Supplementary Information for

Ice-Inclusion Compounds for Energy Gas Storage (from J. Phys. Chem. C 2022, 126, 32, 13585–13594)

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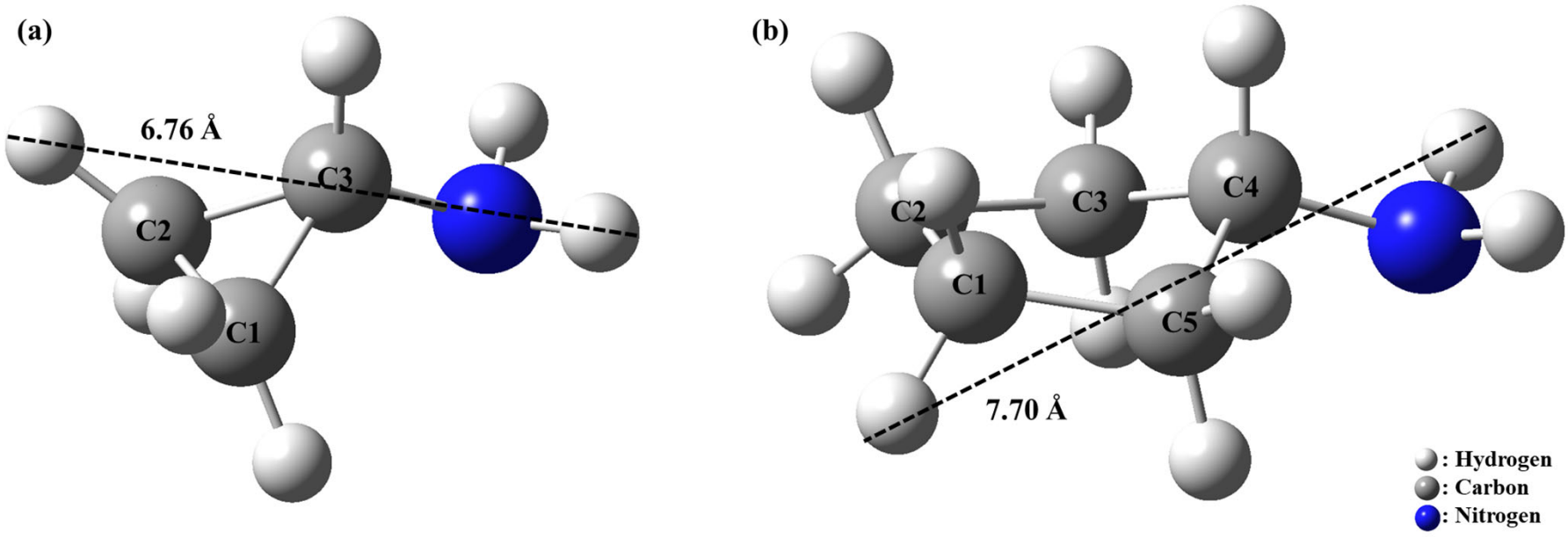

Figure 1. Optimized molecular conformation and size of (a) cyclopropylamine and (b) cyclopentylamine (Grey, carbon; white, hydrogen; blue, nitrogen).

