Supplementary for

Atmospheric implication of synergy in methanesulfonic acid–base trimers. A theoretical investigation

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Contents (31 pages, 5 figures, and 12 tables)

Conformation search

The global minimum (here it refers to energy minimum) sampling technique is an efficient and convenient tool for searching for atmospheric clusters[1-3]. In this study, this method was used to locate global minima for MSA-based clusters (MSA-X and MSA-X-Y); a detailed flow chart is shown in Fig. S1. Herein, the process of calculation is described as follows: to identify the lowest Gibbs free energy structure of the clusters, firstly the initial 1000 structures of clusters were randomly generated and optimized by the CHARMM36 force field in the ABCluster program. Then, up to 100 conformations with relatively low energies were further optimized by the semiempirical PM6-DH$^+$ method in MOPAC2016. Moreover, up to 30 conformations with relatively low energies were chosen for re-optimization using M06-2X/ 6-31+G(d). Finally, approximately 10 lowest-energy resulting structures were optimized at four different DFT/aug-cc-pVTZ level. Theoretical calculations and kinetics simulations were performed using the ABCluster [4, 5], MOPAC [6] and GAUSSIAN 09 [7] programs. The molecular structure of the precursor was described using the CHARMM36 force field [8] in the ABCluster program.

Structure optimization

For four atmospheric precursors including methane sulfonic acid (MSA), ammonia (A), methylamine (M), and dimethylamine (D) have been optimized by B3LYP-D3, M06-2X, ωB97X-D, and PW91PW91 combined with same basis set aug-cc-pVTZ levels (the corresponding structural parameter is shown in Fig. S2). The benchmark results showed that the optimized structural parameters are close to each other by four functional methods. Compared with the other three methods (B3LYP-D3, M06-2X, and ωB97X-D), the O/N−H bond lengths are slightly longer for five optimized molecules, and H−N−H/C−N−H/C−N−C/S−O−H bond angles in four molecules are slightly smaller by the PW91PW91 method. Herein, it should be pointed out that the configuration of MA-A, and A-A is always unsuccessful with M06-2X method.

Thermochemical properties calculation

Herein, four density functional theory (DFT) levels (B3LYP-D3, M06-2X, PW91PW91, and ωB97X-D) were utilized because they have previously been identified to perform well in describing dispersion interaction[9] of atmospheric relevant clusters.[10-13] Structural optimization, frequency analysis, and thermodynamic calculation for all structures were performed by four DFT methods in conjunction with aug-cc-pVTZ basis set for C, H, N and O atoms (aug-cc-pV(T+d)Z for S atom). Herein, two additional options, i.e., "opt = very tight" and "integral = ultrafine", were used to obtain good frequencies and thermochemical corrections to the electronic energies in all optimization.[14, 15] One note is that all of the values of thermochemical properties are the average value based on B3LYP-D3, M06-2X, PW91PW91, and ωB97X-D functional methods. The benchmark shown that the values for thermochemical properties of title dimers are accurate compared with the literature data in Table S6, which further confirmed that the calculated methods chosen in this work is reasonable. All calculation for clusters has been performed using Gaussian 09 program. [16]

AIM, NCI and CT analysis

Atoms in Molecules (AIM) theory is widely used to characterize noncovalent interactions.[17-20] Topological properties, electron density $\rho(r)$ and Laplacian $\nabla^2\rho(r)$ at the critical points (CPs), are very helpful to understand the nature of hydrogen bonding. As an extension of AIM theory, the noncovalent interaction (NCI) index by Yang and coworkers[21] is also a very practical tool to visualize the intermolecular interaction. The $\Delta q(H)$ (change atomic charge q at the H atom) is obtained by natural bond orbit (NBO) module in Gaussian 09. All wavefunctions of relevant structures were obtained at B3LYP-D3/aug-cc-pVTZ level. AIM and NCI analyses have been performed using Multiwfn[22] and VMD programs[23].

Evaporation rate

In addition, as an important indicator to measure the stability of clusters, the low evaporation rate is very favorable for clusters formation and growth. Herein, the evaporation rate has been carried out through ACDC simulations in the MATLAB-

R2013a.[24-26] Evaporation rate (γ) is obtained using the values of Gibbs free energy of formation (ΔG) for clusters as the following Eqs:

$$i + j \underset{\text{Evaporation}}{\overset{\text{Collision}}{\rightleftharpoons}} i-j \quad (1)$$

$$\gamma_{i-j\rightarrow i} C_{i-j} = \beta_{i\text{-}j} C_i C_j \quad (2)$$

$$\beta_{i\text{-}j} = \left(\frac{3}{4\pi}\right)^{1/6} \left[6k_B T\left(\frac{1}{m_i}+\frac{1}{m_j}\right)\right]^{1/2} \left(V_i^{1/3}+V_j^{1/3}\right)^2 \quad (3)$$

$$\gamma_{i-j\rightarrow i} = \beta_{i-j} \times \frac{c_i^e c_j^e}{c_{i-j}^e} = \beta_{i-j} \times c_{ref} \times \exp\left(\frac{\Delta G_{i-j} - \Delta G_i - \Delta G_j}{k_b T}\right) \quad (4)$$

where $\beta_{i\text{-}j}$ is the collision coefficient between cluster i and j; c_i^e, c_j^e, and c_{i-j}^e are the equilibrium concentration of cluster i, j, and i-j, respectively; $\Delta G_{i\text{-}j}$, ΔG_i, and ΔG_j are the Gibbs free energy of the formation of i-j clusters, i, and j monomers, respectively, the value of ΔG_i and ΔG_j equals to zero here; k_b and T are the Boltzmann's constant and temperature, respectively; c_{ref} is the monomer concentration of the reference vapor corresponding to the pressure of 1 atm at which the Gibbs free energies were determined.

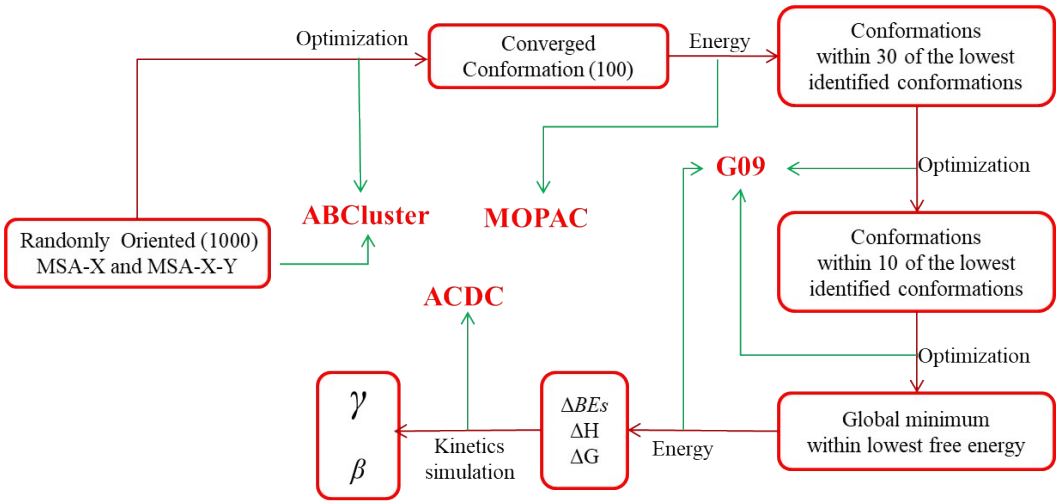
Atmospheric relevance

These complicated reactions, e.g., can be expressed succinctly as following: MSA + X ↔ MSA-X and MSA-X + Y ↔ MSA-X-Y between separate species as monomers and dimers. Under thermodynamic equilibrium conditions, the law of conservation of mass dominates complex concentration relationship involving MSA-based clusters as the following Eqs. 3 and 4:

$$[\text{MSA-X}] = [\text{MSA}] \times [\text{X}] \times e^{-\frac{\Delta G}{RT}} \quad (5)$$

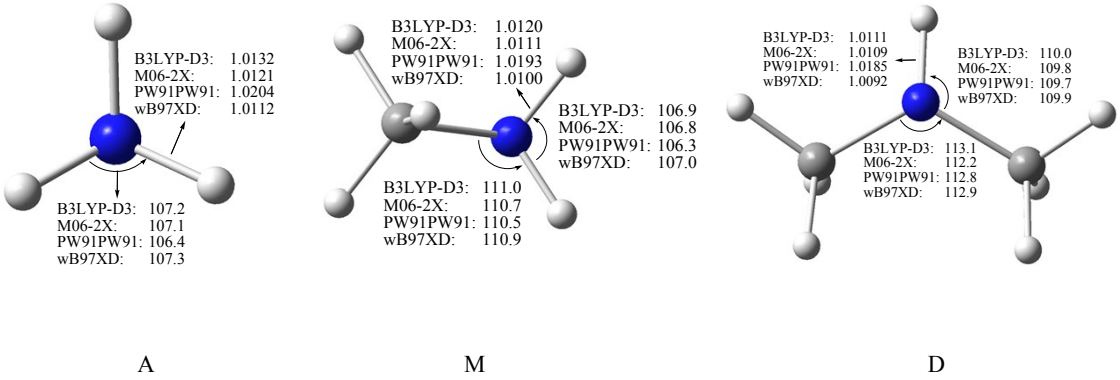
$$[\text{MSA-X-Y}]/[\text{MSA-X}] = [\text{Y}] \times e^{-\frac{\Delta G}{RT}} \quad (6)$$

where R is the molar gas constant; T is the temperature in K; ΔG is the free energies of formation of clusters. For example, the atmospheric concentration of MSA-X clusters is dependent on both the ΔG for MSA-X clusters and the vapor concentration for monomers (MSA and X).

