Contribution: Poster

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Synthesis, Structural and Optical Properties of Lead-Free 0D Halide Perovskites

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In the current era, search for materials with high power conversion efficiency to convert solar to electrical energy is of utmost importance to address the ever-increasing energy demand. In this context, metal halide perovskites are an active area of research because of the excellent optoelectronic properties of these compounds. Cheaper components, easy to fabricate the device and high-power conversion efficiency of lead-based halide perovskites make these compounds very promising as efficient solar absorber. However, the toxicity of lead in these materials inhibit these for large scale applications. Hence search for lead free halide perovskite with high power conversion efficiency has attracted attention of various scientist across the world. Among the lead-free halide perovskites, antimony and bismuth-based halide perovskites are one of the classes of compounds that show promising photovoltaic properties and hence can be explored for solar cell applications. Further, by lowering the dimensionality of these halide perovskites, the stability and efficiency of perovskite solar cell has been increased. To explore 0D lead free halide perovskites, we have synthesized several new hybrid 0D halide perovskite by using sulphur based organic cation. The structure of 0D halide perovskite is confirmed by the single crystal study. $[(CH_3)_3S]_2BiBr_5$.DMSO crystallize in triclinic $P\bar{1}$ space group and contains isolated $BiBr_5$(DMSO) unit as building blocks. The compounds are characterized by using different spectroscopic technique.

Synthesis, Structure and Optical Properties of Lead-Free Bi based 0D Halide Perovskite

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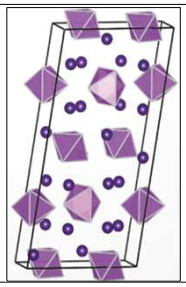
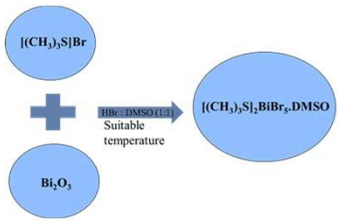
Abstract: Lead free Bi based 0D halide perovskite $[(CH_3)_3S]_2BiBr_5$.DMSO is synthesized and characterized by using single crystal XRD, powder XRD, IR, UV-Vis-DRS, SEM and EDX. The compound adapt triclinic crystal system with S.G. P−1 (2) have a direct band gap of ~2.89 eV and indirect band gap of ~2.79 eV.

Introduction: 0D halide perovskite has isolated metal-halide octahedra surrounded by organic/inorganic cation. Low dimension halide perovskite having higher environmental and thermal stability. 0D halide perovskite restrict the mobility in one or more crystallographic directions.



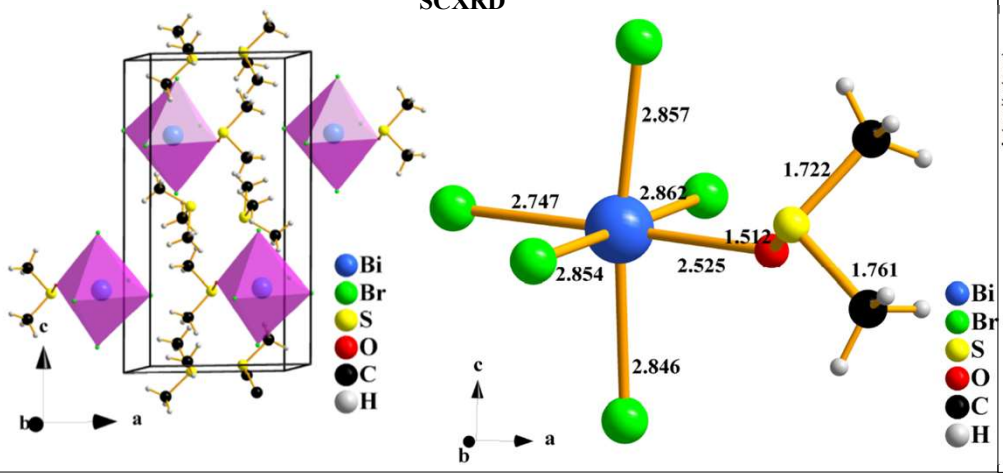
Synthesis:



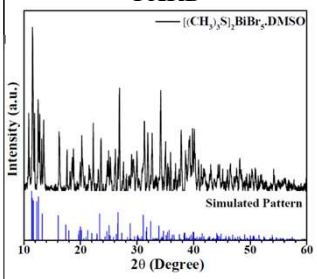
Result and Discussion

Crystal Structure

SCXRD



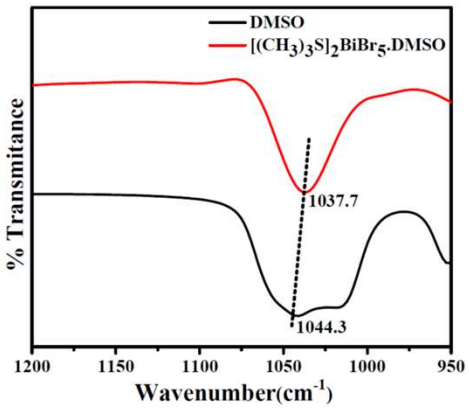
PXRD



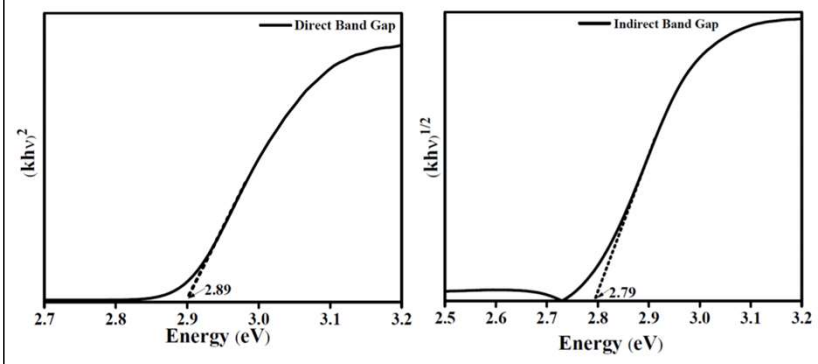
Crystallographic Details

$[(CH_3)_3S]_2BiBr_5$.DMSO
Triclinic; S.G.: $P\bar{1}(2)$
$a = 8.2321(3)$ Å, $\alpha = 89.11°$
$b = 9.2196(3)$ Å, $\beta = 88.20°$
$c = 15.2213(4)$ Å, $\gamma = 78.94°$

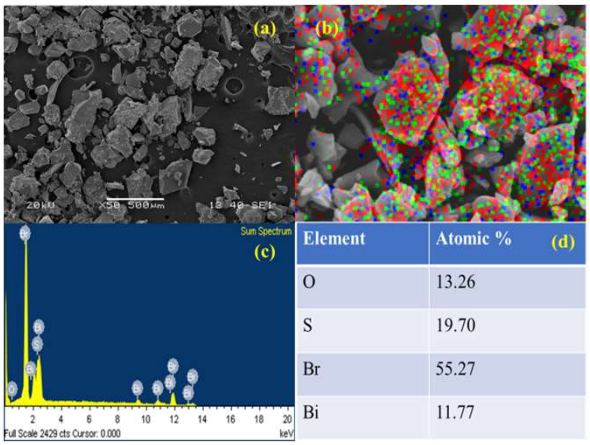
IR



UV-Vis-DRS



SEM and EDX



Element	Atomic % (d)
O	13.26
S	19.70
Br	55.27
Bi	11.77

Conclusion:

- We have synthesized $[(CH_3)_3S]_2BiBr_5$.DMSO via solution method and characterized with different spectroscopic technique.
- The compound $[(CH_3)_3S]_2BiBr_5$.DMSO having isolated metal-halide octahedra In the compound Bi is bonded to five Br ions and oxygen of the DMSO molecule resulting a six coordinated polyhedra.

References:

1. Hong, K., *et al.* Low-dimensional halide perovskites: Review and issues. *J. Mater. Chem. C* **6**, 2189–2209 (2018).
2. Wei, Q. *et al.* Self-Trapped Exciton Emission in a Zero-Dimensional $(TMA)_2SbCl_5$·DMF Single Crystal and Molecular Dynamics Simulation of Structural Stability. *J. Phys. Chem. Lett.* **12**, 7091–7099 (2021)