

Theoretical Analysis of Sulfuric Acid-Dimethylamine-Oxalic Acid-Water Clusters and Implications for Atmospheric Cluster Formation

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S1 Method for Hydrate Distribution

The hydrate distribution can be given as follows:

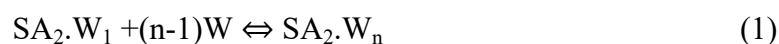
$$\frac{\rho(1,n)}{\rho_{SA.DMA.OA}^{total}} = \frac{\rho(1,m)}{\rho(1,0) + \rho(1,1) + \dots + \rho(1,n)} = \frac{K_1 K_2 \dots \left(S \frac{p_w^{eq}}{p}\right)^m}{1 + K_1 S \frac{p_w^{eq}}{p} + \dots + K_1 K_2 \dots K_n \left(S \frac{p_w^{eq}}{p}\right)^n}$$

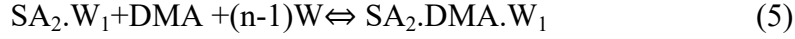
$$K_n = \exp\left(-\frac{\Delta G_n}{RT}\right)$$

Here, K_n represents the equilibrium which is related to the formation of stepwise hydration. S is the saturation ratio, related to the relative humidity. p_w^{eq} (kPa) is the saturation vapor pressure of water, and P is the reference pressure of 1 atm.

S2 Method for Concentration Ratios

For following cluster forming reactions:





According to the law of mass balance, we can get:

$$\begin{aligned} & \frac{[SA_2.DMA.OA.W_1] + [SA_2.DMA.OA.W_2] + \dots + [SA_2.DMA.OA.W_n]}{[SA_2.W_1] + [SA_2.W_2] + \dots + [SA_2.W_n]} \\ &= [DMA][OA]\rho^{-2} \frac{K'_1 + K'_2 \left[\frac{\rho_W^{free}}{\rho}\right] + \dots + K'_n \left[\frac{\rho_W^{free}}{\rho}\right]^{n-1}}{1 + K_1 \left[\frac{\rho_W^{free}}{\rho}\right] + \dots + K_{n-1} \left[\frac{\rho_W^{free}}{\rho}\right]^{n-1}} \\ & \frac{[SA_2.DMA.W_1] + [SA_2.DMA.W_2] + \dots + [SA_2.OA.W_n]}{[SA_2.W_1] + [SA_2.W_2] + \dots + [SA_2.W_n]} \\ &= [DMA]\rho^{-1} \frac{K''_1 + K''_2 \left[\frac{\rho_W^{free}}{\rho}\right] + \dots + K''_n \left[\frac{\rho_W^{free}}{\rho}\right]^{n-1}}{1 + K_1 \left[\frac{\rho_W^{free}}{\rho}\right] + \dots + K_{n-1} \left[\frac{\rho_W^{free}}{\rho}\right]^{n-1}} \end{aligned}$$

Here K_{n-1} , K'_1 , K'_n , K''_1 , K''_n are the equilibrium constants of equation (1) to equation (5), respectively. ρ_W^{free} (cm^{-3}) is the free monomer concentration of water.

$$K_n = \exp\left(-\frac{\Delta G_n}{RT}\right)$$

$$\rho_W^{free} = \frac{S}{k_B T} P_w^{eq}$$

Where, P_w^{eq} (kPa) is the saturation vapor pressure of water, the reference concentration ρ (cm^{-3}) is given by:

$$\rho = \frac{P}{k_B T}$$

Finally, the concentration ratio of $SA_2.DMA.OA.W_n$ to binary $SA_2.W_n$ dimer clusters (A) and $SA_2.DMA.W_n$ to binary $SA_2.W_n$ dimer clusters (B) are calculated as:

$$A = [DMA][OA]\rho^{-2} \frac{K'_1 + K'_2 \left[S \frac{P^{eq}}{W} \right] + \dots + K'_n \left[S \frac{P^{eq}}{W} \right]^{n-1}}{1 + K_1 \left[S \frac{P^{eq}}{W} \right] + \dots + K_{n-1} \left[S \frac{P^{eq}}{W} \right]^{n-1}}$$

$$B = [DMA]\rho^{-1} \frac{K''_1 + K''_2 \left[S \frac{P^{eq}}{W} \right] + \dots + K''_n \left[S \frac{P^{eq}}{W} \right]^{n-1}}{1 + K_1 \left[S \frac{P^{eq}}{W} \right] + \dots + K_{n-1} \left[S \frac{P^{eq}}{W} \right]^{n-1}}$$

