研究简报

$[Bi_2Cl_{10}(H_2\text{-Norf})_4(H_2O)_8]$(H-Norf 是诺氟沙星)

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$[Bi_2Cl_{10}(H_2\text{-Norf})_4(H_2O)_8]$ where H-Norf is Norfloxacin®

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Abstract: The crystal structure of $[Bi_2Cl_{10}(H_2\text{-Norf})_4(H_2O)_8]$ (**1**) comprises $[H_2\text{-Norf}]^+$ cations and $[Bi_2Cl_{10}]_4^-$ anions, that are loosely associated via H-bonding interactions, as well as water molecules that also participate in H-bonding interactions. Strong blue-fluorescent emission of **1** at solid state is observed at the room temperature. CCDC: 238237.

Key words: crystal structure; Norfloxacin®; bismuth(Ⅲ)

Comment

During investigations on various metal complexes with H-Norf[1,2], complexation with Bi was investigated. Fig.1 shows the structure of the first Bi(Ⅲ)$_R$ complex containing the antibacterial drug Norfloxacin○, $[Bi_2Cl_{10}(H_2\text{-Norf})_4(H_2O)_8]$. This is an ionic compound comprising four $[H_2\text{-Norf}]^+$ cations, one $[Bi_2Cl_{10}]_4^-$ anion and eight lattice water molecules. In the cation, the exo-N atom of the piperazine ring is protonated, and thereby loses its coordination ability. The dinuclear and centrosymmetric anion comprises two edge-shared octahedra. The constituents of the structure are connected into a 3D network through H-bonding interactions, as shown in Fig.2. On the other hand, there are intensive investigations about norfloxacin metal complex blue-fluorescent emission[3]. As we know, free ligand also

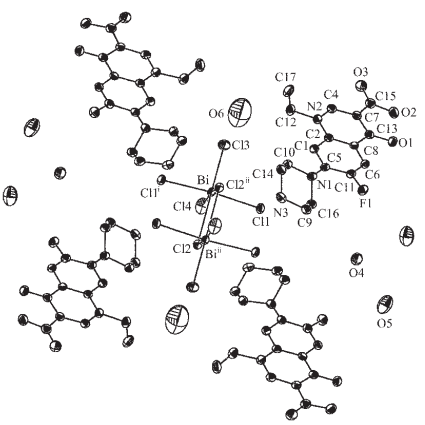

Fig.1　Structure of $[Bi_2Cl_{10}(H_2\text{-Norf})_4(H_2O)_8]$; H atoms are omitted for clarity
Key geometric parameters:
Bi-Cl1 0.268 27(13), Bi-Cl2 0.291 8(2),
Bi-Cl3 0.258 1(2), Bi-Cl4 0.255 7(3) nm,
Cl1-Bi-Cl2^{ii} 89.75(3)°, Cl3-Bi-Cl4 98.01(11)°,
Cl3-Bi-Cl1^{i} 92.42(3)°, Cl4-Bi-Cl2^{ii} 167.64(9)°,
Bi-Cl2-B^{iii} 96.50(6)°.
Symmetry operations ^{i}: x, $-y$, z; ^{ii}: $2-x$, $-y$, $1-z$.

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displays strong blue fluorescent emission. Bi is one kind of main group metal and its coordination to norfloxacin should result in the fluorescent enhancement. As expected, the fluorescent intensity of **1** ($\lambda_{e,max}$=446 nm, Fig.3) is about ten times as that of free ligand, but a red shift in the fluorescent emission of **1** is observed probably due to there existing many supramolecular weak interactions in its solid state.

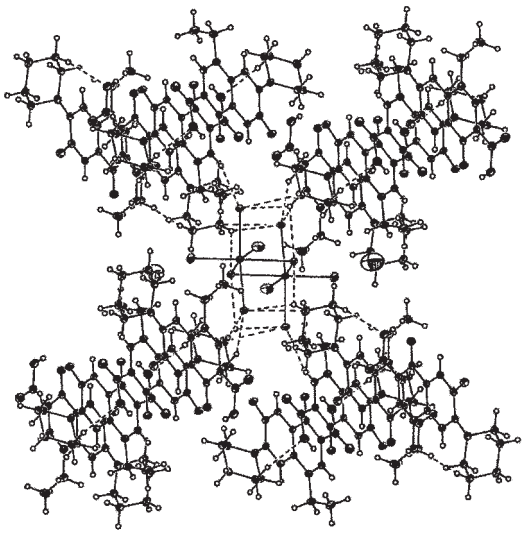

Fig.2 Packing view of **1** along *a*-axis

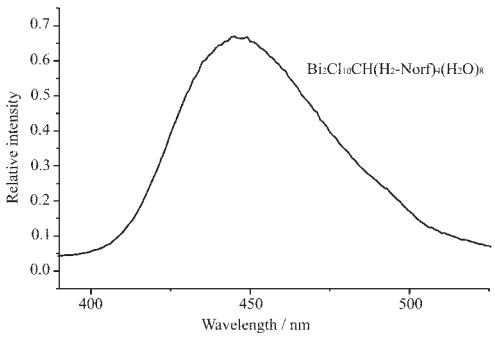

Fig.3 Fluorescent emission of **1** at the solid state at room temperature

Experiment

Hydrothermal treatment of $BiCl_3$ (0.3 mmol), norfloxacin (0.6 mmol), water (1.0 mL) and methanol (1.0 mL) over two days at 130 ℃ yielded pale yellow block crystals. The yield was about 40% based on norfloxacin. Intensity data were collected at 293(2) K on a Bruker AXS SMART CCD for a colorless block 0.10 mm × 0.15 mm × 0.20 mm. $C_{32}H_{46}BiCl_5F_2N_6O_{10}$, M= 1 098.98, monoclinic, C_2/m, a=1.421 6(2) nm, b= 2.576 2(4) nm, c=1.259 8(2) nm, β=95.028(3)°, V= 4.596 0(13) nm^3, Z=4, 6 647 unique data (θ_{max}=30.0°), R=0.042 (4 214 [$I \geqslant 2\sigma(I)$] reflections), wR=0.106 (all data), ρ_{max}=0.013 90 e·nm^{-3}; water-H were not located. Programs used: SAINT, SADABS, SHELX-97, ORTEP.

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