Ammonia clathrate hydrates as new solid phases for Titan, Enceladus, and other planetary systems

Kyuchul Shin*, Rajnish Kumarb, Konstantin A. Udachina*, Saman Alavi, and John A. Ripmeester†

aSteacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON, Canada K1A 0R6; and bNational Chemical Laboratory, Council of Scientific and Industrial Research, Pune 411008, India

Results

As a first step in this study we show that in the presence of other clathrate hydrate forming substances, ammonia indeed can be incorporated in cages within the clathrate lattice. Incorporation of ammonia in a clathrate hydrate phase was accomplished by freezing a solution of the well known clathrate hydrate former tetrahydrofuran (THF) and approximately 5% aqueous ammonia with an approximate THF:water mole ratio of 1:17 at −10°C. Crystals formed were harvested after a few days and those suitable for diffraction were identified and mounted on a diffractometer at low temperatures. The above experimental conditions can be compared with those in the study of Dong et al. (15, 16) who used THF:water ratios of about 1:63 with up to 5% ammonia to study methane hydrate formation in the presence of ammonia. In their experiments, Dong et al. (15, 16) did not use sufficient THF to lead to the direct formation of the binary THF + NH3 clathrate hydrate and ammonia hydrate formation was not observed.

Structural data were recorded at 100 K (see Materials and Methods). The structure was shown to be the usual cubic structure II (sII) clathrate hydrate (28), space group Fd-3m with a unit cell edge of 1.71413(6) nm. The THF molecules occupy the large cages, as expected, and 39% of the small cages are filled with ammonia molecules (Fig. 1). This measured small cage occupancy is likely to be a function of the starting composition. Whether small cages could be completely filled with a more ammonia-rich liquid is uncertain and should be studied separately. One of the water molecules in the small cages which encapsulate the ammonia guests has moved out of its normal position, 0.118 nm inward into the small cage thus forming H⋯O bonds. Nitrogen, hydrogen, and oxygen positional data were determined by difference electrondensity calculations. The unit cell of sII ammonia clathrate hydrate contains one ammonia molecule per unit cell (as suggested by hydrogen positions on the ammonia guest). The formation of HOH⋯NH3 hydrogen bonding could also lead to this water displacement. This displacement breaks the hydrogen bond of this water molecule with another water from an adjacent large (or small) cage (O⋯O distances 0.393 nm), thus distorting both large and small cages. The equivalent O⋯O distance in the undistorted edges of the water polyhedra is 0.279 nm. It should be noted that the minimum heavy atom N⋯O distance in the clathrate hydrate is smaller than in the ammonia hydrates, where the more uniform local environment of the NH3 molecule results in N⋯O distances of 0.305 to 0.330 nm.

Because structural evidence for the mixed THF + NH3 sII hydrate showed that it is possible to incorporate ammonia into...
and Methods

clathrate cages, attempts were made to form clathrate hydrates with only ammonia as guest. Pure ammonia clathrate hydrate synthesis cannot be done by simply cooling aqueous ammonia solutions, as a variety of stoichiometric hydrates of ammonia are known to form preferentially (2, 11, 18, 19). Other ways of forming clathrate hydrates include vapor deposition of water at low temperatures to yield amorphous ice, followed by exposure of the ice to a pressure of guest gas and annealing (29), or vapor codeposition of water and the potential guest material at low temperatures, again, followed by annealing (23, 30, 31). It has been shown that below approximately 140 K ice surfaces are relatively inert to exposure of water and the potential guest material at low temperatures, and will template clathrate hydrate lattices when amorphous ice is annealed (30).

Following the latter procedure, described in detail in Materials and Methods, vapor codeposits of ammonia and water were prepared at $T < 20$ K. The codeposited crystals were harvested at 77 K and kept in liquid nitrogen until appropriate measurements could be made. A portion of each amorphous product was mounted in a low temperature cell on a powder X-ray diffractometer and the samples annealed stepwise, increasing temperature from approximately 100 K. Fig. 2 shows the transformation of the amorphous deposit upon annealing. Fig. 2A shows the powder X-ray diffraction (PXRD) pattern for amorphous ice with traces of ices Ic and Ih at 100 K. At 140 K, the amorphous ice has largely transformed to ices Ic and Ih plus a number of other crystalline phases (the Bragg positions for Ic are omitted). These reflections continue to develop with increase of temperature to 150 K. The inset (Fig. 2B) shows a vertical expansion of the 150 K pattern. For each pattern the profiles are matched to those of known crystalline phases, including the stoichiometric ammonia hydrates (hemi-, mono-, and dihydrates), hexagonal ice Ih, and clathrate hydrates. Eight reflections (shown in Fig. 2) can be assigned to the cubic structure (SI) ammonia clathrate hydrate and indexed to be consistent with SI clathrate hydrate, space group $Pm\text{-}3n$, with unit cell edge 1.818(2) nm at 150 K.

