

Supporting information

-for-

Mechanistic insights into 2-methylglyceric acid enhanced sulfuric acid-dimethylamine particle nucleation in forested and urban industrial regions

Kaiyu Xue ‡, Yaogeng Li ‡, Chengyan Zhang, Heran Cui, Xueping Feng, Jiating Liu, Zhihui Liu, Rui Wang*, Tianlei Zhang*,

Shaanxi Key Laboratory of Catalysis, School of Chemical & Environment Science, Shaanxi University of Technology, Hanzhong, Shaanxi 723001, P. R. China

S. NO	Caption
S3	Figure. S1 The optimized geometries of the important precursors of atmospheric aerosol nucleation (SA, DMA and MGA), especially the main bond lengths and bond angles at two different theoretical levels. MGA, SA and DMA are the shorthand for 2-methylglyceric acid, sulfuric acid, and dimethylamine, respectively. a The values obtained at the M06-2X/6-311+G(2d,2p) level of theory. b The values obtained at the M06-2X/6-311++G(3df,3p d) level of theory. Bond length is in angstrom and angle is in degree.
S4	Table S1 Comparison of calculated formation free energies (ΔG) at the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311+G(2d, 2p) and the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(3df, 3pd) levels.
S5	Table S2 The actual Gibbs free energies (ΔG_{actual} , kcal·mol ⁻¹) of MGA-SA-DMA-based clusters along the main nucleation pathways were calculated at 1 atm and temperatures of 238.15, 258.15 and 278.15 K with fixed concentrations of [SA] = 10 ⁷ molecules·cm ⁻³ and [DMA] = 10 ⁹ molecules·cm ⁻³ , and varying [MGA] (10 ⁹ and 10 ¹⁰ molecules·cm ⁻³).
S6	Table S3 The Gibbs free energy (ΔG , kcal·mol ⁻¹) of MGA-SA-DMA-based clusters at 1 atm and temperatures of 278.15, 268.15, 258.15, 248.15 and 238.15 K
S7-S8	Table S4 Collision coefficients (β , cm ³ ·s ⁻¹) for each cluster investigated in the present study of MGA-SA-DMA system
S9-S11	Table S5 Evaporation rates (s ⁻¹) of the studied clusters in MGA-SA-DMA system at different temperatures of 278.15, 268.15, 258.15, 248.15 and 238.15 K
S12	Table S6 Total evaporation coefficients ($\sum \gamma$, s ⁻¹) for each cluster analyzed in the present study of MGA-SA-DMA system

S13-S14	Table S7 Ratios ($\beta C/\Sigma\gamma$) between monomer molecule collisions and evaporation coefficients for each cluster involving MGS in the present study. [SA] = 1.0×10^6 molecules·cm ⁻³ , [DMA] = 1.0×10^9 molecules·cm ⁻³ , [MGA] = 1.0×10^{10} molecules·cm ⁻³
S15	Figure S2 The influence of (a) [MGA], (b) [SA] and (c) [DMA] on the relative contribution of the pure SA-DMA-based clustering route and the MGA participation route to the system flux is analyzed at $T = 238.15$ K.
S17	Figure S3 (a) The cluster formation rate J (cm ⁻³ s ⁻¹) and (b) the enhancement strength R of MGA are presented [MGA] from 10^8 to 10^{10} molecules·cm ⁻³ under different temperatures (238.15, 248.15, 258.15, 268.15 and 278.15 K) where [SA] = 10^6 molecules·cm ⁻³ and [DMA] = 10^9 molecules·cm ⁻³ . (c) The cluster formation rates J (cm ⁻³ s ⁻¹) and (d) the enhancement strength R as a function of [DMA] with [MGA] = 10^{11} molecules·cm ⁻³ and three different [SA] at 258.15 K
S18	Table S8 Formation rate J (cm ⁻³ s ⁻¹) of MGA at $T = 238.15$ K, with [SA] = 10^6 - 10^8 molecules·cm ⁻³ , [DMA] = 10^7 - 10^{11} molecules·cm ⁻³ , and [MGA] = 0, 10^8 - 10^{10} molecules·cm ⁻³ . SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.
S19	Table S9 Formation rate J (cm ⁻³ s ⁻¹) of MGA at $T = 248.15$ K, with [SA] = 10^6 - 10^8 molecules·cm ⁻³ , [DMA] = 10^7 - 10^{11} molecules·cm ⁻³ , and [MGA] = 0, 10^8 - 10^{10} molecules·cm ⁻³ . SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.
S20	Table S10 Formation rate J (cm ⁻³ s ⁻¹) of MGA at $T = 258.15$ K, with [SA] = 10^6 - 10^8 molecules·cm ⁻³ , [DMA] = 10^7 - 10^{11} molecules·cm ⁻³ , and [MGA] = 0, 10^8 - 10^{10} molecules·cm ⁻³ . SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.
S21	Table S11 Formation rate J (cm ⁻³ s ⁻¹) of MGA at $T = 268.15$ K, with [SA] = 10^6 - 10^8 molecules·cm ⁻³ , [DMA] = 10^7 - 10^{11} molecules·cm ⁻³ , and [MGA] = 0, 10^8 - 10^{10} molecules·cm ⁻³ . SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.
S22	Table S12 Formation rate J (cm ⁻³ s ⁻¹) of MGA at $T = 278.15$ K, with [SA] = 10^6 - 10^8 molecules·cm ⁻³ , [DMA] = 10^7 - 10^{11} molecules·cm ⁻³ , and [MGA] = 0, 10^8 - 10^{10} molecules·cm ⁻³ . SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.
S23-S51	Table S13 Cartesian coordinates of all molecules and clusters in the studied system.

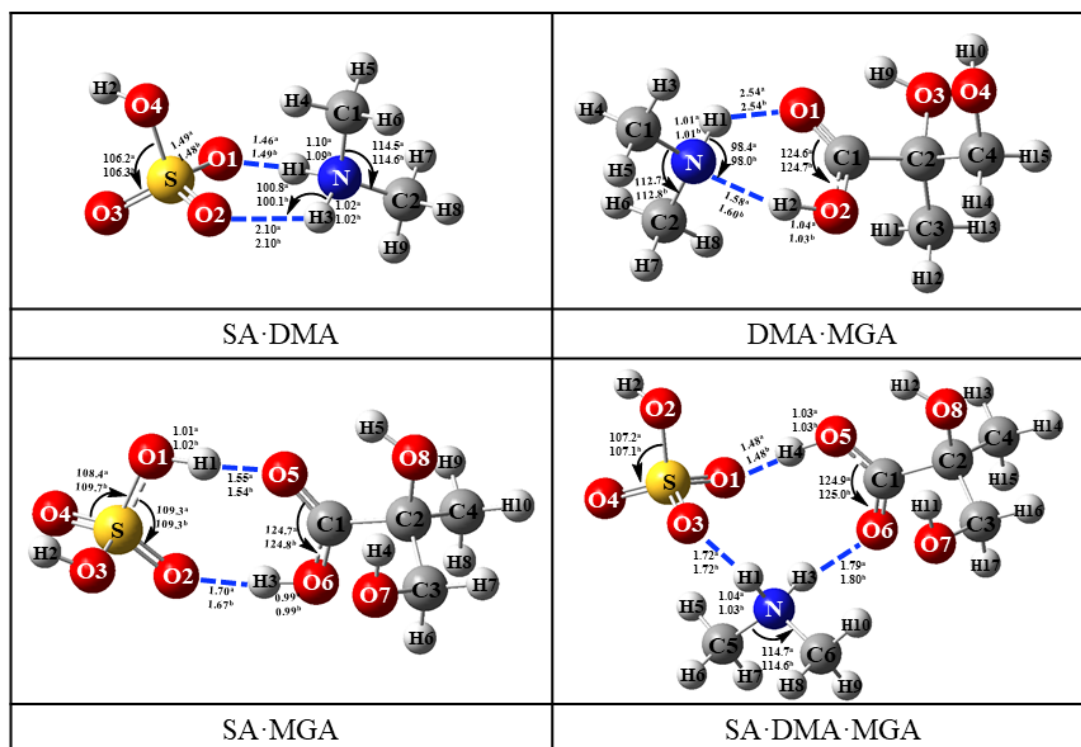


Figure. S1 The optimized geometries of the important precursors of atmospheric aerosol nucleation (SA, DMA and MGA), especially the main bond lengths and bond angles at two different theoretical levels. MGA, SA and DMA are the shorthand for 2-methylglyceric acid, sulfuric acid, and dimethylamine, respectively. ^a The values obtained at the M06-2X/6-311+G(2d,2p) level of theory. ^b The values obtained at the M06-2X/6-311++G(3df,3pd) level of theory. Bond length is in angstrom and angle is in degree.

Table S1 Comparison of calculated formation free energies (ΔG) at the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311+G(2*d*, 2*p*) and the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(3*df*, 3*pd*) levels.

Cluster	DLPNO-CCSD(T)/aug-cc- pVTZ//M06-2X/6-311+G(2 <i>d</i> , 2 <i>p</i>)	DLPNO-CCSD(T)/aug-cc- pVTZ//M06-2X/6-311++G(3 <i>df</i> , 3 <i>pd</i>)
	kcal·mol ⁻¹	
SA·DMA	-13.61	-13.53
SA·MGA	-8.43	-8.21
DMA·MGA	-5.08	-5.22
SA·DMA·MGA	-23.62	-23.85

Table S2 The actual Gibbs free energies (ΔG_{actual} , kcal·mol⁻¹) of MGA-SA-DMA-based clusters along the main nucleation pathways were calculated at 1 atm and temperatures of 238.15, 258.15 and 278.15 K with fixed concentrations of [SA] = 10⁷ molecules·cm⁻³ and [DMA] = 10⁹ molecules·cm⁻³, and varying [MGA] (10⁹ and 10¹⁰ molecules·cm⁻³).

Clusters	$T = 238.15$ K	$T = 258.15$ K	$T = 278.15$ K
SA	15.00	15.89	17.08
SA·DMA	11.82	14.63	17.44
(SA) ₂ ·DMA	4.40	9.33	14.25
(SA) ₂ ·(DMA) ₂	-2.56	4.00	10.54
(SA) ₃ ·(DMA) ₂	-5.53	3.06	11.63
(SA) ₃ ·(DMA) ₃	-14.41	-4.19	6.00
SA·MGA	15.88	18.63	-
SA·DMA·MGA	11.34	15.79	-
(SA) ₂ ·DMA·MGA	14.22	17.73	-
(SA) ₂ ·(DMA) ₂ ·MGA	6.12	10.47	-

Table S3 The Gibbs free energy (ΔG , kcal·mol⁻¹) of MGA-SA-DMA-based clusters at 1 atm and temperatures of 278.15, 268.15, 258.15, 248.15 and 238.15 K

Clusters	$T = 278.15$ K	$T = 268.15$ K	$T = 258.15$ K	$T = 248.15$ K	$T = 238.15$ K
SA·DMA	-12.91	-13.26	-13.61	-13.96	-14.31
(SA) ₂	-9.41	-9.72	-10.03	-10.35	-10.66
(SA) ₂ ·DMA	-33.18	-33.99	-34.80	-35.62	-36.43
(SA) ₂ ·(DMA) ₂	-50.15	-51.31	-52.48	-53.65	-54.82
(SA) ₃	-14.35	-15.11	-15.88	-16.65	-17.42
(SA) ₃ ·DMA	-46.25	-47.44	-48.64	-49.83	-51.03
(SA) ₃ ·(DMA) ₂	-66.14	-67.72	-69.31	-70.90	-72.49
(SA) ₃ ·(DMA) ₃	-85.03	-86.97	-88.91	-90.85	-92.80
(MGA) ₂	-5.91	-6.36	-6.80	-7.24	-7.69
DMA·MGA	-4.36	-4.72	-5.08	-5.43	-5.79
(DMA) ₂ ·(MGA) ₂	-17.61	-18.86	-20.10	-21.35	-22.60
DMA·(MGA) ₂	-7.80	-8.64	-9.48	-10.32	-11.16
SA·MGA	-7.71	-8.07	-8.43	-8.80	-9.16
SA·DMA·MGA	-22.11	-22.86	-23.62	-24.37	-25.13
SA·(DMA) ₂ ·MGA	-31.25	-32.40	-33.56	-34.72	-35.88
(MGA) ₃	-10.81	-11.71	-12.61	-13.51	-14.41
SA ₂ ·DMA·MGA	-29.17	-30.36	-31.56	-32.75	-33.95
(SA) ₂ ·(DMA) ₂ ·MGA	-50.12	-51.71	-52.79	-54.89	-56.48
(SA) ₂ ·(DMA) ₃ ·MGA	-57.36	-59.36	-61.37	-63.38	-65.40
SA·(MGA) ₂	-16.05	-16.92	-17.78	-18.64	-19.51
DMA·(MGA) ₃	-10.60	-11.87	-13.13	-14.40	-15.67
SA·(DMA) ₂ ·(MGA) ₂	-39.08	-40.71	-42.35	-43.99	-45.63
(SA) ₂ ·MGA	-15.15	-15.88	-16.61	-17.34	-18.08
SA·DMA·(MGA) ₂	-25.27	-26.54	-27.81	-29.08	-30.35
(DMA) ₂ ·(MGA) ₃	-27.44	-29.09	-30.75	-32.40	-34.07
SA·(DMA) ₃ ·(MGA) ₂	-41.28	-43.34	-45.41	-47.48	-49.55
(DMA) ₃ ·(MGA) ₃	-29.88	-31.95	-34.02	-36.10	-38.18

*Calculated at M06-2X/6-311+G(2d,2p) level of theory.

Table S4 Collision coefficients (β , $\text{cm}^3\cdot\text{s}^{-1}$) for each cluster investigated in the present study of MGA-SA-DMA system

Collisions	β , $\text{cm}^3\cdot\text{s}^{-1}$				
	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
SA + DMA	1.18×10^{-10}	1.14×10^{-10}	1.10×10^{-10}	1.06×10^{-10}	1.02×10^{-10}
SA + MGA	7.53×10^{-11}	7.27×10^{-11}	7.01×10^{-11}	6.74×10^{-11}	6.48×10^{-11}
MGA + DMA	1.39×10^{-10}	1.34×10^{-10}	1.30×10^{-10}	1.25×10^{-10}	1.20×10^{-10}
SA + SA	6.55×10^{-11}	6.32×10^{-11}	6.09×10^{-11}	5.87×10^{-11}	5.64×10^{-11}
MGA + MGA	8.36×10^{-11}	8.07×10^{-11}	7.78×10^{-11}	7.49×10^{-11}	7.20×10^{-11}
(SA) ₂ + DMA	1.64×10^{-10}	1.58×10^{-10}	1.52×10^{-10}	1.47×10^{-10}	2.31×10^{-10}
SA·DMA + SA	9.22×10^{-11}	8.90×10^{-11}	8.58×10^{-11}	8.26×10^{-11}	7.94×10^{-11}
(SA) ₂ ·A + DMA	1.67×10^{-10}	1.61×10^{-10}	1.55×10^{-10}	1.50×10^{-10}	1.44×10^{-10}
(MGA) ₂ + DMA	2.17×10^{-10}	2.10×10^{-10}	2.02×10^{-10}	1.95×10^{-10}	1.87×10^{-10}
MGA·DMA + MGA	1.12×10^{-10}	1.08×10^{-10}	1.04×10^{-10}	1.01×10^{-10}	9.67×10^{-11}
(MGA) ₂ ·A + DMA	2.10×10^{-10}	2.02×10^{-10}	1.95×10^{-10}	1.88×10^{-10}	1.81×10^{-10}
(SA) ₂ + MGA	8.75×10^{-11}	8.45×10^{-11}	8.14×10^{-11}	7.84×10^{-11}	7.54×10^{-11}
SA·MGA + SA	1.00×10^{-10}	9.66×10^{-11}	9.31×10^{-11}	8.96×10^{-11}	8.62×10^{-11}
(MGA) ₂ + SA	1.09×10^{-10}	1.05×10^{-10}	1.01×10^{-10}	9.74×10^{-11}	9.36×10^{-11}
SA·MGA + MGA	1.03×10^{-10}	9.95×10^{-11}	9.59×10^{-11}	9.24×10^{-11}	8.88×10^{-11}
(SA) ₂ + SA	8.30×10^{-11}	8.01×10^{-11}	7.72×10^{-11}	7.43×10^{-11}	7.15×10^{-11}
(MGA) ₂ + MGA	1.11×10^{-10}	1.07×10^{-10}	1.03×10^{-10}	9.90×10^{-11}	9.52×10^{-11}
SA + (SA) ₂ ·DMA	8.25×10^{-11}	7.97×10^{-11}	7.68×10^{-11}	7.39×10^{-11}	7.39×10^{-11}
(SA) ₃ + DMA	2.12×10^{-10}	2.04×10^{-10}	1.97×10^{-10}	1.90×10^{-10}	1.82×10^{-10}
(SA) ₂ ·(DMA) ₂ + SA	9.42×10^{-11}	9.09×10^{-11}	8.77×10^{-11}	8.44×10^{-11}	8.11×10^{-11}
(SA) ₃ ·DMA + DMA	1.59×10^{-10}	1.54×10^{-10}	1.48×10^{-10}	1.43×10^{-10}	1.37×10^{-10}
(SA) ₃ ·(DMA) ₂ + DMA	2.41×10^{-10}	2.32×10^{-10}	2.24×10^{-10}	2.16×10^{-10}	2.07×10^{-10}
(MGA) ₂ ·DMA + MGA	1.04×10^{-10}	1.00×10^{-10}	9.65×10^{-11}	9.29×10^{-11}	8.93×10^{-11}
(MGA) ₃ + DMA	2.32×10^{-10}	2.24×10^{-10}	2.16×10^{-10}	2.08×10^{-10}	2.00×10^{-10}
(MGA) ₂ ·(DMA) ₂ + MGA	1.00×10^{-10}	9.70×10^{-11}	9.35×10^{-11}	9.00×10^{-11}	8.65×10^{-11}
(MGA) ₃ ·DMA + DMA	2.21×10^{-10}	2.14×10^{-10}	2.06×10^{-10}	1.98×10^{-10}	1.91×10^{-10}
(MGA) ₃ ·(DMA) ₂ + DMA	2.62×10^{-10}	2.53×10^{-10}	2.44×10^{-10}	2.35×10^{-10}	2.26×10^{-10}
MGA·DMA + SA	1.07×10^{-10}	1.04×10^{-10}	9.99×10^{-11}	9.62×10^{-11}	9.25×10^{-11}
SA·DMA + MGA	9.89×10^{-11}	9.54×10^{-11}	9.20×10^{-11}	8.86×10^{-11}	8.51×10^{-11}
SA·MGA + DMA	1.98×10^{-10}	1.91×10^{-10}	1.85×10^{-10}	1.78×10^{-10}	1.71×10^{-10}

