Supporting Information

1 **Structural Effects of Amines in Enhancing**

2 **Methanesulfonic Acid-driven New Particle Formation**

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20 *Totally, 57 pages, 11 figures and 3 tables*

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45 **Basic Formula of ACDC.** Briefly, the birth-death equation (Eq. (1)) is employed to

46 describe the time-dependent cluster distributions in ACDC simulation:

47 $$\frac{dc_i}{dt} = \frac{1}{2}\sum_{j<i}\beta_{j,(i-j)}c_jc_{(i-j)} + \sum_j \gamma_{(i+j)\to i}c_{i+j} - \sum_j \beta_{i,j}c_ic_j - \frac{1}{2}\sum_{j<i}\gamma_{i\to j}c_i + Q_i - S_i \quad (1)$$

48 where subscripts (i, j, i-j, j-i and i+j) denote different clusters or monomers in the

49 system, c_i denotes the number concentration of i, $\beta_{i,j}$ denotes the collision rate

50 coefficient between i and j, $\gamma_{(i+j)\to i}$ denotes the evaporation rate of a cluster i+j into

51 smaller cluster (or monomer) i and j. Q_i denotes an additional outside source term of i

52 and S_i denotes other sink terms for i. Eq. (2) and Eq. (3) were used to calculate $\beta_{i,j}$ and

53 $\gamma_{(i+j)\to i}$, respectively.

54 $$\beta_{i,j} = \left(\frac{3}{4\pi}\right)^{1/6}\left(\frac{6k_bT}{m_i} + \frac{6k_bT}{m_j}\right)^{1/2}\left(V_i^{1/3} + V_j^{1/3}\right)^2 \quad (2)$$

55 where k_b is the Boltzmann constant, T is the temperature, and m_i and V_i are the mass

56 and volume of i, respectively.

57 $$\gamma_{(i+j)\to i} = \beta_{i,j}c_{\text{ref}}\exp\left\{\frac{\Delta G_{i+j} - \Delta G_i - \Delta G_j}{k_bT}\right\} \quad (3)$$

58 where ΔG is the formation free energy of a cluster, c_{ref} is the reference monomer

59 concentration at 1 atm (the pressure at which ΔG was calculated).

60 **Judgement of Cluster Stability.** In the process of base-acid cluster growth, there is a

61 competition between evaporation into smaller cluster and collision with monomers or

62 clusters to form larger one. Such competition determines the stability of a cluster in

63 view of a cluster growth. A cluster with higher collision rate than that of evaporation

64 can be judged to be stable. In general, the collision rate constant of a cluster with

65 base/acid monomers is of the order of 10^{-10} cm^3 s^{-1}, and the collision rate can be

66 considered to be about 10^{-2} s^{-1} under the condition that the concetration of base/acid

67 monomer reaches ppt level. Therefore, a given cluster can be deemed as stable enough

68 to engage in further growth when the evaporation rate is lower than 10^{-2} s^{-1}.

69 **Selection of Boundary Clusters.** The boundary clusters are allowed to leave the

70 simulation box for further growth. Therefore, these clusters are required to be stable

71 enough and therefore prefer to further grow. In the studied DMA/MA-MSA systems,

72 (DMA/MA)$_z$(MSA)$_z$ (z = 1-4) and (DMA/MA)$_z$(MSA)$_{z+1}$ (z = 1-3) clusters have

73 relatively lower evaporation rates than other clusters. Therefore, this allows us to select

74 (DMA/MA)$_4$(MSA)$_5$ and (DMA/MA)$_5$(MSA)$_5$ clusters as the boundary clusters for

75 DMA/MA-MSA systems in the "4 × 4 box" simulation. Similarly, for "2 × 2 box" and

76 "3 × 3 box" simulations, (DMA/MA)$_2$(MSA)$_3$ and (DMA/MA)$_3$(MSA)$_3$, and

77 (DMA/MA)$_3$(MSA)$_4$ and (DMA/MA)$_4$(MSA)$_4$ clusters are assumed to leave the

78 corresponding simulation boxes.

79 **Effect of Coagulation Sink Coefficient.** To examine the effect of coagulation sink

80 coefficient on enhancing potentials of DMA and MA, here, ACDC test runs were

81 performed with various values covering cases of clean and haze days (6×10^{-4}-6×10^{-2}

82 s^{-1}) under the conditions of [MSA] = 10^6 cm^{-3}, [DMA/MA] = 10 ppt and 278.15 K for

83 DMA-MSA and MA-MSA systems. As can be seen in Figure S2, $\sum$[(MSA)$_2$] and J

84 decrease with increasing coagulation sink coefficient for both systems. In addition, the

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85   DMA-MSA system shows a stronger dependence on coagulation sink coefficient than

86   MA-MSA system. More importantly, $\sum[(MSA)_2]$ of DMA-MSA system is significantly

87   higher than that of MA-MSA system within the considered range of coagulation sink

88   coefficients, however, J in DMA-MSA system is lower than that of MA-MSA system

89   in most considered cases (~1.5×10^{-3}-6.0×10^{-2} s^{-1}). The conclusion is consistent with

90   the case where the coagulation sink coefficient 2.6×10^{-3} s^{-1} is used.

91   With two extreme coagulation sink coefficients of 6.0×10^{-4} s^{-1} and 6.0×10^{-2} s^{-1},

92   corresponding clean day condition and haze day condition, respectively, the effect of

93   coagulation sink coefficients on cluster growth pathways were tested. As can be seen

94   in Figure S3, when coagulation sink coefficient is 6.0×10^{-4} s^{-1}, the cluster growth

95   pathways for both systems are similar to those at the condition with coagulation sink

96   coefficient of 2.6×10^{-3} s^{-1}. When coagulation sink coefficient is 6×10^{-2} s^{-1}, the cluster

97   growth pathways change slightly for MA-MSA system, however, they become more

98   complicate for DMA-MSA system than that of the case where coagulation sink

99   coefficient is 2.6×10^{-3} s^{-1}. Still, the dominant growth pathways for both systems are

100   kept when coagulation sink coefficients is changed.

101   **Energy Decomposition Analysis based on Force Field (EDA-FF).** For the selected

102   model clusters $(DMA)_z(MSA)_z$ and $(MA)_z(MSA)_z$ (z = 1-4), energy decomposition

103   analysis based on force field (EDA-FF) was performed using GAFF force field using

104   Multiwfn software version 3.7.[1] The total intermolecular interaction energy (E_{int}) in

105   EDA-FF can be decomposed into three terms including electrostatic (E_{ele}), repulsion

106   (E_{rep}) and dispersion (E_{disp}) energies[1-5]:

$$E_{int} = E_{ele} + E_{rep} + E_{disp} \tag{1}$$

107   E_{ele}, E_{rep} and E_{disp} can be described by following equations:

$$E_{ele} = \frac{q_A q_B}{r_{AB}} \tag{2}$$

$$E_{rep} = \varepsilon_{AB} \left(\frac{R_{AB}^0}{r_{AB}} \right)^{12} \tag{3}$$

$$E_{disp} = -2\varepsilon_{AB} \left(\frac{R_{AB}^0}{r_{AB}} \right)^{6} \tag{4}$$

108   where q_A and q_B are the atomic charge atom A and B, respectively, r_{AB} is the interatomic

109   distance between atom A and B, ε_{AB} represents the depth of the van der Waals

110   interaction potential well and R_{AB} represents the non-bonding contact distance.

111   E_{int}^*, E_{ele}^*, E_{rep}^* and E_{disp}^* for both the studied DMA-MSA and MA-MSA system

112   are presented in Figure S6, along with the obtained total intermolecular interaction

113   energy (E_{int}) at the DLPNO-CCSD(T)/aug-cc-pVTZ level of theory as a comparison. It

114   can be infered from Figure S6 that both E_{int}^*-DMA and E_{int}^*-MA obtained from EDA-

115   FF analysis are compared to E_{int}-DMA and E_{int}-MA from DLPNO-CCSD(T)/aug-cc-

116   pVTZ level of theory, respectively, showing rationality for the force field selection in

117   EDA-FF analysis.

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119   Table S1. Evaporation coefficients (s^{-1}) for all evaporation pathways of clusters at

120   278.15 K.

Evaporation pathways	Evaporation coefficients
$(DMA)_1(MSA)_1 \rightarrow DMA + MSA$	6.86×10^2
$(DMA)_1(MSA)_2 \rightarrow (DMA)_1(MSA)_1 + MSA$	7.42×10^{-4}
$(DMA)_1(MSA)_2 \rightarrow DMA + (MSA)_2$	4.95×10^{-5}
$(DMA)_1(MSA)_3 \rightarrow (DMA)_1(MSA)_2 + MSA$	3.12×10^2
$(DMA)_1(MSA)_3 \rightarrow (DMA)_1(MSA)_1 + (MSA)_2$	1.88×10^{-5}
$(DMA)_1(MSA)_3 \rightarrow DMA + (MSA)_3$	2.10×10^{-8}
$(DMA)_1(MSA)_4 \rightarrow (DMA)_1(MSA)_3 + MSA$	6.77×10^2
$(DMA)_1(MSA)_4 \rightarrow (DMA)_1(MSA)_2 + (MSA)_2$	1.50×10^1
$(DMA)_1(MSA)_4 \rightarrow (DMA)_1(MSA)_1 + (MSA)_3$	1.52×10^{-8}
$(DMA)_1(MSA)_4 \rightarrow DMA + (MSA)_4$	1.10×10^{-12}
$(DMA)_2(MSA)_1 \rightarrow (DMA)_2 + MSA$	4.05×10^{-6}
$(DMA)_2(MSA)_1 \rightarrow (DMA)_1(MSA)_1 + DMA$	1.49×10^5
$(DMA)_2(MSA)_2 \rightarrow (DMA)_2(MSA)_1 + MSA$	2.63×10^{-12}
$(DMA)_2(MSA)_2 \rightarrow (DMA)_2 + (MSA)_2$	8.64×10^{-22}
$(DMA)_2(MSA)_2 \rightarrow (DMA)_1(MSA)_2 + DMA$	5.27×10^{-4}
$(DMA)_2(MSA)_2 \rightarrow (DMA)_1(MSA)_1 + (DMA)_1(MSA)_1$	2.38×10^{-10}
$(DMA)_2(MSA)_3 \rightarrow (DMA)_2(MSA)_2 + MSA$	2.89×10^2
$(DMA)_2(MSA)_3 \rightarrow (DMA)_2(MSA)_1 + (MSA)_2$	5.41×10^{-14}
$(DMA)_2(MSA)_3 \rightarrow (DMA)_2 + (MSA)_3$	2.98×10^{-25}
$(DMA)_2(MSA)_3 \rightarrow (DMA)_1(MSA)_3 + DMA$	4.87×10^{-4}
$(DMA)_2(MSA)_3 \rightarrow (DMA)_1(MSA)_2 + (DMA)_1(MSA)_1$	1.62×10^{-4}
$(DMA)_2(MSA)_4 \rightarrow (DMA)_2(MSA)_3 + MSA$	1.13×10^2
$(DMA)_2(MSA)_4 \rightarrow (DMA)_2(MSA)_2 + (MSA)_2$	2.10×10^0
$(DMA)_2(MSA)_4 \rightarrow (DMA)_2(MSA)_1 + (MSA)_3$	6.61×10^{-18}
$(DMA)_2(MSA)_4 \rightarrow (DMA)_2 + (MSA)_4$	2.35×10^{-30}
$(DMA)_2(MSA)_4 \rightarrow (DMA)_1(MSA)_4 + DMA$	8.13×10^{-5}
$(DMA)_2(MSA)_4 \rightarrow (DMA)_1(MSA)_3 + (DMA)_1(MSA)_1$	5.31×10^{-5}
$(DMA)_2(MSA)_4 \rightarrow (DMA)_1(MSA)_2 + (DMA)_1(MSA)_2$	0.98×10^1
$(DMA)_3(MSA)_1 \rightarrow (DMA)_3 + MSA$	1.91×10^{-7}
$(DMA)_3(MSA)_1 \rightarrow (DMA)_2(MSA)_1 + DMA$	5.78×10^9
$(DMA)_3(MSA)_1 \rightarrow (DMA)_2 + (DMA)_1(MSA)_1$	2.84×10^1
$(DMA)_3(MSA)_2 \rightarrow (DMA)_3(MSA)_1 + MSA$	5.48×10^{-13}
$(DMA)_3(MSA)_2 \rightarrow (DMA)_3 + (MSA)_2$	7.43×10^{-24}
$(DMA)_3(MSA)_2 \rightarrow (DMA)_2(MSA)_2 + DMA$	1.20×10^9
$(DMA)_3(MSA)_2 \rightarrow (DMA)_2(MSA)_1 + (DMA)_1(MSA)_1$	3.37×10^{-6}
$(DMA)_3(MSA)_2 \rightarrow (DMA)_2 + (DMA)_1(MSA)_2$	1.84×10^{-8}

