Supporting Information

for

Formation of Atmospheric Molecular Clusters Consisting of Sulfuric Acid and a $C_8H_{12}O_6$ Tricarboxylic Acid

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Energetics Based on M06-2X Geometries

Table S1: Thermodynamic parameters (G_{corr}, H_{DFT} and S_{DFT}) are calculated at the M06-2X/6-31++G(d,p) level of theory. The DLPNO single point energies (E_{DLPNO}) are calculated on top of the M06-2X/6-31++G(d,p) geometry. S_{DFT} is given in cal mol^{-1} K^{-1} and all other values are in Hartrees.

Cluster	G_{corr}	H_{DFT}	S_{DFT}	G_{DFT}	E_{DFT}	E_{DLPNO}
MBTCA	0.165280	-762.998364	123.505	-763.057045	-763.222325	-762.577352
SA	0.011422	-700.036239	71.917	-700.070393	-700.081815	-699.576295
$(MBTCA)_2$	0.355480	-1526.027556	200.073	-1526.122617	-1526.478097	-1525.182341
$(MBTCA)(SA)$	0.199688	-1463.072875	150.862	-1463.144554	-1463.344242	-1462.186417
$(MBTCA)(SA)_2$	0.234099	-2163.142971	177.843	-2163.227470	-2163.461569	-2161.790063
$(MBTCA)(SA)_3$	0.269684	-2863.218141	201.044	-2863.313664	-2863.583348	-2861.393836
$(MBTCA)(SA)_4$	0.302010	-3563.288979	232.832	-3563.399605	-3563.701615	-3561.002047
$(MBTCA)_2(SA)$	0.391611	-2226.110439	221.714	-2226.215783	-2226.607394	-2224.798234
$(MBTCA)_2(SA)_2$	0.429678	-2926.198579	239.802	-2926.312517	-2926.742195	-2924.414330
$(MBTCA)_2(SA)_3$	0.461948	-3626.278972	268.526	-3626.406557	-3626.868505	-3624.030887
$(MBTCA)_2(SA)_4$	0.493996	-4326.338413	301.024	-4326.481439	-4326.975435	-4323.624260
$(MBTCA)_3(SA)$	0.582302	-2989.149482	294.203	-2989.289268	-2989.871570	-2987.408512
$(MBTCA)_3(SA)_2$	0.616678	-3689.226483	320.203	-3689.378622	-3689.995300	-3687.024120
$(MBTCA)_3(SA)_3$	0.650817	-4389.297339	348.740	-4389.463037	-4390.113854	-4386.621552

Energetics Based on PW91 Geometries

Table S2: Thermodynamic parameters (G_{corr}, H_{DFT} and S_{DFT}) are calculated at the PW91/6-31++G(d,p) level of theory. The DLPNO single point energies (E_{DLPNO}) are calculated on top of the PW91/6-31++G(d,p) geometry. S_{DFT} is given in cal mol^{-1} K^{-1} and all other values are in Hartrees.