Continued table

Collisions	β , cm ³ ·s ⁻¹				
	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
SA·MGA·DMA + DMA	2.06×10 ⁻¹⁰	1.99×10 ⁻¹⁰	1.92×10 ⁻¹⁰	1.85×10 ⁻¹⁰	1.78×10 ⁻¹⁰
SA·MGA·DMA + SA	1.02×10 ⁻¹⁰	9.83×10 ⁻¹¹	9.48×10 ⁻¹¹	9.13×10 ⁻¹¹	8.77×10 ⁻¹¹
(SA) ₂ ·DMA + MGA	8.58×10 ⁻¹¹	8.28×10 ⁻¹¹	7.98×10 ⁻¹¹	7.69×10 ⁻¹¹	7.39×10 ⁻¹¹
(SA) ₂ ·MGA + DMA	2.77×10 ⁻¹⁰	2.67×10 ⁻¹⁰	2.58×10 ⁻¹⁰	2.48×10 ⁻¹⁰	2.38×10 ⁻¹⁰
SA·MGA·(DMA) ₂ + SA	1.10×10 ⁻¹⁰	1.06×10 ⁻¹⁰	1.02×10 ⁻¹⁰	9.82×10 ⁻¹¹	9.44×10 ⁻¹¹
(SA) ₂ ·(DMA) ₂ + MGA	9.58×10 ⁻¹¹	9.25×10 ⁻¹¹	8.92×10 ⁻¹¹	8.58×10 ⁻¹¹	8.25×10 ⁻¹¹
(SA) ₂ ·MGA·DMA + DMA	1.94×10 ⁻¹⁰	1.87×10 ⁻¹⁰	1.80×10 ⁻¹⁰	1.74×10 ⁻¹⁰	1.67×10 ⁻¹⁰
(SA) ₂ ·MGA·(DMA) ₂ + DMA	2.40×10 ⁻¹⁰	2.32×10 ⁻¹⁰	2.24×10 ⁻¹⁰	2.15×10 ⁻¹⁰	2.07×10 ⁻¹⁰
(MGA) ₂ ·DMA + SA	1.03×10 ⁻¹⁰	9.91×10 ⁻¹¹	9.55×10 ⁻¹¹	9.19×10 ⁻¹¹	8.84×10 ⁻¹¹
SA·MGA·DMA + MGA	1.04×10 ⁻¹⁰	9.99×10 ⁻¹¹	9.63×10 ⁻¹¹	9.27×10 ⁻¹¹	8.92×10 ⁻¹¹
SA·(MGA) ₂ + DMA	2.12×10 ⁻¹⁰	2.04×10 ⁻¹⁰	1.97×10 ⁻¹⁰	1.90×10 ⁻¹⁰	1.82×10 ⁻¹⁰
(MGA) ₂ ·(DMA) ₂ + SA	1.00×10 ⁻¹⁰	9.66×10 ⁻¹¹	9.31×10 ⁻¹¹	8.97×10 ⁻¹¹	8.62×10 ⁻¹¹
SA·MGA·(DMA) ₂ + MGA	1.10×10 ⁻¹⁰	1.06×10 ⁻¹⁰	1.02×10 ⁻¹⁰	9.83×10 ⁻¹¹	9.45×10 ⁻¹¹
SA·(MGA) ₂ ·DMA + DMA	2.23×10 ⁻¹⁰	2.15×10 ⁻¹⁰	2.07×10 ⁻¹⁰	1.99×10 ⁻¹⁰	1.92×10 ⁻¹⁰
SA·(MGA) ₂ ·(DMA) ₂ + DMA	2.08×10 ⁻¹⁰	2.01×10 ⁻¹⁰	1.93×10 ⁻¹⁰	1.86×10 ⁻¹⁰	1.79×10 ⁻¹⁰
SA·MGA·DMA + DMA	2.06×10 ⁻¹⁰	1.99×10 ⁻¹⁰	1.92×10 ⁻¹⁰	1.85×10 ⁻¹⁰	1.78×10 ⁻¹⁰
SA·MGA·DMA + SA	1.02×10 ⁻¹⁰	9.83×10 ⁻¹¹	9.48×10 ⁻¹¹	9.13×10 ⁻¹¹	8.77×10 ⁻¹¹
(SA) ₂ ·DMA + MGA	8.58×10 ⁻¹¹	8.28×10 ⁻¹¹	7.98×10 ⁻¹¹	7.69×10 ⁻¹¹	7.39×10 ⁻¹¹
(SA) ₂ ·MGA + DMA	2.77×10 ⁻¹⁰	2.67×10 ⁻¹⁰	2.58×10 ⁻¹⁰	2.48×10 ⁻¹⁰	2.38×10 ⁻¹⁰
SA·MGA·(DMA) ₂ + SA	1.10×10 ⁻¹⁰	1.06×10 ⁻¹⁰	1.02×10 ⁻¹⁰	9.82×10 ⁻¹¹	9.44×10 ⁻¹¹
(SA) ₂ ·(DMA) ₂ + MGA	9.58×10 ⁻¹¹	9.25×10 ⁻¹¹	8.92×10 ⁻¹¹	8.58×10 ⁻¹¹	8.25×10 ⁻¹¹
(SA) ₂ ·MGA·DMA + DMA	1.94×10 ⁻¹⁰	1.87×10 ⁻¹⁰	1.80×10 ⁻¹⁰	1.74×10 ⁻¹⁰	1.67×10 ⁻¹⁰
(SA) ₂ ·MGA·(DMA) ₂ + DMA	2.40×10 ⁻¹⁰	2.32×10 ⁻¹⁰	2.24×10 ⁻¹⁰	2.15×10 ⁻¹⁰	2.07×10 ⁻¹⁰
(MGA) ₂ ·DMA + SA	1.03×10 ⁻¹⁰	9.91×10 ⁻¹¹	9.55×10 ⁻¹¹	9.19×10 ⁻¹¹	8.84×10 ⁻¹¹
SA·MGA·DMA + MGA	1.04×10 ⁻¹⁰	9.99×10 ⁻¹¹	9.63×10 ⁻¹¹	9.27×10 ⁻¹¹	8.92×10 ⁻¹¹
SA·(MGA) ₂ + DMA	2.12×10 ⁻¹⁰	2.04×10 ⁻¹⁰	1.97×10 ⁻¹⁰	1.90×10 ⁻¹⁰	1.82×10 ⁻¹⁰
(MGA) ₂ ·(DMA) ₂ + SA	1.00×10 ⁻¹⁰	9.66×10 ⁻¹¹	9.31×10 ⁻¹¹	8.97×10 ⁻¹¹	8.62×10 ⁻¹¹
SA·MGA·(DMA) ₂ + MGA	1.10×10 ⁻¹⁰	1.06×10 ⁻¹⁰	1.02×10 ⁻¹⁰	9.83×10 ⁻¹¹	9.45×10 ⁻¹¹
SA·(MGA) ₂ ·DMA + DMA	2.23×10 ⁻¹⁰	2.15×10 ⁻¹⁰	2.07×10 ⁻¹⁰	1.99×10 ⁻¹⁰	1.92×10 ⁻¹⁰
SA·(MGA) ₂ ·(DMA) ₂ + DMA	2.08×10 ⁻¹⁰	2.01×10 ⁻¹⁰	1.93×10 ⁻¹⁰	1.86×10 ⁻¹⁰	1.79×10 ⁻¹⁰

Table S5 Evaporation rates (s^{-1}) of the studied clusters in MGA-SA-DMA system at different temperatures of 278.15, 268.15, 258.15, 248.15 and 238.15 K

Evaporation pathways	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
$(\text{SA})_2 \rightarrow \text{SA} + \text{SA}$	6.73×10^1	1.98×10^1	5.31×10^0	1.28×10^0	6.49×10^{-1}
$(\text{SA})_3 \rightarrow (\text{SA})_2 + \text{SA}$	2.77×10^5	8.47×10^4	2.36×10^4	5.92×10^3	1.32×10^3
$(\text{SA})_1 \cdot (\text{DMA})_1 \rightarrow \text{SA} + \text{DMA}$	2.16×10^{-1}	4.70×10^{-2}	9.07×10^{-3}	1.53×10^{-3}	2.22×10^{-4}
$(\text{SA})_2 \cdot (\text{DMA})_1 \rightarrow (\text{SA})_1 \cdot (\text{DMA})_1 + \text{SA}$	2.72×10^{-7}	2.91×10^{-8}	2.61×10^{-9}	1.94×10^{-10}	1.15×10^{-11}
$(\text{SA})_2 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{SA})_2$	8.58×10^{-10}	6.77×10^{-11}	4.38×10^{-12}	3.73×10^{-13}	1.51×10^{-14}
$(\text{SA})_3 \cdot (\text{DMA})_1 \rightarrow (\text{SA})_2 \cdot (\text{DMA})_1 + \text{SA}$	1.14×10^{-1}	2.29×10^{-2}	4.07×10^{-3}	6.52×10^{-4}	8.57×10^{-5}
$(\text{SA})_3 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{SA})_3$	4.57×10^{-16}	2.38×10^{-17}	9.82×10^{-19}	3.13×10^{-20}	7.48×10^{-22}
$(\text{SA})_2 \cdot (\text{DMA})_2 \rightarrow (\text{SA})_2 \cdot (\text{DMA})_1 + \text{DMA}$	1.96×10^{-4}	3.22×10^{-5}	4.57×10^{-6}	5.52×10^{-7}	2.56×10^{-7}
$(\text{SA})_3 \cdot (\text{DMA})_2 \rightarrow (\text{SA})_2 \cdot (\text{DMA})_2 + \text{SA}$	1.81×10^8	7.60×10^7	2.97×10^7	1.08×10^7	3.57×10^6
$(\text{SA})_3 \cdot (\text{DMA})_2 \rightarrow (\text{SA})_3 \cdot (\text{DMA})_1 + \text{DMA}$	9.39×10^{-7}	1.18×10^{-7}	1.26×10^{-8}	1.12×10^{-9}	8.12×10^{-11}
$(\text{SA})_3 \cdot (\text{DMA})_3 \rightarrow (\text{SA})_3 \cdot (\text{DMA})_2 + \text{DMA}$	8.64×10^{-6}	1.25×10^{-6}	1.55×10^{-7}	1.62×10^{-8}	1.40×10^{-9}
$(\text{SA})_1 \cdot (\text{MGA})_1 \rightarrow \text{SA} + \text{MGA}$	1.66×10^3	5.01×10^2	1.38×10^2	3.42×10^1	7.53×10^0
$(\text{SA})_2 \cdot (\text{MGA})_1 \rightarrow (\text{SA})_1 \cdot (\text{MGA})_1 + \text{SA}$	1.32×10^6	1.86×10^5	1.78×10^5	5.79×10^4	1.71×10^4
$(\text{SA})_2 \cdot (\text{MGA})_1 \rightarrow \text{MGA} + (\text{SA})_2$	6.85×10^4	2.12×10^4	5.99×10^3	1.52×10^3	3.46×10^2
$(\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{MGA} + \text{DMA}$	1.32×10^6	1.86×10^5	1.78×10^5	5.79×10^4	1.71×10^4
$(\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{SA} + (\text{MGA})_1 \cdot (\text{DMA})_1$	3.09×10^{-5}	4.43×10^{-6}	5.45×10^{-7}	5.64×10^{-8}	4.83×10^{-9}

Continued table

Evaporation pathways	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
$(\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{SA})_1 \cdot (\text{MGA})_1$	2.45×10^{-2}	4.44×10^{-3}	7.02×10^{-4}	9.55×10^{-5}	1.10×10^{-5}
$(\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{MGA} + (\text{SA})_1 \cdot (\text{DMA})_1$	1.48×10^2	3.71×10^1	8.38×10^0	1.67×10^0	2.91×10^{-1}
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{SA} + (\text{SA})_1 \cdot (\text{DMA})_1 \cdot (\text{MGA})_1$	7.27×10^3	1.98×10^3	4.90×10^2	1.08×10^2	2.08×10^1
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{SA})_2 \cdot (\text{MGA})_1$	3.10×10^{12}	1.99×10^{12}	1.23×10^{12}	7.31×10^{11}	4.13×10^{11}
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1 \rightarrow \text{MGA} + (\text{SA})_2 \cdot (\text{DMA})_1$	3.10×10^{12}	1.99×10^{12}	1.23×10^{12}	7.31×10^{11}	4.13×10^{11}
$(\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_2 \rightarrow \text{DMA} + (\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1$	3.44×10^2	8.76×10^1	2.00×10^1	4.04×10^0	7.13×10^{-1}
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_2 \rightarrow \text{SA} + (\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_2$	4.10×10^{-6}	5.10×10^{-7}	1.46×10^{-7}	4.75×10^{-9}	3.41×10^{-10}
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot \text{DMA}_2 \rightarrow \text{DMA} + (\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1$	2.57×10^9	1.17×10^9	1.35×10^9	1.98×10^8	7.28×10^7
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_2 \rightarrow \text{MGA} + (\text{SA})_2 \cdot (\text{DMA})_2$	2.57×10^9	1.17×10^9	1.35×10^9	1.98×10^8	7.28×10^7
$(\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_3 \rightarrow \text{DMA} + (\text{SA})_2 \cdot (\text{MGA})_1 \cdot (\text{DMA})_2$	1.24×10^4	3.48×10^3	3.26×10^2	1.99×10^2	3.97×10^1
$(\text{MGA})_2 \rightarrow \text{MGA} + \text{MGA}$	4.81×10^4	1.40×10^4	3.71×10^3	8.82×10^2	3.43×10^2
$(\text{SA})_1 \cdot (\text{MGA})_2 \rightarrow \text{SA} + (\text{MGA})_2$	2.95×10^1	6.79×10^0	1.39×10^0	2.51×10^{-1}	3.93×10^{-2}
$(\text{SA})_1 \cdot (\text{MGA})_2 \rightarrow \text{MGA} + (\text{SA})_1 \cdot (\text{MGA})_1$	7.31×10^2	1.62×10^2	3.20×10^1	5.54×10^0	8.28×10^{-1}
$(\text{MGA})_2 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{MGA})_2$	1.81×10^8	7.60×10^7	2.97×10^7	1.08×10^7	3.57×10^6
$(\text{MGA})_2 \cdot (\text{DMA})_1 \rightarrow \text{MGA} + (\text{MGA})_1 \cdot (\text{DMA})_1$	5.69×10^6	1.82×10^6	5.34×10^5	1.41×10^5	3.34×10^4
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_1 \rightarrow \text{SA} + (\text{MGA})_2 \cdot (\text{DMA})_1$	4.89×10^{-5}	6.71×10^{-6}	7.90×10^{-7}	7.82×10^{-8}	6.37×10^{-9}