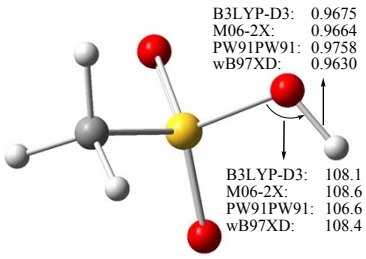


115

116 **Fig. S1.** Flow-chart for the multistep global minimum sampling method.



A M D

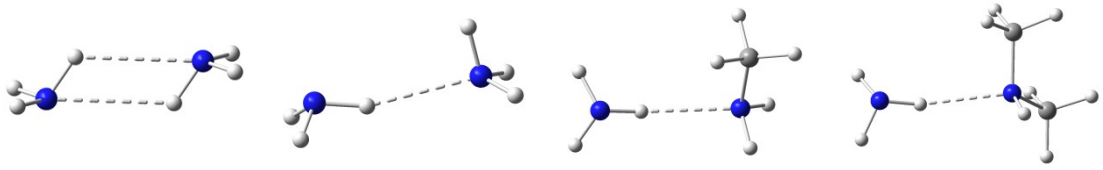


MSA

117 **Fig. S2** The optimized structures of dimers at the DFT/aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur)

118 level (angles in degrees; lengths in Å). The red, yellow, blue, gray, and white balls stand for O, S,

119 N, C, and H atoms, respectively.



A-A A-A-h A-M A-D

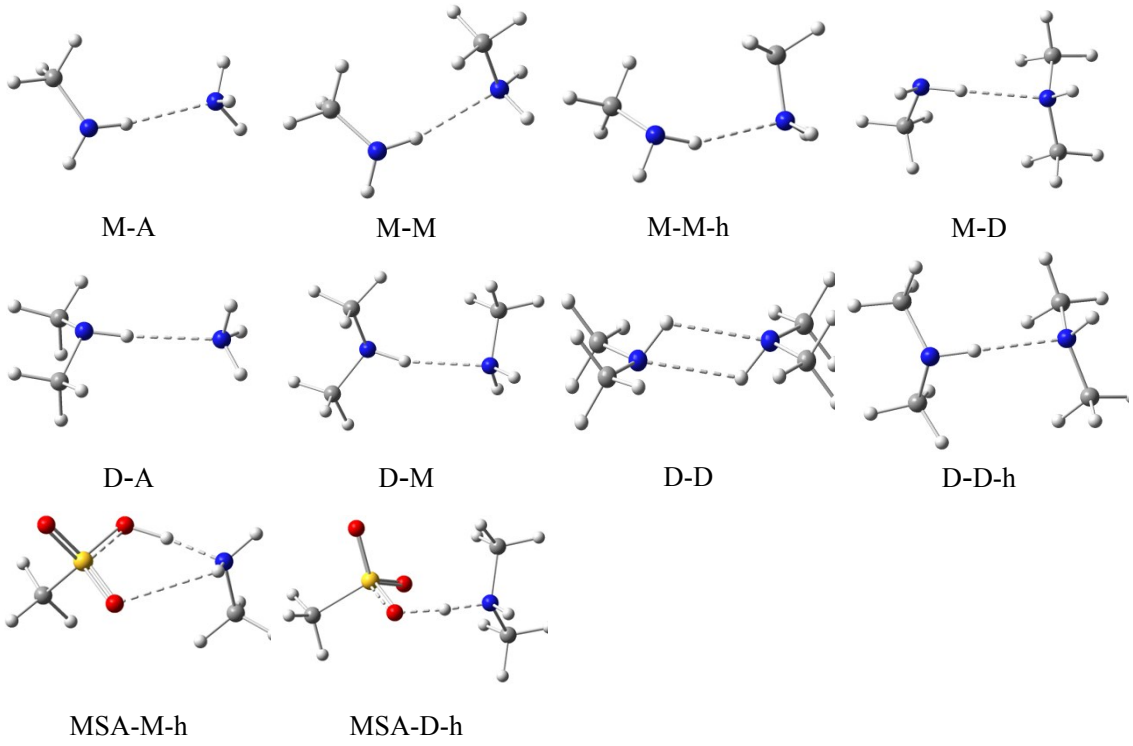


Fig. S3 The optimized structures of the homodimers and other heterodimers with high energy (h) at the B3LYP-D3/aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur) level. The red, yellow, blue, gray, and white balls stand for O, S, N, C, and H atoms, respectively.

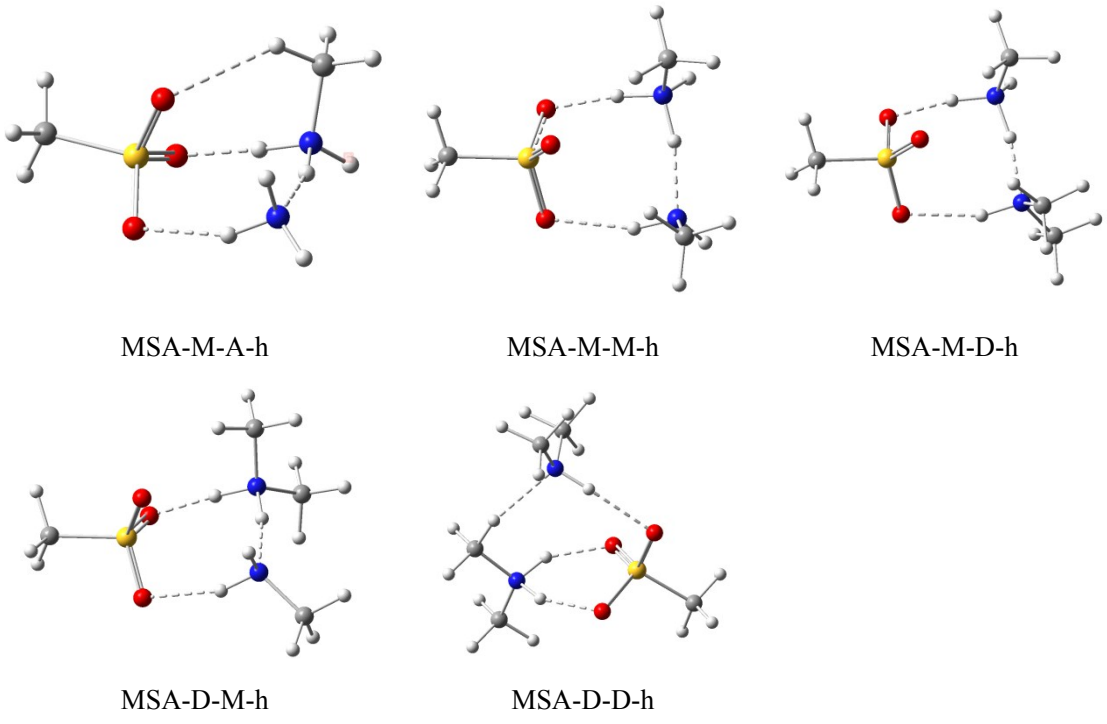
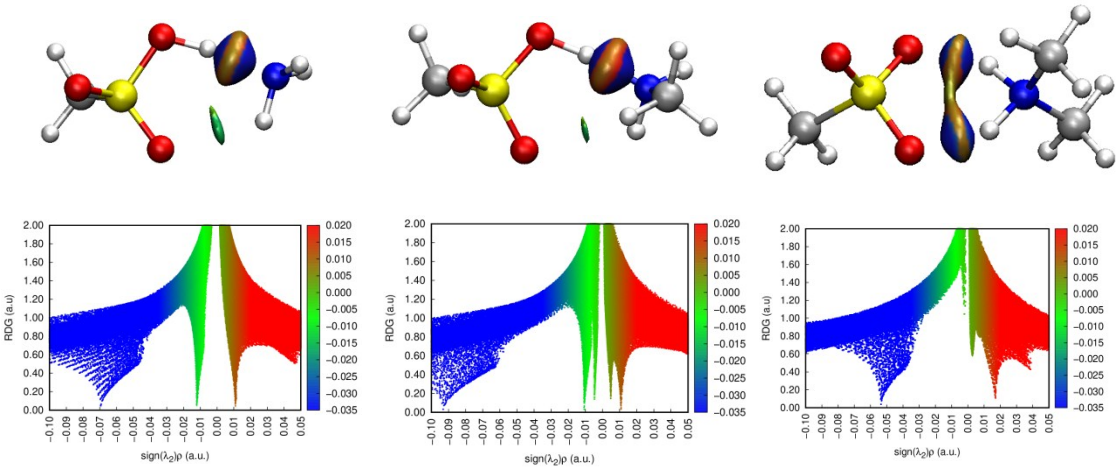
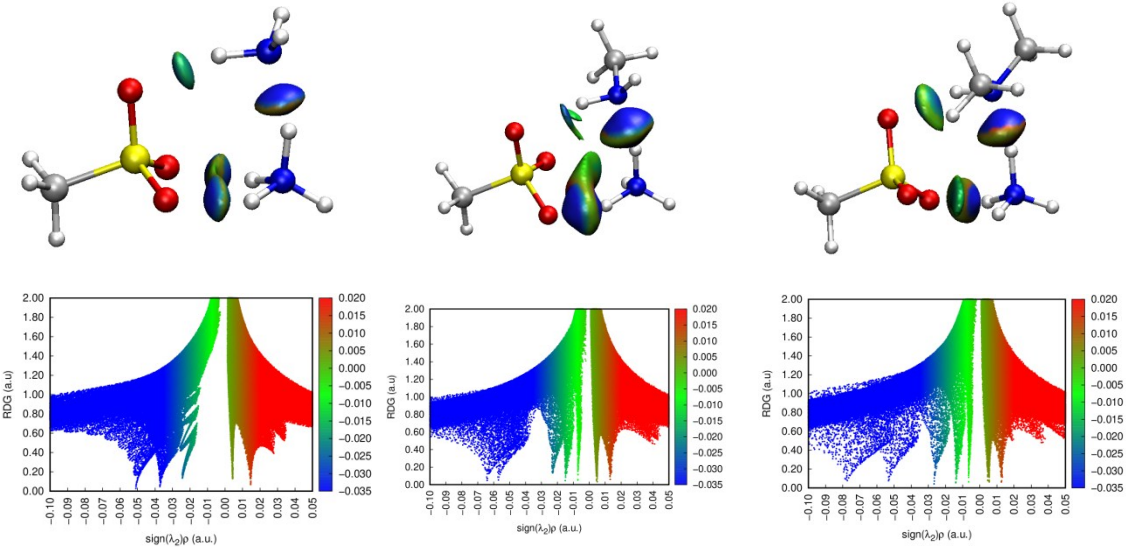


