Title

A new zero-dimensional (0D) hybrid bismuth (III) halide: Synthesis, crystal structure, thermal analysis, photophysical properties and DFT calculations

Abstract

Low-dimensional organic-inorganic hybrid Bi(III) halides, with organic N, O-heterocycles, are promising solid-state photoluminescent materials, but are underexplored. In this work, we present the synthesis and characterization of a novel bismuth (III) hybrid salt, namely (C8H12NO)4[Bi2Cl10] (referred as (1)). (1) was synthesized using a solvent-evaporation method and extensively characterized using various techniques. The crystal structure of (1) was determined to be zero-dimensional (0D). In this structure, the individual bioctahedral [Bi2Cl10]4− dimers, which share edges, are completely isolated from each other. These dimers are separated by large 4-methoxybenzylammonium cations (C8H12NO)+. The latter are crucial for the crystal structural stability by balancing [Bi2Cl10]4-dimer charges and maintaining overall integrity. Solid-state diffuse reflectance UV–Vis spectrum demonstrates that (1) is a semiconductor with a band gap of 3.32 eV. Its photoluminescence spectrum exhibits intense blue emission when exposed to UV light, with CIE chromaticity coordinates of (0.22, 0.21). Theoretical calculations suggest that the emission with multiple centers originates both from a charge transition between (C8H12NO)+ and Bi2Cl104− ions and from excited-state proton transfer (ESPT) processes related to fluorescence properties. These ESPT processes occur through C–H…π and C–H…O intermolecular hydrogen bonding between the organic cations.

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References

Li W., Wang Z., Deschler F., Gao S., Friend R.H., Cheetham A.K., Chemically diverse and multifunctional hybrid organic- inorganic perovskites, Nat. Rev. Mater., 2, (2017); Kojima A., Teshima K., Shirai Y., Miyasaka T., Organometal halide perovskites as visible-light sensitizers for photovoltaic cells, J. Am. Chem. Soc., 131, pp. 6050-6051, (2009); Saidaminov M.I., Mohammed O.F., Bakr O.M., Low-dimensional-networked metal halide perovskites: the next big thing, ACS Energy Lett, 2, pp. 889-896, (2017); Zhou J., Huang J., Photodetectors based on organic–inorganic hybrid lead halide perovskites, Adv. Sci., 5, (2018); Guan X., Lei Z., Yu X., Lin C.-H., Huang J.-K., Huang C.-Y., Hu L., Li F., Vinu A., Yi J., Wu T., Low-dimensional metal-halide perovskites as high performance materials for memory applications, Small, 18, (2022); Jiang X., Chen Z., Tao X., (1-C5H14N2Br)2MnBr4: a lead-free zero-dimensional organic-metal halide with intense green photoluminescence, Front. Chem., 8, (2020); Sun C., Zang J.-P., Liu Y.-Q., Zhong Q.-Q., Xing X.-X., Li J.-P., Yue C.-Y., Lei X.-W., Lead-free hybrid indium perovskites with highly efficient and stable green light emissions, CCS Chem., 4, pp. 3106-3121, (2022); Li Z., Li Y., Liang P., Zhou T., Wang L., Xie R.-J., Dual-band luminescent lead-free antimony chloride halides with near-unity photoluminescence quantum efficiency, Chem. Mater., 31, pp. 9363-9371, (2019); Msaadi I., Rayes A., Benito M., Issaoui N., Molins E., Ayed B., A combined experimental and theoretical studies of two new decavanadate: (C₆N₂H₉)₄[H₂V₁₀O₂₈]·4H₂O and (C₇H₉NF)₄[H₂V₁₀O₂₈]·2H₂O, J. Mol. Struc., 1262, (2022); Zhou C., Tian Y., Yuan Z., Lin H., Chen B., Clark R., Dilbeck T., Zhou Y., Hurley J., Neu J., Besara T., Siegrist T., Djurovich P., Ma B., Highly efficient broadband yellow

