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

ESI for the

Kinetic Instability of the Sulfurous Acid in the Presence of Ammonia and Formic Acid

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Table S1: Optimized geometries in Cartesian coordinates and normal mode frequencies of all species calculate at MP2/aug-cc-pVTZ level of theory

compound	cartesian coordinate(Å)				frequency(cm^{-1})		
WM	O	0.00000000	0.00000000	0.11818900	1627.7613	3824.7049	3950.6088
	H	0.00000000	0.75802500	-0.47275400			
	H	0.00000000	-0.75802500	-0.47275400			
FA	C	-0.13228100	0.40084000	0.00030400	625.8763	674.7693	1059.0209
	O	-1.13878300	-0.26223900	-0.00006900	1130.6399	1301.9831	1409.2658
	O	1.12070900	-0.09253500	-0.00001600	1793.2981	3123.9869	3741.6317
	H	-0.09681300	1.49274100	-0.00082200			
	H	1.03508700	-1.05959000	-0.00032000			
AM	N	0.00000000	0.00000000	0.11400700	1037.5716	1668.9373	1668.9373
	H	0.00000000	0.93809600	-0.26601700	3502.6045	3649.5724	3649.5724
	H	-0.81241500	-0.46904800	-0.26601700			
	H	0.81241500	-0.46904800	-0.26601700			
SO_2	S	0.00000000	0.00000000	0.37256200	493.2718	1099.0853	1305.3854
	O	0.00000000	-1.25968300	-0.37256200			
	O	0.00000000	1.25968300	-0.37256200			
$H_2SO_3(_{cis-trans})$	S	0.04054400	0.14574300	-0.42300500	237.6446	293.2820	396.8364
	O	0.38509500	1.34488900	0.32736000	460.7578	490.6683	735.9567
	O	0.98882000	-1.07344100	0.11868900	773.0322	1095.7975	1110.9230
	H	1.12703400	-0.92866300	1.07281600	1282.1183	3690.1026	3751.9048
	O	-1.38217100	-0.30970000	0.28784800			
	H	-1.70968200	-1.09720200	-0.17589900			
RC_{AM}	O	-0.43622400	1.22290400	0.69705700	50.0590	107.0022	117.3363
	O	0.18597000	-0.16582000	-1.28977900	199.0971	266.9910	316.5524
	H	1.08669300	-0.19682100	-0.78759800	403.1097	419.0865	458.2586
	O	-0.83465500	-1.23587000	0.59967400	552.7854	703.4687	895.9831
	H	-1.30137100	-1.08469000	1.43639300	1073.6178	1112.3537	1140.3763
	N	2.33452600	-0.08538800	0.24145700	1205.3523	1447.2222	1659.0768
	H	1.91541200	0.57775500	0.88762200	1672.7956	2597.8268	3476.7701
	H	3.22707600	0.28480300	-0.05998500	3616.3462	3647.7412	3762.7347
	H	2.50679800	-0.94395500	0.75006500			
	S	-0.94356300	0.21193200	-0.24827000			
TS_{AM}	O	0.71994200	-0.12703000	1.33925900	-211.6355	70.3125	194.0770
	O	0.36197200	-1.06399000	-0.91547900	266.6909	289.5971	372.4990
	H	-1.42132100	-1.07772600	-0.23917300	407.4223	463.0392	505.4948
	O	-0.34863500	1.39364500	-0.51439800	558.1405	636.7119	875.5041
	H	-0.12910100	2.10678800	0.10414700	1095.3482	1202.5648	1236.3947
	N	-2.00138600	-0.35789500	0.21997100	1496.3101	1557.6765	1637.7790
	H	-1.94316900	-0.49961200	1.22350400	1724.2708	1945.3714	3280.9763
	H	-2.96080100	-0.37349700	-0.10212600	3546.3073	3639.4783	3768.2377
	H	-1.41810800	0.57039200	-0.05628300			
	S	1.00099800	0.00987100	-0.10905800			