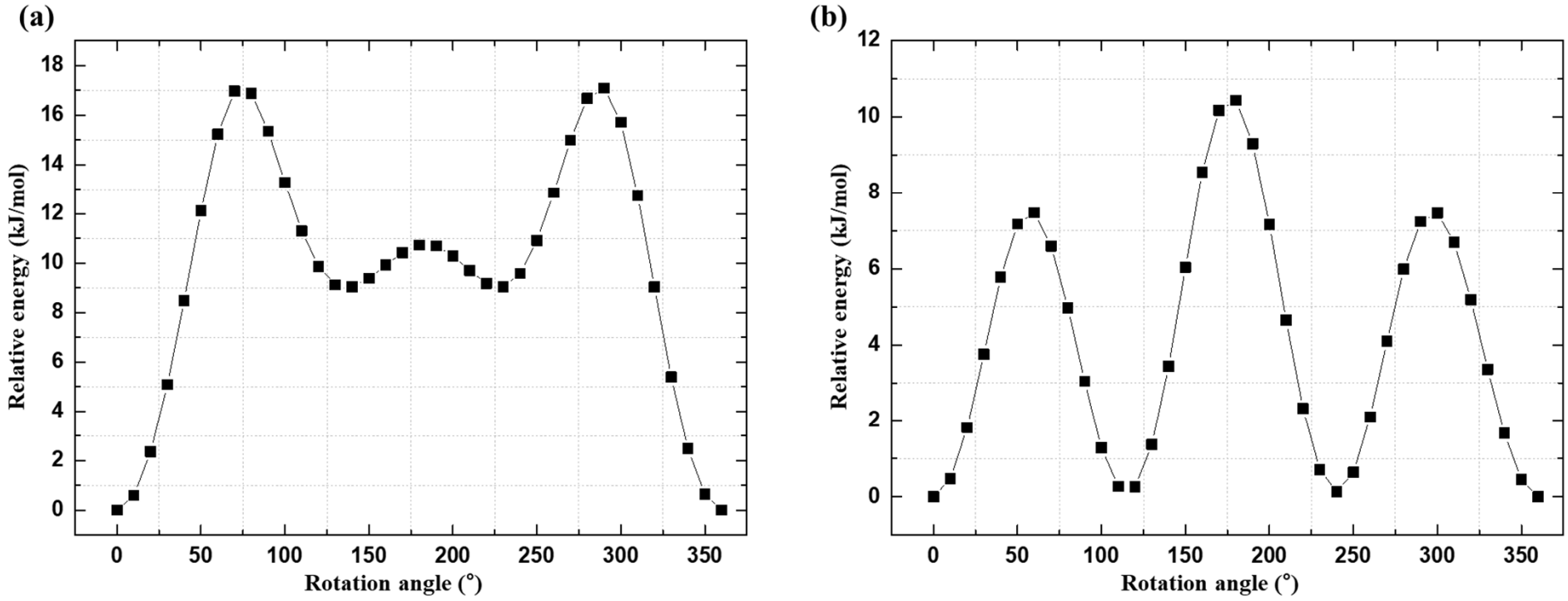

Figure 2. Potential energy surface of (a) cycloproylamine and (b) cyclopentylamine as a function of the dihedral angle (H-N-C3-C1 for cyclopropylamine and H-N-C4-C3 for cyclopentylamine).

