Planetary ices in the H_2O – NH_3 – CO_2 ternary system

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Background

Interactions between simple molecules are of fundamental interest across diverse areas of the physical sciences, and the ternary system H_2O – NH_3 – CO_2 is no exception.

In the outer solar system, interaction of CO_2 with aqueous ammonia is likely to occur, synthesizing 'rock-forming' minerals [1], with CO_2 perhaps playing a role in ammonia-water oceans and cryomagmas inside icy planetary bodies. In the same context, ammonium carbonates may have some astrobiological relevance, since removal of water leads to the formation of urea.

On Earth, combination of CO_2 with aqueous ammonia has relevance to carbon capture schemes [2], and there is interest in using such materials for hydrogen storage in fuel cells [3].

Consequently, from earthly matters of climate change to the study of extraterrestrial ices, understanding the structures and properties of ammonium carbonates are important. Despite this, our knowledge of ammonium carbonates is limited under ambient conditions of pressure and temperature and is entirely absent at the higher pressures, severely limiting our ability to model the behaviour of H_2O – NH_3 – CO_2 solids and fluids in planetary environments.

Methods

We report the results of Density Functional Theory (DFT) calculations on five compounds in the H_2O – NH_3 – CO_2 ternary system and on several polymorphs of urea. We anticipate being able to present complementary variable pressure and temperature neutron diffraction work on ammonium carbonate and ammonium carbamate. These computational and experimental studies provide the structural, thermoelastic and vibrational information required for accurate planetary modelling and remote identification of these material on planetary surfaces.

[1] Kargel (1991) Icarus 94 , 368-390. [2] Han et al. (2013) Int. J. Greenhouse Gas Control 14 , 270-281. [3] Lan et al. (2012) Int. J. Hydrogen Energy 37 (2), 1482-1494.