0.17325600
	H	-2.28447000	1.33308300	-0.20330800
	H	-4.02427300	0.65463100	0.14108500
	O	2.14677200	-0.02344100	-0.80897600
	O	1.21992200	0.06770800	1.43980700
	S	0.91491200	0.10018100	-0.11506900
	C	-2.94352000	0.47203100	-0.00105200
	H	2.02004700	-0.45521000	1.60096100
C1B	O	-2.54526900	0.63651800	0.04469900
	O	-0.00029100	-1.15614300	0.22729700
	O	0.08930100	1.21793000	-0.22794900
	H	-0.87963700	1.03162100	-0.10841500
	H	-4.06952000	-0.66629000	0.03821100
	H	-2.30837900	-1.35654300	-0.12659300
	C	-2.98017900	-0.48833000	-0.01740600
	S	0.91084500	-0.10052600	-0.10622900
	O	1.81201000	0.19110300	1.15741900
	O	1.80208500	-0.20495400	-1.19758200
	H	1.30238500	0.05397300	1.96982900

TS1A	O	-2.27444800	-0.60458400	0.08430500
	O	-0.22734200	0.63824500	-0.96791600
	O	-0.01924900	-1.03623800	0.76273200
	H	-1.34893000	-0.97693900	0.56238700
	H	-2.62565900	1.15831700	-0.83191200
	H	-1.59658600	1.20624300	0.74101200
	C	-2.08272400	0.62632400	-0.04892400
	S	0.72010100	-0.08288400	-0.10775400
	O	1.86872900	-0.63755300	-0.73505400
	O	1.21313000	1.06242500	0.88892800
	H	2.05933200	0.80221400	1.28217300
TS1B	O	2.20995800	-0.67931400	-0.01625000
	O	0.24187000	0.89793200	0.70915600
	O	0.03286300	-0.78991500	-1.00095500
	H	1.32060900	-0.93317500	-0.61884100
	H	2.66080700	1.03858900	0.94098500
	H	1.89578500	1.19151100	-0.76899000
	C	2.16913800	0.57053800	0.08673200
	S	-0.71488200	0.09484200	-0.06868300
	O	-1.34234300	-0.87408700	1.02236800
	O	-1.79039200	0.79551300	-0.68562100
	H	-2.26955500	-1.03866000	0.79581100
TS1C	O	2.23985500	0.63784400	0.11171100
	O	0.23725000	-0.68264900	-0.89950400
	O	0.03038000	0.79181200	0.99704800
	H	1.31559900	0.86794800	0.69675400
	H	2.64075700	-0.97741600	-1.03357400
	H	1.79608700	-1.29186600	0.61275200
	C	2.13609300	-0.58513400	-0.14891400
	S	-0.72224300	-0.09537100	0.06294300
	O	-1.63709100	0.86864100	-0.79422200
	O	-1.61029100	-0.99508100	0.70135200
	H	-1.09393200	1.47353700	-1.32061600
TS1D	O	2.22856700	-0.62696800	-0.12542800
	O	0.23024500	0.80829200	0.80460400
	O	0.02521500	-0.72776200	-1.03804600
	H	1.31957100	-0.84357200	-0.73029900
	H	2.64396200	0.97663600	1.02797600
	H	1.86177100	1.31057700	-0.64634700
	C	2.15557400	0.59860000	0.12806700
	S	-0.71062600	-0.08306000	0.09134300
	O	-1.47599600	-0.95351500	0.90460600
	O	-1.76521500	0.85779800	-0.62215000
	H	-1.33126800	1.43095800	-1.26991100