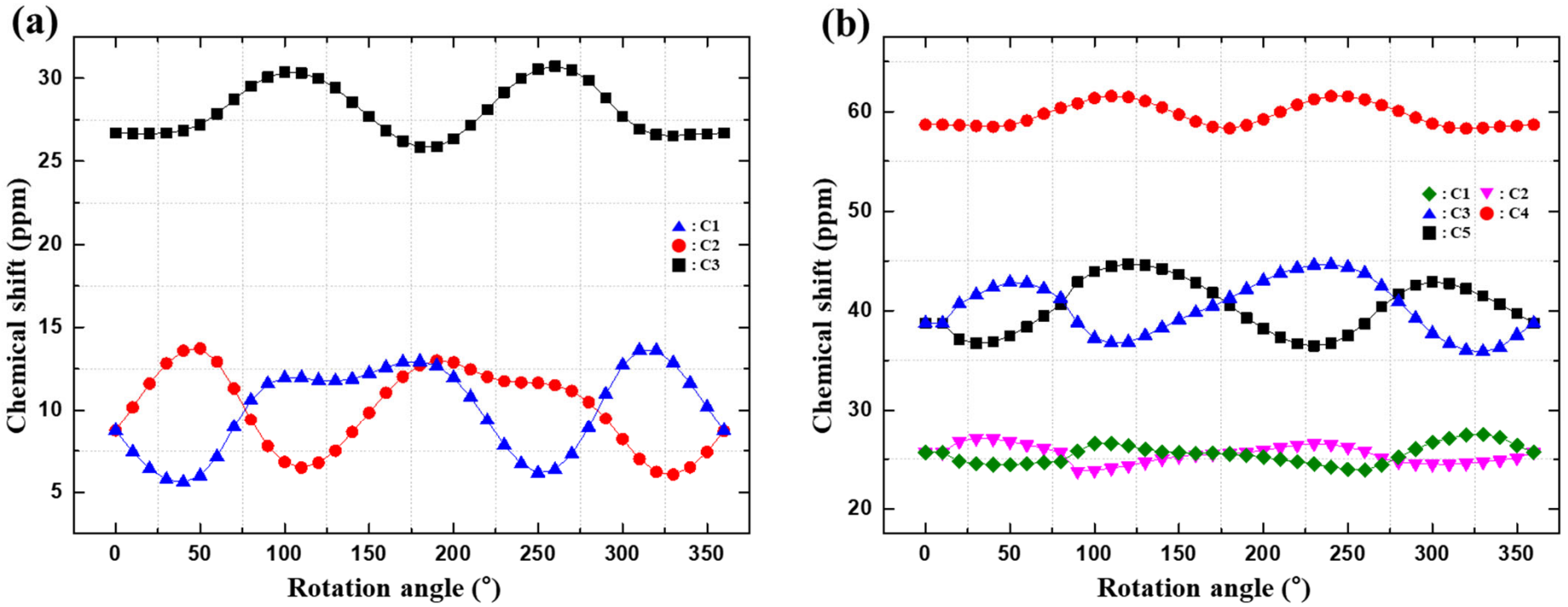

Figure 3. Changes in the chemical shift of the carbon atoms in (a) cyclopropylamine and (b) cyclopentylamine as a function of the dihedral angle (H-N-C3-C1 for cyclopropylamine and H-N-C4-C3 for cyclopentylamine).

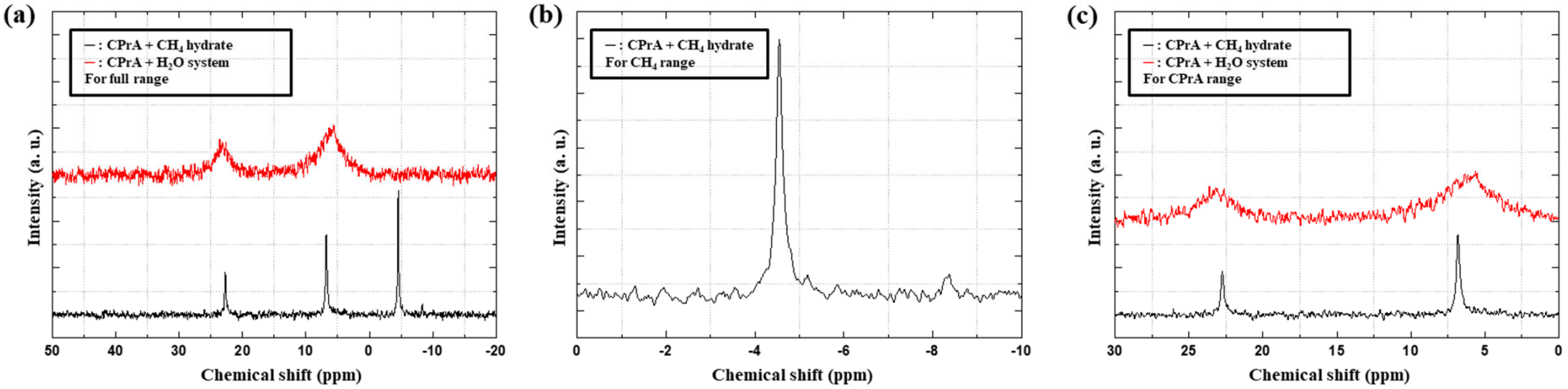

Figure 4. ^{13}C NMR spectra of (cyclopropylamine + CH_4) hydrate and (cyclopropylamine + H_2O) system for (a) full range, (b) CH_4 region, and (c) cyclopropylamine region.