compound	cartesian coordinate(Å)				frequency(cm^{-1})		
PC_{AM}	O	1.68034300	0.28503000	1.00644200	21.8581	85.8251	93.4327
	O	0.33102400	-1.28240300	-0.39967900	118.5825	133.5760	180.2255
	H	-1.84686800	-1.21221000	0.22504400	228.9191	247.5856	267.2352
	O	-0.85527900	1.57713800	-0.42233900	335.5906	504.6608	535.0421
	H	-0.82206000	2.28633700	0.22713600	858.0347	1116.5682	1120.6559
	N	-2.57538200	-0.51371200	0.33554900	1303.2595	1653.7697	1671.7451
	H	-2.95555000	-0.62139300	1.26777700	1678.9387	3378.2487	3486.3360
	H	-3.31570600	-0.74578600	-0.31510300	3621.5648	3644.1521	3876.5851
	H	-1.56134100	0.96567400	-0.10636900			
	S	1.20503200	-0.10717200	-0.32017000			
RC_{FA}	S	-1.36682000	-0.05835500	-0.41748200	49.4258	72.1672	116.9188
	O	-2.72344700	0.10124000	0.08485200	163.9259	201.5166	220.7574
	O	-0.48958300	1.25606300	0.19625100	298.4966	407.8889	435.9692
	H	-0.88969600	1.46055400	1.06159600	497.2693	646.8333	680.7879
	O	-0.72892100	-1.20846200	0.51407700	774.5210	831.8415	923.0801
	H	0.23517000	-1.27700700	0.28203000	1082.8242	1104.7576	1234.0329
	C	2.63298700	-0.16455600	-0.08500300	1254.7570	1311.8392	1392.6972
	O	1.90113400	-1.14007100	-0.08802600	1438.1958	1749.0529	3140.8476
	O	2.25772200	1.09557100	0.03295200	3294.3988	3401.3178	3686.8955
	H	3.71646300	-0.24443000	-0.18625400			
	H	1.27401400	1.14716000	0.11150100			
TS_{FA}	S	-1.39128000	-0.19498200	-0.40062800	-982.7045	51.8597	73.4615
	O	-2.60355600	0.06459800	0.36581200	155.9665	253.8797	290.0760
	O	-0.41072500	1.38377900	-0.07206400	322.9541	429.0778	473.0979
	H	-0.82771400	1.73272400	0.73445300	518.8867	629.2857	677.2540
	O	-0.47880800	-1.14458000	0.37218700	742.5058	919.6018	1079.0721
	H	0.73155900	-1.13502100	0.08288100	1105.7027	1267.4470	1284.5745
	C	2.48917800	-0.06492500	-0.00235300	1352.3748	1365.4610	1422.6975
	O	1.88236100	-1.16754100	-0.06789600	1474.4698	1509.9192	1643.2586
	O	1.98484200	1.09277800	0.09977200	1759.3168	3171.9352	3720.2478
	H	3.57645100	-0.10571300	-0.04042600			
	H	0.85220000	1.18499500	0.06475900			
PC_{FA}	S	-1.78010800	-0.29528400	-0.22616900	25.1721	42.9948	86.4406
	O	-1.93232200	-0.35793700	1.22440800	102.7528	143.5735	162.9746
	O	-0.51844100	1.97481600	-0.33548000	172.7776	196.6905	222.9852
	H	-0.66830400	2.63707900	0.34669700	271.3032	407.2389	507.9122
	O	-0.60695400	-0.96626700	-0.80410500	662.7613	669.1936	849.7047
	H	1.10080100	-1.17154000	-0.23521200	1081.0706	1123.3847	1212.5942
	C	2.60513500	-0.11853000	0.22412700	1301.8678	1370.6668	1428.6805
	O	2.04361600	-1.29877700	0.01108900	1651.4450	1765.8593	3128.0527
	O	2.05927700	0.96401800	0.13702400	3501.0380	3611.3456	3879.3711
	H	3.65602100	-0.23548400	0.49734400			
	H	0.40098800	1.67883500	-0.19838200			

