Supplementary Materials

Interaction between Dicarboxylic Acid and Sulfuric Acid-Base Clusters Enhances New Particle Formation

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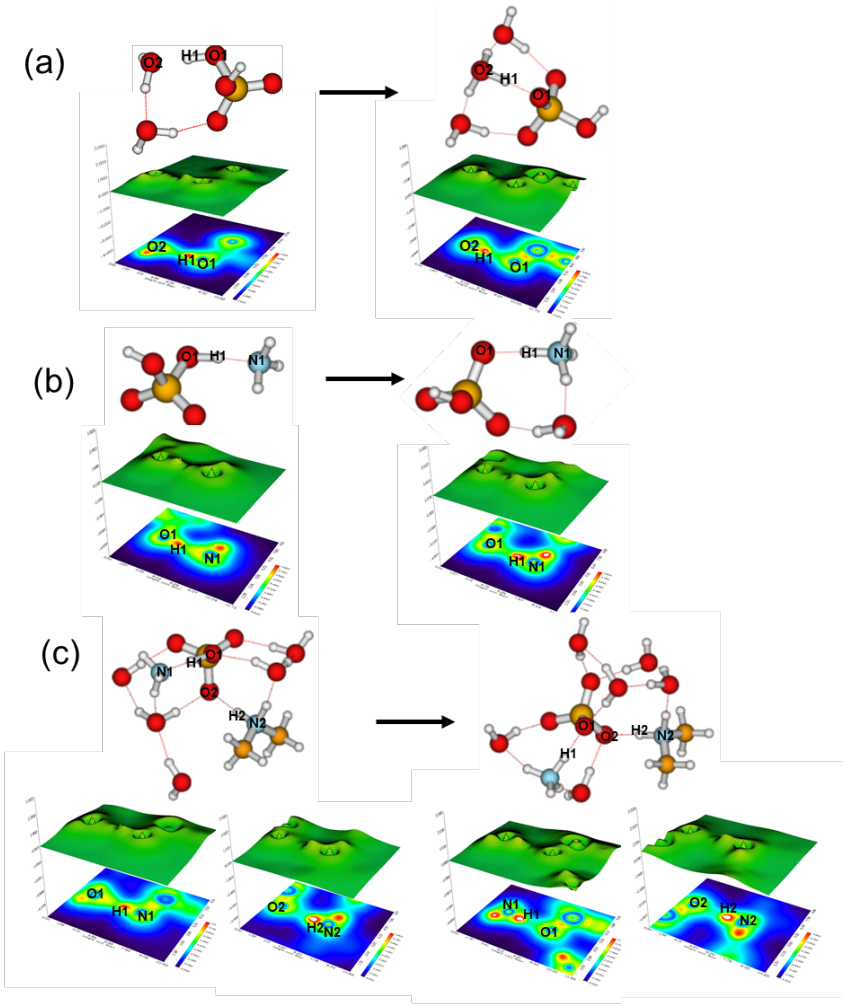

FIG. S1. Relief maps with the projection of localized orbital locator (LOL) for corresponding clusters of (a) SA·$(W)_2$ and SA·$(W)_3$, (b) SA·AM and SA·AM·W, and (c) SA·DMA·AM·$(W)_5$ and SA·DMA·AM·$(W)_6$. Hydrogen bonds are shown as dashed lines. A large LOL value means that electrons are greatly localized, indicating the existence of a covalent bond.

Table S1. Laplacian of electron densities at BCPs of the nitrogen-hydrogen bond in the clusters (a.u.).

Clusters	Bonds	No. of water						
		0	*1*	*2*	*3*	*4*	*5*	*6*
SA•AM	N1-H1	0.028	-1.046	-1.512	-1.535	-1.526	-1.599	-1.625
SA•AM•SUA	N1-H1	-1.278	-1.510	-1.528	-1.597	-1.576	-1.658	-1.582
SA•DMA	N2-H2	-1.443	-1.372	-1.513	-1.524	-1.534	-1.545	-1.592
SA•DMA•SUA	N2-H2	-1.488	-1.480	-1.603	-1.604	-1.544	-1.613	-1.555
SA•DMA•AM	N1-H1	0.076	0.078	0.038	0.016	0.029	0.016	-1.394
	N2-H2	-1.312	-1.324	-1.321	-1.427	-1.524	-1.547	-1.504
SA•DMA•AM•SUA	N1-H1	-1.351	-1.388	-1.304	-0.866	-1.560	-1.528	-1.575
	N2-H2	-1.142	-1.117	-1.396	-1.610	-1.355	-1.510	-1.513

Note: N1 is the nitrogen atom on the ammonia (AM) molecule; N2 is the nitrogen atom on the dimethylamine (DMA) molecule; H1 is the hydrogen atom on one of the hydroxyl functions of sulfuric acid (SA) molecule and bound to N1; H2 is the hydrogen atom on one of the hydroxyl functions of SA (SA) molecule and bound to N2.