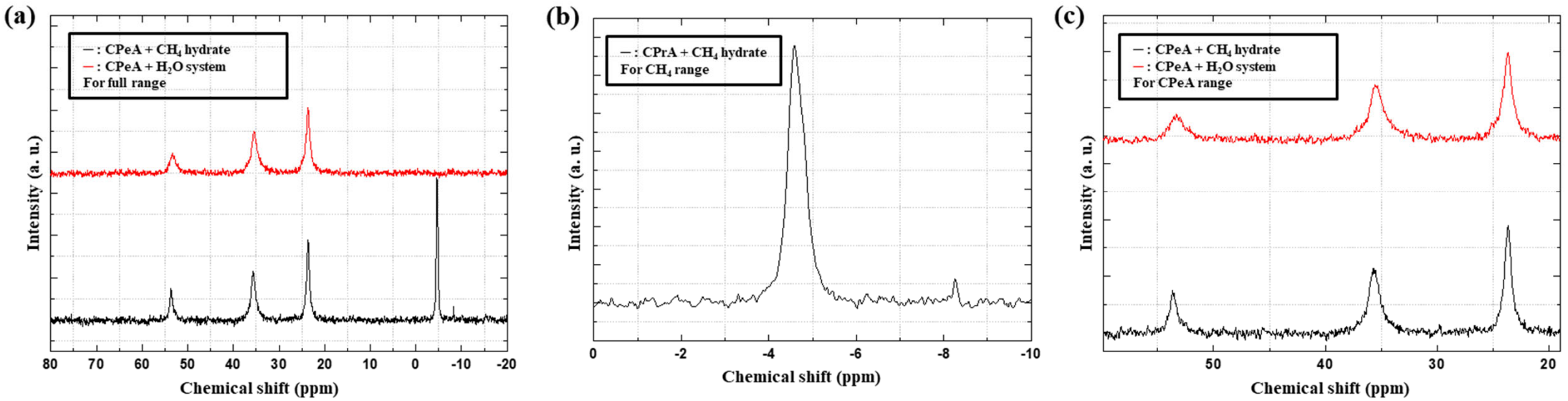

Figure 5. ^{13}C NMR spectra of (cyclopentylamine + CH_4) hydrate and (cyclopentylamine + H_2O) system for (a) full range, (b) CH_4 region, and (c) cyclopentylamine region.