compound	cartesian coordinate(Å)				frequency(cm^{-1})		
RC_{WM}	S	0.87251500	0.07193300	-0.37725900	62.3764	165.3698	183.3682
	O	0.11594100	1.33749400	-0.31260100	234.0332	265.8636	324.7838
	O	1.05238000	-0.39667300	1.21352300	409.3767	424.3108	536.1023
	H	1.50578800	0.33347600	1.66394300	617.7362	724.7685	858.0635
	O	-0.12117500	-1.11452900	-0.74738000	876.9386	1112.7089	1189.9473
	H	-1.01130700	-0.90441600	-0.34082700	1347.8156	1634.8266	3174.3099
	H	-2.57452400	-0.09693100	1.17800900	3670.2138	3758.9520	3887.6727
	O	-2.31091500	0.01091500	0.25863800			
	H	-1.77002900	0.81927400	0.23758200			
TS_{WM}	S	-0.92213400	-0.10490000	-0.30566400	-786.5688	64.9953	276.5646
	O	-1.28392400	0.10832600	1.10060900	361.9459	454.2690	482.9446
	O	0.36245100	1.29104400	-0.52712900	512.4672	534.6199	619.7150
	H	-0.01089900	2.02431800	-0.01401300	658.6590	682.9187	946.8784
	O	0.08621600	-1.22667300	-0.48139300	1062.5621	1230.2755	1402.5021
	H	1.26295800	-0.86490500	0.05290300	1447.9634	1669.6300	1718.1809
	H	1.45825300	0.67917800	0.04911800	2203.4031	3763.1397	3813.7178
	O	2.07325300	-0.17010600	0.34458900			
	H	2.13986600	-0.18091100	1.30920300			
PC_{WM}	S	-1.17402700	-0.10401200	-0.33007800	22.3347	79.0412	128.6276
	O	-1.67048000	0.25214100	0.99746800	141.3135	170.0553	185.7566
	O	0.89388200	1.62177500	-0.37019400	208.4819	234.6266	271.0908
	H	0.89851800	2.34254500	0.26683200	421.5895	453.3708	503.6001
	O	-0.24464700	-1.23616500	-0.41974500	700.7430	1118.4307	1303.9794
	H	1.70428800	-1.16272900	0.17264700	1630.6824	1655.4142	3610.2006
	H	1.60214000	1.01818700	-0.07954400	3751.4088	3888.0210	3909.8747
	O	2.48066100	-0.59379900	0.27207500			
	H	2.90415400	-0.88541900	1.08447800			
TS_{Uncat}	S	-0.35210300	0.03742200	-0.41862000	-1589.0005	228.7607	430.9480
	O	-1.39039100	-0.54637100	0.41259400	489.6202	501.2786	662.7370
	O	0.33213900	1.26278500	0.24519300	817.0385	1016.8424	1239.4487
	H	1.24898400	0.49930000	0.43381600	1292.3417	1932.6476	3747.8109
	O	1.36259900	-0.73877200	0.19491900			
	H	1.94989100	-0.91919100	-0.55753600			
PC_{Uncat}	S	0.64468900	0.00000700	-0.37725000	24.2711	89.7166	105.4362
	O	0.74995200	-1.25490900	0.36820800	129.2983	218.8321	244.6129
	O	-2.18438400	-0.00004500	-0.09376300	500.7708	1111.8266	1308.9823
	H	-2.41907400	-0.76110700	0.44738300	1628.1927	3802.7181	3926.2607
	O	0.74978800	1.25495500	0.36818800			
	H	-2.41879900	0.76098300	0.44755200			
$H_2SO_3(_{cis-cis})$	S	-0.000003	0.111069	-0.438378	126.3792	339.2728	408.2412
	O	0.000123	1.374565	0.309988	442.2980	484.6238	769.1334
	O	1.255834	-0.751948	0.155137	779.4566	1082.2596	1108.1792
	O	-1.255969	-0.751732	0.155140	1254.7515	3696.9858	3698.6878
	H	-1.471241	-0.372119	1.026062			
	H	1.471396	-0.372074	1.025871			
$H_2SO_3(_{trans-trans})$	S	-0.000088	0.140499	0.401265	176.774	249.1102	366.7285
	O	1.250242	-0.678579	-0.299028	431.2504	501.0832	732.1629
	O	-1.249173	-0.680583	-0.298806	757.2215	1071.3886	1117.8083
	H	-1.550805	-1.353581	0.330885	1301.6225	3764.2936	3767.7290
	H	1.554461	-1.349579	0.331544			
	O	-0.001350	1.416058	-0.287499			

Table S2: Bimolecular rate constant k_b in (cm^3 $molecule^{-1}$ sec^{-1}) of AM, FA, and WM catalyzed channel within the temperature of 213-1000 K.

