Variation of H-bond properties with density in astrophysical ice structures

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The interpretation of infrared measurements of remote sources, like in astronomical missions, often relies on the knowledge of the density of the sample measured by other means. For icy samples containing water, the analysis of the infrared spectra may reveal the presence of different kinds of O-H bonding types, from free or nearly free O-H bonds to O-H…O hydrogen bonds of diverse strength. Each bonding type has a different signature, but also this signature may vary with the density of the sample.

We have chosen for this investigation a mixture of water and methane, plus a relevant amount of nitrogen, frozen at 50 K, to simulate the possible content of a spot at the surface of Pluto, the Pulfrich crater [1], recently observed by the New Horizons mission. By varying the size of the cell containing this mixture of molecules, we can study the effect of the corresponding density of the sample on the predicted IR spectra.

We have covered a large density range, from a very low value that simulates a gas-phase mixture, to values corresponding to solids under fairly high internal stress, with a middle range that could be expected to cover the values of mixtures at astronomical conditions.

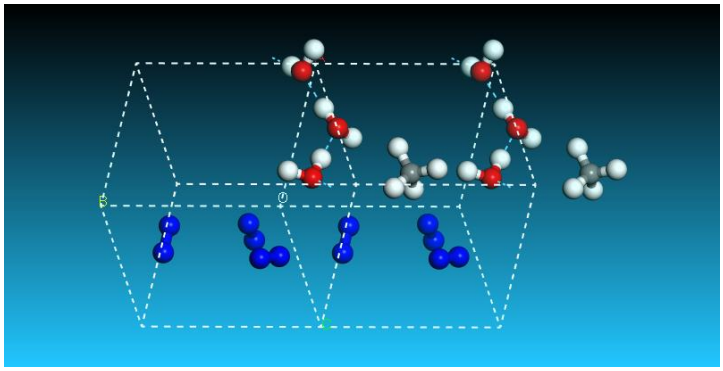

Fig. 1. Sample with density 0.75 g cm^{-3}. Two unit cells are shown to better appreciate the optimized structure. Note the apparent porosity of the sample.

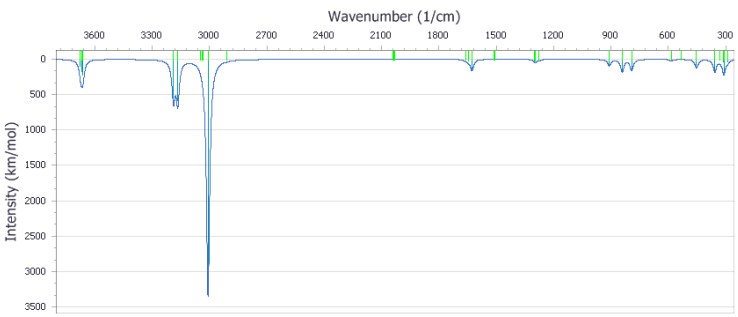

Fig. 2. Predicted IR spectrum of the sample in Fig. 1.

References

[1] W.M. Grundy et al, Science 351, aad9189, 2016.