Crystal structure of tetrakis(1H-benzimidazol-2-amine)-κN)-bis(µ2-sulfonato-κ²O:O‘)dizinc(II) - methanol (1/1), C₃₀H₃₆N₁₂O₁₀S₂Zn₂

Abstract

C₃₀H₃₆N₁₂O₁₀S₂Zn₂, monoclinic, C2/c (no. 15), a = 22.770(11) Å, b = 12.482(6) Å, c = 14.098(7) Å, β = 95.054(8)°, V = 3991(3) Å³, Z = 4, Rgt(F) = 0.0390, wRref(F²) = 0.1120, T = 293(2) K.

CCDC no.: 1863091

The crystal structure is shown in the figure. The solvent molecule methanol is omitted for clarity. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All the reagents were used of chemical or analytical pure grade and obtained from commercial sources. A mixture of 1H-benzimidazol-2-amine (0.0058 g, 0.02 mmol) and ZnSO₄·7H₂O (0.0027 g, 0.02 mmol) was stirred in methanol (4 mL). The resultant solution was allowed to evaporate slowly at room temperature for a week to give colorless crystals of the title complex.

Discussion

Benzimidazoles as organic ligands have attracted interest in syntheses of metalorganic frameworks, not only because of their coordination abilities to metal ions but also significant potential applications in biological systems [5–11]. Each asymmetric unit contains one Zn(II), a SO₄²⁻ anion, two 1H-benzimidazol-2-amine ligands and a methanol molecule. As shown in the figure, Zn(II) is four-coordinated with irregular tetrahedral geometry surrounded by two nitrogen atoms (N1, N4) from two 1H-benzimidazol-2-amine ligands and two oxygen atoms from two sulfato ligands. The distances of Zn–N (1.973(3)–1.980(3) Å) and Zn–O (1.940(3)–2.008(3) Å) are close to those observed in

Table 1: Data collection and handling.

| Crystal: Block, colorless |
| Size: 25.0 × 0.17 × 0.16 mm |
| Wavelength: Mo Kα radiation (λ = 0.71073 Å) |
| μ: 1.374 mm⁻¹ |
| Diffractometer, scan mode: Bruker D8 Venture, Φ and ω-scans |
| θmax, completeness: 26.0°, >99% |
| N(hkl)measured, N(hkl)unique, Rint: 10762, 3913, 0.0314 |
| Criterion for lobs, N(hkl)gt: lobs > 2σ(lobs), 2880 |
| N(param)refined: 291 |
| Programs: Bruker programs [1], SHELX [2, 3], DIAMOND [4] |

slowly at room temperature for a week to give colorless crystals of the title complex.

Experimental details

The disordered sulfato ligand has been modelled by splitting it into two parts (S1, O1, O2, O3, O4 and S1′, O1′, O2′, O3′, O4′). The site occupation factors of which refined in a ratio of 0.840(7):0.160(7). Only one orientation of the sulfato ligand is shown in the figure. Hydrogen atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 Å (aromatic) or 0.96 Å (CH₃), N–H = 0.86 Å and O–H = 0.85 Å. Ueq(H) = 1.5Ueq(C,O) for methyl H atoms and hydroxy H atoms and 1.2Ueq(C,N) for others.

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other Zn(II) complexes [12, 13]. The title complex is a binuclear complex and the two Zn(II) ions are connected through SO$_2^{2-}$. The distance of Zn1···Zn1' (′ = –x, –y, –z) is 4.1634(14) Å. There are two kinds of intramolecular N(3)–H···O(15) and N(6)–H···O(2) hydrogen bonds. Four kinds of N–H···O hydrogen bonds and one kind of O–H···O hydrogen bonds form the 1-D chain.

Acknowledgements: This work was supported by the Key Scientific Research Project of Colleges and Universities in Henan Province (Grant No. 15A350002) and Henan Province Basic and Frontier Technology Research Projects (Grant No. 152300410214).

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