Å Temp (K)	K_{eq}^{AM}	k_{uni}^{AM}	k_b^{AM}	K_{eq}^{FA}	k_{uni}^{FA}	k_b^{FA}	K_{eq}^{WM}	k_{uni}^{WM}	k_b^{WM}
213	7.73×10^{-11}	3.01×10^{3}	2.32×10^{-7}	7.16×10^{-16}	4.47×10^{5}	3.20×10^{-10}	6.89×10^{-17}	3.81×10^{-2}	2.62×10^{-18}
216	4.65×10^{-11}	3.94×10^{3}	1.83×10^{-7}	4.88×10^{-16}	5.28×10^{5}	2.58×10^{-10}	4.99×10^{-17}	5.67×10^{-2}	2.83×10^{-18}
219	2.83×10^{-11}	5.11×10^{3}	1.45×10^{-7}	3.36×10^{-16}	6.21×10^{5}	2.09×10^{-10}	3.65×10^{-17}	8.36×10^{-2}	3.05×10^{-18}
224	1.28×10^{-11}	7.77×10^{3}	9.94×10^{-8}	1.85×10^{-16}	8.11×10^{5}	1.50×10^{-10}	2.20×10^{-17}	1.57×10^{-1}	3.45×10^{-18}
235	2.51×10^{-12}	1.84×10^{4}	4.62×10^{-8}	5.44×10^{-17}	1.42×10^{6}	7.74×10^{-11}	7.86×10^{-18}	5.73×10^{-1}	4.51×10^{-18}
250	3.45×10^{-13}	5.25×10^{4}	1.81×10^{-8}	1.23×10^{-17}	2.90×10^{6}	3.56×10^{-11}	2.24×10^{-18}	2.84	6.35×10^{-18}
259	1.18×10^{-13}	9.29×10^{4}	1.09×10^{-8}	5.47×10^{-18}	4.33×10^{6}	2.37×10^{-11}	1.13×10^{-18}	6.81	7.71×10^{-18}
265	5.97×10^{-14}	1.33×10^{5}	7.94×10^{-9}	3.29×10^{-18}	5.58×10^{6}	1.84×10^{-11}	7.38×10^{-19}	1.18×10^{1}	8.73×10^{-18}
278	1.52×10^{-14}	2.75×10^{5}	4.18×10^{-9}	1.19×10^{-18}	9.41×10^{6}	1.12×10^{-11}	3.11×10^{-19}	3.63×10^{1}	1.13×10^{-17}
280	1.25×10^{-14}	3.05×10^{5}	3.81×10^{-9}	1.02×10^{-18}	1.02×10^{7}	1.04×10^{-11}	2.75×10^{-19}	4.27×10^{1}	1.17×10^{-17}
290	4.83×10^{-15}	5.05×10^{5}	2.44×10^{-9}	5.04×10^{-19}	1.47×10^{7}	7.42×10^{-12}	1.51×10^{-19}	9.34×10^{1}	1.41×10^{-17}
298	2.37×10^{-15}	7.39×10^{5}	1.75×10^{-9}	2.96×10^{-19}	1.95×10^{7}	5.78×10^{-12}	9.61×10^{-20}	1.69×10^{2}	1.62×10^{-17}
300	1.99×10^{-15}	8.10×10^{5}	1.61×10^{-9}	2.61×10^{-19}	2.09×10^{7}	5.45×10^{-12}	8.63×10^{-20}	1.94×10^{2}	1.68×10^{-17}
310	8.72×10^{-16}	1.26×10^{6}	1.10×10^{-9}	1.41×10^{-19}	2.91×10^{7}	4.10×10^{-12}	5.12×10^{-20}	3.86×10^{2}	1.98×10^{-17}
320	4.02×10^{-16}	1.90×10^{6}	7.64×10^{-10}	7.93×10^{-20}	3.98×10^{7}	3.16×10^{-12}	3.15×10^{-20}	7.36×10^{2}	2.32×10^{-17}
330	1.95×10^{-16}	2.80×10^{6}	5.45×10^{-10}	4.63×10^{-20}	5.36×10^{7}	2.48×10^{-12}	2.00×10^{-20}	1.35×10^{3}	2.69×10^{-17}
350	5.19×10^{-17}	5.67×10^{6}	2.94×10^{-10}	1.74×10^{-20}	9.25×10^{7}	1.61×10^{-12}	8.70×10^{-21}	4.08×10^{3}	3.55×10^{-17}
375	1.22×10^{-17}	1.23×10^{7}	1.51×10^{-10}	5.97×10^{-21}	1.70×10^{8}	1.02×10^{-12}	3.52×10^{-21}	1.38×10^{4}	4.86×10^{-17}
400	3.46×10^{-18}	2.43×10^{7}	8.42×10^{-11}	2.37×10^{-21}	2.91×10^{8}	6.88×10^{-13}	1.60×10^{-21}	4.02×10^{4}	6.44×10^{-17}
425	1.15×10^{-18}	4.42×10^{7}	5.07×10^{-11}	1.05×10^{-21}	4.70×10^{8}	4.94×10^{-13}	8.07×10^{-22}	1.03×10^{5}	8.31×10^{-17}
500	8.35×10^{-20}	1.84×10^{8}	1.54×10^{-11}	1.56×10^{-22}	1.50×10^{9}	2.34×10^{-13}	1.61×10^{-22}	9.81×10^{5}	1.58×10^{-16}
550	2.22×10^{-20}	3.83×10^{8}	8.50×10^{-12}	5.99×10^{-23}	2.74×10^{9}	1.64×10^{-13}	7.17×10^{-23}	3.13×10^{6}	2.24×10^{-16}
600	7.46×10^{-21}	7.04×10^{8}	5.25×10^{-12}	2.74×10^{-23}	4.56×10^{9}	1.25×10^{-13}	3.72×10^{-23}	8.20×10^{6}	3.05×10^{-16}
650	3.01×10^{-21}	1.18×10^{9}	3.55×10^{-12}	1.44×10^{-23}	7.04×10^{9}	1.01×10^{-13}	2.17×10^{-23}	1.86×10^{7}	4.02×10^{-16}
700	1.40×10^{-21}	1.83×10^{9}	2.56×10^{-12}	8.39×10^{-24}	1.03×10^{10}	8.60×10^{-14}	1.38×10^{-23}	3.73×10^{7}	5.17×10^{-16}
750	7.31×10^{-22}	2.67×10^{9}	1.95×10^{-12}	5.32×10^{-24}	1.42×10^{10}	7.57×10^{-14}	9.49×10^{-24}	6.85×10^{7}	6.50×10^{-16}
800	4.18×10^{-22}	3.73×10^{9}	1.56×10^{-12}	3.61×10^{-24}	1.90×10^{10}	6.87×10^{-14}	6.89×10^{-24}	1.17×10^{8}	8.03×10^{-16}
850	2.58×10^{-22}	4.99×10^{9}	1.29×10^{-12}	2.59×10^{-24}	2.47×10^{10}	6.38×10^{-14}	5.25×10^{-24}	1.86×10^{8}	9.79×10^{-16}
900	1.69×10^{-22}	6.48×10^{9}	1.10×10^{-12}	1.94×10^{-24}	3.11×10^{10}	6.04×10^{-14}	4.16×10^{-24}	2.84×10^{8}	1.18×10^{-15}
950	1.17×10^{-22}	8.17×10^{9}	9.57×10^{-13}	1.52×10^{-24}	3.84×10^{10}	5.82×10^{-14}	3.40×10^{-24}	4.13×10^{8}	1.41×10^{-15}
1000	8.46×10^{-23}	1.01×10^{10}	8.53×10^{-13}	1.22×10^{-24}	4.65×10^{10}	5.68×10^{-14}	2.86×10^{-24}	5.80×10^{8}	1.66×10^{-15}

