Polymorphic transformations and melting of ice XVII: Molecular dynamics modeling

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Depending on temperature and pressure water molecules in the solid state may give rise to more than 17 different forms of ices. In 2016 del Rosso et al [1,2] were able to empty the Co clathrate of hydrogen and to identify the obtained structure as a new form of ice, ice XVII. Recently del Rosso et al [3] have described a new method to obtain pure cubic ice Ic in large quantities from ice XVII.
It is known that the TIP4P/Ice model used in this work describes different characteristics of the solid phase of water with high precision. In this work, the transition of ice XVII into cubic ice Ic was obtained using molecular dynamics methods. The mechanism of such a transition was shown. The latent heat of the phase transition and the rate of formation of cubic ice Ic have been calculated. The probability of the formation of cubic (Ic) or hexagonal (Ih) ices depending on the temperature was obtained. Also, different characteristics of ice XVII were determined by molecular dynamics methods and compared with experimental data.

[1] del Rosso L, Celli M and Ulivi L 2016 *Nat. Commun.* **7** 13394
[2] Smirnov G S and Stegailov V V 2013 *J. Phys. Chem. Lett.* **4** 3560–3564
[3] del Rosso L, Celli M and Grazzi F 2020 *Nat. Mater.* **19** 663–668