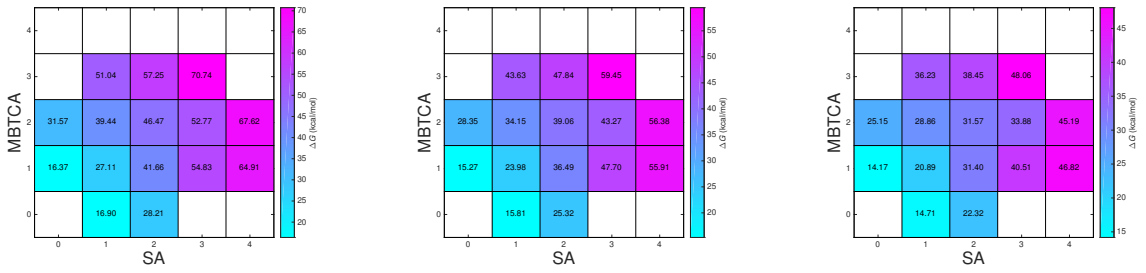
Cluster	G_{corr}	H_{DFT}	S_{DFT}	G_{DFT}	E_{DFT}	E_{DLPNO}
MBTCA	0.155518	-763.066861	127.400	-763.127393	-763.282911	-762.573695
SA	0.008248	-700.101318	73.625	-700.136300	-700.144548	-699.566676
$(MBTCA)_2$	0.338577	-1526.168897	199.798	-1526.263827	-1526.602404	-1525.174933
$(MBTCA)(SA)$	0.187075	-1463.202299	154.722	-1463.275813	-1463.462888	-1462.173929
$(MBTCA)(SA)_2$	0.219365	-2163.331519	180.756	-2163.417402	-2163.636767	-2161.767627
$(MBTCA)(SA)_3$	0.249714	-2863.462119	210.063	-2863.561927	-2863.811641	-2861.363467
$(MBTCA)(SA)_4$	0.276061	-3563.596325	247.139	-3563.713748	-3563.989809	-3560.962286
$(MBTCA)_2(SA)$	0.370043	-2226.309632	225.732	-2226.416884	-2226.786927	-2224.779327
$(MBTCA)_2(SA)_2$	0.403715	-2926.450035	248.269	-2926.567996	-2926.971711	-2924.387651
$(MBTCA)_2(SA)_3$	0.436876	-3626.596330	271.375	-3626.725269	-3627.162145	-3623.995685
$(MBTCA)_2(SA)_4$	0.460279	-4326.718654	313.855	-4326.867776	-4327.328055	-4323.584172
$(MBTCA)_3(SA)$	0.549355	-2989.412658	305.324	-2989.557727	-2990.107082	-2987.385521
$(MBTCA)_3(SA)_2$	0.581656	-3689.558481	328.827	-3689.714717	-3690.296373	-3686.991555
$(MBTCA)_3(SA)_3$	0.608654	-4389.689205	363.980	-4389.862144	-4390.470798	-4386.586896

Energetics Based on ωB97X-D Geometries

Table S3: Thermodynamic parameters (G_{corr}, H_{DFT} and S_{DFT}) are calculated at the ωB97X-D/6-31++G(d,p) level of theory. The DLPNO single point energies (E_{DLPNO}) are calculated on top of the ωB97X-D/6-31++G(d,p) geometry. S_{DFT} is given in cal mol^{-1} K^{-1} and all other values are in Hartrees.

Cluster	G_{corr}	H_{DFT}	S_{DFT}	G_{DFT}	E_{DFT}	E_{DLPNO}
MBTCA	0.165676	-763.080598	123.821	-763.139429	-763.305105	-762.577306
SA	0.011180	-700.080489	72.473	-700.114924	-700.126104	-699.575880
$(MBTCA)_2$	0.358290	-1526.196418	196.292	-1526.289682	-1526.647972	-1525.184451
(MBTCA)(SA)	0.201050	-1463.198089	149.640	-1463.269188	-1463.470238	-1462.186822
$(MBTCA)(SA)_2$	0.235832	-2163.310573	176.756	-2163.394555	-2163.630387	-2161.790203
$(MBTCA)(SA)_3$	0.270105	-2863.424836	203.500	-2863.521525	-2863.791630	-2861.396668
$(MBTCA)(SA)_4$	0.305391	-3563.536722	231.186	-3563.646566	-3563.951957	-3561.004231
$(MBTCA)_2(SA)$	0.394420	-2226.318999	220.102	-2226.423576	-2226.817996	-2224.799047
$(MBTCA)_2(SA)_2$	0.431264	-2926.445277	241.248	-2926.559901	-2926.991165	-2924.418437
$(MBTCA)_2(SA)_3$	0.466312	-3626.569655	266.880	-3626.696458	-3627.162770	-3624.033050
$(MBTCA)_2(SA)_4$	0.492484	-4326.671108	311.151	-4326.818946	-4327.311430	-4323.630630
$(MBTCA)_3(SA)$	0.587278	-2989.438524	292.185	-2989.577351	-2990.164629	-2987.410128
$(MBTCA)_3(SA)_2$	0.618714	-3689.560423	324.276	-3689.714497	-3690.333211	-3687.025728
$(MBTCA)_3(SA)_3$	0.651621	-4389.672169	353.946	-4389.840340	-4390.491961	-4386.631363

