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## Discovery of a symmetric (L-Orn(H)-H-L-OrnH) (3+)-cation in the structure of (L-Orn(H)-H-L-OrnH)(I3)3•4H2O

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L-Ornithine is one of the amino acids able to establish both singly and doubly charged cations. Under certain conditions it can form salts with a dimeric cation (L-OrnH2•••L-OrnH)<sup>3+</sup>, as seen in the structures of (L-OrnH2•••L-OrnH)(Cl)2(ClO4) and (L-OrnH2•••L-OrnH)(Cl)2(NO3) [1], where doubly charged L-OrnH2 and singly charged L-OrnH cations are linked through a short O–H•••O type hydrogen bond. This study reports the first identification of a symmetric (L-Orn(H)-H-L-OrnH)<sup>3+</sup> dimeric cation, stabilized by an O-H-O symmetric hydrogen bond, within the new crystal structure of (L-Orn(H)-H-L-OrnH)(I<sub>3</sub>)<sub>3</sub>•4H<sub>2</sub>O. The O•••O distance is quite short, i.e. 2.436(3) Å. The salt crystallizes in the monoclinic space group C2, with an ordered chain arrangement of triiodide anions formed through supramolecular halogen bonding. The powder of black, shiny crystals exhibits strong absorption in the visible light region, thus having narrow bandgap of 1.41 eV. DFT calculations confirm the indirect bandgap of 1.374 eV, claiming the contribution of incorporated triiodide.

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