

Crystal Engineering of a New Layered Polyiodide Using 1,9-Diammoniononane as a Flexible Template Cation

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The reaction of 1,9-diaminononane with hydroiodic acid in the presence of iodine gave a compound best described as 1,9-diammoniononane bis-triiodide iodine, $(\text{H}_3\text{N}-(\text{CH}_2)_9-\text{NH}_3)[\text{I}_3]_2 \cdot \text{I}_2$. The structure is built from two crystallographically independent I_3^- anions, which are connected *via* secondary $\text{I} \cdots \text{I}$ interactions to the iodine molecules, and the 1,9-diammonioalkane cations are connected *via* weak hydrogen bonds to neighbouring iodine atoms. By a cooperative phenomenon, the shape and the functionality of the cation lead to a solid state structure that includes a polyiodide substructure with the formula ${}_{\infty}^2[\text{I}_8]^{2-}$ or ${}_{\infty}^2[\text{I}_3 \cdot \text{I}_2 \cdot \text{I}_3]^{2-}$, is best described as a brick-shaped layered array. Its rectangular pores fit excellently with the hydrogen bonding functionality as well as with the conformational needs of the 1,9-diammoniononane template. The Raman spectrum shows typical bands of coordinated triiodide anions and iodine molecules. The thermal analysis (DSC/TG) of the title compound indicates decomposition at temperatures above 210 °C.

Key words: Structure Determination, Crystal Engineering, Polyiodide, Diammonioalkane, Hydrogen Bonding