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Acetatobis(1,10-phenanthroline)zinc(II) tetrafluoroborate

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Key indicators

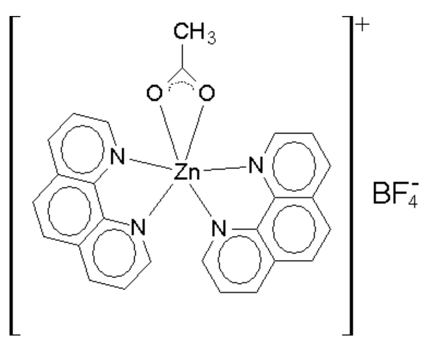
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.050
wR factor = 0.116
Data-to-parameter ratio = 12.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Zn(C_2H_3O_2)(phen)_2]BF_4$, where phen is 1,10-phenanthroline ($C_{12}H_8N_2$), crystallizes in the monoclinic space group $P2_1/n$. Zinc is in a general crystallographic position and is coordinated by one acetate and two phenanthroline ligands in an approximate *mm*2 point-group symmetry. The two Zn—O bond distances are similar to each other, as are the Zn—N bond distances.

Comment

This work reports the crystal structure of $[Zn(ac)(phen)_2]BF_4$, (I), where phen is 1,10-phenanathroline and ac is the acetate ion. This new structure is of the type $ML_2(OXO)Y$, where *M* is a transition metal, *L* is the bidentate ligand phen (1,10-phenanthroline) or bipy (2,2′-bipyridyl), OXO is a ligand such as acetate (ac), carbonate (COO) or nitrite (ONO), which can be mono- or bicoordinated to the metal atom, and *Y* is a negatively charged counter-ion, such as BF_4^-, PF_6^- or Cl^-. The Zn atom in (I) is hexacoordinated by two bidentate phenanthroline groups, *viz*. phen12 (containing atoms N1 and N2) and phen34 (containing atoms N3 and N4), and one bidentate acetate group. The dihedral angle between phen12 and phen34 is of 58.20 (4)°. Atom N2, which belongs to phen12, lies approximately in the plane formed by phen34 and Zn. Considering the zinc coordination, atoms N2 and N3 are in *trans* positions; the N2—Zn—N3 angle is 175.29 (12)° (Table 1). Phen34, on the other hand, does not have an N atom close to the least-squares plane of phen12. The carboxylate group (C41, O1 and O2) and the Zn atom are coplanar, the maximum deviation being 0.049 (3) Å for C41. N1 and N4 are displaced on opposite sides of this plane by 0.313 (5) and 0.369 (5) Å, respectively.



(I)

The mean value of the Zn—N1 and Zn—N2 distances is 2.121 (3) Å, and the mean value of the Zn—N3 and Zn—N4 distances is 2.134 (3) Å. The N1—Zn—N2 and N3—Zn—N4 angles are 78.94 (12) and 77.92 (12)°, respectively (Table 1). These geometric parameters suggest that the Zn–phen12 and Zn–phen34 interactions have similar strengths. This is also observed in other [Zn(*ac*)(phen)$_2$]*Y* structures (Tables 2 and 3). Similar features have also been observed in Zn–bipyridine complexes. On the other hand, copper coordination in bipyridine or phenanthroline complexes results in the metal being more strongly coordinated to one bidentate ligand than to the other. As pointed out by Rodrigues (2004), this feature is in agreement with the more symmetrical electron distribution of Zn^{2+} (d^{10}) in comparison to Cu^{2+} (d^9).

Experimental

An ethanol mixture (12 ml) containing Zn(ac)$_2$·4H$_2$O (0.090 g), phenanthroline (0.095 g) and NaBF$_4$ (0.113 g) was heated to 333 K for 1 h, then left at 298 K and filtered. Slow evaporation of the filtrate resulted in single crystals of (I).

