Supplementary Material (ESI) for PCCP

Supporting Information for: Molecular Dynamics Simulation of NMR Powder Lineshapes of Linear Guests in Structure I Clathrate Hydrate

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Figure S1. Two of the large structure I cages extracted from the unit cell showing the different proton orientations in water for the two cages. Guest molecules in each cage will experience a slightly different net intermolecular potential from the cage as a result of the differing proton orientations. In a) the hexagonal faces are aligned in the *x*-direction, while in b), they are aligned in the *z*-direction.

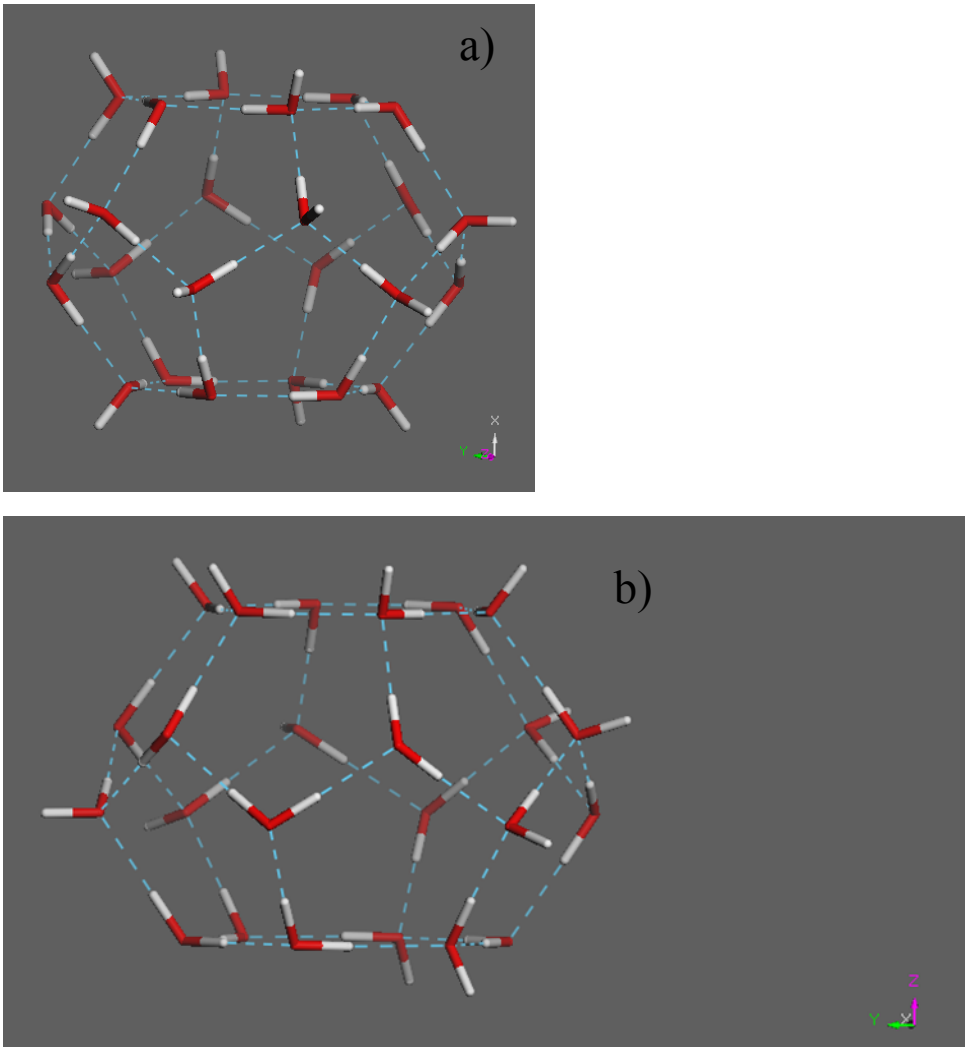


Figure S2. Snapshots of the distributions of CS in the small sI cages at 70, 150 and 200 K during a 100 ps trajectory (left hand column) and a 6 ns trajectory (right hand column). The carbon atoms are shown with blue spheres and the sulfur with yellow spheres