Table S3: Half life time in sec. for the catalyzed and uncatalyzed channel at room temperature.

Temp (K)	AM catalyzed			FA catalyzed		WM catalyzed		Uncat
	0.1ppbv	10pppv	2900ppbv	0.01ppbv	10ppbv	20%RH	100%RH	
280	2.18×10^{-1}	2.18×10^{-3}	7.50×10^{-6}	7.48×10^{5}	7.48×10^{2}	1.22	2.44×10^{-1}	5.70×10^{5}
290	2.76×10^{-1}	2.76×10^{-3}	9.52×10^{-6}	7.25×10^{5}	7.25×10^{2}	4.95×10^{-1}	9.90×10^{-2}	2.15×10^{5}
298	3.77×10^{-1}	3.77×10^{-3}	1.30×10^{-5}	7.08×10^{5}	7.08×10^{2}	2.96×10^{-1}	5.93×10^{-2}	9.87×10^{4}
300	4.08×10^{-1}	4.08×10^{-3}	1.41×10^{-5}	7.03×10^{5}	7.03×10^{2}	2.33×10^{-1}	4.67×10^{-2}	8.12×10^{4}
310	4.77×10^{-1}	4.77×10^{-3}	1.65×10^{-5}	6.81×10^{5}	6.81×10^{2}	1.07×10^{-1}	2.13×10^{-2}	3.09×10^{4}
320	6.63×10^{-1}	6.63×10^{-3}	2.29×10^{-5}	6.59×10^{5}	6.59×10^{2}	5.82×10^{-2}	1.16×10^{-2}	1.19×10^{4}