S3 Method for Rayleigh Light Scattering Properties

The Rayleigh light scattering properties of the natural light (R_n , a.u.), and the parallel ($R_{p\parallel}$, a.u.) and perpendicular ($R_{p\perp}$, a.u.) components of the linearly polarized light are calculated as follows:

$$R_n = 45(\bar{\alpha})^2 + 13(\Delta\alpha)^2$$

$$R_{p\perp} = 45(\bar{\alpha})^2 + 7(\Delta\alpha)^2$$

$$R_{p\parallel} = 6(\Delta\alpha)^2$$

Here, $\bar{\alpha}$ (a.u.) and $\Delta\alpha$ (a.u.) represent the isotropic mean and anisotropic polarizabilities, respectively, which can be expressed as:

$$\bar{\alpha} = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$(\Delta\alpha)^2 = \frac{1}{2}[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2] + 3[(\alpha_{xy})^2 + (\alpha_{yz})^2 + (\alpha_{zx})^2]$$

For Rayleigh scattering, σ_n , σ_p , and σ_c represent the depolarization ratio of natural, plane-polarized, and circular-polarized light, respectively. The detailed computational methods are given by:

$$\sigma_n = \frac{6(\Delta \alpha)^2}{45(\bar{\alpha})^2 + 7(\Delta \alpha)^2}$$

$$\sigma_p = \frac{3(\Delta \alpha)^2}{45(\bar{\alpha})^2 + 4(\Delta \alpha)^2}$$

$$\sigma_c = \frac{\sigma_n}{1 - \sigma_n}$$

Table S1 Binding energies at 0 K (ΔE), and enthalpies at 298.15 K (ΔH) for $SA_m.DMA.OA.W_n$ ($m=1-2, n=0-4$) according to reaction path 1. Energies are calculated at DF-LMP2-F12/VDZ-F12//M06-2x/6-311+G(2d, p) level of theory (in kcal/mol).

Reactions	ΔE	ΔH	ΔG
$SA + DMA + OA \Leftrightarrow SA.DMA.OA$	-43.78	-41.01	-19.83
$SA + DMA + OA + W \Leftrightarrow SA.DMA.OA.W_1$	-58.44	-53.46	-21.30
$SA + DMA + OA + 2W \Leftrightarrow SA.DMA.OA.W_2$	-68.20	-61.68	-20.75
$SA + DMA + OA + 3W \Leftrightarrow SA.DMA.OA.W_3$	-76.74	-67.78	-16.19
$SA + DMA + OA + 4W \Leftrightarrow SA.DMA.OA.W_4$	-88.5	-77.46	-16.82
$2SA + DMA + OA \Leftrightarrow SA_2.DMA.OA$	-67.20	-62.50	-29.85
$2SA + DMA + OA + W \Leftrightarrow SA_2.DMA.OA.W_1$	-77.70	-71.59	-29.44
$2SA + DMA + OA + 2W \Leftrightarrow SA_2.DMA.OA.W_2$	-93.41	-85.51	-30.14
$2SA + DMA + OA + 3W \Leftrightarrow SA_2.DMA.OA.W_3$	-104.7	-86.49	-33.27
$2SA + DMA + OA + 4W \Leftrightarrow SA_2.DMA.OA.W_4$	-112.40	-101.14	-27.45

Table S2 Binding energies at 0 K (ΔE), and enthalpies at 298.15 K (ΔH) for $SA_m.DMA.OA.W_n$ ($m=1-2, n=0-4$) according to reaction path 2. Energies are calculated at DF-LMP2-F12/VDZ-F12//M06-2x/6-311+G(2d, p) level of theory (in kcal/mol).

Reactions	ΔE	ΔH	ΔG
$SA.DMA.OA + W \rightleftharpoons SA.DMA.OA.W_1$	-14.70	-12.50	-1.47
$SA.DMA.OA.W_1 + W \rightleftharpoons SA.DMA.OA.W_2$	-9.75	-8.22	0.56
$SA.DMA.OA.W_2 + W \rightleftharpoons SA.DMA.OA.W_3$	-7.74	-6.34	2.84
$SA.DMA.OA.W_3 + W \rightleftharpoons SA.DMA.OA.W_4$	-11.80	-9.68	-0.63
$SA_2.DMA.OA + W \rightleftharpoons SA_2.DMA.OA.W_1$	-9.19	-8.26	-0.11
$SA_2.DMA.OA.W_1 + W \rightleftharpoons SA_2.DMA.OA.W_2$	-13.20	-11.40	-1.26
$SA_2.DMA.OA.W_2 + W \rightleftharpoons SA_2.DMA.OA.W_3$	-11.30	-9.63	1.00
$SA_2.DMA.OA.W_3 + W \rightleftharpoons SA_2.DMA.OA.W_4$	-7.69	-5.99	1.69