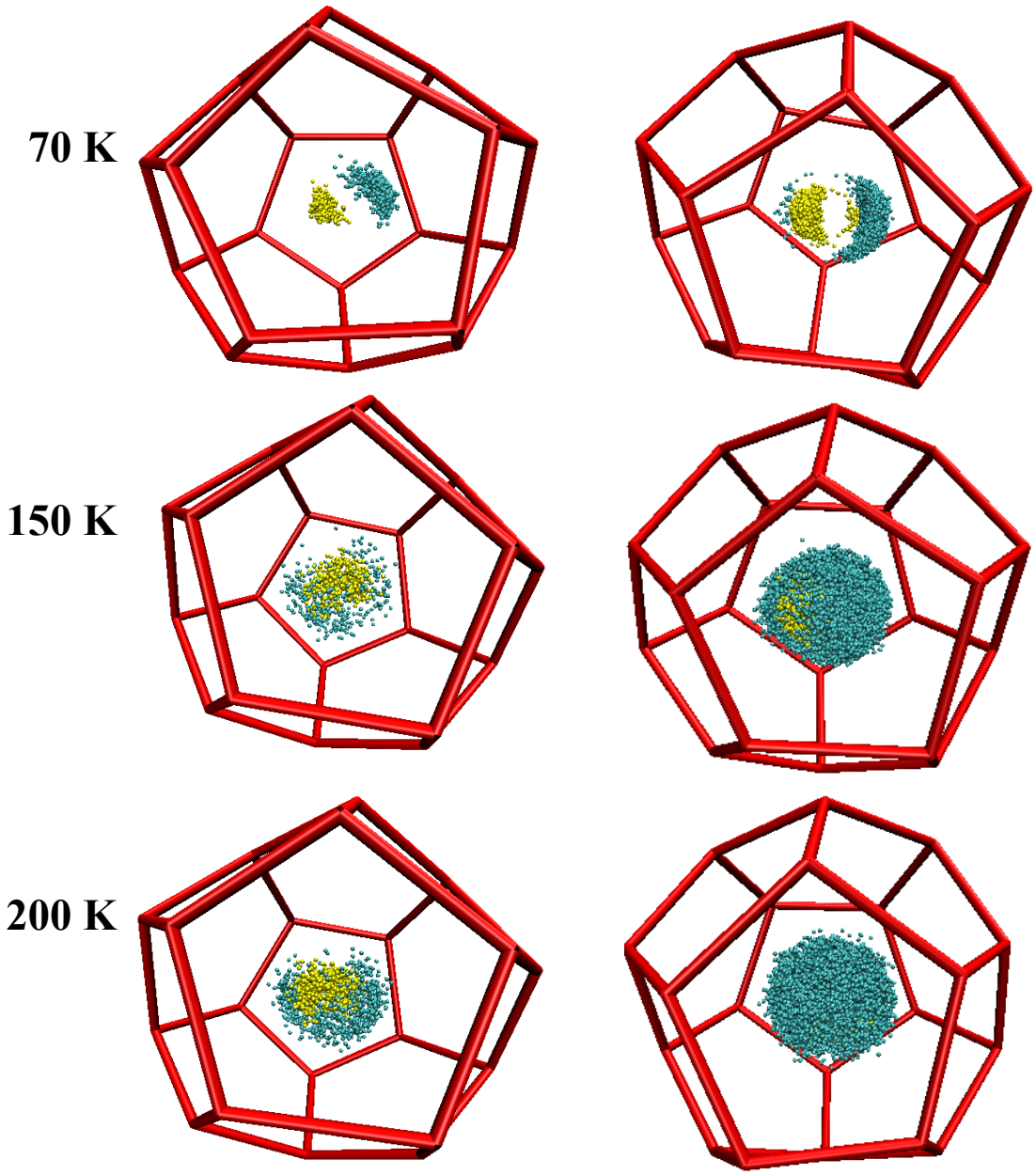
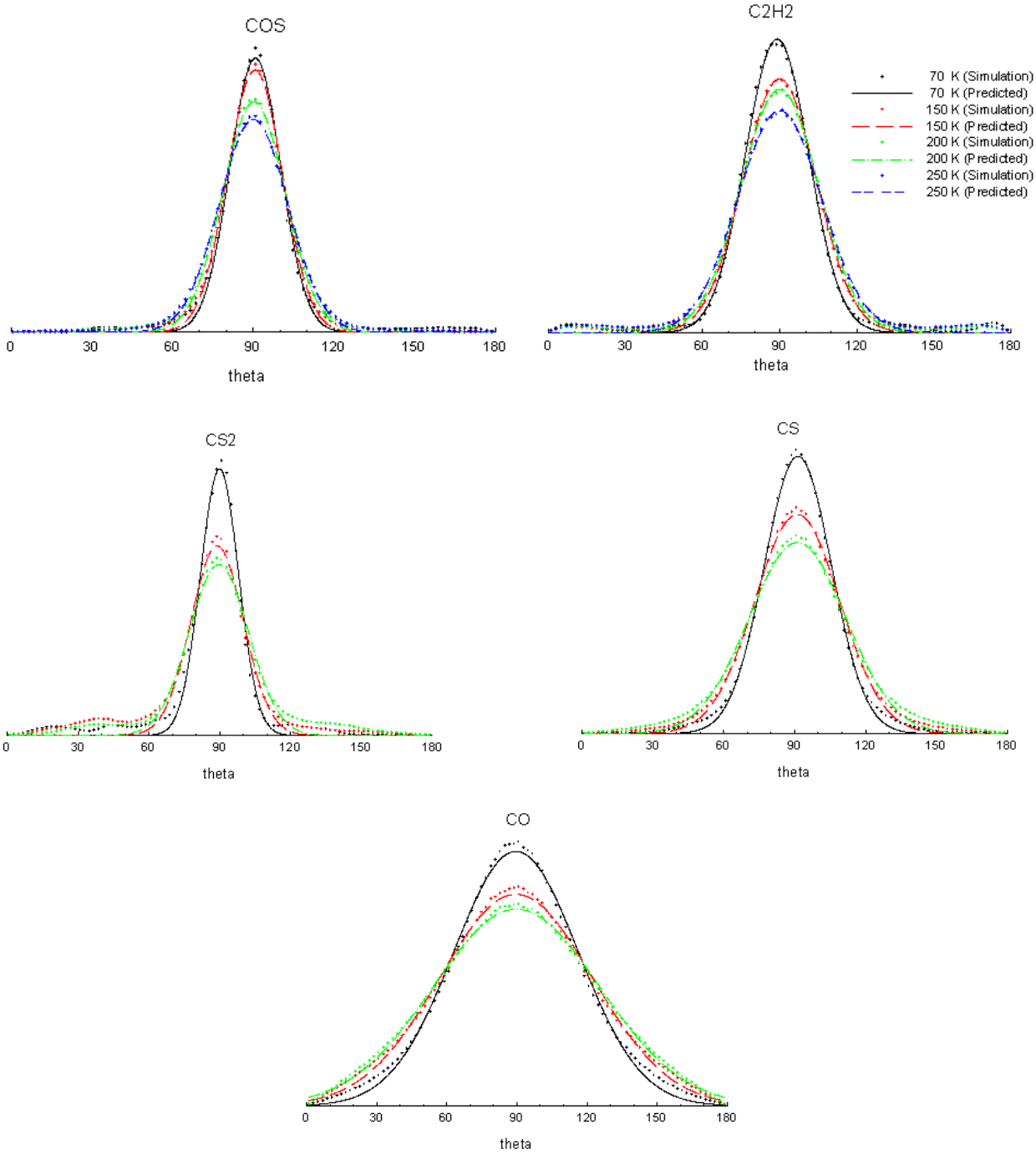


