New Class of Stable NaCl Hydrates: On the Role of Pressure in Hydration and Ionic Dissociation in Hydrogen Bonded Solids

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We report the discovery and structural characterization of two new stable phases of NaCl hydrates at high pressures and low temperatures [1]: disodium chloride decaheptahydrate, $2NaCl{\cdot}17H_2O$ (SC8.5); and sodium chloride decatriahydrate, $NaCl{\cdot}13H_2O$ (SC13). Both differentiate themselves from the only previously known form of sodium chloride hydrate, hydrohalite, $NaCl{\cdot}2H_2O$ (SC2), by having ions fully dissociated in the structure, allowing for the high incorporation of water molecules, which we refer to as "hyperhydration". Experimental thermodynamic constraints suggest that SC8.5 should be stable at 1 atmosphere below 235 K, resulting in the first update to the canonical phase diagram of H_2O-NaCl in over 150 years. These results show that very large hydration numbers are possible even for diatomic alkali halide solids. It also provides evidence of a greater diversity of hydrates and hydrogen-bonded crystal structures than previously recognized and suggests that other hyperhydrated crystalline phases of common salts might be found at higher pressures and low temperatures.

References

1. Journaux, B., Pakhomova, A., Collings, I.E., Petitgirard, S., Boffa Ballaran, T., Brown, J.M., Vance, S.D., Chariton, S., Prakapenka, V.B., Huang, D., Ott, J., Glazyrin, K., Garbarino, G., Comboni, D., Hanfland, M., 2023. On the identification of hyperhydrated sodium chloride hydrates, stable at icy moon conditions. Proceedings of the National Academy of Sciences 120, e2217125120. https://doi.org/10.1073/pnas.2217125120