Table S2. Electron densities at BCPs of the nitrogen-hydrogen bond in the clusters (a.u.).

Clusters	Bonds	No. of water						
		0	*1*	*2*	*3*	*4*	*5*	*6*
SA•AM	N1-H1	0.091	0.248	0.300	0.302	0.301	0.315	0.322
SA•AM•SUA	N1-H1	0.271	0.298	0.301	0.311	0.308	0.321	0.307
SA•DMA	N2-H2	0.295	0.285	0.302	0.303	0.304	0.306	0.313
SA•DMA•SUA	N2-H2	0.297	0.297	0.311	0.313	0.306	0.314	0.305
SA•DMA•AM	N1-H1	0.063	0.060	0.085	0.095	0.090	0.094	0.287
	N2-H2	0.281	0.281	0.280	0.294	0.304	0.307	0.301
SA•DMA•AM•SUA	N1-H1	0.283	0.284	0.275	0.230	0.306	0.302	0.312
	N2-H2	0.258	0.260	0.288	0.314	0.284	0.300	0.301

Note: N1 is the nitrogen atom on the ammonia (AM) molecule; N2 is the nitrogen atom on the dimethylamine (DMA) molecule; H1 is the hydrogen atom on one of the hydroxyl functions of sulfuric acid (SA) molecule and bound to N1; H2 is the hydrogen atom on one of the hydroxyl functions of SA (SA) molecule and bound to N2.

Table S3 Potential energy densities at BCPs of the nitrogen-hydrogen bond in the clusters (a.u.).

Clusters	Bonds	No. of water						
		0	*1*	*2*	*3*	*4*	*5*	*6*
SA•AM	N1-H1	-0.087	-0.373	-0.478	-0.483	-0.481	-0.499	-0.508
SA•AM•SUA	N1-H1	-0.424	-0.476	-0.482	-0.499	-0.493	-0.513	-0.493
SA•DMA	N2-H2	-0.466	-0.449	-0.481	-0.484	-0.486	-0.488	-0.499
SA•DMA•SUA	N2-H2	-0.475	-0.473	-0.500	-0.500	-0.487	-0.503	-0.489
SA•DMA•AM	N1-H1	-0.053	-0.050	-0.078	-0.091	-0.085	-0.090	-0.452
	N2-H2	-0.437	-0.439	-0.438	-0.461	-0.484	-0.488	-0.479
SA•DMA•AM•SUA	N1-H1	-0.443	-0.448	-0.431	-0.332	-0.488	-0.482	-0.496
	N2-H2	-0.394	-0.394	-0.453	-0.502	-0.446	-0.478	-0.479

Note: N1 is the nitrogen atom on the ammonia (AM) molecule; N2 is the nitrogen atom on the dimethylamine (DMA) molecule; H1 is the hydrogen atom on one of the hydroxyl functions of sulfuric acid (SA) molecule and bound to N1; H2 is the hydrogen atom on one of the hydroxyl functions of SA (SA) molecule and bound to N2.

Table S4 Thermochemical properties for addition of SA and SUA to pure SA, hydrated SA, and SA·base clusters (kcal mol^{-1}).

Reactions	ΔE(ZPE)	ΔH	ΔG
SA+SA→$(SA)_2$	-14.59	-14.66	-3.72
SA+SUA→SA•SUA	-19.14	-18.95	-8.61
SA•AM+SA →SA•AM•SA	-22.23	-22.78	-9.46
SA•AM+SUA →SA•AM•SUA	-34.19	-34.69	-6.20
SA•DMA+SA → $(SA)_2$•DMA	-23.40	-23.64	-10.53
SA•DMA+SUA → SA•DMA•SUA	-20.85	-20.32	-9.86