P1A	O	2.42579200	-0.45560100	0.03633800
	O	0.44265300	0.53963800	0.79909300
	O	-0.16207500	-1.11758800	-0.87345300
	H	2.23575800	1.46315000	0.59705000
	H	1.41955800	1.04922200	-0.96139200
	C	1.69034700	0.69782500	0.04397000
	S	-0.72260200	-0.16999000	0.03147100
	O	-1.71141300	-0.51012100	0.98692800
	O	-1.28034300	0.99482600	-0.88559700
	H	1.97528400	-1.10766700	-0.52052700
	H	-1.92796900	1.51894000	-0.38896000
P1B	O	2.19731200	0.62526700	-0.07024400
	O	0.41094600	-0.79581900	-0.65987800
	O	-0.26826600	0.24999500	1.42476000
	H	1.80907300	1.06885000	0.69693700
	H	2.37142800	-1.23865600	-0.81151900
	H	1.73956300	-1.14558700	0.88265900
	C	1.76022200	-0.67492400	-0.10598600
	S	-0.73638300	-0.05864100	0.11434900
	O	-0.82026800	1.32722800	-0.63565300
	O	-1.93710600	-0.77386800	-0.12463400
	H	-1.36022100	1.24076700	-1.43656800
P1C	O	2.04692700	0.61901500	-0.02159500
	O	0.36667900	-0.91440400	-0.60427100
	O	-0.30432700	0.23366500	1.42683700
	H	1.81396900	0.93361700	0.86371200
	H	2.34251600	-1.21528900	-0.84282900
	H	1.77469000	-1.21982900	0.87630700
	C	1.70826200	-0.73008800	-0.10019600
	S	-0.74813100	-0.03572400	0.09280900
	O	-0.66351500	1.28571100	-0.75548200
	O	-2.00474200	-0.61701100	-0.17323700
	H	0.26116500	1.59780900	-0.75897400
P1D	O	-2.40083200	-0.49932500	0.04835700
	O	-0.45160200	0.42823400	-0.86938400
	O	0.22619700	-1.01399300	0.98524300
	H	-1.92295100	-1.06722500	0.67093600
	H	-2.26307600	1.33254200	-0.76511600
	H	-1.41699300	1.14833000	0.82053200
	C	-1.69446200	0.65929300	-0.12328300
	S	0.73125800	-0.15054700	-0.04224100
	O	1.72545900	-0.59188200	-0.94334900
	O	1.20613500	1.18610300	0.67521900
	H	1.62681400	0.96626000	1.52052500

NH_3	H	0.00000000	0.94703700	-0.25544100
	H	0.82015800	-0.47351900	-0.25544100
	N	0.00000000	0.00000000	0.10947500
	H	-0.82015800	-0.47351900	-0.25544100
M1A	H	-3.43567900	-0.71460100	-0.15407900
	H	-1.35697900	-0.19150100	-0.76212300
	O	-0.38179100	-0.36917900	-1.07143500
	S	0.60303500	-0.11211300	0.08738200
	O	1.05419700	1.39245200	-0.15946700
	O	-0.11860900	-0.09027100	1.31930600
	O	1.74876900	-0.93501600	-0.09309000
	H	-2.46495200	0.07948400	0.92175300
	N	-2.77053500	0.04595100	-0.05026800
	H	-3.24421800	0.91701000	-0.27012200
	H	1.82649100	1.39787500	-0.74418100
C2A	C	1.91695900	-1.53238300	0.20285600
	H	1.86391800	-2.48362200	-0.35174400
	O	2.52014700	-0.58185300	-0.24748000
	H	2.13170100	1.17377100	-0.00141500
	H	1.41792700	-1.49116900	1.18451100
	H	0.74195900	1.79683400	-0.68913400
	O	-0.66080400	0.84267000	-1.12911700
	S	-0.92719100	-0.07772100	-0.02101700
	O	-2.50182800	-0.01490200	0.24298700
	O	-0.62505300	-1.45861400	-0.33317800
	O	-0.35422800	0.40345300	1.23077000
	H	1.91617600	2.87810700	-0.01160500
	N	1.46564400	1.96990300	0.05199900
	H	0.91958100	1.82947100	0.91863700
	H	-2.94334200	-0.58091000	-0.40597200
C2B	C	1.91360300	-1.53893300	0.18755400
	H	1.84727800	-2.48288800	-0.37798800
	O	2.51904700	-0.58752400	-0.25727000
	H	2.15381300	1.17817900	0.01156000
	H	1.42451900	-1.50530400	1.17456600
	H	0.90557600	1.76452400	0.92933200
	O	-0.35757500	0.39244200	1.22985400
	S	-0.93063800	-0.07016000	-0.03754700
	O	-2.51798300	0.02306100	0.11995100
	O	-0.64346300	0.85543300	-1.12605300