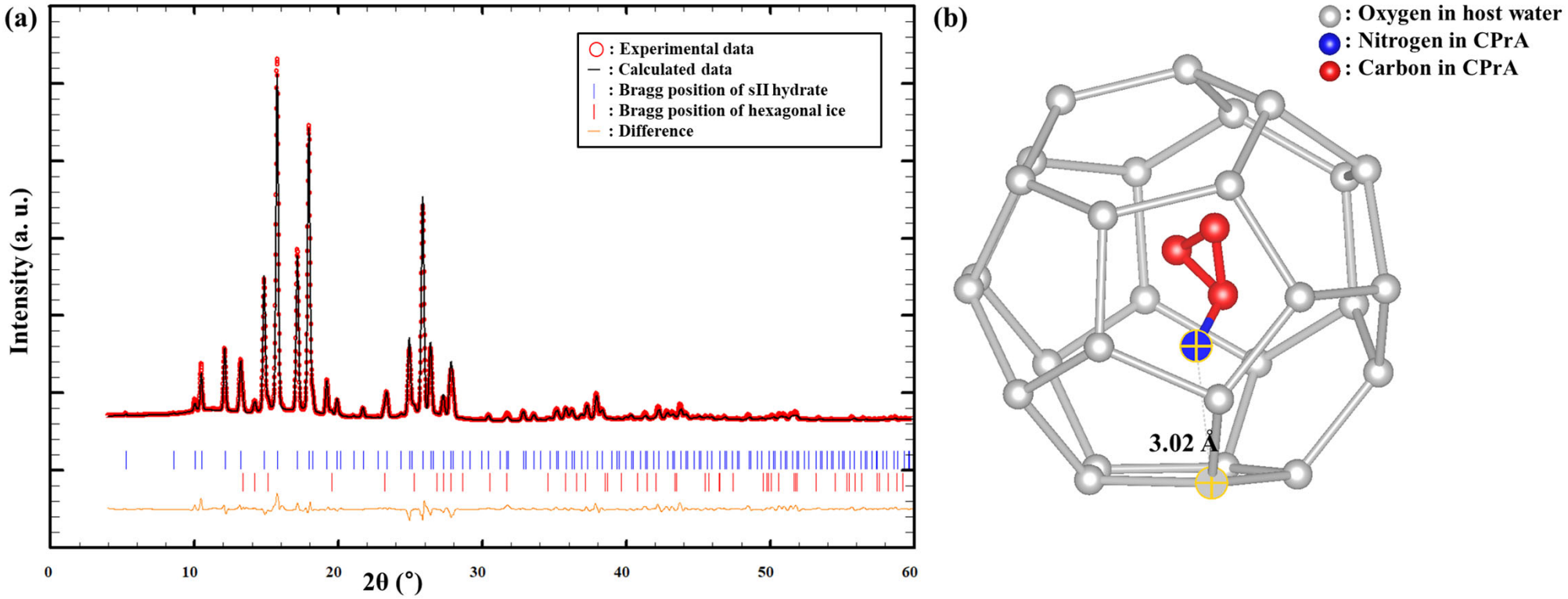

Figure 6. (a) Supramolecular crystallography pattern of (cyclopropylamine + CH_4) hydrate measured at 100 K and the Rietveld refinement results (background corrected R_{wp} = 11.5 % and χ^2 = 18.1). Tick marks indicate the Bragg position for sII hydrate (top) and the hexagonal ice (bottom) and (b) the cyclopropylamine in the large ($5^{12}6^4$) cage of sII hydrate (grey, oxygen in water host molecule; blue, nitrogen in guest molecule; red, carbon in guest molecule).