$(DMA)_3(MSA)_3 \rightarrow (DMA)_3(MSA)_2 + MSA$	2.17×10^{-9}
$(DMA)_3(MSA)_3 \rightarrow (DMA)_3(MSA)_1 + (MSA)_2$	7.64×10^{-26}
$(DMA)_3(MSA)_3 \rightarrow (DMA)_3 + (MSA)_3$	1.74×10^{-38}
$(DMA)_3(MSA)_3 \rightarrow (DMA)_2(MSA)_3 + DMA$	9.02×10^{-3}
$(DMA)_3(MSA)_3 \rightarrow (DMA)_2(MSA)_2 + (DMA)_1(MSA)_1$	2.51×10^{-3}
$(DMA)_3(MSA)_3 \rightarrow (DMA)_2(MSA)_1 + (DMA)_1(MSA)_2$	7.81×10^{-12}
$(DMA)_3(MSA)_3 \rightarrow (DMA)_2 + (DMA)_1(MSA)_3$	1.15×10^{-19}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_3(MSA)_3 + MSA$	1.44×10^{1}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_3(MSA)_2 + (MSA)_2$	1.84×10^{-12}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_3(MSA)_1 + (MSA)_3$	1.09×10^{-30}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_3 + (MSA)_4$	1.60×10^{-44}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_2(MSA)_4 + DMA$	1.15×10^{-3}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_2(MSA)_3 + (DMA)_1(MSA)_1$	1.15×10^{-4}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_2(MSA)_2 + (DMA)_1(MSA)_2$	3.54×10^{1}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_2(MSA)_1 + (DMA)_1(MSA)_3$	2.99×10^{-13}
$(DMA)_3(MSA)_4 \rightarrow (DMA)_2 + (DMA)_1(MSA)_4$	2.24×10^{-21}
$(DMA)_4(MSA)_1 \rightarrow (DMA)_4 + MSA$	4.80×10^{-8}
$(DMA)_4(MSA)_1 \rightarrow (DMA)_3(MSA)_1 + DMA$	3.51×10^{10}
$(DMA)_4(MSA)_1 \rightarrow (DMA)_3 + (DMA)_1(MSA)_1$	7.14×10^{0}
$(DMA)_4(MSA)_1 \rightarrow (DMA)_2(MSA)_1 + (DMA)_2$	5.88×10^{6}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_4(MSA)_1 + MSA$	1.72×10^{-12}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_4 + (MSA)_2$	5.27×10^{-24}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_3(MSA)_2 + DMA$	1.10×10^{11}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_3(MSA)_1 + (DMA)_1(MSA)_1$	5.78×10^{-5}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_3 + (DMA)_1(MSA)_2$	1.30×10^{-8}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_2(MSA)_2 + (DMA)_2$	3.45×10^{6}
$(DMA)_4(MSA)_2 \rightarrow (DMA)_2(MSA)_1 + (DMA)_2(MSA)_1$	0.98×10^{0}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_4(MSA)_2 + MSA$	1.05×10^{-11}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_4(MSA)_1 + (MSA)_2$	1.06×10^{-27}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_4 + (MSA)_3$	5.46×10^{-41}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_3(MSA)_3 + DMA$	5.28×10^{8}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_3(MSA)_2 + (DMA)_1(MSA)_1$	1.01×10^{-3}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_3(MSA)_1 + (DMA)_1(MSA)_2$	5.93×10^{-13}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_3 + (DMA)_1(MSA)_3$	3.61×10^{-22}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_2(MSA)_3 + (DMA)_2$	1.14×10^{-7}
$(DMA)_4(MSA)_3 \rightarrow (DMA)_2(MSA)_2 + (DMA)_2(MSA)_1$	6.48×10^{0}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_4(MSA)_3 + MSA$	1.49×10^{-9}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_4(MSA)_2 + (MSA)_2$	8.50×10^{-25}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_4(MSA)_1 + (MSA)_3$	1.45×10^{-42}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_4 + (MSA)_4$	4.82×10^{-57}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_3(MSA)_4 + DMA$	5.43×10^{-2}

$(DMA)_4(MSA)_4 \rightarrow (DMA)_3(MSA)_3 + (DMA)_1(MSA)_1$	6.43×10^{-4}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_3(MSA)_2 + (DMA)_1(MSA)_2$	1.37×10^{-9}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_3(MSA)_1 + (DMA)_1(MSA)_3$	2.17×10^{-24}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_3 + (DMA)_1(MSA)_4$	6.75×10^{-34}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_2(MSA)_4 + (DMA)_2$	1.39×10^{-18}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_2(MSA)_3 + (DMA)_2(MSA)_1$	2.84×10^{-11}
$(DMA)_4(MSA)_4 \rightarrow (DMA)_2(MSA)_2 + (DMA)_2(MSA)_2$	1.41×10^3
$(MA)_1(MSA)_1 \rightarrow MA + MSA$	2.31×10^5
$(MA)_1(MSA)_2 \rightarrow (MA)_1(MSA)_1 + MSA$	3.56×10^{-3}
$(MA)_1(MSA)_2 \rightarrow MA + (MSA)_2$	8.58×10^{-2}
$(MA)_1(MSA)_3 \rightarrow (MA)_1(MSA)_2 + MSA$	4.12×10^0
$(MA)_1(MSA)_3 \rightarrow (MA)_1(MSA)_1 + (MSA)_2$	1.25×10^{-6}
$(MA)_1(MSA)_3 \rightarrow MA + (MSA)_3$	5.05×10^{-7}
$(MA)_1(MSA)_4 \rightarrow (MA)_1(MSA)_3 + MSA$	5.02×10^4
$(MA)_1(MSA)_4 \rightarrow (MA)_1(MSA)_2 + (MSA)_2$	1.53×10^1
$(MA)_1(MSA)_4 \rightarrow (MA)_1(MSA)_1 + (MSA)_3$	7.75×10^{-8}
$(MA)_1(MSA)_4 \rightarrow MA + (MSA)_4$	2.03×10^{-9}
$(MA)_2(MSA)_1 \rightarrow (MA)_2 + MSA$	3.93×10^{-2}
$(MA)_2(MSA)_1 \rightarrow (MA)_1(MSA)_1 + MA$	6.22×10^6
$(MA)_2(MSA)_2 \rightarrow (MA)_2(MSA)_1 + MSA$	9.91×10^{-12}
$(MA)_2(MSA)_2 \rightarrow (MA)_2 + (MSA)_2$	3.48×10^{-17}
$(MA)_2(MSA)_2 \rightarrow (MA)_1(MSA)_2 + MA$	1.82×10^{-2}
$(MA)_2(MSA)_2 \rightarrow (MA)_1(MSA)_1 + (MA)_1(MSA)_1$	1.14×10^{-10}
$(MA)_2(MSA)_3 \rightarrow (MA)_2(MSA)_2 + MSA$	2.71×10^0
$(MA)_2(MSA)_3 \rightarrow (MA)_2(MSA)_1 + (MSA)_2$	2.06×10^{-15}
$(MA)_2(MSA)_3 \rightarrow (MA)_2 + (MSA)_3$	1.21×10^{-22}
$(MA)_2(MSA)_3 \rightarrow (MA)_1(MSA)_3 + MA$	1.24×10^{-2}
$(MA)_2(MSA)_3 \rightarrow (MA)_1(MSA)_2 + (MA)_1(MSA)_1$	1.57×10^{-7}
$(MA)_2(MSA)_4 \rightarrow (MA)_2(MSA)_3 + MSA$	2.03×10^3
$(MA)_2(MSA)_4 \rightarrow (MA)_2(MSA)_2 + (MSA)_2$	3.74×10^{-1}
$(MA)_2(MSA)_4 \rightarrow (MA)_2(MSA)_1 + (MSA)_3$	4.76×10^{-18}
$(MA)_2(MSA)_4 \rightarrow (MA)_2 + (MSA)_4$	1.81×10^{-26}
$(MA)_2(MSA)_4 \rightarrow (MA)_1(MSA)_4 + MA$	5.17×10^{-4}
$(MA)_2(MSA)_4 \rightarrow (MA)_1(MSA)_3 + (MA)_1(MSA)_1$	7.10×10^{-5}
$(MA)_2(MSA)_4 \rightarrow (MA)_1(MSA)_2 + (MA)_1(MSA)_2$	3.57×10^{-2}
$(MA)_3(MSA)_1 \rightarrow (MA)_3 + MSA$	2.61×10^{-8}
$(MA)_3(MSA)_1 \rightarrow (MA)_2(MSA)_1 + MA$	8.55×10^6
$(MA)_3(MSA)_1 \rightarrow (MA)_2 + (MA)_1(MSA)_1$	1.24×10^0
$(MA)_3(MSA)_2 \rightarrow (MA)_3(MSA)_1 + MSA$	1.23×10^{-10}
$(MA)_3(MSA)_2 \rightarrow (MA)_3 + (MSA)_2$	2.56×10^{-22}
$(MA)_3(MSA)_2 \rightarrow (MA)_2(MSA)_2 + MA$	1.11×10^8

$(MA)_3(MSA)_2 \rightarrow (MA)_2(MSA)_1 + (MA)_1(MSA)_1$	3.48×10^{-9}
$(MA)_3(MSA)_2 \rightarrow (MA)_2 + (MA)_1(MSA)_2$	4.03×10^{-8}
$(MA)_3(MSA)_3 \rightarrow (MA)_3(MSA)_2 + MSA$	8.95×10^{-9}
$(MA)_3(MSA)_3 \rightarrow (MA)_3(MSA)_1 + (MSA)_2$	7.75×10^{-23}
$(MA)_3(MSA)_3 \rightarrow (MA)_3 + (MSA)_3$	2.70×10^{-36}
$(MA)_3(MSA)_3 \rightarrow (MA)_2(MSA)_3 + MA$	3.77×10^{-1}
$(MA)_3(MSA)_3 \rightarrow (MA)_2(MSA)_2 + (MA)_1(MSA)_1$	2.88×10^{-6}
$(MA)_3(MSA)_3 \rightarrow (MA)_2(MSA)_1 + (MA)_1(MSA)_2$	7.21×10^{-15}
$(MA)_3(MSA)_3 \rightarrow (MA)_2 + (MA)_1(MSA)_3$	8.32×10^{-17}
$(MA)_3(MSA)_4 \rightarrow (MA)_3(MSA)_3 + MSA$	1.35×10^{1}
$(MA)_3(MSA)_4 \rightarrow (MA)_3(MSA)_2 + (MSA)_2$	7.68×10^{-12}
$(MA)_3(MSA)_4 \rightarrow (MA)_3(MSA)_1 + (MSA)_3$	1.12×10^{-27}
$(MA)_3(MSA)_4 \rightarrow (MA)_3 + (MSA)_4$	2.51×10^{-42}
$(MA)_3(MSA)_4 \rightarrow (MA)_2(MSA)_4 + MA$	2.58×10^{-3}
$(MA)_3(MSA)_4 \rightarrow (MA)_2(MSA)_3 + (MA)_1(MSA)_1$	1.34×10^{-5}
$(MA)_3(MSA)_4 \rightarrow (MA)_2(MSA)_2 + (MA)_1(MSA)_2$	8.18×10^{-3}
$(MA)_3(MSA)_4 \rightarrow (MA)_2(MSA)_1 + (MA)_1(MSA)_3$	2.04×10^{-14}
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$(MA)_4(MSA)_1 \rightarrow (MA)_4 + MSA$	1.06×10^{-10}
$(MA)_4(MSA)_1 \rightarrow (MA)_3(MSA)_1 + MA$	1.03×10^{10}
$(MA)_4(MSA)_1 \rightarrow (MA)_3 + (MA)_1(MSA)_1$	8.84×10^{-4}
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$(MA)_4(MSA)_2 \rightarrow (MA)_4 + (MSA)_2$	9.65×10^{-28}
$(MA)_4(MSA)_2 \rightarrow (MA)_3(MSA)_2 + MA$	1.08×10^{7}
$(MA)_4(MSA)_2 \rightarrow (MA)_3(MSA)_1 + (MA)_1(MSA)_1$	3.87×10^{-9}
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$(MA)_4(MSA)_3 \rightarrow (MA)_3 + (MA)_1(MSA)_3$	5.31×10^{-24}
$(MA)_4(MSA)_3 \rightarrow (MA)_2(MSA)_3 + (MA)_2$	7.22×10^{-9}
$(MA)_4(MSA)_3 \rightarrow (MA)_2(MSA)_2 + (MA)_2(MSA)_1$	3.80×10^{-7}
$(MA)_4(MSA)_4 \rightarrow (MA)_4(MSA)_3 + MSA$	5.88×10^{-10}
$(MA)_4(MSA)_4 \rightarrow (MA)_4(MSA)_2 + (MSA)_2$	3.28×10^{-23}
$(MA)_4(MSA)_4 \rightarrow (MA)_4(MSA)_1 + (MSA)_3$	4.52×10^{-42}

$(MA)_4(MSA)_4 \rightarrow (MA)_4 + (MSA)_4$	3.76×10^{-59}
$(MA)_4(MSA)_4 \rightarrow (MA)_3(MSA)_4 + MA$	5.16×10^{-5}
$(MA)_4(MSA)_4 \rightarrow (MA)_3(MSA)_3 + (MA)_1(MSA)_1$	1.68×10^{-9}
$(MA)_4(MSA)_4 \rightarrow (MA)_3(MSA)_2 + (MA)_1(MSA)_2$	3.17×10^{-15}
$(MA)_4(MSA)_4 \rightarrow (MA)_3(MSA)_1 + (MA)_1(MSA)_3$	9.03×10^{-26}
$(MA)_4(MSA)_4 \rightarrow (MA)_3 + (MA)_1(MSA)_4$	5.61×10^{-38}
$(MA)_4(MSA)_4 \rightarrow (MA)_2(MSA)_4 + (MA)_2$	2.02×10^{-21}
$(MA)_4(MSA)_4 \rightarrow (MA)_2(MSA)_3 + (MA)_2(MSA)_1$	7.24×10^{-17}
$(MA)_4(MSA)_4 \rightarrow (MA)_2(MSA)_2 + (MA)_2(MSA)_2$	0.88×10^{-5}

121

122

123   Table S2. Number of H-bonds formed by DMA/MA and MSA/SA in the

124    $(DMA/MA)_z(MSA/SA)_z$ (z = 1-4) clusters.

Clusters Systems	1:1	2:2	3:3	4:4
DMA-MSA	2	4	6	8
MA-MSA	1	4	8	12
DMA-SA[a]	2	4	6	8
MA-SA[a]	2	4	8	10

125   [a]data are obtained from reference 6.[6]

126

127   Table S3. The thermochemical information including enthalpy change ΔH (kcal mol^{-1})

128   and entropy change ΔS (cal (mol·K)$^{-1}$) for the optimized DMA/MA-MSA clusters at

129   298.15 K and 1 atm.

