Supporting information

A theoretical study on the formation mechanism of carboxylic sulfuric anhydride and the potential role in new particle formation

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I. Supplementary figures.

Figure S1. Flowchart for the multistep global minimum sampling method.

Figure S2. The most stable configurations at M06-2X/6-311++G(3df,3pd) level of theory of (a) DTAA (b) DTASA-1 and (c) DTASA-2.

II. Supplementary tables.

Table S1. The Gibbs free energies (G_{DFT}) and Gibbs free energy correction terms (G_{Therm}) at M06-2X/6-311++G(3df,3pd) level of theory, single point energies (E_{DLPNO}) at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, the corrected Gibbs free energies (G_{DLPNO}), and imaginary frequency (v_{im}) of transition state calculated for the cycloaddition reaction of SO_3 to the -COOH group containing C1 in DTAA molecule. All energies are in Hartrees and T = 298 K.

Table S2. The Gibbs free energies (G_{DFT}) and Gibbs free energy correction terms (G_{Therm}) at M06-2X/6-311++G(3df,3pd) level of theory, single point energies (E_{DLPNO}) at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, the corrected Gibbs free energies (G_{DLPNO}), and imaginary frequency (v_{im}) of transition state calculated for the cycloaddition reaction of SO_3 to the -COOH group containing C5 in DTAA molecule. All energies are in Hartrees and T = 298 K.

Table S3. The Gibbs free energy G of H_2O, NH_3, DMA and SA molecules at M062X/6-311++G(3df,3pd) level of theory and pressure of 1 atm, T = 298 K.

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III. Cartesian coordinates of all optimized structures.

I. Supplementary Figure.

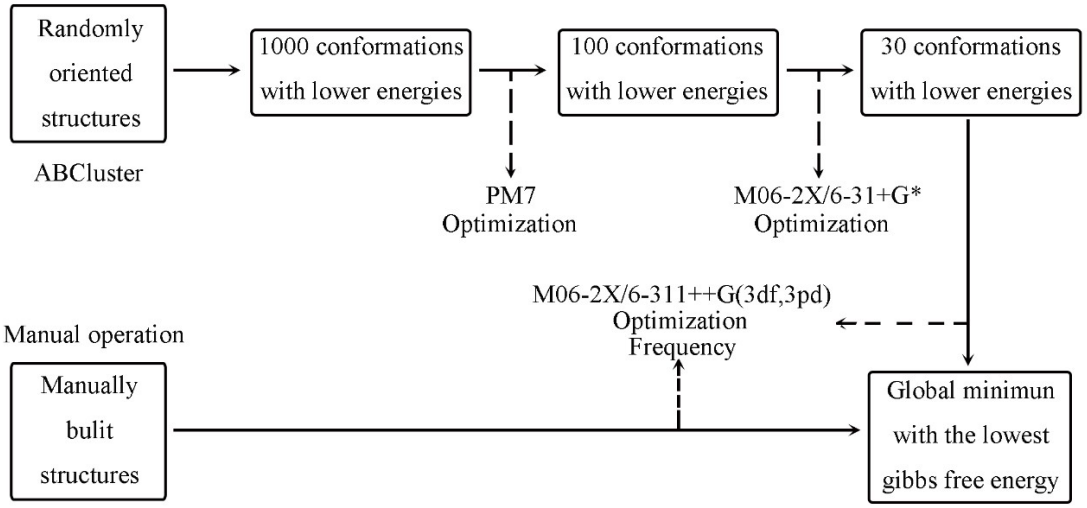

Figure S1. Flowchart for the multistep global minimum sampling method.

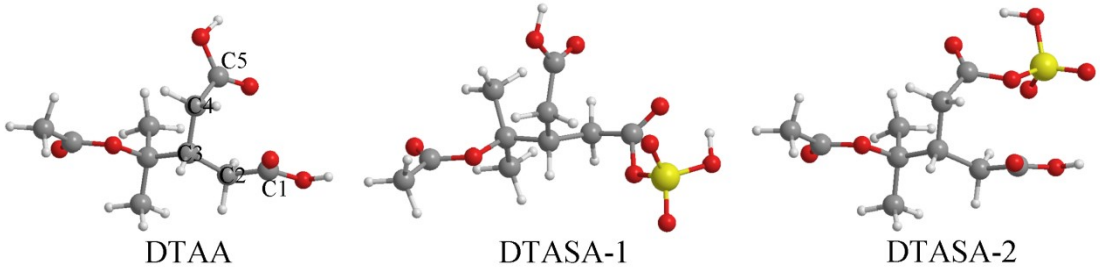

Figure S2. The most stable configurations at M06-2X/6-311++G(3df,3pd) level of theory of (a) DTAA (b) DTASA-1 and (c) DTASA-2.

II. Supplementary tables.

Table S1. The Gibbs free energies (G_{DFT}) and Gibbs free energy correction terms (G_{Therm}) at M06-2X/6-311++G(3df,3pd) level of theory, single point energies (E_{DLPNO}) at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, the corrected Gibbs free energies (G_{DLPNO}), and imaginary frequency (ν_{im}) of transition state calculated for the cycloaddition reaction of SO_3 to the -COOH group containing C1 in DTAA molecule. All energies are in Hartrees and T = 298 K.