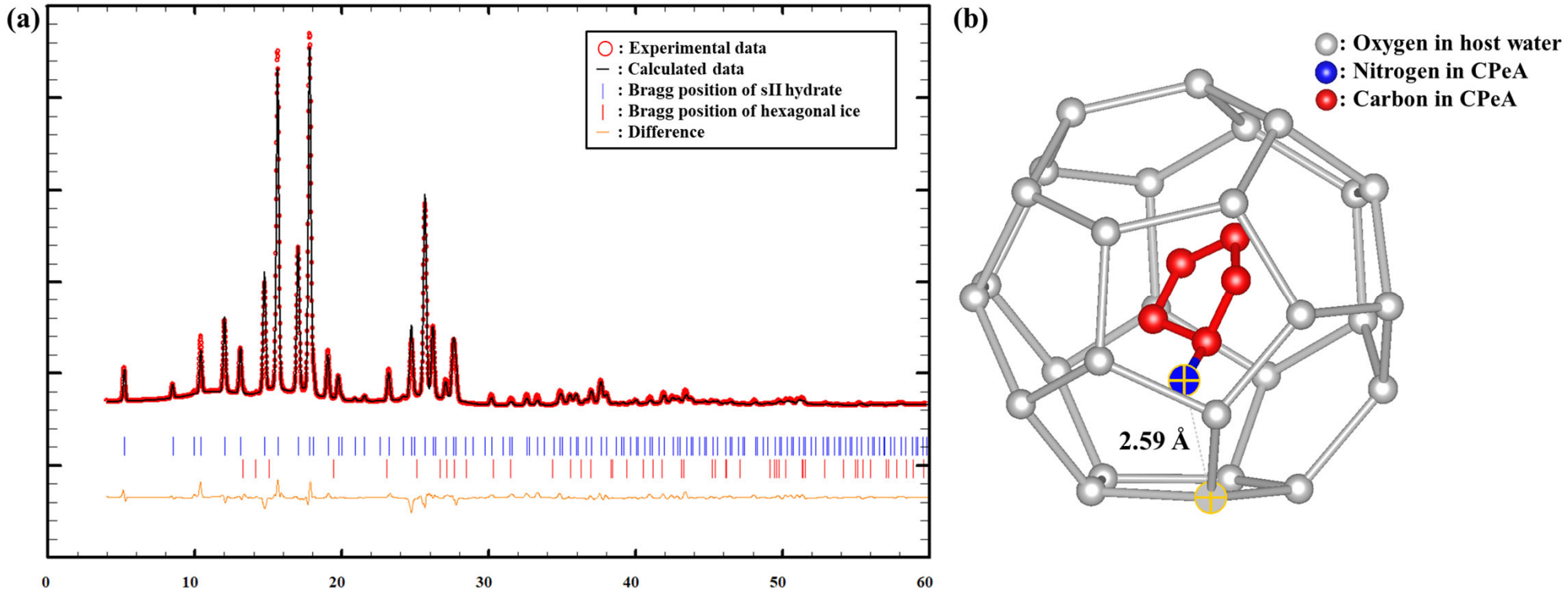

Figure 7. (a) Supramolecular crystallography pattern of (cyclopentylamine + CH_4) hydrate measured at 100 K and the Rietveld refinement results (background corrected R_{wp} = 11.8 % and χ^2 = 16.9). Tick marks indicate the Bragg position for sII hydrate (top) and the hexagonal ice (bottom) and (b) the cyclopentylamine in the large ($5^{12}6^4$) cage of sII hydrate (grey, oxygen in water host molecule; blue, nitrogen in guest molecule; red, carbon in guest molecule).