Species	ΔH	ΔS
$(DMA)_1(MSA)_1$	-19.44	-36.64
$(DMA)_1(MSA)_2$	-48.45	-80.49
$(DMA)_1(MSA)_3$	-69.61	-121.76
$(DMA)_1(MSA)_4$	-91.15	-165.78
$(DMA)_2(MSA)_1$	-36.38	-74.59
$(DMA)_2(MSA)_2$	-74.24	-111.41
$(DMA)_2(MSA)_3$	-97.77	-160.84
$(DMA)_2(MSA)_4$	-119.72	-202.62
$(DMA)_3(MSA)_1$	-46.12	-107.37
$(DMA)_3(MSA)_2$	-84.13	-141.48
$(DMA)_3(MSA)_3$	-124.34	-199.83
$(DMA)_3(MSA)_4$	-149.14	-247.63
$(DMA)_4(MSA)_1$	-56.46	-145.74
$(DMA)_4(MSA)_2$	-96.93	-190.81
$(DMA)_4(MSA)_3$	-137.28	-238.93
$(DMA)_4(MSA)_4$	-174.10	-284.11
$(MA)_1(MSA)_1$	-16.16	-36.35
$(MA)_1(MSA)_2$	-44.38	-80.57
$(MA)_1(MSA)_3$	-66.60	-117.12
$(MA)_1(MSA)_4$	-85.63	-160.73
$(MA)_2(MSA)_1$	-31.68	-76.61
$(MA)_2(MSA)_2$	-68.48	-112.39
$(MA)_2(MSA)_3$	-92.73	-155.24
$(MA)_2(MSA)_4$	-114.46	-202.03
$(MA)_3(MSA)_1$	-43.66	-104.57
$(MA)_3(MSA)_2$	-81.17	-147.74
$(MA)_3(MSA)_3$	-117.53	-195.20
$(MA)_3(MSA)_4$	-142.45	-243.43
$(MA)_4(MSA)_1$	-54.43	-142.07
$(MA)_4(MSA)_2$	-94.03	-178.95
$(MA)_4(MSA)_3$	-132.42	-229.11
$(MA)_4(MSA)_4$	-172.23	-283.37

130

131

132
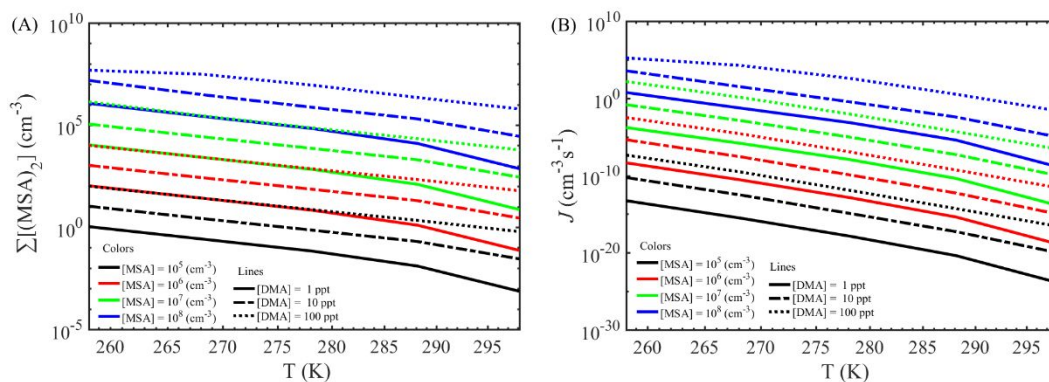
Figure S1. Simulated steady-state MSA dimer concentration $\Sigma[(MSA)_2]$ (cm^{-3}) (A) and

cluster formation rate J (cm^{-3} s^{-1}) (B) as a function of temperature for the DMA-MSA

system.

136
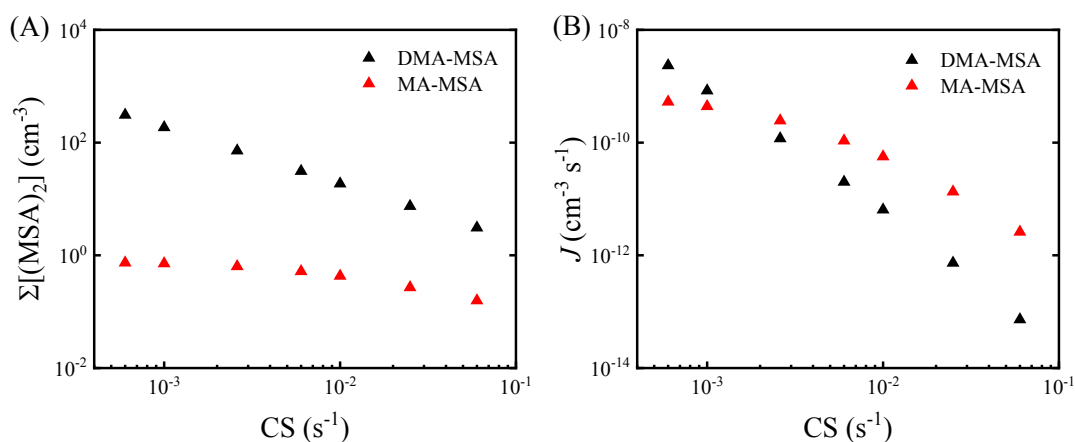
Figure S2. Simulated steady-state MSA dimer concentration ($\Sigma[(MSA)_2]$) (cm^{-3}) (A)

and the cluster formation rate (J) (cm^{-3}s^{-1}) (B) as a function of condensation sink

coefficient for both DMA-MSA and MA-MSA systems at 278.15 K, [MSA] = 10^6 cm^{-3},

and [base] (DMA or MA) = 10 ppt.

141
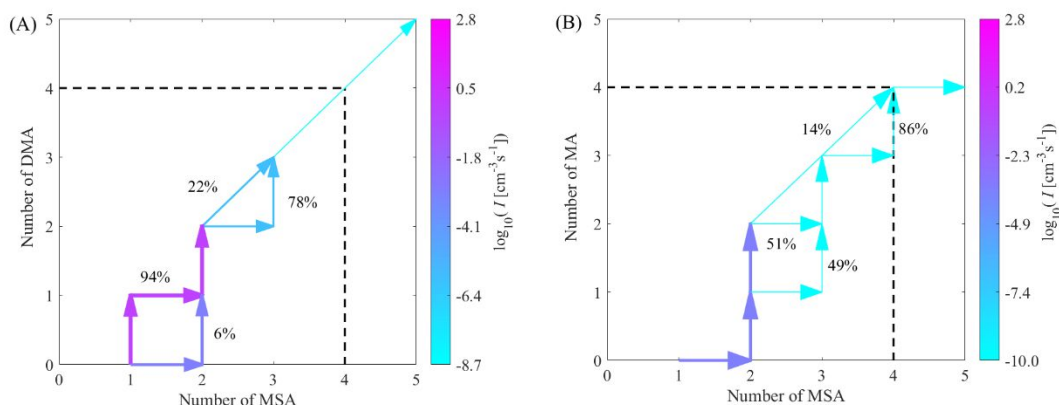
142

143 Figure S3. Cluster formation pathways for the DMA-MSA system (A) and the MA-

144 MSA system (B) at 278.15 K, [MSA] = 10^6 cm^{-3}, [DMA/MA] = 10 ppt, and coagulation

145 sink coefficient = 6.0×10^{-4} s^{-1}. For clarity, pathways contributing less than 5% to the

146 flux of the cluster are not shown.
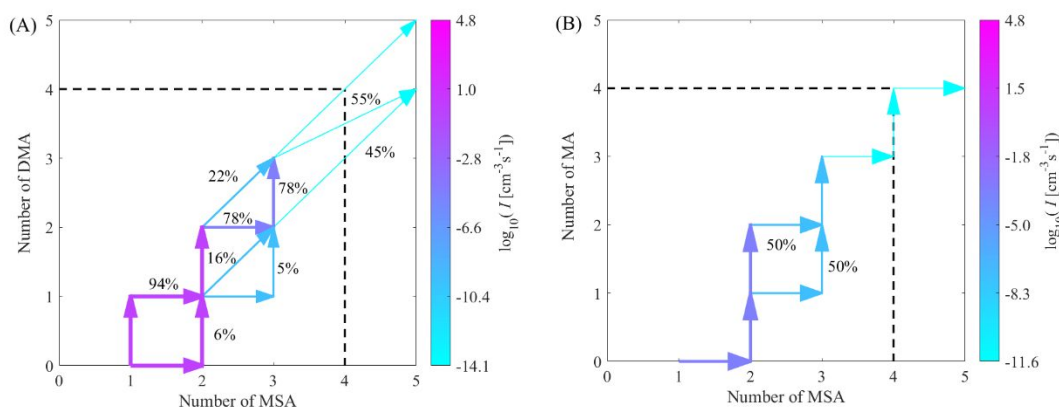
147

148 Figure S4. Cluster formation pathways for the DMA-MSA system (A) and the MA-

149 MSA system (B) at 278.15 K, [MSA] = 10^6 cm^{-3}, [DMA/MA] = 10 ppt, and coagulation

150 sink coefficient = 6.0×10^{-2} s^{-1}. For clarity, pathways contributing less than 5% to the

151 flux of the cluster are not shown.

152

153
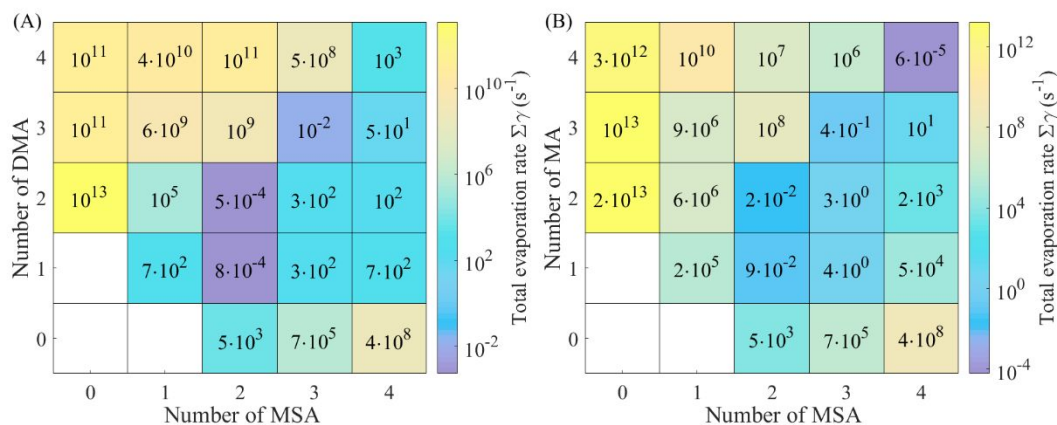
Figure S5. Evaporation rates of $(DMA)_m(MSA)_n$ ($m = 0-4$ and $n = 0-4$) (A) and

$(MA)_x(MSA)_y$ clusters ($x = 0-4$ and $y = 0-4$) (B) at 278.15 K.

156
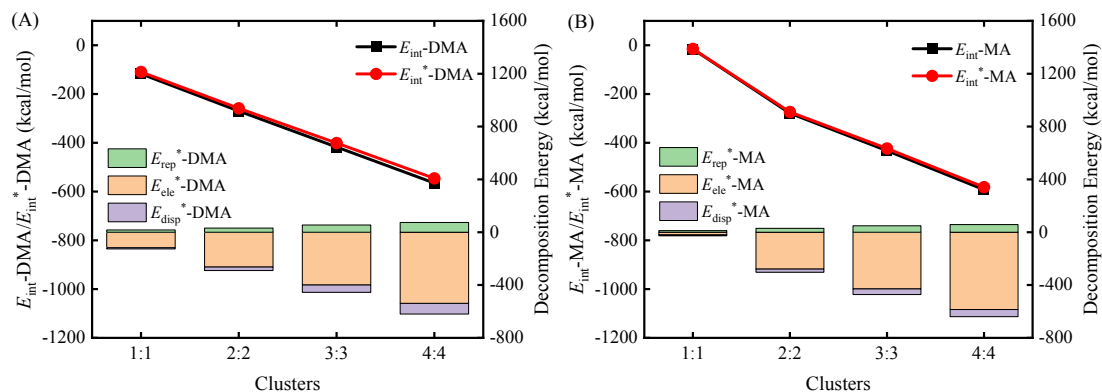
Figure S6. Interaction energy and interaction energy decomposition of $(DMA)_z(MSA)_z$

($z = 1-4$) clusters (A) and $(MA)_z(MSA)_z$ ($z = 1-4$) clusters (B). The black line represents

the interaction energy (E_{int}) obtained from the DLPNO-CCSD(T)/aug-cc-

pVTZ//ωB97X-D/6-31++G(d,p) level of theory, and the red line represents the total

energy (E_{int}^*) obtained from EDA-FF analysis.

162

163

164
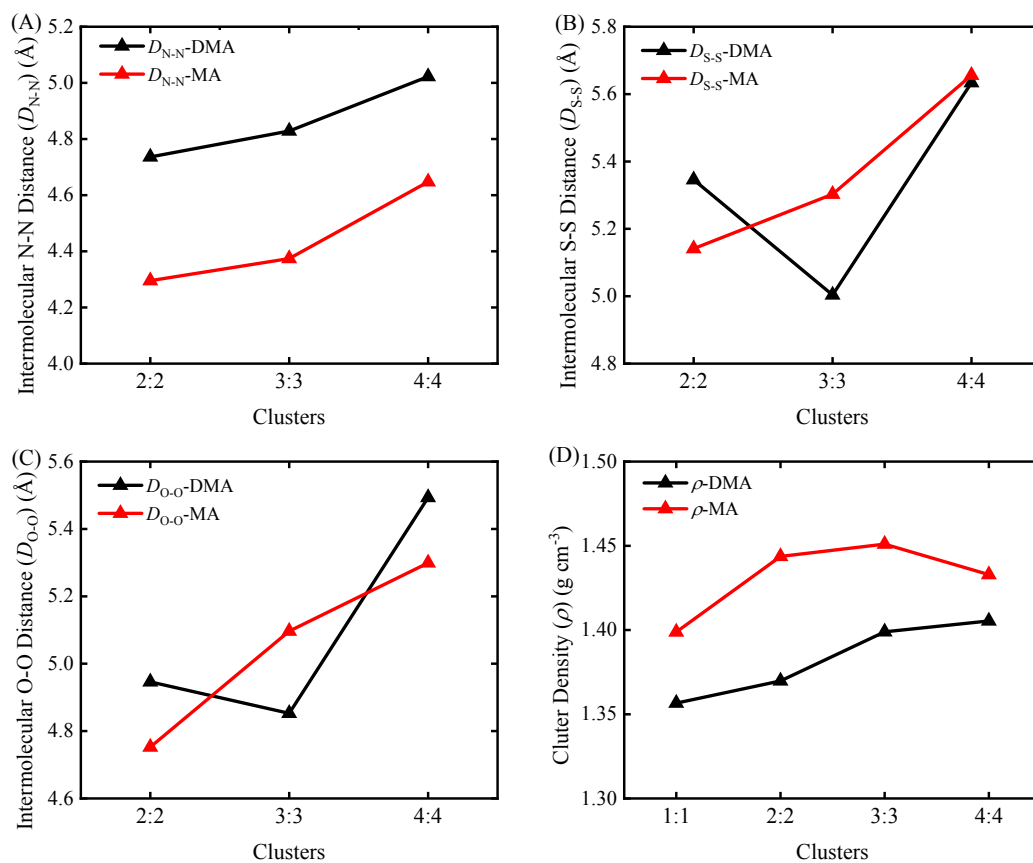
Figure S7. Variation of average intermolecular nitrogen-nitrogen distance (D_{N-N}) (Å)

(A), sulfur-sulfur distance (D_{S-S}) (Å) (B) and oxygen-oxygen distance (D_{O-O}) (Å) (C),

and cluster density (ρ) (g cm^{-3}) (D) with cluster size for the $(DMA)_z(MSA)_z$ and

$(MA)_z(MSA)_z$ clusters (z = 1-4).