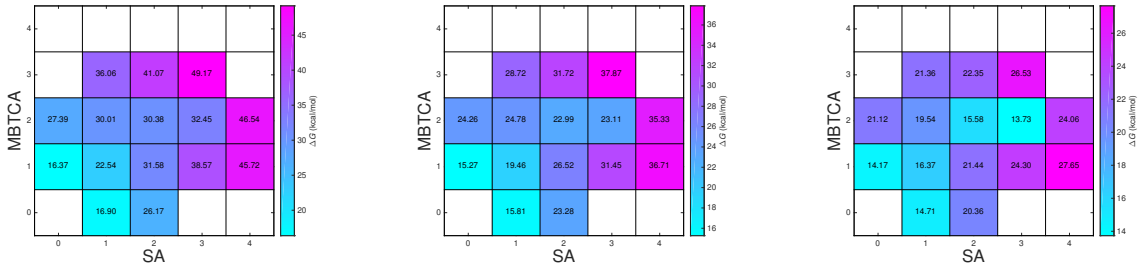
Actual Free Energy Surface - DLPNO-CCSD(T)//DFT/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S1: Free energy surface (kcal/mol) of the MBTCA-SA system calculated with DLPNO. $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

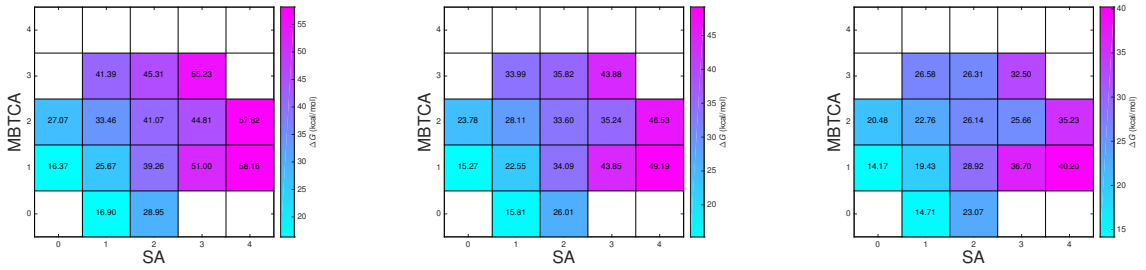
Actual Free Energy Surface - M06-2X/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S2: Free energy surface (kcal/mol) of the MBTCA-SA system calculated with M06-2X/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

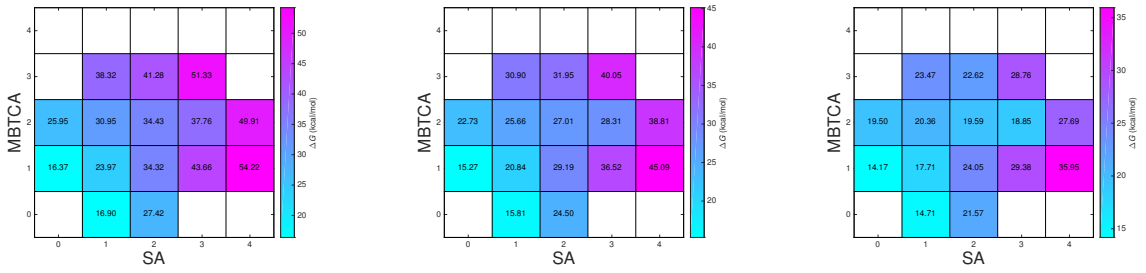
Actual Free Energy Surface - PW91/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S3: Free energy surface (kcal/mol) of the MBTCA-SA system calculated with PW91/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

