

Scientific paper

In Situ Preparation, Structure, Photoluminescence and Theoretical Study of an Unusual Bismuth Complex

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Abstract

A novel bismuth photoluminescent material, (*N,N'*-dimethyl-2,2'-bipy)₂(Bi₂Cl₁₀) · 2H₂O (**1**) (bipy = bipyridine), with the *N,N'*-dimethyl-2,2'-bipy²⁺ moiety obtained *in situ*, has been synthesized under solvothermal conditions and characterized by single-crystal X-ray diffraction. Compound **1** is characterized by an isolated structure, consisting of *N,N'*-dimethyl-2,2'-bipy²⁺ cations, Bi₂Cl₁₀⁴⁻ anions and lattice water molecules. Photoluminescence experiments with solid-state samples discover that compound **1** exhibits a strong emission in the green region. Time-dependent density functional theory (TDDFT) calculation reveals that the essence of the photoluminescence of **1** can be assigned to the combination of the metal-to-ligand charge transfer (MLCT) (from the HOMO of the bismuth ion to the LUMO of the *N,N'*-dimethyl-2,2'-bipy²⁺ moiety) and the ligand-to-ligand charge transfer (LLCT) (from the HOMO of the chloride ions to the LUMO of the *N,N'*-dimethyl-2,2'-bipy²⁺ moiety).

Keywords: Bismuth; photoluminescence; *in situ*; TDDFT; X-ray diffraction

1. Introduction

In recent years, bismuth compounds have gained increasing interest and have been broadly investigated because they can generally exhibit attractive properties for applications in the fields of medicine, biology, chemistry and so forth.^{1,2} To our knowledge, as a heavy p-block element of the group 15, bismuth displays variable stereochemical activity, large ionic radius and flexible coordination geometries which allow it to be applied to build different crystal architectures. The good deformation and polarization ability of bismuth make it to conquer the steric hindrance and achieve high coordination number compounds. Bismuth is a green metal due to its non-toxic and non-carcinogenic character.^{2–5} Therefore, some bismuth compounds have been applied in medicine to destroy cancer cells in high efficiency without side effect.^{6,7} Bismuth compounds have attracted increasing attention due to their

interesting properties and structural diversities and, nowadays, numbers of bismuth compounds have been documented.^{8–10}

Organic ligands with various functional groups are important in the construction of metal compounds. N-containing heterocyclic ligands (e.g., 2,2'-bipy, 4,4'-bipy) have been broadly exploited for the syntheses of metal compounds due to their plenty of coordination sites and different coordination patterns.¹¹ 2,2'-bipy has been proved to be a good chelating and bridging ligand to construct metal compounds. As a very strong N-ligating ligand, 2,2'-bipy is also important to offer potential supramolecular recognition sites to give attractive supramolecular structures. As a result, 2,2'-bipy is an important and useful building block to construct extended structures or supramolecular structures. Moreover, the pyridyl rings of the 2,2'-bipy have delocalized π -electrons which allow it to become a nice candidate to design photoluminescent

materials in the areas of organic light emitting diodes (OLEDs), solar energy conversion, chemical sensors, and so on.^{12–15}

Recently we become interested in the crystal engineering of bismuth compounds. For the sake of exploring novel bismuth compounds with new structural motifs and interesting properties, we aim at the design and synthesis of novel bismuth compounds with different organic ligands under solvothermal conditions. In this work, we report the preparation, crystal structure, photoluminescence, TDDFT study of a novel bismuth photoluminescent compound, i.e. (*N,N'*-dimethyl-2,2'-bipy)₂(Bi₂Cl₁₀) · 2H₂O (1) (bipy = bipyridine) that is synthesized by a solvothermal reaction. The *N,N'*-dimethyl-2,2'-bipy²⁺ moiety is obtained *in situ*. It should be pointed out that this is the first bismuth compound with a methylated 2,2'-bipy moiety.

2. Experimental

2.1. Materials and Instrumentation.

The reagents and chemicals were commercially purchased and directly used for the reactions. FT-IR was conducted with KBr pellets on a PE Spectrum-One spectrometer. Photoluminescence measurements were performed with solid state samples at room temperature on a JY FluoroMax-3 spectrometer. Time-dependent density functional theory (TDDFT) investigations were carried out by means of Gaussian03 suite of program packages.