	O	-0.64092900	-1.46214900	-0.31287400
	H	0.77691300	1.82548100	-0.67804000
	N	1.47791800	1.96301300	0.08748700
	H	1.91781500	2.87852500	0.08741800
	H	-2.83553400	-0.81354900	0.48729300
C2C	C	1.93310400	-1.37832900	0.06717400
	H	1.75271000	-2.20733800	-0.63901600
	O	2.87616900	-0.63108600	-0.06449100
	H	2.36409200	1.16275100	0.23149300
	H	1.22138300	-1.27784400	0.90613500
	H	0.78336400	1.58836700	0.69740500
	O	-0.62987200	0.79019400	1.11876900
	S	-1.11878700	0.05534800	-0.05844600
	O	-2.44175400	0.40755500	-0.47941300
	O	-0.08633600	0.01478500	-1.09352400
	O	-1.19936200	-1.48376000	0.41764700
	H	1.18808700	1.52725400	-0.87086100
	N	1.58413100	1.81288100	0.03957900
	H	1.86639500	2.78896900	0.06493200
	H	-2.11372600	-1.66943200	0.67303500
TS2A	C	1.43933600	-1.53185500	0.26363500
	H	1.39741600	-2.58786100	-0.01132300
	O	2.19357400	-0.77762300	-0.40272600
	H	2.12474200	0.39323200	-0.11544300
	H	1.14872900	-1.26088600	1.28460600
	H	1.16641700	1.88027300	-0.60849400
	O	-0.68444500	0.98669100	-1.09327200
	S	-0.90019300	0.06132300	-0.00243500
	O	-2.47224100	-0.11798000	0.14416200
	O	-0.39598100	-1.30316100	-0.31574100
	O	-0.44873800	0.51005100	1.29346300
	H	2.67764600	2.27000400	0.01768800
	N	1.88053700	1.64491300	0.08932500
	H	1.42142800	1.74205400	0.99617300
	H	-2.87041800	-0.12506200	-0.73842400

TS2B	C	-1.39849900	1.55218600	0.26533200
	H	-1.34514800	2.60742500	-0.01135600
	O	-2.16176600	0.80540500	-0.39950700
	H	-2.12259800	-0.36828600	-0.09505200
	H	-1.12093200	1.28250700	1.29078700
	H	-1.27612400	-1.90832400	-0.61448600
	O	0.60616000	-0.99934700	-1.10604900
	S	0.89578000	-0.08432500	-0.03726000
	O	2.47915600	0.03247100	-0.02646100
	O	0.42995600	1.30686200	-0.30112800
	O	0.47579400	-0.51667400	1.28424500
	H	-2.73085400	-2.21158500	0.17280300
	N	-1.91017400	-1.61491500	0.13470000
	H	-1.36425000	-1.68379700	0.99648100
	H	2.75524000	0.59281200	0.71328800
TS2C	C	1.33745700	-1.47227600	0.22981100
	H	1.07565300	-2.50941200	0.00941600
	O	2.35564500	-0.98178600	-0.31088100
	H	2.48211500	0.22481400	-0.07013900
	H	0.94234100	-1.04058700	1.15898900
	H	1.42297200	1.62971900	0.32697800
	O	-2.08043700	0.73049800	-0.96475900
	S	-1.08429900	0.16167900	-0.11331200
	O	-1.83976000	-0.74458700	0.97809100
	O	-0.22222400	-0.84651400	-0.76970400
	O	-0.29250100	1.11074700	0.66046600
	H	2.67225900	1.96989400	-0.73462200
	N	2.42296900	1.46743800	0.11378400
	H	3.00004100	1.80430400	0.87941600
	H	-2.59791500	-0.25085400	1.32187900
C2PA	C	-0.98304400	1.58872800	0.35873600
	H	-0.95506000	2.67890600	0.39856700
	O	-1.94944900	1.17082100	-0.49332500
	H	-2.16504000	0.22170000	-0.31870600
	H	-1.04866800	1.14554000	1.36102400
	H	-1.67888200	-1.97491600	-0.67633500
	O	0.56188600	-0.95043500	-1.17075000
	S	0.87245100	-0.20572200	0.00705100
	O	2.42606800	0.04329000	0.03159700
	O	0.38247600	1.26637400	-0.13359400
	O	0.50099000	-0.71322500	1.28579900
	H	-3.11783700	-2.04558700	0.12978200
	N	-2.21975100	-1.57431300	0.08707600
	H	-1.70854800	-1.77182600	0.94427100