Continued table

Evaporation pathways	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{SA})_1 \cdot (\text{MGA})_2$	3.10×10^2	7.76×10^1	1.74×10^1	3.46×10^0	5.98×10^{-1}
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_1 \rightarrow \text{MGA} + (\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_1$	8.67×10^6	2.66×10^6	7.46×10^5	1.89×10^5	4.25×10^4
$(\text{MGA})_2 \cdot (\text{DMA})_2 \rightarrow \text{DMA} + (\text{MGA})_2 \cdot (\text{DMA})_1$	1.04×10^2	2.50×10^1	5.39×10^0	1.03×10^0	1.70×10^{-1}
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_2 \rightarrow \text{SA} + (\text{MGA})_2 \cdot (\text{DMA})_2$	3.41×10^{-8}	3.87×10^{-9}	3.69×10^{-10}	2.91×10^{-11}	1.85×10^{-12}
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_2 \rightarrow \text{DMA} + (\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_1$	7.88×10^{-2}	1.57×10^{-2}	2.74×10^{-3}	4.15×10^{-4}	5.35×10^{-5}
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_2 \rightarrow \text{MGA} + (\text{SA})_1 \cdot (\text{MGA})_1 \cdot (\text{DMA})_2$	1.95×10^3	4.69×10^2	1.01×10^2	1.91×10^1	3.14×10^0
$(\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_3 \rightarrow \text{DMA} + (\text{SA})_1 \cdot (\text{MGA})_2 \cdot (\text{DMA})_2$	9.89×10^7	3.81×10^7	1.36×10^7	4.46×10^6	1.33×10^6
$(\text{MGA})_3 \rightarrow (\text{MGA})_2 + \text{MGA}$	3.94×10^5	1.21×10^5	3.39×10^4	8.53×10^3	1.91×10^3
$(\text{MGA})_3 \cdot (\text{DMA})_1 \rightarrow \text{DMA} + (\text{MGA})_3$	8.73×10^9	4.44×10^9	2.13×10^9	9.65×10^8	4.08×10^8
$(\text{MGA})_3 \cdot (\text{DMA})_1 \rightarrow \text{MGA} + (\text{MGA})_2 \cdot (\text{DMA})_1$	1.67×10^7	6.19×10^6	2.13×10^6	6.71×10^5	1.91×10^5
$(\text{MGA})_3 \cdot (\text{DMA})_2 \rightarrow \text{DMA} + (\text{MGA})_3 \cdot (\text{DMA})_1$	3.27×10^{-4}	5.08×10^{-5}	6.82×10^{-6}	7.78×10^{-7}	7.37×10^{-8}
$(\text{MGA})_3 \cdot (\text{DMA})_2 \rightarrow \text{MGA} + (\text{MGA})_2 \cdot (\text{DMA})_2$	4.81×10^1	1.15×10^1	2.47×10^0	4.67×10^{-1}	7.64×10^{-2}
$(\text{MGA})_3 \cdot (\text{DMA})_3 \rightarrow \text{DMA} + (\text{MGA})_3 \cdot (\text{DMA})_2$	8.12×10^7	3.14×10^7	1.12×10^7	3.69×10^6	1.10×10^6

Table S6 Total evaporation coefficients ($\sum\gamma$, s⁻¹) for each cluster analyzed in the present study of MGA-SA-DMA system

Clusters	$\sum\gamma$, s ⁻¹				
	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
SA·DMA	2.16×10^{-1}	4.70×10^{-2}	9.07×10^{-3}	1.53×10^{-3}	2.22×10^{-4}
SA·MGA	1.66×10^3	5.01×10^2	1.38×10^2	3.42×10^1	7.53×10^0
DMA·MGA	1.32×10^6	1.86×10^5	1.78×10^5	5.79×10^4	1.71×10^4
(SA) ₂	6.73×10^1	1.98×10^1	5.31×10^0	1.28×10^0	6.49×10^{-1}
(MGA) ₂	4.81×10^4	1.40×10^4	3.71×10^3	8.82×10^2	3.43×10^2
(SA) ₂ ·DMA	2.73×10^{-7}	2.92×10^{-8}	2.62×10^{-9}	1.94×10^{-10}	1.16×10^{-11}
(SA) ₂ ·(DMA) ₂	1.96×10^{-4}	3.22×10^{-5}	4.57×10^{-6}	5.52×10^{-7}	2.56×10^{-7}
DMA·(MGA) ₂	1.87×10^8	7.78×10^7	3.03×10^7	1.09×10^7	3.61×10^6
(DMA) ₂ ·(MGA) ₂	1.04×10^2	2.50×10^1	5.39×10^0	1.03×10^0	1.70×10^{-1}
(SA) ₂ ·MGA	7.22×10^4	2.23×10^4	6.29×10^3	1.60×10^3	3.62×10^2
SA·(MGA) ₂	7.60×10^2	1.69×10^2	3.34×10^1	5.80×10^0	8.68×10^{-1}
(SA) ₃	2.77×10^5	8.47×10^4	2.36×10^4	5.92×10^3	1.32×10^3
(MGA) ₃	3.94×10^5	1.21×10^5	3.39×10^4	8.53×10^3	1.91×10^3
(SA) ₃ ·DMA	1.14×10^{-1}	2.29×10^{-2}	4.07×10^{-3}	6.52×10^{-4}	8.57×10^{-5}
(SA) ₃ ·(DMA) ₂	6.51×10^{-4}	1.00×10^{-4}	1.34×10^{-5}	1.52×10^{-6}	1.44×10^{-7}
(SA) ₃ ·(DMA) ₃	8.64×10^{-6}	1.25×10^{-6}	1.55×10^{-7}	1.62×10^{-8}	1.40×10^{-9}
DMA·(MGA) ₃	8.74×10^9	4.44×10^9	2.14×10^9	9.66×10^8	4.08×10^8
(DMA) ₂ ·(MGA) ₃	4.81×10^1	1.15×10^1	2.48×10^0	4.67×10^{-1}	7.64×10^{-2}
(DMA) ₃ ·(MGA) ₃	8.12×10^7	3.14×10^7	1.12×10^7	3.69×10^6	1.10×10^6
SA·DMA·MGA	1.48×10^2	3.71×10^1	8.38×10^0	1.67×10^0	2.91×10^{-1}
SA·(DMA) ₂ ·MGA	3.44×10^2	8.76×10^1	2.00×10^1	4.04×10^0	7.13×10^{-1}
SA ₂ ·DMA·MGA	3.10×10^{12}	1.99×10^{12}	1.23×10^{12}	7.31×10^{11}	4.13×10^{11}
(SA) ₂ ·(DMA) ₂ ·MGA	2.57×10^9	1.17×10^9	1.35×10^9	1.98×10^8	7.28×10^7
(SA) ₂ ·(DMA) ₃ ·MGA	1.24×10^4	3.48×10^3	3.26×10^2	1.99×10^2	3.97×10^1
SA·DMA·(MGA) ₂	8.67×10^6	2.66×10^6	7.47×10^5	1.89×10^5	4.25×10^4
SA·(DMA) ₂ ·(MGA) ₂	1.95×10^3	4.69×10^2	1.01×10^2	1.91×10^1	3.14×10^0
SA·(DMA) ₃ ·(MGA) ₂	9.89×10^7	3.81×10^7	1.36×10^7	4.46×10^6	1.33×10^6

Table S7 Ratios ($\beta C/\Sigma\gamma$) between monomer molecule collisions and evaporation coefficients for each cluster involving MGS in the present study. [SA] = 1.0×10^6 molecules $\cdot\text{cm}^{-3}$, [DMA] = 1.0×10^9 molecules $\cdot\text{cm}^{-3}$, [MGA] = 1.0×10^{10} molecules $\cdot\text{cm}^{-3}$

Clusters	$\beta C/\Sigma\gamma$				
	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
Collision with SA monomer: $C = [\text{SA}]$					
SA $\cdot$ DMA	4.12×10^{-10}	1.83×10^{-9}	9.11×10^{-9}	5.19×10^{-8}	3.43×10^{-7}
SA $\cdot$ MGA	5.82×10^{-14}	1.86×10^{-13}	6.49×10^{-13}	2.52×10^{-12}	1.10×10^{-11}
DMA $\cdot$ MGA	7.87×10^{-17}	5.38×10^{-16}	5.40×10^{-16}	1.60×10^{-15}	5.19×10^{-15}
(SA) $_2$	1.19×10^{-12}	3.89×10^{-12}	1.40×10^{-11}	5.59×10^{-11}	1.06×10^{-10}
(MGA) $_2$	2.18×10^{-15}	7.22×10^{-15}	2.62×10^{-14}	1.06×10^{-13}	2.62×10^{-13}
(SA) $_2$ $\cdot$ DMA	2.92×10^{-4}	2.63×10^{-3}	2.82×10^{-2}	3.80×10^{-1}	6.14×10^0
(SA) $_2$ $\cdot$ (DMA) $_2$	4.63×10^{-7}	2.73×10^{-6}	1.85×10^{-5}	1.47×10^{-4}	3.04×10^{-4}
DMA $\cdot$ (MGA) $_2$	5.31×10^{-19}	1.23×10^{-18}	3.04×10^{-18}	8.10×10^{-18}	2.35×10^{-17}
(DMA) $_2$ $\cdot$ (MGA) $_2$	9.30×10^{-13}	3.73×10^{-12}	1.66×10^{-11}	8.40×10^{-11}	4.88×10^{-10}
SA $\cdot$ DMA $\cdot$ MGA	6.66×10^{-13}	2.55×10^{-12}	1.09×10^{-11}	5.24×10^{-11}	2.89×10^{-10}
SA $\cdot$ (DMA) $_2$ $\cdot$ MGA	3.08×10^{-13}	1.17×10^{-12}	4.92×10^{-12}	2.34×10^{-11}	1.27×10^{-10}
Collision with A monomer: $C = [\text{DMA}]$					
SA $\cdot$ MGA	1.15×10^{-10}	3.69×10^{-10}	1.29×10^{-9}	5.00×10^{-9}	2.18×10^{-8}
(SA) $_2$	2.35×10^{-9}	7.68×10^{-9}	2.76×10^{-8}	1.81×10^{-7}	3.42×10^{-7}
(MGA) $_2$	4.36×10^{-12}	1.44×10^{-11}	5.24×10^{-11}	2.12×10^{-10}	5.23×10^{-10}
(SA) $_2$ $\cdot$ DMA	5.91×10^{-1}	5.33×10^0	5.72×10^1	7.41×10^2	1.20×10^4
DMA $\cdot$ (MGA) $_2$	1.08×10^{-15}	2.51×10^{-15}	6.20×10^{-15}	1.66×10^{-14}	4.81×10^{-14}
(SA) $_2$ $\cdot$ MGA	3.70×10^{-12}	1.15×10^{-11}	3.94×10^{-11}	1.49×10^{-10}	6.31×10^{-10}
SA $\cdot$ (MGA) $_2$	2.69×10^{-10}	1.17×10^{-9}	5.68×10^{-9}	3.15×10^{-8}	2.02×10^{-7}
(SA) $_3$	7.37×10^{-13}	2.33×10^{-12}	8.03×10^{-12}	3.08×10^{-11}	1.32×10^{-10}
(MGA) $_3$	5.69×10^{-13}	1.79×10^{-12}	6.15×10^{-12}	2.35×10^{-11}	1.00×10^{-10}
(SA) $_3$ $\cdot$ DMA	1.36×10^{-6}	6.48×10^{-6}	3.51×10^{-5}	2.11×10^{-4}	1.54×10^{-3}
(SA) $_3$ $\cdot$ (DMA) $_2$	3.57×10^{-4}	2.23×10^{-3}	1.61×10^{-2}	1.36×10^{-1}	1.38×10^0
DMA $\cdot$ (MGA) $_3$	2.44×10^{-17}	4.64×10^{-17}	9.29×10^{-17}	1.97×10^{-16}	4.48×10^{-16}
(DMA) $_2$ $\cdot$ (MGA) $_3$	5.25×10^{-9}	2.11×10^{-8}	9.48×10^{-8}	4.83×10^{-7}	2.83×10^{-6}
SA $\cdot$ DMA $\cdot$ MGA	1.35×10^{-9}	5.17×10^{-9}	2.21×10^{-8}	1.06×10^{-7}	5.85×10^{-7}

Continued table

Clusters	$\beta C/\sum \gamma$				
	278.15 K	268.15 K	258.15 K	248.15 K	238.15 K
(SA) ₂ ·DMA·MGA	6.04×10 ⁻²⁰	9.07×10 ⁻²⁰	1.41×10 ⁻¹⁹	2.28×10 ⁻¹⁹	3.88×10 ⁻¹⁹
(SA) ₂ ·(DMA) ₂ ·MGA	9.01×10 ⁻¹⁷	1.91×10 ⁻¹⁶	1.60×10 ⁻¹⁶	1.04×10 ⁻¹⁵	2.73×10 ⁻¹⁵
SA·DMA·(MGA) ₂	2.48×10 ⁻¹⁴	7.78×10 ⁻¹⁴	2.67×10 ⁻¹³	1.01×10 ⁻¹²	4.32×10 ⁻¹²
SA·(DMA) ₂ ·(MGA) ₂	1.03×10 ⁻¹⁰	4.13×10 ⁻¹⁰	1.85×10 ⁻⁹	9.38×10 ⁻⁹	5.47×10 ⁻⁸
Collision with MGA monomer: $C = [\text{MGA}]$					
SA·DMA	4.41×10 ⁻⁶	1.96×10 ⁻⁵	9.77×10 ⁻⁵	5.57×10 ⁻⁴	3.68×10 ⁻³
SA·MGA	6.00×10 ⁻¹⁰	1.92×10 ⁻⁹	6.69×10 ⁻⁹	2.60×10 ⁻⁸	1.13×10 ⁻⁷
DMA·MGA	8.23×10 ⁻¹³	5.63×10 ⁻¹²	5.65×10 ⁻¹²	1.67×10 ⁻¹¹	5.43×10 ⁻¹¹
(SA) ₂	1.26×10 ⁻⁸	4.11×10 ⁻⁸	1.48×10 ⁻⁷	5.89×10 ⁻⁷	1.11×10 ⁻⁶
(MGA) ₂	2.22×10 ⁻¹¹	7.35×10 ⁻¹¹	2.67×10 ⁻¹⁰	1.08×10 ⁻⁹	2.66×10 ⁻⁹
(SA) ₂ ·DMA	3.03×10 ⁰	2.74×10 ¹	2.94×10 ²	3.80×10 ³	6.14×10 ⁴
(SA) ₂ ·(DMA) ₂	4.71×10 ⁻³	2.77×10 ⁻²	1.88×10 ⁻¹	1.50×10 ⁰	3.09×10 ⁰
DMA·(MGA) ₂	5.36×10 ⁻¹⁵	1.24×10 ⁻¹⁴	3.07×10 ⁻¹⁴	8.19×10 ⁻¹⁴	2.38×10 ⁻¹³
(DMA) ₂ ·(MGA) ₂	9.34×10 ⁻⁹	3.74×10 ⁻⁸	1.67×10 ⁻⁷	8.44×10 ⁻⁷	4.90×10 ⁻⁶
SA·DMA·MGA	6.77×10 ⁻⁹	2.60×10 ⁻⁸	1.11×10 ⁻⁷	5.33×10 ⁻⁷	2.94×10 ⁻⁶
SA·(DMA) ₂ ·MGA	3.08×10 ⁻⁹	1.17×10 ⁻⁸	4.92×10 ⁻⁸	2.34×10 ⁻⁷	1.27×10 ⁻⁶

Research has shown that it is important to consider the concentration of precursors when evaluating the cluster stability, because a larger concentration of precursors increases the collision probability for a cluster, resulting in higher stability of the cluster. Therefore, the ratio of the collision frequency to the total evaporation rate ($\beta \cdot C/\sum \gamma$, in Table S5) was investigated. The $\beta \cdot C/\sum \gamma$ increases with the decrease of temperature, this indicates that the lower temperature is more MGA vorable for the formation of clusters.

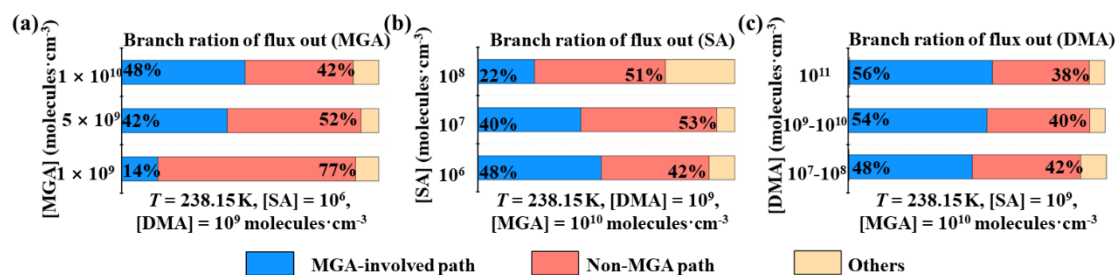


Figure S2 The influence of (a) [MGA], (b) [SA] and (c) [DMA] on the relative contribution of the pure SA-DMA-based clustering route and the MGA participation route to the system flux is analyzed at $T = 238.15 \text{ K}$.

Part S1. Enhancement of cluster formation rates

To quantify the aerosol formation capability of the SA-DMA-MGA system and the enhancing effect of MGA on SA-DMA-driven nucleation, ACDC simulations of the aerosol formation rate (J , $\text{cm}^{-3} \text{ s}^{-1}$) were performed. Meanwhile, for further evaluation of the relative enhancement contributed by MGA, the enhancement factor, R , is defined as the ratio of $(\text{SA})_x(\text{DMA})_y(\text{MGA})_z$ ($0 < z \leq x + y \leq 3$) clusters to that of $(\text{SA})_x(\text{DMA})_y$ ($0 < x + y \leq 3$) clusters, as shown in Eq. (2):

$$R = \frac{J([\text{SA}] = x, [\text{DMA}] = y, [\text{MGA}] = z)}{J([\text{SA}] = x, [\text{DMA}] = y, [\text{MGA}] = 0)} \quad (2)$$

Here, x , y and z denote the atmospheric concentrations of SA (10^6 to 10^8 molecules $\cdot\text{cm}^{-3}$), DMA (10^7 to 10^{11} molecules $\cdot\text{cm}^{-3}$), and MGA (10^8 to 10^{10} molecules $\cdot\text{cm}^{-3}$), respectively.