	G_{DFT}	G_{Therm}	E_{DLPNO}	G_{DLPNO}	ν_{im} (cm^{-1})
SO_3	-623.830402	-0.012729	-623.0814757	-623.0942047	
DTAA	-841.866528	0.218982	-840.8798912	-840.6609092	
$React_1$	-1465.705124	0.230018	-1463.987555	-1463.757537	
TS_1	-1465.705893	0.225402	-1463.98234	-1463.756938	-851.9145*i*
$Prod_1$	-1465.70872	0.228556	-1463.990469	-1463.761913	

Table S2. The Gibbs free energies (G_{DFT}) and Gibbs free energy correction terms (G_{Therm}) at M06-2X/6-311++G(3df,3pd) level of theory, single point energies (E_{DLPNO}) at DLPNO-CCSD(T)/aug-cc-pVTZ level of theory, the corrected Gibbs free energies (G_{DLPNO}), and imaginary frequency (ν_{im}) of transition state calculated for the cycloaddition reaction of SO_3 to the -COOH group containing C5 in DTAA molecule. All energies are in Hartrees and T = 298 K.

	G_{DFT}	G_{Therm}	E_{DLPNO}	G_{DLPNO}	ν_{im} (cm^{-1})
$React_5$	-1465.706209	0.22876	-1463.987852	-1463.759092	
TS_5	-1465.706437	0.225671	-1463.98374	-1463.758069	-887.2504*i*
$Prod_5$	-1465.710709	0.229317	-1463.992394	-1463.763077	

Table S3. The Gibbs free energy G of H_2O, NH_3, DMA and SA molecules at M062X/6-311++G(3df,3pd) level of theory and pressure of 1 atm, T = 298 K.

Monomers	G_{DFT} (Hartree)
H_2O	-76.423003
NH_3	-56.535518
DMA	-135.073214
SA	-700.276484

Table S4. The reaction free energy for forming these clusters (ΔG), potential energy density $V(\mathbf{r})$ at corresponding BCPs and hydrogen bond energy (E_H) for clusters DTAA-H_2O, DTASA-H_2O and SA-H_2O.

Cluster	ΔG (kcal/mol)	hydrogen bond	$V(\mathbf{r})$ (a.u)	E_H (kcal/mol)
DTAA-H_2O	0.21	O1-H1---O3	-0.03264	-10.24
		O3-H2---O2	-0.02090	-6.56
DTASA-H_2O	-2.76	O1-H1---O3	-0.08608	-27.01
		O3-H2---O2	-0.01867	-5.86
SA-H_2O	-2.93	O1-H1---O3	-0.05864	-18.40
		O3-H2---O2	-0.01453	-4.56

Table S5. The reaction free energy for forming these clusters (ΔG), potential energy density $V(\mathbf{r})$ at

correspondingBCPs and hydrogen bond energy (E_H) for clusters DTAA-NH_3, DTASA-NH_3 and SA-NH_3.

Cluster	ΔG (kcal/mol)	hydrogen bond	$V(\mathbf{r})$ (a.u)	E_H (kcal/mol)
DTAA-NH_3	-0.71	O1-H1---N	-0.04604	-14.44
		N-H2---O2	-0.00916	-2.88
DTASA-NH_3	-8.34	N-H1---O1	-0.08609	-27.01
		N-H2---O2	-0.01335	-4.19
		N-H3---O3	-0.01759	-5.52
SA-NH_3	-7.33	O1-H1---N	-0.07955	-24.96
		N-H2---O2	-0.00894	-2.81

Table S6. The reaction free energy for forming these clusters (ΔG), potential energy density $V(\mathbf{r})$ at corresponding BCPs, hydrogen bond energy (E_H) for clusters DTAA-DMA, DTASA-DMA and SA-DMA.

Cluster	ΔG (kcal/mol)	hydrogen bond	$V(\mathbf{r})$ (a.u)	E_H (kcal/mol)
DTAA-DMA	-1.90	O1-H1---N	-0.05995	-18.81
DTASA-DMA	-15.53	N-H1---O1	-0.06806	-21.35
		N-H2---O2	-0.01429	-4.48
SA-DMA	-11.25	N-H1---O1	-0.09464	-29.69
		N-H2---O2	-0.01743	-5.47

Table S7. The reaction free energy for forming these clusters (ΔG), potential energy density $V(\mathbf{r})$ at corresponding BCPs and hydrogen bond energy (E_H) for clusters DTAA-SA, DTASA-SA and SA-SA.

Cluster	ΔG (kcal/mol)	hydrogen bond	$V(\mathbf{r})$ (a.u)	E_H (kcal/mol)
DTAA-SA	-7.88	O1-H1---O2	-0.08734	-27.40
		O3-H2---O4	-0.04111	-12.90
DTASA-SA	-7.99	O1-H1---O2	-0.06277	-19.70
		O3-H2---O4	-0.05281	-16.57
		O5-H3---O6	-0.02660	-8.35
SA-SA	-8.42	O1-H1---O2	-0.05362	-16.82
		O3-H2---O4	-0.05363	-16.83

III. Coordinates of the clusters in the system.

Table S8. Geometry of SO_3. Units are in angstrom.

Atom	X	Y	Z
S	0.000000	0.000000	0.000060
O	0.000000	0.000000	1.413527
O	0.000000	1.224138	-0.706824
O	0.000000	-1.224138	-0.706824

Table S9. Geometry of DTAA. Units are in angstrom.

