Supplementary Information for

Managing Hydrogen Bonding in the Clathrate Hydrate of the 1-Pentanol Guest Molecule

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Table S1. Atomic point charges and Lennard-Jones parameters for H_2O, NH_4F, CH_3OH, and 1-PeOH. The Lorentz-Berthelot combination rules are used for the Lennard-Jones parameters of unlike atom types.

Atom	q / e	σ_{ii} / Å	ε_{ii} / kcal·mol^{-1}
O_W (H_2O)	0.0	3.1668	0.2108
H_W (H_2O)	+0.5897	0.000	0.000
EE (H_2O)	-1.1794	0.000	0.000
F_H (F^-)	-1.0000	2.997	0.050
N_H (NH_4^+)	-0.4000	3.250	0.1700
H_N (NH_4^+)	+0.3500	0.000	0.000
CH_3 (CH_3OH)	+0.265	3.740	0.2090
O (CH_3OH)	-0.700	3.030	0.1719
H (CH_3OH)	+0.435	0.000	0.000
C_1 (1-PeOH)	-0.079	3.400	0.1094
H(C_1) (1-PeOH)	+0.010	2.650	0.0157
C_2 (1-PeOH)	+0.136	3.400	0.1094
H(C_2) (1-PeOH)	-0.036	2.650	0.0157
C_3 (1-PeOH)	+0.030	3.400	0.1094
H(C_3) (1-PeOH)	-0.015	2.650	0.0157
C_4 (1-PeOH)	0.069	3.400	0.1094
H(C_4) (1-PeOH)	-0.026	2.650	0.0157
C_5 (1-PeOH)	0.297	3.400	0.1094
H(C_5) (1-PeOH)	-0.038	2.471	0.0157
O (1-PeOH)	-0.632	3.066	0.2104
H (1-PeOH)	0.371	0.000	0.000

Figure S1. The comparison of $\Delta\delta_{expt.,liq.}$ with $\Delta\delta_{calc.}$ for the chemical shifts of each conformer of 1-PeOH. The definitions of the conformers are given in Table 1 of the text.