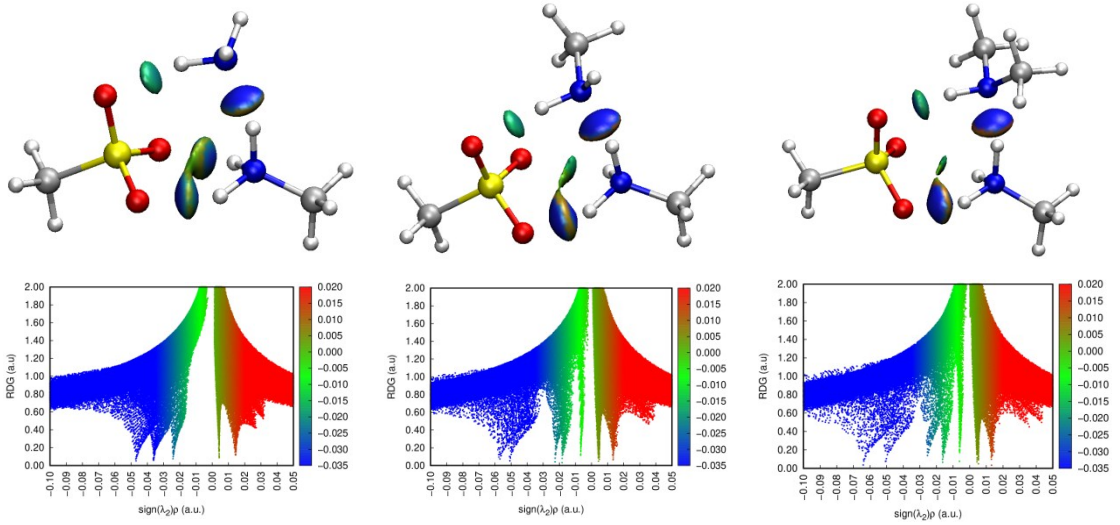
Fig. S4. The optimized structures of the heterotrimers with high energy (h) at the B3LYP-D3 /aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur) level. The red, yellow, blue, gray, and white balls stand for O, S, N, C, and H atoms, respectively.



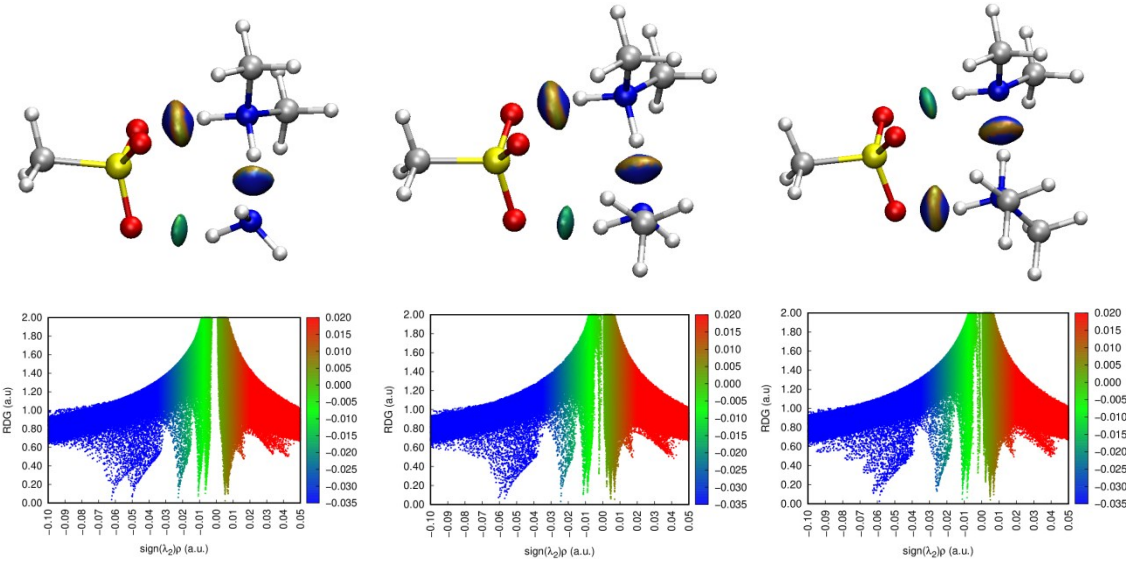
MSA-A MSA-M MSA-D



MSA-A-A MSA-A-M MSA-A-D



MSA-M-A MSA-M-M MSA-M-D



MSA-D-A MSA-D-M MSA-D-D

Fig. S5. Noncovalent interactions(NCI): the electron density ($sign(\lambda_2)\rho$) as a function of the reduced density gradient (RDG) and the visualized weak intermolecular interactions of the global minima calculated at the B3LYP/aug-cc-pVTZ level. The upper is the RDG plot, and the lower is the scatter plot (all reduced gradient isosurface plots in Fig. S4 are obtained at s = 0.03 a.u.).

Table S1. Selected optimized geometric parameters in dimers at the B3LYP-D3/aug-cc-pVTZ level (aug-cc-pV(T+d)Z for sulfur; angles in degrees; length in Å).

Dimer	N–H···N		
	R [a]	ΔR [b]	θ [c]
A-A	2.263	0.005	161.3
A-M	2.213	0.006	157.0
A-D	2.196	0.007	161.3
M-A	2.254	0.004	163.8
M-M	2.214	0.005	156.3
M-D	2.197	0.005	159.5
D-A	2.223	0.004	174.2
D-M	2.181	0.005	160.9
D-D	2.172	0.005	163.8

[a] Inter-molecular hydrogen bond distance.

[b] $\Delta R = R_{\mathrm{O/N-H}}(\mathrm{dimer}) - R_{\mathrm{O/N-H}}(\mathrm{monomer})$

[c] Inter-molecular hydrogen bond angle.

Table S2. Calculated binding energy (*BE*), enthalpy of formation ($^{\Delta H^{\theta}_{298K}}$) and Gibbs free energy of formation ($^{\Delta G^{\theta}_{298K}}$) for the dimers and hetero-trimers at the B3LYP-D3/aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur) level under 298 K (in kJ mol^{-1}).