Atom	X	Y	Z
C	-3.25682800	-0.15178000	0.25281000
C	-4.07202800	0.23506500	1.45675800
C	1.25647600	1.85885900	-0.12332600
C	-0.95166800	-0.60921700	-0.40784600
C	0.35307700	-0.49699600	0.41735100
O	0.70861800	3.08693400	-0.13055100
O	2.18790600	1.57813400	-0.82789700
H	-5.11524200	0.31348000	1.17330900
H	-3.71478900	1.18505300	1.84979100
H	-3.94705200	-0.51258200	2.23752800
H	1.21163200	3.61946600	-0.76082400
O	-3.70555500	-0.34018800	-0.84326300
O	-1.96183000	-0.25742800	0.57895100
C	-1.19400900	-2.03980200	-0.87321200
H	-1.07077200	-2.73896200	-0.04558200
H	-2.19801800	-2.13268500	-1.27630900
H	-0.48988500	-2.30093300	-1.66097000
C	-0.98035100	0.37246700	-1.57642800
H	-1.09619900	1.39451000	-1.21599200
H	-0.04663500	0.30955900	-2.13417800
H	-1.80555100	0.15138200	-2.24512900
C	0.60839000	0.94787700	0.88274200
H	-0.32037100	1.39316300	1.22754900
H	1.29778500	0.91671400	1.72668900
C	1.53424600	-1.15327800	-0.29969600
H	1.35826900	-2.22634900	-0.39270600
H	1.68732800	-0.76736900	-1.30412700
C	2.83680200	-1.02223600	0.44184000
O	3.88080300	-1.32289100	-0.34372400
H	4.67902400	-1.23520300	0.19260700
O	2.96438700	-0.73798200	1.60055100
H	0.17120900	-1.06763800	1.32986500

Table S10. Geometry of $React_1$ for DTAA. Units are in angstrom.

Atom	X	Y	Z
S	3.67335300	0.24638000	0.74346400
O	3.29474600	1.52683000	0.26713300
O	4.35488200	-0.62214500	-0.18720800
O	3.94292700	0.05734900	2.11689200
C	-4.36663600	0.24091300	0.73216500
C	-4.86635300	1.09258700	1.86575100
C	0.16969400	1.40237400	-1.14608000
C	-2.30121100	-0.68892500	-0.17169300
C	-0.83679200	-0.48824200	0.29605800
O	-0.06825300	2.68640000	-1.42434700
O	0.81540100	0.69469700	-1.87477300
H	-4.35299300	2.05191600	1.86047400
H	-4.64273100	0.60426900	2.81239600
H	-5.93567600	1.23539200	1.76139600
H	0.40890600	2.90413000	-2.23660000
O	-5.05700200	-0.23848600	-0.12176700
O	-3.03464400	0.08691200	0.81202200
C	-2.71861700	-2.15082800	-0.06530800
H	-2.46813400	-2.54846800	0.91884000
H	-3.78824200	-2.24256900	-0.22682600
H	-2.21296800	-2.74513000	-0.82434900
C	-2.53124400	-0.13359000	-1.57495100
H	-2.48155900	0.95531000	-1.57025400
H	-1.76595200	-0.50453700	-2.25552200
H	-3.50598500	-0.42762200	-1.94971400
C	-0.41232500	0.98710400	0.17619800
H	-1.25681600	1.62862400	0.41249300
H	0.36421800	1.21480200	0.90724900
C	0.08227700	-1.51898400	-0.38518800
H	-0.06174400	-2.49689100	0.08005000
H	-0.12504800	-1.63664100	-1.44550300
C	1.53948100	-1.22718500	-0.28245000
O	2.30153900	-1.75250800	-1.16721800
H	3.24435200	-1.46204800	-0.99519900
O	1.96267500	-0.54547500	0.68243200
H	-0.84108100	-0.71255000	1.36330700

Table S11. Geometry of TS_1 for DTAA. Units are in angstrom.

Atom	X	Y	Z
S	3.54044300	0.19377000	0.75775400
O	3.30511200	1.47449000	0.20182400
O	4.27100800	-0.73779000	-0.14709500
O	3.88433300	0.05305900	2.11759300
C	-4.35692600	0.19835300	0.71609700
C	-4.86999000	1.00857200	1.87390900
C	0.19543200	1.46622600	-1.07973100
C	-2.27752300	-0.68462300	-0.20475600
C	-0.81711000	-0.48592300	0.27833100
O	0.02344000	2.77672600	-1.26902700
O	0.80289600	0.77669300	-1.85601400
H	-4.37056700	1.97500600	1.89792200
H	-4.64017900	0.49571800	2.80594500
H	-5.94112600	1.13932300	1.77222400
H	0.51416500	3.02549600	-2.06413400
O	-5.03900000	-0.26039800	-0.15555700
O	-3.02376300	0.05520300	0.79727400
C	-2.68418000	-2.15235800	-0.14388800
H	-2.43869800	-2.57614500	0.83056800
H	-3.75175000	-2.24734600	-0.31669500
H	-2.16823900	-2.72118900	-0.91534600
C	-2.50389600	-0.09072300	-1.59246000
H	-2.45569900	0.99774500	-1.55787200
H	-1.73576700	-0.44141800	-2.28018800
H	-3.47721500	-0.37563600	-1.97760200
C	-0.41032900	0.99727600	0.21351600
H	-1.26898100	1.62073600	0.44901200
H	0.34042800	1.21758600	0.97266400
C	0.11129300	-1.49018800	-0.43149100
H	-0.02493900	-2.47922100	0.01221100
H	-0.10245500	-1.58622900	-1.49260600
C	1.57337400	-1.21239300	-0.35197200
O	2.36638900	-1.67185600	-1.18112600
H	3.45809200	-1.28197000	-0.81826000
O	1.96988100	-0.52128800	0.68655900
H	-0.82737800	-0.74680600	1.33731900

Table S12. Geometry of $Prod_1$ for DTAA. Units are in angstrom.