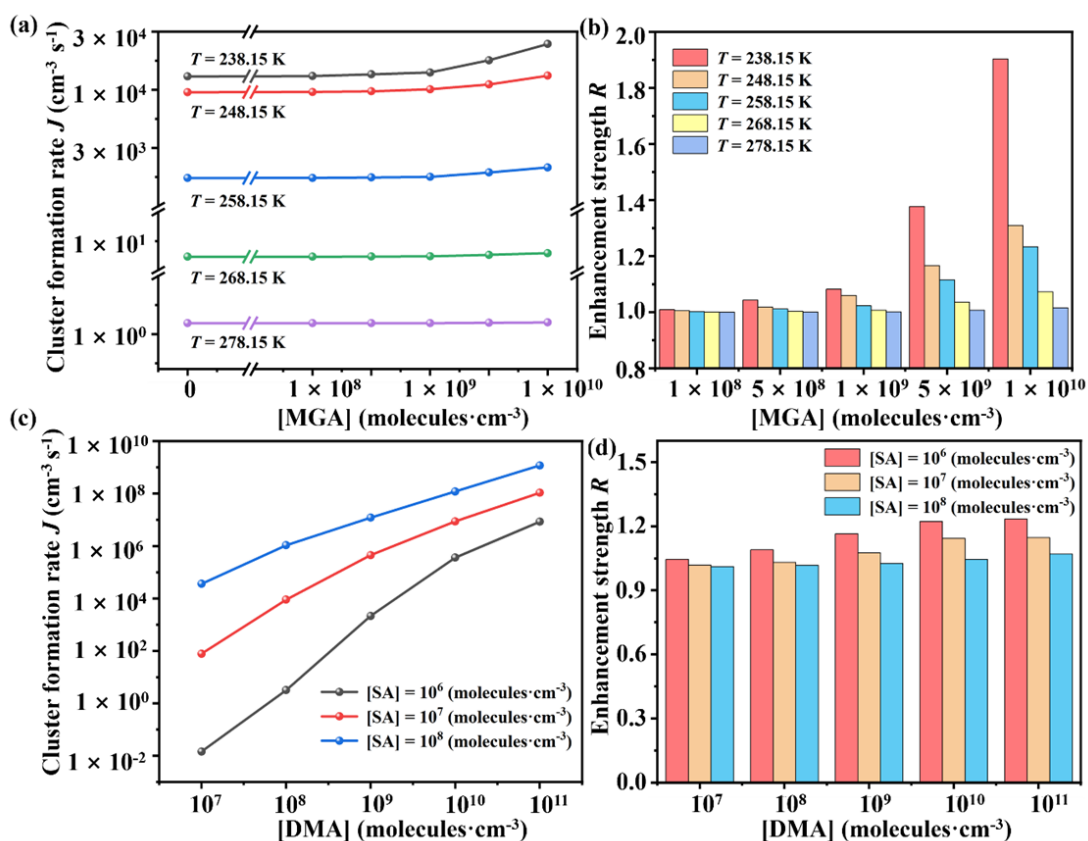


Figure S3 The cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) and (b) the enhancement strength R of MGA are presented [MGA] from 10^8 to 10^{10} $\text{molecules} \cdot \text{cm}^{-3}$ under different temperatures (238.15, 248.15, 258.15, 268.15 and 278.15 K) where [SA] = 10^6 $\text{molecules} \cdot \text{cm}^{-3}$ and [DMA] = 10^9 $\text{molecules} \cdot \text{cm}^{-3}$. (c) The cluster formation rates J ($\text{cm}^{-3} \text{s}^{-1}$) and (d) the enhancement strength R as a function of [DMA] with [MGA] = 10^{11} $\text{molecules} \cdot \text{cm}^{-3}$ and three different [SA] at 258.15 K

Table S8 Formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of MGA at $T = 238.15 \text{ K}$, with $[\text{SA}] = 10^6\text{-}10^8 \text{ molecules}\cdot\text{cm}^{-3}$, $[\text{DMA}] = 10^7\text{-}10^{11} \text{ molecules}\cdot\text{cm}^{-3}$, and $[\text{MGA}] = 0, 10^8\text{-}10^{10} \text{ molecules}\cdot\text{cm}^{-3}$. SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[DMA]	[MGA] = 0	[MGA] = 10^5	[MGA] = 10^6	[MGA] = 10^7	[MGA] = 10^8	[MGA] = 5×10^8	[MGA] = 10^9	[MGA] = 5×10^9	[MGA] = 10^{10}
[SA] = 10^6	[DMA] = 10^7	8.00×10^{-2}	8.00×10^{-2}	8.00×10^{-2}	8.01×10^{-2}	8.12×10^{-2}	8.59×10^{-2}	9.14×10^{-2}	1.41×10^{-1}	8.12×10^{-2}
[SA] = 10^6	[DMA] = 10^8	3.26×10^1	3.26×10^1	3.26×10^1	3.26×10^1	3.31×10^1	3.50×10^1	3.73×10^1	5.72×10^1	3.31×10^1
[SA] = 10^6	[DMA] = 10^9	1.30×10^4	1.30×10^4	1.30×10^4	1.30×10^4	1.31×10^4	1.36×10^4	1.41×10^4	1.79×10^4	1.31×10^4
[SA] = 10^6	[DMA] = 10^{10}	6.00×10^5	6.00×10^5	6.00×10^5	6.00×10^5	6.03×10^5	6.13×10^5	6.22×10^5	6.81×10^5	6.03×10^5
[SA] = 10^6	[DMA] = 10^{11}	9.31×10^6	9.31×10^6	9.31×10^6	9.31×10^6	9.32×10^6	6.13×10^5	9.41×10^6	9.64×10^6	9.32×10^6
[SA] = 10^7	[DMA] = 10^7	2.97×10^2	2.97×10^2	2.97×10^2	2.97×10^2	3.00×10^2	3.13×10^2	3.27×10^2	4.54×10^2	3.00×10^2
[SA] = 10^7	[DMA] = 10^8	2.67×10^4	2.67×10^4	2.67×10^4	2.67×10^4	2.69×10^4	2.76×10^4	2.84×10^4	3.57×10^4	2.69×10^4
[SA] = 10^7	[DMA] = 10^9	6.93×10^5	6.93×10^5	6.93×10^5	6.94×10^5	6.96×10^5	7.05×10^5	7.16×10^5	8.16×10^5	6.96×10^5
[SA] = 10^7	[DMA] = 10^{10}	9.66×10^6	9.66×10^6	9.66×10^6	9.66×10^6	9.68×10^6	9.75×10^6	9.84×10^6	1.05×10^7	9.68×10^6
[SA] = 10^7	[DMA] = 10^{11}	1.07×10^8	1.07×10^8	1.07×10^8	1.07×10^8	1.07×10^8	1.08×10^8	1.08×10^8	1.10×10^8	1.07×10^8
[SA] = 10^8	[DMA] = 10^7	5.55×10^4	5.55×10^4	5.55×10^4	5.55×10^4	5.57×10^4	5.65×10^4	5.75×10^4	6.72×10^4	5.57×10^4
[SA] = 10^8	[DMA] = 10^8	1.35×10^6	1.35×10^6	1.35×10^6	1.35×10^6	1.36×10^6	1.37×10^6	1.39×10^6	1.58×10^6	1.36×10^6
[SA] = 10^8	[DMA] = 10^9	1.32×10^7	1.32×10^7	1.32×10^7	1.32×10^7	1.33×10^7	1.34×10^7	1.36×10^7	1.51×10^7	1.33×10^7
[SA] = 10^8	[DMA] = 10^{10}	1.19×10^8	1.19×10^8	1.19×10^8	1.19×10^8	1.19×10^8	1.20×10^8	1.21×10^8	1.29×10^8	1.19×10^8
[SA] = 10^8	[DMA] = 10^{11}	1.15×10^9	1.15×10^9	1.15×10^9	1.15×10^9	1.15×10^9	1.15×10^9	1.15×10^9	1.18×10^9	1.15×10^9

Table S9 Formation rate J ($\text{cm}^{-3} \text{ s}^{-1}$) of MGA at $T = 248.15 \text{ K}$, with $[\text{SA}] = 10^6\text{-}10^8 \text{ molecules}\cdot\text{cm}^{-3}$, $[\text{DMA}] = 10^7\text{-}10^{11} \text{ molecules}\cdot\text{cm}^{-3}$, and $[\text{MGA}] = 0, 10^8\text{-}10^{10} \text{ molecules}\cdot\text{cm}^{-3}$. SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[DMA]	[MGA] = 0	[MGA] = 10^5	[MGA] = 10^6	[MGA] = 10^7	[MGA] = 10^8	[MGA] = 5×10^8	[MGA] = 10^9	[MGA] = 5×10^9	[MGA] = 10^{10}
[SA] = 10^6	[DMA] = 10^7	5.23×10^{-2}	5.23×10^{-2}	5.23×10^{-2}	5.24×10^{-2}	5.26×10^{-2}	5.36×10^{-2}	5.66×10^{-2}	6.47×10^{-2}	8.47×10^{-2}
[SA] = 10^6	[DMA] = 10^8	1.87×10^1	1.87×10^1	1.87×10^1	1.87×10^1	1.88×10^1	1.92×10^1	2.05×10^1	2.38×10^1	3.25×10^1
[SA] = 10^6	[DMA] = 10^9	9.53×10^3	9.53×10^3	9.53×10^3	9.53×10^3	9.58×10^3	9.70×10^3	1.01×10^4	1.11×10^4	1.25×10^4
[SA] = 10^6	[DMA] = 10^{10}	5.61×10^5	5.61×10^5	5.61×10^5	5.61×10^5	5.62×10^5	5.65×10^5	5.73×10^5	5.97×10^5	6.33×10^5
[SA] = 10^6	[DMA] = 10^{11}	9.27×10^6	9.27×10^6	9.27×10^6	9.27×10^6	9.28×10^6	9.32×10^6	9.40×10^6	9.59×10^6	9.79×10^6
[SA] = 10^7	[DMA] = 10^7	2.20×10^2	2.20×10^2	2.20×10^2	2.20×10^2	2.21×10^2	2.24×10^2	2.28×10^2	2.59×10^2	3.15×10^2
[SA] = 10^7	[DMA] = 10^8	2.19×10^4	2.19×10^4	2.19×10^4	2.19×10^4	2.19×10^4	2.21×10^4	2.24×10^4	2.45×10^4	2.79×10^4
[SA] = 10^7	[DMA] = 10^9	6.54×10^5	6.54×10^5	6.54×10^5	6.54×10^5	6.55×10^5	6.58×10^5	6.65×10^5	6.89×10^5	7.27×10^5
[SA] = 10^7	[DMA] = 10^{10}	9.63×10^6	9.63×10^6	9.63×10^6	9.63×10^6	9.63×10^6	9.66×10^6	9.69×10^6	9.91×10^6	1.02×10^7
[SA] = 10^7	[DMA] = 10^{11}	1.09×10^8	1.09×10^8	1.09×10^8	1.09×10^8	1.09×10^8	1.09×10^8	1.09×10^8	1.11×10^8	1.12×10^8
[SA] = 10^8	[DMA] = 10^7	5.10×10^4	5.10×10^4	5.10×10^4	5.10×10^4	5.11×10^4	5.13×10^4	5.16×10^4	5.41×10^4	5.74×10^4
[SA] = 10^8	[DMA] = 10^8	1.29×10^6	1.29×10^6	1.29×10^6	1.29×10^6	1.29×10^6	1.29×10^6	1.30×10^6	1.34×10^6	1.40×10^6
[SA] = 10^8	[DMA] = 10^9	1.30×10^7	1.30×10^7	1.30×10^7	1.30×10^7	1.31×10^7	1.31×10^7	1.31×10^7	1.34×10^7	1.38×10^7
[SA] = 10^8	[DMA] = 10^{10}	1.21×10^8	1.21×10^8	1.21×10^8	1.21×10^8	1.21×10^8	1.21×10^8	1.21×10^8	1.24×10^8	1.26×10^8
[SA] = 10^8	[DMA] = 10^{11}	1.17×10^9	1.17×10^9	1.17×10^9	1.17×10^9	1.17×10^9	1.17×10^9	1.17×10^9	1.18×10^9	1.20×10^9

Table S10 Formation rate J ($\text{cm}^{-3} \text{ s}^{-1}$) of MGA at $T = 258.15 \text{ K}$, with $[\text{SA}] = 10^6\text{-}10^8 \text{ molecules}\cdot\text{cm}^{-3}$, $[\text{DMA}] = 10^7\text{-}10^{11} \text{ molecules}\cdot\text{cm}^{-3}$, and $[\text{MGA}] = 0, 10^8\text{-}10^{10} \text{ molecules}\cdot\text{cm}^{-3}$. SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[DMA]	[MGA] = 0	[MGA] = 10^5	[MGA] = 10^6	[MGA] = 10^7	[MGA] = 10^8	[MGA] = 5×10^8	[MGA] = 10^9	[MGA] = 5×10^9	[MGA] = 10^{10}
[SA] = 10^6	[DMA] = 10^7	1.25×10^{-2}	1.25×10^{-2}	1.25×10^{-2}	1.25×10^{-2}	1.25×10^{-2}	1.26×10^{-2}	1.27×10^{-2}	1.35×10^{-2}	1.46×10^{-2}
[SA] = 10^6	[DMA] = 10^8	2.63×10^0	2.63×10^0	2.63×10^0	2.63×10^0	2.64×10^0	2.66×10^0	2.69×10^0	2.92×10^0	3.22×10^0
[SA] = 10^6	[DMA] = 10^9	1.75×10^3	1.75×10^3	1.75×10^3	1.75×10^3	1.75×10^3	1.77×10^3	1.79×10^3	1.95×10^3	2.15×10^3
[SA] = 10^6	[DMA] = 10^{10}	3.34×10^5	3.34×10^5	3.34×10^5	3.34×10^5	3.35×10^5	3.36×10^5	3.38×10^5	3.50×10^5	3.64×10^5
[SA] = 10^6	[DMA] = 10^{11}	8.11×10^6	8.11×10^6	8.11×10^6	8.11×10^6	8.12×10^6	8.13×10^6	8.15×10^6	8.31×10^6	8.48×10^6
[SA] = 10^7	[DMA] = 10^7	6.80×10^1	6.80×10^1	6.80×10^1	6.80×10^1	6.81×10^1	6.85×10^1	6.90×10^1	7.29×10^1	7.79×10^1
[SA] = 10^7	[DMA] = 10^8	7.91×10^3	7.91×10^3	7.91×10^3	7.91×10^3	7.92×10^3	7.96×10^3	8.02×10^3	8.47×10^3	9.03×10^3
[SA] = 10^7	[DMA] = 10^9	4.18×10^5	4.18×10^5	4.18×10^5	4.18×10^5	4.19×10^5	4.20×10^5	4.22×10^5	4.34×10^5	4.50×10^5
[SA] = 10^7	[DMA] = 10^{10}	8.47×10^6	8.47×10^6	8.47×10^6	8.47×10^6	8.47×10^6	8.48×10^6	8.50×10^6	8.60×10^6	8.73×10^6
[SA] = 10^7	[DMA] = 10^{11}	1.06×10^8	1.06×10^8	1.06×10^8	1.06×10^8	1.06×10^8	1.06×10^8	1.06×10^8	1.07×10^8	1.08×10^8
[SA] = 10^8	[DMA] = 10^7	3.38×10^4	3.38×10^4	3.38×10^4	3.38×10^4	3.38×10^4	3.39×10^4	3.40×10^4	3.50×10^4	3.61×10^4
[SA] = 10^8	[DMA] = 10^8	1.03×10^6	1.03×10^6	1.03×10^6	1.03×10^6	1.03×10^6	1.03×10^6	1.04×10^6	1.05×10^6	1.08×10^6
[SA] = 10^8	[DMA] = 10^9	1.18×10^7	1.18×10^7	1.18×10^7	1.18×10^7	1.18×10^7	1.18×10^7	1.19×10^7	1.20×10^7	1.21×10^7
[SA] = 10^8	[DMA] = 10^{10}	1.18×10^8	1.18×10^8	1.18×10^8	1.18×10^8	1.18×10^8	1.18×10^8	1.18×10^8	1.19×10^8	1.20×10^8
[SA] = 10^8	[DMA] = 10^{11}	1.18×10^9	1.18×10^9	1.18×10^9	1.18×10^9	1.18×10^9	1.18×10^9	1.18×10^9	1.18×10^9	1.19×10^9