Types	Complexes	*BEs* [a]	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}
Dimers	MSA-A	–56.39	–58.94	–19.06
	MSA-M	–69.38	–70.35	–29.98
	MSA-D	–81.67	–82.38	–38.84
	A-A	–7.54	–7.48	16.70
	A-M	–10.06	–9.94	19.20
	A-D	–11.01	–10.41	17.07
	M-A	–10.06	–9.94	19.20
	M-M	–12.60	–11.39	20.08
	M-D	–14.17	–12.51	18.30
	D-A	–11.00	–9.34	12.98
	D-M	–14.64	–12.74	17.65
	D-D	–16.92	–17.16	23.98
Trimers	MSA-A-A	–99.38	–105.54	–21.00
	MSA-A-M	–109.82	–114.77	–24.91
	MSA-A-D	–115.63	–119.42	–30.02
	MSA-M-A	–121.44	–125.33	–39.64
	MSA-M-M	–131.22	–133.46	–44.55
	MSA-M-D	–135.96	–137.13	–48.16
	MSA-D-A	–136.85	–139.65	–52.33
	MSA-D-M	–147.43	–148.79	–56.58
	MSA-D-D	–152.53	–152.72	–60.62

[a] *BEs* corrected with ZPVE.

Table S3. Calculated binding energy (*BE*), enthalpy of formation (ΔH^{θ}_{298K}) and Gibbs free energy of formation (ΔG^{θ}_{298K}) for the dimers and hetero-trimers at the M06-2X/aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur) level under 298 K (in kJ mol^{-1}).

Types	Complexes	*BEs* [a]	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}
Dimers	MSA-A	–57.72	–60.41	–19.94
	MSA-M	–70.98	–72.30	–29.63
	MSA-D	–76.29	–77.12	–31.65
	A-A[b]	–	–	–
	A-M	–9.37	–9.38	20.69
	A-D	–12.20	–12.37	20.72
	M-A[b]	–	–	–
	M-M	–11.04	–10.56	25.13
	M-D	–12.19	–10.78	22.36
	D-A	–12.12	–12.32	20.80
	D-M	–12.98	–11.40	21.93
	D-D	–13.44	–11.19	18.74
Trimers	MSA-A-A	–96.31	–102.92	–15.28
	MSA-A-M	–106.24	–111.08	–21.23
	MSA-A-D	–110.48	–113.95	–25.46
	MSA-M-A	–113.60	–119.40	–27.64

	MSA-M-M	–125.69	–128.40	–36.70
	MSA-M-D	–127.15	–128.00	–39.68
	MSA-D-A	–130.60	–133.36	–45.29
	MSA-D-M	–137.91	–138.68	–49.25
	MSA-D-D	–141.23	–140.91	–51.04

[a] *BEs* corrected with ZPVE.

[b] Optimization of the related structures are unsuccessful at the M06-2X/ aug-cc-pVTZ.

Table S4. Calculated binding energy (*BE*), enthalpy of formation (ΔH^{θ}_{298K}) and Gibbs free energy of formation (ΔG^{θ}_{298K}) for the dimers and hetero-trimers at the PW91PW91/aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur) level under 298 K (in kJ mol^{-1}).

Types	Complexes	*BEs* [a]	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}
Dimers	MSA-A	–57.51	–60.26	–19.48
	MSA-M	–69.93	–70.99	–29.50
	MSA-D	–74.52	–75.42	–30.14
	A-A	–8.19	–8.27	16.46
	A-M	–9.73	–9.48	18.44
	A-D	–9.94	–9.28	17.56
	M-A	–9.73	–9.48	18.44
	M-M	–11.25	–9.57	17.49
	M-D	–11.66	–9.91	20.35
	D-A	–11.10	–9.65	14.99
	D-M	–13.01	–10.87	16.80
	D-D	–13.25	–10.67	15.89
Trimers	MSA-A-A	–97.62	–106.19	–14.32
	MSA-A-M	–105.76	–110.64	–22.04
	MSA-A-D	–123.90	–126.90	–38.94
	MSA-M-A	–114.93	–118.91	–33.72
	MSA-M-M	–121.34	–123.49	–35.48
	MSA-M-D	–123.57	–124.55	–38.64
	MSA-D-A	–123.85	–126.88	–38.77
	MSA-D-M	–130.26	–131.46	–40.22
	MSA-D-D	–132.02	–132.15	–40.52

[a] *BEs* corrected with ZPVE.

Table S5. Calculated binding energy (*BE*), enthalpy of formation (ΔH^{θ}_{298K}) and Gibbs free energy of formation (ΔG^{θ}_{298K}) for the dimers and hetero-trimers at the ωB97X-D/aug-cc-pVTZ (aug-cc-pV(T+d)Z for sulfur) level under 298 K (in kJ mol^{-1}).

Types	Complexes	*BEs* [a]	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}

Dimers	MSA-A	–54.33	–56.74	–17.22
	MSA-M	–65.74	–66.69	–25.18
	MSA-D	–76.54	–77.18	–33.48
	A-A	–7.25	–7.37	17.90
	A-M	–10.26	–10.16	19.09
	A-D	–12.12	–12.25	20.51
	M-A	–10.26	–10.16	19.09
	M-M	–12.73	–11.35	18.54
	M-D	–14.38	–12.91	19.73
	D-A	–10.89	–9.28	13.88
	D-M	–14.75	–13.24	20.11
	D-D	–16.09	–13.96	16.97
Trimers	MSA-A-A	–94.65	–102.87	–12.00
	MSA-A-M	–103.95	–108.80	–19.17
	MSA-A-D	–107.90	–112.08	–20.96
	MSA-M-A	–116.59	–122.59	–30.00
	MSA-M-M	–125.42	–127.59	–38.13
	MSA-M-D	–129.36	–130.54	–40.45
	MSA-D-A	–131.30	–134.01	–46.61
	MSA-D-M	–141.23	–142.46	–50.67
	MSA-D-D	–145.61	–145.82	–53.48

[a] *BEs* corrected with ZPVE.

Table S6. Comparison of various computational approaches for calculating *BEs*, ΔH^{θ}_{298K} and ΔG^{θ}_{298K} (in kJ·mol^{-1}).

Reactions	Our work [a]			Others methods		
	BEs	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}	*BEs*	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}
MSA-A	–56.49	–59.09	–18.93	–61.45 [b]		–15.47 [b]
				–61.86 [b]		–18.39 [b]
				–65.63 [b]		
MSA-M	–69.01	–70.08	–28.57	–75.87 [c]		
MSA-D	–77.26	–78.03	–33.53			–31.02 [d]
						–36.53 [d]
						–38.83 [e]
						–34.23 [d]
						–35.82 [d]

[a] *BEs*, ΔH^{θ}_{298K}, and ΔG^{θ}_{298K} are mean calculated values by four functional methods in our work.

[b] see reference [27]; [c] see reference [28]; [d] see reference [29]; [e] see reference [30]

Table S7. Calculated binding energy (*BEs*), enthalpy of formation (ΔH^{θ}_{298K}), and Gibbs free energy of formation (ΔG^{θ}_{298K}) at 298 K for MSA-free dimers (in kJ·mol^{-1}).[a]

	Complexes	*BEs* [b]	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}
Dimers	A-A[c]	–7.66	–7.71	17.02
	A-M	–9.86	–9.74	19.36
	A-D	–11.32	–11.08	18.97
	M-A[c]	–10.02	–9.86	18.91
	M-M	–11.91	–10.72	20.31
	M-D	–13.10	–11.53	20.19
	D-A	–11.28	–10.15	15.66
	D-M	–13.85	–12.06	19.12
	D-D	–14.93	–13.25	18.90

[a] The results are the mean of which were obtained by four DFT level; energies are in kJ·mol^{-1}.

[b] *BEs* corrected with ZPVE.

[c] These thermodynamic values of A-A and MA-A dimers are the average of which were obtained by three DFT level (B3LYP-D3, PW91PW91 and wB97X-D).

Table S8 Calculated binding energy (*BEs*), enthalpy of formation (ΔH^{θ}_{298K}), and Gibbs free energy of formation (ΔG^{θ}_{298K}) at 298 K for MSA-based clusters [a].

Complexes	*BEs* [b]	ΔH^{θ}_{298K}	ΔG^{θ}_{298K}
MSA-A	–56.49	–59.09	–18.93
MSA-M	–69.01	–70.08	–28.57
MSA-D	–77.26	–78.03	–33.53
MSA-A-A	–96.99	–104.38	–15.65
MSA-A-M	–106.44	–111.32	–21.84
MSA-A-D	–114.48	–118.09	–28.85
MSA-M-A	–116.64	–121.56	–32.75
MSA-M-M	–125.92	–128.24	–38.72
MSA-M-D	–129.01	–130.06	–41.73
MSA-D-A	–130.65	–133.48	–45.75
MSA-D-M	–139.21	–140.35	–49.18
MSA-D-D	–142.85	–142.90	–51.42

[a] The results are the mean of which were obtained by four DFT level; energies are in kJ·mol^{-1}.