Table S4: Concentration of Ammonia, Formic acid and Water (in molecules cm^{-3}) within the temperature range of 280-320 K

Temp (K)	Ammonia			Formic acid		Water	
	0.1ppv	10ppbv	2900ppbv	0.01ppbv	10ppbv	20%H	100%H
280	2.62×10^{9}	2.62×10^{11}	7.60×10^{13}	2.62×10^{8}	2.62×10^{11}	5.16×10^{16}	2.58×10^{17}
290	2.53×10^{9}	2.53×10^{11}	7.34×10^{13}	2.53×10^{8}	2.53×10^{11}	9.56×10^{16}	4.78×10^{17}
298	2.46×10^{9}	2.46×10^{11}	7.13×10^{13}	2.46×10^{8}	2.46×10^{11}	1.55×10^{17}	7.73×10^{17}
300	2.44×10^{9}	2.44×10^{11}	7.08×10^{13}	2.44×10^{8}	2.44×10^{11}	1.72×10^{17}	8.58×10^{17}
310	2.36×10^{9}	2.36×10^{11}	6.84×10^{13}	2.36×10^{8}	2.36×10^{11}	2.92×10^{17}	1.46×10^{18}
320	2.29×10^{9}	2.29×10^{11}	6.64×10^{13}	2.29×10^{8}	2.29×10^{11}	4.70×10^{17}	2.35×10^{18}

Table S5: Average concentration of Ammonia, Formic acid and Water (in molecules cm^{-3}) at higher altitude.

Altitude (km)	Temp (K)	Ammonia	Formic acid	Water
15	213	1.20×10^{8}	3.20×10^{9}	2.00×10^{13}
10	230	8.50×10^{8}	8.30×10^{9}	4.90×10^{15}
5	259	7.60×10^{9}	2.00×10^{10}	2.40×10^{16}

Table S6: Absolute energies in Hartree for the AM, FA, and WM catalyzed species aw well as for the uncatalyzed species optimized at MP2/aug-cc-pVTZ level of theory.

Catalyst	Species	MP2/aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ	CCSD(T)/aug-cc-pVDZ	CCSD(T)/CBS
	cis-cis	-624.2865771	-624.3314174	-624.0543806	-624.4602388813
	cis-trans	-624.2852928	-624.3298599	-624.0527504	-624.4587371021
	trans-trans	-624.2788033	-624.3231526	-624.0457362	-624.4520617652
None	TS_{uncat}	-624.2437867	-624.2834554	-624.0093838	-624.4114112324
	PC_{uncat}	-624.3009192	-624.3404773	-624.0671367	-624.4684902367
	RC_{AM}	-680.7687116	-680.8326127	-680.499944	-680.9881799874
AM	TS_{AM}	-680.7603585	-680.8192494	-680.4892874	-680.9745445486
	PC_{AM}	-680.7785951	-680.837934	-680.5098007	-680.9924957142
	RC_{FA}	-813.7940338	-813.7940338	-813.4310599	-814.0765183028
FA	TS_{FA}	-813.7802465	-813.7802465	-813.4124196	-814.05851221
	PC_{FA}	-813.8072671	-813.8072671	-813.44302	-814.0846538875
	RC_{WM}	-700.6328388	-700.6909988	-700.3450377	-700.8537825188
WM	TS_{WM}	-700.6127721	-700.6658186	-700.3207028	-700.8281029186
	PC_{WM}	-700.6446555	-700.6977199	-700.3561171	-700.859440685

Table S7: Product branching ratio (γ) of catalyzed channels at 1 atm pressure.