Atom	X	Y	Z
S	3.41663100	-0.89239200	0.49344600
O	3.15423500	0.07165900	1.49631900
O	4.51557300	-0.38356900	-0.47907500
O	3.68931500	-2.23895100	0.78777100
C	-4.04612500	-1.05121900	0.50590600
C	-4.38591200	-1.71150900	1.81355700
C	-0.34872800	2.19304300	0.67419100
C	-2.12781500	-0.21269900	-0.75080300
C	-0.63468300	-0.17201900	-0.34466700
O	-0.66058500	2.85134100	1.80176700
O	-0.06218000	2.76303000	-0.34083800
H	-4.06047300	-1.07962800	2.63775300
H	-3.85536700	-2.65811000	1.89427100
H	-5.45627400	-1.87362100	1.86519000
H	-0.56687400	3.79555800	1.61871500
O	-4.84334100	-0.74799100	-0.33582400
O	-2.72220400	-0.85111000	0.41220000
C	-2.32954300	-1.10300400	-1.97135500
H	-1.82012900	-2.05831900	-1.83961200
H	-3.38866800	-1.28128000	-2.12905800
H	-1.93585800	-0.61296600	-2.86038600
C	-2.72847000	1.17171200	-0.96600000
H	-2.80654500	1.70891700	-0.02034400
H	-2.09663400	1.75278300	-1.63472800
H	-3.72310200	1.09097000	-1.39222100
C	-0.36738000	0.70072500	0.88872400
H	-1.08903900	0.46857500	1.66815800
H	0.61531400	0.45871500	1.30823500
C	0.28695100	0.14371600	-1.53773200
H	0.23643800	-0.67583600	-2.25533800
H	0.03704900	1.07773700	-2.02934700
C	1.71538000	0.24568200	-1.10498500
O	2.46558200	1.15706000	-1.26868000
H	4.25575100	0.50401900	-0.79564500
O	2.11246800	-0.91814600	-0.46588000
H	-0.40464400	-1.19237800	-0.03386600

Table S13. Geometry of $React_5$ for DTAA. Units are in angstrom.

Atom	X	Y	Z
S	3.04221900	-1.19053400	0.37629000
O	4.17871600	-0.40144400	0.10048800
O	2.88993700	-2.41670000	-0.37433200
O	2.44181500	-1.15513900	1.66065000
C	-4.07725400	-0.70416800	-0.02780200
C	-5.02478500	-0.84607100	-1.18645800
C	0.72670400	-0.64295800	-1.06866400
C	-1.96075700	0.33878700	0.57900300
C	-0.95857200	1.13189700	-0.29261100
O	0.61906000	-1.89023700	-1.35004100
O	1.74692500	-0.15360600	-0.52128000
H	-5.87759400	-1.44105600	-0.88074300
H	-4.51344700	-1.32412600	-2.02004100
H	-5.34874200	0.13815100	-1.51844000
H	1.45759100	-2.36339800	-1.05550500
O	-4.23623200	-1.19587700	1.05306100
O	-3.02202600	0.05242700	-0.37179700
C	-2.51736500	1.20948300	1.69909000
H	-2.84572300	2.17407900	1.31075100
H	-3.35643000	0.70813000	2.17184000
H	-1.75541400	1.37474700	2.45851000
C	-1.35457000	-0.95517000	1.12000900
H	-1.31012300	-1.71364900	0.33969200
H	-0.34365200	-0.77851500	1.49258400
H	-1.95250300	-1.35206400	1.93360900
C	-0.38967200	0.26588600	-1.44330900
H	-1.18228100	-0.32382300	-1.89398600
H	0.02319300	0.94277800	-2.19293100
C	0.09546900	1.84209200	0.55971800
H	-0.39174600	2.60410700	1.16925900
H	0.61152200	1.17590300	1.24895800
C	1.13311000	2.57156500	-0.25299900
O	2.20991400	2.86291300	0.48089500
H	2.84557800	3.31788200	-0.08688000
O	1.01852100	2.88990500	-1.40479300
H	-1.54262800	1.90340900	-0.79599100

Table S14. Geometry of TS_5 for DTAA. Units are in angstrom.

Atom	X	Y	Z
S	2.96521100	-1.10591300	0.35461100
O	4.17492600	-0.43784800	0.08463900
O	2.81415300	-2.40692800	-0.34853900
O	2.39034200	-1.08124100	1.64995800
C	-4.09089200	-0.64967500	-0.05181500
C	-5.02022000	-0.79745600	-1.22434100
C	0.72794200	-0.74040500	-1.02710000
C	-1.96030600	0.35418000	0.56973700
C	-0.92175100	1.09882800	-0.30201200
O	0.64146600	-1.97251600	-1.16787400
O	1.80584700	-0.17909700	-0.55084000
H	-5.88364200	-1.38045600	-0.92531100
H	-4.50045900	-1.28846100	-2.04492200
H	-5.33028600	0.18625900	-1.57120400
H	1.68369200	-2.40892100	-0.79544000
O	-4.28333100	-1.10741700	1.03839900
O	-3.01042900	0.07113300	-0.39438200
C	-2.51540900	1.26800600	1.65584500
H	-2.80804000	2.23170100	1.23783500
H	-3.37796500	0.80086200	2.12157800
H	-1.76523600	1.42976700	2.42763900
C	-1.40006000	-0.94012200	1.15670300
H	-1.36195500	-1.72100300	0.39896700
H	-0.39047800	-0.78117500	1.54144400
H	-2.02233500	-1.29538200	1.97141300
C	-0.35627000	0.19521400	-1.42766800
H	-1.15713300	-0.38606500	-1.87437200
H	0.08012800	0.84993000	-2.18357800
C	0.13770600	1.80086600	0.54953100
H	-0.34189800	2.57380900	1.15136800
H	0.64340400	1.13420500	1.24625700
C	1.18259500	2.51394100	-0.26882400
O	2.27460700	2.77546200	0.45450700
H	2.91202300	3.22462100	-0.11607900
O	1.06143900	2.84218700	-1.41678900
H	-1.47538300	1.87475800	-0.83233600

Table S15. Geometry of $Prod_5$ for DTAA. Units are in angstrom.

