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A cluster-of-functional-groups approach for studying organic enhanced atmospheric cluster formation

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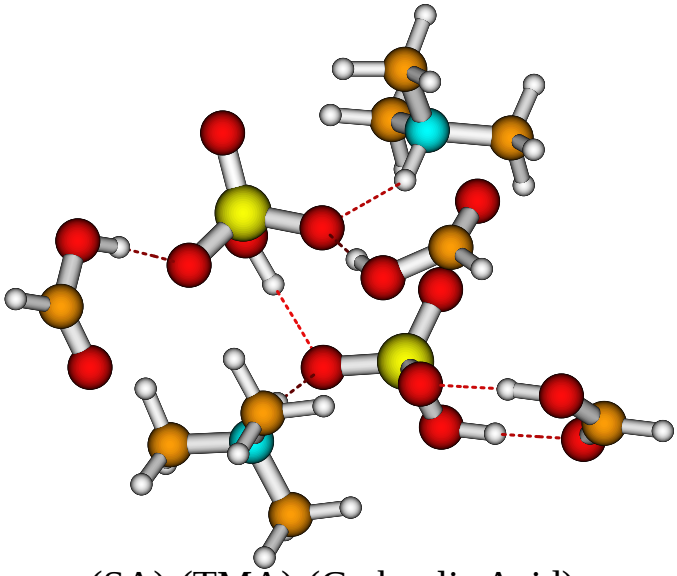
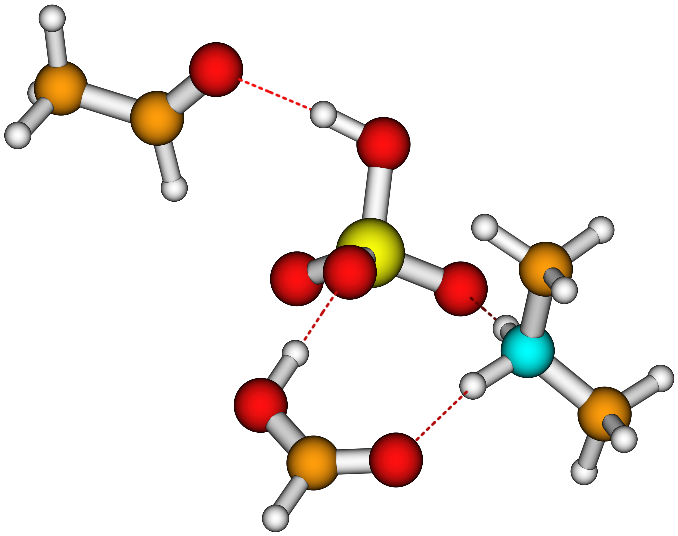
S1 Cluster Structures



$(SA)_2(TMA)_2(Carboxlic\ Acid)_3$

Figure S1. The $(SA)_2(TMA)_2(Carboxlic\ Acid)_3$ cluster geometry lowest in free energy. Calculated at the DLPNO-CCSD(T_0)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory with quasi-harmonic cutoff of 100 cm^{-1}, at 298.15 K and 1 atm. White = hydrogen, brown = carbon, red = oxygen, yellow = sulfur, blue = nitrogen.



$(SA)_1(DMA)_1(Aldehyde)_1(CA)_1$

Figure S2. The $(SA)_1(DMA)_1(Aldehyde)_1(Carboxlic\ Acid)_1$ cluster geometry second lowest in free energy ($+0.62$ kcal/mol). Calculated at the DLPNO-CCSD(T_0)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory with quasi-harmonic cutoff of 100 cm^{-1}, at 298.15 K and 1 atm. White = hydrogen, brown = carbon, red = oxygen, yellow = sulfur, blue = nitrogen.

S2 Fluxes

Table S1. Sum of outgrowing channels that contribute over 2 % to the total flux and contain OOM. The SA concentration was fixed at 10^6 cm^{-3}.

System	C_{OOM}(ppt)	C_{base} (ppt)	Outgrowing (%)
SA-AM-OOM	1	10	97.96
	1	10000	97.95
	10	10	99.80
	10	10000	99.81
SA-MA-OOM	1	1	98.86
	1	100	99.05
	10	1	99.72
	10	100	99.74
SA-DMA-OOM	1	1	72.44
	1	10	83.77
	10	1	99.03
	10	10	99.67
SA-TMA-OOM	1	1	7.52
	1	10	12.39
	10	1	78.97
	10	10	87.22