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Polyiodide of dimethylglycine ($\text{DMG-}\frac{1}{2}\text{H} \cdots \frac{1}{2}\text{H-DMG})(\text{I}_3)(\text{I}_2)$)

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Polyiodides have emerged as compounds of interest both for their practical application and in the context of supramolecular chemistry. In the synthesis of halogenometallates the incorporation of polyiodide anions leads to an increase of absorption in the visible region and helps to achieve a narrower bandgap which was additional motivation to investigate polyiodides independently. We have previously reported on polyiodides of betaine, L-proline, L-arginine and L-cystine. In the present work the salt of dimethylglycine ($\text{DMG-H-DMG})(\text{I}_3)(\text{I}_2)$, crystallizing in the monoclinic space group C2/c , is studied. The structure exhibits a symmetric dimeric cation of dimethylglycine formed through strong hydrogen bonding with a short $\text{O} \cdots \text{O}$ distance of $2.459(3) \text{ \AA}$. In this $\text{O-H} \cdots \text{O}$ moiety the hydrogen atom position is disordered and split into two positions separated by a two-fold axis, each with a 50% H-atom occupancy. The compound further contains a triiodide anion (centered at the Wyckoff position 4d with site symmetry 1^-) and a diatomic iodine (centered around a 2-fold axis). The compound features an ordered chain arrangement of cations stabilized via aforementioned hydrogen contact as well as $\text{N-H} \cdots \text{O}$ hydrogen bonds. The powder of black, shiny crystals exhibits strong absorption in the UV-Vis region, thus exhibiting narrow bandgaps of 1.87 eV and 1.62 eV for direct and indirect transitions, respectively.

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