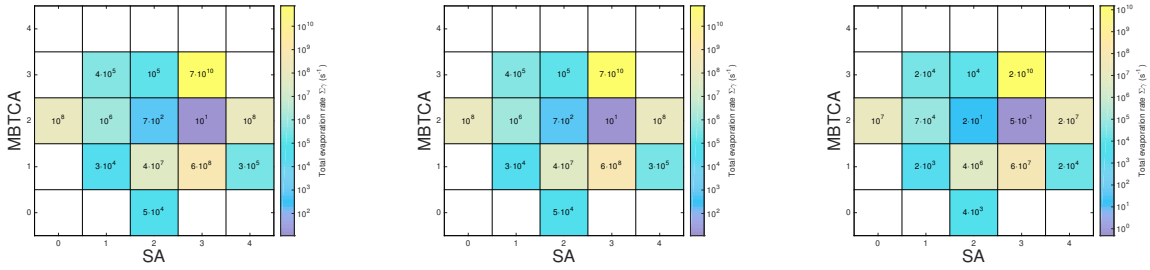
Actual Free Energy Surface - ωB97X-D/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S4: Free energy surface (kcal/mol) of the MBTCA-SA system calculated with ωB97X-D/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

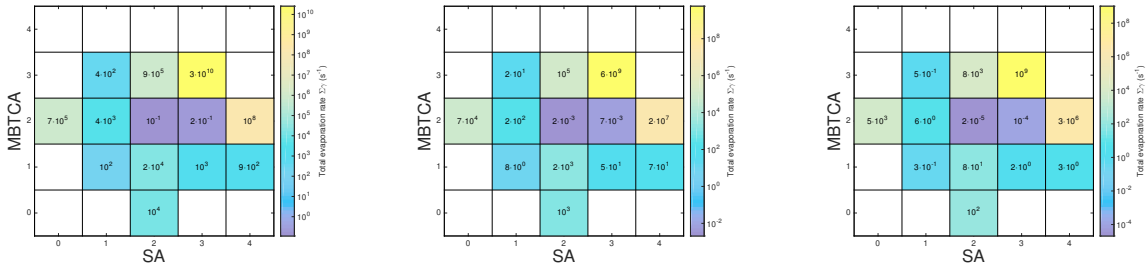
Total Evaporation Rates - DLPNO-CCSD(T)//DFT/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S5: Evaporation rate (s^{-1}) of the MBTCA-SA system calculated with DLPNO.

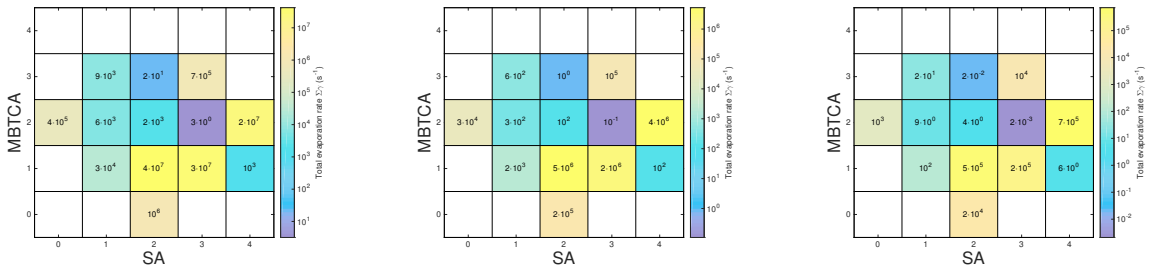
Total Evaporation Rates - M06-2X/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S6: Evaporation rate (s^{-1}) of the MBTCA-SA system calculated with M06-2X/6-31++G(d,p).

