metal-organic papers

Bis[3-dimethylamino-1-(2-pyridyl)prop-2-enonato]-diperchloratozinc(II)

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The title compound, [Zn(C$_{10}$H$_{12}$N$_2$O)$_2$(ClO$_4$)$_2$], crystallizes as mononuclear molecules with distorted octahedral Zn^{II} coordination. 3-Dimethylamino-l-(2-pyridyl)prop-2-enone ions are coordinated to Zn^{II} as bidentate ligands, while the perchlorate ions are monodentate. The Zn atom lies on a centre of symmetry.

Comment

The structures of a large number of complexes obtained from the reactions of Zn^{II} ions with different pyridine derivatives as ligands have been reported: examples are diphenyl(2-pyridyl)methanol Zn^{II} (Doering *et al.*, 1986), [Zn(CH$_2$SiMe$_3$){OCH$_2$(2-py)}]$_4$ (van der Schaaf *et al.*, 1993), Zn^{II}/X/(py)$_2$CO [X = Cl$^-$, N$_3^-$ and SO$_4^{2-}$, and (py)$_2$CO is di-2-pyridyl ketone; Katsoulakou *et al.*., 2002].

(I)
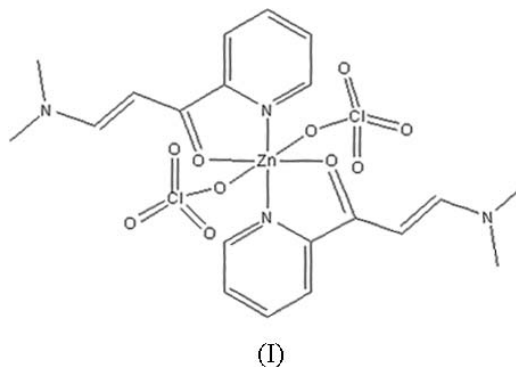
In the monomeric title complex, [Zn(C$_{10}$H$_{12}$N$_2$O)$_2$](ClO$_4$)$_2$, (I), the Zn^{II} atom is surrounded by two bidentate 3-dimethylamino-l-(2-pyridyl)prop-2-enone and two monodentate perchlorate ligands. The Zn atom lies on a centre of symmetry (Fig. 1).

Although the Zn^{II} atom has four-coordination, close contact of atom O2 [Zn1$\cdots$O2 = 2.44 (3) Å] may be considered to give six-coordination. The six-coordination around the Zn^{II} ion can be described as distorted octahedral.

The O1—Zn1$\cdots$O2 and N2—Zn1$\cdots$O2 angles are 86.4 (6) and 85.3 (8)°, respectively. The configuration around atom Zn1 is given by the torsion angles listed in Table 1.

Experimental

The slow diffusion of a CH$_3$OH solution (5 ml) of Zn(NO$_3$)$_2$ (1.0 mmol) into a CHCl$_3$ solution (5 ml) of 3-dimethylamino-l-(2-pyridyl)prop2-enone (1.0 mmol) resulted in the formation of the single crystals of (I).

Crystal data

$[Zn(C_{10}H_{12}N_2O)_2(ClO_4)_2]$
$M_r = 616.70$
Triclinic, $P\bar{1}$
$a = 7.5449 (19)$ Å
$b = 9.187 (2)$ Å
$c = 9.5884 (19)$ Å
$\alpha = 79.358 (3)°$
$\beta = 78.130 (2)°$
$\gamma = 70.887 (3)°$
$V = 609.6 (2)$ Å^3

$Z = 1$
$D_x = 1.680$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2384
    reflections
$\theta = 2.4–27.0°$
$\mu = 1.29$ mm^{-1}
$T = 298 (2)$ K
Block, pink
$0.52 \times 0.34 \times 0.31$ mm

Data collection

Bruker SMART CCD area-detector
    diffractometer
φ and ω scans
Absorption correction: multi-scan
    (*SADABS*; Sheldrick, 1996)
    $T_{min} = 0.554$, $T_{max} = 0.691$
3200 measured reflections

2166 independent reflections
1988 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.3°$
$h = -6 \rightarrow 9$
$k = -9 \rightarrow 11$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.101$
$S = 1.12$
2166 reflections
182 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.1968P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.025$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: *SHELXL97*
    (Sheldrick, 1997)
Extinction coefficient: 0.027 (4)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.0216 (16)	Zn1—O2	2.44 (3)
Zn1—N2	2.0448 (19)		
O1—Zn1—N2	80.22 (7)	N2—Zn1—O2	85.3 (8)
O1—Zn1—O2	93.6 (6)		
O1—Zn1—N2—C6	−3.04 (15)	O2—Zn1—O1—C1	−85.0 (8)
O2—Zn1—N2—C6	91.4 (5)	O1—Zn1—O2—Cl1	−27 (3)
O1—Zn1—N2—C10	179.5 (2)	N2—Zn1—O2—Cl1	−107 (3)
O2—Zn1—N2—C10	−86.0 (5)		

Atom O2 of the perchlorate ligand is disordered and was modelled with split positions, having site occupation factors of 0.62 (13) and 0.38 (13) with common isotropic displacement parameters. H atoms were positioned geometrically at distances of 0.93 (CH) and 0.96 Å (CH$_3$) from their parent C atoms; a riding model was used during the
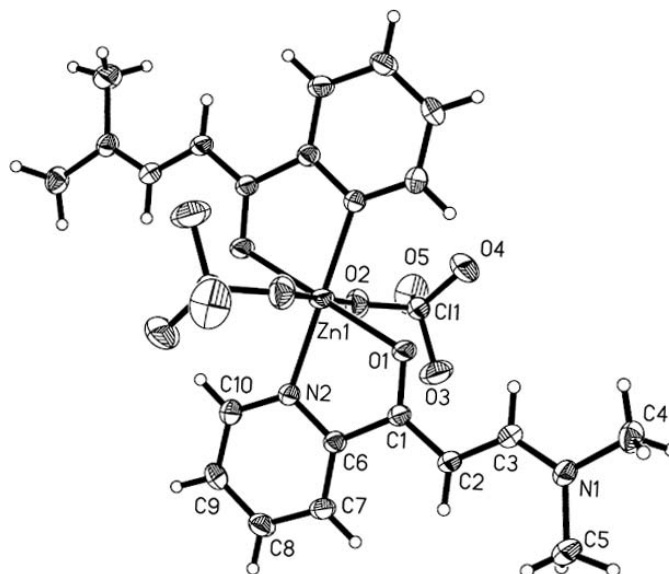

Figure 1
Drawing of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: $2 - x$, $-y$, $-z$.]

refinement process. The $U_{iso}(H)$ values were constrained to be 1.2 (1.5 for methyl) times U_{eq} of the carrier atom.

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

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