

Supplementary Materials to
“Hydrate phase equilibrium of CH₄+N₂+CO₂ gas mixtures and cage
occupancy behaviors”

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Figure S1. The mole ratio of CH₄ in large cages and small cages ($3x/\theta$) (calculated by CSMHYD program).

Figure S2. Relationship of values of θ/x of N₂ and CO₂ molecules with temperature.

Figure S3. Occupancy ratios of N₂ and CO₂ in hydrate cages (calculated by CSMHYD program).

Figure S4. Mole ratios of N₂/CO₂ in small and large cages(calculated by CSMHYD program).

Figure S5. Relative occupancies of CH₄/N₂/CO₂ in small cages (a), large cages (b) and hydrate cages(c) (calculated by CSMHYD program).

Figure S6. Variation of occupancy of CO₂ in large cages with the concentration of CH₄ in gas phase.

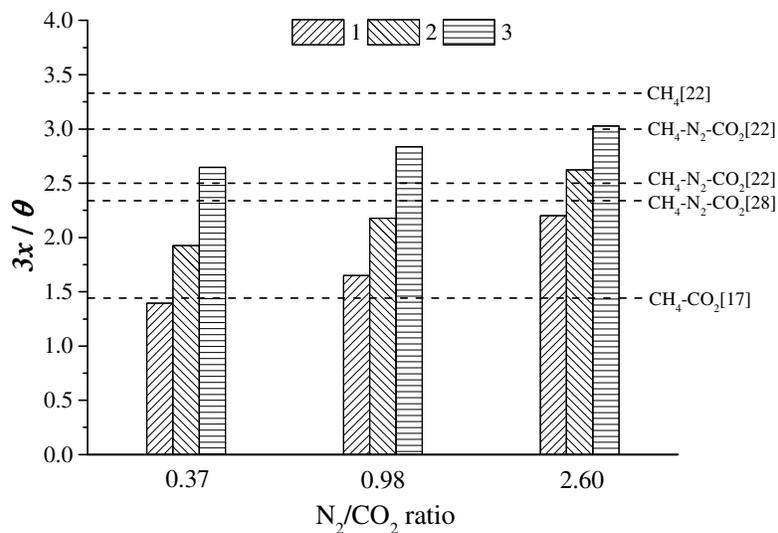


Figure S1. The mole ratio of CH₄ in large cages and small cages ($3x/\theta$) (calculated by CSMHYD program) The numbers of 1, 2 and 3 respectively represent the CH₄ levels of 20%, 50% and 80% in each group with different N₂/CO₂ ratios.

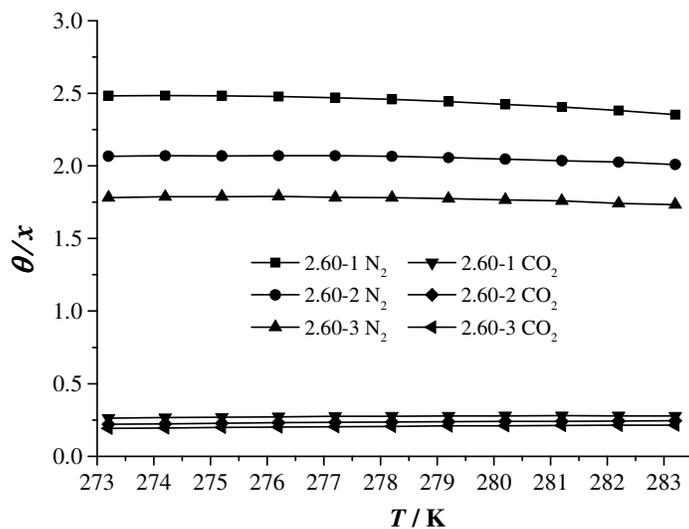


Figure S2. Relationship of values of θ/x of N₂ and CO₂ molecules with temperature. The numbers of 1, 2 and 3 respectively represent the CH₄ levels of 20%, 50% and 80% in each group with different N₂/CO₂ ratios.