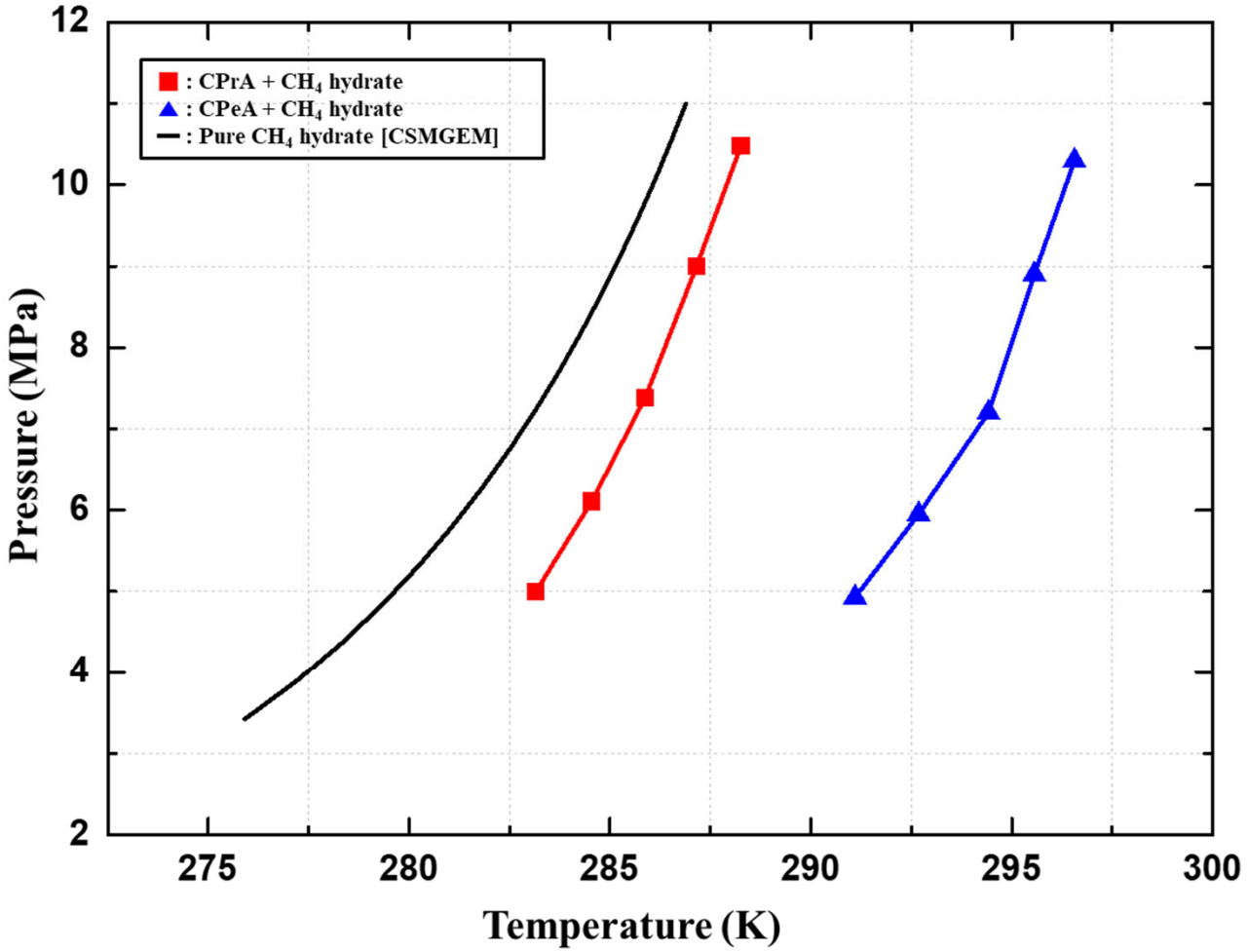

Figure 8. Phase equilibria of (cyclopropylamine + CH_4), (cyclopentylamine + CH_4), and pure CH_4 hydrate from CSMGEM.

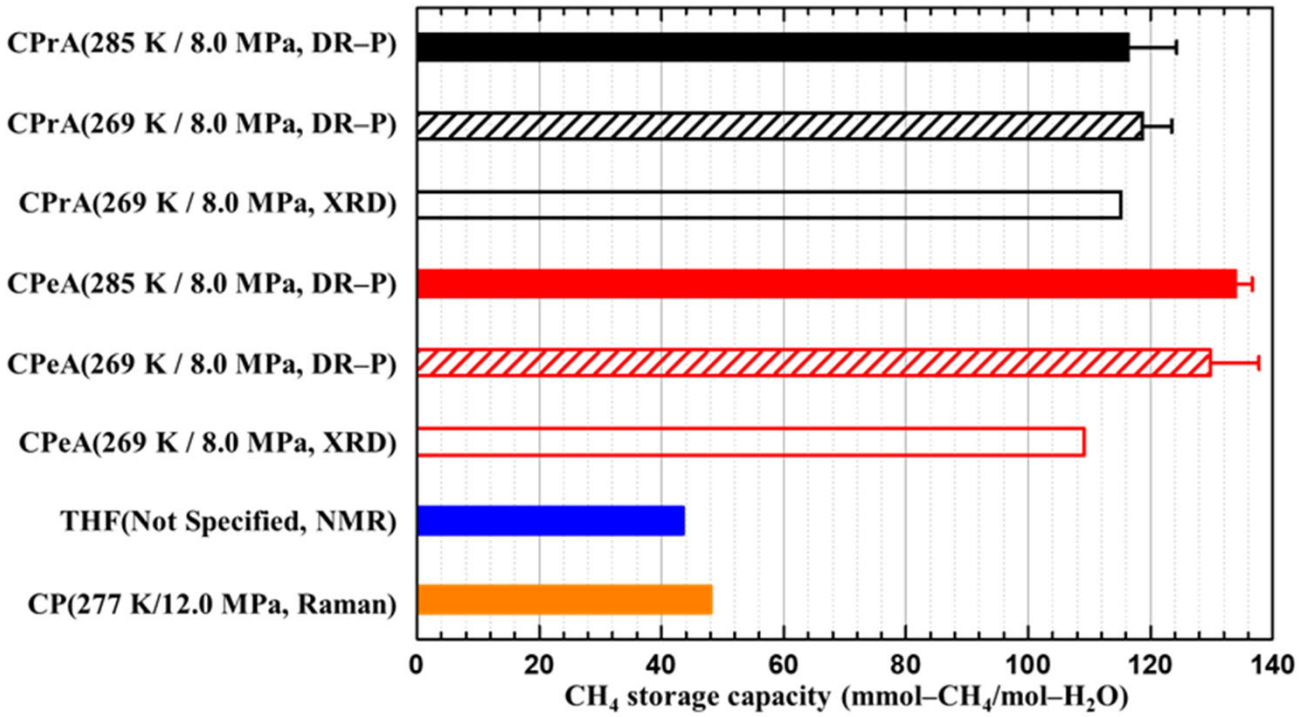

Figure 9. CH_4 storage capacity of the binary (cyclopropylamine + CH_4) and (cyclopentylamine + CH_4) hydrate and other CH_4 hydrate from different conditions.