



**SYNTHESIS AND STRUCTURE OF NEW SUPRAMOLECULAR
COMPLEX BIS((PYRIDIN-1-IUM-4-YL)METHANAMINIUM)
HEXAHALOSTANNATE(IV) DIBROMO**

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The nonlinear optical materials, which widely used in different areas in physical and chemistry sciences, calls great interest. Nonlinear optical materials are materials whose optical properties, such as refractive index, can be altered by light. They play a crucial role in advanced light functionalities, such as all-optical switching. Based on this, was synthesized new supramolecular complex (I) on the base of bis((pyridin-1-ium-4-yl)methanaminium) with SnBr_2 . New supramolecular compound $\text{SnBr}_6 \cdot [\text{C}_6\text{N}_2\text{H}_{10}]^{+4} \cdot 2\text{Br}^{-2}$ was determinate by Single crystal X-ray diffraction. The hole structure shown in Fig.1. The asymmetric unit of complex consists of a single diprotonated cation, one bromide ion, and half of a hexabromostannate(IV) anion. These components are intricately connected through a network of hydrogen bonds, specifically N-H...Br interactions. The cation donates two protons that form strong hydrogen bonds with the bromide ion, creating a robust network of intermolecular interactions. These hydrogen bonds stabilize the structure and influence the packing and arrangement of ions within the crystal lattice. In the crystal structure, the Sn-Cl

bond distances range from 2.5908(4) Å to 2.6194(5) Å, indicating a uniform bonding environment around the tin atom. The Br-Sn-Br bond angles vary between 87.344(14)° and 92.657(14)°, reflecting slight deviations from ideal octahedral geometry. The compound exhibits extensive hydrogen-bonding interactions, significantly contributing to its stability and structural organization. The Sn atom is six-coordinated, forming a quasi-regular octahedral arrangement. This coordination geometry is stabilized by the surrounding chloride ions, which, along with the hydrogen bonds, create a robust three-dimensional network within the crystal lattice.

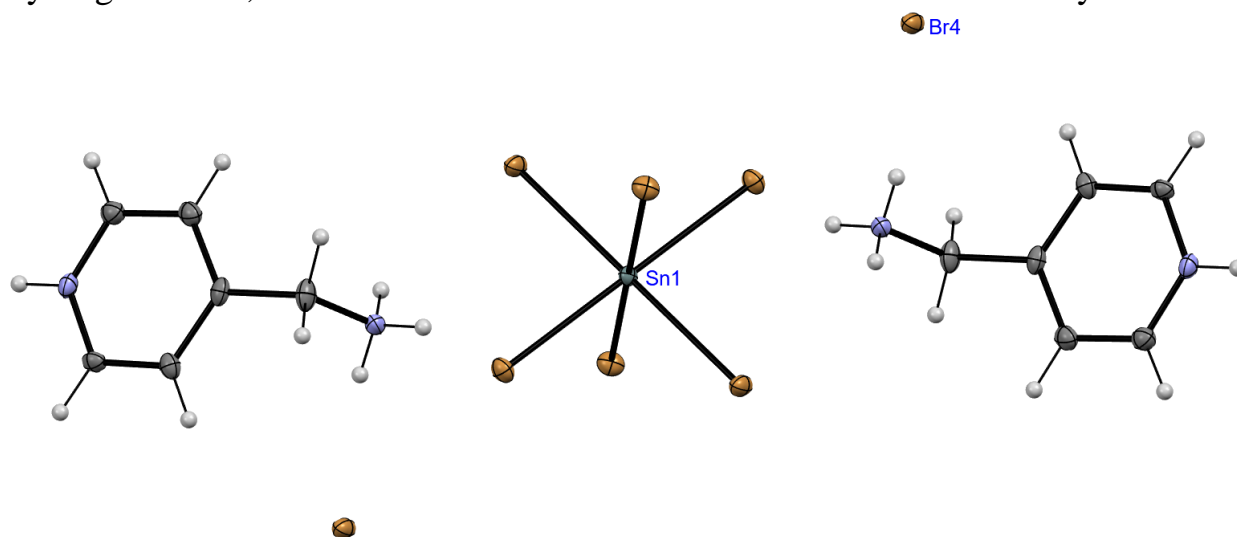


Fig.1. $\text{SnBr}_6 \cdot [\text{C}_6\text{N}_2\text{H}_{10}]^{4+} \cdot 2\text{Br}^{2-}$.

The nearly regular octahedral configuration of the SnBr_6^{2-} anion, combined with the extensive hydrogen bonding, highlights the intricate balance of forces that define the structural characteristics of this compound. The bond angle variance is measured at 2.9376°, indicating only minor deviations from the ideal octahedral angles of 90°. Furthermore, the effective coordination number is calculated to be 5.9950, which is nearly perfect compared to the ideal value of 6. These measurements collectively demonstrate that the SnBr_6^{2-} anion maintains nearly perfect octahedral geometry.



References

- [1] F. Hao, C.C. Stoumpos, R.P.H. Chang, M.G. Kanatzidis, Anomalous band gap behavior in mixed Sn and Pb perovskites enables broadening of absorption spectrum in solar cells, *J. Am. Chem. Soc.* 136 (2014) 8094-8099.
- [2] C.C. Stoumpos, C.D. Malliakas, M.G. Kanatzidis, Semiconducting tin and lead iodide perovskites with organic cations: phase transitions, high mobilities, and near-infrared photoluminescent properties, *Inorg. Chem.* 52 (2013) 9019-9038.
- [3] W.-Q. Liao, Y. Zhang, C.-L. Hu, J.-G. Mao, H.-Y. Ye, P.-F. Li, S.D. Huang, R.-G. Xiong, A lead-halide perovskite molecular ferroelectric semiconductor, *Nat. Commun.* 6 (1) (2015) 1-7.