

## **Supporting Information**

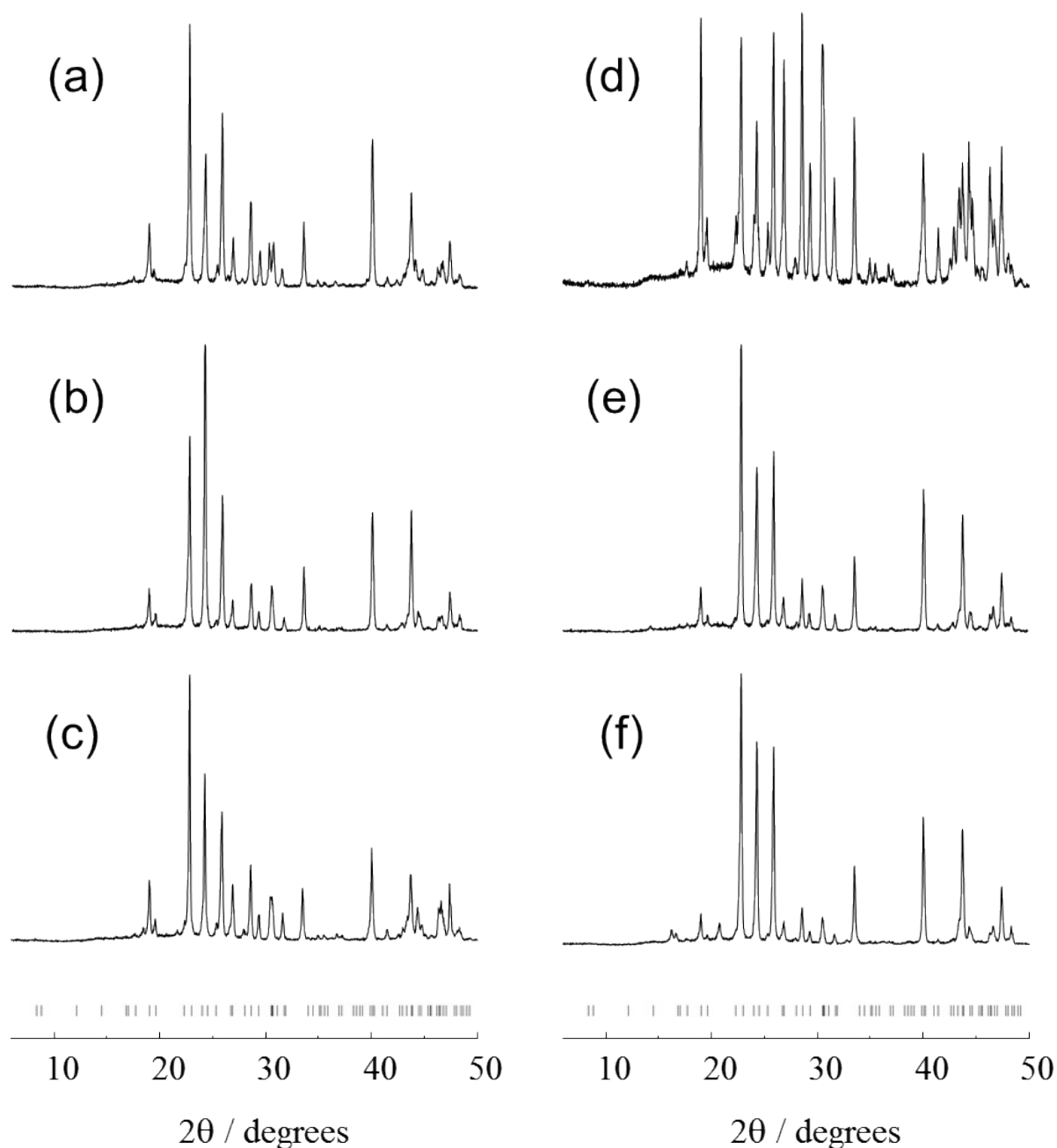
# **Effect of Temperature and Large Guest Molecules on the C–H Symmetric Stretching Vibrational Frequencies of Methane in Structure H and I Clathrate Hydrates**

