Complexity in low-temperature phase diagrams of planetary ices: phase transition in bischofite, MgCl2.6H2O

Ema Bobocioiu[1], Razvan Caracas[2]
[1] ENS de Lyon, Univ. Claude Bernard Lyon, Laboratoire de Geologie, UMR 5276, Lyon, France
[2] CNRS, ENS de Lyon, Univ. Claude Bernard Lyon, Laboratoire de Geologie, UMR 5276, Lyon, France

Bischofite, $MgCl_2.6H_2O$ is a marine evaporite that may be present also on or inside icy satellites. It has a monoclinic structure formed of $[Mg(H_2O)_6]^{2-}$ octahedral cations and individual chlorine ions. The structure is quasihexagonal with a distorted hexagonal-close packed arrangement of the two structural groups. . This structure has C2/m space group.
First-principles calculations based on density functional perturbation theory indicate the presence of unstable imaginary phonon modes in the zone-center. They are characterized by 153*i* cm^{-1} and 57*i* cm^{-1} imaginary wavenumbers. Both these modes correspond to tilting of the water molecules.
We then investigate these lattice instabilities and find a new structure that is present at low temperatures. The phase transition to this new structure involves the break of the symmetry with the loss of the m symmetry plane and of the inversion center. The new structure is polar with C2 space group.