The interactions of ammonia with methane clathrate hydrates are also considered to be important in determining the phase equilibria on Titan and Enceladus. Several vapor deposits of methane, ammonia, and water were prepared as described in Materials and Methods and annealing of the vapor codeposits was followed by PXRD. Fig. 3A shows the PXRD pattern at 112 K, indicating the material to be mainly amorphous except for some crystalline Ih. At 143 K (Fig. 3A, second trace) most of the pattern for the amorphous deposit has transformed into ice Ic plus other crystalline phases that upon closer inspection suggested the presence of both cubic SI and SIH clathrate hydrates. At 160 K, this pattern is well developed and a vertically expanded detail is given in Fig. 3B. Profile matching for each powder pattern shows that a good fit is obtained by considering the presence of ices Ic and Ih, as well as cubic SI [$Pm\text{-}3n$, $a = 1.1847(8)$ nm] and cubic SIH clathrate hydrates [$Fd\text{-}3m$, $a = 1.7161(9)$ nm]. To observe both common cubic clathrate hydrate structures is surprising. Structure I is the usual clathrate that forms for methane at low pressures although metastable SIH methane hydrate has been observed as well (30). A blank run for a vapor codeposited of water and methane but without ammonia did not reveal any clathrate hydrate under similar conditions of annealing (Fig. S1). Further annealing of the three-component codeposit at 180 K showed (Fig. 3A) that the SIH clathrate hydrate pattern had largely disappeared, and reflections for the stoichiometric ammonia hydrates were absent. The transformation from mixed SI and SIH hydrates to SI hydrate was confirmed by observing methane C-H symmetric stretch frequencies around 2,905 cm$^{-1}$ by Raman spectroscopy (32) (Fig. S2). At low temperature, the deposited methane peak appeared at 2,908 cm$^{-1}$, which is close to the Raman shift of dissolved methane in water (33). This peak splits into a doublet at 160 K; one peak at 2,903 cm$^{-1}$ representing the methane in the large cages and the second at 2,914 cm$^{-1}$ representing methane in the small cages. As temperature increases, the ratio of methane in the large cages to that of the guest in the small cages increases, which implies the transformation to SI phase (six large cages to two small cages) which has a greater proportion of large cages than SIH (8 large cages to 16 small cages). Similar enhanced processes of CO$_2$ clathrate hydrate formation on ice
simulate the pure NH cages) binary sII clathrate hydrate from 100 to 240 K. We also recorded at 112, 143, 160, and 180 K; (c) clathrates are mechanically stable at simulation temperatures.

**Materials and Methods**

The molecular dynamics simulation methodology is described in detail in Materials and Methods. For the duration of the simulations, all the clathrates are mechanically stable at simulation temperatures up to 200 K and did not show signs of decomposition and cage collapse.

In the molecular simulations of the sI and sII pure ammonia hydrate phases, we observe hydrogen bonding between the ammonia guest molecules and the water molecules in both the small and large clathrate hydrate cages. Cases where ammonia is the hydrogen donor (H₂N-H⋯OH₂) and hydrogen acceptor (H₂N⋯-H-OH) are both common but the latter is more frequent (Fig. S3 and S4). On the other hand, in the binary sII hydrate phases with THF or methane in the large cages, ammonia showed either no hydrogen bonding or only a small probability for hydrogen bond formation with water molecules of the small cages (see Figs. S5 and S6). From integrating the hydrogen bonding peak in the radial distribution functions (RDF), we calculated the probability of hydrogen bonding, p, in the pure NH sI, sII, and binary NH₃ + CH₄ sII clathrate hydrates for ammonia molecules and the results are given in Table 1. Peaks in the RDF with H₂N-H⋯OH₂ or H₂N⋯-H-OH distances less than 0.25 nm were assigned to hydrogen bonding. The areas underneath the hydrogen bond peaks in the RDF give a measure of the hydrogen bond probability (see Materials and Methods). The probability of hydrogen bonding increases with temperature, which shows that the ammonia-water hydrogen bonding in the clathrate hydrates is endothermic. The temperature dependence of the hydrogen bonding probability is evaluated using the van’ Hoff plot of ln K [where K = p/(1 − p)] as a function of 1/T (Fig. S7). The slopes of the linear plots are used to determine the enthalpies of hydrogen bond formation for ammonia in the different environments which are also given in Table 1. The formation of hydrogen bonds in the sII clathrate hydrate is less endothermic and the more facile formation of these bonds may destabilize the sII clathrate hydrate water lattice to a greater extent than the sI case.