$(MA)_1(MSA)_1$ $(MA)_1(MSA)_2$ $(MA)_1(MSA)_3$ $(MA)_1(MSA)_4$

$(MA)_2(MSA)_1$ $(MA)_2(MSA)_2$ $(MA)_2(MSA)_3$ $(MA)_2(MSA)_4$

$(MA)_3(MSA)_1$ $(MA)_3(MSA)_2$ $(MA)_3(MSA)_3$ $(MA)_3(MSA)_4$

$(MA)_4(MSA)_1$ $(MA)_4(MSA)_2$ $(MA)_4(MSA)_3$ $(MA)_4(MSA)_4$
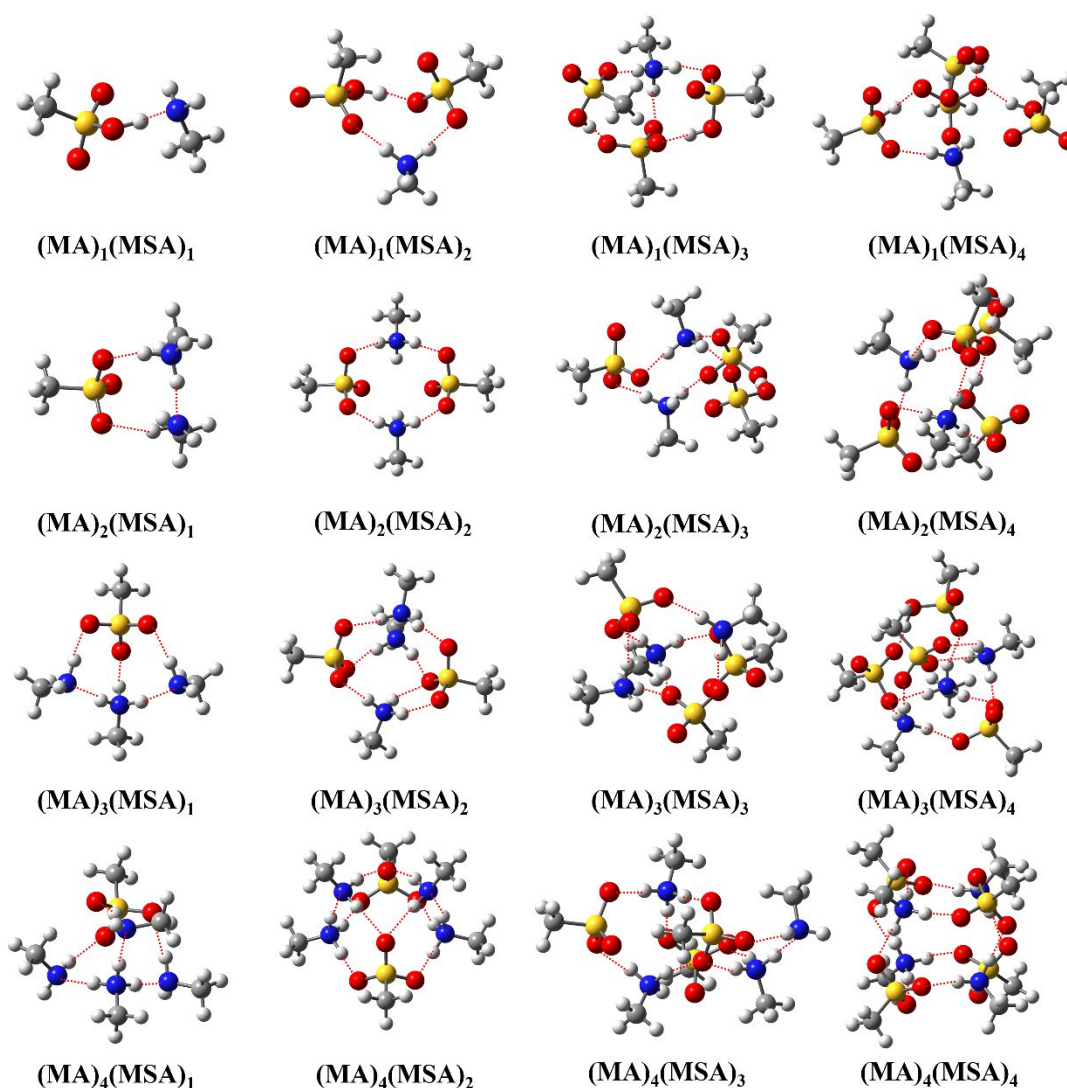
Figure S8. Cluster conformations of $(MA)_x(MSA)_y$ (x = 1-4, y = 1-4) at ωB97X-D/6-31++G(d,p) level of theory. The red balls stand for O atoms, the blue ones for N atoms, the gray ones for C atoms and white ones for H atoms. Dashed red lines indicate hydrogen bonds (defined by the configurational criteria).

176

177
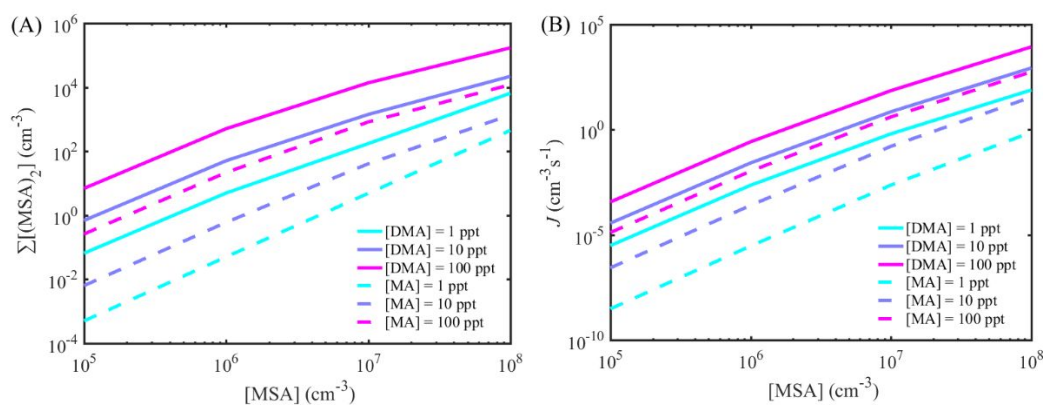
Figure S9. Simulated steady-state MSA dimer concentration ($\Sigma[(MSA)_2]$) (cm^{-3}) (A)

and the cluster formation rate (J) (cm^{-3}s^{-1}) (B) as a function of monomer concentration

at 278.15 K with a "2 × 2 box".

181
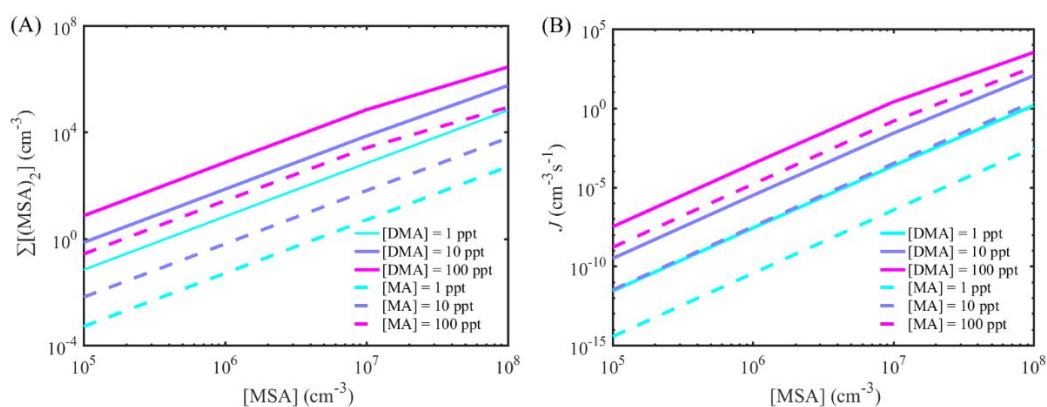
Figure S10. Simulated steady-state MSA dimer concentration ($\Sigma[(MSA)_2]$) (cm^{-3}) (A)

and the cluster formation rate (J) (cm^{-3}s^{-1}) (B) as a function of monomer concentration

at 278.15 K with a "3 × 3 box".

185

186

187
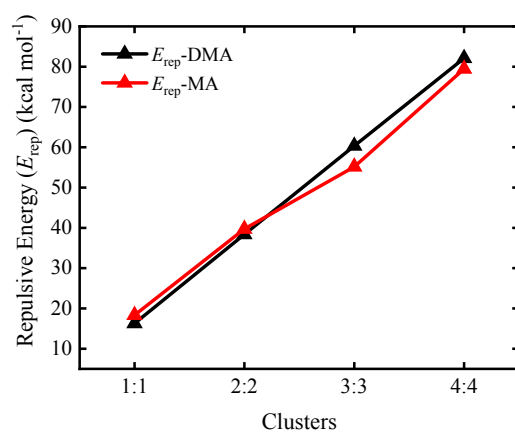
Figure S11. Repulsive energy (E_{rep}) (kcal mol^{-1}) obtained from EDA-FF analysis for

(DMA/MA)$_z$(SA)$_z$ (z = 1-4) clusters.

190

191 **Coordinates of all optimized clusters**

192 (DMA)$_1$(MSA)$_1$

N	-1.897591	0.127560	0.000197
H	-1.218638	0.289820	0.787956
C	-2.286995	-1.298629	-0.000207
H	-2.872744	-1.514873	-0.894979
H	-2.872894	-1.515466	0.894318
H	-1.374153	-1.896723	-0.000402
C	-3.011192	1.089809	-0.000024
H	-3.620752	0.942000	-0.892984
H	-2.600546	2.099589	0.001228
H	-3.622507	0.940507	0.891497
S	1.210251	-0.083698	0.000051
O	1.630667	-1.486234	-0.000435
O	0.441871	0.317279	1.227420
O	0.441451	0.318107	-1.226853
H	-1.218135	0.289956	-0.787099
C	2.683041	0.923146	-0.000124
H	3.253704	0.680195	0.896544
H	3.254033	0.678998	-0.896262
H	2.390725	1.973065	-0.000940

193

194 (DMA)$_1$(MSA)$_2$

N	-0.744416	2.202596	-0.109272
H	-1.479229	1.498559	-0.378128
C	-0.713661	3.308518	-1.086227
H	0.090878	3.998527	-0.828003
H	-1.672231	3.829308	-1.071962
H	-0.536302	2.890846	-2.077063
C	-0.969852	2.615929	1.291942
H	-0.158676	3.272311	1.610629
H	-0.991829	1.712609	1.901598
H	-1.925310	3.138200	1.362344
S	-1.778051	-1.009529	-0.114565
O	-1.012315	-1.798427	-1.085102
O	-2.461804	0.188460	-0.683093
O	-0.955193	-0.596738	1.078095
H	0.153122	1.679110	-0.162781
C	-3.069066	-2.053290	0.530685
H	-3.706129	-2.349735	-0.302901

H	-2.599664	-2.925681	0.985414
H	-3.636235	-1.487012	1.269098
S	2.364458	-0.272861	0.065491
O	3.746397	-0.130428	0.465593
O	1.661086	0.930447	-0.418086
O	1.569920	-0.875394	1.282481
H	0.558049	-0.807549	1.166503
C	2.214540	-1.514182	-1.195078
H	2.727554	-1.136198	-2.080133
H	2.697062	-2.418830	-0.824940
H	1.150865	-1.679623	-1.386636

195

196   (DMA)₁(MSA)₃

N	0.014960	-1.307574	1.760676
H	0.848880	-0.934065	1.278301
C	0.092267	-2.786655	1.732105
H	-0.814201	-3.196037	2.178346
H	0.976349	-3.105349	2.284554
H	0.173747	-3.104424	0.694647
C	-0.091889	-0.728703	3.118568
H	-0.983229	-1.130873	3.601549
H	-0.169826	0.351788	3.020121
H	0.799345	-0.997780	3.686675
S	-0.023101	1.924902	0.350779
O	-0.049369	1.575003	-1.078264
O	1.184964	1.409502	1.065573
O	-1.249327	1.502057	1.091608
H	-0.799994	-1.024933	1.188957
C	0.047396	3.699816	0.473192
H	0.074958	3.967487	1.529376
H	0.950192	4.037676	-0.036226
H	-0.841937	4.107587	-0.007703
S	-3.177141	-0.716823	-0.706778
O	-4.450088	-1.378856	-0.879219
O	-2.105078	-1.427845	0.004672
O	-3.443340	0.658084	0.024765
H	-2.592037	1.025498	0.422392
C	-2.533435	-0.220033	-2.286905
H	-2.314711	-1.131682	-2.844518
H	-3.302732	0.364520	-2.791494
H	-1.630059	0.369680	-2.113880

S	3.208243	-0.684585	-0.695929
O	2.265602	-1.425680	0.152818
O	4.517412	-1.247186	-0.937308
O	3.408755	0.759325	-0.081958
H	2.557818	1.069755	0.359334
C	2.395417	-0.360479	-2.243528
H	2.208389	-1.325844	-2.715637
H	1.464322	0.172656	-2.036284
H	3.067201	0.242544	-2.854489

197

198   (DMA)$_1$(MSA)$_4$

N	0.026167	-0.630592	2.089018
H	0.746038	-0.479507	1.369046
C	0.221572	-1.965532	2.688758
H	-0.552607	-2.133583	3.438599
H	1.210948	-2.001349	3.145792
H	0.151934	-2.708609	1.896438
C	0.082221	0.485292	3.059574
H	-0.710582	0.348172	3.795832
H	-0.069883	1.413330	2.511250
H	1.063360	0.486514	3.533143
S	0.041256	-1.984879	-1.342558
O	0.075014	-0.954781	-2.408429
O	-1.272408	-2.077720	-0.646571
O	1.151001	-1.855426	-0.359225
H	-0.888070	-0.592142	1.615003
C	0.271582	-3.547605	-2.161141
H	-0.530692	-3.669701	-2.888814
H	1.242673	-3.527153	-2.656168
H	0.236776	-4.333251	-1.406672
S	3.800518	0.191480	0.603332
O	5.113682	-0.080358	1.148083
O	2.641716	0.150932	1.499497
O	3.537328	-0.815969	-0.596385
H	2.611039	-1.190789	-0.555030
C	3.829208	1.762523	-0.223980
H	4.000095	2.523335	0.538226
H	4.647975	1.743844	-0.943195
H	2.872465	1.921698	-0.720510
S	-0.129650	2.132834	-0.899507
O	0.525503	3.332914	-0.420300

O	-0.474045	1.081043	0.052352
O	0.828654	1.507547	-2.004664
H	0.579579	0.548602	-2.172720
C	-1.593805	2.556886	-1.807696
H	-2.315893	2.937631	-1.083657
H	-1.326620	3.307054	-2.551343
H	-1.982125	1.647008	-2.266329
S	-3.588982	0.203518	0.619406
O	-3.728118	1.645749	0.560473
O	-2.750481	-0.394937	1.661608
O	-3.125228	-0.322483	-0.793290
H	-2.361439	-0.990213	-0.731180
C	-5.211037	-0.512533	0.760863
H	-5.635732	-0.168719	1.704566
H	-5.811004	-0.163901	-0.079626
H	-5.111075	-1.597655	0.749990