Atom	X	Y	Z
S	3.07292600	-0.81310700	0.25589300
O	4.20830300	-0.04723200	-0.05851600
O	3.31562400	-2.25681600	-0.26607900
O	2.49729300	-0.84324000	1.54861100
C	-4.23640800	-0.56262700	-0.14160500
C	-5.07061500	-0.77016100	-1.37564000
C	0.70718400	-0.97450100	-0.80859200
C	-2.08304500	0.34656300	0.56098800
C	-0.93915400	0.93950500	-0.29503200
O	0.63197400	-2.12817400	-0.50841100
O	1.91196200	-0.29518900	-0.74746000
H	-6.00482800	-1.24594200	-1.10073200
H	-4.52610100	-1.39189100	-2.08383400
H	-5.25959400	0.18823000	-1.85507600
H	2.47979600	-2.75594700	-0.18472700
O	-4.55876100	-0.88915200	0.96535200
O	-3.07970500	0.04195400	-0.45380800
C	-2.64765500	1.39630700	1.51132200
H	-2.82273500	2.33806400	0.99038500
H	-3.58161100	1.03968800	1.93523600
H	-1.95355700	1.56964200	2.33138800
C	-1.66909700	-0.91768800	1.30723700
H	-1.56181400	-1.75425200	0.61987600
H	-0.71010900	-0.76311300	1.80301700
H	-2.40953400	-1.17844500	2.05628800
C	-0.37834500	-0.08140000	-1.32164200
H	-1.18402700	-0.71251300	-1.68405900
H	0.04479500	0.48168900	-2.15228600
C	0.14095400	1.60681200	0.55361300
H	-0.30306800	2.38924200	1.17005700
H	0.64002100	0.91834400	1.23518600
C	1.18895600	2.29402300	-0.28569200
O	2.33168900	2.44533400	0.39192300
H	2.98084200	2.85722400	-0.19381300
O	1.03258700	2.67860900	-1.41024600
H	-1.39965600	1.71993400	-0.90187400

Table S16. Geometry of DTASA-5-H_2O. Units are in angstrom.

Atom	X	Y	Z
S	3.13684100	-0.24296000	-0.04130100
O	3.98841200	0.82973400	-0.37006400
O	3.60168300	-1.50765000	-0.75880100
O	2.77557500	-0.53742300	1.30219100
C	-4.41257000	-0.73926100	-0.28283200
C	-5.15774900	-0.94019700	-1.57391100
C	0.64147700	-0.65956100	-0.76789100
C	-2.36376600	0.27353900	0.58324100
C	-1.23086000	0.99851400	-0.17883400
O	0.67269200	-1.79237100	-0.38770900
O	1.75890400	0.13085800	-0.82524600
H	-6.09527600	-1.44514400	-1.37209100
H	-4.55054900	-1.53764500	-2.25194600
H	-5.33634700	0.02112700	-2.05078600
H	3.28911200	-2.34687600	-0.25058100
O	-4.77401900	-1.14452400	0.78569700
O	-3.28503700	-0.04471700	-0.49693500
C	-3.05259000	1.22479900	1.55676800
H	-3.26175800	2.18227800	1.07899600
H	-3.98263100	0.78585800	1.90434500
H	-2.42246800	1.39566100	2.42741300
C	-1.89630700	-0.99779100	1.28162300
H	-1.63103900	-1.76275800	0.55486200
H	-1.01398200	-0.78352000	1.88499200
H	-2.67584600	-1.38447800	1.92996100
C	-0.55768400	0.10185200	-1.25434700
H	-1.27873100	-0.61436400	-1.63693000
H	-0.22202400	0.74712000	-2.06307000
C	-0.22000500	1.66480300	0.75064700
H	-0.72861100	2.32524000	1.45349500
H	0.34970500	0.95216900	1.34835200
C	0.75378000	2.53713400	-0.00533600
O	1.87346400	2.73265100	0.69666300
H	2.49834800	3.22531400	0.14760600
O	0.55649900	3.01291100	-1.08736500
H	-1.72086800	1.79480800	-0.73985800
O	2.69363600	-3.44051700	0.59945700
H	2.90211200	-3.19991200	1.50833800
H	1.77455400	-3.16212600	0.46985100

Table S17. Geometry of DTASA-5-NH_3. Units are in angstrom.

Atom	X	Y	Z
S	3.17495700	-0.29587000	-0.08264300
O	3.97016900	0.85804200	-0.29404400
O	3.59590500	-1.48548400	-0.82326900
O	2.77700900	-0.61034400	1.26908700
C	-4.40922500	-0.72976100	-0.27858900
C	-5.17319300	-0.90111700	-1.56363100
C	0.65374600	-0.63258800	-0.80268300
C	-2.35409900	0.27577500	0.58283700
C	-1.22870700	1.01319600	-0.17795000
O	0.66928700	-1.78704200	-0.46289100
O	1.74567400	0.15250800	-0.82096300
H	-6.10562200	-1.41528400	-1.36122300
H	-4.57337400	-1.47706100	-2.26632600
H	-5.36269900	0.07145400	-2.01273400
H	3.08984100	-2.70133100	-0.07017300
O	-4.75696800	-1.16434800	0.78394900
O	-3.28917600	-0.02777500	-0.49163500
C	-3.03777100	1.20694000	1.57898400
H	-3.25285400	2.17209100	1.11968700
H	-3.96367200	0.75961900	1.92735800
H	-2.39928300	1.36477200	2.44586800
C	-1.87707000	-1.00611500	1.25515200
H	-1.61380300	-1.75463600	0.51078900
H	-0.98817200	-0.79650300	1.85038200
H	-2.64861300	-1.40629600	1.90508300
C	-0.55854200	0.13209000	-1.26697900
H	-1.28070300	-0.57932100	-1.65672600
H	-0.23126700	0.79076000	-2.06814000
C	-0.21789800	1.66920800	0.75914500
H	-0.72479900	2.32607700	1.46661400
H	0.34967000	0.94797400	1.34815700
C	0.76707600	2.54003200	0.01527700
O	1.87334700	2.73251800	0.73530700
H	2.53503600	3.16576000	0.17964800
O	0.58299800	3.01781600	-1.06890400
H	-1.72571700	1.81625300	-0.72349500
N	2.58828900	-3.30828700	0.68154500
H	1.66527700	-3.53569000	0.31946200
H	2.47304900	-2.62398200	1.43783000
H	3.10850800	-4.12580500	0.97692800

Table S18. Geometry of DTASA-5-DMA. Units are in angstrom.