Sample hydrogen bonded configurations of the ammonia guests in the large and small cages of the sI and sII clathrate hydrates are shown in Fig. 4. Hydrogen bond configurations with ammonia acting as the proton donor and the proton acceptor (often simultaneously) are observed. The ammonia guest remains mostly in the cage but in some configurations the ammonia molecule displaces one of the water molecules from a lattice site. The water molecules in the hexagonal faces of the large clathrate hydrate cages are less hindered and may also have less stable water-water hydrogen bonds which require less energy to break compared to the water molecules forming hydrogen bonds in pentagonal faces. Snapshots from the simulations show that the ammonia molecules preferentially hydrogen bond with the water molecules in the hexagonal faces. Ammonia-water hydrogen bonding severely distorts the small and large cage structures. At temperatures below 200 K, the hydrate phase maintains its mechanical stability without framework collapse despite the ammonia-water hydrogen bonds and the defects they induce in the hydrate lattice hydrogen-bonding network. As we only performed a molecular dynamics simulation and not a full free energy calculation comparing the thermodynamic stability of the clathrate hydrate phase to the products, we cannot comment on the thermodynamic stability of the ammonia clathrate hydrate phase. By mechanical stability we imply that the hydrate structure did not

![Fig. 3. PXRD patterns of NH₃, CH₄, and H₂O co-deposition sample (A) recorded at 112, 143, 160, and 180 K, (B) expansion of the pattern at 160 K. Vertical thin red lines and arrows indicate the peaks from sII hydrate and blue lines and arrows indicate the peaks from sI hydrate. Lattice parameter (160 K): a = 0.4491(3) nm and c = 0.7333(5) nm for Ih (space group P6₃/mmc), a = 0.6361(3) nm for Ic (space group Fd-3m), a = 1.1847(8) nm for sI hydrate (space group Pm-3n), and a = 1.7161(9) nm for sII hydrate (space group Fd-3m).](image)

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<th>140 K</th>
<th>160 K</th>
<th>170 K</th>
<th>ΔHformation/KJ mol⁻¹</th>
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<tr>
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<td>6.1</td>
<td>24.4</td>
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<td>1.3</td>
<td>1.8</td>
<td>2.9</td>
<td>5.09</td>
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Table 1. The average percent (H₂N–H–OH) hydrogen bonding configurations calculated from RDFs and the enthalpy of hydrogen bond formation for pure sI and sII NH₃ hydrates and binary sII CH₄ (large cages) + NH₃ (small cages) hydrate at different temperatures.
decompose under the pressure-temperature conditions of the simulation. As temperature and vibrational amplitudes of the water molecules in the hydrate lattice increase, these lattice defects lead to the breakdown of the water framework structure and instability of the hydrate phase.

From Table 1, the ammonia molecules in the large sI and sII cages form hydrogen bonds more readily than in the corresponding small cages. In addition, the larger hydrogen bonding formation enthalpy in the sI hydrate compared to the sII hydrate, reveals that the water lattice in the sI phase is less susceptible to hydrogen bonding with ammonia and is preferred when the ammonia forms a clathrate phase with amorphous ice upon annealing.

In contrast to the pure NH$_3$ hydrates, binary CH$_4$ + NH$_3$ sII hydrate shows a H$_3$N⋯–H–OH hydrogen bond probability of only approximately 3% even at 170 K. Incorporating methane in the cages of the binary clathrate hydrate apparently stabilizes the cages which encapsulate ammonia. The molecular dynamics simulation results are consistent within the framework of experimental knowledge of the ammonia hydrate system described above. Strong hydrogen bonding of ammonia with water in the solid phase is expected. The stability of the ammonia hydrate is dependent on the low temperature and/or stabilizing effect of methane help gas.

**Discussion**

The presence of both ammonia and methane give a clathrate hydrate that is much more stable than that of the pure ammonia hydrate (stability up to 180 K for the mixed clathrate as compared to 150 K for the pure NH$_3$ clathrate). On the other hand, the presence of ammonia is critical in forming a clathrate in a temperature region where methane by itself does not form a clathrate hydrate. The activation of ice surfaces by ammonia at low temperatures is a well known phenomenon (35), so it may well be that synergistic behavior of ammonia and methane on the amorphous ice surface produce a reasonably stable clathrate: ammonia to initiate the reaction by introducing defects and methane to stabilize the clathrate lattice by limiting guest-host hydrogen bonding. Experiments with ethane and ammonia gave similar results (Fig. S8). From the work presented it is clear that ammonia plays an important role, so far unrealized, in forming solid clathrate phases at low temperatures in planetary environments. It may be difficult to quantify the effects of ammonia on a clathrate hydrate-forming environment as it is clear that some ammonia phases have time and temperature-limited regions of existence.