phosphor based on zerodimensional tin mixed-halide perovskite, ACS Appl. Mater. Interfaces, 9, 51, pp. 44579-44583, (2017); Sun N., Lin J., He S., Cao J., Guo Z., Zhao J., Liu Q., Yuan W., High-efficiency intrinsic yellow-orange emission in hybrid indium bromide with double octahedral configuration, Inorg. Chem., 62, pp. 3018-3025, (2023); Filip M.R., Volonakis G., Giustino F., Hybrid halide perovskites: fundamental theory and materials design, Handbook of Materials Modeling, pp. 295-324, (2020); Wani A.L., Ara A., Usman J.A., Lead toxicity: a review, Interdiscip. Toxicol., 8, 2, pp. 55-64, (2015); Yang J., Kelly T.L., Decomposition and cell failure mechanisms in lead halide perovskite solar cells, Inorg. Chem., 56, pp. 92-101, (2017); Boix P.P., Agarwala S., Koh T.M., Mathews N., Mhaisalkar S.G., Perovskite solar cells: beyond methylammonium lead iodide, J. Phys. Chem. Lett., 6, pp. 898-907, (2015); Shi Z., Guo J., Chen Y., Li Q., Pan Y., Zhang H., Xia Y., Huang W., Lead-free organic–inorganic hybrid perovskites for photovoltaic applications: recent advances and perspectives, Adv. Mater., 29, (2017); Mohan R., Green bismuth, Nat. Chem., 2, (2010); Slavney A.H., Hu T., Lindenberg A.M., Karunadasa H.I., A bismuth-halide double perovskite with long carrier recombination lifetime for photovoltaic applications, J. Am. Chem. Soc., 138, pp. 2138-2141, (2016); Lyu M., Yun J.-H., Cai M., Jiao Y., Bernhardt P.V., Zhang M., Wang Q., Du A., Wang H., Liu G., Wang L., Organic–inorganic bismuth (III)-based material: a lead-free, air-stable and solution-processable light-absorber beyond organo-lead perovskites, Nano Res., 9, 3, pp. 692-702, (2016); Park B.-W., Philippe B., Zhang X., Rensmo H., Boschloo G., Johansson E.M.J., Bismuth based hybrid perovskites A₃Bi₂I₉ (A: methylammonium or cesium) for solar cell application, Adv. Mater., 27, pp. 6806-6813, (2015); Adonin S.A., Sokolov M.N., Rakhmanova M.E., Smolentsev A.I., Korolkov I.V., Kozlova S.G., Fedin V.P., Luminescent properties of 4,4-bipyridinium chlorobismuthate salt: strong influence of solvation, Inorg. Chem. Commun., 54, pp. 89-91, (2015); Garcia-Fernandez A., Marcos-Cives I., Platas-Iglesias C., Castro-Garcia S.,

Vazquez-Garcia D., Fernandez A., Sanchez-Andujar M., Diimidazolium halobismuthates [Dim]2[Bi₂X₁₀] (X = Cl[–], Br[–], or I[–]): a new class of thermochromic and photoluminescent materials, Inorg. Chem., 57, 13, pp. 7655-7664, (2018); Moon T.H., Oh S.-J., Ok K.M., [((R) C₈H₁₂N)₄][Bi₂Br₁₀] and [((S) C₈H₁₂N)₄][Bi₂Br₁₀]: chiral hybrid bismuth bromides templated by chiral organic cations, ACS Omega, 3, pp. 17895-17903, (2018); Lin R.-G., Xu G., Wang M.-S., Lu G., Li P.-X., Guo G.-C., Photochromic hybrid containing in situ -generated benzyl viologen and novel trinuclear [Bi₃Cl₁₄]^{5–}: improved photoresponsive behavior by the π-π interactions and size effect of inorganic oligomer, Inorg. Chem., 53, pp. 5538-5545, (2014); Liu Y.-H., Peng H., Liao W.-Q., A lead-free bismuth iodide organic–inorganic ferroelectric semiconductor, Chem. Commun., 57, pp. 647-650, (2021); Li M.-Q., Hu Y.-Q., Bi L.-Y., Zhang H.-L., Wang Y., Zheng Y.-Z., Structure tunable organic-inorganic bismuth halides for an enhanced two-dimensional lead-free light-harvesting material, Chem. Mater., 29, pp. 5463-5467, (2017); Ya. Heng H., Rosli M.M., Wong Q.A., Anizaim A.H., Abdullah M., Razak I.A., Single crystal, a lead-free hybrid organic-inorganic perovskite material: {[(C₆H₅)NH₃]⁺}4.I.[BiI₆]^{3–}.H₂O with optical and third-order nonlinear properties, J. Solid State Chem., 312, (2022); Sun D., Wang D., Chen H., Hou R., Dang Y., Wu K., Wang J., Shen C., New low-dimensional lead-free perovskite (2-AMP)₂BiX₇·H₂O (X = Cl, Br) crystals: synthesis, stability, and nonlinear optical properties, Inorg. Chem., 61, pp. 15247-15255, (2022); Yao L., Zeng Z., Cai C., Xu P., Gu H., Gao L., Han J., Zhang X., Wang X., Wang X., Pan A., Wang J., Liang W., Liu S., Chen C., Tang J., Strong second-