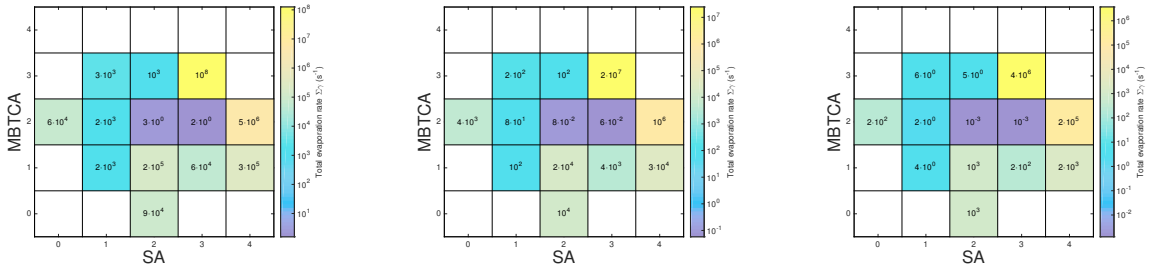
Total Evaporation Rates - PW91/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S7: Evaporation rate (s^{-1}) of the MBTCA-SA system calculated with PW91/6-31++G(d,p).

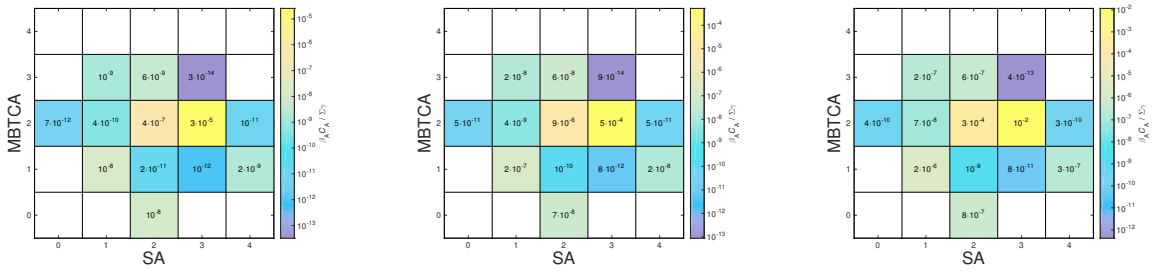
Total Evaporation Rates - ωB97X-D/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S8: Evaporation rate (s^{-1}) of the MBTCA-SA system calculated with ωB97X-D/6-31++G(d,p).

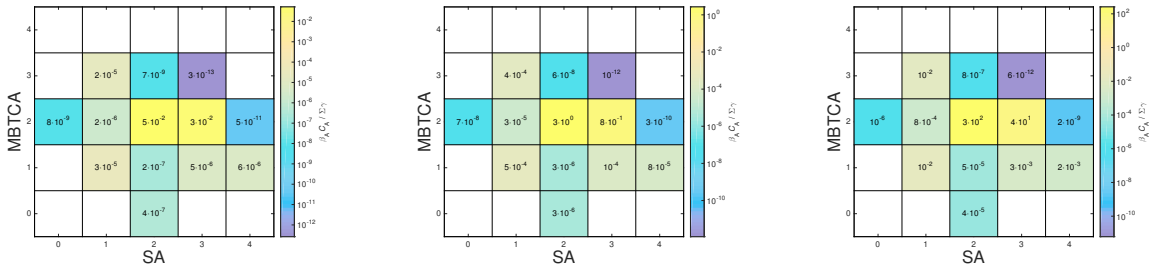
Ratio between the Collision Rate of Sulfuric acid Molecules and Total Evaporation Rate - DLPNO-CCSD(T)//DFT/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S9: $\beta_{SA} c_{SA} / \sum \gamma$ of the MBTCA-SA system calculated with DLPNO. $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