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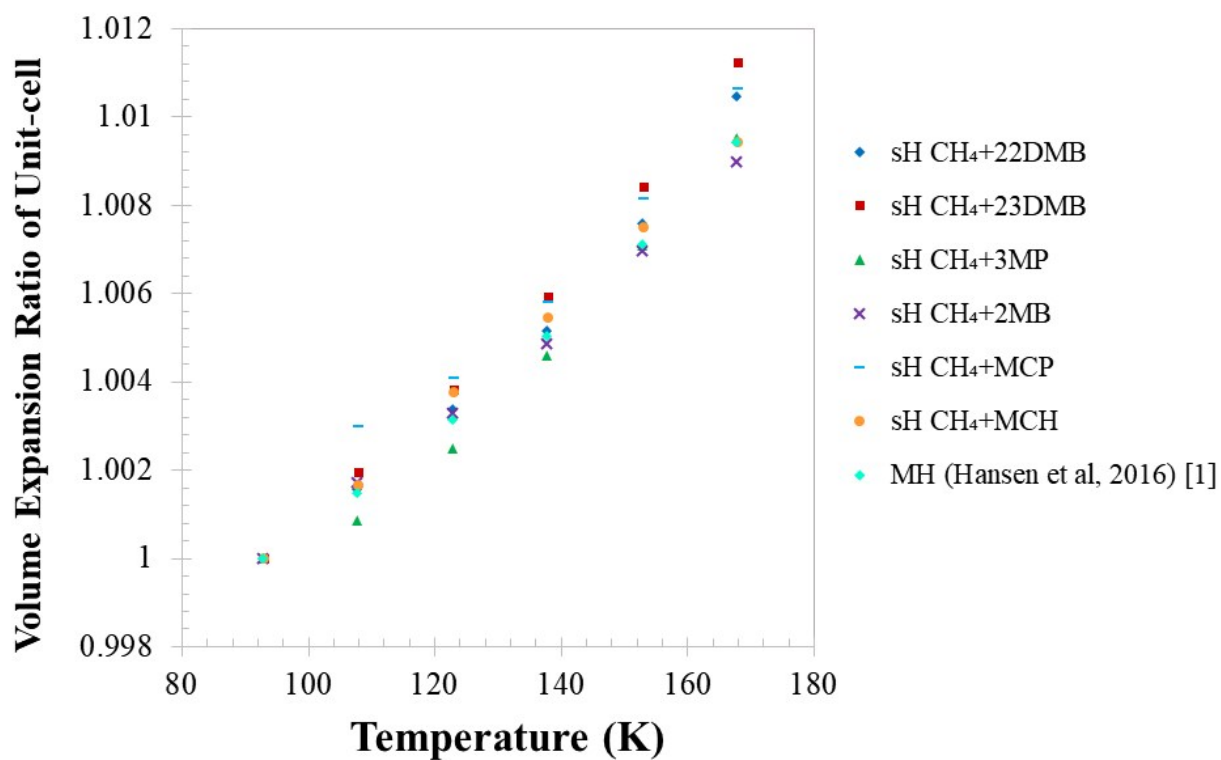
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**Fig. S1.** X-ray diffraction patterns of the structure H hydrates at 93 K: (a)  $\text{CH}_4$  + 2,2-dimethylbutane hydrate; (b)  $\text{CH}_4$  + 2,3-dimethylbutane hydrate; (c)  $\text{CH}_4$  + 3-methylpentane hydrate; (d)  $\text{CH}_4$  + 2-methylbutane hydrate; (e)  $\text{CH}_4$  + methylcyclopentane hydrate; (f)  $\text{CH}_4$  + methylcyclohexane hydrate. The curves in each pattern represent the observed intensities. The line marks below each pattern show the calculated peak positions for hexagonal ice.



**Fig. S2.** Temperature effect on volume expansion ratio of unit-cell for six types sH hydrates and sI CH<sub>4</sub> hydrate (MH).<sup>1</sup>

## Reference

- [1] Hansen, T. C.; Falenty, A.; Kuhs, W. F. Lattice Constants and Expansivities of Gas Hydrates from 10 K up to the Stability Limit. *J. Chem. Phys.* **2016**, 145, 7066–7070.