

Poster Presentation

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Two Reversible Phase Transitions in the Fluorophosphate (NH₄)₂PO₃F•(NH₄)NO₃

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Fluorophosphates have multiple applications, e.g. as wood preservatives, as corrosion inhibitors or as toothpaste additives [1]. Fluorophosphates contain the tetrahedral anion PO₃F²⁻ that is characterized by three P-O bonds of similar length (ca. 1.51 Å) and one considerably longer P-F bond (ca. 1.60 Å). In the course of systematic crystal growth experiments of new fluorophosphates, we have isolated the double salt (NH₄)₂PO₃F•(NH₄)NO₃. Temperature-dependent X-ray diffraction studies on polycrystalline and single-crystalline samples revealed two reversible phase transitions. The room-temperature polymorph I (space group P2₁/n) transforms at ca. 170 K into the intermediate polymorph II (space group P-1) that in turn transforms at ca. 140 K into the low-temperature polymorph III (space group P2₁/n). The driving force of the phase transitions I->II and II->III is a tilting of the nitrate groups within the structure relative to the other building blocks. The two phase transitions are accompanied by an increase of the unit cell volume on cooling. The three-dimensional structural set-up in the three polymorphs of (NH₄)₂PO₃F•(NH₄)NO₃ is dominated by an intricate N-H...O hydrogen-bonding system between ammonium donor groups and nitrate and fluorophosphates acceptor groups. It is interesting to note that hydrogen-bonding of the type N-H...F plays a minor role.

[1] Stöger, B., Weil, M. & Skibsted, J. (2013). *Dalton Trans.* 42, 11672-11682.

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