Supplemental Information

Novel Methodology for the Calculation of the Enthalpy of Enclathration of Methane Hydrates using Molecular Dynamics Simulations

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Table S1. Enthalpy of enclathration per methane molecule ($\Delta H^{encl.}$) for the sI methane hydrate. Statistical uncertainties are given in the parenthesis.

T **[K]**	($\Delta H^{encl.}$) **per CH_4 Small Cages [kJ/mol]**	($\Delta H^{encl.}$) **per CH_4 Large Cages [kJ/mol]**
274	-25.2 (0.3)	-25.4 (0.2)
278	-25.1 (0.2)	-25.3 (0.3)
282	-24.9 (0.2)	-25.2 (0.3)
286	-24.7 (0.4)	-25.1 (0.2)
290	-24.6 (0.1)	-24.8 (0.2)
294	-24.4 (0.2)	-24.6 (0.1)
298	-24.2 (0.3)	-24.3 (0.3)
302	-23.8 (0.1)	-23.9 (0.2)
306	-23.3 (0.4)	-23.5 (0.3)
310	-22.1 (0.5)	-23.2 (0.4)

Table S2. Total enthalpy per hydrate unit cell (UC) for the sI methane hydrate, as a function of temperature, along the three-phase (H–L_w–V) equilibrium line. Statistical uncertainties are given in the parenthesis.

T **[K]**	**Empty Lattice Enthalpy/UC [kJ/mol]**	**Full Occupancy Enthalpy/UC [kJ/mol]**	**Partial Occupancy Enthalpy/UC [kJ/mol]**	**Small Cages Empty Enthalpy/UC [kJ/mol]**	**Large Cages Empty Enthalpy/UC [kJ/mol]**
274	-2438 (1)	-2587.9 (0.6)	-2574 (2)	-2545.0 (0.4)	-2472.4 (0.4)
278	-2426 (3)	-2576 (1)	-2564 (2)	-2533.5 (0.4)	-2460.9 (0.2)
282	-2414 (1)	-2565 (1)	-2559.6 (0.7)	-2522 (2)	-2448.4 (0.2)
286	-2400 (1)	-2549.5 (0.4)	-2546 (2)	-2506 (1)	-2434.8 (0.2)
290	-2384 (1)	-2531 (1)	-2529 (2)	-2490 (2)	-2418.5 (0.2)
294	-2363 (2)	-2510.5 (0.3)	-2508.3 (0.6)	-2469.3 (0.6)	-2397.7 (0.2)
298	-2337 (2)	-2480.7 (0.5)	-2479.6 (0.6)	-2440.7 (0.8)	-2369.8 (0.3)
302	-2301 (2)	-2446.0 (0.3)	-2436.4 (0.3)	-2406 (1)	-2334.6 (0.2)
306	-2255 (2)	-2399 (1)	-2390 (1)	-2358 (1)	-2289.0 (0.2)
310	-2200 (2)	-2342 (1)	-2338 (1)	-2302 (1)	-2233.2 (0.2)