199

200 (DMA)₂(MSA)₁

N	-1.183310	1.438994	-0.051162
H	-1.413723	0.380789	-0.065429
C	-2.069824	2.147395	-0.986082
H	-1.812718	3.208240	-1.014080
H	-3.108621	2.031709	-0.668325
H	-1.942813	1.719040	-1.981207
C	-1.231307	1.922101	1.341614
H	-0.990591	2.987055	1.370414
H	-0.486994	1.359128	1.907403
H	-2.231067	1.759655	1.751250
S	1.726664	-0.125634	-0.101316
O	1.273963	-1.314067	-0.858337
O	1.261429	-0.110399	1.305019
O	1.387057	1.160044	-0.799571
H	-0.182411	1.472259	-0.390083
C	3.510069	-0.186476	-0.069905
H	3.872926	0.686765	0.472242
H	3.804865	-1.106193	0.435851
H	3.870109	-0.180482	-1.098862
N	-1.589054	-1.282982	-0.092113
H	-0.670231	-1.525275	-0.477959
C	-2.646533	-1.818557	-0.941400
H	-3.621584	-1.465557	-0.586773

H	-2.667110	-2.918397	-0.949425
H	-2.504951	-1.469675	-1.967835
C	-1.649569	-1.771036	1.285435
H	-2.551318	-1.385147	1.775142
H	-0.765316	-1.411825	1.817365
H	-1.675145	-2.869213	1.339415

201

202 (DMA)$_2$(MSA)$_2$

N	-0.009660	2.407134	0.078250
H	-0.898335	1.971089	-0.268909
C	0.078424	3.786551	-0.437290
H	1.004445	4.243846	-0.085298
H	-0.781732	4.359412	-0.086794
H	0.077972	3.752427	-1.526686
C	0.012747	2.304678	1.553237
H	-0.803680	2.902997	1.962163
H	0.974982	2.660226	1.923641
H	-0.123581	1.257521	1.818283
S	2.660513	-0.021154	-0.205486
O	2.230244	-1.213737	-0.989583
O	2.244167	-0.096215	1.210327
O	2.259064	1.261681	-0.851691
H	0.803769	1.866438	-0.305726
C	4.443701	-0.034082	-0.251167
H	4.789671	-0.960968	0.206521
H	4.757848	0.022704	-1.293433
H	4.804193	0.829593	0.307838
N	0.025007	-2.328274	0.162407
H	0.815946	-1.875659	-0.355779
C	-0.639302	-3.316904	-0.711209
H	-1.427891	-3.819673	-0.148641
H	0.099118	-4.043660	-1.054121
H	-1.087912	-2.787514	-1.551120
C	0.572331	-2.882577	1.417892
H	-0.246531	-3.267662	2.027973
H	1.098283	-2.079280	1.935260
H	1.272056	-3.685350	1.178455
S	-2.684979	0.016284	-0.234525
O	-2.705460	-0.969403	-1.323230
O	-2.424779	1.418997	-0.667397
O	-1.753999	-0.375898	0.875382

H	-0.655061	-1.567795	0.402970
C	-4.316934	0.042762	0.489165
H	-5.022735	0.343699	-0.285294
H	-4.546668	-0.960537	0.848456
H	-4.319834	0.758083	1.311594

203

204 (DMA)$_2$(MSA)$_3$

N	-0.272494	-2.391043	-0.295387
H	0.402145	-1.846048	0.279470
C	0.441249	-2.810178	-1.517114
H	-0.259143	-3.302933	-2.193701
H	1.246900	-3.491985	-1.242250
H	0.871865	-1.926071	-1.985963
C	-0.798582	-3.506954	0.516284
H	0.037737	-4.103725	0.883708
H	-1.457865	-4.119154	-0.101642
H	-1.360618	-3.075173	1.344211
S	-2.924276	-0.240280	0.373976
O	-2.620827	1.213872	0.288378
O	-2.310480	-0.883096	1.559147
O	-2.617811	-0.982290	-0.883687
H	-1.063133	-1.759061	-0.547660
C	-4.695666	-0.349035	0.573076
H	-5.166799	0.114049	-0.294074
H	-4.966738	-1.402686	0.642775
H	-4.967664	0.179839	1.486809
N	-0.225928	1.793095	1.637219
H	-1.050476	1.538553	1.051113
C	-0.009477	3.253102	1.564388
H	0.878057	3.508080	2.145496
H	-0.886935	3.762399	1.965905
H	0.140527	3.519505	0.518187
C	-0.421590	1.268594	3.004451
H	0.490880	1.437599	3.577670
H	-0.643699	0.204921	2.928269
H	-1.266793	1.781696	3.465962
S	2.816562	-0.426320	0.700362
O	3.100916	-0.440617	-0.767928
O	1.915075	-1.532867	1.114992
O	2.385223	0.896960	1.204877
H	0.603777	1.323808	1.229568

C	4.391466	-0.762883	1.465309
H	4.753297	-1.722072	1.094839
H	5.077187	0.039166	1.192396
H	4.241623	-0.795887	2.544575
S	0.360462	1.198190	-1.879593
O	0.410082	2.632131	-1.645280
O	0.115752	0.329542	-0.729714
O	1.683860	0.692138	-2.579336
H	2.286460	0.277844	-1.863063
C	-0.857370	0.862880	-3.122357
H	-0.628116	1.460216	-4.004612
H	-0.847025	-0.203844	-3.342139
H	-1.814957	1.141807	-2.680429

205

206   (DMA)₂(MSA)₄

N	-2.006919	-1.932520	-1.260749
H	-1.128997	-2.076930	-0.723692
C	-1.792266	-2.433303	-2.631849
H	-2.674264	-2.213791	-3.235321
H	-1.610439	-3.508369	-2.596078
H	-0.919040	-1.927586	-3.044247
C	-3.118570	-2.583115	-0.540189
H	-4.041293	-2.447420	-1.105639
H	-3.226997	-2.102390	0.431639
H	-2.896103	-3.644571	-0.419618
S	1.457943	-1.958157	-0.400753
O	1.100985	-0.815603	-1.277162
O	0.336314	-2.911840	-0.209170
O	2.032487	-1.512351	0.909340
H	-2.212714	-0.912784	-1.307557
C	2.757474	-2.850897	-1.225308
H	3.044739	-3.688357	-0.588969
H	2.370429	-3.205746	-2.180918
H	3.589852	-2.159463	-1.365180
S	-3.524797	1.379878	-0.585849
O	-4.077752	0.551950	0.526829
O	-3.038452	0.543327	-1.719170
O	-2.518037	2.369363	-0.145784
H	0.542073	0.832202	-0.571913
C	-4.915721	2.302024	-1.209608
H	-5.679716	1.593874	-1.529869

H	-5.287457	2.934274	-0.403278
H	-4.571190	2.907412	-2.048110
N	0.178674	1.798649	-0.627821
H	-0.843505	1.746492	-0.469536
C	0.438752	2.310781	-1.989666
H	1.517314	2.356778	-2.142727
H	-0.011497	3.299940	-2.084944
H	-0.016328	1.626472	-2.705421
C	0.731138	2.648988	0.452801
H	1.799085	2.777143	0.286583
H	0.542326	2.160120	1.408376
H	0.213361	3.608872	0.422709
S	-1.212618	-0.280291	2.263160
O	-0.602189	0.796901	3.021274
O	-1.034547	-0.274393	0.808915
O	-2.767682	-0.366178	2.550280
H	-3.278907	0.061139	1.782303
C	-0.652661	-1.834770	2.903299
H	0.419961	-1.872541	2.701034
H	-0.867003	-1.865062	3.971500
H	-1.158144	-2.635914	2.365142
S	4.256462	0.978116	-0.193803
O	3.640210	1.998827	-1.034532
O	4.705956	-0.259384	-0.818307
O	3.307111	0.663475	1.024192
H	2.815447	-0.238529	0.942422
C	5.620969	1.728326	0.665401
H	6.343601	2.036070	-0.090887
H	5.248401	2.592302	1.215264
H	6.052956	0.989772	1.339916

207

208 $(DMA)_3(MSA)_1$

N	-0.266175	1.949987	-0.736490
H	-0.956759	1.415237	-0.081698
C	-0.957110	2.266729	-1.994481
H	-0.263714	2.735813	-2.695808
H	-1.791637	2.943867	-1.796707
H	-1.335841	1.339780	-2.428625
C	0.275792	3.115323	-0.016957
H	0.958904	3.668076	-0.666049
H	0.817341	2.739308	0.852010

H	-0.544437	3.768510	0.291463
S	2.049161	-0.402607	0.234801
O	1.570331	-1.774967	0.484421
O	1.689479	0.577288	1.285664
O	1.660779	0.107841	-1.126406
H	0.514843	1.265604	-0.923376
C	3.833397	-0.497489	0.203447
H	4.231404	0.499315	0.012621
H	4.166180	-0.865598	1.174414
H	4.124354	-1.188704	-0.587734
N	-1.957174	0.535257	0.850748
H	-1.734952	-0.413005	0.494332
C	-3.383439	0.777368	0.672486
H	-3.624893	1.817640	0.920366
H	-4.005812	0.126549	1.305439
H	-3.656072	0.600719	-0.372444
C	-1.524650	0.632943	2.244732
H	-1.689976	1.652159	2.613585
H	-0.455634	0.412197	2.300933
H	-2.076705	-0.057960	2.899225
N	-1.253559	-2.052794	-0.360293
H	-0.316854	-2.171217	0.030065
C	-1.127549	-1.839598	-1.794363
H	-2.077451	-1.472147	-2.205708
H	-0.857950	-2.756893	-2.343824
H	-0.342829	-1.098948	-1.974293
C	-2.098321	-3.185315	-0.020379
H	-3.130985	-2.987781	-0.332559
H	-2.095535	-3.333843	1.062987
H	-1.776632	-4.125175	-0.499519

209

210   (DMA)$_3$(MSA)$_2$

N	0.027195	-2.081131	-1.049434
H	-0.818527	-1.736751	-0.545830
C	0.130717	-3.533024	-0.818079
H	1.031189	-3.912394	-1.304032
H	-0.754145	-4.024833	-1.225118
H	0.188879	-3.691380	0.258394
C	-0.055983	-1.684193	-2.470676
H	0.852851	-2.006282	-2.980351
H	-0.146844	-0.599581	-2.517449

H	-0.938182	-2.144456	-2.917884
S	2.558846	0.553596	-0.546197
O	2.007582	1.016098	0.773171
O	1.942353	1.265781	-1.676674
O	2.516465	-0.926760	-0.658636
H	0.860260	-1.625093	-0.631341
C	4.290933	0.983381	-0.513855
H	4.373995	2.065945	-0.415940
H	4.753752	0.482690	0.336675
H	4.737822	0.647127	-1.449664
N	-0.288610	2.476292	0.587853
H	0.568229	1.873212	0.573126
C	-0.217101	3.337638	1.782911
H	-1.126843	3.936361	1.851280
H	0.655901	3.988254	1.709968
H	-0.128966	2.703783	2.665516
C	-0.390615	3.209606	-0.692560
H	-1.260677	3.867837	-0.655280
H	-0.509659	2.478513	-1.489778
H	0.523075	3.784277	-0.847819
N	0.657026	-1.587335	1.850408
H	1.023514	-0.659348	1.649566
C	1.755483	-2.416770	2.316568
H	1.414652	-3.453695	2.433963
H	2.167811	-2.095335	3.289470
H	2.557560	-2.396986	1.573431
C	-0.437287	-1.493892	2.804208
H	-0.914117	-2.474952	2.913700
H	-1.194350	-0.801021	2.429110
H	-0.111370	-1.166300	3.808316
S	-2.765226	0.062127	-0.241059
O	-2.436854	-1.374882	-0.045370
O	-2.161606	0.633761	-1.461202
O	-2.462551	0.884079	0.971343
H	-1.116337	1.838942	0.689908
C	-4.538175	0.130508	-0.431798
H	-4.807433	-0.460363	-1.307620
H	-4.995348	-0.281925	0.467645
H	-4.824861	1.173264	-0.569019

211

212   (DMA)$_3$(MSA)$_3$

N	-0.744339	-0.658288	-2.137365
H	-1.519831	-0.037400	-1.816570
C	-1.334652	-1.836451	-2.800080
H	-0.538835	-2.536160	-3.058019
H	-1.868826	-1.514058	-3.695444
H	-2.025657	-2.297590	-2.094438
C	0.220381	0.095217	-2.962257
H	1.069498	-0.552348	-3.188439
H	0.557729	0.960763	-2.390681
H	-0.270942	0.415800	-3.882841
S	-3.471329	0.026149	-0.105460
O	-2.690886	-1.226550	0.147691
O	-3.072365	0.640433	-1.405136
O	-3.462928	0.947049	1.040857
H	-0.257677	-0.983832	-1.287307
C	-5.164432	-0.501308	-0.330671
H	-5.764199	0.381527	-0.553772
H	-5.201019	-1.210545	-1.157856
H	-5.501956	-0.969373	0.594359
S	2.133065	-2.007363	0.002786
O	2.950742	-1.214281	-0.958004
O	0.783298	-2.335256	-0.518953
O	2.089578	-1.400595	1.356432
H	-1.299530	-0.869805	1.203399
C	2.979051	-3.570141	0.175850
H	3.054182	-4.030230	-0.809544
H	3.969763	-3.379890	0.589084
H	2.396454	-4.198483	0.849994
N	-0.675255	-1.020947	2.021240
H	0.293085	-0.893267	1.685961
C	-0.851150	-2.420972	2.450142
H	-1.887497	-2.569057	2.755670
H	-0.172503	-2.632586	3.277970
H	-0.619600	-3.063405	1.600593
C	-0.989448	-0.014721	3.059888
H	-2.066249	-0.014600	3.231017
H	-0.672146	0.963888	2.699623
H	-0.449405	-0.270073	3.973929
S	0.183282	2.296388	0.252103
O	0.581744	2.637835	1.629689
O	-0.098394	0.848028	0.072964
O	1.187284	2.755804	-0.772905

H	2.552331	1.936488	-0.490512
C	-1.317372	3.176633	-0.116920
H	-2.085119	2.821939	0.572957
H	-1.119199	4.241543	0.007005
H	-1.616071	2.940367	-1.138161
N	3.435969	1.398437	-0.257165
H	3.252883	0.405044	-0.522767
C	3.654941	1.476771	1.203934
H	3.736389	2.524750	1.494596
H	4.564945	0.930711	1.459694
H	2.797504	1.025363	1.700051
C	4.546685	1.928550	-1.067125
H	4.687118	2.986283	-0.838626
H	4.299761	1.814013	-2.122898
H	5.461114	1.375818	-0.843514