Table S11 Formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of MGA at $T = 268.15 \text{ K}$, with $[\text{SA}] = 10^6\text{-}10^8 \text{ molecules}\cdot\text{cm}^{-3}$, $[\text{DMA}] = 10^7\text{-}10^{11} \text{ molecules}\cdot\text{cm}^{-3}$, and $[\text{MGA}] = 0, 10^8\text{-}10^{10} \text{ molecules}\cdot\text{cm}^{-3}$. SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[DMA]	[MGA] = 0	[MGA] = 10^5	[MGA] = 10^6	[MGA] = 10^7	[MGA] = 10^8	[MGA] = 5×10^8	[MGA] = 10^9	[MGA] = 5×10^9	[MGA] = 10^{10}
[SA] = 10^6	[DMA] = 10^7	1.84×10^{-3}	1.84×10^{-3}	1.84×10^{-3}	1.84×10^{-3}	1.85×10^{-3}	1.85×10^{-3}	1.85×10^{-3}	1.88×10^{-3}	1.91×10^{-3}
[SA] = 10^6	[DMA] = 10^8	2.00×10^{-1}	2.00×10^{-1}	2.00×10^{-1}	2.00×10^{-1}	2.00×10^{-1}	2.00×10^{-1}	2.01×10^{-1}	2.04×10^{-1}	2.09×10^{-1}
[SA] = 10^6	[DMA] = 10^9	4.13×10^1	4.13×10^1	4.13×10^1	4.13×10^1	4.13×10^1	4.14×10^1	4.16×10^1	4.27×10^1	4.43×10^1
[SA] = 10^6	[DMA] = 10^{10}	3.86×10^4	3.86×10^4	3.86×10^4	3.86×10^4	3.86×10^4	3.87×10^4	3.88×10^4	3.97×10^4	4.09×10^4
[SA] = 10^6	[DMA] = 10^{11}	3.97×10^6	3.97×10^6	3.97×10^6	3.97×10^6	3.97×10^6	3.98×10^6	3.99×10^6	4.03×10^6	4.09×10^6
[SA] = 10^7	[DMA] = 10^7	1.11×10^1	1.11×10^1	1.11×10^1	1.11×10^1	1.11×10^1	1.11×10^1	1.11×10^1	1.13×10^1	1.15×10^1
[SA] = 10^7	[DMA] = 10^8	1.04×10^3	1.04×10^3	1.04×10^3	1.04×10^3	1.04×10^3	1.04×10^3	1.04×10^3	1.06×10^3	1.08×10^3
[SA] = 10^7	[DMA] = 10^9	7.59×10^4	7.59×10^4	7.59×10^4	7.59×10^4	7.59×10^4	7.60×10^4	7.62×10^4	7.76×10^4	7.93×10^4
[SA] = 10^7	[DMA] = 10^{10}	4.29×10^6	4.29×10^6	4.29×10^6	4.29×10^6	4.29×10^6	4.30×10^6	4.30×10^6	4.34×10^6	4.39×10^6
[SA] = 10^7	[DMA] = 10^{11}	8.61×10^7	8.61×10^7	8.61×10^7	8.61×10^7	8.61×10^7	8.61×10^7	8.62×10^7	8.65×10^7	8.70×10^7
[SA] = 10^8	[DMA] = 10^7	1.05×10^4	1.05×10^4	1.05×10^4	1.05×10^4	1.05×10^4	1.05×10^4	1.05×10^4	1.07×10^4	1.08×10^4
[SA] = 10^8	[DMA] = 10^8	4.66×10^5	4.66×10^5	4.66×10^5	4.66×10^5	4.66×10^5	1.05×10^4	4.67×10^5	4.71×10^5	4.77×10^5
[SA] = 10^8	[DMA] = 10^9	7.34×10^6	7.34×10^6	7.34×10^6	7.34×10^6	7.34×10^6	7.35×10^6	7.35×10^6	7.40×10^6	7.47×10^6
[SA] = 10^8	[DMA] = 10^{10}	9.79×10^7	9.79×10^7	9.79×10^7	9.79×10^7	9.79×10^7	9.80×10^7	9.80×10^7	9.84×10^7	9.88×10^7
[SA] = 10^8	[DMA] = 10^{11}	1.12×10^9	1.12×10^9	1.12×10^9	1.12×10^9	1.12×10^9	1.12×10^9	1.12×10^9	1.12×10^9	1.12×10^9

Table S12 Formation rate J ($\text{cm}^{-3} \text{ s}^{-1}$) of MGA at $T = 278.15 \text{ K}$, with $[\text{SA}] = 10^6\text{-}10^8 \text{ molecules}\cdot\text{cm}^{-3}$, $[\text{DMA}] = 10^7\text{-}10^{11} \text{ molecules}\cdot\text{cm}^{-3}$, and $[\text{MGA}] = 0, 10^8\text{-}10^{10} \text{ molecules}\cdot\text{cm}^{-3}$. SA, DMA and MGA denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[DMA]	[MGA] = 0	[MGA] = 10^5	[MGA] = 10^6	[MGA] = 10^7	[MGA] = 10^8	[MGA] = 5×10^8	[MGA] = 10^9	[MGA] = 5×10^9	[MGA] = 10^{10}
[SA] = 10^6	[DMA] = 10^7	3.28×10^{-4}	3.28×10^{-4}	3.28×10^{-4}	3.28×10^{-4}	3.28×10^{-4}	3.28×10^{-4}	3.28×10^{-4}	3.30×10^{-4}	3.31×10^{-4}
[SA] = 10^6	[DMA] = 10^8	2.71×10^{-2}	2.71×10^{-2}	2.71×10^{-2}	2.71×10^{-2}	2.71×10^{-2}	2.72×10^{-2}	2.72×10^{-2}	2.73×10^{-2}	2.74×10^{-2}
[SA] = 10^6	[DMA] = 10^9	1.24×10^0	1.24×10^0	1.24×10^0	1.24×10^0	1.24×10^0	1.24×10^0	1.24×10^0	1.25×10^0	1.26×10^0
[SA] = 10^6	[DMA] = 10^{10}	6.54×10^2	6.54×10^2	6.54×10^2	6.54×10^2	6.54×10^2	6.54×10^2	6.55×10^2	6.61×10^2	6.68×10^2
[SA] = 10^6	[DMA] = 10^{11}	4.23×10^5	4.23×10^5	4.23×10^5	4.23×10^5	4.23×10^5	4.24×10^5	4.24×10^5	4.27×10^5	4.30×10^5
[SA] = 10^7	[DMA] = 10^7	2.02×10^0	2.02×10^0	2.02×10^0	2.02×10^0	2.02×10^0	2.02×10^0	2.02×10^0	2.03×10^0	2.04×10^0
[SA] = 10^7	[DMA] = 10^8	1.58×10^2	1.58×10^2	1.58×10^2	1.58×10^2	1.58×10^2	1.58×10^2	1.58×10^2	1.59×10^2	1.60×10^2
[SA] = 10^7	[DMA] = 10^9	5.56×10^3	5.56×10^3	5.56×10^3	5.56×10^3	5.56×10^3	5.56×10^3	5.57×10^3	5.60×10^3	5.63×10^3
[SA] = 10^7	[DMA] = 10^{10}	5.59×10^5	5.59×10^5	5.59×10^5	5.59×10^5	5.59×10^5	5.60×10^5	5.60×10^5	5.63×10^5	5.67×10^5
[SA] = 10^7	[DMA] = 10^{11}	3.52×10^7	3.52×10^7	3.52×10^7	3.52×10^7	3.52×10^7	3.53×10^7	3.53×10^7	3.54×10^7	3.55×10^7
[SA] = 10^8	[DMA] = 10^7	2.15×10^3	2.15×10^3	2.15×10^3	2.15×10^3	2.15×10^3	2.15×10^3	2.15×10^3	2.16×10^3	2.17×10^3
[SA] = 10^8	[DMA] = 10^8	1.23×10^5	1.23×10^5	1.23×10^5	1.23×10^5	1.23×10^5	1.23×10^5	1.23×10^5	1.23×10^5	1.24×10^5
[SA] = 10^8	[DMA] = 10^9	2.09×10^6	2.09×10^6	2.09×10^6	2.09×10^6	2.09×10^6	2.09×10^6	2.09×10^6	2.09×10^6	2.10×10^6
[SA] = 10^8	[DMA] = 10^{10}	4.53×10^7	4.53×10^7	4.53×10^7	4.53×10^7	4.53×10^7	4.53×10^7	4.54×10^7	4.55×10^7	4.56×10^7
[SA] = 10^8	[DMA] = 10^{11}	8.47×10^8	8.47×10^8	8.47×10^8	8.47×10^8	8.47×10^8	8.47×10^8	8.47×10^8	8.48×10^8	8.49×10^8

Table S13 Cartesian coordinates of all molecules and clusters in the studied system.**SA:**

Atoms	X	Y	Z
S	-0.00000100	0.00000200	-0.15819500
O	0.66661200	-1.06395900	-0.82004100
O	-0.66662200	1.06398200	-0.82000300
O	1.02237300	0.68616100	0.84170500
O	-1.02236200	-0.68618400	0.84169900
H	1.69216400	0.03658000	1.09211300
H	-1.69215100	-0.03661100	1.09213100

DMA:

Atoms	X	Y	Z
N	0.00000000	0.57071400	-0.14992000
H	-0.00000100	1.33069300	0.51694100
C	1.20463300	-0.22468800	0.02036500
H	1.26337800	-0.95968400	-0.78356100
H	2.08342000	0.41428500	-0.04677400
H	1.23814500	-0.76931700	0.97439600
C	-1.20463300	-0.22468800	0.02036500
H	-2.08342300	0.41427800	-0.04681700
H	-1.26335500	-0.95971200	-0.78353700
H	-1.23816400	-0.76928400	0.97441400

MGA:

Atoms	X	Y	Z
O	-1.85357800	0.47694100	-1.41347100
O	-1.52693600	1.07456000	0.94651900
O	-2.75313600	0.98357400	0.25771500
S	-1.72743600	0.02870600	0.06314200
H	-1.06184400	1.02595400	-1.58976800
C	0.89293700	0.35870100	0.48933900
C	1.90624200	1.40075200	-0.00818400
C	0.91386900	0.29004400	2.00905500
C	1.24466900	0.96299400	-0.18430800
H	2.89431200	1.12802300	0.35636100
H	1.61773900	2.36244000	0.42457700
H	0.23677000	0.47101300	2.38224700
H	0.60948200	1.25942400	2.40051200
H	1.92352500	0.06911100	2.34835200
H	1.11758000	1.71157300	-1.74827200
H	2.56996600	2.28300300	-0.16729300
O	-0.35330900	0.85891300	-0.02185700

O	1.97669200	1.44640200	-1.40689300
O	2.36232700	1.47659100	0.32394500
O	0.64608200	1.47691100	-1.09250800

(SA)₁·(DMA)₁:

Atoms	X	Y	Z
N	1.89113100	-0.11329900	0.16945900
H	1.54361500	-0.28453900	1.11468000
C	2.04415500	1.34438600	-0.01804100
H	2.29979200	1.53244600	-1.05767000
H	1.09248700	1.81258500	0.21980000
H	2.82949800	1.72246400	0.63266300
C	3.09746000	-0.89799200	-0.13568300
H	2.88750300	-1.95107200	0.02711200
H	3.36044000	-0.73835400	-1.17822600
H	3.92124800	-0.58031200	0.49989600
S	1.26892100	-0.17507500	0.05787500
O	2.49404200	-0.91778400	0.08482300
O	0.56815800	0.05771100	1.30884000
O	0.31520000	-0.64357000	-0.98543900
H	1.01842500	-0.42029800	-0.43058300
O	1.66048200	1.32539300	-0.41277800
H	2.43481700	1.24901000	-0.98111600

(SA)₁·(MGA)₁:

Atoms	X	Y	Z
C	-2.65942500	-0.34106800	0.08303500
C	-3.23010100	0.87868900	-0.64002300
C	-3.19992700	-1.64035000	-0.50847900
C	-1.14478800	-0.32162500	-0.03166600
H	-2.95821400	0.85341400	-1.69294900
H	-4.31984000	0.83203100	-0.55148000
H	-2.77288800	-2.49911400	0.00757500
H	-4.27914600	-1.65849100	-0.36856300
H	-2.97017000	-1.71151700	-1.56999800
H	-2.23410400	-0.37747300	1.97818900
H	-2.92153500	2.06567400	0.84056500
H	0.28529200	-0.31734300	-1.27376300
O	-3.01938700	-0.22069500	1.44155000
O	-2.71277700	2.06818300	-0.09876700
O	-0.70122600	-0.31446400	-1.25660400
O	-0.43752200	-0.34260000	0.96627100
S	2.82720600	-0.05882300	-0.06884000

O	1.98540100	-0.37008100	-1.19234900
O	4.16956500	-0.51278600	-0.00704300
O	2.81537900	1.52634300	-0.00832100
O	2.11101800	-0.47314100	1.23643700
H	3.54994000	1.82400200	0.54430900
H	1.10720500	-0.40997200	1.12096700

(SA)₁·(MGA)₁·(DMA)₁:

Atoms	X	Y	Z
S	2.31631600	-0.71154000	-0.34042500
O	1.87018700	-0.60614000	1.16838500
O	2.56814600	-2.05971700	-0.70082800
O	3.36043300	0.28038100	-0.46184000
O	1.09040500	-0.13623900	-1.09371000
H	2.73717400	1.72327500	0.17984800
H	0.28707000	-0.81059200	-1.12655000
N	2.19361900	2.43055200	0.73147900
H	1.34374900	2.73503100	0.20634300
H	2.77511400	3.22537000	0.97732200
H	1.85774300	1.95938700	1.57232200
C	-0.82723300	1.82741200	0.09721900
O	-0.28470900	2.77543700	-0.42797300
H	-0.80928600	0.56406600	1.54371100
O	-0.47853100	1.46259200	1.32008200
C	-1.92190000	1.05496000	-0.62825200
C	-3.07805800	1.98924900	-0.95019300
H	-3.82258200	1.44203200	-1.52207300
H	-3.53514900	2.35135300	-0.03086800
H	-2.71567800	2.83346200	-1.53111900
H	-1.47784400	0.67594700	-1.54956800
O	-0.68731700	-1.19485800	1.32848800
O	-0.93386000	-1.55495500	-1.05844400
O	-2.65227200	-2.39795200	0.48388300
O	-2.44682900	-0.01630100	0.14302300
S	-1.64364000	-1.43632500	0.22574600
H	0.95947100	-0.99507800	1.27397500

(SA)₁·(MGA)₁·(DMA)₂:

Atoms	X	Y	Z
N	-0.86137400	1.94802100	0.12620900
H	-1.25297300	1.27213200	-0.56450600
C	0.02402000	2.92945100	-0.53690600
H	0.41636800	3.61083800	0.21380600
H	0.84085900	2.39330000	-1.01543600

H	-0.55354200	3.48237000	-1.27335100
C	-2.01013700	2.54069400	0.84643400
H	-2.58555500	1.73623600	1.29724500
H	-1.63793700	3.21791400	1.61074300
H	-2.62673700	3.08141900	0.13363200
C	2.97752100	-0.63342600	0.14552700
C	3.45260200	0.64562600	-0.53379900
C	3.84836500	-0.98549000	1.34629100
C	1.54404600	-0.39543200	0.61400900
H	3.42076000	1.47300600	0.17122400
H	4.48122700	0.49401500	-0.87216300
H	3.50688500	-1.91686000	1.79602700
H	4.87562800	-1.12110700	1.01190500
H	3.80787600	-0.19489000	2.09391200
H	2.25505000	-2.20452800	-0.75434300
H	2.56169500	0.20236100	-2.18331900
H	-0.29085900	1.37667700	0.77157400
O	3.03424000	-1.64597400	-0.84144300
O	2.60215800	0.97764900	-1.61270100
O	1.25203700	0.59399300	1.26262200
O	0.70728500	-1.33051800	0.25983100
S	-2.68366300	-0.76379000	-0.12882800
O	-2.28798000	0.08256100	-1.24851100
O	-4.00655500	-0.57508100	0.39644200
O	-1.64337000	-0.73875900	0.92858500
O	-2.62769100	-2.24172000	-0.75088900
H	-0.25787700	-1.11966600	0.55580200
H	-3.25212900	-2.78446700	-0.25578200

(SA)₁·(MGA)₂:

Atoms	X	Y	Z
C	-2.96942400	-1.19797900	0.26231500
C	-3.62857000	-0.43610100	-0.88002800
C	-3.47829200	-2.63626600	0.33169600
C	-1.45705200	-1.22391600	0.08026200
H	-3.40914100	-0.90212100	-1.83699600
H	-4.70759300	-0.43774600	-0.71315500
H	-2.99839700	-3.16103300	1.15627000
H	-4.55125400	-2.61707800	0.51422300
H	-3.27691900	-3.16867400	-0.59664900
H	-2.45921000	-0.39435700	1.95473200
H	-3.17636500	1.25819400	-0.03306500
H	-0.07047800	-1.53413300	-1.17740900
O	-3.27339200	-0.49632200	1.44636500

O	-3.14098900	0.89370100	-0.93074600
O	-1.06386100	-1.57124500	-1.11462500
O	-0.71252100	-0.96443300	1.01111300
C	0.88474700	2.95370800	0.01713300
C	2.04178500	1.99458000	-0.23117600
C	0.91977400	4.10771400	-0.98078700
C	-0.45535400	2.23489800	-0.10100300
H	1.90689700	1.44816300	-1.16155200
H	2.97011800	2.56901200	-0.26834200
H	0.07453700	4.77308700	-0.81177400
H	1.83855800	4.67174900	-0.83110000
H	0.88159500	3.73745500	-2.00394300
H	0.14796300	3.37842100	1.75090600
H	2.03086800	1.51801400	1.64992200
H	-1.54274900	1.25458000	-1.28168000
O	1.02269200	3.42405900	1.34143900
O	2.09862700	1.03456100	0.81664100
O	-0.61488700	1.60702000	-1.24718200
O	-1.28948900	2.30305200	0.77389100
S	2.43352500	-2.02454300	-0.19075600
O	3.06365600	-3.24549100	-0.52878700
O	1.56749100	-1.36221600	-1.15223300
O	1.59942600	-2.22251100	1.11536600
O	3.54022300	-1.02065400	0.23469700
H	0.78994000	-1.64365300	1.09813600
H	3.09373900	-0.17320500	0.52558600

(SA)₁·(MGA)₂·(DMA)₁:

Atoms	X	Y	Z
N	-0.46835700	1.92106500	-1.46368100
H	-0.37287500	2.33579900	-0.52113600
C	-1.85417100	2.08625800	-1.96247100
H	-1.95182500	1.53061500	-2.89117200
H	-2.55965900	1.70812900	-1.22949900
H	-2.02990300	3.14371100	-2.14172100
C	0.55374500	2.51423400	-2.36282700
H	1.52683900	2.37088700	-1.90709200
H	0.50449100	2.00026100	-3.31833300
H	0.33161000	3.57099200	-2.48398700
C	-3.74387000	-1.14587100	0.44896100
C	-4.57810300	-0.37984700	-0.57121000
C	-3.83534000	-2.65161500	0.22045300
C	-2.28575600	-0.71725200	0.29572500
H	-4.19121500	-0.55699500	-1.57261300