Table S3 Binding energies at 0 K (ΔE), and enthalpies at 298.15 K (ΔH) for $SA_m.DMA.OA.W_n$ ($m=1-2$, $n=0-4$) according to the reaction path 3. Energies are calculated at DF-LMP2-F12/VDZ-F12//M06-2x/6-311+G(2d, p) level of theory (in kcal/mol).

Reactions	ΔE	ΔH	ΔG
$SA.DMA + OA \rightleftharpoons SA.DMA.OA$	-18.42	-17.37	-6.14
$SA.DMA.W_1 + OA \rightleftharpoons SA.DMA.OA.W_1$	-18.38	-17.47	-4.66
$SA.DMA.W_2 + OA \rightleftharpoons SA.DMA.OA.W_2$	-16.40	-16.17	-4.53
$SA.DMA.W_3 + OA \rightleftharpoons SA.DMA.OA.W_3$	-14.32	-13.01	-0.63
$SA.DMA.W_4 + OA \rightleftharpoons SA.DMA.OA.W_4$	-14.09	-13.31	-2.02
$SA_2.DMA + OA \rightleftharpoons SA_2.DMA.OA$	-11.23	-10.52	-0.09
$SA_2.DMA.W_1 + OA \rightleftharpoons SA_2.DMA.OA.W_1$	-10.44	-9.91	-0.31
$SA_2.DMA.W_2 + OA \rightleftharpoons SA_2.DMA.OA.W_2$	-16.19	-15.32	-0.76
$SA_2.DMA.W_3 + OA \rightleftharpoons SA_2.DMA.OA.W_3$	-10.15	-9.37	3.62
$SA_2.DMA.W_4 + OA \rightleftharpoons SA_2.DMA.OA.W_4$	-5.715	-5.07	6.55

Table S4 Binding energies at 0 K (ΔE), and enthalpies at 298.15 K (ΔH) for $SA_m.DMA.OA.W_n$ ($m=1-2, n=0-4$) according to reaction path 4. Energies are calculated at DF-LMP2-F12/VDZ-F12//M06-2x/6-311+G(2d, p) level of theory (in kcal/mol).

Reactions	ΔE	ΔH	ΔG
$SA.DMA + OA \rightleftharpoons SA.DMA.OA$	-18.42	-17.37	-6.14
$SA.DMA + OA + W \rightleftharpoons SA.DMA.OA.W_1$	-33.08	-29.82	-7.61
$SA.DMA + OA + 2W \rightleftharpoons SA.DMA.OA.W_2$	-42.83	-38.04	-7.06
$SA.DMA + OA + 3W \rightleftharpoons SA.DMA.OA.W_3$	-51.38	-44.14	-2.50
$SA.DMA + OA + 4W \rightleftharpoons SA.DMA.OA.W_4$	-63.16	-53.82	-3.12
$SA.DMA + SA + OA \rightleftharpoons SA_2.DMA.OA$	-41.82	-38.85	-16.15
$SA.DMA + SA + OA + W \rightleftharpoons SA_2.DMA.OA.W_1$	-52.35	-47.95	-15.75
$SA.DMA + SA + OA + 2W \rightleftharpoons SA_2.DMA.OA.W_2$	-68.04	-61.87	-16.44
$SA.DMA + SA + OA + 3W \rightleftharpoons SA_2.DMA.OA.W_3$	-79.36	-71.51	-15.44
$SA.DMA + SA + OA + 4W \rightleftharpoons SA_2.DMA.OA.W_4$	-87.05	-77.5	-13.76

Table S5 Binding energies at 0 K (ΔE), and enthalpies at 298.15 K (ΔH) for $SA_m.DMA.OA.W_n$ ($m=1-2$, $n=0-4$) according to the reaction path 5. Energies are calculated at DF-LMP2-F12/VDZ-F12//M06-2x/6-311+G(2d, p) level of theory (in kcal/mol).

