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Supporting Information for: Network Analysis and Percolation Transition in Hydrogen Bonded Clusters: Nitric Acid and Water Extracted by Tributyl Phosphate

Michael J. Servis, David T. Wu,* and Jenifer C. Braley†

The force field parameters used for the TBP and dodecane molecules are given in Tables 1, 2, 3, 4. Parameters which have been modified from the default GAFF values, as described in the main article, are denoted with an asterisk. Table 5 gives the partial atomic charges used in the dodecane and TBP models.

Table 1 GAFF Lennard Jones parameters for the TBP and dodecane atom types.

Atom	σ [Å]	ε [kcal mol^{-1}]
O2	2.9599	0.2100
P	3.7418	0.2000
OS	3.0000	0.1700
CT* (TBP)	3.2297	0.1127
CT* (dodecane)	3.1324	0.1444
H1	2.4714	0.0157
HC	2.6495	0.0157

Table 2 GAFF equilibrium bond length and bond energy parameters.

Bond	l_0 [Å]	k_l [kcal mol^{-1} Å^{-2}]
O2-P	1.481	487.7
P-OS	1.602	342.5
P-CT	1.813	259.7
OS-CT	1.439	301.5
CT-CT	1.535	303.1
CT-H1	1.093	335.9
CT-HC	1.092	337.3

Table 3 GAFF equilibrium angle and angle energy parameters.

Angle	θ_0 [deg]	k_θ [kcal mol^{-1} deg^{-2}]
O2-P-OS	116.09	44.0
O2-P-CT	112.50	39.9
OS-P-OS	102.46	45.2
OS-P-CT	103.83	40.6
P-OS-CT	118.00	78.5
P-CT-CT	114.24	77.0
P-CT-H1	109.64	53.8
OS-CT-CT	108.42	67.8
OS-CT-H1	108.82	50.8
CT-CT-CT	110.63	63.2
CT-CT-H1	110.07	46.4
CT-CT-HC	110.05	46.4
H1-CT-H1	109.55	39.2
HC-CT-HC	108.35	39.4

Colorado School of Mines, 1500 Illinois St., Golden, CO.
† *E-mail: jbraley@mines.edu*
* *E-mail: dwu@mines.edu*
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Table 4 GAFF equilibrium dihedral angle and dihedral energy parameters. Asterisk indicates modified parameters.

Dihedral	n=1		n=2		n=3	
	V_n [kcal mol^{-1}]	γ_n [deg]				
O2-P-OS-CT*	2.00	180	3.00	180		
O2-P-CT-CT*			0.80	180		
O2-P-CT-H1*			0.80	180		
OS-P-OS-CT*	2.00	180	3.00	180		
OS-P-CT-CT*			0.80	180		
OS-P-CT-H1*			0.80	180		
CT-P-OS-CT*			2.40	0		
P-OS-CT-CT					1.15	0
P-CT-CT-CT					1.40	0
P-CT-CT-HC					1.40	0
P-OS-CT-H1					1.15	0
OS-CT-CT-CT					1.40	0
OS-CT-CT-HC	0.25	0				
CT-CT-CT-CT	0.20	180	0.25	180	0.18	0
CT-CT-CT-H1					0.16	0
CT-CT-CT-HC					0.16	0
H1-CT-CT-HC					0.15	0
HC-CT-CT-HC					0.15	0

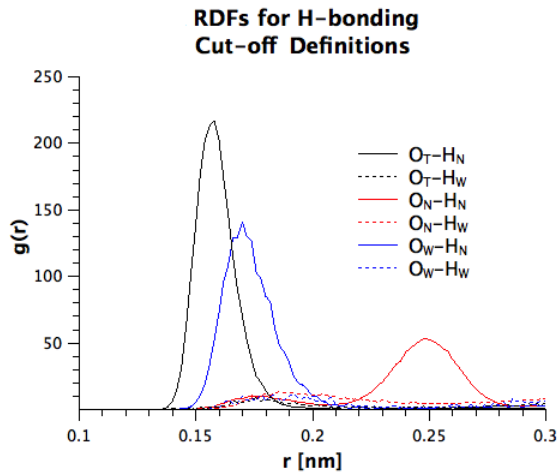

Fig. 1 The RDFs used to determine the distance cut-off given in the text for the hydrogen bond definitions of each hydrogen bond type.