H	-5.60946000	-0.73853100	-0.51244000
H	-3.23578600	-3.18244300	0.95895000
H	-4.87247600	-2.96240500	0.33324400
H	-3.48295200	-2.91143800	-0.77642100
H	-3.51563000	-0.66494300	2.32372500
H	-4.73655400	1.13811000	0.59931800
H	-0.25006000	0.91862900	-1.35095900
O	-4.25440200	-0.79484800	1.72019400
O	-4.50391200	1.00850300	-0.32666400
O	-1.72956700	-0.76268900	-0.79394000
O	-1.72074100	-0.34623400	1.40371200
S	1.28078200	1.52501300	1.17140900
O	0.27491500	2.56859600	1.23414300
O	2.32367700	1.75237900	0.18700000
O	0.66670800	0.18267900	0.98879500
O	1.95271000	1.48034400	2.59761800
H	-0.72080600	-0.08840300	1.26573000
H	2.56280400	0.71307500	2.56278200
C	3.00285300	-1.48409100	-0.60757200
C	3.07532200	-1.74273900	0.92907500
C	3.48312400	-2.72749700	-1.35300400
C	1.58603100	-1.19334800	-1.09445800
H	2.10316900	-2.03500700	1.31594500
H	3.78826000	-2.55299100	1.10099200
H	3.36790600	-2.59130800	-2.42703300
H	4.53806800	-2.87646200	-1.12892500
H	2.91983300	-3.60438100	-1.03728800
H	3.33895400	0.40390200	-0.86715400
H	4.12495700	-0.13376300	1.07152300
H	-0.18274800	-1.76255800	-0.92345100
O	3.84807500	-0.41795700	-0.95571000
O	3.50009900	-0.59755400	1.64404300
O	0.70686400	-2.10749700	-0.71128000
O	1.30658200	-0.26191400	-1.81238800

(SA)₁·(MGA)₂·(DMA)₂:

Atoms	X	Y	Z
N	-0.60229300	-1.18865800	2.19461500
H	-1.28090000	-0.53795900	1.76889800
C	0.02159000	-0.56587200	3.37944000
H	0.77679100	-1.24392800	3.77066300
H	0.47206300	0.37522300	3.08441000
H	-0.74193200	-0.39681900	4.13509900
C	-1.26883500	-2.47277100	2.50531700

H	-1.66953800	-2.88055700	1.58456700
H	-0.53187600	-3.14872300	2.93183400
H	-2.07138300	-2.29424100	3.21722600
C	3.24427300	-1.66184900	0.20137500
C	3.10036600	-0.22778800	0.70209600
C	3.57696000	-2.60056800	1.35268600
C	1.92932100	-2.09111500	0.47749500
H	2.20761500	-0.11561400	1.31310600
H	3.98463700	0.03615700	1.28910600
H	3.65747000	-3.62359400	0.98887600
H	4.53110900	-2.31350900	1.79288500
H	2.79957900	-2.56091100	2.11528200
H	3.89244600	-2.04576500	1.55476500
H	3.66914300	0.41709900	1.01094200
H	0.11601000	-1.38074700	1.45241100
O	4.28602700	-1.66148400	0.75648100
O	2.96357500	0.66359900	0.39846900
O	0.88693900	-2.10768000	0.22115400
O	1.99199900	-2.38365600	1.69121100
S	-3.43418000	-0.59264700	0.09919300
O	-2.77978800	0.32532800	1.05334100
O	-4.80446000	-0.88222400	0.40410900
O	-2.57084200	-1.72388000	0.20735700
O	-3.45060800	0.23514800	1.30187300
H	0.32902400	-2.10900100	2.13586200
H	-4.30343600	0.68216800	1.35699400
N	-0.56287100	-1.56712200	2.13766800
H	-1.04368300	-1.79292800	1.25810200
C	-1.45067200	-1.91037200	3.26370500
H	-0.95623000	-1.65192700	4.19641800
H	-1.66495000	-2.97468900	3.23738100
H	-2.37362000	-1.34647700	3.15505000
C	-0.19347700	-0.13063300	2.09059300
H	0.46326300	0.02494200	1.24063700
H	0.32422100	0.13218800	3.00811600
H	-1.09573900	0.46647100	1.98405900
C	0.71503900	3.46690800	0.20944300
C	0.75463100	3.64964700	1.31090600
C	0.19839000	4.72774400	0.88609200
C	-0.18628900	2.27150900	0.51091600
H	-0.22692900	3.94202900	1.68008400
H	1.47342700	4.44643300	1.52286600
H	0.19773700	4.59429900	1.96631500
H	0.86570200	5.55379200	0.64418800
H	-0.80917700	4.96377800	0.55284500

H	2.26969500	2.31328000	0.49831700
H	1.86924300	2.05968500	1.55017900
H	-1.97745400	1.67569600	0.44725600
O	2.00964200	3.22242200	0.69991100
O	1.09707500	2.45206300	1.97536500
O	-1.44965500	2.47676400	0.19752700
O	0.23296200	1.23084100	0.97026900

(SA)₁·(MGA)₂·(DMA)₃:

Atoms	X	Y	Z
N	0.19584300	-0.68463500	2.25135400
H	-0.38909000	-0.22714700	1.54475200
C	0.10598100	0.09460800	3.50016200
H	0.77298400	-0.35139400	4.23407800
H	0.40503300	1.11307900	3.27616800
H	-0.91960300	0.07454400	3.86025400
C	-0.19078500	-2.10202800	2.39602200
H	-0.05520000	-2.58916600	1.43387800
H	0.46472800	-2.55908700	3.13331800
H	-1.23243200	-2.17482300	2.69526000
C	4.24695800	-1.03135700	-0.21183800
C	4.88989400	0.28698400	0.20222300
C	5.08844600	-2.21558200	0.23820800
C	2.84101500	-1.09422000	0.42102600
H	4.91796100	0.36611400	1.28591100
H	5.90540700	0.33564600	-0.19945000
H	4.61721600	-3.14720400	-0.07201900
H	6.07441200	-2.15900400	-0.22229500
H	5.19002900	-2.21691400	1.32196400
H	3.19853100	-1.18913700	-1.80241200
H	3.97255200	1.19226300	-1.22339700
H	1.19703100	-0.67459800	1.92352900
O	4.13129100	-1.00385800	-1.62598900
O	4.11790200	1.37851900	-0.28641100
O	2.77627200	-1.03786600	1.65946000
O	1.86289600	-1.17050500	-0.37687700
S	-2.86273500	-2.13851600	0.15515600
O	-2.09432600	-0.92102800	0.41102300
O	-3.22425400	-2.92146200	1.30605100
O	-2.29756100	-2.90627800	-0.95794300
O	-4.25321400	-1.51082400	-0.41780900
H	0.08909400	-0.81087700	-1.20104100
H	-4.92390500	-2.20103100	-0.35797500
N	-0.46425900	-1.17403800	-1.98471200

H	-1.06583500	-1.93380900	-1.59395300
C	0.47018000	-1.71488800	-2.99312200
H	1.10207800	-0.90180600	-3.34219300
H	1.07301600	-2.48662900	-2.52534700
H	-0.10673000	-2.12845800	-3.81656500
C	-1.36129000	-0.12578300	-2.52133300
H	-1.93997800	0.27292100	-1.69501800
H	-0.75717300	0.65813300	-2.96543100
H	-2.01914700	-0.58640400	-3.25469800
C	0.85869100	2.65067900	0.14013000
C	1.34542000	2.50534300	-1.29893000
C	1.02348500	4.09633700	0.60873300
C	-0.62041300	2.27950900	0.25924300
H	0.71913700	3.10139600	-1.95886400
H	2.37014700	2.88919200	-1.35197300
H	0.68640200	4.18498100	1.64011900
H	2.07674300	4.37406900	0.56259900
H	0.44631000	4.77697000	-0.01637400
H	2.49134000	1.75614000	0.74141600
H	1.67994700	0.58673600	-1.07233400
H	-2.36118900	2.35561000	-0.54202300
O	1.55265800	1.75595300	0.98747900
O	1.28533900	1.16678800	-1.74465700
O	-1.37771900	2.74357300	-0.70202100
O	-1.04603300	1.64577500	1.20464800
N	-3.65404900	1.67568700	-0.16831600
H	-3.31453400	0.76705200	0.15003500
C	-4.67002600	1.48931000	-1.20273900
H	-4.95469000	2.46171700	-1.60457300
H	-4.26869700	0.87759400	-2.00780800
H	-5.56207000	0.99446900	-0.81061800
C	-4.17454200	2.40563100	0.98970100
H	-3.38436400	2.49577700	1.73142700
H	-4.48344800	3.40234700	0.67419100
H	-5.03508700	1.90033800	1.43613600

(MGA)₁·(DMA)₁:

Atoms	X	Y	Z
N	2.79187600	-0.15244500	0.12739800
H	2.60895600	-0.50832700	1.06010300
C	2.82247600	1.31092700	0.18836600
H	2.91667700	1.70401000	-0.82328700
H	1.88689000	1.66668100	0.61557000
H	3.65973900	1.68246100	0.78584000

C	4.02927000	-0.72058900	-0.40147200
H	3.96918500	-1.80671400	-0.39100400
H	4.15645700	-0.39301800	-1.43249700
H	4.90830800	-0.40634100	0.16933800
C	-1.84038700	-0.36998600	0.01812800
C	-2.18251600	0.73240500	-0.98145700
C	-2.28409700	-1.73486700	-0.49469400
C	-0.33620600	-0.36458800	0.27408300
H	-1.66145600	0.56152200	-1.92085900
H	-3.26238800	0.70014800	-1.15960800
H	-2.03573600	-2.50755500	0.23155800
H	-3.36449500	-1.72732100	-0.63105500
H	-1.80087100	-1.96774800	-1.44198400
H	-1.81800500	-0.06816500	1.91945000
H	-2.16134500	2.08135700	0.38188600
H	1.39043000	-0.47552400	-0.52267100
O	-2.49592500	-0.05649800	1.23035900
O	-1.77979100	1.99236800	-0.49755300
O	0.39273100	-0.55372700	-0.79627100
O	0.10964500	-0.20566300	1.39467900

(SA)₂:

Atoms	X	Y	Z
S	-2.04477400	0.06723500	-0.12328700
O	-1.06465200	-0.10002200	-1.16035000
O	-3.34330500	0.55514100	-0.41024300
O	-2.14575700	-1.36599300	0.54165000
H	-2.93029500	-1.40135000	1.10567500
O	-1.45320300	0.94593800	1.01385100
H	-0.49746000	0.72003200	1.13904700
O	1.06515100	0.09142600	1.16155400
S	2.04527800	-0.06744200	0.12310800
O	1.45732200	-0.94577800	-1.01622500
O	3.34662100	-0.54928500	0.40739400
O	2.13766200	1.36844300	-0.53740800
H	0.50053800	-0.72392900	-1.14016600
H	2.92043800	1.40957700	-1.10347700

(SA)₂·(DMA)₁:

Atoms	X	Y	Z
S	1.36653300	-1.28225400	-0.11546100
O	2.20849000	-0.41429700	-0.91573000
O	0.87266000	-0.59500700	1.09245900
O	2.37029200	-2.41378200	0.38241100

O	0.30425400	-1.98085200	-0.82228100
H	1.78638300	1.20692600	-0.44924600
H	1.85231200	-3.17720000	0.66580600
S	-2.24217800	0.09786000	0.04115000
O	-1.70949100	-0.52543600	1.36568600
O	-3.59330900	0.47664600	0.22616200
O	-2.21444300	-1.08775500	-0.97072600
O	-1.27784900	1.08886900	-0.39985200
H	-0.70934300	-0.60246300	1.32104100
H	-1.29117200	-1.44105500	-1.03340700
N	1.26507500	2.01658700	-0.05669000
H	0.32901000	1.62157600	0.13202100
C	1.11361400	3.07625700	-1.07614900
H	2.09626100	3.44664200	-1.35519800
H	0.51272200	3.88083800	-0.66107900
H	0.60912100	2.64963800	-1.93774900
C	1.90570300	2.45550500	1.20089500
H	2.89891500	2.83552800	0.97722300
H	1.96825500	1.59702400	1.86241400
H	1.30160500	3.23909600	1.65045800

(SA)₂·(MGA)₁:

Atoms	X	Y	Z
C	-4.41759800	-0.42947200	-0.37856700
C	-5.00235000	-0.56855200	1.02653800
C	-5.26899900	0.49213100	-1.24825700
C	-3.00894300	0.12915600	-0.27431700
H	-5.06207200	0.40489100	1.50809600
H	-6.01173400	-0.97780900	0.92196600
H	-4.82898700	0.59269600	-2.23949800
H	-6.25617200	0.04640600	-1.35603600
H	-5.36385100	1.47841500	-0.79764400
H	-3.48409000	-1.85600500	-1.31316700
H	-4.11613100	-2.23794500	1.38492200
H	-2.00122200	1.59699400	0.37773400
O	-4.35906100	-1.72611900	-0.93016500
O	-4.18670700	-1.38632800	1.82709500
O	-2.93165800	1.27553900	0.33954900
O	-2.05925500	-0.46432000	-0.76801600
S	0.76794800	1.21063800	0.11127000
O	2.01819800	1.79825800	-0.28174200
O	-0.34875000	2.07859800	0.35621200
O	0.40439400	0.17081500	-0.96778000
O	0.95970800	0.38477600	1.41378400

H	-0.57425500	-0.09164700	-0.87976500
H	1.81152300	-0.11467300	1.36446000
S	4.32626400	-0.70936500	0.05653300
O	3.32769600	-0.81106000	1.08338900
O	5.62818600	-1.23728800	0.23931000
O	3.64938100	-1.38880000	-1.20383000
O	4.47855900	0.77441700	-0.37893700
H	4.32771500	-1.56774100	-1.86895200
H	3.59370000	1.21856700	-0.37028700

(SA)₂·(MGA)₁·(DMA)₁:

Atoms	X	Y	Z
N	0.88050400	-0.95313000	2.14126900
H	1.07435300	-1.68285300	1.43883800
C	-0.33045900	-1.31936300	2.91183800
H	-0.60083600	-0.48019000	3.54767100
H	-1.13903500	-1.54268400	2.22083300
H	-0.10148300	-2.18772900	3.52439600
C	2.07482900	-0.68862900	2.97338500
H	2.88732900	-0.40574500	2.31293000
H	1.84148500	0.12368900	3.65633300
H	2.32318900	-1.58822600	3.53018600
C	-3.14611200	-0.10600900	-0.48318100
C	-3.53773200	-0.37961600	0.95988900
C	-3.43680100	1.34063600	-0.87370500
C	-1.64737700	-0.33294800	-0.64310600
H	-2.96761900	0.27046700	1.62038100
H	-4.60361500	-0.16241200	1.07228600
H	-3.18667400	1.50096200	-1.92200000
H	-4.49859400	1.53887600	-0.73510900
H	-2.84650800	2.02740600	-0.26749700
H	-3.41169300	-1.18675100	-2.08698200
H	-3.63993300	-2.27694900	0.64678800
H	0.68908300	-0.11470400	1.57605800
O	-3.88822700	-1.02327800	-1.26740500
O	-3.24736600	-1.71311300	1.32166400
O	-0.84654400	-0.01990300	0.20549300
O	-1.32265700	-0.83339500	-1.82013700
S	2.05229300	-1.50381600	-0.91233000
O	1.14019600	-2.43514100	-0.28260300
O	2.95183500	-0.80841600	-0.02383300
O	1.35609200	-0.56666700	-1.83694000
O	2.92669400	-2.43108100	-1.87491700
H	-0.33737400	-0.87559500	-1.89204300

H	3.62022400	-1.88774100	-2.26833400
S	0.78799000	2.49210900	0.08117300
O	-0.50429200	3.07028700	0.26623800
O	1.35694300	1.61984900	1.06450600
O	1.82665700	3.68847000	-0.04295900
O	0.86468300	1.87177700	-1.32838900
H	1.36388300	4.45265700	-0.40770800
H	1.15557300	0.89720000	-1.37385600

(SA)₂·(GMA)₁·(DMA)₂:

Atoms	X	Y	Z
N	3.66504500	-0.65305100	0.87865200
H	3.89402200	0.18867900	0.32366800
C	4.56244700	-1.78011800	0.56353300
H	4.21504900	-2.65376800	1.10972400
H	4.51354300	-1.96522600	-0.50490400
H	5.57635500	-1.52981400	0.86480000
C	3.61902900	-0.29762600	2.31239100
H	2.90770100	0.51303200	2.43074300
H	3.28020300	-1.16623200	2.86896200
H	4.61081600	0.00903100	2.63443300
C	0.01503600	-2.28514300	-0.64573000
C	1.35889800	-2.59350500	-1.29033100
C	-0.82228400	-3.55869200	-0.54395800
C	0.23753500	-1.72768900	0.77434300
H	1.89925100	-3.32201100	-0.68824300
H	1.15934500	-3.02130100	-2.27633800
H	-1.80744900	-3.34056800	-0.13390200
H	-0.94941900	-3.97984400	-1.54064900
H	-0.32800400	-4.29067500	0.09438400
H	-1.54320000	-1.28015000	-1.30523900
H	1.66625300	-0.72339300	-1.77620900
H	2.71373900	-0.90169700	0.57318000
O	-0.58936600	-1.31551500	-1.47764700
O	2.18012500	-1.44951400	-1.39676600
O	1.25212800	-1.95062900	1.39722500
O	-0.74280500	-1.02457800	1.30680400
S	2.13243600	1.93293500	-0.50615300
O	3.58324600	1.81160800	-0.44167500
O	1.61112200	3.27391700	-0.41320600
O	1.44315400	0.96048300	0.34546700
O	1.72191000	1.38523600	-1.98520300
H	-1.85014500	1.41908600	0.98833300
H	2.22532900	1.88434400	-2.63964000

