Tai Xi-Shi*, Zhou Xiao-Jing, Liu Li-Li, Cao Shu-Hua and Wang Li-Hua

The crystal structure of *catena*-poly[(μ_2 -2-((3-bromo-2-oxidobenzylidene)amino)acetato- $\kappa^4 O, N, O': O''$)-(dimethylformamide- $\kappa^1 O$)]zinc(II), $C_{12}H_{13}N_2O_4BrZn$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.12 × 0.11 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.76 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5869, 2402, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2162
$N(\text{param})_{\text{refined}}$:	183
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3, 4]

Source of material

5-Bromosalicylaldehyde, glycine, sodium hydroxide, zinc acetate dihydrate and ethanol are of analytical grade and used as received. An amount of 0.201 g 5-bromosalicylaldehyde (1.0 mmol), 0.075 g glycine (1.0 mmol) and 0.08 g sodium hydroxide (2.0 mmol) were dissolved in ethanol-water (15 mL, v:v = 4:1) at room temperature. The mixture was stirred for 2.5 h at 75 °C. Then 0.110 g zinc acetate dihydrate (0.5 mmol) was added to the above solution and the white precipitate immediately formed. The reactants were stirred at 75 °C for 4 hours. After cooling to room temperature, the white precipitate was received by filtration. A small amount of precipitation was dissolved in DMF and the colorless crystals of the title compound were obtained within 30 days.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93–0.96 Å). Their U_{iso} values were set to 1.2 U_{eq} or 1.5 U_{eq} of the parent atoms.

Comment

Many studies have been devoted to the synthesis, structure and properties of metal coordination polymers, because they exhibit widespread applications [5–8]. In our previous work, we have been explored the synthesis, structure and property of metal coordination polymers [9–12].

The result of single crystal analysis on the title compound indicates that there is one Zn(II) ion, one 2-((3-bromo-2-oxidobenzylidene)amino)acetate ligand and one

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Abstract

$C_{12}H_{13}N_2O_4BrZn$, monoclinic, $P2_1/n$ (no. 14), $a = 12.0182(12)$ Å, $b = 6.9735(7)$ Å, $c = 16.2510(14)$ Å, $\beta = 93.572(9)^\circ$, $V = 1359.3(2)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0279$, $wR_{\text{ref}}(F^2) = 0.0613$, $T = 293(2)$ K.

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A part of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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