Poster Presentation

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Reinvestigation of hypoxanthinium nitrate monohydrate structure

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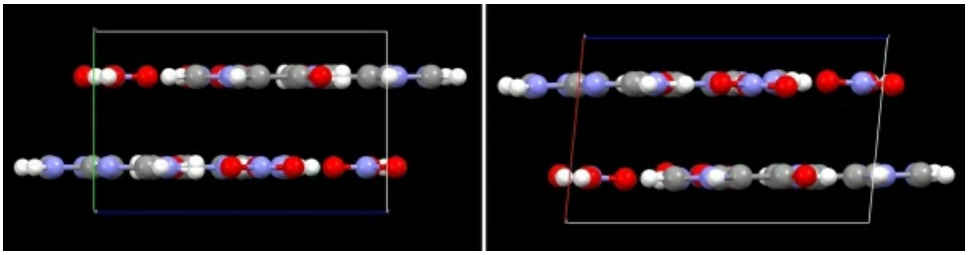
As a part of our study on nucleobases, we investigated the structure of hypoxanthinium nitrate monohydrate, which proved to be more challenging than previously thought.
In room temperature, hypoxanthinium nitrate monohydrate crystallizes in Pnma group in orthorhombic crystal system, which has already been reported [1][2]. Cooling crystal to 100 K caused it to undergo phase transition, resulting in non-merohedral twin with half of molecules forming a new lattice, turned by 180o around c axis with respect to the original lattice.
To determine clearly the point of transition, we conducted a series of measurements starting from 385 K and ending at 105 K, with a step of 15 K.
Both phases have layered structure with hypoxantiniu cations surrounded by three nitrate anions and three water molecules placed alternately. Looking along c axis there are ribbons of hypoxanthinium cations held together by nitrate anion paired with water molecule. Such pair (nitrate anion and water) is oriented in the same direction both along the ribbon, and across it. The ribbons aren't placed precisely on top of each other, and hypoxanthinium cation doesn't form any stacking interactions. Instead, there are water molecules directly below and above every cation.
Additionally, we conducted TGA/DSC experiments and electrostatic energy calculations to characterize phrase transition not only geometrically, but also from the energetic point of view.
[1] Rosenstein, R. D. et al., (1982). Cryst. Struct. Commun. 11, 1507-1513.
[2] Schmalle H. et al., (1990). Acta Cryst. C46, 340-342.



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