P (atm)	Temp (K)	AM catalyzed	FA catalyzed	WM catalyzed
	213	5.47×10^{-3}	8.95×10^{-1}	1.30×10^{-5}
	216	5.34×10^{-3}	9.16×10^{-1}	2.70×10^{-5}
	219	5.21×10^{-3}	9.16×10^{-1}	3.10×10^{-5}
	224	4.80×10^{-3}	9.25×10^{-1}	3.10×10^{-5}
	235	4.60×10^{-3}	9.44×10^{-1}	4.60×10^{-5}
	250	3.52×10^{-3}	9.56×10^{-1}	7.00×10^{-5}
	259	3.51×10^{-3}	9.58×10^{-1}	6.10×10^{-5}
1.0	265	2.99×10^{-3}	9.60×10^{-1}	9.60×10^{-5}
	278	2.92×10^{-3}	9.60×10^{-1}	1.09×10^{-4}
	280	2.55×10^{-3}	9.61×10^{-1}	1.08×10^{-4}
	290	2.33×10^{-3}	9.61×10^{-1}	1.39×10^{-4}
	298	1.92×10^{-3}	9.61×10^{-1}	1.40×10^{-4}
	300	1.83×10^{-3}	9.62×10^{-1}	1.59×10^{-4}
	310	1.81×10^{-3}	9.62×10^{-1}	1.98×10^{-4}
	320	1.50×10^{-3}	9.62×10^{-1}	2.18×10^{-4}

Table S8: Product branching ratio (γ) of catalyzed channels at higher altitudes.

P (atm)	Temp (K)	AM catalyzed	FA catalyzed	WM catalyzed
0.12	213	3.81×10^{-3}	9.91×10^{-1}	3.00×10^{-5}
0.27	230	3.65×10^{-3}	9.80×10^{-1}	4.70×10^{-5}
0.54	259	2.89×10^{-3}	9.78×10^{-1}	8.60×10^{-5}

Table S9: Product branching ratio (γ) of catalyzed channels at 298K.

P (atm)	Temp (K)	AM catalyzed	FA catalyzed	WM catalyzed
0.10		1.12×10^{-3}	9.67×10^{-1}	1.70×10^{-4}
0.50		1.79×10^{-3}	9.69×10^{-1}	1.80×10^{-4}
1.0	298	1.92×10^{-3}	9.70×10^{-1}	1.50×10^{-4}
5.0		4.70×10^{-3}	9.72×10^{-1}	1.70×10^{-4}
10.0		5.23×10^{-3}	9.80×10^{-1}	1.70×10^{-4}