	H	2.77557100	-0.00904600	-0.87118800
C2PB	C	-0.95322400	1.59576900	0.36423700
	H	-0.91509300	2.68573500	0.40662400
	O	-1.93332400	1.18875600	-0.47616600
	H	-2.16108600	0.24373000	-0.29395400
	H	-1.01264500	1.15002600	1.36629400
	H	-1.76431500	-1.96309500	-0.65918900
	O	0.48695300	-0.96933400	-1.17871300
	S	0.86767300	-0.22290000	-0.03374800
	O	2.42211000	-0.01220300	-0.14121100
	O	0.40474000	1.26383300	-0.14395600
	O	0.54506100	-0.71061200	1.27422200
	H	-3.14211500	-1.99316700	0.25017700
	N	-2.23893700	-1.54372300	0.13733500
	H	-1.67102900	-1.74670400	0.95697500
	H	2.77110900	0.33780800	0.69286200
C2PC	C	-0.84751600	1.48102000	0.29213600
	H	-0.62118300	2.54333000	0.40199800
	O	-2.03174700	1.31528600	-0.33403500
	H	-2.37549700	0.39702300	-0.19683000
	H	-0.76786700	0.94948300	1.25045500
	H	-1.90647400	-1.77149500	0.25552000
	O	0.18870600	-1.24490400	0.47153300
	S	1.05745700	-0.26615700	-0.11482500
	O	1.93787500	-0.63815200	-1.15935000
	O	0.27238500	0.98257400	-0.56212600
	O	1.88203700	0.38484000	1.08274900
	H	2.22063200	-0.31634500	1.65972500
	H	-3.21155500	-1.77555400	-0.74937200
	N	-2.81966300	-1.35249100	0.08676000
	H	-3.42867700	-1.58376100	0.86540600

TS3	H	1.64173400	-0.13187000	-0.83859500
	O	-1.10539900	-0.43400600	-0.00014000
	H	0.21403500	-1.00772100	0.00001600
	C	-0.27131800	0.61280900	-0.00002600
	H	-0.25824000	1.25456000	-0.90300600
	H	-0.25846000	1.25454000	0.90297200
	N	1.07007200	-0.20606000	0.00012800
	H	1.64153100	-0.13188800	0.83899100
H_2CNH_2OH	H	-1.37579600	-0.70093300	0.85131400
	O	1.21468500	-0.24245700	0.05014400
	H	1.09485600	-0.95232100	-0.59259200
	C	0.04410100	0.54052400	0.01667000
	H	0.09188500	1.17227100	0.91499800
	H	0.02998600	1.19792900	-0.86639800
	N	-1.12734700	-0.31172800	-0.05176400
	H	-1.93158200	0.16166100	-0.44614500
C4A	C	-2.21336500	-1.00234400	0.51435700
	O	-1.70755700	-1.45956100	-0.49107100
	H	-3.27893800	-1.16681100	0.73377000
	H	-1.61870700	-0.46798800	1.27260000
	H	-0.15425500	-1.16919100	-0.84304400
	O	0.18351800	1.16939800	0.05829200
	H	-1.92052900	1.66997800	-0.15270700
	O	0.81795200	-0.93651600	-0.98663800
	S	1.24344600	0.22224600	-0.05599600
	O	1.29741300	-0.48116000	1.37037300
	O	2.55930300	0.60995800	-0.41795200
	H	-3.30703300	1.37786100	-0.98843300
	H	2.13313300	-0.96393500	1.46163900
	N	-2.89970200	1.40447600	-0.05820300
	H	-3.37573100	2.12992600	0.46936300
C4B	C	-2.46090800	-0.81596600	0.43340000
	O	-1.87253300	-1.45593500	-0.41572400
	H	-3.53836700	-0.61302900	0.33738600
	H	-1.95917500	-0.47501200	1.35200000
	H	-0.25561800	-1.52651300	-0.38177300
	O	0.78115200	0.93628900	-1.12391300
	H	-1.57517700	1.63593800	-0.94117500
	O	0.74444500	-1.38688000	-0.34066000
	S	1.04095400	0.09792600	-0.00573500
	O	0.46232100	0.42368600	1.26441300
	O	2.60393100	0.02215700	0.14948200
	H	-2.82480900	2.42146800	-0.21244300
	H	2.83346500	-0.34117200	1.01838500