[b] *BEs* corrected with ZPVE.

Table S9. The evaporation rate (in molecules·s^{-1}) of dimers and trimers under 298.15 K and 1atm.

Complexes	γ_{MSA}	γ_{M}	γ_{N}	γ_{Total}
MSA-A				6.77×10^{6}
MSA-M				1.26×10^{5}
MSA-D				1.66×10^{4}
MSA-A-A	9.41×10^{3}	5.62×10^{10}	5.62×10^{10}	1.12×10^{11}
MSA-A-M	7.50×10^{2}	2.38×10^{11}	4.18×10^{9}	2.42×10^{11}

MSA-A-D	5.16×10^{1}	1.08×10^{11}	2.37×10^{8}	1.08×10^{11}
MSA-M-A	1.09×10^{1}	5.08×10^{7}	2.89×10^{9}	2.94×10^{9}
MSA-M-M	5.56×10^{-1}	2.34×10^{8}	2.34×10^{8}	4.67×10^{8}
MSA-M-D	1.74×10^{-1}	5.27×10^{8}	6.60×10^{7}	5.93×10^{8}
MSA-D-A	2.13×10^{-1}	2.57×10^{5}	1.17×10^{8}	1.17×10^{8}
MSA-D-M	1.32×10^{-2}	3.26×10^{6}	2.61×10^{7}	2.94×10^{7}
MSA-D-D	5.94×10^{-3}	1.01×10^{7}	1.01×10^{7}	2.01×10^{7}

Table S10. Calculated Gibbs free energies of formation (in kJ·mol^{-1}) at different temperatures (in K) and heights (in km) in the Earth atmosphere when the atmospheric pressure is equal to 1 atm. [a]

Complexes	0 Km 298.15 K 1 atm	2 Km 275.21 K 1 atm	4 Km 262.23 K 1 atm	6 Km 249.49 K 1 atm	8 Km 236.27 K 1 atm	10 Km 223.29 K 1 atm	12 Km 216.69 K 1 atm
MSA-A	–19.06	–22.13	–23.87	–25.61	–27.35	–29.08	–29.97
MSA-M	–29.98	–33.09	–34.85	–36.62	–38.38	–40.15	–41.05
MSA-D	–38.84	–42.19	–44.09	–45.99	–47.90	–49.80	–50.77
MSA-A-A	–21.00	–27.51	–31.20	–34.88	–38.57	–42.25	–44.12
MSA-A-M	–24.91	–31.83	–35.74	–39.66	–43.58	–47.50	–49.50
MSA-A-D	–30.02	–36.90	–40.81	–44.71	–48.61	–52.52	–54.51
MSA-M-A	–39.65	–46.25	–49.99	–53.74	–57.48	–61.23	–63.14
MSA-M-M	–44.56	–51.40	–55.29	–59.18	–63.07	–66.97	–68.96
MSA-M-D	–48.16	–55.01	–58.90	–62.80	–66.70	–70.61	–72.61
MSA-D-A	–52.33	–59.06	–62.88	–66.69	–70.52	–74.35	–76.30
MSA-D-M	–56.58	–63.69	–67.72	–71.75	–75.80	–79.85	–81.92
MSA-D-D	–60.62	–67.72	–71.75	–75.79	–79.84	–83.89	–85.96

[a] Obtained at the B3LYP-D3/aug-cc-pVTZ level (aug-cc-pV(T+d)Z for sulfur)

[b] In the troposphere, the temperature drops about 6.49 K for every 1 km increase in altitude. In the stratosphere (from 11 km height above the earth surface), the constant temperature is 216.69 K. [31, 32] U.S. standard atmosphere, 1976.[33]

Table S11. Calculated Gibbs free energies of formation (in kJ mol^{-1}) at different atmospheric pressures (in atm) and heights (in km) in the Earth atmosphere when the atmospheric temperature is equal to 298.15 K. [a]

Complexes	0 Km 298.15 K 1 atm	2 Km 298.15 K 0.78 atm	4 Km 298.15 K 0.61 atm	6 Km 298.15 K 0.47 atm	8 Km 298.15 K 0.35 atm	10 Km 298.15 K 0.26 atm	12 Km 298.15 K 0.26 atm
MSA-A	–19.06	–18.45	–17.85	–17.21	–16.48	–15.75	–14.98
MSA-M	–29.98	–29.37	–28.77	–28.13	–27.40	–26.67	–25.90
MSA-D	–38.84	–38.22	–37.62	–36.98	–36.26	–35.53	–34.76
MSA-A-A	–21.00	–19.79	–18.58	–17.30	–15.85	–14.39	–12.85
MSA-A-M	–24.91	–23.69	–22.48	–21.20	–19.76	–18.29	–16.76
MSA-A-D	–30.02	–28.80	–27.59	–26.31	–24.87	–23.41	–21.87
MSA-M-A	–39.65	–38.43	–37.22	–35.94	–34.50	–33.04	–31.50

MSA-M-M	–44.56	–43.33	–42.12	–40.85	–39.40	–37.94	–36.40
MSA-M-D	–48.16	–46.94	–45.73	–44.45	–43.01	–41.54	–40.01
MSA-D-A	–52.33	–51.11	–49.91	–48.63	–47.18	–45.72	–44.18
MSA-D-M	–56.58	–55.36	–54.16	–52.88	–51.43	–49.97	–48.43
MSA-D-D	–60.62	–59.40	–58.19	–56.91	–55.47	–54.01	–52.47

[a] Obtained at the B3LYP-D3/aug-cc-pVTZ level (aug-cc-pV(T+d)Z for sulfur)

[b] In the troposphere, the temperature drops about 6.49 K for every 1 km increase in altitude. In the stratosphere (from 11 km height above the earth surface), the constant temperature is 216.69 K. [31, 32] U.S. standard atmosphere, 1976.[33]

Table S12. Calculated Gibbs free energies of formation (in $kJ \cdot mol^{-1}$) at different temperatures (in K), atmospheric pressures (in atm), and heights (in km) in the Earth atmosphere [a].

Complexes	0 Km 298.15 K 1 atm	2 Km 275.21 K 0.78 atm	4 Km 262.23 K 0.61 atm	6 Km 249.49 K 0.47 am	8 Km 236.27 K 0.35 atm	10 Km 223.29 K 0.26 atm	12 Km 216.69 K 0.26 atm
MSA-A	–19.06	–21.57	–22.80	–24.02	–25.30	–26.61	–27.01
MSA-M	–29.98	–32.53	–33.78	–35.03	–35.76	–37.67	–38.08
MSA-D	–38.84	–41.63	–43.02	–44.40	–45.85	–47.32	–47.81
MSA-A-A	–21.00	–26.39	–29.06	–31.71	–34.48	–37.30	–38.19
MSA-A-M	–24.91	–30.70	–33.61	–36.49	–39.50	–42.55	–43.57
MSA-A-D	–30.02	–35.78	–38.67	–41.53	–44.53	–47.57	–48.58
MSA-M-A	–39.65	–45.12	–47.85	–50.56	–53.40	–56.28	–57.21
MSA-M-M	–44.56	–50.28	–53.15	–56.00	–58.99	–62.02	–63.03
MSA-M-D	–48.16	–53.89	–56.77	–59.62	–62.62	–65.66	–66.68
MSA-D-A	–52.33	–57.94	–60.74	–63.52	–66.43	–69.40	–70.38
MSA-D-M	–56.58	–62.56	–65.58	–68.58	–71.72	–74.90	–75.99
MSA-D-D	–60.62	–66.60	–69.61	–72.61	–75.75	–78.94	–80.03

[a] Obtained at the B3LYP-D3/aug-cc-pVTZ level (aug-cc-pV(T+d)Z for sulfur)

[b] In the troposphere, the temperature drops about 6.49 K for every 1 km increase in altitude. In the stratosphere (from 11 km height above the earth surface), the constant temperature is 216.69 K.[31, 32] U.S. standard atmosphere, 1976.3

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Coordinates

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259	M-M			
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	1	2.805740000	-0.465438000	0.898539000
	1	1.381631000	0.427758000	1.449129000
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	1	2.010870000	-0.017634000	-1.391192000
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	1	-1.988928000	-0.250536000	-1.511680000
	1	-0.526140000	0.094272000	-0.863150000
260	M-M-h			
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261	M-D			
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	1	-0.787285000	-1.802814000	3.007578000
	1	-1.177982000	-0.937944000	4.500194000
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	1	0.277857000	0.439407000	3.165834000
	1	-0.772016000	0.408126000	1.908598000
262	D-A			
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	6	-2.243987000	-1.323338000	-0.184116000
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	1	1.788342000	1.100052000	-0.001902000
263	D-M			
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	1	-2.994424000	1.317749000	-0.912857000
	1	-3.669021000	0.865329000	0.658647000
	1	-2.369848000	2.053920000	0.577519000
	6	1.641729000	-0.681146000	0.413312000
	1	2.678715000	-0.761602000	0.757055000
	1	0.981970000	-0.839107000	1.265595000

