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Single-crystal-to-single-crystal phase transitions of commensurately modulated sodium saccharinate 1.875-hydrate

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This contribution reports reversible, single-crystal-to-single-crystal phase transitions of commensurately modulated sodium saccharinate 1.875-hydrate [Na(sac)(15/8)H₂O]. The phases were studied in the temperature range 298 to 20 K. They exhibit complex disordered states. An unusual reentrant disorder has been discovered upon cooling through a phase transition at 120 K. The disordered region involves three sodium cations, four water molecules and one saccharinate anion. At room temperature, the structure is an eightfold superstructure that can be described by the superspace group C2/c(0b0)s0 with **q** = (0, 3/4, 0). It demonstrates maximum disorder with the disordered chemical entities having slightly different but close to 0.50:0.50 disorder component ratios. Upon cooling, the crystal tends to an ordered state, smoothly reaching a unified disorder component ratio of around 0.90:0.10 for each of the entities. Between 130 and 120 K a phase transition occurs involving a sudden increase of the disorder towards the disorder component ratio 0.65:0.35. Meanwhile, the space group and general organization of the structure are retained. Between 60 and 40 K there is another phase transition leading to a twinned triclinic phase. After heating the crystal back to room temperature its structure is the same as before cooling, indicating a complete reversibility of the phase transitions.

Primary authors: REKIS, Toms (University of Bayreuth); Mr SCHALLER, Achim M. (University of Bayreuth); Mr KOTLA, Surya Rohith (University of Bayreuth); Dr SCHÖNLEBER, Andreas (University of Bayreuth); Dr NOOHINEJAD, Leila (DESY); Dr TOLKIEHN, Martin (DESY); Dr PAULMANN, Carsten (DESY); VAN SMAALEN, Sander (University of Bayreuth)

Presenter: REKIS, Toms (University of Bayreuth)

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