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Bis[2-(4-methylanilinomethyl)-6-methoxyphenolato-κ^2O,O']bis(nitrato-κO)cobalt(II)

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Key indicators

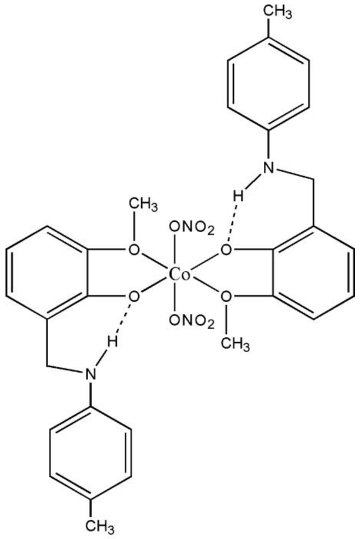
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.097
Data-to-parameter ratio = 15.3

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

The centrosymmetric title complex, $[Co(NO_3)_2(C_{15}H_{15}NO_2)_2]$, is a neutral molecule whose Co atom is six-coordinated in an octahedral geometry by four O atoms of the phenoxy and methoxy groups of the 2-(4-methylanilinomethyl)-6-methoxyphenolate Schiff base ligands, and by two O atoms of nitrate groups.

Comment

Schiff base complexes are useful chemicals (Tümer *et al.*, 1999), and metal complexes of Schiff bases synthesized by condensing salicylaldehyde and its derivatives are the best known. They include complexes with a methoxy group in the *ortho* position (West, 1960; Polishchuk *et al.*, 1990) as the methoxy group can also bind to the metal. Such Schiff bases behave as bidentate ligands to divalent first-row transition metals (Calvin *et al.*, 1946; Sacconi *et al.*, 1962; Nishikawa *et al.*,1965; Lane *et al.*, 1961). The title compound, (I), also has the deprotonated ligand binding in this manner.



(I)

The Co atom exists in an octahedral coordination environment (Fig. 1). It lies on an inversion center. The structure features an intramolecular hydrogen bond (Table 2).

Experimental

The ligand was prepared by the direct solid-phase reaction of *o*-vanillin (10 mmol, 1.5251 g) and *p*-toluidine (10 mmol, 1.0700 g). The reactants were ground in an agate mortar. The color of the mixture changed from light yellow to orange. A solution of $Co(NO_3)_2 \cdot 6H_2O$ (1.0 mmol, 0.29 g) in methanol (10 ml) was added to a methanol

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solution of the Schiff base ligand (2 mmol, 0.48 g). Dark-red crystals were isolated after two weeks.

Crystal data

$[Co(NO_3)_2(C_{15}H_{15}NO_2)_2]$
$M_r = 665.51$
Triclinic, $P\overline{1}$
$a = 8.3029$ (17) Å
$b = 9.4201$ (19) Å
$c = 9.5979$ (19) Å
$\alpha = 84.32$ (3)°
$\beta = 80.47$ (3)°
$\gamma = 82.01$ (3)°
$V = 730.9$ (3) Å^3
$Z = 1$
$D_x = 1.512$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.65$ mm^{-1}
$T = 296$ (2) K
Block, red
0.24 × 0.19 × 0.10 mm

Data collection

Bruker APEX-II area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.859$, $T_{\max} = 0.940$
9334 measured reflections
3227 independent reflections
2733 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.097$
$S = 1.02$
3227 reflections
211 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.2339P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.32$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0118 (13)	Co1—O2	2.1815 (14)
Co1—O3	2.0885 (18)		
O1^{i}—Co1—O1	180	O3—Co1—O2^{i}	85.72 (7)
O1—Co1—O3^{i}	90.64 (7)	O1—Co1—O2	77.00 (5)
O1—Co1—O3	89.36 (7)	O3—Co1—O2	94.28 (7)
O3^{i}—Co1—O3	180	O2^{i}—Co1—O2	180
O1—Co1—O2^{i}	103.00 (5)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.91 (2)	1.84 (2)	2.597 (2)	139 (2)

The H atoms bonded to C atoms were positioned geometrically and refined using a riding model [C—H = 0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$] and methyl groups were allowed to rotate to fit the electron density [C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$]. The H atom bonded to N atoms was located in a difference Fourier map and refined with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm N})$.

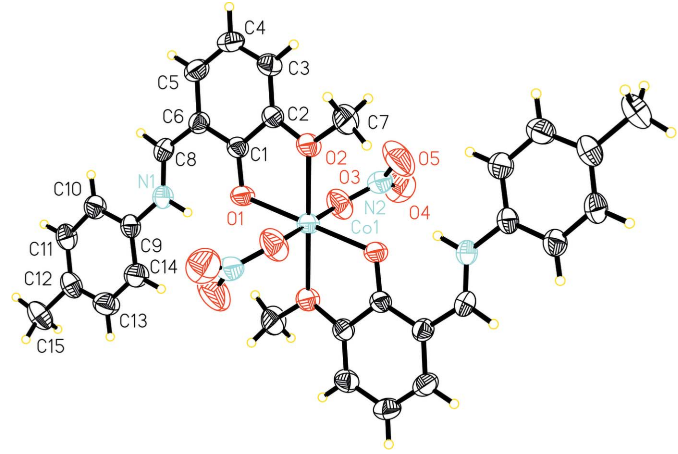

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. The unlabeled atoms are related to the labeled ones by the symmetry operation $(1 - x, 1 - y, 1 - z)$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2002); software used to prepare material for publication: *SHELXL97*.

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