

## Poster Presentation

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### *Common Packing Motif in Salts of H-Acid, and the Incommensurate Sodium Hydrate*

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"H-Acid" (4-ammonio-5-hydroxynaphthalene-2,7-disulfonate) is a coal tar derivative and important intermediate in the manufacture of hundreds of dyes. Despite the fact that on the order of one million metric tons of the sodium salt have been manufactured in the past century, no crystal structures incorporating this organosulfonate have been reported. Diffraction quality needles of the hydrated sodium salt are prepared by slow cooling a concentrated aqueous solution under anaerobic conditions. Variable temperature X-ray diffraction studies revealed the structure exhibits positional disorder of donor atoms around aqua-bridged Na<sup>+</sup> dimers between room temperature and 180 K. Upon further cooling the structure undergoes a reversible phase transition to an ordered, incommensurately modulated structure with retention of crystal quality. Structure elucidation of over a dozen other salts of H-Acid revealed in all cases the adoption of a stacking motif reinforced by hydrogen bonds involving a "keystone" water molecule. This water molecule is also retained during in situ dehydration of the sodium salt at elevated temperature; surprisingly, a sodium-coordinated water molecule is the first to be released.

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