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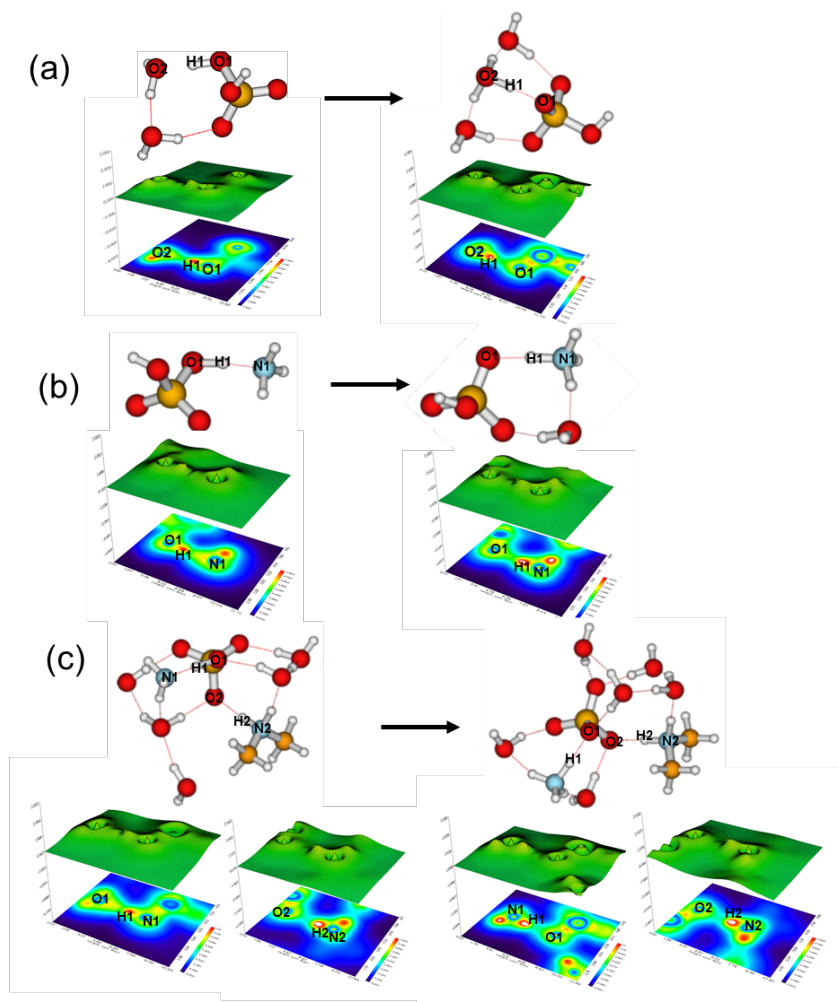
*Supplement of*

## **Interaction between succinic acid and sulfuric acid–base clusters**

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

21

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

Clusters	Bonds	No. of water						
		<i>0</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>	<i>6</i>
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

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

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

Clusters	Bonds	No. of water						
		<i>0</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>	<i>6</i>
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

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

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

Clusters	Bonds	No. of water						
		<i>0</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>	<i>6</i>
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

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

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