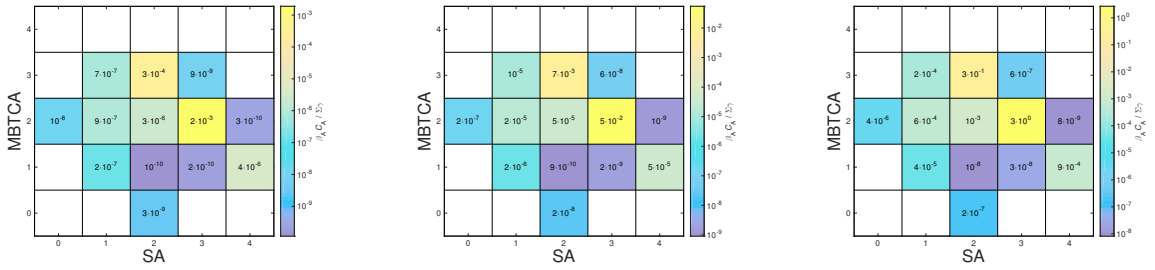
Ratio between the Collision Rate of Sulfuric acid Molecules and Total Evaporation Rate - M06-2X/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S10: $\beta_{SA}C_{SA}/\sum\gamma$ of the MBTCA-SA system calculated with M06-2X/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

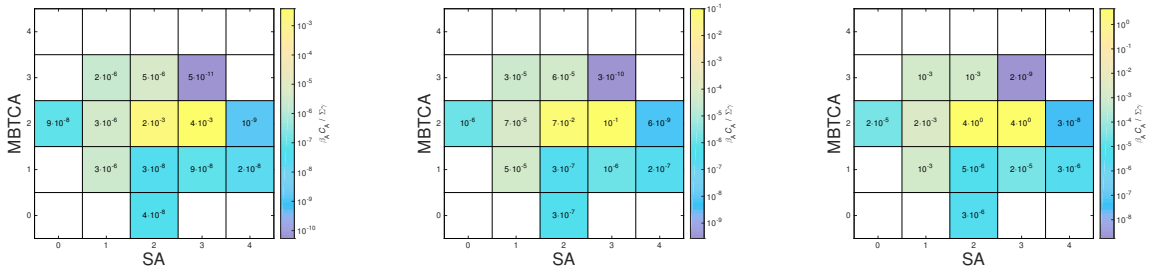
Ratio between the Collision Rate of Sulfuric acid Molecules and Total Evaporation Rate - PW91/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S11: $\beta_{SA}C_{SA}/\sum\gamma$ of the MBTCA-SA system calculated with PW91/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

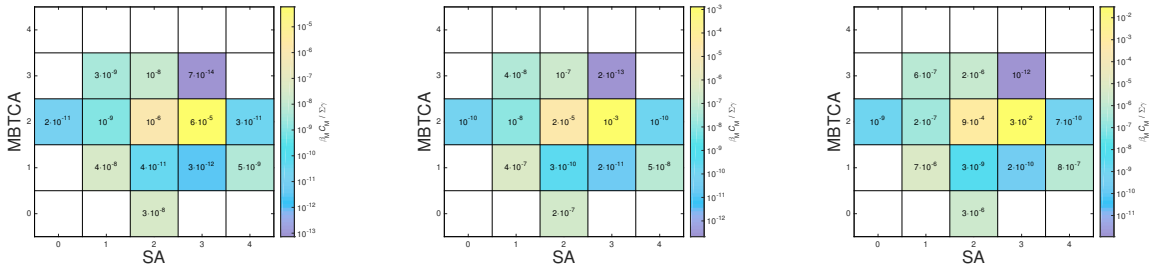
Ratio between the Collision Rate of Sulfuric acid Molecules and Total Evaporation Rate - ωB97X-D/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S12: $\beta_{SA}C_{SA}/\sum\gamma$ of the MBTCA-SA system calculated with ωB97X-D/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

