Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects.

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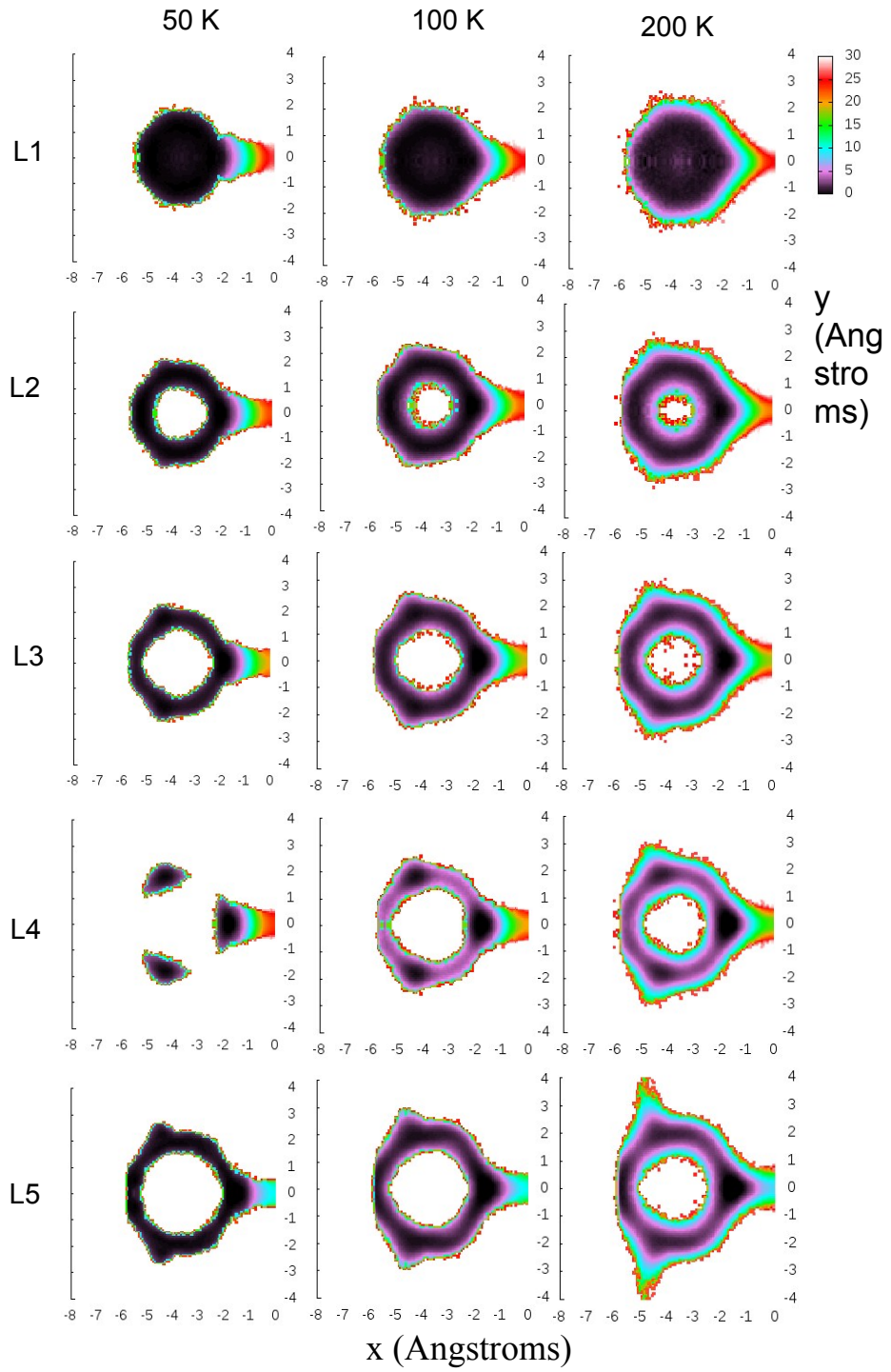


Figure S1. Free-energy surfaces F(x,y) for the different occupations and different temperatures, where the colour corresponds to the free-energy value in kJ/mol, and x and y are the perpendicular and parallel distances from the center of the bridging hexamer.