Reactions	ΔE	ΔH	ΔG
$SA.OA + DMA \rightleftharpoons SA.DMA.OA$	-31.19	-29.32	-17.45
$SA.OA + DMA + W \rightleftharpoons SA.DMA.OA.W_1$	-45.85	-41.78	-18.92
$SA.OA + DMA + 2W \rightleftharpoons SA.DMA.OA.W_2$	-55.6	-49.99	-18.37
$SA.OA + DMA + 3W \rightleftharpoons SA.DMA.OA.W_3$	-64.15	-56.09	-13.81
$SA.OA + DMA + 4W \rightleftharpoons SA.DMA.OA.W_4$	-75.93	-65.77	-14.43
$SA.OA + SA + DMA \rightleftharpoons SA_2.DMA.OA$	-54.59	-50.81	-27.46
$SA.OA + SA + DMA + W \rightleftharpoons SA_2.DMA.OA.W_1$	-65.12	-59.9	-27.06
$SA.OA + SA + DMA + 2W \rightleftharpoons SA_2.DMA.OA.W_2$	-80.81	-73.83	-27.75
$SA.OA + SA + DMA + 3W \rightleftharpoons SA_2.DMA.OA.W_3$	-92.13	-83.46	-26.75
$SA.OA + SA + DMA + 4W \rightleftharpoons SA_2.DMA.OA.W_4$	-99.82	-89.45	-25.07

Table S6 Binding energies at 0 K (ΔE), and enthalpies at 298.15 K (ΔH) for SA_m .DMA.OA.W_n (m=1-2, n=0-4) according to the reaction path 6. Energies are calculated at DF-LMP2-F12/VDZ-F12//M06-2x/6-311+G(2d, p) level of theory (in kcal/mol).

Reactions	ΔE	ΔH	ΔG
DMA.OA + SA \Leftrightarrow SA.DMA.OA	-28.72	-26.82	-15.68
DMA.OA + SA + W \Leftrightarrow SA.DMA.OA.W ₁	-43.38	-39.27	-17.14
DMA.OA + SA + 2W \Leftrightarrow SA.DMA.OA.W ₂	-53.14	-47.49	-16.59
DMA.OA + SA + 3W \Leftrightarrow SA.DMA.OA.W ₃	-61.68	-53.59	-12.03
DMA.OA + SA + 4W \Leftrightarrow SA.DMA.OA.W ₄	-73.46	-63.26	-12.66
DMA.OA + 2SA \Leftrightarrow SA ₂ .DMA.OA	-52.13	-48.3	-25.69
DMA.OA + 2SA + W \Leftrightarrow SA ₂ .DMA.OA.W ₁	-62.65	-57.39	-25.28
DMA.OA + 2SA + 2W \Leftrightarrow SA ₂ .DMA.OA.W ₂	-78.35	-71.32	-25.98
DMA.OA + 2SA + 3W \Leftrightarrow SA ₂ .DMA.OA.W ₃	-89.66	-80.95	-24.97
DMA.OA + 2SA + 4W \Leftrightarrow SA ₂ .DMA.OA.W ₄	-97.35	-86.94	-23.29

Table S7 The isotropic mean polarizability ($\bar{\alpha}$) and Rayleigh scattering intensity (R_n) of different isomer.

cluster	$\bar{\alpha}$ (a.u.)	R_n (a.u.)
SA.W ₁	47	101559
SA.W ₂	57	149497
SA.W ₃	67	208501
SA.W ₄	77	275196
DMA.OA.W ₁	88	358182
DMA.OA.W ₂	97	432831
DMA.OA.W ₃	107	531651
DMA.OA.W ₄	116	613278
SA.DMA.W ₁	85	325585
SA.DMA.W ₂	94	397929
SA.DMA.W ₃	104	491654
SA.DMA.W ₄	113	578366

Cartesian coordinates of optimized structures:

SA.DMA.OA

16	2.446833000	-0.521582000	-0.017725000
8	1.932345000	0.842661000	-0.067582000
8	3.812110000	-0.720732000	-0.385860000
8	2.308424000	-0.861971000	1.551417000
8	1.521899000	-1.473163000	-0.688222000
1	2.785143000	-1.686773000	1.716964000
1	-1.290118000	1.581228000	0.243155000
6	-0.435629000	2.456801000	-1.404324000
7	-0.421370000	2.096825000	0.031502000
6	-0.239232000	3.251725000	0.932453000
1	-0.581301000	1.543510000	-1.975509000
1	0.524700000	2.901094000	-1.657404000
1	-1.246511000	3.158443000	-1.590394000
1	0.375049000	1.432044000	0.155187000
1	-0.250530000	2.902457000	1.961915000
1	-1.043827000	3.966643000	0.772199000
1	0.722421000	3.712298000	0.714597000
8	-4.061299000	-1.182542000	0.368242000
6	-2.979452000	-0.460981000	0.177365000
8	-2.947126000	0.735728000	0.303840000
6	-1.749131000	-1.317994000	-0.210146000
8	-0.714461000	-0.597044000	-0.463255000
8	-1.880541000	-2.518490000	-0.228596000
1	-3.802839000	-2.112950000	0.223891000
1	0.257912000	-1.103331000	-0.593485000