2.2. Synthesis of (*N,N'*-dimethyl-2,2'-bipy)₂(Bi₂Cl₁₀) · 2H₂O (1)

BiCl₃ (1.00 mmol, 315 mg), 2,2'-bipy (1.00 mmol, 156 mg), methanol (2 mL), concentrated hydrochloric acid (0.5 mL) and distilled water (10 mL) were loaded into a 25 mL Teflon-lined stainless steel autoclave. The autoclave was heated at 473 K for 7 days and then powered off. After cooling down to room temperature, colorless crystals suitable for single-crystal X-ray diffraction were collected, washed with distilled water and dried in air. The yield was 27% (based on Bi). IR peaks (KBr, cm⁻¹): 3847(m), 3739(m), 3473(vs), 3049(m), 2941(w), 2360(m), 1690(m), 1617(vs), 1504(m), 1449(m), 1277(m), 1173(m), 947(w), 888(w), 780(s), 519(m) and 425(m).

2.3. X-ray Structure Determination

The crystal data of the title compound were obtained from a Rigaku Mercury CCD X-ray diffractometer equipped with graphite monochromated Mo-K α radiation source ($\lambda = 0.71073$ Å) at room temperature. The data reduction and the empirical absorption corrections were carried out using the CrystalClear software.¹⁶ We solved the crystal structure by virtue of the direct method. The Siemens SHELXTLTM Version 5 software package was applied to

solve the structure.¹⁷ The non-hydrogen atoms were located from the subsequent difference electron density maps and refined anisotropically, while the hydrogen atoms were added theoretically. The final structure was refined by applying the full-matrix least-squares refinement on F^2 . Crystallographic data and structural parameters for the title compound are summarised in Table 1. Selected bond lengths and bond angles are depicted in Table 2.

Table 1. Crystallographic data and structural analysis

Formula	C ₂₄ H ₃₆ Bi ₂ Cl ₁₀ N ₄ O ₂
M_r	1185.03
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	9.4841(15)
b (Å)	15.777(2)
c (Å)	12.832(2)
β (°)	104.738(4)
V (Å ³)	1856.9(5)
Z	2
Reflections collected	15533
Independent, observed reflections (R_{int})	4187, 3586 (0.0261)
$d_{calcd.}$ (g/cm ³)	2.119
μ /mm ⁻¹	10.213
$F(000)$	1120
R1, wR2	0.0179, 0.0380
S	1.007

Table 2. Selected bond lengths (Å) and bond angles (°)

Bond Lengths (Å)	
Cl(2)–Bi(1)–Cl(3)	87.93(3)
Bi(1)–Cl(1)	2.5594(8)
Bi(1)–Cl(2)	2.6230(8)
Bi(1)–Cl(3)	2.7112(9)
Bi(1)–Cl(4)	2.8490(8)
Bi(1)–Cl(4) ⁱ	2.9350(8)
Bi(1)–Cl(5)	2.6829(9)
Bond Angles (°)	
Cl(2)–Bi(1)–Cl(4) ⁱ	88.93(3)
Cl(1)–Bi(1)–Cl(2)	95.64(3)
Cl(1)–Bi(1)–Cl(5)	85.43(3)
Cl(2)–Bi(1)–Cl(5)	94.65(3)
Cl(1)–Bi(1)–Cl(3)	87.19(3)
Cl(5)–Bi(1)–Cl(3)	172.39(3)
Cl(1)–Bi(1)–Cl(4)	93.16(2)
Cl(2)–Bi(1)–Cl(4)	168.87(2)
Cl(5)–Bi(1)–Cl(4)	92.83(3)
Cl(3)–Bi(1)–Cl(4)	85.70(3)
Cl(1)–Bi(1)–Cl(4) ⁱ	174.41(2)
Cl(5)–Bi(1)–Cl(4) ⁱ	91.00(3)
Cl(3)–Bi(1)–Cl(4) ⁱ	96.21(3)
Cl(4)–Bi(1)–Cl(4) ⁱ	82.70(2)
Bi(1)–Cl(4)–Bi(1) ⁱ	97.30(2)

Symmetry codes: (i) $-x, -y, -z$.