213

214 (DMA)$_3$(MSA)$_4$

S	-2.463919	2.078761	-0.431633
O	-1.495064	1.093456	0.073933
O	-2.029530	3.469310	-0.452225
O	-3.770334	1.992403	0.427364
H	-3.924359	1.039291	0.796283
C	-2.958276	1.587683	-2.060358
H	-2.042326	1.523849	-2.652977
H	-3.444812	0.613318	-1.972198
H	-3.642970	2.345063	-2.442063
N	-0.487963	-1.186437	1.622426
H	-1.369002	-1.537094	1.187044
C	-0.868310	-0.361872	2.790120
H	0.038527	0.000811	3.272132
H	-1.455700	-0.980752	3.469993
H	-1.481825	0.462898	2.431509
C	0.357398	-2.351754	1.957931
H	1.279572	-1.994133	2.414691
H	0.587970	-2.881243	1.033686
H	-0.197506	-3.004293	2.633748
S	-4.009066	-1.526178	0.504528
O	-4.112193	-0.318719	1.390082
O	-2.827082	-2.356879	0.859430
O	-4.091736	-1.189089	-0.925559
H	0.006282	-0.632103	0.903587

C	-5.433406	-2.519576	0.907679
H	-6.326221	-1.944382	0.661907
H	-5.386823	-3.433109	0.314562
H	-5.401012	-2.746724	1.973218
S	3.442652	0.222321	1.685745
O	3.788166	-1.156697	1.240467
O	2.138596	0.310266	2.372637
O	3.582941	1.218439	0.583740
H	0.386518	1.678883	-0.249533
C	4.685872	0.651365	2.893817
H	4.630035	-0.072198	3.707375
H	5.662563	0.612055	2.411290
H	4.476428	1.657197	3.258453
N	1.123680	2.368859	-0.042743
H	2.005494	1.828613	0.074291
C	0.812234	3.033358	1.242985
H	-0.148021	3.540489	1.148937
H	1.606529	3.748085	1.465006
H	0.784209	2.268542	2.018130
C	1.249483	3.306116	-1.181471
H	0.314642	3.860257	-1.273853
H	1.420122	2.723225	-2.085486
H	2.081562	3.984130	-0.984274
S	0.543745	-0.577325	-2.077349
O	0.204127	0.753419	-2.612865
O	0.998770	-0.526069	-0.653139
O	1.549452	-1.317520	-2.899449
H	2.893280	-1.505773	-1.969992
C	-0.937182	-1.564008	-2.108946
H	-1.705373	-1.079891	-1.506108
H	-1.266228	-1.648800	-3.145109
H	-0.707098	-2.549422	-1.702722
N	3.806846	-1.580152	-1.452523
H	3.619498	-1.402330	-0.439285
C	4.701003	-0.512963	-1.945392
H	4.834621	-0.625781	-3.022357
H	5.661623	-0.583150	-1.432283
H	4.241035	0.446381	-1.711943
C	4.348028	-2.942031	-1.608877
H	4.535243	-3.137742	-2.666018
H	3.616038	-3.655657	-1.230488
H	5.274995	-3.032133	-1.040187

215

216 (DMA)$_4$(MSA)$_1$

N	1.614174	-0.863464	2.033169
H	1.665455	0.045420	1.574650
C	2.642336	-0.936294	3.058309
H	2.662868	-1.942259	3.494104
H	2.491494	-0.216892	3.881739
H	3.621890	-0.742669	2.611175
C	0.275487	-1.038749	2.571834
H	0.168602	-2.052058	2.979019
H	-0.457973	-0.909546	1.772521
H	0.028442	-0.321968	3.373397
N	1.627232	-1.012703	-1.318375
H	0.593284	-1.278756	-1.119317
C	2.503310	-2.108298	-0.869733
H	3.546626	-1.857584	-1.076186
H	2.237464	-3.024341	-1.403336
H	2.352407	-2.224105	0.206478
C	1.748841	-0.665898	-2.745688
H	2.777983	-0.374860	-2.967591
H	1.073203	0.167951	-2.940965
H	1.472983	-1.530475	-3.354214
S	0.466967	2.046793	-0.219031
O	-0.335513	2.067087	1.019179
O	-0.234852	1.476407	-1.393301
O	1.807237	1.399358	-0.018968
H	1.799428	-0.147491	-0.758581
C	0.826890	3.752673	-0.611573
H	-0.121876	4.265074	-0.773674
H	1.360306	4.191576	0.231707
H	1.438302	3.779494	-1.513823
N	-0.992013	-1.718433	-0.959171
H	-1.425009	-1.034216	-0.316693
C	-1.188416	-3.049687	-0.395716
H	-0.741902	-3.805177	-1.052612
H	-2.252558	-3.298806	-0.265173
H	-0.696386	-3.107710	0.578952
C	-1.638893	-1.552032	-2.258577
H	-1.186292	-2.227958	-2.994221
H	-1.498006	-0.520126	-2.589041
H	-2.717597	-1.766716	-2.220612
N	-2.594033	0.154814	0.736303

H	-1.883105	0.818390	1.047153
C	-3.377616	-0.317208	1.865257
H	-4.066702	-1.103876	1.535795
H	-3.978137	0.477151	2.340356
H	-2.715005	-0.744245	2.623761
C	-3.403167	0.807869	-0.283723
H	-4.074619	0.076922	-0.751142
H	-2.737929	1.216623	-1.048517
H	-4.024247	1.625987	0.118285

217

218    $(DMA)_4(MSA)_2$

N	-1.244997	-2.626934	-0.033456
H	-0.327795	-2.290121	-0.404612
C	-2.068698	-3.114303	-1.157726
H	-3.016055	-3.491494	-0.767225
H	-1.535257	-3.914625	-1.674608
H	-2.261147	-2.274065	-1.824278
C	-1.002538	-3.631809	1.019990
H	-1.953272	-3.894914	1.487041
H	-0.318641	-3.199312	1.749653
H	-0.549509	-4.519909	0.573996
N	0.825367	0.908861	-2.377923
H	0.997421	1.802944	-0.926422
C	-0.310506	1.326334	-3.195187
H	-0.367901	0.774401	-4.146910
H	-0.213570	2.392548	-3.432304
H	-1.236679	1.166185	-2.639154
C	2.096979	0.955318	-3.091219
H	2.086462	0.360620	-4.017974
H	2.883889	0.579432	-2.433214
H	2.326095	1.993141	-3.362631
S	2.143304	-1.528130	0.097842
O	1.487182	-1.719735	1.411071
O	2.821944	-0.228798	-0.058945
O	1.196841	-1.823928	-1.030117
H	0.685599	-0.040861	-2.032891
C	3.416600	-2.777119	-0.025591
H	4.138959	-2.604830	0.772837
H	2.952453	-3.757777	0.082911
H	3.893237	-2.682263	-1.001507
N	1.144465	2.460334	-0.094030

H	0.929594	1.907321	0.799960
C	0.203019	3.588084	-0.220960
H	0.407012	4.125400	-1.151001
H	0.330331	4.268278	0.625160
H	-0.811333	3.187534	-0.225910
C	2.559608	2.869565	-0.059360
H	2.809360	3.398376	-0.982746
H	3.170701	1.972452	0.034090
H	2.727049	3.532821	0.793115
N	0.742881	1.108839	2.299878
H	0.575395	0.138630	2.034955
C	-0.385739	1.618552	3.074052
H	-0.230203	2.684378	3.278721
H	-0.501715	1.101383	4.039074
H	-1.300709	1.507998	2.490369
C	2.007681	1.158756	3.026966
H	2.271441	2.204090	3.228354
H	2.788707	0.706093	2.412080
H	1.962910	0.628795	3.990490
S	-2.897844	0.476908	0.043693
O	-2.675302	-0.049001	-1.321622
O	-2.296202	1.798793	0.296272
O	-2.522319	-0.535108	1.086601
H	-1.716721	-1.788038	0.399401
C	-4.664434	0.695235	0.223660
H	-5.152002	-0.265935	0.058515
H	-4.863071	1.059873	1.231768
H	-4.991399	1.423840	-0.518760

219

220 (DMA)$_4$(MSA)$_3$

N	3.042629	1.892771	1.405995
H	3.267011	1.375420	0.550620
C	4.130176	1.694956	2.355412
H	3.867926	2.140372	3.322138
H	5.075365	2.147537	2.018199
H	4.290111	0.622847	2.497959
C	2.796860	3.295757	1.085602
H	2.490385	3.830924	1.991955
H	1.984116	3.363873	0.356872
H	3.688942	3.797531	0.680091
N	-0.201284	-2.319836	-1.046209

H	0.727068	-1.896355	-1.268976
C	-1.075595	-2.188739	-2.230009
H	-2.049142	-2.622725	-2.002072
H	-0.601802	-2.697953	-3.071430
H	-1.193993	-1.126790	-2.447899
C	0.019253	-3.705695	-0.597034
H	0.471249	-4.275536	-1.410538
H	-0.936142	-4.145311	-0.307238
H	0.696660	-3.678532	0.256639
S	-2.883323	-1.257914	1.198988
O	-3.173989	0.177739	1.497319
O	-1.453753	-1.601381	1.411605
O	-3.390365	-1.673513	-0.125028
H	-0.601206	-1.783903	-0.259381
C	-3.793848	-2.182681	2.426953
H	-3.446381	-1.879783	3.414948
H	-4.853881	-1.958806	2.305896
H	-3.604999	-3.243661	2.261336
N	0.704229	0.587694	2.028956
H	0.427503	0.151691	1.136465
C	-0.290311	1.630065	2.350717
H	0.014403	2.138745	3.268779
H	-1.272691	1.169468	2.471197
H	-0.315844	2.336644	1.518587
C	0.892224	-0.424693	3.082668
H	1.635256	-1.139498	2.730540
H	-0.056345	-0.931067	3.261305
H	1.242230	0.073234	3.990390
S	3.177516	-1.232484	-0.671327
O	3.697536	0.145525	-0.827365
O	2.340312	-1.678992	-1.822862
O	2.506076	-1.474220	0.628336
H	1.641000	1.068795	1.814192
C	4.620009	-2.291151	-0.701679
H	5.121780	-2.154434	-1.659900
H	5.275434	-1.997721	0.118990
H	4.293523	-3.324635	-0.581731
S	-0.110543	1.556565	-1.546514
O	-0.004882	0.367592	-0.660331
O	-0.112739	2.830486	-0.794947
O	-1.295736	1.422812	-2.456060
H	-2.652888	1.426901	-1.494250

C	1.320042	1.539544	-2.601928
H	2.211070	1.551782	-1.971966
H	1.307676	0.608561	-3.169419
H	1.268688	2.408809	-3.257897
N	-3.448238	1.607976	-0.828178
H	-3.239091	1.085373	0.053494
C	-4.704012	1.069162	-1.386961
H	-4.887143	1.523800	-2.362014
H	-5.526170	1.298214	-0.706399
H	-4.594460	-0.012134	-1.475752
C	-3.464723	3.057955	-0.543068
H	-3.740787	3.596375	-1.451270
H	-2.458114	3.355397	-0.244048
H	-4.186206	3.262387	0.249942

221

222   (DMA)$_4$(MSA)$_4$

S	3.986388	1.331959	0.635984
O	3.308647	2.630988	0.504893
O	4.633892	0.818073	-0.586354
O	3.072356	0.284544	1.231018
C	5.276321	1.543974	1.855652
H	5.982874	2.279044	1.468882
H	4.821819	1.901814	2.779764
H	5.768401	0.583783	2.012009
N	-1.639877	-1.220199	-1.978814
H	-1.778770	-2.049048	-1.358598
C	-0.847223	-1.610456	-3.162632
H	-0.577949	-0.704971	-3.708084
H	-1.447835	-2.272999	-3.788543
H	0.037248	-2.141791	-2.813487
C	-2.947001	-0.617980	-2.315248
H	-2.762850	0.274797	-2.913584
H	-3.462160	-0.354653	-1.391126
H	-3.533588	-1.346229	-2.878613
S	-0.466017	-3.734874	0.172062
O	0.570152	-3.381846	-0.849919
O	-1.833102	-3.430507	-0.337943
O	-0.172597	-3.182876	1.503497
H	-1.082937	-0.555294	-1.415639
C	-0.401024	-5.513491	0.322286
H	0.590941	-5.786890	0.683018

H	-1.164474	-5.818397	1.038348
H	-0.592654	-5.952299	-0.656877
S	0.140768	1.846965	-1.643536
O	-0.854127	1.745222	-2.738480
O	0.569372	0.506419	-1.154536
O	-0.344382	2.721760	-0.531508
H	1.400052	0.710650	1.462575
C	1.593044	2.647049	-2.285458
H	2.003060	2.019151	-3.077498
H	1.290217	3.615803	-2.683994
H	2.306081	2.760016	-1.464831
N	0.480932	0.811863	1.934888
H	-0.267257	0.651840	1.233827
C	0.375504	2.179275	2.483788
H	1.163500	2.320498	3.225776
H	-0.608233	2.286115	2.944351
H	0.502385	2.884398	1.663856
C	0.373463	-0.252909	2.957666
H	1.231509	-0.182490	3.628373
H	0.359366	-1.222004	2.455629
H	-0.558998	-0.108177	3.505272
S	-2.992397	0.052302	1.465129
O	-2.739632	0.853287	2.679583
O	-1.791652	-0.019534	0.579220
O	-4.170203	0.531401	0.676429
H	-3.503475	1.971780	-0.074193
C	-3.344639	-1.616503	1.968236
H	-4.211335	-1.598311	2.629395
H	-3.525687	-2.214503	1.075076
H	-2.458277	-2.000886	2.475454
N	-3.023064	2.881489	-0.253835
H	-1.990250	2.686863	-0.312572
C	-3.271564	3.750341	0.916597
H	-2.996489	3.194162	1.814512
H	-4.332176	4.003836	0.958885
H	-2.669279	4.655355	0.822741
C	-3.444843	3.449715	-1.549562
H	-3.090958	2.788771	-2.341351
H	-2.978541	4.428088	-1.675839
H	-4.531718	3.546273	-1.570029
N	2.643035	-1.639342	-0.725128
H	2.586395	-0.769463	-0.163037

C	3.689562	-2.480673	-0.109522
H	3.744604	-3.429025	-0.646193
H	4.638609	-1.946164	-0.164398
H	3.422369	-2.656852	0.931974
C	2.905317	-1.312915	-2.143246
H	2.081847	-0.693195	-2.495264
H	3.839572	-0.754088	-2.200239
H	2.960656	-2.244030	-2.710830
H	1.736030	-2.147610	-0.657449