SA.DMA.OA.W₁

16	2.194129000	-0.921173000	-0.040280000
8	3.601491000	-0.980014000	0.119387000
8	1.551462000	-0.473080000	1.310881000
8	1.635963000	-0.064849000	-1.074438000
8	1.654540000	-2.359440000	-0.250676000
1	0.607494000	1.274456000	-0.491363000
1	0.641292000	-2.334966000	-0.250153000
6	0.841846000	2.578311000	1.090297000
7	0.384669000	2.263865000	-0.283790000
6	1.033213000	3.089369000	-1.323804000
1	0.258424000	1.981751000	1.786523000
1	0.676018000	3.637390000	1.277591000
1	1.897750000	2.330092000	1.177203000

1	-0.650481000	2.367758000	-0.296873000
1	0.660142000	2.785316000	-2.298711000
1	2.107082000	2.919622000	-1.279672000
1	0.807355000	4.138268000	-1.142446000
8	-3.493171000	-2.032575000	-0.553280000
6	-2.955545000	-0.931052000	-0.066315000
8	-3.580403000	0.072131000	0.142883000
6	-1.431588000	-1.051108000	0.199030000
8	-0.886809000	-0.065468000	0.736070000
8	-0.924445000	-2.128079000	-0.163733000
1	-2.768448000	-2.677621000	-0.647975000
1	0.543133000	-0.340024000	1.155703000
8	-2.289797000	2.537084000	0.232224000
1	-3.032079000	3.017921000	-0.142938000
1	-2.624624000	1.632960000	0.394348000

SA.DMA.OA.W₂

16	2.194129000	-0.921173000	-0.040280000
8	3.601491000	-0.980014000	0.119387000
8	1.551462000	-0.473080000	1.310881000
8	1.635963000	-0.064849000	-1.074438000
8	1.654540000	-2.359440000	-0.250676000
1	0.607494000	1.274456000	-0.491363000
1	0.641292000	-2.334966000	-0.250153000
6	0.841846000	2.578311000	1.090297000
7	0.384669000	2.263865000	-0.283790000
6	1.033213000	3.089369000	-1.323804000
1	0.258424000	1.981751000	1.786523000
1	0.676018000	3.637390000	1.277591000
1	1.897750000	2.330092000	1.177203000
1	-0.650481000	2.367758000	-0.296873000
1	0.660142000	2.785316000	-2.298711000
1	2.107082000	2.919622000	-1.279672000
1	0.807355000	4.138268000	-1.142446000
8	-3.493171000	-2.032575000	-0.553280000
6	-2.955545000	-0.931052000	-0.066315000
8	-3.580403000	0.072131000	0.142883000
6	-1.431588000	-1.051108000	0.199030000
8	-0.886809000	-0.065468000	0.736070000
8	-0.924445000	-2.128079000	-0.163733000
1	-2.768448000	-2.677621000	-0.647975000
1	0.543133000	-0.340024000	1.155703000
8	-2.289797000	2.537084000	0.232224000
1	-3.032079000	3.017921000	-0.142938000

1	-2.624624000	1.632960000	0.394348000
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SA.DMA.OA.W₃