N	-1.12138100	2.02650800	0.57457600
H	-0.19262100	1.61429200	0.75250900
C	-1.23023400	3.37245300	1.17758100
H	-2.22756900	3.75527900	0.97715700
H	-1.07636200	3.29228700	2.24977900
H	-0.47001100	4.00822000	0.73359700
C	-1.33772400	2.03102800	-0.89589300
H	-1.07237800	1.04857300	-1.27938700
H	-2.38581100	2.24319700	-1.08964000
H	-0.68663500	2.78214900	-1.33264600
S	-3.93500100	-0.06568600	0.09297500
O	-4.31470100	0.58033300	-1.12641000
O	-3.49219500	0.80259400	1.18620800
O	-2.96895200	-1.17660200	-0.08879400
O	-5.27706600	-0.76225100	0.61857700
H	-1.58208400	-1.05716300	0.77343400
H	-5.12354500	-1.06141500	1.52208800

(SA)₂·(MGA)₁·(DMA)₃:

Atoms	X	Y	Z
N	-2.94446200	1.88557100	-0.10929100
H	-3.49411200	1.00261000	-0.18855600
C	-3.72722000	2.97124100	-0.73020900
H	-3.15494600	3.89216200	-0.67296600
H	-3.92437700	2.71274400	-1.76688800
H	-4.67078400	3.06549100	-0.19825500
C	-2.63332500	2.12196000	1.31636300
H	-1.97504400	1.32511800	1.65046300
H	-2.15238500	3.09305000	1.40303300
H	-3.56025400	2.10063600	1.88435200
C	1.29947200	2.44956200	-0.33361800
C	0.47826200	3.67768600	0.07334300
C	2.65176200	2.49161500	0.35741900
C	0.48173900	1.18564600	0.01780000
H	0.21661600	3.62021500	1.13130300
H	1.09883300	4.56533100	-0.08676400
H	3.24323100	1.61422600	0.09310000
H	3.19066100	3.37916000	0.02798000
H	2.52536900	2.53964500	1.43961500
H	1.72710700	1.70451100	-2.07068800
H	-0.48387500	3.47011900	-1.55761700
H	-2.03864100	1.73884700	-0.58669300
O	1.43978500	2.56486300	-1.73639600
O	-0.71950700	3.77697000	-0.67133700

O	-0.47645200	0.90637800	-0.72250600
O	0.79986000	0.52279700	1.05103100
S	-3.94734000	-1.38986900	0.35178600
O	-4.64698100	-0.24924200	-0.24655900
O	-4.77829900	-2.28453700	1.10609200
O	-2.68478700	-0.98285900	0.96089700
O	-3.40307100	-2.26397800	-0.92635600
H	0.44486400	-1.29557100	-0.10559400
H	-4.16290800	-2.73425600	-1.28795000
N	-0.38552000	-1.80928800	-0.41825900
H	-1.18366000	-1.20814000	-0.17135300
C	-0.49059500	-3.07274000	0.33667100
H	0.40793500	-3.65558800	0.15362400
H	-0.59522100	-2.83224400	1.39082800
H	-1.38117000	-3.59765900	0.00315200
C	-0.30310700	-1.99675600	-1.88259000
H	-0.24246300	-1.01495300	-2.33952200
H	0.59866000	-2.56199900	-2.10210400
H	-1.19284100	-2.52871400	-2.20599300
S	3.12533900	-1.14898600	-1.03092800
O	2.24551200	-0.21638500	-1.70361200
O	2.41712700	-2.10652700	-0.17947100
O	4.26408700	-0.55888800	-0.32930700
O	3.74978900	-1.99504800	-2.24706700
H	2.15178600	0.14992800	1.65189500
H	4.51125200	-2.47908100	-1.90824700
N	2.94733100	-0.36726100	2.17060500
H	3.56515400	-0.71466600	1.42425300
C	2.31337600	-1.48912500	2.89152500
H	1.57537600	-1.08601200	3.58080500
H	1.83445500	-2.12741100	2.15666700
H	3.07022000	-2.04758400	3.43775100
C	3.69596700	0.55085600	3.04736000
H	4.23677000	1.26240900	2.43086100
H	2.99415800	1.07577200	3.69131200
H	4.39631100	-0.01759400	3.65543300

(SA)₂·(DMA)₂:

Atoms	X	Y	Z
S	-1.51266600	1.43380600	-0.54070000
O	-0.55640200	2.46070800	-0.94804600
O	-1.33743500	0.21499400	-1.57181400
O	-1.09392600	0.86139600	0.76905800
O	-2.90556300	1.75588000	-0.61475000
H	-1.40949200	-0.70101400	0.78768900

N	1.54336600	1.82865100	0.70504500
H	0.89444500	2.06493300	-0.07701900
H	1.33554000	0.84192600	0.92530600
O	0.54984800	-2.48022800	-0.74461500
O	1.49934300	-1.02515500	0.98585600
S	1.47456300	-1.40477100	-0.41879400
O	1.35395800	-0.25244900	-1.31433600
O	2.94835800	-1.99367000	-0.65770600
H	2.96783700	-2.39402100	-1.53517300
H	-0.37645100	0.04992500	-1.68467500
H	-1.20180100	-2.05155800	-0.14038600
N	-1.74052800	-1.70007600	0.66095500
C	-3.18695700	-1.64226800	0.36155600
C	-1.38370200	-2.50235900	1.84822500
C	1.18863300	2.68385800	1.85680500
C	2.95373600	1.93930800	0.28208000
H	3.10706400	1.27538800	-0.56237600
H	3.59329000	1.64722300	1.11112200
H	3.15762300	2.96923600	0.00030100
H	1.37329000	3.72175400	1.59242400
H	1.80014600	2.40285300	2.71065500
H	0.13557300	2.53127100	2.06994800
H	-1.86049400	-2.06334300	2.72095800
H	-1.73094200	-3.52343900	1.71088300
H	-0.30276900	-2.47990100	1.95459200
H	-3.55912700	-2.64635700	0.17371400
H	-3.69752800	-1.20772300	1.21704100
H	-3.33212000	-1.00478500	-0.50627000

(MGA)₂:

Atoms	X	Y	Z
C	-2.66301200	-0.06294500	0.15128600
C	-2.62068400	1.09711100	-0.83506300
C	-3.86228600	-0.96530000	-0.12707800
C	-1.38479700	-0.89504500	0.07884700
H	-2.52978000	0.72987600	-1.85408100
H	-3.55055900	1.66143000	-0.73344200
H	-3.89658700	-1.77029700	0.60518000
H	-4.77623600	-0.37971300	-0.03934600
H	-3.80232500	-1.39517300	-1.12634900
H	-2.12623700	0.01435300	2.00585500
H	-1.43044100	2.05308400	0.37153300
H	-0.08392400	-1.56073100	-1.09394200
O	-2.73999200	0.50348100	1.44184600

O	-1.50874300	1.94225200	-0.58663000
O	-0.98798000	-1.16117800	-1.15149400
O	-0.81788800	-1.26941300	1.07808300
C	2.66300700	0.06293200	0.15137000
C	2.62070800	-1.09704600	-0.83507100
C	3.86229000	0.96530700	-0.12688800
C	1.38479600	0.89504000	0.07895800
H	2.52983500	-0.72973100	-1.85406300
H	3.55057900	-1.66137500	-0.73346700
H	3.89657100	1.77024600	0.60543500
H	4.77623700	0.37971300	-0.03917600
H	3.80235900	1.39525900	-1.12612600
H	2.12618400	-0.01450700	2.00591900
H	1.43042800	-2.05311600	0.37141200
H	0.08395200	1.56081300	-1.09381400
O	2.73994700	-0.50359600	1.44188700
O	1.50875800	-1.94220500	-0.58673900
O	0.98800900	1.16126200	-1.15137300
O	0.81786400	1.26934000	1.07820800

(MGA)₂·(DMA)₁:

Atoms	X	Y	Z
C	2.94575400	-0.77533700	0.18877600
C	3.11947100	-0.17654600	-1.20403000
C	4.19281200	-0.57126500	1.04058100
C	1.74991700	-0.07722600	0.83815400
H	3.41392900	0.86871300	-1.12179400
H	3.91546400	-0.73521700	-1.70598200
H	4.06693600	-1.05327800	2.00908700
H	5.04523200	-1.02756100	0.53907700
H	4.38421700	0.48952500	1.19333400
H	1.92959300	-2.39538200	0.54253800
H	1.49215400	-1.07212500	-1.79705000
H	0.10038200	2.10744200	0.75271600
O	2.68881600	-2.15490300	0.00241000
O	1.91707900	-0.21594400	-1.93701200
O	1.69259700	1.13741800	0.91087200
O	0.83814600	-0.89795600	1.27932600
C	-2.71855100	-1.14945800	0.02772800
C	-1.54675000	-2.03348400	-0.37198300
C	-3.54840300	-1.80781700	1.12481100
C	-2.21795500	0.21955800	0.52055200
H	-0.91855500	-2.25872600	0.48484900
H	-1.94963900	-2.96914100	-0.76989700

H	-4.40659400	-1.18226800	1.36640900
H	-3.91455100	-2.77158000	0.77237500
H	-2.95289400	-1.95178500	2.02541200
H	-3.71260700	-0.01784800	-1.15915700
H	-1.31848400	-1.15271800	-2.06426100
H	-0.09023000	-0.42607900	1.41483300
O	-3.49229000	-0.95943900	-1.14309900
O	-0.73199300	-1.38714000	-1.33617800
O	-1.32038100	0.26732800	1.40739700
O	-2.75258600	1.22881300	0.01631100
N	-0.46982800	2.63307100	0.07293800
H	-1.45874200	2.31488700	0.21599900
C	-0.05944800	2.16025500	-1.27081200
H	0.98641000	2.40500400	-1.43118400
H	-0.17192400	1.07922400	-1.30295400
H	-0.69379100	2.63586100	-2.01467000
C	-0.31022000	4.08370000	0.27088400
H	-0.64695400	4.34848200	1.26879600
H	0.73910400	4.34247600	0.15365900
H	-0.90452800	4.61090600	-0.47089300

(MGA)₂·(DMA)₂:

Atoms	X	Y	Z
C	-2.74829200	0.14150600	-1.15423500
C	-2.59489800	-1.33471000	-0.83016100
C	-4.20070900	0.58279200	-0.98806600
C	-1.86055900	0.98790300	-0.22356400
H	-3.06115900	-1.54422300	0.13392500
H	-3.12244900	-1.90299100	-1.60270900
H	-4.30417000	1.62067500	-1.30121300
H	-4.84066000	-0.03221000	-1.62119000
H	-4.52023100	0.49042600	0.04948000
H	-1.80799900	1.12410200	-2.50892600
H	-0.73690800	-1.37986300	-1.48623600
H	-0.94861900	-0.90914800	1.34948300
O	-2.33277500	0.31383900	-2.49495100
O	-1.24471600	-1.73138400	-0.73649900
O	-1.77914900	0.68955300	0.98319200
O	-1.28222800	1.96634700	-0.78109000
C	2.75156200	-0.57237900	-0.87901400
C	1.79849200	0.05275800	-1.90647300
C	3.92440900	0.35914000	-0.60947800
C	1.98314700	-0.86089000	0.42361100
H	1.22342700	0.86311800	-1.45672700

H	2.39271700	0.45395500	-2.73444400
H	4.57564200	-0.06455900	0.15327900
H	4.50008000	0.48798900	-1.52519300
H	3.57362500	1.33182800	-0.26555900
H	2.91998300	-2.47301300	-0.80236800
H	1.38923800	-1.70017500	-2.55304300
H	-0.20901700	2.42591100	0.15560600
O	3.21742000	-1.79153600	-1.42474400
O	0.87490700	-0.90012900	-2.38796700
O	1.56507500	0.11619000	1.09194200
O	1.81773600	-2.06208200	0.72977200
N	-0.54758200	-1.60850000	2.00116700
H	0.37781200	-1.88079700	1.58334900
C	-1.43147900	-2.78589700	2.07690600
H	-2.40958600	-2.47365100	2.43673900
H	-1.51201500	-3.21476500	1.08341300
H	-1.00120100	-3.50686300	2.76811200
C	-0.33871400	-0.94427300	3.30054500
H	0.39198400	-0.15621100	3.15171300
H	-1.28649700	-0.53243400	3.63927000
H	0.03399600	-1.67172300	4.01820400
N	0.64877100	2.58701100	0.80677900
H	1.09509300	1.63555500	0.85540900
C	0.18512700	2.95911600	2.15281000
H	-0.27465700	3.94490700	2.11515300
H	-0.55321600	2.22389600	2.46127400
H	1.02893700	2.97424200	2.84039500
C	1.57727900	3.55388500	0.20570300
H	1.84213800	3.21622500	-0.79362800
H	1.09601100	4.52727000	0.13845500
H	2.47703800	3.63286000	0.81360500

(SA)₃:

Atoms	X	Y	Z
S	0.17426200	1.31596300	-0.06476400
O	-0.08217600	0.09590100	-0.81882000
O	1.38482400	2.00273400	-0.38324000
H	3.13370100	1.29355300	-0.27042800
O	0.09966900	0.98021400	1.45254600
O	-1.00013900	2.28564200	-0.20812400
O	3.84231800	0.62362700	-0.22208300
S	3.21803200	-0.77744600	0.09351200
O	4.28504900	-1.68708900	0.24489200
O	2.45229200	-1.14099900	-1.22872600

O	-2.39588100	-1.33394400	-0.97313800
H	1.54409100	-0.78336800	-1.19969400
H	-1.52359800	-0.87709200	-0.97493100
O	2.22912700	-0.61245800	1.13338900
O	-3.17205500	0.85052700	-0.20017600
H	0.83585800	0.35330700	1.64323200
H	-1.86875700	1.78854200	-0.19624900
O	-4.66998200	-1.13261200	-0.23286500
S	-3.38757600	-0.56429100	-0.05270900
O	-2.85090900	-0.88295500	1.39931700
H	-3.17386300	-1.75125600	1.67768000

(SA)₃·(DMA)₁:

Atoms	X	Y	Z
S	-1.25160400	1.60425100	-0.89283600
O	-2.00283500	1.40763400	0.35326400
O	0.16829500	1.83109000	-0.63427900
O	-1.84781700	2.97508100	-1.42716100
O	-1.51098500	0.60966800	-1.91717100
H	-0.64630100	1.11512600	1.67025400
H	-1.54274400	3.11675400	-2.33260200
S	-1.58021100	-1.93551000	0.16653500
O	-2.76970600	-1.08222000	0.69524400
O	-0.36435600	-1.16948100	0.41831400
O	-1.78841100	-1.99512200	-1.37300800
O	-1.70006100	-3.24558600	0.68312200
H	-2.59210500	-0.11295100	0.53892300
H	-1.66415700	-1.08557700	-1.74202600
N	0.27518100	1.04093600	2.11833500
H	0.89810800	0.63839400	1.39792000
C	0.23313400	0.12042100	3.27608900
H	-0.42086400	0.53546000	4.03821700
H	1.24239200	0.01443400	3.66443800
H	-0.13673200	-0.84179500	2.93714100
C	0.78212700	2.39351500	2.44386900
H	0.14173600	2.84120200	3.19900600
H	0.77471500	2.98411900	1.53346100
H	1.79761200	2.29559300	2.81767900
S	2.80215300	-0.43824600	-0.53907300
O	4.15653100	-0.64129300	-0.89022900
O	2.10458800	0.36229800	-1.67924800
O	2.46224700	0.19528100	0.71932500
H	1.35079800	0.89963900	-1.32109300
O	2.10059000	-1.83593700	-0.58267800

H	1.18966200	-1.74981200	-0.22738500
---	------------	-------------	-------------

(SA)₃·(DMA)₂:

Atoms	X	Y	Z
S	-3.84770100	-0.58218000	-0.52476700
O	-5.14646700	-0.44317800	-1.07116000
O	-3.29844700	0.45500700	0.31919600
O	-3.80367200	-1.92819400	0.26100700
H	-2.89556900	-2.04072300	0.63521000
O	-2.84743800	-0.80853400	-1.70885700
H	-1.91828400	-0.70006000	-1.37981200
N	3.73643100	-1.51028700	-0.16684500
H	3.41374400	-0.70109500	0.40779600
C	4.83168500	-1.07967400	-1.06708700
H	5.11666000	-1.91775400	-1.69778700
H	5.67484300	-0.76732000	-0.45730400
H	4.48290300	-0.24126100	-1.66190400
C	4.08054800	-2.64861900	0.71389300
H	4.37570300	-3.49494900	0.09931100
H	3.20281400	-2.89859600	1.30113900
H	4.90551700	-2.35297000	1.35613000
S	2.46339200	1.53528200	-0.30173800
O	1.38845400	2.50992900	-0.20242100
O	3.75104400	1.99526800	-0.72316700
O	2.53100100	0.69968900	0.93589800
H	1.11987900	0.13971100	1.51012900
O	2.03591800	0.49602700	-1.44862500
H	1.11162100	0.19940300	-1.28994300
S	-0.09846900	-1.27692400	0.53171100
O	0.21968700	-0.25652200	1.69985700
O	-0.43302800	-0.40374400	-0.63545600
O	1.10901600	-2.03881100	0.28547600
H	2.88879400	-1.73912600	-0.69354300
O	-1.24136500	-2.02810500	0.99572200
H	-1.44466800	1.19116200	0.39750900
N	-1.18875200	2.15412500	0.63794600
H	-0.15828200	2.21258100	0.56482700
C	-1.66328800	2.43652000	2.00904400
H	-2.74346300	2.32383800	2.02260000
H	-1.37820300	3.45010000	2.27809300
H	-1.20754500	1.71833300	2.68347200
C	-1.76434400	3.04838900	-0.39145500
H	-2.84329700	2.92676300	-0.38667600
H	-1.35368200	2.76340600	-1.35583200