Atom	X	Y	Z
S	-2.87103500	-0.65437300	-0.26336600
O	-3.40065800	-1.96495900	-0.38924000
O	-3.48199500	0.35355700	-1.12163200
O	-2.60146200	-0.15587500	1.06372200
C	4.51693100	1.23031800	-0.27573100
C	5.30904500	1.40584000	-1.54305900
C	-0.42401000	0.11362800	-0.91633500
C	2.64446100	-0.05441600	0.62612900
C	1.70948200	-1.05852300	-0.08654500
O	-0.67440900	1.26417300	-0.65675500
O	-1.33764100	-0.86635200	-0.91682900
H	6.07081200	2.16140300	-1.38872800
H	4.64487000	1.69834200	-2.35395900
H	5.76750100	0.45839900	-1.81969400
H	-3.22237900	1.75530700	-0.38355200
O	4.72018400	1.83050300	0.74285600
O	3.56022400	0.30989000	-0.44621300
C	3.43907800	-0.73951500	1.73330100
H	3.84976300	-1.68697200	1.38325800
H	4.24939300	-0.09311000	2.05767300
H	2.80006800	-0.93014300	2.59328400
C	1.90968100	1.17497900	1.14765600
H	1.56708100	1.79665100	0.32328200
H	1.03450800	0.86046100	1.71587200
H	2.55507200	1.76296600	1.79202400
C	0.93772800	-0.42353600	-1.27628400
H	1.52369400	0.38621500	-1.70119200
H	0.79142000	-1.19625500	-2.02720900
C	0.79375700	-1.79901900	0.88450000
H	1.37744800	-2.26416900	1.67911200
H	0.06387500	-1.14733300	1.36681900
C	0.03668500	-2.91813800	0.20813300
O	-1.04660700	-3.25414400	0.90988100
H	-1.58899500	-3.85227800	0.37819500
O	0.36614700	-3.45403500	-0.81239100
H	2.36977800	-1.80307100	-0.53271000
N	-2.92876600	2.51403300	0.29800300
H	-2.09143400	2.08247100	0.69780600
C	-3.97274400	2.67454700	1.32803600
H	-4.88286600	3.02668700	0.85042700
H	-3.64211300	3.39712300	2.06977800

H	-4.13786100	1.70469000	1.78680300
C	-2.57166500	3.74860700	-0.42268800
H	-3.45251400	4.11899100	-0.93987500
H	-1.78893300	3.50982700	-1.13519800
H	-2.22110500	4.49484600	0.28575400

Table S19. Geometry of DTASA-5-SA. Units are in angstrom.

Atom	X	Y	Z
S	-1.36621800	2.34999200	0.16626800
O	-2.72360200	1.95659800	0.22917000
O	-1.26611900	3.45923100	-0.91216400
O	-0.62729300	2.69329500	1.31787800
C	5.28868000	-0.85672900	-0.63559200
C	5.77858100	-1.48371400	-1.91110900
C	0.71529600	1.23952100	-0.92494400
C	3.22874600	-0.46237700	0.61440900
C	1.76751600	-0.80132300	0.23421100
O	1.20127500	2.31352400	-1.09663800
O	-0.62086600	1.11580700	-0.54444700
H	6.85436300	-1.36878900	-1.97550700
H	5.29796200	-1.00570600	-2.76266800
H	5.50866200	-2.53780300	-1.92827000
H	-0.32563000	3.68168000	-1.04877800
O	5.98486500	-0.31274200	0.17291700
O	3.95575000	-0.99298300	-0.52632700
C	3.64894000	-1.22069300	1.86885300
H	3.35100300	-2.26776000	1.80688100
H	4.72629300	-1.16083500	1.98824800
H	3.19342200	-0.77460100	2.75077400
C	3.46991700	1.03614500	0.75877900
H	3.42110800	1.53324700	-0.20800700
H	2.71138900	1.47669100	1.40598800
H	4.44570900	1.22384100	1.19459800
C	1.33072000	-0.11337900	-1.08982000
H	2.18826300	-0.01235100	-1.74779700
H	0.58090800	-0.74263600	-1.56582100
C	0.79472900	-0.57495800	1.38953800
H	1.10863500	-1.15429600	2.25889500
H	0.74528900	0.46481200	1.71507500
C	-0.60917700	-1.03073100	1.08749500
O	-1.50176200	-0.45548900	1.84710200
H	-2.42478900	-0.73865600	1.60904200
O	-0.86024100	-1.85660800	0.22700400
H	1.76268900	-1.86830700	0.00997000

S	-4.16053300	-1.43618800	-0.34874900
O	-5.44893400	-1.82967300	-0.75592800
O	-3.92850000	-1.08481200	1.03055700
O	-3.16610200	-2.53317500	-0.76630200
H	-2.26053200	-2.33389200	-0.38287600
O	-3.68144200	-0.22042900	-1.21033000
H	-3.47664100	0.55356700	-0.65089700

