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Grand Canonical Monte Carlo Simulations of the Ammonia clathrate hydrate

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Overcoming the important deficiencies of the clathrate equilibrium data at low temperatures by using theoretical approaches such as the van der Waals & Platteeuw method seems truly tempting. However, this thermodynamic route is usually based on descriptions with simplified intermolecular potentials calibrated using equilibrium data obtained at high temperatures. As a consequence, the theoretical model's ability to predict the composition of clathrates in the outer Solar System could be easily questioned. In the current work, we show that Monte Carlo simulations performed on the Grand Canonical ensemble (GCMC) can be efficiently used to determine theoretically the amount of gas species trapped in the clathrate hydrates at low temperature in various situations as encountered in the Solar System.
In this study, the NH3 molecule has been considered which is thought to contribute to the outgassing of methane clathrate hydrates into the atmosphere of Titan and Encleadus due to its role as a water-ice antifreeze and methane clathrate thermodynamic inhibitor. However, recent experimental results have indicated that NH3 clathrate of structure I could be stable at the very low temperatures
typcial of these Moon's atmospheres (i.e., below 150 K). GCMC simulations have thus been performed to determine the amount of NH3 trapped in clathrate as a function of the partial pressure at different temperatures. The obtained results show that the strong tendency of hydrogen bond formation between NH3 and water molecules leads to the destabilization of the clathrate cages. As a consequence, stabilizing the ammonia clathrate in molecular simulations appears very challenging, indicating that this clathrate could be stable only under very specific conditions.
This application illustrates the efficiency of the GCMC method for studying gas trapping in clathrates at low temperatures of interest for planetary sciences.

Significance statement

Grand Canonical Monte Carlo simulations of the ammonia clathrate are performed for the first time. Results show that this clathrate could be stable in specific conditions relevant to planetary sciences.

Primary author: Dr PICAUD, Sylvain (Institut UTINAM - UMR 6213 CNRS/Univ Franche Comte)

Co-authors: Mr FABIAN, Balazs (Institut UTINAM - Besançon, France / ELTE Univ. of Budapest - Hungary); Prof. JEDLOVSZKY, Pal (EKF Department of Chemistry, Leányka utca 6, H-3300 Eger, Hungary)

Presenters: Mr FABIAN, Balazs (Institut UTINAM - Besançon, France / ELTE Univ. of Budapest - Hungary); Dr PICAUD, Sylvain (Institut UTINAM - UMR 6213 CNRS/Univ Franche Comte)

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