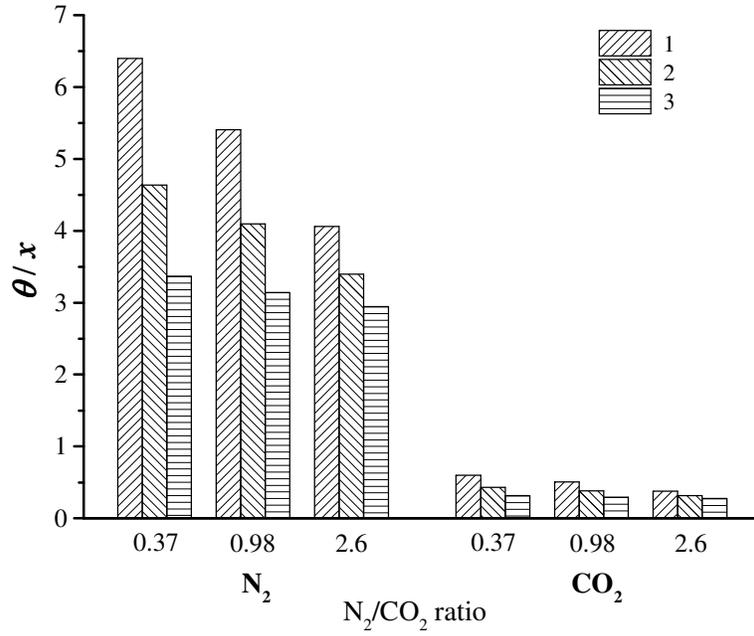
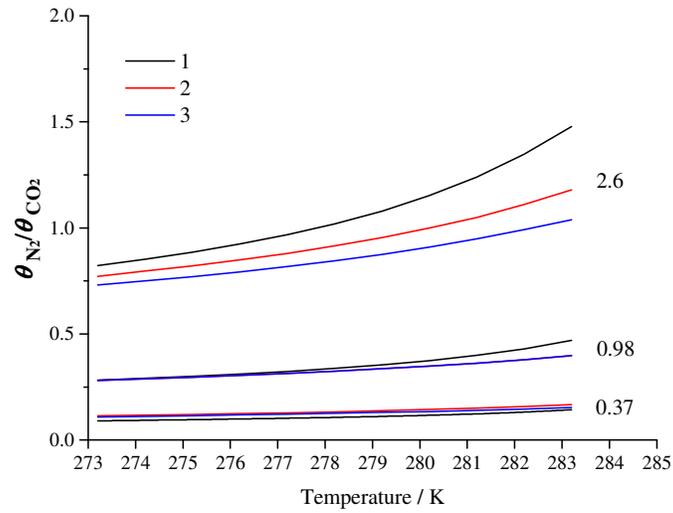
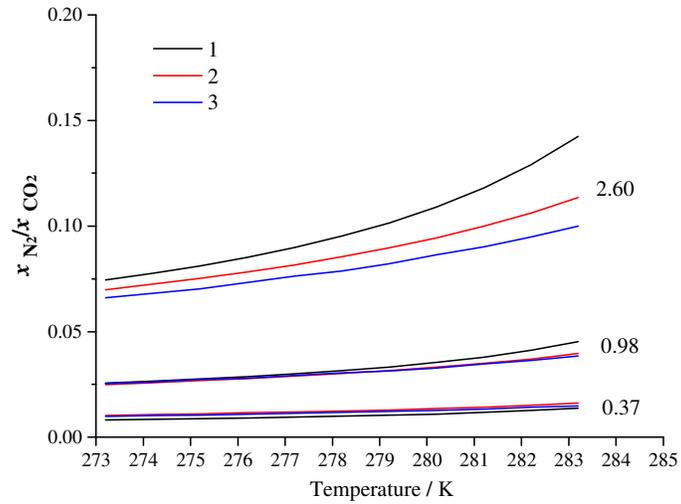


Figure S3. Occupancy ratios of N_2 and CO_2 in hydrate cages (calculated by CSMHYD program). The numbers of 1, 2 and 3 respectively represent the CH_4 levels of 20%, 50% and 80% in each group with different N_2/CO_2 ratios.