3. Results and Discussion

For the sake of getting deep insight into the crystal structure, we carried out the FT-IR spectra of the title compound. The FT-IR peaks of the title compound are mainly located in the frequency region of 780–1690 cm^{-1} . The peaks at 3847 cm^{-1} and 3739 cm^{-1} should be attributed to the stretching and bending vibrations of the methyl groups of the N,N' -dimethyl-2,2'-bipy $^{2+}$ cations. The very strong intensity peak of 3473 cm^{-1} and 1617 cm^{-1} can be ascribed to the O–H stretching and bending vibration of the water molecules, respectively.¹⁸ The peaks at 3049 cm^{-1} and 2941 cm^{-1} are probably assigned to the N–H and C–H bent vibrations, respectively.¹⁹ The peaks at 2360 cm^{-1} and 1690 cm^{-1} should be assigned to the stretching and bending vibrations of the C–N bonds.²⁰ The peaks at 1504, 1449 and 1277 cm^{-1} can be attributed to the stretching vibrations of the pyridyl rings of the N,N' -dimethyl-2,2'-bipy $^{2+}$ cations.²¹ The peaks residing in the region of 888–1173 cm^{-1} can be ascribed to the bending vibration of the pyridyl rings.¹⁸ The peaks at 425, 519 and 780 cm^{-1} should be attributed to the stretching vibrations of the Bi–Cl bonds.²² The N,N' -dimethyl-2,2'-bipy $^{2+}$ cations in the title compound was synthesized with the existence of methanol, 2,2'-bipy and concentrated hydrochloric acid. The methyl groups of the N,N' -dimethyl-2,2'-bipy $^{2+}$ cations must come from the methanol. Therefore, we deem that the *in situ* reaction has happened during the solvothermal process.

As revealed by the single-crystal X-ray diffraction, compound **1** crystallized in the monoclinic space group $P2_1/n$ with two formula units in a unit cell. The asymmetric unit is consisted of half $\text{Bi}_2\text{Cl}_{10}^{4-}$ anion, one N,N' -di-

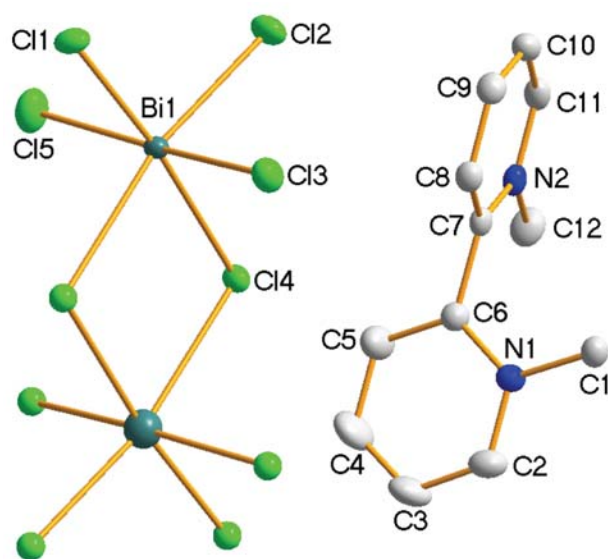


Fig. 1. An ORTEP figure of **1** with 30% thermal ellipsoids. Hydrogen atoms and lattice water molecules were omitted for clarity

methyl-2,2'-bipy $^{2+}$ cation and one lattice water molecule, as presented in Fig. 1. All of the crystallographic independent atoms are located in the general positions. There are two types of chloride ions, i.e. μ_2 -bridging Cl4 and terminal Cl1, Cl2, Cl3 and Cl5 ions. The Bi^{3+} cation is surrounded by two μ_2 -bridging chloride ions and four terminal chloride ions, giving a distorted octahedron. Two octahedra link together through edge-sharing to yield a $\text{Bi}_2\text{Cl}_{10}^{4-}$ anion. The bond lengths of Bi–Cl are in the range of 2.5594(8)–2.9350(8) Å, with an average value of 2.7267(9) Å, which is normal and comparable with those documented in the literature.^{23–27} The bond angle of Bi–Cl–Bi is 97.30(2) $^\circ$. The bond angles of Cl–Bi–Cl are in the wide range of 82.70(2) $^\circ$ –174.41(2) $^\circ$. It is noteworthy that the N,N' -dimethyl-2,2'-bipy $^{2+}$ moiety is synthesized *in situ*. The dihedral angle of the pyridyl rings is 79.37 $^\circ$. The deviation of the six atoms of the pyridyl ring is –0.006 to 0.007 Å Å apart from their average ring plane. In compound **1**, there are abundant hydrogen bonding interactions, including O–H...Cl, C–H...Cl and C–H...O interactions (Table 3). The N,N' -dimethyl-2,2'-bipy $^{2+}$ cations, $\text{Bi}_2\text{Cl}_{10}^{4-}$ anions and lattice water molecules interlink together *via* electrostatic interactions, van der Waals interactions and hydrogen bonding interactions to complete a three-dimensional (3-D) structure, as given in Fig. 2. To the best of my knowledge, this is the first bismuth compound with a methylated 2,2'-bipy moiety, although several bismuth compounds with a 2,2'-bipy moiety have been reported.^{28–31}