Recent spectrophotometric studies by Nelson and coworkers have shown variations in the surface reflectance on Titan which have been attributed to episodic cryovolcanic effusion events which bring NH$_3$ from the interior of Titan to its surface in the form of a fog or frost (36). Most work on ammonia present in Titan focuses on ammonia in aqueous solution in the “magma” and its effect on methane clathrate hydrate inhibition and decomposition in that region (5). Our work shows that under temperature and pressure conditions similar to those found on Titan’s surface (5) ($T \approx 90$ K and $P_{\text{atm}} \approx 1.6$ bar), considering the presence of methane in the atmosphere of Titan and availability of ice on its surface, it is possible that the extruded ammonia vapor forms binary clathrate hydrate phases with methane. Clathrate hydrate formation after ammonia vapor deposition in the presence of methane gas and annealing to about 100 K can provide a mechanism for the removal of ammonia and methane from Titan’s atmosphere. Ethane clathrate hydrate formation may also be catalyzed by the presence of ammonia.

Similar cryovolcanic activity is also seen in Saturn’s moon Enceladus where plumes of ammonia, methane, and water vapor are extruded from the South Pole (37). The sources of these methane extrusions in both moons have been related to clathrate hydrate dissociation (5, 38, 39).

The broader significance of the catalyzing effect of ammonia on methane hydrate formation under vapor deposition conditions may be to the conditions of primordial ices in planets, comets, and planetesimals in solar system formation models. The ammonia can catalyze the formation of nonstoichiometric gas hydrates which are then trapped in icy grains and accreted into planetary objects.

In addition to subsurface processes, ammonia-bearing liquids and vapors may interact directly with surface clathrate hydrate phases on Titan. In situ clathrate hydrate formations (not involving ammonia) have been considered important in determining the surface composition and structures of this moon (40–42) and the presence of ammonia may play a role in these processes. Polar, water miscible molecules such as ammonia are traditionally considered as clathrate hydrate formation inhibitors. Our experiments and computations show that the inhibition effect is not due to inherent instability of the solid clathrate hydrate phase of these guest molecules, but is rather the stabilizing effect of these guests on the aqueous phase from which the clathrate hydrate is formed.

**Materials and Methods**

**Sample Preparation.** Vapor codepositions of water and guest materials (ammonia, methane, and 50 mole % ammonia/methane mixture) were performed in an evacuated chamber at approximately 0.01 mbar. The water was vaporized from a pipette into the evacuation chamber by low pressure
and deposited on a copper plate which was cooled down to approximately 16 K by DISPLEX (Air Products). In each experiment a total of 600 mmHg of the guest gas (ammonia, methane or 1:1 ammonia:methane mixture) was injected into a 1 L bulb and slowly injected into the deposition chamber. The water and guest gas vapor flows were controlled by leak valve and after 24 h approximately 2 g of water and 0.5 g of guest vapors were deposited on the copper plate. The copper plate covered with the product deposit was removed from the evaporation chamber and quickly immersed in liquid nitrogen with minimal exposure to air. Significant moisture condensation on the sample during the short transfer period is not expected. For the various characterization experiments the materials were transferred to the powder X-ray diffraction and Raman instruments.

In the single crystal experiments, a THF + NH₃ binary silt hydrate was prepared from a 1:17 solution of THF in 5% aqueous ammonia. The synthesis conditions give an approximate mole ratio of 1:0.946:17 for THF:NH₃:H₂O in this solution. Upon cooling the solution to 263 K masses of crystals appeared. Crystals suitable for diffraction were identified by examination under a microscope mounted in a cold box. The structure obtained from the single crystal diffraction experiment was used to determine that 39% of the small cages were occupied by ammonia which gives an approximate clathrate hydrate composition of 1:0.78:17 for THF: NH₃: H₂O. Different ammonia small cage occupancies are likely to be found starting from different initial compositions. Whether small cages could be filled with a more ammonia-rich liquid is uncertain and should be the subject of a separate study.