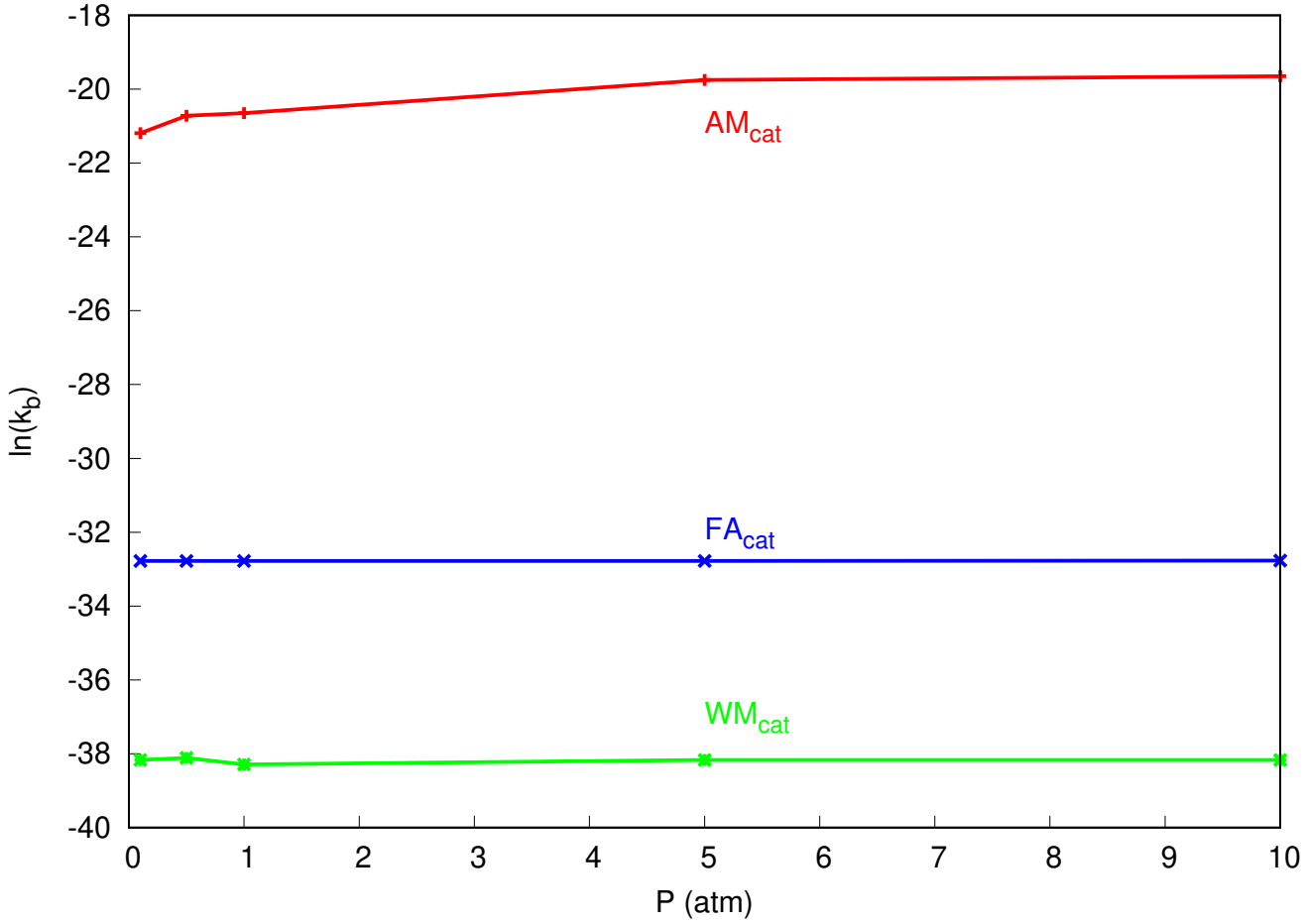
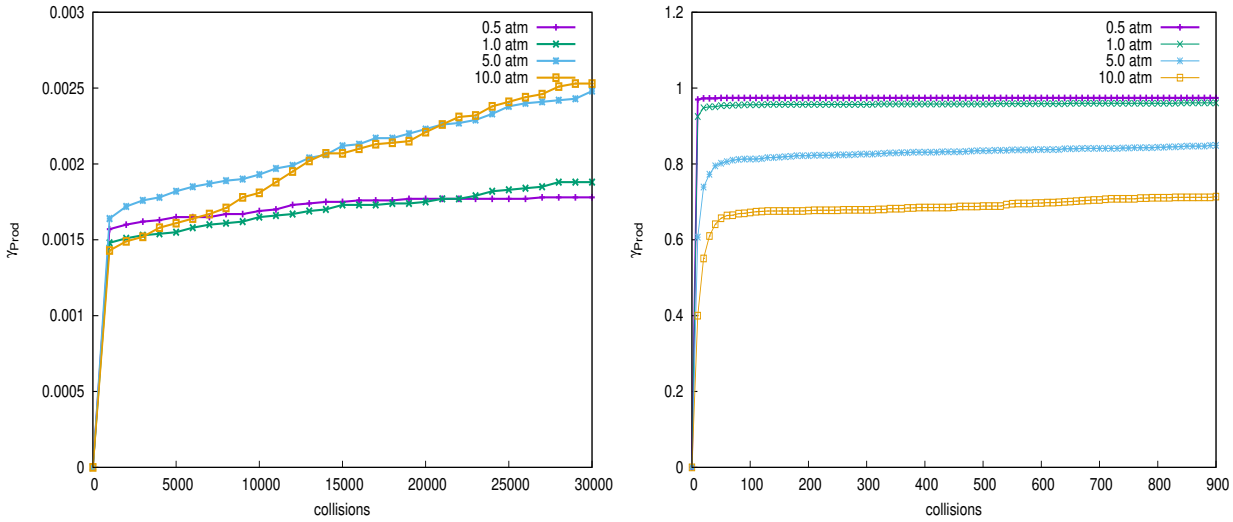


Figure S1: Pressure dependence plot for the decomposition reaction of H_2SO_3 in the presence of AM, FA, and WM at 298 K.



AM catalyzed FA catalyzed

Figure S2: Time evolution of the relative population of the product complex for AM and FA catalyzed channels at 298 K.