

Qing Wang<sup>a\*</sup> and Xiao-Niu Fang<sup>b</sup><sup>a</sup>Office of Organisation, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, and <sup>b</sup>College of Chemistry and Chemical Engineering, JiangXi Province Key Laboratory of Coordination Chemistry, JingGangShan University, Ji'an JiangXi 343009, People's Republic of ChinaCorrespondence e-mail:  
wangqing\_fy@126.com

## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.017\text{ \AA}$   
 $R$  factor = 0.089  
 $wR$  factor = 0.240  
Data-to-parameter ratio = 19.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis{4-Bromo-2-[3-(methylammonio)propyl-  
iminomethyl]phenolato}zinc(II) dinitrate

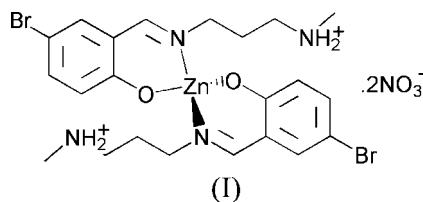
The title compound,  $[\text{Zn}(\text{C}_{11}\text{H}_{15}\text{BrN}_2\text{O})_2](\text{NO}_3)_2$ , is a centrosymmetric mononuclear Schiff base zinc(II) complex. The  $\text{Zn}^{\text{II}}$  atom, lying on a twofold rotation axis, is four-coordinated by two phenolate O atoms and two imine N atoms from two Schiff base ligands, forming a tetrahedral coordination.

Received 30 May 2006

Accepted 8 June 2006

## Comment

Zinc(II) complexes are very important in biological chemistry (Weston, 2005; Henkel & Krebs, 2004). They function as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase (Bertini *et al.*, 1994). We report here the crystal structure of the new title zinc(II) complex, (I), derived from the Schiff base 4-bromo-2-[(3-methylamino-propylimino)methyl]phenol.



The complex molecule of (I) lies on a twofold rotation axis, and thus the asymmetric unit contains only one half of the  $[\text{Zn}(\text{C}_{11}\text{H}_{15}\text{BrN}_2\text{O})_2]^{2+}$  complex cation (Fig. 1). The  $\text{Zn}^{\text{II}}$  atom located on the rotation axis is four-coordinated by two phenolate O atoms and two imine N atoms from two Schiff base ligands, forming a tetrahedral coordination. The  $\text{Zn}-\text{O}$  and  $\text{Zn}-\text{N}$  bond lengths (Table 1) are comparable with the corresponding values observed in other Schiff base zinc(II) complexes (Tatar *et al.*, 1999; Qiu, 2006). As expected, the N1/N2/C8-C11 chain adopts an extended conformation to minimize steric effects.

In the crystal structure, the molecules are linked through intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2), forming chains running along the  $c$  axis. In addition, a short  $\text{Br1}\cdots\text{O2}(x, y, 1+z)$  contact of  $3.214(10)\text{ \AA}$  is observed.

## Experimental

A mixture of 5-bromosalicylaldehyde (1.0 mmol, 202.3 mg), *N*-methyl-1,3-diaminopropane (1.0 mmol, 88.3 mg) and  $\text{Zn}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$  (1.0 mmol, 297.5 mg) was dissolved in ethanol (100 ml). The mixture was stirred for about 1 h at room temperature to give a clear yellow solution. After allowing this solution to stand in air for 18 d, yellow block-shaped crystals of (I) were formed at the bottom of the vessel.

## Crystal data

[Zn(C<sub>11</sub>H<sub>15</sub>BrN<sub>2</sub>O)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub>  
*M<sub>r</sub>* = 731.71  
 Orthorhombic, *Fdd2*  
*a* = 22.010 (4) Å  
*b* = 47.491 (5) Å  
*c* = 5.436 (2) Å  
*V* = 5682 (2) Å<sup>3</sup>

*Z* = 8  
*D<sub>x</sub>* = 1.711 Mg m<sup>-3</sup>  
 Mo *Kα* radiation  
 $\mu$  = 3.73 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Block, yellow  
 0.33 × 0.30 × 0.28 mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.372, *T<sub>max</sub>* = 0.421  
 (expected range = 0.311–0.352)

12087 measured reflections  
 3444 independent reflections  
 1463 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.186  
 $\theta_{\max}$  = 29.0°

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.089  
*wR*(*F*<sup>2</sup>) = 0.240  
*S* = 0.95  
 3444 reflections  
 178 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0824P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho_{\max} = 1.17 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{Å}^{-3}$   
 Extinction correction: *SHELXL97* (Sheldrick, 1997a)  
 Extinction coefficient: 0.0033 (4)  
 Absolute structure: Flack (1983), with 1362 Friedel pairs  
 Flack parameter: 0.00 (4)

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.914 (8)	Zn1—N1	1.953 (9)
O1 <sup>i</sup> —Zn1—O1	114.3 (5)	O1—Zn1—N1	95.9 (3)
O1 <sup>i</sup> —Zn1—N1	116.6 (4)	N1—Zn1—N1 <sup>i</sup>	119.0 (5)

Symmetry code: (i)  $-x + 1, -y + 1, z$ .

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2A...O2 <sup>ii</sup>	0.90	2.00	2.830 (19)	152
N2—H2A...O3 <sup>ii</sup>	0.90	2.23	2.976 (18)	140
N2—H2B...O2 <sup>iii</sup>	0.90	2.08	2.882 (19)	148

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

All H atoms were placed in calculated positions and constrained to ride on their parent atoms, with N—H distances of 0.90 Å and C—H

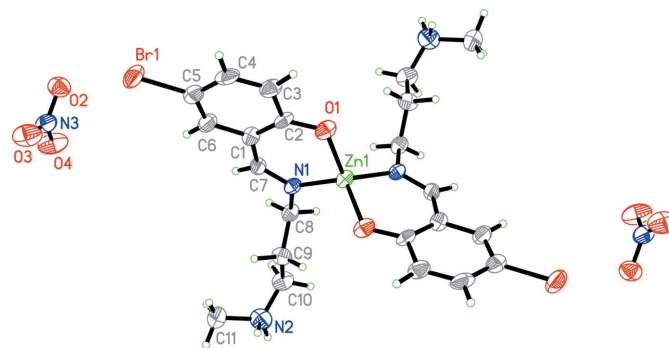


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operation (1 - *x*, 1 - *y*, *z*).

distances of 0.93–0.97 Å, and with *U*<sub>iso</sub>(H) = 1.2 or 1.5*U*<sub>eq</sub>(C,N). The high *R<sub>int</sub>* value and the low ratio of observed to unique reflections (42%) are probably due to the poor diffraction quality of the crystal. The highest peak in the final difference map is located 1.31 Å from atom N1 (1.42 Å from Zn1).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

The authors thank Fuyang Normal College for a research grant.

## References

- Bertini, I., Gray, H. B., Lippard, S. J. & Valentine, J. S. (1994). In *Bioinorganic Chemistry*. Mills Valley, California: University Science Books.
- Bruker (1998). *SMART* (Version 5.628) and *SAINTE* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Henkel, G. & Krebs, B. (2004). *Chem. Rev.* **104**, 801–824.
- Qiu, X.-Y. (2006). *Acta Cryst.* **E62**, m717–m718.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Tatar, L., Ülkü, D. & Atakol, O. (1999). *Acta Cryst.* **C55**, 508–510.
- Weston, J. (2005). *Chem. Rev.* **105**, 2151–2174.