16	2.354285000	-0.824236000	0.049984000
8	3.057427000	0.302909000	-0.519526000
8	1.934896000	-1.826103000	-0.934075000
8	3.368052000	-1.582978000	1.029760000
8	1.273807000	-0.427546000	0.954026000
1	4.087048000	-1.947124000	0.495416000
1	0.850668000	1.183089000	0.016305000
8	-0.605215000	-2.037694000	-0.905353000
6	-1.192594000	-0.891131000	-1.046327000
8	-0.691570000	0.163276000	-1.357905000
6	-2.694245000	-0.981526000	-0.712175000
8	-3.336566000	0.126355000	-1.086096000
8	-3.197698000	-1.908891000	-0.155415000
1	0.408125000	-1.950663000	-0.991651000
1	-4.226727000	0.085676000	-0.705107000
6	1.602704000	2.782372000	1.030633000
7	0.779353000	2.207645000	-0.052887000
6	1.192012000	2.644192000	-1.405120000
1	1.239977000	2.401912000	1.982448000
1	1.524493000	3.867602000	1.000763000
1	2.631705000	2.463116000	0.877934000
1	-0.238519000	2.416340000	0.078859000
1	0.563038000	2.136351000	-2.131471000
1	2.231000000	2.361727000	-1.554709000
1	1.064023000	3.722992000	-1.476098000
8	-1.944125000	2.525914000	0.028011000
1	-2.127332000	1.950291000	-0.727609000
1	-2.348674000	2.038282000	0.772396000
8	-2.993255000	0.726499000	1.845353000
1	-2.348543000	-0.005527000	1.967878000
1	-3.427933000	0.846849000	2.692906000
8	-1.200638000	-1.303660000	1.964516000
1	-1.498699000	-2.069971000	1.459658000
1	-0.275852000	-1.154784000	1.704110000

SA.DMA.OA.W₄

16	0.605551000	-1.314494000	-0.644222000
8	1.851167000	-1.545020000	-1.356513000
8	-0.172867000	-0.173304000	-1.082363000
8	-0.345533000	-2.559411000	-1.010309000
8	0.777659000	-1.370446000	0.813586000

1	0.198256000	-3.358890000	-1.030429000
1	2.643775000	-1.238897000	1.286092000
8	-3.311084000	0.123810000	-1.697777000
6	-2.755567000	0.777633000	-0.691734000
8	-2.535346000	1.952774000	-0.705093000
6	-2.394326000	-0.078372000	0.540230000
8	-2.774191000	-1.325556000	0.412426000
8	-1.812498000	0.404816000	1.475570000
1	-3.314468000	-0.824003000	-1.490990000
1	-2.305215000	-1.891906000	1.126394000
6	-0.339779000	3.126356000	1.437842000
7	0.248500000	2.248194000	0.406701000
6	0.381925000	2.896132000	-0.917525000
1	-0.382154000	2.580648000	2.376436000
1	-1.346540000	3.393855000	1.125011000
1	0.286577000	4.010787000	1.540165000
1	-0.328919000	1.406100000	0.314329000
1	0.741345000	2.151209000	-1.623417000
1	1.096731000	3.712337000	-0.826229000
1	-0.591533000	3.262995000	-1.231822000
8	2.861446000	1.736192000	0.846707000
1	3.286464000	1.561948000	-0.009016000
1	1.213665000	1.939654000	0.688485000
8	3.516484000	-0.861345000	1.479684000
1	3.083769000	0.919516000	1.338815000
1	4.000035000	-0.914626000	0.645791000
8	3.924522000	0.255827000	-1.285998000
1	3.181593000	-0.347578000	-1.475928000
1	4.464722000	0.288523000	-2.078947000
8	-1.329872000	-2.556463000	2.095973000
1	-1.417015000	-2.139685000	2.959711000
1	-0.492028000	-2.202905000	1.726170000

SA₂.DMA.OA

16	2.428883000	-0.781363000	-0.630894000
8	1.823831000	-2.009692000	-1.139350000
8	2.927309000	-0.829975000	0.724658000
8	3.746142000	-0.575340000	-1.503002000
8	1.588745000	0.401624000	-0.881235000
1	3.517387000	-0.688805000	-2.436055000
1	0.477690000	1.022418000	1.198642000
16	-1.452970000	1.846287000	-0.906692000
8	-0.863285000	2.019657000	0.401917000
8	-1.396944000	2.924181000	-1.827195000

8	-0.891420000	0.525093000	-1.523045000
8	-2.953506000	1.451301000	-0.750050000
1	0.096711000	0.435301000	-1.319365000
1	-3.037430000	0.667645000	-0.159777000
6	0.643810000	0.982751000	3.240101000
7	1.238363000	1.073321000	1.892031000
6	1.988020000	2.324068000	1.642962000
1	0.126518000	0.030728000	3.321547000
1	-0.063693000	1.801111000	3.358949000
1	1.432753000	1.056447000	3.986018000
1	1.846884000	0.262165000	1.687583000
1	2.380264000	2.282366000	0.630184000
1	2.797896000	2.403811000	2.365379000
1	1.299612000	3.160714000	1.740456000
8	-0.612973000	-2.559789000	-0.588702000
6	-1.028866000	-1.780691000	0.359074000
8	-0.378878000	-1.025592000	1.038233000
6	-2.545029000	-1.868108000	0.560899000
8	-2.976733000	-3.107444000	0.707180000
8	-3.254500000	-0.897067000	0.603847000
1	0.370327000	-2.386750000	-0.775999000
1	-3.937987000	-3.082957000	0.835332000

