

Aziridinium Cation as a Universal Building Block for HOIPs of Variable Dimensionality

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Hybrid organic–inorganic perovskites remain at the forefront of materials research due to their tunable optoelectronic properties and structural diversity. In this work, we present a family of aziridinium-based hybrid perovskite-like materials of general formula $(\text{AzrH})_3\text{M}_2\text{X}_9$ ($\text{M} = \text{Sb, Bi}$; $\text{X} = \text{Cl, Br, I}$), where the aziridinium cation $(\text{AzrH})^+$ acts as a versatile structure-directing template enabling the formation of perovskite of all dimensionalities—0D, 1D, 2D, and even 3D. Single-crystal X-ray diffraction revealed discrete bi-octahedral 0D units in iodides, 1D polymeric chains in antimony chloride, and layered 2D structures in bromides and bismuth chloride. Furthermore, heterovalent Bi^{3+} doping in aziridinium lead halides enabled the stabilization of mixed-metal 3D perovskites with the band gap of 1.49 eV, which is the lowest value observed for this raw of materials. Across the $(\text{AzrH})_3\text{M}_2\text{X}_9$ series, the optical absorption features strong excitonic transitions (330–499 nm) with binding energies ranging from 0.06 to 0.61 eV, and band gaps varying from 2.61 to 4.09 eV depending on the halogen and metal composition. Density functional theory calculations support these findings, showing that valence and conduction band edges are primarily derived from halide p- and metal s-orbitals, respectively. The established correlations among dimensionality, composition, and optical behavior provide valuable insights into the design of hybrid perovskites with controllable electronic structures.

(1) Kucheriv, O. I.; Semenikhin, O. A.; Bibik, Y. S.; Bardyk, I.; Shova, S.; Gural'skiy, I. A. Aziridinium Cation as a Versatile Template for Hybrid Organic–Inorganic Perovskites of All Dimensionalities. *Inorg. Chem. Front.* 2025. <https://doi.org/10.1039/d5qi01090j>.

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