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Bis(4,6-dibromo-2-formylphenolato-κ^2O,O')-bis(dimethyl sulfoxide-κO)nickel(II)

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Key indicators

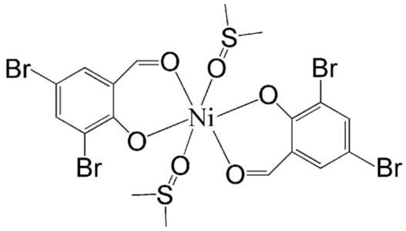
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 16.2

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

In the title compound, $[Ni(C_7H_3Br_2O_2)_2(C_2H_6OS)_2]$, the Ni^{II} atom lies on a centre of inversion and is coordinated in an octahedral geometry by four O atoms from two bidentate 4,6-dibromo-2-formylphenolate ligands and two O atoms from two dimethyl sulfoxide molecules. Short Br···Br contacts exist between molecules.

Comment

Interest in packing arrangements of halogenated compounds goes back many years to what Schmidt called the 'chloro effect', where the presence of chloro substituents on aromatic compounds frequently results in stacking arrangements with a short (*ca* 4 Å) crystallographic axis (Cohen *et al.*, 1964; Zordan *et al.*, 2005; Desiraju, 1989). The title compound, (I), contains the dibrominated ligand 4,6-dibromo-2-formylphenolate, with two Br atoms accessible at the periphery of each ligand.



(I)

In (I), the Ni^{II} atom lies on a centre of inversion and is coordinated by four O atoms from two bidentate 4,6-dibromo-2-formylphenolate ligands and two O atoms from two dimethyl sulfoxide molecules, forming a slightly distorted octahedral geometry (Fig. 1 and Table 1). The shortest Br···Br contacts (Zordan *et al.*, 2005; Zaman *et al.*, 2004; Sarma & Desiraju, 1986) are $Br2\cdots Br2^{ii}$ = 3.5631 (14) Å and $Br1\cdots Br2^{iii}$ = 3.8214 (9) Å [symmetry codes: (ii) $1 - x, -y, -z$; (iii) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$].

Experimental

A solution of taurine ($H_2N(CH_2)_2SO_3H$, 0.253 g, 2 mmol) and KOH (0.112 g, 2 mmol) in distilled water (10 ml) was added slowly to a solution of 4,6-dibromo-2-formylphenol (0.560 g, 2 mmol) in methanol (10 ml). The mixture was stirred for 30 min at room temperature, then added slowly to a solution of nickel(II) nitrate (0.291 g, 1 mmol) in distilled water (10 ml). The resulting mixture was stirred at room temperature for 4 h. The crude product was washed three times with methanol and dried under vacuum. Green prismatic crystals of (I) were obtained by slow evaporation of a solution of the product in dimethyl sulfoxide.

Crystal data

$[Ni(C_7H_3Br_2O_2)_2(C_2H_6OS)_2]$
$M_r = 772.79$
Monoclinic, $P2_1/c$
$a = 12.969$ (2) Å
$b = 12.547$ (2) Å
$c = 7.764$ (1) Å
$\beta = 95.865$ (1)°
$V = 1256.7$ (3) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 7.33$ mm^{-1}
$T = 293$ (2) K
0.27 × 0.14 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.244$, $T_{\max} = 0.697$
9406 measured reflections
2335 independent reflections
1637 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.122$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.102$
$S = 1.00$
2335 reflections
144 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.75$ e Å^{-3}
$\Delta\rho_{\min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.998 (3)	Ni1—O3	2.105 (3)
Ni1—O2	2.049 (3)		
O1—Ni1—O2	89.86 (12)	O1—Ni1—O3$^{\rm i}$	88.95 (12)
O1—Ni1—O3	91.05 (12)	O2—Ni1—O3	87.52 (12)
O1—Ni1—O2$^{\rm i}$	90.14 (12)	O2—Ni1—O3$^{\rm i}$	92.48 (12)

Symmetry code: (i) $-x+2, -y+1, -z$.

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl), and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ (aromatic) or $1.5U_{\rm eq}({\rm C})$ (methyl). The methyl groups were allowed to rotate about their local threefold axes.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 1997); software used to prepare material for publication: *SHELXTL*.

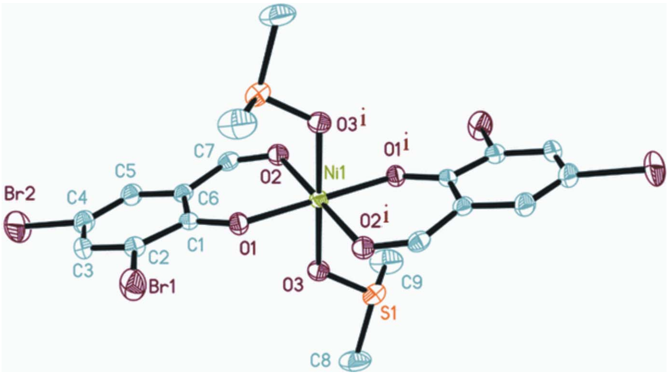


Figure 1
The molecular structure of (I), showing displacement ellipsoids at 30% probability for non-H atoms. H atoms have been omitted. Symmetry code as in Table 1.

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