X-Ray Data Collection and Structure Solution. Single crystal X-ray diffraction data were measured on a Bruker Apex 2 Kappa diffractometer at 100 K, using graphite monochromatized Mo Kα radiation (λ = 0.71073 Å). The unit cell was determined from randomly selected reflections obtained using the Bruker Apex2 automatic search, center, index, and least squares routines. Integration was carried out using the program SAINT, and an absorption correction was performed using SADABS (43). The crystal structures were solved by direct methods and the structure was refined by full-matrix least-squares routines using the SHELXTL program suite (44). All atoms were refined anisotropically. Hydrogen atoms on guest molecules were placed in calculated positions and allowed to ride on the host atoms.

Powder X-Ray Diffraction (PXRD). The PXRD pattern was recorded on a BRUKER AXS model D8 Advance diffractometer in the 2θ scan mode using Cu Kα radiation (λ = 1.5406 Å, 2θ = 1.5444 Å, and λ/λ = 0.3). The samples stored in liquid nitrogen were quickly transferred to the X-ray stage cooled down to approximately 100 K in air and diffraction patterns were measured with increasing temperature. The experiment was carried out in the step mode with a fixed time of 2 s and a step size of 0.03014° for 2θ = 8 to 42° at each temperature. The powder pattern was refined by the Le Bail method using the profile matching method within FULLPROF (45).

Raman Spectroscopy. The Raman spectra were measured using a dispersive Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating spectrometer (1,200 grating) and detected with a CCD detector (laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument with the focused 514.5 nm line of an Ar-ion laser for excitation. The scattered light was dispersed using a single-grating Raman microscope instrument!
46. Smith W, Forester TR, Todorov IT DL_POLY 2.20 (CCLRC, Daresbury Laboratory, Daresbury).
Fig. S1. PXRD patterns of CH₄ and H₂O co-deposition sample. No evidence of methane hydrate formation is seen. The diffraction lines of Ih and Ic are shown for reference below the patterns.

Fig. S2. Raman spectra of NH₃, CH₄, and H₂O co-deposition sample. The peak at 2,908 cm⁻¹ represents the deposited CH₄ in amorphous phase, that at 2,903 cm⁻¹ represents the CH₄ in the large cages, and that at 2,914 cm⁻¹ represents CH₄ in the small cages. As temperature increases, the ratio of CH₄ in the large cages to that of the guest in the small cages increases, which implies the transformation from sI and sII mixture to sI phase which has a greater proportion of large cages than sII case.
Fig. S3. Calculated RDFs for ammonia atoms in the pure NH₃ sl clathrate hydrates. The peaks at \( r = 1.9 \) Å in the first and second plots indicate H₃N⋯H-OH hydrogen bonding and the shoulders at \( r = 2.1 \) Å in the third and fourth plots indicate the H₂N-H⋯OH₂ hydrogen bonding in the large and small cages, respectively. The relative area under these peaks is related to the probability of the corresponding hydrogen bonding interaction.
Fig. S4. Calculated RDFs for ammonia atoms in the pure NH$_3$ sII clathrate hydrates. Peaks and shoulders in the range of $r < 2.5$ Å show the presence of hydrogen bonding between the ammonia guest and cage water.

Fig. S5. Calculated RDFs for ammonia atoms in the binary CH$_4$(L) + NH$_3$(S) sII clathrate hydrates. The Top RDF plot shows that the probabilities of hydrogen bonding between the ammonia N atom and the host water H atom are quite low.
Fig. S6. Calculated RDFs for ammonia atoms in the binary THF + NH$_3$ sII clathrate hydrates at 183 K. The RDFs for methane in the small cages of a binary sII THF + CH$_4$ hydrate are given for reference.

Fig. S7. The logarithm of the equilibrium constants of H$_3$N⋯H-OH hydrogen bonding configurations as a function of inverse temperature in the form of a van't Hoff plot. The slope of these plots is $-\Delta H_{\text{HB}}/R$.

Fig. S8. PXRD patterns of NH$_3$ + C$_2$H$_6$ + H$_2$O (red) and C$_2$H$_6$ + H$_2$O (blue) co-deposition samples recorded at 180 K. Vertical thin red lines indicate the reflections from the sII hydrate. Lattice parameter: $a = 1.7195(2)$ nm for sII hydrate (space group Fd-3m) and $a = 1.1989(1)$ nm for sI hydrate (space group Pm-3n) from NH$_3$ + C$_2$H$_6$ + H$_2$O co-deposition sample (red pattern), $a = 1.1996(2)$ nm for sI hydrate (space group Pm-3n) from C$_2$H$_6$ + H$_2$O co-deposition sample (blue pattern).

Table S1. Atomic point charges and Lennard-Jones parameters for H₂O, THF, CH₄, NH₃

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