	N	-2.12121500	1.70043200	-0.08417500
	H	-1.47615000	2.00974600	0.63942400
C4C	C	-2.46056700	-0.79967300	0.41708200
	O	-1.87492500	-1.45261800	-0.42453700
	H	-3.53555800	-0.58768100	0.31639800
	H	-1.95877400	-0.45587300	1.33501300
	H	-0.27001300	-1.54024900	-0.31033400
	O	0.77482800	0.82622900	-1.16625800
	H	-1.51993100	1.61041400	-0.95414500
	O	0.72735100	-1.41427900	-0.19345800
	S	1.03461700	0.08819400	0.03103500
	O	0.46844700	0.53290100	1.26049100
	O	2.58992600	0.00575700	0.24870400
	H	-2.80299600	2.41881100	-0.31133300
	H	3.04067700	-0.01690400	-0.60929900
	N	-2.10489600	1.70501100	-0.12589300
	H	-1.49461400	2.03943400	0.61635900
TS4A	C	-2.24061900	-0.70470600	0.53341000
	O	-1.78054400	-1.29647700	-0.45825700
	H	-3.28404000	-0.87682800	0.82582400
	H	-1.57238200	-0.31702600	1.31684300
	H	-0.42984100	-1.18047800	-0.64356800
	O	0.26688900	1.22867000	-0.11769600
	H	-1.68255600	1.54700500	-0.26914200
	O	0.64502200	-1.07887000	-0.77000600
	S	1.21804600	0.15532000	-0.09043300
	O	1.26621700	-0.26372900	1.45087100
	O	2.55430700	0.36557200	-0.52747700
	H	-3.12614200	1.14040900	-0.98842300
	H	2.06026100	-0.79582800	1.60922000
	N	-2.64255700	1.23788600	-0.10010000
	H	-3.12754400	1.91934200	0.47691900