and third-harmonic generation in 1D chiral hybrid bismuth halides, J. Am. Chem. Soc., 143, (2021); Xu G., Guo G.-C., Wang M.-S., Zhang Z.-J., Chen W.-T., Huang J.-S., Photochromism of a methyl viologen bismuth(III) chloride: structural variation before and after UV, Angew. Chem., Int. Ed., 46, pp. 3249-3251, (2007); Goforth A.M., Tershansy M.A., Smith M.D., Peterson L., Kelley J.G., DeBenedetti W.J.I., zure Loye H.-C., Structural diversity and thermochromic properties of iodobismuthate materials containing D-metal coordination cations: observation of a high symmetry [Bi₃I₁₁]^{2–} anion and of isolated I[–] anions, J. Am. Chem. Soc., 133, pp. 603-612, (2011); Adonin S.A., Sokolov M.N., Abramov P.A., Kozlova S.G., Pishchur D.P., Sheludyakova L.A., Fedin V.P., Thermochromic behavior and phase transition of new octanuclear polyiodobismuth (III) ate, Inorg. Chim. Acta, 419, pp. 19-25, (2014); Li G., Hao P., Shen J., Yu T., Li H., Fu Y., Bipyridyltriazolium chlorobismuthate with thermo-/photochromic and photoluminescent switching behaviors based on ET and CT, Inorg. Chem., 55, pp. 11342-11347, (2016); Adonin S.A., Sokolov M.N., Fedina V.P., Polynuclear halide complexes of Bi(III): from structural diversity to the new properties, Coord. Chem. Rev., 312, pp. 1-21, (2016); Qi Z., Gao H.I., Zhu X., Lu Z., Zhang X.-M., Blue light-excitable broadband yellow emission in a zero-dimensional hybrid bismuth halide with type-II band alignment, Inorg. Chem., 61, pp. 19483-19491, (2022); Yangui A., Roccanova R., McWhorter T.M., Wu Y., Du M.-H., Saparov B., Hybrid organic-inorganic halides (C₅H₇N₂)₂MBr₄ (M = Hg, Zn) with high color rendering index and high-efficiency white-light emission, Chem. Mater., 31, pp. 2983-2991, (2019); Zhou C., Lin H., Tian Y., Yuan Z., Clark R., Chen B., van de Burgt L.J., Wang J.C., Zhou Y., Hanson K., Meisner Q.J., Neu J., Besara T., Siegrist T., Lambers E., Djurovich P., Ma B., Luminescent zero-dimensional organic metal halide hybrids with near-unity quantum efficiency, Chem. Sci., 9, pp. 586-593, (2018); Kefi R., Matthias Z., Nasr C.B.,