223

224 (MA)$_1$(MSA)$_1$

N	2.298093	-0.758447	0.021260
H	2.938974	-1.486010	-0.279277
H	2.019624	-0.958436	0.980007
C	2.921434	0.571969	-0.062293
H	3.832902	0.655294	0.538320
H	3.158893	0.788840	-1.105576
H	2.200493	1.315791	0.283201
S	-0.890703	0.150662	0.070316
O	-1.060193	1.557941	-0.251222
O	-0.337175	-0.197506	1.380731
O	-0.034291	-0.572112	-1.039618
H	0.953163	-0.710991	-0.674398
C	-2.457003	-0.666628	-0.139348
H	-3.146694	-0.224836	0.580648
H	-2.801545	-0.488885	-1.157944
H	-2.324534	-1.730861	0.051848

225

226 (MA)$_1$(MSA)$_2$

N	0.591767	2.385102	-0.743496
H	-0.287947	1.824653	-0.737457
H	0.551870	3.038011	-1.522782
C	0.769870	3.072394	0.557325
H	0.840895	2.298777	1.321138
H	1.690115	3.655941	0.534347
H	-0.085800	3.719398	0.749534
S	1.877154	-0.661720	-0.071010
O	1.167415	-1.708320	-0.812128
O	1.049753	-0.071216	1.040281
O	2.429078	0.438926	-0.916216
H	1.374395	1.689230	-0.902816

C	3.281199	-1.415911	0.723332
H	2.912565	-2.205864	1.377741
H	3.923364	-1.827934	-0.055339
H	3.807629	-0.651808	1.294926
S	-2.298305	-0.208417	0.048922
O	-1.681313	0.876770	-0.737411
O	-3.681594	-0.054350	0.439142
O	-1.452494	-0.438889	1.355310
H	-0.448449	-0.343822	1.200196
C	-2.082357	-1.712589	-0.868832
H	-1.012398	-1.856083	-1.042245
H	-2.502967	-2.524270	-0.275192
H	-2.626272	-1.596483	-1.806942

227

228   (MA)₁(MSA)₃

N	0.222658	-0.091641	2.281355
H	-0.511802	-0.575161	1.729763
H	0.187079	0.910168	1.998131
C	0.002315	-0.279984	3.729836
H	-0.973876	0.125458	3.993377
H	0.030318	-1.344336	3.961176
H	0.782262	0.241725	4.284007
S	-0.513276	2.257865	-0.209346
O	0.180129	1.219952	-1.043753
O	0.124738	2.412099	1.117828
O	-1.968302	1.999240	-0.147917
H	1.140702	-0.447145	1.966973
C	-0.308324	3.809236	-1.054726
H	0.758807	4.018638	-1.130014
H	-0.758741	3.714825	-2.042820
H	-0.814686	4.577551	-0.470480
S	-2.538866	-1.531460	-0.320884
O	-3.503043	-2.603826	-0.410420
O	-1.847360	-1.328332	0.961718
O	-3.283820	-0.194139	-0.713727
H	-2.754221	0.622961	-0.473269
C	-1.306084	-1.709274	-1.585693
H	-0.701211	-2.581488	-1.336692
H	-1.824667	-1.847353	-2.534402
H	-0.686988	-0.810335	-1.593223
S	2.788659	-0.873426	-0.344442

O	1.916773	-1.843222	-0.986747
O	2.699710	-0.771101	1.119424
O	2.621653	0.550369	-0.990493
H	1.641191	0.855440	-0.996091
C	4.481963	-1.190061	-0.765500
H	4.735726	-2.157025	-0.330400
H	4.565477	-1.218876	-1.851439
H	5.098712	-0.399028	-0.340145

229

230　　(MA)$_1$(MSA)$_4$

N	-0.110801	-0.910374	2.032088
H	0.520044	-0.115989	1.888650
H	-0.035999	-1.464567	1.158647
C	0.256900	-1.712131	3.215566
H	1.289702	-2.038327	3.102612
H	0.158474	-1.099520	4.111337
H	-0.409644	-2.571708	3.281620
S	-0.010588	-1.498981	-1.662682
O	-1.246052	-0.703033	-1.896634
O	-0.027349	-2.275351	-0.410749
O	1.205585	-0.625528	-1.793601
H	-1.079530	-0.558821	2.067947
C	0.115002	-2.670021	-2.994432
H	-0.748031	-3.333827	-2.940492
H	0.124002	-2.117247	-3.933685
H	1.042113	-3.228092	-2.862454
S	0.031921	2.429005	-0.367335
O	0.454072	3.697917	0.185192
O	-0.269503	1.316034	0.528466
O	1.194625	1.965701	-1.362911
H	1.118717	0.989907	-1.559552
C	-1.344107	2.658718	-1.462939
H	-2.200764	2.940108	-0.850398
H	-1.078036	3.440389	-2.174079
H	-1.536402	1.704512	-1.955794
S	-3.693696	-0.079207	0.702852
O	-3.659789	1.295732	0.236673
O	-2.898801	-0.427456	1.883849
O	-3.372850	-1.082302	-0.474322
H	-2.516899	-0.879270	-0.973858
C	-5.371385	-0.565037	1.019358

H	-5.386050	-1.625422	1.269162
H	-5.716228	0.036972	1.860530
H	-5.961087	-0.359023	0.126760
S	3.786233	-0.270643	0.760770
O	4.982144	-0.846414	1.334563
O	2.529055	-0.345718	1.503681
O	3.583473	-0.956494	-0.659915
H	2.651303	-0.871219	-0.997724
C	4.088564	1.432993	0.351457
H	4.982399	1.473413	-0.270976
H	3.219183	1.835034	-0.171193
H	4.249683	1.960711	1.292238

231

232 (MSA)$_2$(MSA)$_1$

N	1.935662	-1.308589	0.691361
H	0.958870	-1.538729	0.906822
H	2.522032	-1.792369	1.364255
C	2.233565	-1.757971	-0.677073
H	1.506445	-1.296358	-1.349507
H	3.240771	-1.438802	-0.962563
H	2.166156	-2.845698	-0.795421
N	1.578322	1.424116	0.683739
H	1.835316	0.376527	0.754840
H	2.040610	1.940471	1.427663
C	1.912298	1.949017	-0.659117
H	1.296249	1.403449	-1.375601
H	1.676446	3.012462	-0.710936
H	2.972270	1.791181	-0.863664
S	-1.292638	-0.073954	0.008314
O	-1.027050	-1.309490	0.777176
O	-0.554035	-0.004097	-1.273485
O	-1.072252	1.166917	0.828518
H	0.523980	1.448730	0.830078
C	-3.034508	-0.072611	-0.378394
H	-3.244838	-0.957766	-0.979101
H	-3.590051	-0.102570	0.559039
H	-3.261372	0.836788	-0.934793

233

234 (MA)$_2$(MSA)$_2$

N	-0.015895	2.147765	-0.053651
H	0.856613	1.966477	0.489032

H	-0.861262	1.955282	0.525039
C	-0.040535	3.496146	-0.648694
H	0.828575	3.618113	-1.294828
H	-0.955529	3.613408	-1.229079
H	-0.013464	4.240413	0.146672
N	0.015310	-2.147625	-0.053273
H	0.031453	-1.413036	-0.773378
H	-0.858257	-1.967984	0.487971
C	0.043632	-3.495629	-0.649113
H	0.961180	-3.611572	-1.225704
H	0.013999	-4.240427	0.145662
H	-0.822627	-3.617962	-1.298997
S	2.570295	0.013201	0.176028
O	2.391552	1.269316	0.952631
O	1.717858	-0.004056	-1.045174
O	2.392888	-1.220135	0.988024
H	0.859363	-1.954197	0.526947
C	4.269693	0.007113	-0.363346
H	4.439107	0.895033	-0.972423
H	4.903396	0.022019	0.523692
H	4.441366	-0.899766	-0.943210
S	-2.570789	-0.013416	0.175988
O	-2.393225	-1.269696	0.952498
O	-1.717497	0.003719	-1.044626
O	-2.393292	1.219777	0.988215
H	-0.031667	1.413592	-0.774204
C	-4.269847	-0.006508	-0.364468
H	-4.904031	-0.021546	0.522227
H	-4.440931	0.900647	-0.944068
H	-4.439215	-0.894155	-0.973960

235

236 (MA)$_2$(MSA)$_3$

N	-0.768399	-0.611296	1.946672
H	-0.640749	0.266717	1.432693
H	-0.107333	-1.302911	1.534918
C	-0.492534	-0.423536	3.383463
H	0.528932	-0.063503	3.502494
H	-1.195218	0.302841	3.791805
H	-0.610355	-1.378569	3.894590
N	-0.579340	0.586190	-1.922658
H	0.088799	1.367938	-1.917407

H	-1.297073	0.775260	-1.181723
C	-1.219836	0.370590	-3.237990
H	-0.463218	0.068906	-3.962168
H	-1.980560	-0.400885	-3.122285
H	-1.694871	1.297618	-3.558939
S	1.957282	-2.039008	-0.185178
O	1.087130	-2.392069	0.957992
O	3.142830	-1.220325	0.231501
O	1.230906	-1.424439	-1.319555
H	-0.028992	-0.242834	-1.633008
C	2.645873	-3.567449	-0.780222
H	3.304254	-3.338848	-1.618076
H	3.200936	-4.028445	0.036656
H	1.819440	-4.204686	-1.095190
S	-3.490726	-0.066170	0.016363
O	-3.583216	-0.688552	-1.311328
O	-2.398761	0.967936	0.079926
O	-3.363851	-1.019662	1.152545
H	-1.752427	-0.907833	1.757549
C	-5.014651	0.818686	0.296604
H	-5.137179	1.551338	-0.501284
H	-5.827426	0.092289	0.280060
H	-4.956264	1.309699	1.267888
S	2.009127	2.049893	0.086402
O	1.067792	1.372449	0.981007
O	1.489181	2.441553	-1.226134
O	3.314344	1.221923	-0.060121
H	3.186695	0.174959	0.050766
C	2.627053	3.513665	0.877196
H	3.047422	3.232855	1.842242
H	3.387487	3.950821	0.230312
H	1.784694	4.195324	0.997648

237

238 $(MA)_2(MSA)_4$

N	0.063308	-0.470507	-2.138049
H	-0.769665	-0.998268	-1.796738
H	0.906407	-0.845427	-1.678157
C	0.170476	-0.569641	-3.607583
H	0.283319	-1.617039	-3.885230
H	-0.737694	-0.163793	-4.051983
H	1.036494	-0.000275	-3.944272

N	-2.395675	1.671227	1.124106
H	-2.100570	0.931259	1.779138
H	-2.506501	1.234902	0.180528
C	-3.674656	2.272407	1.551627
H	-3.556567	2.717253	2.539510
H	-3.965599	3.037267	0.832132
H	-4.427838	1.485483	1.580984
S	0.943774	2.636489	-0.148316
O	0.523395	2.265937	-1.511358
O	1.554094	1.440449	0.569596
O	-0.104573	3.257351	0.680230
H	-1.625290	2.358400	1.055588
C	2.275810	3.805826	-0.287204
H	3.077946	3.346164	-0.865672
H	1.886270	4.687028	-0.797092
H	2.612268	4.056042	0.718812
S	-3.255970	-0.898358	-1.027726
O	-3.620798	-1.059529	0.394610
O	-2.234167	-1.870921	-1.502141
O	-2.852095	0.506498	-1.343690
H	-0.023342	0.517429	-1.852561
C	-4.725359	-1.228865	-1.983452
H	-5.502546	-0.533554	-1.665899
H	-4.491062	-1.088113	-3.038685
H	-5.027180	-2.258343	-1.789838
S	-0.325606	-1.117102	2.228621
O	-1.230019	-0.241277	2.977491
O	0.975839	-1.407399	2.812528
O	-0.130796	-0.493642	0.775820
H	0.560789	0.243951	0.782986
C	-1.171865	-2.611225	1.806506
H	-1.350957	-3.130553	2.749075
H	-2.109188	-2.339452	1.314831
H	-0.526777	-3.196157	1.151687
S	3.738749	-1.167196	-0.451235
O	4.902458	-1.523415	-1.231676
O	2.407381	-1.515927	-0.958774
O	3.800514	0.399534	-0.213879
H	2.917198	0.776472	0.083143
C	3.876816	-1.838487	1.187669
H	3.900753	-2.923987	1.082968
H	4.806961	-1.473197	1.622662

H	3.006607	-1.531219	1.772732

239

240 (MA)₃(MSA)₁

N	-2.411523	-1.148501	-1.033960
H	-1.466878	-1.518990	-1.177596
H	-2.934517	-1.267933	-1.894809
C	-3.034384	-1.891280	0.066081
H	-2.395661	-1.800899	0.949168
H	-4.014466	-1.463250	0.299271
H	-3.162232	-2.960811	-0.140525
N	0.581027	2.589168	-1.078385
H	0.593779	3.246053	-1.851045
H	1.053641	1.730716	-1.375920
C	1.304772	3.124965	0.080366
H	2.344210	3.397272	-0.139766
H	0.788780	4.008798	0.468720
H	1.321099	2.356795	0.858933
N	-1.444117	1.165755	0.216102
H	-1.926441	0.433642	-0.375620
H	-0.864685	1.801678	-0.398844
C	-2.377082	1.909517	1.074455
H	-2.938635	1.213329	1.699091
H	-1.818003	2.593655	1.714435
H	-3.072009	2.480962	0.457370
S	1.250383	-0.990360	0.058315
O	0.644541	-0.267717	1.225317
O	1.810298	-0.056913	-0.944406
O	0.329615	-1.998622	-0.511985
H	-0.726098	0.632240	0.763637
C	2.633943	-1.893233	0.736511
H	2.257332	-2.586359	1.488775
H	3.112552	-2.433248	-0.080865
H	3.325281	-1.176651	1.180364

241

242 (MA)₃(MSA)₂

N	-0.080626	-1.884237	1.751796
H	-0.855642	-1.218633	1.721293
H	0.761076	-1.327724	1.892123
C	-0.268284	-2.876148	2.807629
H	-1.187191	-3.438025	2.618725
H	0.563553	-3.586308	2.801261

H	-0.338669	-2.440574	3.813280
N	0.070609	2.354549	0.271942
H	0.912872	2.519574	-0.305276
H	0.310513	1.489315	0.778506
C	-0.249483	3.452796	1.200865
H	-0.475912	4.353360	0.630335
H	-1.120105	3.162612	1.788857
H	0.601265	3.634874	1.857701
N	0.091909	-2.073882	-1.003711
H	-0.765782	-1.541461	-1.246507
H	0.055269	-2.167112	0.059828
C	0.123910	-3.381426	-1.679585
H	1.008962	-3.931903	-1.358786
H	-0.773642	-3.943279	-1.418725
H	0.160436	-3.238044	-2.759791
S	2.688530	0.420236	-0.312571
O	2.519148	1.771725	-0.901149
O	2.497956	-0.684704	-1.284744
O	1.848416	0.244747	0.910217
H	0.939337	-1.511855	-1.217669
C	4.388282	0.314431	0.219434
H	4.570346	1.108128	0.944124
H	4.545157	-0.665133	0.671456
H	5.023042	0.439891	-0.657889
S	-2.625191	0.371402	-0.370481
O	-2.049149	0.271870	0.994596
O	-2.392099	-0.840588	-1.194631
O	-2.195281	1.627910	-1.050079
H	-0.752457	2.132732	-0.338954
C	-4.394898	0.496865	-0.185868
H	-4.614099	1.377211	0.418519
H	-4.833695	0.592605	-1.179118
H	-4.750401	-0.408258	0.306824