SA₂.DMA.OA.W₁

16	0.363452000	1.911125000	0.624766000
8	1.562264000	1.568835000	1.390085000
8	0.568549000	2.350698000	-0.729615000
8	-0.664647000	0.863820000	0.777585000
8	-0.232494000	3.204062000	1.348447000
1	-2.048409000	0.978208000	0.143541000
1	-0.236993000	3.049146000	2.303043000
16	2.900846000	-1.007741000	-0.459281000
8	3.100433000	-2.407704000	-0.284270000
8	1.581362000	-0.541714000	-0.852675000
8	3.257060000	-0.296974000	0.881313000
8	3.923951000	-0.465191000	-1.471080000
1	2.617434000	0.465563000	1.047023000
1	3.632625000	0.489917000	-1.722439000
6	-0.283744000	-3.295305000	0.140347000
7	-0.232010000	-1.928401000	0.707454000
6	0.504690000	-1.846014000	1.990878000
1	-0.896384000	-3.276176000	-0.757616000
1	-0.725156000	-3.966919000	0.873669000
1	0.733155000	-3.602530000	-0.098666000

1	-1.185870000	-1.549940000	0.801472000
1	0.568258000	-0.799059000	2.279337000
1	1.501766000	-2.258218000	1.842252000
1	-0.032149000	-2.421048000	2.742731000
8	-5.435378000	0.788013000	-1.134007000
6	-4.940191000	-0.358778000	-0.670074000
8	-5.539430000	-1.383059000	-0.659133000
6	-3.491986000	-0.268547000	-0.131572000
8	-2.931116000	-1.241606000	0.303983000
8	-3.001774000	0.941662000	-0.216838000
1	-4.770574000	1.487160000	-1.051079000
1	0.251402000	-1.305489000	0.036838000
8	3.018860000	1.846458000	-1.950750000
1	3.486572000	2.624985000	-1.635012000
1	2.105907000	1.922533000	-1.606849000

SA₂.DMA.OA.W₂

16	-2.578415000	0.744540000	0.320508000
8	-1.522056000	1.203103000	1.190315000
8	-2.247674000	0.891973000	-1.109493000
8	-3.123184000	-0.567870000	0.651711000
8	-3.809672000	1.750233000	0.473256000
1	-2.411853000	-1.933493000	0.190410000
1	-4.268768000	1.541096000	1.298534000
16	0.987803000	-1.751122000	1.098373000
8	0.734270000	-1.088090000	2.353605000
8	0.228086000	-2.993445000	0.876600000
8	0.944336000	-0.872528000	-0.063528000
8	2.508634000	-2.247022000	1.246721000
1	0.600364000	0.830488000	1.852753000
1	2.703528000	-2.855906000	0.521520000
8	3.105262000	0.181443000	-2.609184000
6	2.388319000	0.951930000	-1.812275000
8	2.847840000	1.660137000	-0.965330000
6	0.875224000	0.837218000	-2.074318000
8	0.177417000	1.620893000	-1.314889000
8	0.478505000	0.068137000	-2.921150000
1	2.486154000	-0.304836000	-3.180683000
1	-0.814961000	1.375669000	-1.312471000
6	0.809030000	2.896925000	2.034997000
7	1.239494000	1.574048000	1.531306000
6	2.624359000	1.219202000	1.923526000
1	-0.215293000	3.068340000	1.719431000
1	1.474482000	3.653024000	1.623512000

1	0.874567000	2.894169000	3.121160000
1	1.159399000	1.560653000	0.507270000
1	2.906033000	0.299448000	1.419742000
1	2.647946000	1.076037000	3.001400000
1	3.287068000	2.024365000	1.616526000
8	-1.936895000	-2.668285000	-0.296730000
1	-1.811907000	-2.285680000	-1.249908000
1	-1.019018000	-2.824645000	0.173287000
8	-1.847277000	-1.512612000	-2.525139000
1	-2.329253000	-0.708240000	-2.269404000
1	-0.977469000	-1.163707000	-2.780019000