Table 5 TBP and dodecane AM1-BCC charges. For dodecane, the carbon and hydrogen atoms are denoted by position in the chain.

Atom	AM1-BCC [e]
TBP	
O2	-0.7963
P	1.5955
OS	-0.5682
CT_1	0.1644
CT_2	-0.0834
CT_3	-0.0814
CT_4	-0.0921
$H1_1$	0.0467
HC_2	0.0567
HC_3	0.0417
HC_4	0.0347
dodecane	
$CT_{1,12}$	-0.0891
CT_{2-11}	-0.0744
$HC_{1,12}$	0.0317
HC_{2-11}	0.0367

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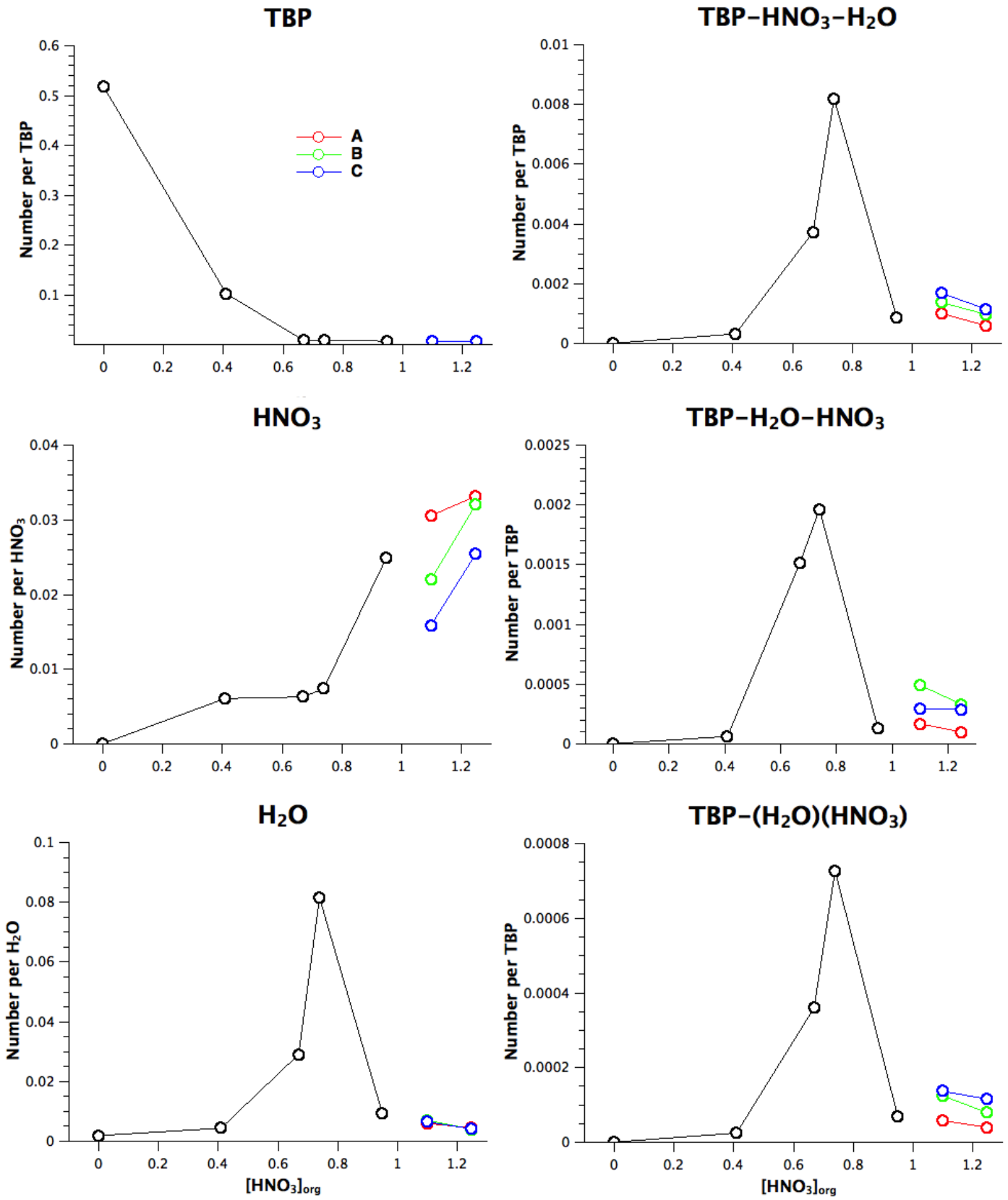

Fig. 2 The average observed number of the TBP, TBP-HNO_3-H_2O, HNO_3, TBP-H_2O-HNO_3, H_2O and TBP(HNO_3)(H_2O) structures.