Table S20. Geometry of DTAA-H_2O. Units are in angstrom

Atom	X	Y	Z
C	-3.65042900	-0.31191300	0.45881700
C	-4.36847500	-0.04603900	1.75407000
C	0.72786300	1.96828200	-0.18176500
C	-1.39660700	-0.59131200	-0.43676000
C	-0.02752500	-0.45682500	0.27262500
O	0.12182700	3.16488500	-0.08181100
O	1.62398800	1.77658500	-0.95802800
H	-5.43588400	-0.00541900	1.57064400
H	-4.02141000	0.89427600	2.17810900
H	-4.13752800	-0.83463500	2.46756900
H	0.55468300	3.75660100	-0.71133000
O	-4.18996200	-0.46308300	-0.60161900
O	-2.32683000	-0.35832000	0.65845400
C	-1.60832500	-2.00175200	-0.97294600
H	-1.37714500	-2.74170200	-0.20598000
H	-2.63847300	-2.12530000	-1.29308200
H	-0.96421200	-2.17533600	-1.83289000
C	-1.58321500	0.45888000	-1.52837400
H	-1.71262500	1.44865800	-1.09071600
H	-0.70442900	0.48042000	-2.17211900
H	-2.45649100	0.23600800	-2.13259500
C	0.19328300	0.96982900	0.80801700
H	-0.72847200	1.34842600	1.24025800
H	0.94120000	0.92496500	1.59958500
C	1.11094900	-1.00147900	-0.59231500
H	0.98639000	-2.07787400	-0.72379200
H	1.13631400	-0.56389300	-1.58693100
C	2.48005200	-0.83052000	0.00806300
O	3.44046000	-1.02701300	-0.87986500
H	4.30924700	-0.92298500	-0.43551600
O	2.69082300	-0.59441400	1.17805300
H	-0.09315000	-1.09244600	1.15742600
O	5.45007900	-0.64336000	0.93354900

H	4.63576400	-0.50189500	1.44152500
H	5.95770600	0.16700400	1.00338200

Table S21. Geometry of DTAA-NH_3. Units are in angstrom

Atom	X	Y	Z
C	-3.65458700	-0.36966100	0.45284100
C	-4.37530700	-0.11946700	1.75021700
C	0.63963800	2.01400900	-0.16185000
C	-1.39528700	-0.60174400	-0.44621600
C	-0.02931800	-0.44483800	0.26377500
O	0.00817000	3.19337300	-0.00558300
O	1.51119400	1.87016400	-0.97502900
H	-5.44363500	-0.09714000	1.56886700
H	-4.04379700	0.82588000	2.17552000
H	-4.12904700	-0.90531100	2.46161100
H	0.40697300	3.81181000	-0.63188000
O	-4.19491000	-0.52663200	-0.60674900
O	-2.33138600	-0.39411500	0.65070200
C	-1.58037800	-2.01294200	-0.99033100
H	-1.32469200	-2.75262200	-0.23091500
H	-2.61043800	-2.15769400	-1.30211700
H	-0.93986200	-2.16516700	-1.85688400
C	-1.60514000	0.44959700	-1.53206400
H	-1.74930700	1.43514000	-1.08919100
H	-0.72896000	0.48805500	-2.17827000
H	-2.47734300	0.21479900	-2.13345100
C	0.16242400	0.97813900	0.81825000
H	-0.75800100	1.32131200	1.28192700
H	0.93271000	0.93753600	1.58875000
C	1.12534900	-0.95433700	-0.59954800
H	1.00710200	-2.02496200	-0.77440800
H	1.16862600	-0.47805900	-1.57553200
C	2.48417400	-0.80331800	0.03870300
O	3.46280200	-0.99816600	-0.82591700
H	4.33648700	-0.89792400	-0.35171000
O	2.66335900	-0.57955900	1.21517300
H	-0.08161100	-1.09061500	1.14240500
N	5.63345500	-0.60560500	0.78091600
H	6.15873100	0.25256400	0.66996400
H	6.28394000	-1.33566000	1.04167700
H	4.97469500	-0.47585600	1.54377900

Table S22. Geometry of DTAA-DMA. Units are in angstrom.

Atom	X	Y	Z
C	-4.33408000	-0.22075400	0.49257200
C	-5.03526100	0.09551000	1.78608000
C	0.13713200	1.87142900	-0.23615400
C	-2.09801600	-0.60931400	-0.40746200
C	-0.71931900	-0.50859800	0.28727800
O	-0.46297900	3.07620500	-0.21922200
O	1.06188400	1.63970200	-0.96762400
H	-6.10072000	0.17881300	1.60532300
H	-4.64715200	1.02612400	2.19562300
H	-4.83583800	-0.69183200	2.51046600
H	-0.00387100	3.63113800	-0.86320200
O	-4.88617900	-0.37137000	-0.56182400
O	-3.01321100	-0.31333500	0.68666700
C	-2.36946100	-2.02369800	-0.90467900
H	-2.16215300	-2.75145400	-0.11954000
H	-3.40607300	-2.11422400	-1.21526100
H	-1.73881100	-2.24608800	-1.76326600
C	-2.25360900	0.41900700	-1.52469400
H	-2.35724000	1.42171000	-1.11087000
H	-1.37221200	0.40204400	-2.16532700
H	-3.13062300	0.20574200	-2.12709100
C	-0.44021800	0.92522100	0.77951200
H	-1.34554200	1.35407800	1.19914000
H	0.30867500	0.86846600	1.56893800
C	0.39084800	-1.12051000	-0.56843200
H	0.22385200	-2.19382600	-0.67131900
H	0.42099500	-0.71033200	-1.57509200
C	1.77588200	-0.97530500	0.01360000
O	2.71760100	-1.24575500	-0.86681900
H	3.61721700	-1.05836000	-0.43759900
O	2.00043000	-0.68050000	1.16770100
H	-0.80122500	-1.11318100	1.19226400
N	4.85012100	-0.37340300	0.45627500
H	4.41429500	-0.55413200	1.35476000
C	4.68219200	1.04069300	0.12966700
H	5.05382800	1.21594800	-0.87957100
H	5.22638100	1.69663100	0.81667800
H	3.62286100	1.29120800	0.15336900
C	6.24550900	-0.78944500	0.46397300
H	6.65322100	-0.69186300	-0.54161200
H	6.31878800	-1.83304700	0.76160600
H	6.86053800	-0.18474100	1.13906200

Table S23. Geometry of DTAA-SA. Units are in angstrom.