SA₂.DMA.OA.W₃

16	-2.392312000	1.120212000	-0.552657000
8	-2.497420000	0.258550000	0.621744000
8	-2.038082000	0.357453000	-1.765034000
8	-3.894658000	1.598373000	-0.764044000
8	-1.574165000	2.298068000	-0.370620000
1	-3.928525000	2.201321000	-1.520594000
1	0.241332000	2.204533000	0.333844000
16	0.519121000	-1.857041000	1.121276000
8	-0.466286000	-2.367172000	2.048849000
8	1.890548000	-1.802857000	1.544825000
8	0.382649000	-2.486515000	-0.226104000
8	0.132673000	-0.313874000	0.876749000
1	-0.918426000	-2.369057000	-0.825770000
1	-0.846532000	-0.208838000	0.926447000
8	2.730206000	-1.820513000	-1.534637000
6	2.840759000	-0.512339000	-1.504618000
8	3.879172000	0.067232000	-1.365872000
6	1.540018000	0.309854000	-1.675287000
8	0.557582000	-0.383537000	-2.217477000
8	1.484014000	1.462177000	-1.350382000
1	1.811735000	-2.114715000	-1.362862000
1	-0.273291000	0.141872000	-2.198114000
6	1.534255000	3.754746000	0.702862000
7	0.879919000	2.486288000	1.087779000
6	0.121119000	2.571692000	2.351994000
1	2.059958000	3.593542000	-0.234392000
1	2.235046000	4.036855000	1.486279000
1	0.773876000	4.524161000	0.582208000
1	1.619337000	1.743018000	1.155834000
1	-0.307887000	1.596598000	2.568133000
1	-0.671784000	3.307800000	2.236918000

1	0.800604000	2.863187000	3.150623000
8	-1.913771000	-2.252361000	-1.142462000
1	-2.032695000	-1.316895000	-1.450226000
1	-2.484634000	-2.383931000	-0.270685000
8	3.003780000	0.810378000	1.392532000
1	3.566788000	0.778256000	0.606550000
1	2.757656000	-0.114365000	1.569731000
8	-3.071854000	-2.501326000	1.054359000
1	-2.282231000	-2.635672000	1.613394000
1	-3.360726000	-1.598748000	1.251226000

SA₂.DMA.OA.W₄

16	-0.059481000	1.814020000	-0.471023000
8	-0.884631000	2.961308000	-0.651895000
8	-0.695721000	0.512650000	-0.514330000
8	1.061518000	1.872696000	-1.551279000
8	0.725574000	1.859445000	0.862001000
1	1.547252000	0.979453000	-1.583351000
1	1.584577000	2.442416000	0.782967000
16	3.013831000	-0.625602000	-0.280807000
8	2.186535000	-0.424452000	-1.487576000
8	3.855986000	0.515640000	0.019105000
8	2.233144000	-1.165450000	0.813772000
8	4.000425000	-1.827962000	-0.650338000
1	1.615315000	-0.245102000	2.412627000
1	4.709497000	-1.482451000	-1.210084000
8	-0.993782000	-1.374568000	1.916852000
6	-1.888999000	-0.405149000	1.865494000
8	-1.854937000	0.619202000	2.484306000
6	-2.993911000	-0.708011000	0.838761000
8	-4.066871000	-0.012812000	1.031621000
8	-2.809046000	-1.495211000	-0.072005000
1	0.444231000	-1.404439000	-0.358804000
1	-4.682650000	-0.106470000	0.230447000
6	-0.254997000	-2.170242000	-2.138369000
7	-0.132435000	-2.196962000	-0.665135000
6	0.455991000	-3.443568000	-0.132423000
1	-0.664310000	-1.205701000	-2.428343000
1	-0.923946000	-2.972002000	-2.445012000
1	0.732188000	-2.299080000	-2.574782000
1	-1.066207000	-2.024725000	-0.249584000
1	0.488016000	-3.369988000	0.950844000
1	1.466328000	-3.545499000	-0.523991000
1	-0.161901000	-4.284429000	-0.441648000

8	0.933295000	-0.188310000	3.100670000
1	0.529601000	0.685539000	3.004151000
1	-0.215736000	-1.026627000	2.474723000
8	-5.367311000	-0.043521000	-1.180099000
1	-5.378707000	-0.910560000	-1.595790000
1	-4.644963000	0.455367000	-1.620442000
8	-3.087811000	1.205422000	-1.974703000
1	-2.365367000	0.752688000	-1.514253000
1	-2.932078000	2.135811000	-1.772218000
8	2.920180000	3.024606000	0.636429000
1	3.438215000	2.227118000	0.408842000
1	2.977219000	3.615077000	-0.122104000