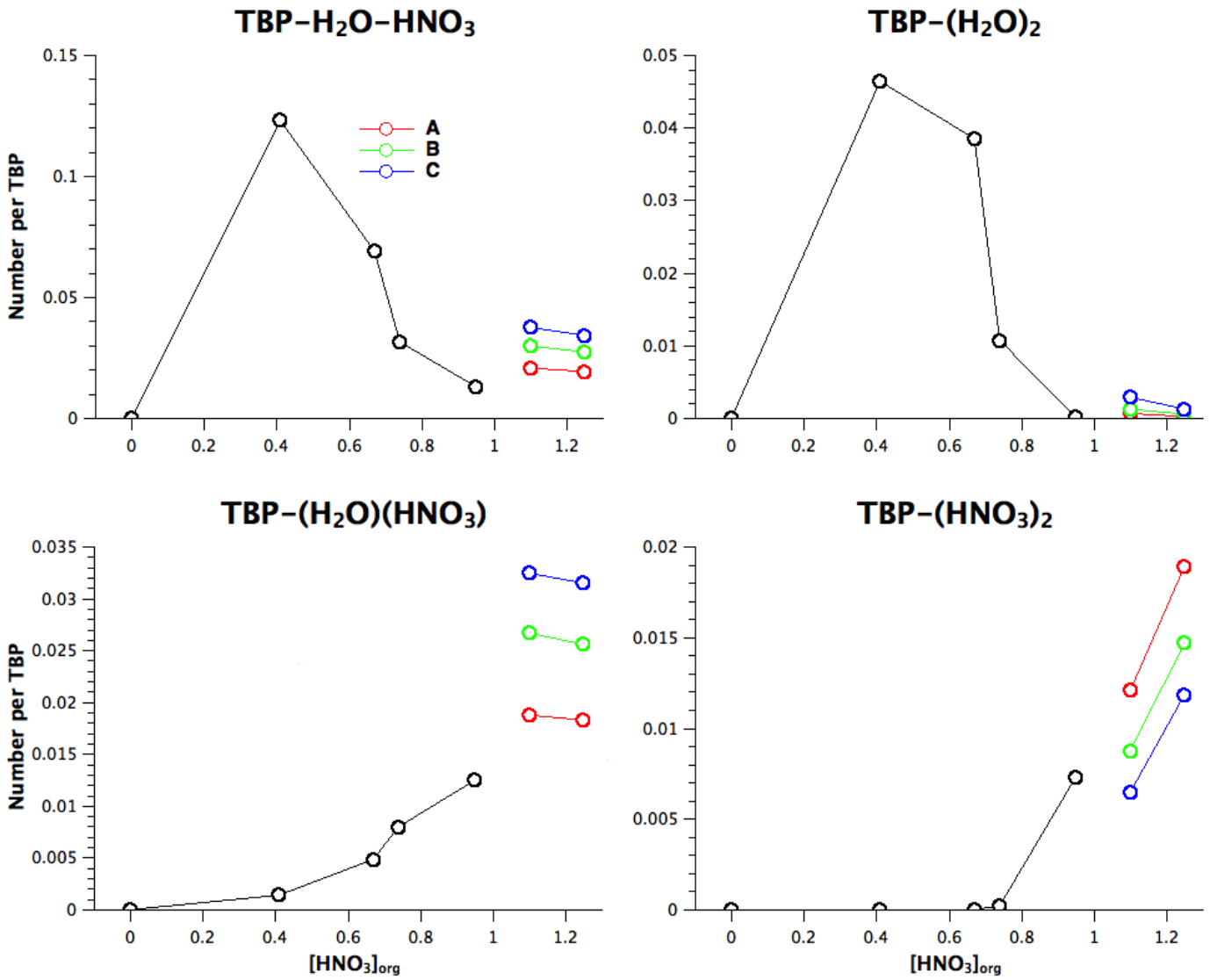

Fig. 3 The average observed number of the TBP-H_2O-HNO_3, TBP$(H_2O)_2$, TBP$(H_2O)(HNO_3)$ and TBP$(HNO_3)_2$ substructures.

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