(4-Methoxyphenyl)methanaminium chloride, Acta Cryst, E67, (2011); Macrae C.F., Bruno I.J., Chisholm J.A., Edgington P.R., McCabe P., Pidcock E., Rodriguez-Monge L., Taylor R., van de Streek J., Wood P.A., New features for the visualization and investigation of crystal structures, J. Appl. Crystallogr., 41, pp. 466-470, (2008); Turner M.J., McKinnon J.J., Wolff S.K., Grimwood D.J., Spackman P.R., Jayatilaka D., Spackman M.A., CrystalExplorer 17.5, (2007); Perdew J.P., Burke K., Ernzerhof M., Generalized gradient approximation made simple, Phys. Rev. Lett., 77, pp. 3865-3868, (1996); van Setten M.J., Giantomassi M., Bousquet E., Verstraete M.J., Hamann D.R., Gonze X., Rignanese G.-M., The PseudoDojo: training and grading a 85 element optimized norm-conserving pseudopotential table, Comput. Phys. Commun., 226, pp. 39-54, (2018); Monkhorst H.J., Pack J.D., Special points for Brillouin-zone integrations, Phys. Rev. B., 13, pp. 5188-5192, (1976); Furness J.W., Kaplan A.D., Ning J., Perdew J.P., Sun J., Accurate and numerically efficient r2SCAN meta-generalized gradient approximation, J. Phys. Chem. Lett., 11, pp. 8208-8215, (2020); Fu C.L., Ho K.M., First-principles calculation of the equilibrium ground-state properties of transition metals: applications to Nb and Mo, Phys. Rev. B., 28, pp. 5480-5486, (1983); Blochl P.E., Jepsen O., Andersen O.K., Improved tetrahedron method for Brillouin-zone integrations, Phys. Rev. B., 49, pp. 16223-16233, (1994); Grimme S., Antony J., Ehrlich S., Krieg H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, J. Chem. Phys., 132, (2010); Sm idstrup S., Markussen T., Vancraeyveld P., Wellendorff J., Schneider J., Gunst T., Verstichel B., Stradi D., Khomyakov P.A., Vej-Hansen U.G., Lee M.-E., Chill S.T., Rasmussen F., Penazzi G., Corsetti F., Ojanpera A., Jensen K., Palsgaard M.L.N., Martinez U., Blom A., Brandbyge M., Stokbro K., QuantumATK: an integrated platform of electronic and atomic-scale modelling tools, J. Phys. Condens. Matter., 32, (2020); Becke A.D., Density-functional thermochemistry. III. The role of exact exchange, J. Chem. Phys., 98, pp. 5648-5652, (1993); Lee C., Yang W., Parr R.G., Development of the

Colle-Salvetti correlation-energy formula into a functional of the electron density, Phys. Rev. B., 37, pp. 785-789, (1988); Stephens P.J., Devlin F.J., Chabalowski C.F., Frisch M.J., Ab Initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields, J. Phys. Chem., 98, pp. 11623-11627, (1994); Weigend F., Ahlrichs R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: design and assessment of accuracy, Phys. Chem. Chem. Phys., 7, (2005); Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Scalmani G., Barone V., Petersson G.A., Nakatsuji H., Li X., Caricato M., Marenich A., Bloino J., Janesko B.G., Gomperts R., Mennucci B., Hratchian H.P., Ortiz J.V., Izmaylov A.F., Sonnenberg J.L., Williams-Young D., Ding F., Lipparini F., Egidi F., Goings J., Peng B., Petrone A., Henderson T., Ranasinghe D., Zakrzewski V.G., Gao J., Rega N., Zheng G., Liang W., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Throssell K., Montgomery J.A., Peralta J.E., Ogliaro F., Bearpark M., Heyd J.J., Brothers E., Kudin K.N., Staroverov V.N., Keith T., Kobayashi R., Normand J., Raghavachari K., Rendell A., Burant J.C., Iyengar S.S., Tomasi J., Cossi M., Millam J.M., Klene M., Adamo C., Cammi R., Ochterski J.W., Martin R.L., Morokuma K., Farkas O., Foresman J.B., Fox D.J., Wallingford, (2016); Fredj D., Ben Hassen C., Elleuch S., Feki H., Chniba N., B T., Boujelbene M.M., Structural, vibrational and optical properties of a new organic–inorganic material: (C₅H₈N₃)₂[BiCl₅], Mater. Res. Bull., 85, pp. 23-29, (2017); Ouerghi Z., Guionneau P., Brandan S.A., Temel E., Kefi R., Crystal structure, computational study, optical and vibrational properties of a new luminescent material based on bismuth(III): (C₁₀H₂₈N₄)[Bi₂Cl₁₀], J. Solid State Chem., 303, (2021); Chouri M., Boughzala H., Crystal structure of the new hybrid material bis(1,4-diazoniabicyclo[2.2.2]octane) di-L-chloridobis[tetrachloridobismuthate(III)] dehydrate, Acta Cryst., E71, pp.