H	-1.48401500	4.07249600	-0.16054500
---	-------------	------------	-------------

(SA)₃·(DMA)₃:

Atoms	X	Y	Z
S	-0.60219000	-1.90053200	-0.76113300
O	0.58310300	-2.74012500	-0.74832500
O	-1.75331500	-2.52481800	-1.40365500
O	-0.95575500	-1.33609600	0.54782100
O	-0.18543400	-0.66149900	-1.67333800
H	0.38392500	2.30187700	-0.25076800
N	2.59761400	-2.32339000	1.01763200
H	1.90606700	-2.21058900	0.25056800
H	3.32423000	-1.59648400	0.86758100
O	1.74537600	0.43671400	0.36292800
O	4.11670100	-0.13758700	0.23923000
S	2.96892800	0.44091700	-0.44388100
O	3.22679900	1.73436400	-1.06550000
O	2.68402800	-0.61093100	-1.61678500
H	1.72615900	-0.61468500	-1.80065800
H	-3.12589700	-1.78922300	-0.73172900
H	1.90214300	2.75339800	-0.62889700
N	1.01098900	3.11340600	-0.23062700
C	1.23766000	3.50727800	1.17941700
C	0.43345500	4.18414600	-1.07054000
C	3.17101700	-3.67712000	0.88875900
C	1.88694200	-2.08309500	2.29195800
H	1.54468500	-1.05295000	2.28967700
H	2.56795700	-2.26478200	3.11965300
H	1.03550300	-2.75690500	2.34186800
H	2.36379000	-4.40185300	0.95358600
H	3.89293900	-3.84067900	1.68458100
H	3.65558000	-3.75534300	-0.08006500
H	-0.52903400	4.46232200	-0.65123600
H	1.11634900	5.02963000	-1.07735600
H	0.30166800	3.80002300	-2.07757900
H	1.95979100	4.31967700	1.19634300
H	0.28721000	3.81617600	1.60410200
H	1.62017200	2.63850600	1.70532400
S	-1.94039100	1.80503200	0.54382900
O	-1.94351200	3.21289300	0.83795300
O	-1.40621700	1.49567500	-0.80382100
O	-3.19839100	1.10770900	0.79974200
H	-0.65780900	0.15354100	-1.34297300
O	-0.85095800	1.20782900	1.54290200

H	-0.66700400	0.28521700	1.26169600
N	-3.84021100	-1.28898700	-0.16083200
C	-4.07593800	-2.05294500	1.08109100
C	-5.06077500	-1.02275400	-0.94409900
H	-3.42452200	-0.36869700	0.12140100
H	-4.53853400	-3.00562500	0.83539200
H	-3.11367200	-2.20950700	1.55895300
H	-4.72726300	-1.47209400	1.72944800
H	-5.52410700	-1.96493200	-1.22591900
H	-5.74457100	-0.43495600	-0.33685000
H	-4.78962100	-0.46101700	-1.83309700

(MGA)₃:

Atoms	X	Y	Z
C	3.39138400	-1.55557200	0.13809600
C	4.26686300	-0.32566000	0.33646100
C	3.67966800	-2.60983100	1.20300600
C	1.91230800	-1.18008200	0.19196600
H	4.07226400	0.13393900	1.30233500
H	5.31195200	-0.63972800	0.28670400
H	3.05453200	-3.48567500	1.03594600
H	4.72337500	-2.91074200	1.12887400
H	3.48351500	-2.21871200	2.20033900
H	2.83952800	-2.31162200	-1.55372800
H	3.92589800	0.18673300	-1.50317000
H	0.64824400	-0.13385100	1.23572500
O	3.67760800	-2.04278600	-1.15591300
O	4.00027700	0.64914300	-0.65900500
O	1.60365800	-0.42473800	1.21106700
O	1.14445300	-1.60046500	-0.64897700
C	-0.30993100	2.66280900	-0.07536800
C	-0.48993300	2.23626400	1.38771000
C	-0.21575300	4.17793700	-0.17627900
C	0.95118800	1.99082200	-0.60499100
H	0.38235100	2.51951500	1.97504000
H	-1.37381200	2.74180500	1.78096900
H	-0.04585600	4.47349100	-1.20976600
H	-1.15886600	4.61012400	0.15536900
H	0.59462600	4.55936800	0.44152700
H	-1.14870800	1.38474500	-1.25376600
H	-1.59654200	0.62875200	1.34698700
H	2.80736000	1.85073800	-0.32793400
O	-1.41046700	2.21230900	-0.82597000
O	-0.65524500	0.83292400	1.49785100

O	2.06306600	2.43150500	-0.03955200
O	0.91346000	1.10864900	-1.42833100
C	-3.60351700	-1.26509400	-0.29104400
C	-3.88366300	0.21385900	-0.03705900
C	-4.13259800	-1.70387300	-1.64952400
C	-2.09940100	-1.50307300	-0.18186200
H	-3.39288300	0.84963700	-0.76829300
H	-4.96387200	0.37063300	-0.08121800
H	-3.92677600	-2.76124800	-1.80751000
H	-5.21124800	-1.55708500	-1.67274300
H	-3.67119600	-1.12915100	-2.45048800
H	-3.55658000	-2.54372000	1.15457300
H	-3.75634800	-0.03896300	1.87127800
H	-0.43284000	-1.06260500	-0.95537100
O	-4.23284100	-1.98256600	0.75152400
O	-3.38185200	0.58622000	1.23866500
O	-1.39326100	-0.85772100	-1.09329200
O	-1.62983200	-2.20589900	0.67963900

(MGA)₃·(DMA)₁:

Atoms	X	Y	Z
C	2.86990100	-2.16258700	-0.82260300
C	3.63499500	-1.77796600	0.45059400
C	2.87549100	-3.66766400	-1.02555400
C	1.45656000	-1.62227800	-0.62381700
H	3.28499500	-2.38263200	1.28811100
H	4.69160500	-1.99285200	0.26822900
H	2.39165000	-3.91519000	-1.96833100
H	3.90552200	-4.01999900	-1.06631700
H	2.35309900	-4.16463300	-0.21104800
H	3.02119800	-0.73396700	-2.13553000
H	3.47947800	0.14897000	0.03538100
H	-0.65191600	-0.49631000	1.91915800
O	3.49357800	-1.54846700	-1.93029200
O	3.43198300	-0.42983400	0.81023300
O	0.70088000	-2.10348800	0.21818900
O	1.16938100	-0.59281900	-1.35412100
C	0.83473500	3.00301100	-0.52544500
C	1.80716200	2.40204800	-1.52892800
C	-0.38245000	3.58903400	-1.23661300
C	0.33307600	1.96511400	0.49070500
H	1.33893200	1.61089800	-2.10633900
H	2.11280500	3.19904600	-2.21231700
H	-1.02422600	4.08625100	-0.51002400

H	-0.05204600	4.32918700	-1.96471500
H	-0.95819900	2.80819500	-1.73226100
H	1.29474600	3.93625200	1.08998500
H	3.26388100	2.54256600	-0.28502800
H	0.50899800	0.07906400	-0.81745100
O	1.55829300	4.00765100	0.16298300
O	2.94123200	1.85287000	-0.87728000
O	-0.11412000	0.85430600	0.07918400
O	0.32654400	2.31021200	1.68914700
N	-0.22648700	-0.07748800	2.75611500
H	-0.06940200	0.92923600	2.47002400
C	1.08741900	-0.69864700	3.02662200
H	0.95754000	-1.77276000	3.13412300
H	1.75298000	-0.48312100	2.19420100
H	1.48814200	-0.27398200	3.94413200
C	-1.18367700	-0.17882700	3.87177800
H	-2.11030500	0.30533300	3.58103000
H	-1.37400200	-1.22755300	4.08556600
H	-0.76021300	0.30879200	4.74600800
C	-3.91513400	-0.81383800	-0.66058500
C	-3.68779200	0.10664400	-1.85778400
C	-4.56903000	-2.12235200	-1.09550800
C	-2.59064200	-1.11555700	0.03061100
H	-2.99826900	-0.35781600	-2.55928800
H	-4.65499700	0.25199200	-2.35022700
H	-4.71655200	-2.77432400	-0.23555500
H	-5.54262900	-1.89930300	-1.52867400
H	-3.95440900	-2.63840600	-1.83104600
H	-4.34000200	-0.20143800	1.11929200
H	-3.67244700	1.67151100	-0.74563500
H	-0.83338600	-1.80694300	-0.27438400
O	-4.74638800	-0.11996600	0.24779800
O	-3.12449000	1.33260100	-1.46064200
O	-1.69490700	-1.64327400	-0.75674100
O	-2.43834000	-0.91484900	1.22220500

(MGA)₃·(DMA)₂:

Atoms	X	Y	Z
C	4.56069300	-0.05464600	0.25023200
C	4.81393100	-0.67450100	-1.11858400
C	5.30085200	1.26955700	0.39384600
C	3.05267200	0.17945700	0.42587500
H	4.39494300	-0.03971600	-1.89650800
H	5.89359400	-0.76742000	-1.26873100

H	5.11481900	1.69819100	1.37795200
H	6.37147300	1.09569200	0.29403600
H	4.97300600	1.97476900	-0.36817100
H	4.28188400	-1.08958000	1.84213400
H	4.48425700	-2.43339300	-0.43747100
H	1.05580100	-0.37750300	-1.07719300
O	5.01128600	-0.98683300	1.21623800
O	4.18505300	-1.93971400	-1.20967300
O	2.47799100	0.86467400	-0.45995500
O	2.51015700	-0.32343900	1.43522000
C	-3.58499800	-1.71821800	-0.02526600
C	-3.37570500	-2.26422600	1.37624800
C	-4.68777600	-0.66536600	-0.04979400
C	-2.27087600	-1.10644100	-0.54460300
H	-3.10509200	-1.45456900	2.05060600
H	-4.31095100	-2.71656200	1.72040300
H	-4.81380600	-0.27955200	-1.06004200
H	-5.62473400	-1.12091000	0.26989800
H	-4.45651400	0.17242700	0.60892200
H	-3.46201900	-2.67692500	-1.67831300
H	-2.51620500	-3.83952200	0.70145400
H	-0.60444100	0.65805700	1.57899500
O	-3.93114900	-2.82209200	-0.84523900
O	-2.32026100	-3.20720600	1.40150500
O	-1.58759000	-0.40966700	0.24051700
O	-1.97917500	-1.35027300	-1.74005300
N	0.68943900	-1.18761500	-1.58670800
H	-0.33915200	-1.02492100	-1.73732000
C	0.83047600	-2.41365000	-0.77388300
H	1.88097300	-2.56327600	-0.54261700
H	0.24006800	-2.29323600	0.13130000
H	0.44329700	-3.25048400	-1.35042500
C	1.38183800	-1.25186700	-2.89030800
H	1.28224800	-0.28156000	-3.36745000
H	2.42615900	-1.50097900	-2.72043700
H	0.90437500	-2.01916500	-3.49500100
C	-1.82296300	2.75743900	-0.80744800
C	-2.18210100	3.06474200	0.64012700
C	-1.74959800	4.05624300	-1.61206800
C	-0.47978800	2.04402900	-0.96906200
H	-1.44494500	3.74610500	1.06402400
H	-3.15596400	3.56387900	0.63057800
H	-1.53929300	3.82546500	-2.65471700
H	-2.71086400	4.56446900	-1.55213800
H	-0.96982300	4.71506200	-1.22929600

H	-2.41781400	1.28876300	-1.93079500
H	-2.49524600	1.16300600	0.90529900
H	1.24403900	1.72696200	-0.20111900
O	-2.83552400	1.91287000	-1.32091300
O	-2.22938700	1.91498900	1.45823100
O	0.39232900	2.25587200	-0.00556500
O	-0.25727700	1.37838600	-1.95563300
N	0.06657800	0.39411600	2.30965800
H	0.96267000	0.10659700	1.84244700
C	-0.47987300	-0.75934800	3.05423900
H	-1.38473700	-0.44324200	3.56873300
H	-0.71851200	-1.55197900	2.34957000
H	0.26143400	-1.09368900	3.77616400
C	0.33803500	1.57233500	3.15520000
H	0.71965200	2.36662100	2.52063300
H	-0.59143000	1.89009600	3.61943400
H	1.07419100	1.30275100	3.90855800

(GMA)₃·(DMA)₃:

Atoms	X	Y	Z
C	4.45104300	-1.41182300	0.42028800
C	4.64343900	-1.75940500	-1.05117200
C	5.46851200	-0.37183500	0.87306700
C	3.02408200	-0.87350100	0.61816600
H	4.45701700	-0.88161200	-1.66699000
H	5.67382500	-2.09551200	-1.20268500
H	5.31296300	-0.12945800	1.92373500
H	6.47333300	-0.77751500	0.76157900
H	5.37942600	0.53778200	0.28049400
H	3.82424800	-2.67873500	1.71464500
H	3.83893800	-3.48575000	-0.82983600
H	0.87098100	-0.55455800	-0.60186700
O	4.61080500	-2.60962400	1.15553900
O	3.72433100	-2.75709200	-1.45023300
O	2.66483900	0.10021100	-0.08691400
O	2.31095100	-1.45653400	1.46757500
C	-4.10752500	-1.82737700	-0.22615600
C	-3.95501500	-3.14118700	0.53192200
C	-5.05093700	-0.87220000	0.49364000
C	-2.72190200	-1.18077200	-0.36119100
H	-3.50628900	-2.95682500	1.50576500
H	-4.94765600	-3.58291700	0.66896700
H	-5.10317100	0.07378400	-0.04503000
H	-6.04781100	-1.30984700	0.53401700

H	-4.70008300	-0.68143400	1.50774800
H	-4.01036300	-1.71145000	-2.13559300
H	-3.43293100	-4.03475200	-1.07450800
H	-0.58069600	0.13532900	1.29085100
O	-4.60674800	-2.14925300	-1.51257000
O	-3.10161700	-4.02285000	-0.16987600
O	-2.10729300	-0.89598100	0.69145700
O	-2.30215500	-0.97080300	-1.52874800
N	0.33206300	-1.16981400	-1.22113600
H	-0.66080300	-0.82603700	-1.26630300
C	0.30175500	-2.55901800	-0.71344300
H	1.31523700	-2.94854700	-0.69670900
H	-0.13205400	-2.55570600	0.28194100
H	-0.33483300	-3.14472700	-1.37188100
C	0.92339900	-1.06028200	-2.56948200
H	0.93775400	-0.00942300	-2.84506900
H	1.92918200	-1.47325100	-2.54735400
H	0.29745700	-1.61593000	-3.26354000
C	-2.22063800	2.83733100	-0.23301200
C	-2.62348600	2.86821800	1.24295100
C	-2.59266300	4.15077700	-0.90790100
C	-0.70509800	2.59804200	-0.31308800
H	-2.08815400	3.66367500	1.76065000
H	-3.69850700	3.06811700	1.29431700
H	-2.29721900	4.12667600	-1.95614600
H	-3.67313700	4.28282200	-0.86237200
H	-2.09887700	4.98856600	-0.42016500
H	-2.28173700	1.11365400	-1.14412000
H	-2.64250600	0.91943900	1.34903800
H	1.35315000	3.16317700	-0.31664800
O	-2.92120100	1.77452700	-0.83808600
O	-2.30964500	1.65235900	1.89173900
O	0.03816000	3.55696500	0.05796600
O	-0.29052900	1.49403100	-0.71887000
N	0.11103300	0.03322000	2.05013900
H	0.88371100	-0.59880200	1.72723900
C	-0.57164800	-0.60216500	3.19883800
H	-1.35198600	0.06941100	3.54553300
H	-1.01258200	-1.53403300	2.86022300
H	0.16351000	-0.78233800	3.97963200
C	0.72005700	1.33587700	2.38393600
H	1.20307100	1.71879700	1.49220700
H	-0.06396300	2.01625000	2.70033400
H	1.45202400	1.18021900	3.17357800
N	2.30971200	2.76804200	-0.75674400

H	2.32001500	1.76121700	-0.53765400
C	3.50020900	3.39750400	-0.16960900
H	3.44903600	4.47361700	-0.31907900
H	3.52600800	3.17979100	0.89522100
H	4.40086700	3.00544200	-0.63904800
C	2.20593700	2.93812300	-2.21527100
H	1.26343000	2.50142700	-2.53564000
H	2.21435600	4.00014700	-2.45072300
H	3.03983900	2.44421600	-2.71128400

Communications in Computational Chemistry

Communications in Computational Chemistry