Bismuthate compounds are well-known for their interesting photoluminescent behaviors and they have been found applications in the fields of chemical sensors, electrochemical displays, light-emitting diodes

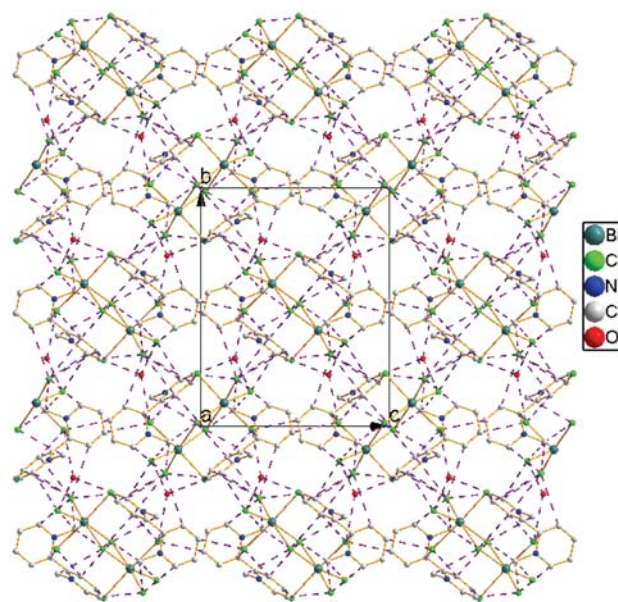


Fig. 2. Packing diagram of **1** with the dashed lines representing the hydrogen bonding interactions.

Table 3. Hydrogen bonding interactions

<i>D</i> –H... <i>A</i>	<i>D</i> –H, Å	H... <i>A</i> , Å	<i>D</i> ... <i>A</i> , Å	<i>D</i> –H... <i>A</i> , °
O1W–H1WA...Cl2 ⁱ	0.90(7)	2.54(7)	3.315(5)	144(5)
O1W–H1WB...Cl3 ⁱⁱ	0.90(6)	2.36(6)	3.223(5)	161(6)
C1–H1C...Cl4	0.96	2.75	3.681(3)	163
C8–H8A...Cl3 ⁱⁱⁱ	0.93	2.83	3.679(3)	153
C12–H12B...Cl4	0.96	2.78	3.442(4)	127
C10–H10A...O1W	0.93	2.53	3.187(6)	128

Symmetry codes: (i) $-1 + x, y, z$; (ii) $-\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iii) $-1 - x, -y, -z$.

(LEDs), photoluminescent materials, and so on.^{32,33} Taking into account the good photoluminescent properties of bismuthate and 2,2'-bipy, in the present work, we investigate the photoluminescent behaviors of compound **1** with solid-state samples at room temperature. The result of the photoluminescent measurement of compound **1** is depicted in Fig. 3. As presented in the figure, the emission spectrum of compound **1** displays a broad and strong emission band. The excitation spectrum of compound **1** exhibits that the effective energy absorption dominantly locates in the ultraviolet range of 350–400 nm. The excitation spectrum shows one peak at 385 nm. When excited at 385 nm, the emission spectrum displays one strong emission band at 551 nm in the green region, accompanied by a shoulder band at 479 nm. As a result, compound **1** could be a candidate of potential green photoluminescent materials.

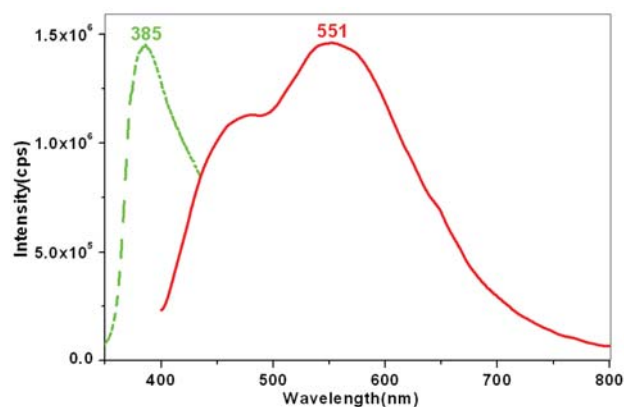


Fig. 3. Photoluminescence spectra of **1** with the green and red lines representing excitation and emission spectra, respectively.