Figure S3. The simulated and fitted Gaussian distributions of polar angle probability distribution function $P(\theta,T)$ of the guest molecules in large sI cages at 1 bar and different temperatures. The temperature dependence of the FWHM is also shown.



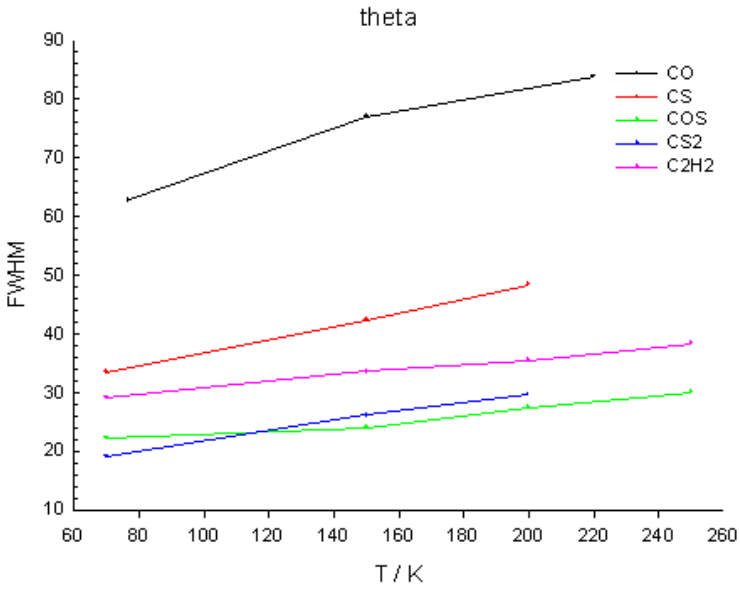

theta
FWHM
T / K
CO
CS
COS
CS2
C2H2
90
80
70
60
50
40
30
20
10
60
80
100
120
140
160
180
200
220
240
260

Figure S4. The simulated ^{13}C powder NMR lineshape at 70, 150 and 200 K and 1 bar for CS in the spherical small sI cages. Trajectories of 6 ns length were used for determining the angle distributions of the CS guests.