Supplementary Material

Computation of the dissociation temperature of TBAB semi-clathrate in an aqueous solution using molecular simulations

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Table 1: Parameters for intramolecular bond potential in the TBAB molecule. The bond potential is modeled as $E_{bond} = k_r(r - r_0)^2$.

Bond (harmonic)	k_r (kcal/mol/Å^2)		r_0 (Å)	
	OPLS	GAFF	OPLS	GAFF
C-H_C	340	340	1.090	1.090
C-H_N	340	240	1.090	1.090
C-C	268	310	1.529	1.526
C-N	367	367	1.471	1.471

Table 2: Parameters for intramolecular bending potential in the TBAB molecule. The bending potential is modeled as $E_{bend} = k_\theta(\theta - \theta_0)^2$.

Angle (harmonic)	k_θ (kcal/mol/rad^2)		θ_0 (degree)	
	OPLS	GAFF	OPLS	GAFF
H_C-C-H_C	33.00	35.00	107.8	109.5
H_N-C-H_N	33.00	35.00	107.8	109.5
C-C-H_C	37.50	50.00	110.7	109.5
C-C-C	58.35	40.00	112.7	109.5
C-C-N	80.00	80.00	111.2	111.2
H_N-C-N	35.00	50.00	109.5	109.5
C-N-C	50.00	50.00	113.0	109.5

Table 3: Parameters for intramolecular dihedral potential in TBAB molecule. The dihedral potential is modeled as $E^{OPLS}_{dihedral} = \frac{k_1}{2}[1 + \cos(\phi)] + \frac{k_2}{2}[1 - \cos(2\phi)] + \frac{k_3}{2}[1 + \cos(3\phi)]$ for the OPLS forcefield and $E^{GAFF}_{dihedral} = \frac{k}{2}[1 + \cos(\phi - d)]$ for the GAFF forcefield. The units of k's are in kcal/mol and d in degree.

Dihedral angle	OPLS-AA			GAFF	
	k_1	k_2	k_3	k	d
H_C-C-C-H_C	0.0000	0.0000	0.3000	0.15	0
H_C-C-C-C	0.0000	0.0000	0.3000	0.16	0
H_C-C-C-H_N	0.0000	0.0000	0.3000	0.15	0
H_N-C-C-C	0.0000	0.0000	0.3000	0.16	180
C-C-C-C	1.3000	-0.0500	0.2000	0.18	0
C-C-C-N	2.7320	-0.2290	0.4850	0.15	0
C-C-N-C	1.4379	-0.1238	0.2639	0.15	0
H_C-C-C-N	0.0000	0.0000	0.3840	0.15	0
H_C-C-N-C	0.0000	0.0000	0.3017	0.15	0