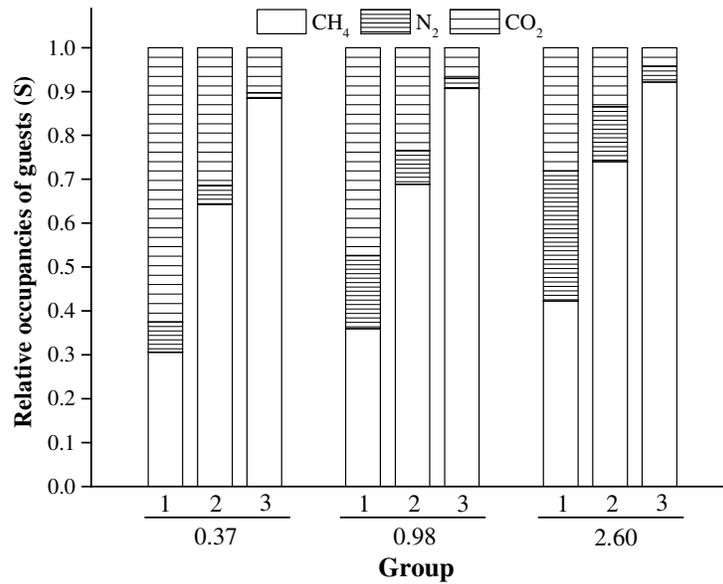


a. In small cage

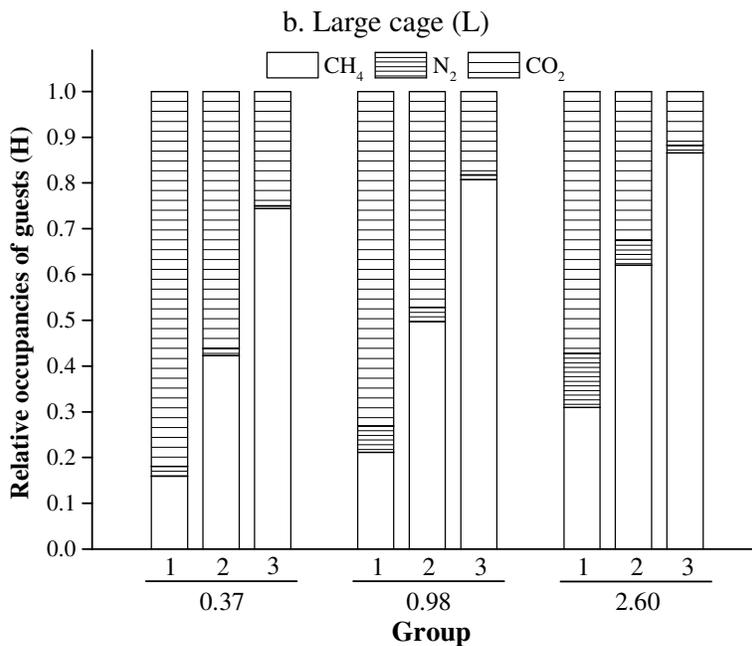
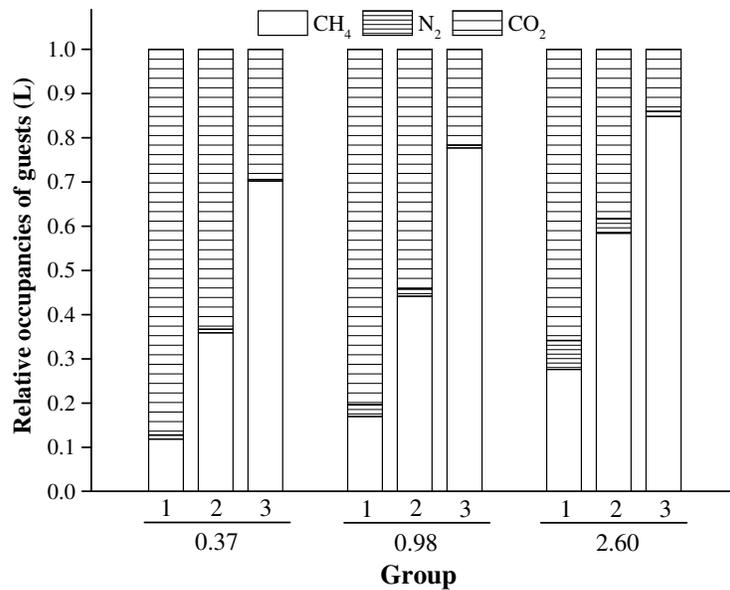


b. In large cage

Figure S4. Mole ratios of N_2/CO_2 in small and large cages (calculated by CSMHYD program). The numbers of 1, 2 and 3 respectively represent the CH_4 levels of 20%, 50% and 80% in each group with different N_2/CO_2 ratios.



a. Small cage (S)



c. Hydrate cages (H)

Figure S5. Relative occupancies of CH₄/N₂/CO₂ in small cages (a), large cages (b) and hydrate cages (c) (calculated by CSMHYD program). The numbers of 1, 2 and 3 respectively represent the CH₄ levels of 20%, 50% and 80% in each group with different N₂/CO₂ ratios.

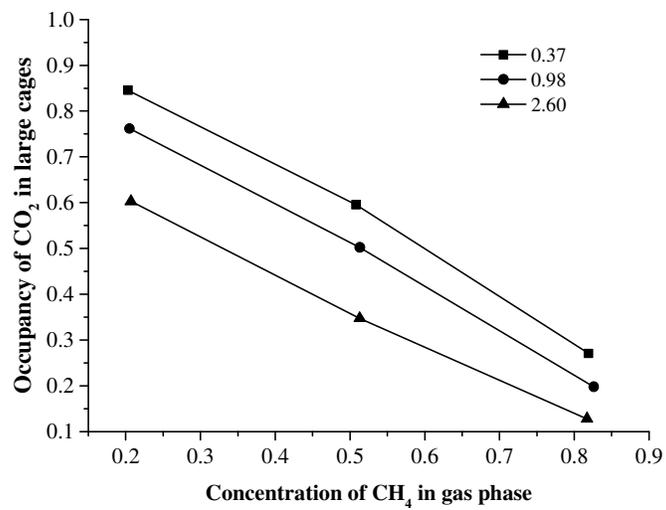


Figure S6. Variation of occupancy of CO₂ in large cages with the concentration of CH₄ in gas phase