TS4B	C	-2.28748100	-0.64272500	0.50680800
	O	-1.84224800	-1.32149300	-0.43715600
	H	-3.37099900	-0.60160400	0.66801700
	H	-1.64486000	-0.38305400	1.35899200
	H	-0.52103900	-1.35445500	-0.44867300
	O	0.63490300	1.09041200	-0.93067200
	H	-1.29387300	1.49969200	-0.46145100
	O	0.59075100	-1.28812100	-0.40221100
	S	1.04760200	0.09869200	0.01855300
	O	0.74053200	0.33668500	1.40162000
	O	2.61368000	-0.01979100	-0.13059600
	H	-2.89365500	1.48355100	-0.89335500
	N	-2.24999300	1.37412500	-0.11452400
	H	-2.44394000	2.09010700	0.58051300
	H	2.98062000	-0.45737400	0.65204800
TS4C	C	-2.35124300	-0.56411300	0.45315000
	O	-1.85124800	-1.31855100	-0.40265900
	H	-3.43648200	-0.41561200	0.46329700
	H	-1.80512500	-0.33910400	1.37928700
	H	-0.55764100	-1.42102900	-0.22702600
	O	0.73376400	0.71926000	-1.23266400
	H	-1.38849700	1.30989500	-0.96877300
	O	0.54115200	-1.36778000	-0.00555500
	S	1.00957700	0.07774700	0.02534200
	O	0.57510200	0.74609700	1.21434500
	O	2.57121800	-0.09167200	0.17133300
	H	-2.81424800	1.98730500	-0.43638000
	N	-2.01127000	1.42651700	-0.16685100
	H	-1.47312400	1.91161700	0.54937600
	H	2.94832800	-0.37678700	-0.67460700
C4PA	C	-2.32109800	-0.11848700	0.56450800
	O	-2.32946700	-1.18008500	-0.29694600
	H	-3.30622000	-0.00979400	1.02873400
	H	-1.53314100	-0.17474800	1.32774200
	H	-1.39242000	-1.43772200	-0.44871400
	O	0.51441900	1.18932100	-0.57778600
	H	-0.96171400	1.17958400	-0.46179800
	O	0.35381300	-1.20323400	-0.29306500
	S	1.20470600	-0.03327600	-0.12746600
	O	1.27422200	0.21355100	1.46860800
	O	2.55432100	-0.17061300	-0.57545600
	H	-2.58574200	1.11641800	-1.09200300
	H	2.04824400	-0.25511400	1.81103200

	N	-2.04013400	1.14831000	-0.22932600
	H	-2.27524200	1.99502900	0.28984800
C4PB	C	2.18677400	0.14929800	0.52567600
	O	2.11790400	1.18881200	-0.35895600
	H	3.20613100	0.04240800	0.90894700
	H	1.45701700	0.21685600	1.33998500
	H	1.19543000	1.52424700	-0.35342200
	O	-0.55489700	-0.51057800	-1.28612500
	H	1.00736600	-0.98338600	-0.81774900
	O	-0.59262700	1.37249200	0.25946800
	S	-1.00223400	-0.00478200	0.00993000
	O	-0.64928000	-0.90734200	1.09424600
	O	-2.58719400	0.01572300	-0.11820400
	H	2.63250800	-1.49040800	-0.76186500
	H	-2.94791300	0.59684800	0.56673300
	N	1.84948200	-1.16065200	-0.19852500
	H	1.54693500	-1.87413600	0.47067700
C4PC	C	-2.19012400	0.12422100	-0.52536000
	O	-2.11509500	1.20500800	0.30794000
	H	-3.21155600	0.00120500	-0.89802500
	H	-1.46572300	0.15169200	-1.34693200
	H	-1.19000500	1.53375800	0.28650800
	O	0.55100300	-0.44528800	1.29828300
	H	-1.00076300	-0.94105600	0.86268200
	O	0.59566800	1.36531700	-0.30222400
	S	1.00330700	-0.00792900	-0.02950400
	O	0.65097800	-0.96190800	-1.05921900
	O	2.59228700	-0.00709900	-0.00186700
	H	-2.62940900	-1.44566100	0.84639000
	H	2.89708200	0.77176800	0.48561600
	N	-1.85033200	-1.14871200	0.25985400
	H	-1.55820500	-1.89744700	-0.37429000

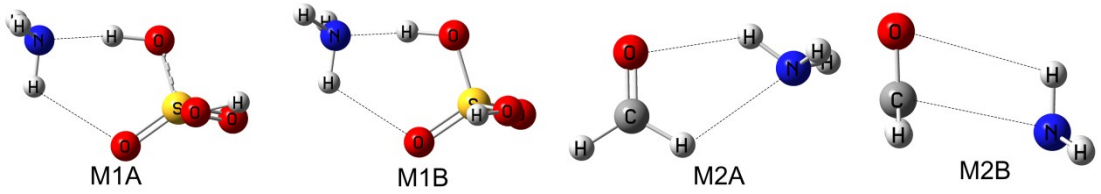

Figure S1. The optimized geometries of the $H_2SO_4\cdots NH_3$ (M1A and M1B) and $HCHO\cdots NH_3$ (M2A and M2B) complexes at the M08-SO/maug-cc-pVTZ level.