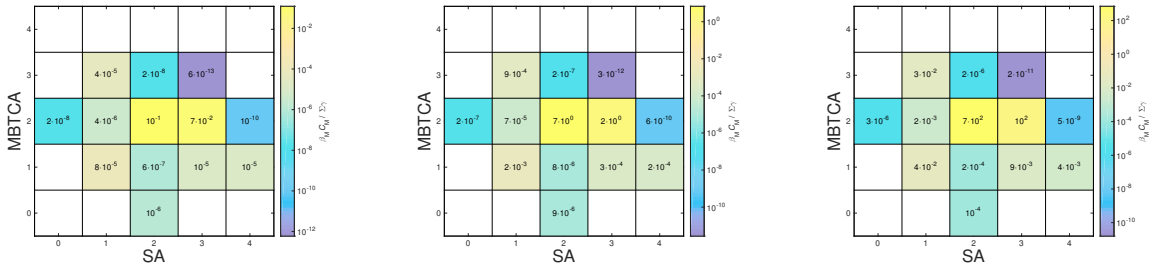
Ratio between the Collision Rate of MBTCA Molecules and Total Evaporation Rate - DLPNO-CCSD(T)//DFT/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S13: $\beta_{MBTCA} C_{MBTCA} / \sum \gamma$ of the MBTCA-SA system calculated with DLPNO. $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

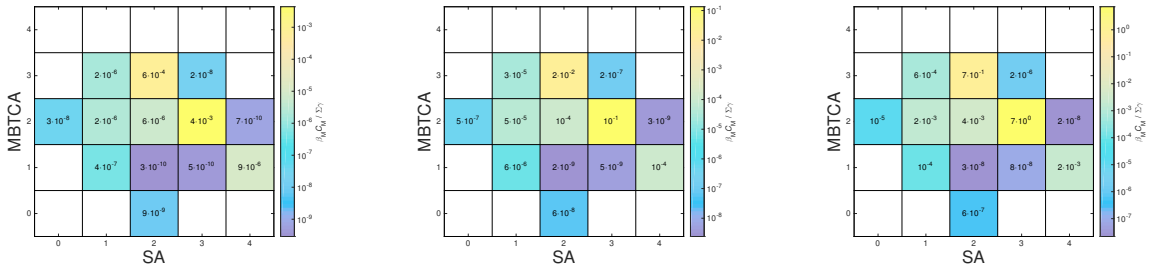
Ratio between the Collision Rate of MBTCA Molecules and Total Evaporation Rate - M06-2X/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S14: $\beta_{MBTCA} C_{MBTCA} / \sum \gamma$ of the MBTCA-SA system calculated with M06-2X/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

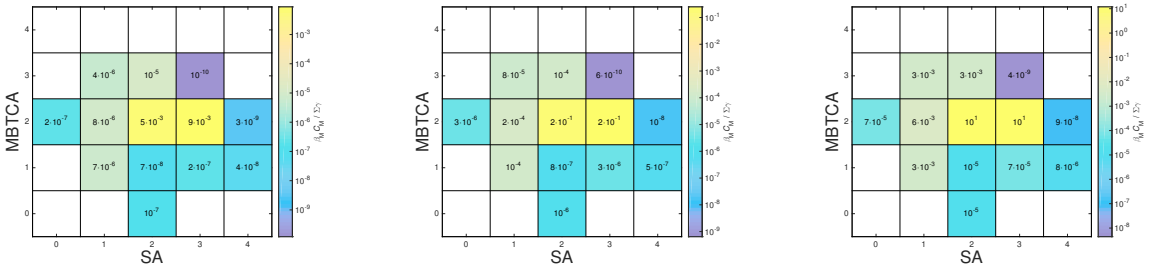
Ratio between the Collision Rate of MBTCA Molecules and Total Evaporation Rate - PW91/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S15: $\beta_{MBTCA} C_{MBTCA} / \sum \gamma$ of the MBTCA-SA system calculated with PW91/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.

Ratio between the Collision Rate of MBTCA Molecules and Total Evaporation Rate - ωB97X-D/6-31++G(d,p)



298.15 K **278.15 K** **258.15 K**

Figure S16: $\beta_{MBTCA} C_{MBTCA} / \sum \gamma$ of the MBTCA-SA system calculated with ωB97X-D/6-31++G(d,p). $[H_2SO_4] = 10^7$ molecules cm^{-3} and [MBTCA] = 1ppt.