Crystal data

[Zn(C$_2$H$_3$O$_2$)(C$_{12}$H$_8$N$_2$)$_2$]BF$_4$
M_r = 571.63
Monoclinic, $P2_1/n$
a = 8.2289 (5) Å
b = 19.2134 (11) Å
c = 15.6534 (5) Å
β = 95.803 (3)°
V = 2462.2 (2) Å^3
Z = 4
D_x = 1.542 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5441 reflections
θ = 1.0–27.5°
μ = 1.06 mm^{-1}
T = 293 (2) K
Prism, colorless
0.13 × 0.10 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
7832 measured reflections
4329 independent reflections
2440 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 25°
$h = -9 \rightarrow 9$
$k = -21 \rightarrow 22$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.116
S = 0.94
4329 reflections
343 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.4 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.293 (3)	Zn1—N2	2.151 (3)
Zn1—O2	2.149 (3)	Zn1—N3	2.148 (3)
Zn1—N1	2.091 (3)	Zn1—N4	2.119 (3)
N1—Zn1—O1	88.41 (11)	N2—Zn1—N4	98.37 (12)
N1—Zn1—O2	145.25 (11)	N3—Zn1—O1	93.56 (11)
N1—Zn1—N2	78.94 (12)	N3—Zn1—O2	91.95 (11)
N1—Zn1—N3	99.82 (12)	N3—Zn1—N4	77.92 (12)
N1—Zn1—N4	113.81 (12)	N4—Zn1—O1	157.13 (11)
N2—Zn1—O1	90.95 (11)	N4—Zn1—O2	100.56 (11)
N2—Zn1—O2	91.59 (11)	O1—Zn1—O2	58.12 (11)
N2—Zn1—N3	175.29 (12)		

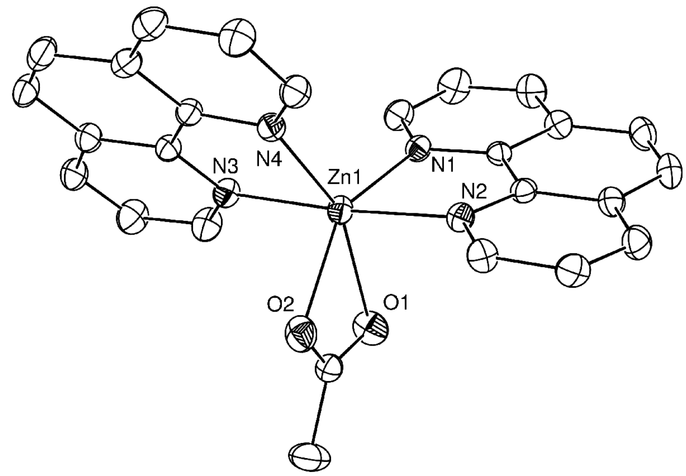


Figure 1
ORTEP-3 (Farrugia, 1997) drawing of the zinc coordination in (I), shown with 20% probability displacement ellipsoids. H atoms have been omitted for clarity, as has the anion.

Table 2
Comparative bond lengths (Å) for [Zn(ac)(phen)$_2$]*Y* complexes.

Y	Zn—N1	Zn—N2	Zn—N3	Zn—N4	Zn—O1	Zn—O2
BF$_4$[a]	2.091 (3)	2.151 (3)	2.148 (3)	2.119 (3)	2.293 (3)	2.149 (3)
BF$_4$·2H$_2$O[b]	2.116 (2)	2.147 (2)	2.147 (2)	2.116 (2)	2.184 (2)	2.184 (2)
ClO$_4$[c]	2.135 (6)	2.143 (6)	2.160 (5)	2.100 (5)	2.296 (5)	2.156 (5)

Notes: (*a*) [Zn(ac)(phen)$_2$]BF$_4$ (this work); (*b*) [Zn(ac)(phen)$_2$]BF$_4$·2H$_2$O (Fitzgerald *et al.*, 1985); (*c*) [Zn(ac)(phen)$_2$]ClO$_4$ (Chen *et al.*, 1994).

Table 3
Comparative bond angles (°) for [Zn(ac)(phen)$_2$]*Y* complexes.

	N1—Zn—N2	N3—Zn—N4	O1—Zn—O2
[Zn(ac)(phen)$_2$]BF$_4$[a]	78.94 (12)	77.92 (12)	58.12 (11)
[Zn(ac)(phen)$_2$]BF$_4$·2H$_2$O[b]	78.47	78.47	57.2
[Zn(ac)(phen)$_2$]ClO$_4$[c]	78.1 (2)	78.6 (2)	57.8 (2)

Notes: (*a*) this work; (*b*) Fitzgerald *et al.* (1985); (*c*) Chen *et al.* (1994).

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å for CH and 0.96 Å for CH$_3$. U_{iso}(H) = 1.2 (CH) or 1.5 (CH$_3$) times U_{eq} of the parent atom.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *COLLECT*; data reduction: *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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