1384-1387, (2015); Ferjania H., Boughzalab H., A new hybrid material: (C₃H₆N₃)₄Bi₂Cl₁₀. Synthesis, structural study and spectroscopic behavior, Russ. J. Inorg. Chem., 63, pp. 349-356, (2018); Turel I., Golic L., Bukovec P., Gubina M., Crystal structure, computational study, optical and vibrational properties of a new luminescent material based on bismuth(III): (C₁₀H₂₈N₄)[Bi₂Cl₁₀], J. Solid State Chem., 303, (2021); Brown I.D., Bond valence as an aid to understanding the stereochemistry of O and F complexes of Sn(II), Sb(III), Te(IV), I(V) and Xe(VI), J. Solid State Chem., 11, pp. 214-233, (1974); Rayes A., Mezzadri F., Issaoui N., Ayed B., Calestani G., Synthesis, physico-chemical studies, non-linear optical properties and DFT calculations of a new non-centrosymmetric compound: (3-ammoniumpyridinium)tetrachloridozincate (II), J. Mol. Struct., 1184, pp. 524-531, (2019); Vassilyeva O.Y., Buvaylo E.A., Kokozay V.N., Skelton B.W., Organic–inorganic hybrid mixed-halide ZnII and CdII tetrahalometallates with the 2-methylimidazo[1,5-a]pyridinium cation, Acta Cryst., E78, pp. 359-364, (2022); Yu. Vassilyeva O., Buvaylo E.A., Kokozay V.N., Skelton B.W., Sobolev A.N., Crystal structures of an imidazo[1,5-a]pyridiniumbased ligand and its (C₁₃H₁₂N₃)₂[CdI₄] hybrid salt, Acta Cryst., E75, pp. 1209-1214, (2019); Kaiba A., Al Otaibi F., Geesi M.H., Riadi Y., Aljohani T.A., Guionneau P., A new organic–inorganic hybrid compound (NH₃(CH₂)C₆H₄CO₂H)[SnCl₆]: synthesis, crystal structure, vibrational, optical, magnetic properties and theoretical study, J. Mol. Struct., 1234, (2021); Mason W.R., Electronic Absorption and MCD Spectra for BiX₆ 3–, X) Cl[–], Br[–], and I[–], in acetonitrile solution: metal-centered vs ligand-to-metal charge-transfer assignments, Inorg. Chem., 38,

pp. 2742-2745, (1999); Huang Z., Ma X., Tailoring tunable luminescence via supramolecular assembly strategies, Cell Rep. Phys. Sci., 1, (2020); Gassara M., Msalmi R., Liu X., Hassen F., Moliterni A., Ben Hamadi N., Guesmi A., Khezami L., Soltani T., Naili H., A promising 1D Cd-based hybrid perovskite-type for white-light emission with high-color-rendering index, RSC Adv, 12, pp. 33516-33524, (2022); Zamora P.P., Bieger K., Cuchillo A., Tello A., Muena J.P., Theoretical determination of a reaction intermediate: Fukui function analysis, dual reactivity descriptor and activation energy, J. Mol. Struct., 1227, (2021); Bulat F.A., Chamorro E., Fuentealba P., Toro-Labbe A., Condensation of frontier molecular orbital fukui functions, J. Phys. Chem. A., 108, 2, pp. 342-349, (2004); Cederbaum L.S., One-body green’s function for atoms and molecules: theory and application, J. Phys. B., 8, pp. 290-303, (1975); Roy K., Moholkar V.S., Sulfadiazine degradation by combination of hydrodynamic cavitation and Fenton–Persulfate: parametric optimization and deduction of chemical mechanism, Environ. Sci. Pollut. Res., 30, pp. 25569-25581, (2023)

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