In order to reveal the nature of the photoluminescence of compound **1**, we conducted the time-dependent density functional theory (TDDFT) calculations based on the ground state geometry of compound **1** obtained from the single-crystal X-ray diffraction data. TDDFT calculations with B3LYP function were carried out by means of the Gaussian03 program package. The final electron-population diagrams were drawn by the

ChemOffice Ultra 7.0 graphics program, as depicted in Fig. 4. We can easily observe from this figure that the characteristics of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of compound **1**. The electron-population of the singlet state of the HOMO dominantly locates at the $\text{Bi}_2\text{Cl}_{10}^{4-}$ anions. However, the electron-population of the singlet state of the LUMO mainly resides on the N,N' -dimethyl-2,2'-bipy²⁺ moiety. As a result, the essence of the photoluminescence of compound **1** can be assigned to the metal-to-ligand charge transfer (MLCT) (from the HOMO of the bismuth ion to the LUMO of the N,N' -dimethyl-2,2'-bipy²⁺ moiety) and ligand-to-ligand charge transfer (LLCT) (from the HOMO of the chloride ions to the LUMO of the N,N' -dimethyl-2,2'-bipy²⁺ moiety).

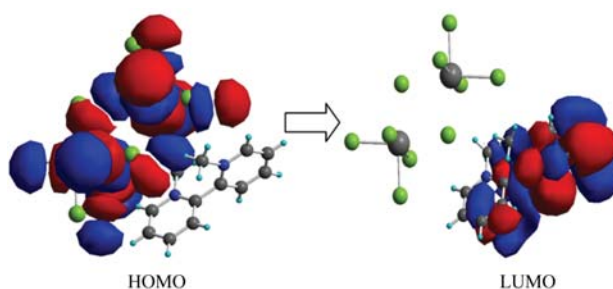


Fig. 4. The electron-density population of **1**. The isosurfaces correspond to the electronic density differences of $-15 e \text{ nm}^{-3}$ (blue) and $+15 e \text{ nm}^{-3}$ (red).

4. Conclusions

In conclusion, we have prepared a novel photoluminescent bismuth compound via a solvothermal in situ reaction. The title compound is characterized by an isolated structure. It exhibits a strong photoluminescent emission in the green region. TDDFT calculation reveals that the essence of the photoluminescence can be assigned to the combination of the MLCT and LLCT. The title compound is a potential green-light photoluminescent material.

5. Acknowledgements

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6. Supplementary Material

Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1499913. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (44) 1223 336-033; e-mail:).

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Povzetek

Z uporabo solvotermalnih pogojev smo sintetizirali nov bizmutov fotoluminiscentni material, $(N,N'$ -dimetil-2,2'-bipy) $_2(\text{Bi}_2\text{Cl}_{10}) \cdot 2\text{H}_2\text{O}$ (**1**) (bipy = bipyridin), z N,N' -dimetil-2,2'-bipy $^{2+}$ kationom dobljenim *in situ*, ter ga okarakterizirali z monokristalno rentgensko difrakcijo. Spojina **1** ima izolirano strukturo zgrajeno iz N,N' -dimetil-2,2'-bipy $^{2+}$ kationov, $\text{Bi}_2\text{Cl}_{10}^{4-}$ anionov in mrežno molekulo vode. Fotoluminiscenčni eksperiment na trdnem vzorcu razkrije, da spojina **1** močno emitira v zelenem območju. Računski pristop s časovno-odvisnim gostotnostnim funkcionalom (TDDFT) razkrije, da je vzrok za fotoluminiscenco spojine **1** možno pripisati kombinaciji prenosa naboja s kovine na ligand (MLCT) (iz HOMO bizmutovega kationa na LUMO N,N' -dimetil-2,2'-bipy $^{2+}$ kationa) in prenosu naboja z liganda na ligand (LLCT) (iz HOMO kloridnega aniona na LUMO N,N' -dimetil-2,2'-bipy $^{2+}$ kationa).