	1	1.456955000	-1.487047000	-0.296408000
	7	1.304968000	0.599504000	-0.218113000
	1	1.491503000	1.369471000	0.412126000
	1	1.864799000	0.754590000	-1.046755000
264	D-D			
	7	1.461074000	0.318951000	-0.066920000
	1	0.734182000	0.380427000	0.635900000
	1	-0.781249000	-0.534816000	-0.680062000
	7	-1.465929000	-0.368269000	0.047435000
	6	-1.961812000	0.991249000	-0.077904000
	6	-2.532713000	-1.350305000	-0.017633000
	6	2.433416000	1.382350000	0.104214000
	6	2.069330000	-0.997840000	-0.001764000
	1	1.293590000	-1.762407000	-0.035177000
	1	2.669167000	-1.155454000	0.905527000
	1	2.724880000	-1.138482000	-0.862759000
	1	3.129083000	1.373273000	-0.736396000
	1	3.023933000	1.288677000	1.026488000
	1	1.930542000	2.348350000	0.111426000
	1	-3.186794000	-1.228000000	0.847045000
	1	-3.153039000	-1.259977000	-0.920294000
	1	-2.115764000	-2.355555000	0.017969000
	1	-2.585980000	1.145259000	-0.969046000
	1	-2.564016000	1.239613000	0.797533000
	1	-1.121946000	1.683854000	-0.125462000
265	D-D-h			
	7	1.609699000	-0.180266000	-0.563290000
	1	0.621737000	-0.130303000	-0.795411000
	1	-2.036489000	0.381377000	-1.508266000
	7	-1.538965000	0.066039000	-0.686307000
	6	-1.625394000	1.070087000	0.365910000
	6	-2.036880000	-1.239280000	-0.272778000
	6	2.130751000	1.157600000	-0.352461000
	6	1.798745000	-1.045880000	0.585500000
	1	1.336041000	-2.014835000	0.397968000
	1	1.379190000	-0.639595000	1.522395000
	1	2.864780000	-1.214521000	0.755359000
	1	3.218355000	1.124069000	-0.253695000
	1	1.733986000	1.650900000	0.551402000
	1	1.894838000	1.784437000	-1.212383000
	1	-1.401450000	-1.630339000	0.523242000
	1	-3.069389000	-1.215970000	0.104911000
	1	-1.988633000	-1.933812000	-1.110381000
	1	-2.637002000	1.186305000	0.780802000

	1	-0.960232000	0.790575000	1.184483000
	1	-1.293736000	2.034310000	-0.016880000
266	MSA-A			
	16	0.087016000	1.757848000	1.867145000
	8	-0.086585000	2.910361000	1.033567000
	8	1.556718000	1.229619000	1.714515000
	8	-0.228069000	1.847409000	3.276641000
	1	1.985623000	1.076877000	2.641221000
	6	-0.854557000	0.423533000	1.163914000
	1	-0.531256000	0.280625000	0.136762000
	1	-0.691673000	-0.473806000	1.753814000
	1	-1.899800000	0.720219000	1.196209000
	7	2.481795000	0.975668000	4.170584000
	1	2.723684000	0.067546000	4.547388000
	1	1.620561000	1.291133000	4.608077000
	1	3.219805000	1.625160000	4.414300000
267	MSA-M			
	16	-0.953063000	0.221930000	0.050235000
	8	-1.390624000	1.534786000	-0.332446000
	8	-0.060756000	-0.392671000	-1.070826000
	8	-0.274866000	0.060577000	1.320930000
	1	0.915132000	-0.607488000	-0.688577000
	6	-2.365481000	-0.857510000	0.021161000
	1	-2.805063000	-0.819739000	-0.971537000
	1	-2.045008000	-1.865252000	0.268630000
	1	-3.067294000	-0.483539000	0.762169000
	6	2.919234000	0.555032000	-0.010462000
	1	3.820267000	0.572035000	0.604556000
	1	3.182850000	0.816501000	-1.033198000
	1	2.221954000	1.300134000	0.365413000
	7	2.244313000	-0.755841000	-0.005200000
	1	2.855491000	-1.490320000	-0.340135000
	1	1.945446000	-0.992444000	0.935185000
268	MSA-M-h			
	16	-1.139115000	0.258316000	0.133879000
	8	-1.734197000	1.519554000	-0.201789000
	8	-0.034686000	-0.097555000	-0.909875000
	8	-0.595046000	0.068632000	1.462843000
	1	0.876225000	-0.334389000	-0.417377000
	6	-2.349431000	-1.011784000	-0.161625000
	1	-2.677510000	-0.938504000	-1.194605000
	1	-1.901907000	-1.981280000	0.037456000
	1	-3.179507000	-0.825912000	0.515076000
	6	2.020651000	-2.039607000	0.928926000

	1	2.808610000	-2.281218000	1.644393000
	1	1.055774000	-2.171091000	1.412898000
	1	2.086083000	-2.728518000	0.088743000
	7	2.098213000	-0.656733000	0.428613000
	1	1.977136000	-0.000670000	1.192835000
	1	2.992305000	-0.468390000	-0.008137000
269	MSA-D			
	16	-1.281632000	0.121500000	0.000866000
	8	-1.939226000	1.407532000	-0.047087000
	8	-0.479894000	-0.193325000	-1.213018000
	8	-0.456549000	-0.090684000	1.221316000
	1	1.137172000	-0.126554000	-0.793608000
	6	-2.553969000	-1.125711000	0.065630000
	1	-3.166451000	-1.024850000	-0.826292000
	1	-2.086756000	-2.105845000	0.102311000
	1	-3.149123000	-0.949838000	0.957645000
	6	2.855264000	-1.058870000	0.010060000
	1	3.468573000	-1.015502000	-0.887270000
	1	3.486554000	-0.940664000	0.887967000
	1	2.343129000	-2.016109000	0.055573000
	7	1.846199000	0.013834000	-0.024932000
	1	1.152839000	-0.061001000	0.766733000
	6	2.379348000	1.390375000	-0.088037000
	1	2.993209000	1.585254000	0.788318000
	1	2.975329000	1.510662000	-0.989777000
	1	1.537476000	2.077082000	-0.108394000
270	MSA-D-h			
	16	-1.172937000	0.170373000	-0.035933000
	6	-2.625640000	-0.852438000	0.112277000
	1	-3.247893000	-0.667382000	-0.759318000
	1	-2.319835000	-1.894202000	0.150420000
	1	-3.150648000	-0.570332000	1.020730000
	8	-1.613360000	1.548956000	-0.057886000
	8	-0.447430000	-0.278149000	-1.226816000
	8	-0.373139000	-0.155674000	1.199731000
	1	1.017905000	-0.090840000	0.878687000
	7	2.081240000	-0.007258000	0.541188000
	1	2.664056000	0.032439000	1.372041000
	6	2.204100000	1.261129000	-0.222351000
	1	1.524079000	1.201114000	-1.066912000
	1	3.229985000	1.396363000	-0.558996000
	1	1.901854000	2.084187000	0.419162000
	6	2.407629000	-1.214326000	-0.256851000
	1	1.676703000	-1.274761000	-1.058031000

	1	2.319340000	-2.089424000	0.381609000
	1	3.418421000	-1.140530000	-0.653506000
271	MSA-A-A			
	16	0.789669000	-0.087001000	0.000058000
	8	0.397488000	0.652542000	-1.219592000
	8	0.397427000	0.652431000	1.219749000
	8	0.326006000	-1.473410000	-0.000020000
	1	-1.180005000	1.467637000	0.801042000
	6	2.569520000	-0.140039000	0.000093000
	1	2.944075000	0.879723000	0.000149000
	1	2.890820000	-0.668229000	0.893618000
	1	2.890860000	-0.668146000	-0.893466000
	7	-2.641326000	-1.163485000	-0.000072000
	1	-3.083994000	-1.570776000	-0.815671000
	1	-3.084024000	-1.570816000	0.815491000
	1	-1.660236000	-1.465235000	-0.000061000
	7	-1.842817000	1.504794000	0.000020000
	1	-2.447196000	2.316901000	-0.000035000
	1	-2.363348000	0.574533000	-0.000018000
	1	-1.179866000	1.467617000	-0.800901000
272	MSA-A-M			
	16	1.004357000	-0.222093000	0.050474000
	8	0.375147000	0.042815000	-1.251180000
	8	1.125699000	1.028991000	0.845976000
	8	0.364353000	-1.301492000	0.799847000
	1	-0.220987000	1.876321000	0.450990000
	6	2.676759000	-0.743711000	-0.272048000
	1	3.182685000	0.043210000	-0.824406000
	1	3.167143000	-0.921719000	0.681020000
	1	2.635068000	-1.658277000	-0.857430000
	7	-2.415383000	-0.267872000	0.686860000
	1	-3.103504000	-0.346730000	1.425635000
	1	-1.560180000	-0.731686000	1.002939000
	7	-1.152640000	2.049780000	-0.029940000
	1	-1.539671000	2.969211000	0.144997000
	1	-1.794898000	1.234363000	0.299696000
	1	-0.951456000	1.898693000	-1.017323000
	6	-2.882378000	-0.934157000	-0.541426000
	1	-3.751740000	-0.411006000	-0.940665000
	1	-2.078827000	-0.894371000	-1.274152000
	1	-3.150193000	-1.981242000	-0.384374000
273	MSA-A-D			
	16	1.355774000	-0.224223000	0.006462000
	8	1.408111000	0.819375000	-1.049451000

