Low-temperature Thermodynamic Study of the Metastable Empty Clathrate Hydrates using Molecular Simulations

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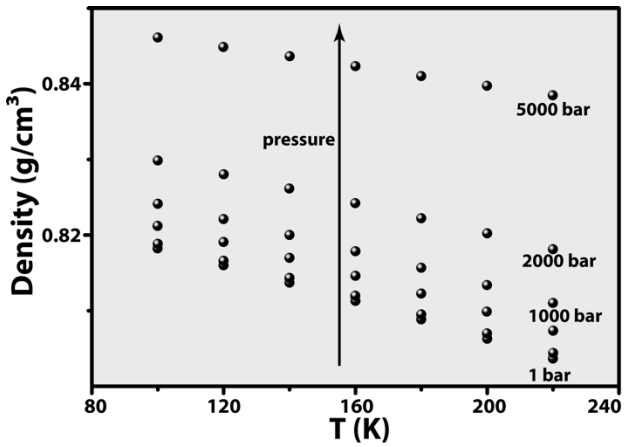

Figure SI1. Isobaric $\rho - T$ data obtained in the calculations for the empty sI clathrate hydrate phase.

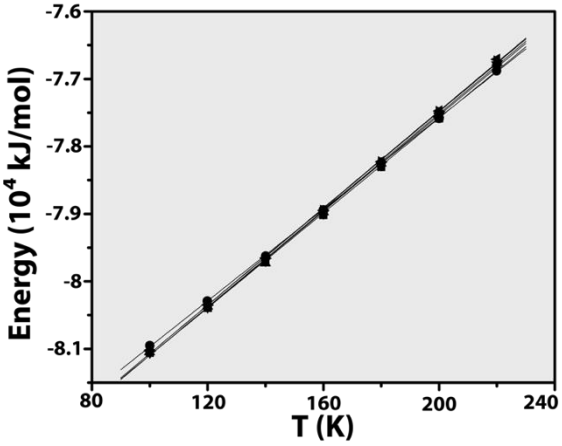

Figure SI2. Potential energy obtained from the calculations (symbols) and corresponding linear correlations (lines): ◀) 1 bar, ▶) 100 bar, ▲) 500 bar, ▼) 1000 bar, ■) 2000 bar and ●) 5000 bar for the empty sI clathrate hydrate phase.

Table SI1. Isobaric thermal expansivity maxima, α_p, for the curves in Figure 3b.

P (bar)	1	100	500	1000	2000	5000
T^{max} (K)	194.7	193.0	193.8	189.6	183.0	166.2
α_p (10^{-5}K^{-1})	5.306	5.235	5.025	4.710	4.148	2.630

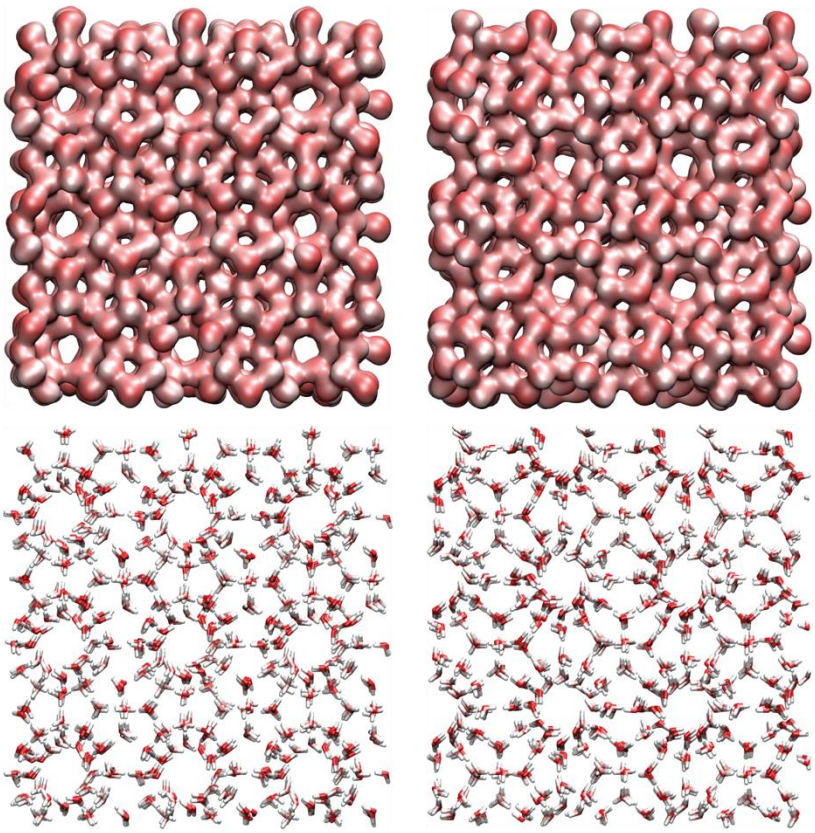

Figure SI3. Snapshots of two different views of the final configuration of the (5000 bar, 220 K) simulation after 50 ns reveal clathrate integrity. *top)* volumetric representation of the atomic clouds (not to scale) and *bottom)* ball and stick model for water (O – red, H – white).