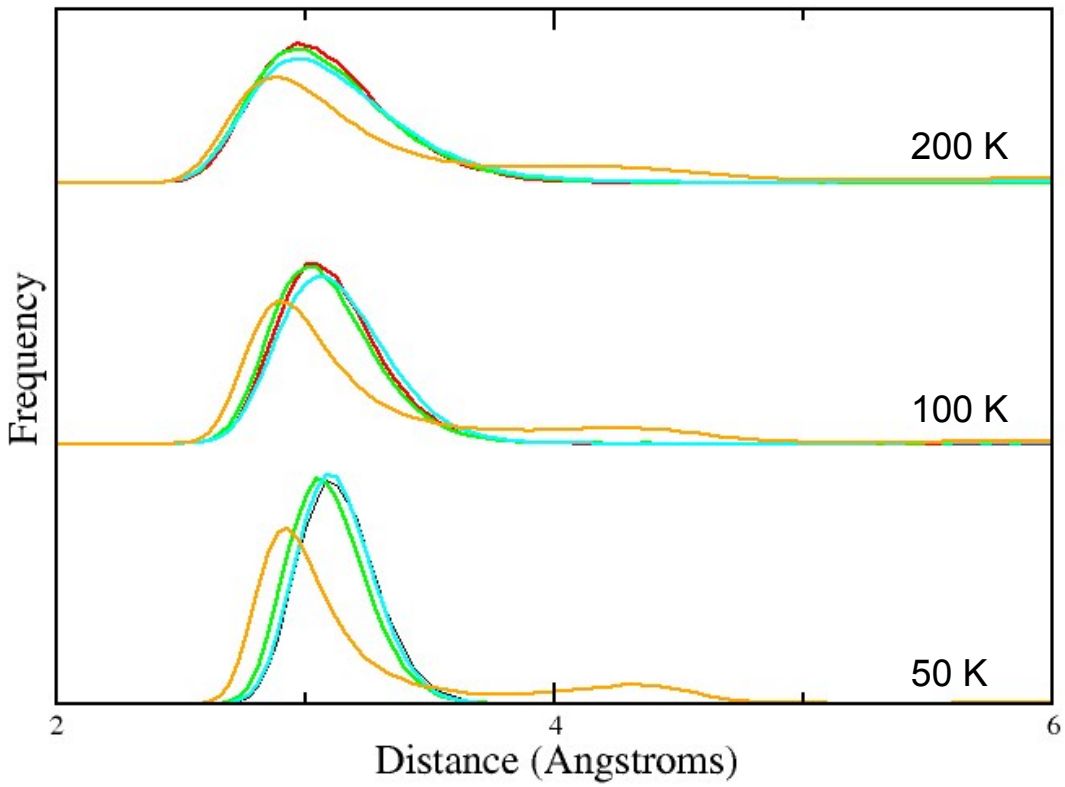
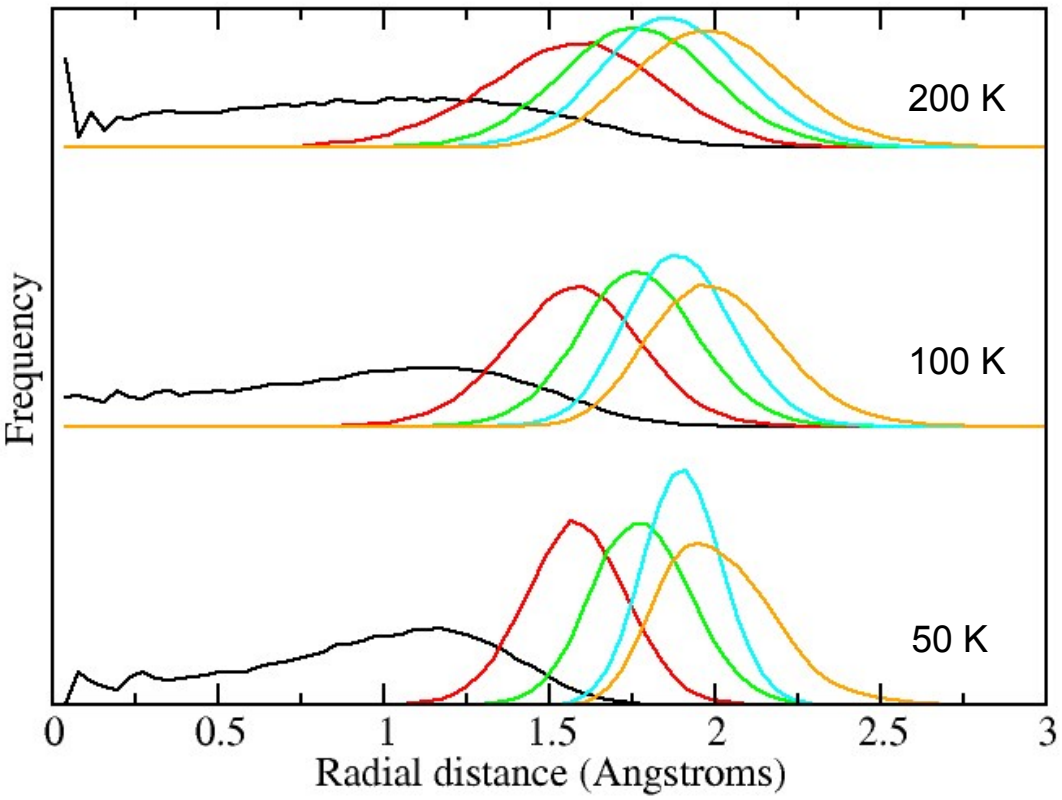


Figure S2. H_2 centre-of-mass distribution functions (path-integral). (a): above - Intermolecular separation between H_2 centres of mass inside each cage. (b): overleaf - Radial distance of H_2 centres of mass from the cage centre. (Divided by r^2 to give the frequency per unit shell volume.) Colour scheme: Black, red, green, cyan, orange corresponds to L1, L2, L3, L4, L5



See figure caption for bottom part of Figure S2 on the previous page (marked “overleaf”).