	8	0.897896000	0.337869000	1.284270000
	8	0.599776000	-1.405683000	-0.412111000
	1	-0.437545000	2.204599000	0.801207000
	6	3.040548000	-0.754384000	0.238685000
	1	3.631831000	0.104028000	0.545095000
	1	3.047846000	-1.520627000	1.009160000
	1	3.403962000	-1.155566000	-0.703378000
	7	-2.088385000	-0.236795000	-0.182952000
	1	-1.264418000	-0.799025000	-0.413193000
	7	-0.751581000	2.103942000	-0.161762000
	1	-1.169139000	2.956811000	-0.513737000
	1	-1.422212000	1.214273000	-0.202273000
	1	0.113791000	1.807401000	-0.691864000
	6	-3.150208000	-0.478018000	-1.156981000
	1	-3.989486000	0.193360000	-0.966705000
	1	-2.774501000	-0.286210000	-2.161204000
	1	-3.525193000	-1.506533000	-1.119108000
	6	-2.475479000	-0.550580000	1.194737000
	1	-1.603838000	-0.432751000	1.835447000
	1	-3.260948000	0.132316000	1.524496000
	1	-2.850120000	-1.574430000	1.295231000
274	MSA-M-A			
	16	-1.048027000	0.064197000	0.099714000
	8	-0.384878000	-0.133498000	-1.191058000
	8	-0.494764000	-0.853567000	1.135864000
	8	-1.062883000	1.456767000	0.545587000
	1	1.080273000	-0.775124000	0.986533000
	6	-2.748385000	-0.432662000	-0.092136000
	1	-2.769901000	-1.470853000	-0.411673000
	1	-3.249556000	-0.313502000	0.864452000
	1	-3.200659000	0.209318000	-0.843270000
	7	2.094069000	-0.601013000	0.688427000
	1	2.716066000	-0.739418000	1.478014000
	1	2.115120000	0.422235000	0.394285000
	7	1.760029000	2.032145000	-0.203837000
	1	2.264575000	2.877030000	0.035219000
	1	0.797860000	2.115906000	0.136548000
	1	1.684472000	1.990279000	-1.214299000
	6	2.431933000	-1.478597000	-0.458814000
	1	2.406113000	-2.518052000	-0.143100000
	1	1.675425000	-1.308431000	-1.219459000
	1	3.420174000	-1.230908000	-0.838435000
275	MSA-M-A-h			
	16	-1.146243000	-0.047618000	0.000134000

	8	-0.515018000	-0.595461000	-1.219620000
	8	-0.515032000	-0.595100000	1.220046000
	8	-1.215862000	1.412940000	-0.000088000
	1	1.265645000	-0.760645000	0.794992000
	6	-2.826084000	-0.640154000	0.000201000
	1	-2.807875000	-1.726417000	0.000361000
	1	-3.316576000	-0.263535000	0.893632000
	1	-3.316557000	-0.263798000	-0.893352000
	7	1.904980000	-0.567086000	0.000158000
	1	1.265440000	-0.760786000	-0.794499000
	1	2.030714000	0.483358000	0.000041000
	7	1.652725000	2.238970000	-0.000171000
	1	1.905322000	2.785532000	0.814953000
	1	0.630961000	2.143423000	-0.000127000
	1	1.905266000	2.785302000	-0.815467000
	6	3.160946000	-1.336486000	0.000074000
	1	3.739814000	-1.089384000	0.886239000
	1	2.939327000	-2.400389000	0.000190000
	1	3.739593000	-1.089534000	-0.886276000
276	MSA-M-M			
	16	1.281055000	-0.176663000	-0.046655000
	8	0.964484000	-1.405887000	-0.771283000
	8	1.044516000	1.043438000	-0.858987000
	8	0.611752000	-0.079337000	1.260709000
	1	-0.534061000	1.486487000	-0.446813000
	6	3.033929000	-0.208034000	0.271886000
	1	3.551574000	-0.259200000	-0.682049000
	1	3.303208000	0.697996000	0.807596000
	1	3.250346000	-1.087711000	0.872024000
	7	-2.002617000	-1.238668000	-0.668767000
	1	-1.049676000	-1.422651000	-0.990139000
	1	-2.639079000	-1.530791000	-1.400003000
	7	-1.441560000	1.372005000	0.074395000
	1	-1.119380000	1.215972000	1.031234000
	6	-2.393996000	2.484682000	-0.079788000
	1	-1.940413000	3.413407000	0.256768000
	1	-2.661868000	2.579029000	-1.128905000
	1	-3.291833000	2.288996000	0.501512000
	6	-2.233808000	-2.005806000	0.566826000
	1	-1.475710000	-1.717095000	1.292444000
	1	-3.218283000	-1.770228000	0.972511000
	1	-2.169937000	-3.086667000	0.420851000
	1	-1.817001000	0.422716000	-0.259135000
277	MSA-M-M-h			

	16	1.264215000	-0.119163000	0.029770000
	8	0.534274000	-0.021424000	-1.235906000
	8	1.093220000	1.112128000	0.849540000
	8	0.966881000	-1.334863000	0.787844000
	1	-0.471092000	1.448851000	0.833157000
	6	3.001300000	-0.174158000	-0.363146000
	1	3.256884000	0.724258000	-0.918066000
	1	3.561164000	-0.224969000	0.566580000
	1	3.179457000	-1.060756000	-0.965713000
	7	-1.527319000	1.475627000	0.684530000
	1	-1.828686000	0.442027000	0.733595000
	7	-1.987708000	-1.256572000	0.687653000
	1	-2.566149000	-1.706648000	1.386634000
	1	-1.013102000	-1.491678000	0.892316000
	6	-1.835215000	2.055953000	-0.645406000
	1	-1.546741000	3.103649000	-0.665174000
	1	-1.250894000	1.503824000	-1.375588000
	1	-2.897995000	1.961243000	-0.854343000
	6	-2.323500000	-1.744130000	-0.661313000
	1	-3.325937000	-1.415368000	-0.937411000
	1	-1.606422000	-1.321416000	-1.361484000
	1	-2.282493000	-2.832863000	-0.745767000
	1	-1.966855000	1.990705000	1.440189000
278	MSA-M-D			
	16	1.552102000	-0.266991000	-0.009832000
	8	1.040730000	0.132045000	-1.329789000
	8	1.417985000	0.837934000	0.972437000
	8	0.983288000	-1.523770000	0.476933000
	1	-0.027289000	1.588086000	0.511205000
	6	3.303891000	-0.537950000	-0.191049000
	1	3.759469000	0.381674000	-0.547637000
	1	3.707017000	-0.816045000	0.778853000
	1	3.446913000	-1.340895000	-0.909140000
	7	-1.880303000	-0.854651000	0.151032000
	1	-0.977667000	-1.240815000	0.436804000
	7	-0.895133000	1.703526000	-0.072130000
	1	-1.409820000	0.754142000	0.040400000
	1	-0.527186000	1.704298000	-1.023429000
	6	-2.163072000	-1.334412000	-1.202712000
	1	-3.046678000	-0.829878000	-1.599404000
	1	-1.307808000	-1.111317000	-1.837799000
	1	-2.347918000	-2.414070000	-1.232020000
	6	-2.909921000	-1.215886000	1.120837000
	1	-2.606168000	-0.890270000	2.115028000