243

244 (MA)$_3$(MSA)$_3$

N	2.858667	1.836976	-0.427026
H	3.197687	1.125635	0.257008
H	2.688603	2.740639	0.026538
C	3.761987	1.916745	-1.590874
H	3.835254	0.919328	-2.024405
H	3.352339	2.617286	-2.318688

H	4.746182	2.254089	-1.265755
N	-0.184252	-1.028599	-1.742362
H	-0.282821	-0.046760	-1.425065
H	-0.854890	-1.560331	-1.153012
C	-0.501885	-1.173335	-3.177092
H	0.172175	-0.544705	-3.759356
H	-0.372337	-2.215793	-3.468795
H	-1.536199	-0.863502	-3.324052
N	-0.633957	-0.737189	1.992379
H	-0.580347	0.294249	1.845231
H	0.295984	-1.143946	1.794942
C	-1.113025	-1.028064	3.356593
H	-2.096526	-0.574758	3.478754
H	-1.181202	-2.107131	3.495822
H	-0.417918	-0.604315	4.081390
S	-0.234017	2.526322	0.379513
O	-3.385407	0.209830	0.755664
O	0.730790	3.639840	0.285701
O	-0.403854	1.993410	1.750810
H	-1.286142	-1.128549	1.283353
C	-1.827338	3.096408	-0.161220
H	-2.120645	3.914090	0.498060
H	-1.736054	3.441214	-1.191119
H	-2.525021	2.259541	-0.078078
S	2.860925	-1.533176	0.303311
O	1.665129	-2.017100	1.032553
O	3.559133	-0.408335	0.978110
O	2.558616	-1.219330	-1.124850
H	0.793405	-1.291601	-1.521003
C	4.012107	-2.894316	0.292572
H	3.532562	-3.742285	-0.196494
H	4.904345	-2.585439	-0.252173
H	4.256137	-3.134032	1.327614
S	-3.299760	-0.777053	-0.335413
O	-2.228419	-1.807991	-0.039310
O	-3.133107	-0.212493	-1.686637
O	0.156294	1.421283	-0.579493
H	1.898669	1.526969	-0.693332
C	-4.829212	-1.698422	-0.337060
H	-4.772747	-2.460495	-1.114359
H	-4.959273	-2.155109	0.644129
H	-5.637985	-0.997091	-0.544580

245

246 (MA)₃(MSA)₄

N	-1.369710	-2.444858	0.815309
H	-2.308560	-1.997837	0.810910
H	-1.054157	-2.511002	1.796967
C	-1.340073	-3.705065	0.054562
H	-1.617342	-3.490244	-0.977280
H	-0.332644	-4.116911	0.097983
H	-2.052970	-4.405383	0.490574
N	-0.295505	0.239242	-1.996630
H	0.362591	-0.437802	-1.586097
H	-0.148508	1.133243	-1.502170
C	-0.015110	0.400000	-3.435377
H	-0.143905	-0.561811	-3.931208
H	-0.708713	1.128654	-3.854861
H	1.011692	0.746066	-3.551698
N	-1.441653	2.528568	0.977030
H	-1.073178	2.005001	1.811355
H	-2.136850	1.928387	0.496619
C	-2.031425	3.823865	1.359536
H	-1.267047	4.438111	1.835636
H	-2.412771	4.327957	0.471263
H	-2.847653	3.650699	2.060696
S	0.228926	-0.103496	2.448711
O	2.380142	2.561011	0.769984
O	-0.286664	-1.351166	3.055987
O	-0.384127	1.127019	3.019230
H	-0.641612	2.648957	0.333376
C	1.962761	-0.023812	2.828204
H	2.054201	0.044819	3.912646
H	2.426894	-0.934968	2.452482
H	2.372143	0.860097	2.337379
S	-3.665594	-0.277146	-0.705568
O	-3.339047	1.164760	-0.566939
O	-3.763471	-1.000597	0.582945
O	-2.738285	-0.964335	-1.655505
H	-1.258881	-0.122854	-1.836638
C	-5.284113	-0.349962	-1.449267
H	-5.247666	0.175772	-2.403379
H	-5.541600	-1.399141	-1.594371
H	-5.988593	0.129352	-0.769336
S	2.045381	2.430221	-0.645360

O	0.608276	2.706837	-0.969645
O	2.460167	1.124940	-1.268495
O	0.109243	-0.111286	0.949264
H	-0.721743	-1.729522	0.445942
C	2.969298	3.666251	-1.539677
H	2.740806	3.574447	-2.601364
H	2.671041	4.644093	-1.161073
H	4.029084	3.490208	-1.354336
S	2.373104	-2.264424	-0.475033
O	1.367606	-1.964989	-1.504433
O	1.916405	-2.950153	0.722080
O	3.159978	-0.971371	-0.091589
H	2.818179	-0.094883	-0.528514
C	3.649927	-3.245442	-1.229496
H	3.204441	-4.200458	-1.509436
H	4.021890	-2.715710	-2.106043
H	4.441089	-3.390878	-0.493959

247

248   (MA)$_4$(MSA)$_1$

N	0.904431	0.277943	-2.413754
H	1.004801	0.831315	-3.258021
H	-0.095254	0.199414	-2.203337
C	1.480776	-1.059381	-2.588461
H	2.570615	-0.987700	-2.669151
H	1.221995	-1.655761	-1.709939
H	1.102707	-1.586418	-3.473735
N	1.716946	-1.233135	1.632375
H	0.873978	-1.612243	1.188785
H	1.522944	-1.173759	2.626603
C	2.865362	-2.098516	1.367879
H	3.016008	-2.167676	0.286534
H	3.770736	-1.666158	1.805171
H	2.750020	-3.119425	1.755131
N	-0.669272	2.669210	1.084458
H	-0.658910	3.298313	1.880136
H	-1.149836	1.809255	1.365899
C	-1.361751	3.274101	-0.057717
H	-2.369014	3.638413	0.182749
H	-0.776508	4.113291	-0.447515
H	-1.458049	2.513003	-0.835767
N	1.560703	1.188938	0.179503

H	1.609370	0.309883	0.766427
H	0.770333	1.789419	0.544975
C	2.841253	1.907816	0.231967
H	3.637506	1.270336	-0.156783
H	2.783422	2.816416	-0.369905
H	3.071174	2.176481	1.264484
S	-1.586396	-0.827850	0.101052
O	-1.690249	0.120467	-1.037798
O	-1.446748	-0.144566	1.412164
O	-0.546147	-1.867964	-0.110056
H	1.331374	0.905068	-0.813351
C	-3.147846	-1.698579	0.156655
H	-3.940004	-0.966764	0.317593
H	-3.286132	-2.210766	-0.795837
H	-3.112205	-2.415164	0.977522

249

250 $(MA)_4(MSA)_2$

N	0.002840	-1.864247	1.835058
H	-0.817525	-1.260977	1.762733
H	0.822704	-1.260305	1.762068
C	0.003757	-2.629935	3.078548
H	-0.879191	-3.274483	3.113006
H	0.887575	-3.273324	3.112331
H	0.003686	-2.004979	3.981971
N	-0.001006	1.866961	1.834254
H	0.820033	1.264532	1.762791
H	-0.820269	1.262160	1.761891
C	-0.002946	2.634830	3.076334
H	0.878978	3.280853	3.109556
H	-0.887776	3.276881	3.109113
H	-0.001798	2.011579	3.980945
N	0.001607	-2.523835	-0.846144
H	-0.848224	-2.005291	-1.145610
H	0.001613	-2.463110	0.218681
C	-0.005259	-3.913126	-1.331562
H	-0.006905	-3.924874	-2.421905
H	0.884545	-4.426811	-0.965962
H	-0.898626	-4.418780	-0.963478
N	-0.002390	2.522703	-0.847965
H	0.847407	2.003603	-1.146746
H	-0.002308	2.463247	0.216981

C	0.004805	3.911353	-1.335193
H	-0.884908	4.425770	-0.970402
H	0.898248	4.417306	-0.967703
H	0.006577	3.921610	-2.425552
S	-2.738417	0.001099	-0.516828
O	-2.405399	-1.231986	-1.276226
O	-2.420247	1.245241	-1.264506
O	-2.179122	-0.002155	0.859747
H	-0.857407	2.012040	-1.145934
C	-4.514630	-0.010296	-0.338807
H	-4.956017	-0.007767	-1.335438
H	-4.795827	-0.911839	0.205842
H	-4.806351	0.882341	0.214922
S	2.738135	-0.002156	-0.516989
O	2.181030	0.004199	0.860429
O	2.402672	1.228519	-1.279222
O	2.420054	-1.248592	-1.260945
H	0.856832	-2.013488	-1.144258
C	4.514600	0.011498	-0.341734
H	4.808055	-0.879377	0.213911
H	4.954536	0.006821	-1.338999
H	4.795636	0.914749	0.200158

251

252 $(MA)_4(MSA)_3$

N	4.332279	-2.160901	0.355586
H	5.284982	-2.467717	0.190338
H	3.699098	-2.825998	-0.093040
C	4.038500	-2.114483	1.794135
H	4.603674	-1.303149	2.262155
H	2.971013	-1.917691	1.922631
H	4.271791	-3.051003	2.315230
N	3.125675	0.088612	-0.807830
H	3.699218	-0.699064	-0.386837
H	2.983194	0.842038	-0.108345
C	3.730107	0.632605	-2.038354
H	4.733770	0.997922	-1.817704
H	3.784565	-0.155234	-2.790394
H	3.109188	1.455115	-2.394527
N	-1.094547	0.993375	-1.710341
H	-1.865318	1.216545	-1.042962
H	-0.628544	0.126422	-1.383845

C	-1.648211	0.781303	-3.062274
H	-2.401901	-0.003286	-2.994546
H	-2.103546	1.706774	-3.415068
H	-0.847448	0.479497	-3.737824
N	-0.744942	0.051274	2.084044
H	-0.200523	-0.738680	1.678761
H	-1.754064	-0.168454	1.919577
C	-0.450676	0.207400	3.521289
H	0.606090	0.443585	3.647498
H	-1.057740	1.017454	3.924925
H	-0.685800	-0.723124	4.037742
S	1.222225	2.838917	0.218535
O	1.190071	2.616674	-1.255230
O	2.408046	2.212366	0.857217
O	-0.060306	2.455546	0.860658
H	-0.504615	0.922227	1.573599
C	1.390296	4.596205	0.465471
H	0.523524	5.085479	0.021197
H	1.431866	4.784168	1.538393
H	2.310876	4.921942	-0.018964
S	-3.729269	-0.236001	0.142483
O	-3.258829	-1.149625	-0.921943
O	-3.336968	1.178539	-0.120659
O	-3.337002	-0.673768	1.510819
H	-0.370765	1.730300	-1.671854
C	-5.512701	-0.272979	0.119898
H	-5.847238	0.043709	-0.868207
H	-5.831587	-1.294832	0.326128
H	-5.877544	0.408953	0.887978
S	0.657450	-2.418800	-0.370480
O	0.601596	-2.153463	1.093467
O	1.815841	-3.233016	-0.773070
O	0.596075	-1.121876	-1.139362
H	2.185259	-0.305540	-1.004442
C	-0.817954	-3.310252	-0.805386
H	-0.835962	-4.223757	-0.210120
H	-1.688069	-2.679990	-0.601971
H	-0.757562	-3.546809	-1.868194

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254 (MA)$_4$(MSA)$_4$

S	-1.999725	1.999725	-1.999725

O	-0.868279	1.552909	-2.852771
O	-1.552909	2.852771	-0.868279
C	-3.029223	3.029223	-3.029223
H	-3.883900	3.356007	-2.436684
H	-2.436684	3.883900	-3.356007
H	-3.356007	2.436684	-3.883900
O	-2.852771	0.868279	-1.552909
H	-1.532658	2.075110	0.703473
N	-1.643150	1.643150	1.643150
H	-2.075110	0.703473	1.532658
H	-0.703473	1.532658	2.075110
C	-2.495068	2.495068	2.495068
H	-2.018733	3.467830	2.615615
H	-3.467830	2.615615	2.018733
H	-2.615615	2.018733	3.467830
S	1.999725	-1.999725	-1.999725
O	2.852771	-0.868279	-1.552909
O	0.868279	-1.552909	-2.852771
C	3.029223	-3.029223	-3.029223
H	2.436684	-3.883900	-3.356007
H	3.356007	-2.436684	-3.883900
H	3.883900	-3.356007	-2.436684
O	1.552909	-2.852771	-0.868279
H	-0.703473	-1.532658	-2.075110
N	-1.643150	-1.643150	-1.643150
H	-1.532658	-2.075110	-0.703473
H	-2.075110	-0.703473	-1.532658
C	-2.495068	-2.495068	-2.495068
H	-2.615615	-2.018733	-3.467830
H	-2.018733	-3.467830	-2.615615
H	-3.467830	-2.615615	-2.018733
S	-1.999725	-1.999725	1.999725
O	-0.868279	-1.552909	2.852771
O	-1.552909	-2.852771	0.868279
C	-3.029223	-3.029223	3.029223
H	-3.883900	-3.356007	2.436684
H	-2.436684	-3.883900	3.356007
H	-3.356007	-2.436684	3.883900
O	-2.852771	-0.868279	1.552909
H	2.075110	0.703473	-1.532658
N	1.643150	1.643150	-1.643150
H	0.703473	1.532658	-2.075110

H	1.532658	2.075110	-0.703473
C	2.495068	2.495068	-2.495068
H	3.467830	2.615615	-2.018733
H	2.615615	2.018733	-3.467830
H	2.018733	3.467830	-2.615615
S	1.999725	1.999725	1.999725
O	1.552909	2.852771	0.868279
O	2.852771	0.868279	1.552909
C	3.029223	3.029223	3.029223
H	3.356007	2.436684	3.883900
H	3.883900	3.356007	2.436684
H	2.436684	3.883900	3.356007
O	0.868279	1.552909	2.852771
H	1.532658	-2.075110	0.703473
N	1.643150	-1.643150	1.643150
H	2.075110	-0.703473	1.532658
H	0.703473	-1.532658	2.075110
C	2.495068	-2.495068	2.495068
H	2.018733	-3.467830	2.615615
H	3.467830	-2.615615	2.018733
H	2.615615	-2.018733	3.467830

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