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Tetra-μ-acetato-κ^8*O*:*O*′-bis[(2-benzylidene-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one-κ*N*)cobalt(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.033
wR factor = 0.194
Data-to-parameter ratio = 15.2

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

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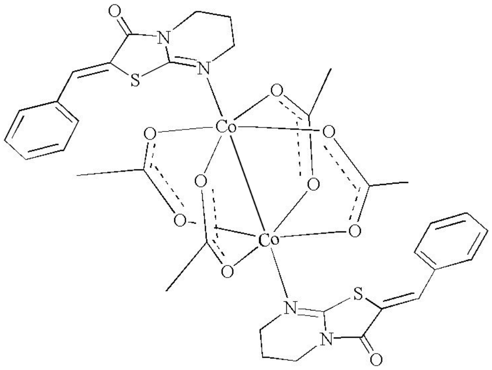
The title compound, $[Co_2(C_2H_3O_2)_4(C_{13}H_{12}N_2OS)_2]$, is a binuclear complex, which occupies a special position at an inversion centre. Each Co atom has a distorted octahedral coordination, which involves four O atoms of four μ-acetate groups [Co—O = 1.9617 (19)–1.977 (2) Å] and the N atom of the 2-benzylidene-6,7-dihydro-5*H*-thiazolo[3,2-*a*]-pyrimidin-3-one ligand [Co—N = 2.214 (2) Å]; the coordination octahedron is completed by the Co—Co bond of 2.6708 (8) Å.

Comment

Thiazolidinones have been the subject of extensive studies and in the recent past numerous reports highlighting their chemistry and applications have appeared (*e.g.* Russowsky & da Silveira Neto, 2004). Transition metal complexes with thiazolidinone ligands have also received substantial attention (Tong *et al.*, 2003).



(I)

The title compound, (I), is a neutral binuclear cobalt complex which occupies a special position at an inversion centre. Atom Co1 (Fig. 1) has a distorted octahedral coordination, which involves four O atoms of four μ-acetate groups and atom N1 of the 2-benzylidene-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one ligand; the coordination octahedron is completed by the Co1—Co1^{i} bond [symmetry code: (i) $-x, 1-y, -z$].

As has been noted (Campos-Fernandez *et al.*, 2002), the basicity of the axial ligand and the strength of the axial *M*—*L* coordination influences the geometry of the rest of the complex. Indeed, the axial Co—N bond in (I) [Co1—N1 = 2.214 (2) Å] is considerably longer than the axial Co—N bond (2.085 Å) in tetrakis(μ-phenylacetato-*O*:*O*′)bis(quinoline-*N*)cobalt(II) (Cui *et al.*, 1999), whereas the Co—O and Co—Co distances in (I) [Co—O = 1.9617 (19)–1.977 (2) Å and

Co1—Co1^{i} = 2.6708 (8) Å] are substantially shorter than corresponding distances in its quinoline analogue (2.010–2.047 and 2.813 Å, respectively; Cui *et al.*, 1999).

Atoms S1, C6, C5, N2, C4, N1, C1 and C3 of the thiazolodihydropyrimidine ligand form an approximately (within 0.07 Å) planar system, with C2 deviating from the mean plane (plane *A*) by 0.6673 (2) Å. Plane *A* approximately bisects the angle between the two carboxylate planes: the angles between plane *A* and the Co1/O2/C14/O3/Co1^{i} and Co1/O4/C16/O5/Co1^{i} planes are 40.3 (3) and 51.1 (4)°, respectively, and the two carboxylate planes are mutually almost orthogonal. The C8–C13 mean plane forms a dihedral angle of 16.900 (8)° with plane *A*.

Experimental

The ligand 2-benzylidene-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one was prepared (m.p. 421–422 K, yield 89%) according to Mohan & Kumar (1998). 2-Benzylidene-6,7-dihydro-5*H*-thiazolo[3,2-*a*]-pyrimidin-3-one (488 mg, 2 mmol) and Co($CH_3COO)_2$ (195 mg, 1 mmol) were added to 20 ml of refluxing acetonitrile, and the reaction mixture was stirred at room temperature for 12 h. The blue precipitate was filtered off and dissolved in 50 ml of hot acetonitrile. Single crystals of the title compound suitable for X-ray analysis were grown by slow evaporation of the solvent (m.p. 554–556 K).

Crystal data

$[Co_2(C_2H_3O_2)_4(C_{13}H_{12}N_2OS)_2]$
M_r = 842.65
Monoclinic, $C2/c$
a = 22.268 (6) Å
b = 12.924 (4) Å
c = 14.674 (4) Å
β = 123.375 (4)°
V = 3526.5 (17) Å^3
Z = 4

D_x = 1.587 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1020 reflections
θ = 3.1–26.0°
μ = 1.12 mm^{-1}
T = 293 (2) K
Block, blue
0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.821, T_{max} = 1.000
10 022 measured reflections

3625 independent reflections
2816 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.4°
$h = -23 \rightarrow 27$
$k = -16 \rightarrow 14$
$l = -18 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.194$
S = 1.04
3625 reflections
238 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.084P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0031 (2)

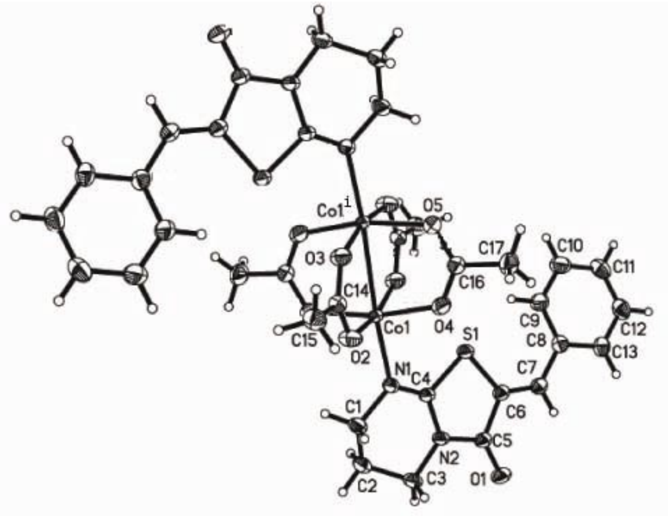


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level [symmetry code: (i) $-x$, $1 - y$, $-z$].

H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined in a riding model, with U_{iso}(H) = $1.5U_{eq}$(carrier) for methyl H atoms and $1.2U_{eq}$(carrier) for all other H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SADABS, SMART, SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Campos-Fernandez, C. S., Thomson, L. M., Galan-Mascaros, J. R., Ouyan, X. & Dunbar, K. R. (2002). *Inorg. Chem.* **41**, 1523–1533.

Cui, Y., Zheng, F. & Huang, J. (1999). *Acta Cryst.* C**55**, 1067–1069.

Mohan, J. & Kumart, V. (1998). *Indian J. Chem. Sect. B*, **37**, 183–186.

Russowsky, D. & da Silveira Neto, B. A. (2004). *Tetrahedron Lett.* **45**, 1437–1440.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Tong, W.-J., Liu, L., Meng, Q.-J., Li, Y.-Z. & Yao, Y.-G. (2003). *Acta Cryst.* E**59**, m3–m5.