	1	-3.849872000	-0.721527000	0.868135000
	1	-3.096472000	-2.295774000	1.154106000
	6	-1.717928000	2.877259000	0.265173000
	1	-2.049542000	2.791395000	1.296724000
	1	-1.136813000	3.789279000	0.153676000
	1	-2.587911000	2.921384000	-0.385764000
279	MSA-M-D-h			
	16	1.492761000	-0.301798000	0.045862000
	8	0.994990000	0.205857000	-1.234413000
	8	1.474054000	0.754712000	1.093241000
	8	0.828507000	-1.530330000	0.485999000
	1	0.024514000	1.461412000	0.989651000
	6	3.214067000	-0.704882000	-0.176256000
	1	3.738743000	0.192150000	-0.493243000
	1	3.606041000	-1.065921000	0.770544000
	1	3.280967000	-1.477489000	-0.937483000
	7	-1.973298000	-0.717810000	0.090568000
	1	-1.090456000	-1.198966000	0.278817000
	7	-0.965283000	1.754716000	0.733919000
	1	-1.409598000	2.194634000	1.532843000
	1	-1.467781000	0.814877000	0.505471000
	6	-2.246094000	-0.804525000	-1.345428000
	1	-3.094307000	-0.166528000	-1.602308000
	1	-1.364729000	-0.469127000	-1.887574000
	1	-2.484461000	-1.826768000	-1.660664000
	6	-3.035353000	-1.285458000	0.915870000
	1	-2.740027000	-1.256595000	1.964277000
	1	-3.951192000	-0.702689000	0.798640000
	1	-3.262721000	-2.324831000	0.651784000
	6	-0.938274000	2.642187000	-0.453716000
	1	-0.447316000	3.579467000	-0.204709000
	1	-0.370150000	2.126449000	-1.222341000
	1	-1.952478000	2.836238000	-0.794360000
280	MSA-D-A			
	16	-1.333413000	-0.015374000	0.158976000
	8	-0.882977000	0.101095000	-1.230163000
	8	-0.543578000	-1.039379000	0.897503000
	8	-1.384393000	1.262648000	0.868554000
	1	0.980108000	-0.742435000	0.482849000
	6	-2.998232000	-0.650855000	0.126642000
	1	-2.991104000	-1.609166000	-0.385268000
	1	-3.341038000	-0.764230000	1.151398000
	1	-3.618538000	0.064288000	-0.406935000
	7	1.913966000	-0.398403000	0.108561000

	1	1.760131000	0.641841000	-0.025111000
	7	1.179039000	2.296873000	-0.241685000
	1	0.903080000	2.389211000	-1.213193000
	1	1.642376000	3.154049000	0.033791000
	1	0.301951000	2.213241000	0.279397000
	6	2.146215000	-1.023254000	-1.210886000
	1	2.272012000	-2.096403000	-1.085149000
	1	1.271102000	-0.823786000	-1.823056000
	1	3.039997000	-0.600005000	-1.665403000
	6	2.978889000	-0.625383000	1.101390000
	1	2.701955000	-0.132561000	2.029738000
	1	3.091058000	-1.692395000	1.280192000
	1	3.919425000	-0.216791000	0.736780000
281	MSA-D-M			
	16	1.492761000	-0.301798000	0.045862000
	8	0.994990000	0.205857000	-1.234413000
	8	1.474054000	0.754712000	1.093241000
	8	0.828507000	-1.530330000	0.485999000
	1	0.024514000	1.461412000	0.989651000
	6	3.214067000	-0.704882000	-0.176256000
	1	3.738743000	0.192150000	-0.493243000
	1	3.606041000	-1.065921000	0.770544000
	1	3.280967000	-1.477489000	-0.937483000
	7	-1.973298000	-0.717810000	0.090568000
	1	-1.090456000	-1.198966000	0.278817000
	7	-0.965283000	1.754716000	0.733919000
	1	-1.409598000	2.194634000	1.532843000
	1	-1.467781000	0.814877000	0.505471000
	6	-2.246094000	-0.804525000	-1.345428000
	1	-3.094307000	-0.166528000	-1.602308000
	1	-1.364729000	-0.469127000	-1.887574000
	1	-2.484461000	-1.826768000	-1.660664000
	6	-3.035353000	-1.285458000	0.915870000
	1	-2.740027000	-1.256595000	1.964277000
	1	-3.951192000	-0.702689000	0.798640000
	1	-3.262721000	-2.324831000	0.651784000
	6	-0.938274000	2.642187000	-0.453716000
	1	-0.447316000	3.579467000	-0.204709000
	1	-0.370150000	2.126449000	-1.222341000
	1	-1.952478000	2.836238000	-0.794360000
282	MSA-D-M-h			
	16	1.552102000	-0.266991000	-0.009832000
	8	1.040730000	0.132045000	-1.329789000
	8	1.417985000	0.837934000	0.972437000

	8	0.983288000	-1.523770000	0.476933000
	1	-0.027289000	1.588086000	0.511205000
	6	3.303891000	-0.537950000	-0.191049000
	1	3.759469000	0.381674000	-0.547637000
	1	3.707017000	-0.816045000	0.778853000
	1	3.446913000	-1.340895000	-0.909140000
	7	-1.880303000	-0.854651000	0.151032000
	1	-0.977667000	-1.240815000	0.436804000
	7	-0.895133000	1.703526000	-0.072130000
	1	-1.409820000	0.754142000	0.040400000
	1	-0.527186000	1.704298000	-1.023429000
	6	-2.163072000	-1.334412000	-1.202712000
	1	-3.046678000	-0.829878000	-1.599404000
	1	-1.307808000	-1.111317000	-1.837799000
	1	-2.347918000	-2.414070000	-1.232020000
	6	-2.909921000	-1.215886000	1.120837000
	1	-2.606168000	-0.890270000	2.115028000
	1	-3.849872000	-0.721527000	0.868135000
	1	-3.096472000	-2.295774000	1.154106000
	6	-1.717928000	2.877259000	0.265173000
	1	-2.049542000	2.791395000	1.296724000
	1	-1.136813000	3.789279000	0.153676000
	1	-2.587911000	2.921384000	-0.385764000
283	MSA-D-D			
	16	-1.387398000	0.736786000	0.235405000
	8	0.064472000	0.927303000	0.205102000
	8	-1.929122000	0.170174000	-1.001453000
	8	-1.808538000	-0.029840000	1.438190000
	1	0.040295000	-2.092297000	0.305347000
	6	-2.128951000	2.346219000	0.424745000
	1	-1.847435000	2.947689000	-0.435416000
	1	-3.207568000	2.223176000	0.468593000
	1	-1.754671000	2.791114000	1.342597000
	7	-0.007775000	-2.035452000	-1.388888000
	1	-0.750237000	-1.336010000	-1.458325000
	7	-0.017154000	-2.015081000	1.380121000
	1	-0.750312000	-1.266106000	1.527219000
	6	-0.474829000	-3.295822000	1.945120000
	1	-1.434366000	-3.550728000	1.502447000
	1	0.248340000	-4.078346000	1.722630000
	1	-0.589945000	-3.205258000	3.023232000
	6	1.274608000	-1.528789000	1.906960000
	1	2.064648000	-2.229662000	1.643525000
	1	1.461800000	-0.554775000	1.463979000

	1	1.215610000	-1.435772000	2.989597000
	6	-0.406613000	-3.256079000	-2.082192000
	1	0.331795000	-4.041818000	-1.910202000
	1	-1.367920000	-3.597898000	-1.699713000
	1	-0.499380000	-3.114869000	-3.165792000
	6	1.226988000	-1.449451000	-1.912247000
	1	1.391343000	-0.491617000	-1.423574000
	1	2.070477000	-2.111191000	-1.703944000
	1	1.184039000	-1.288501000	-2.995863000
284	MSA-D-D-h			
	16	-1.103348000	1.139251000	-0.085493000
	8	-0.044221000	2.085857000	-0.389670000
	8	-1.426890000	0.226114000	-1.208371000
	8	-0.872533000	0.369738000	1.161482000
	1	-0.824672000	-1.326001000	-0.807499000
	6	-2.580011000	2.095221000	0.200614000
	1	-2.794374000	2.659823000	-0.702709000
	1	-3.397159000	1.417934000	0.432967000
	1	-2.389196000	2.766538000	1.033467000
	7	2.397815000	0.261977000	-0.250725000
	1	1.692713000	0.955815000	-0.480955000
	7	-0.532009000	-1.987095000	-0.047454000
	1	-0.482896000	-1.277461000	0.717840000
	6	-1.621735000	-2.945476000	0.223604000
	1	-2.535513000	-2.385729000	0.402070000
	1	-1.752120000	-3.599097000	-0.635545000
	1	-1.374822000	-3.539475000	1.100328000
	6	0.794556000	-2.584348000	-0.321077000
	1	0.731897000	-3.196952000	-1.217857000
	1	1.501342000	-1.761052000	-0.455180000
	1	1.087530000	-3.204130000	0.523940000
	6	3.575955000	0.451848000	-1.081459000
	1	4.278647000	-0.371112000	-0.926860000
	1	3.288148000	0.455865000	-2.132586000
	1	4.113438000	1.388244000	-0.869004000
	6	2.684754000	0.349373000	1.174094000
	1	1.748381000	0.331340000	1.729439000
	1	3.295793000	-0.502697000	1.485452000
	1	3.228369000	1.264448000	1.451438000
285				