Atom	X	Y	Z
C	-4.98160900	-0.38274500	0.85459000
C	-5.47614200	-0.22154000	2.26587000
C	-0.75035100	1.99128900	-0.33155000
C	-2.90716500	-0.56399900	-0.41819900
C	-1.43927900	-0.45932800	0.06298100
O	-1.34574200	3.16992900	-0.08977800
O	0.03931300	1.84851700	-1.22571900
H	-6.55984800	-0.21257000	2.26675300
H	-5.09226200	0.70832900	2.68173600
H	-5.10285100	-1.03722500	2.88159300
H	-1.00321400	3.80307000	-0.73510400
O	-5.68653200	-0.45943200	-0.11201000
O	-3.64152400	-0.42745600	0.82951100
C	-3.19913000	-1.93530400	-1.01510600
H	-2.83937400	-2.72497500	-0.35466100
H	-4.26810400	-2.05308600	-1.16509000
H	-2.71208900	-2.03731100	-1.98320500
C	-3.27610000	0.56073800	-1.38209800
H	-3.34034100	1.51292900	-0.85565100
H	-2.51644900	0.65000800	-2.15822200
H	-4.23457400	0.36752200	-1.85224200
C	-1.14176000	0.92930800	0.65899800
H	-1.99310900	1.26835200	1.24167900
H	-0.29145300	0.84315300	1.33490200
C	-0.46533100	-0.92060500	-1.02499000
H	-0.59526400	-1.99121600	-1.19734200
H	-0.62609200	-0.42774500	-1.98011200
C	0.98501200	-0.75549000	-0.67981500
O	1.77248300	-0.82927600	-1.71604500
H	2.71857300	-0.74771600	-1.45210900
O	1.38140500	-0.62914800	0.47150000
H	-1.35416000	-1.16168000	0.89363600
S	4.78408300	-0.25095200	0.41059800
O	6.03423100	-0.69559200	0.89777800
O	4.32959600	-0.63658800	-0.89025200
O	4.79505100	1.32628700	0.36700000
O	3.70471100	-0.57699100	1.44415500
H	5.34631100	1.66353300	1.08470600
H	2.76613700	-0.58409200	1.02594700

Table S24. Geometry of SA-H_2O. Units are in angstrom.

Atom	X	Y	Z
S	0.57427700	-0.07595500	0.12159100
O	-0.21560500	0.28880800	1.24846000
O	1.73770000	-0.87044400	0.24743700
O	-0.33853300	-0.73229600	-0.94176200
O	0.97912100	1.29126500	-0.55273900
H	-1.28989000	-0.46901700	-0.77380000
H	1.73614800	1.15035600	-1.13565000
O	-2.66195900	0.10598500	-0.10975800
H	-2.25927400	0.36134000	0.73181200
H	-3.38119900	-0.49394900	0.09908600

Table S25. Geometry of SA-NH_3. Units are in angstrom.

Atom	X	Y	Z
S	-0.59870500	-0.11256700	0.08524700
O	0.10265000	-0.10743600	1.32425800
O	-1.75716300	-0.90622700	-0.10955500
O	0.38798200	-0.38892900	-1.05713200
O	-1.00872200	1.40007000	-0.15516000
H	1.36768300	-0.20347800	-0.74044000
H	-1.74400800	1.42970200	-0.77955700
N	2.73195900	0.04327500	-0.05125300
H	3.19562900	0.91429100	-0.27855800
H	3.40590000	-0.70670600	-0.14509700
H	2.43238300	0.08452300	0.91917700

Table S26. Geometry of SA-DMA. Units are in angstrom.

Atom	X	Y	Z
S	-1.26717000	-0.17444900	0.04935400
O	-0.55303500	0.01477400	1.29329000
O	-2.47253700	-0.93652700	0.07870500
O	-1.69112200	1.32457000	-0.34716300
H	-2.47666900	1.27230700	-0.90279200
O	-0.33408600	-0.58638100	-1.02046000
H	1.04041000	-0.40387800	-0.47189000
N	1.89038900	-0.11189200	0.15003100
H	1.50173900	-0.28839600	1.08018800
C	2.05507200	1.34602100	-0.01704800

H	2.34477000	1.54536200	-1.04521900
H	2.81928400	1.71350900	0.66344800
H	1.09835400	1.81525600	0.19621800
C	3.10083700	-0.90096300	-0.11961800
H	3.40294100	-0.73456800	-1.15005600
H	2.87986900	-1.95367900	0.02709200
H	3.90207800	-0.59331900	0.54813300

Table S27. Geometry of SA-SA. Units are in angstrom.

Atom	X	Y	Z
S	-2.03548700	-0.07317300	0.11417400
O	-1.06716200	0.08449600	1.15674100
O	-3.31102400	-0.60315200	0.39613000
O	-2.18063600	1.36956700	-0.49185400
H	-2.95953500	1.41530400	-1.06305500
O	-1.42366900	-0.89022200	-1.03840600
H	-0.46245000	-0.65740800	-1.15787100
O	1.06711100	-0.08504100	-1.15665100
S	2.03544700	0.07316900	-0.11418100
O	1.42339800	0.89015600	1.03831400
O	3.31076000	0.60360000	-0.39631800
O	2.18123300	-1.36941800	0.49205900
H	0.46224000	0.65707100	1.15783700
H	2.96028900	-1.41477800	1.06307600