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Interaction between succinic acid and sulfuric acid–base clusters

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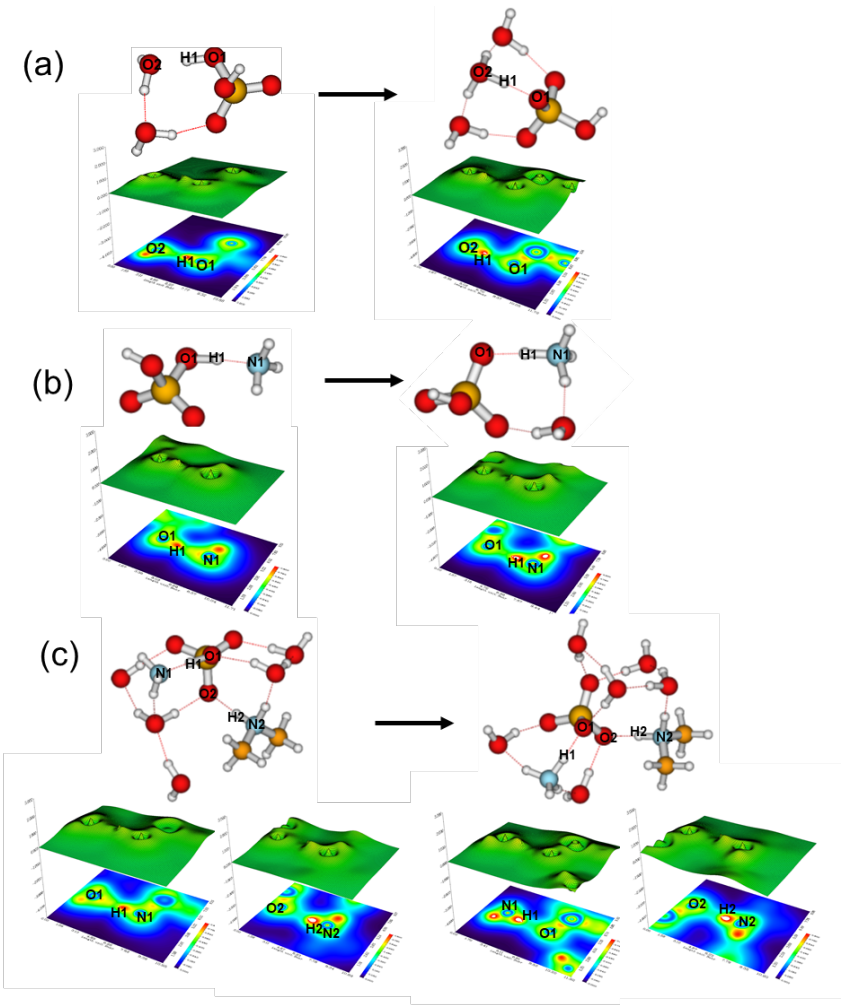

FIG. S1. Relief maps with the projection of localized orbital locator (LOL) for corresponding clusters of (a) SA·$(W)_2$ and SA·$(W)_3$, (b) SA·AM and SA·AM·W, and (c) SA·DMA·AM·$(W)_5$ and SA·DMA·AM·$(W)_6$. Hydrogen bonds are shown as dashed lines. A large LOL value means that electrons are greatly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