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Acetonitrile[2-(3,5-dimethylpyrazol-1-yl)-1,3-benzothiazole]dinitratocobalt(II)

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Key indicators

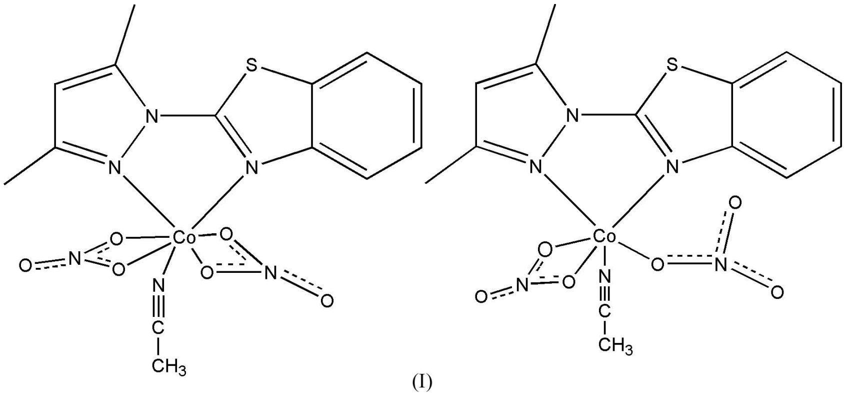
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.098
wR factor = 0.208
Data-to-parameter ratio = 11.9

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

The asymmetric unit of the title complex, [Co(NO_3)$_2$(C_2H_3N)($C_{12}H_{11}N_3S$)], comprises two Co^{II} complexes with the same chemical formula but with different coordination behaviour of the nitrate ligands. The geometry of the Co^{II} ion can be described as being intermediate between distorted pentagonal bipyramidal and distorted octahedral, whereby O atoms of one of the bidentate coordinating nitrate groups are considered as occupying one coordination site.

Comment

The coordination chemistry of pyrazole-containing ligands has received much attention, owing to their potential role in modelling the active sites of metalloenzymes (Sorrell *et al.*, 1982; Arali *et al.*, 1993). In this paper, we report the crystal structure of the title 2-(3,5-dimethylpyrazol-1-yl)-benzothiazole complex of cobalt(II), (I).



(I)

Molecular views of each of the two 2-(3,5-dimethylpyrazol-1-yl)benzothiazole cobalt complexes in (I) are shown in Figs. 1 and 2. All bond lengths and angles are within reasonable ranges .

The coordination of Co1 includes atoms N3, O1, O3, O4, O6 forming a plane, with Co1—N6 = 2.090 (7) and Co1—N1 = 2.118 (6) Å. The coordination sphere of Co2 has atoms N7, O7, O9, O10 in a plane, with Co2—N9 = 2.101 (6) and Co2—N12 = 2.097 (7) Å. The two Co^{II} complexes differ in that one of the coordinating nitrate groups binds to Co in either a monodentate or a bidentate mode. However, as shown in Figs. 1 and 2, the two Co^{II} atoms present almost the same geometry if the N atoms of the NO_3 groups are considered instead of the coordinating O atoms. Several authors have proposed that the bidentate nitrate anion could be considered as occupying one coordination site (Cotton *et al.*, 1963; Locher *et al.*, 1987), so in such a case, the two Co atoms might be regarded as having a trigonal–bipyramidal environment. However, we prefer to

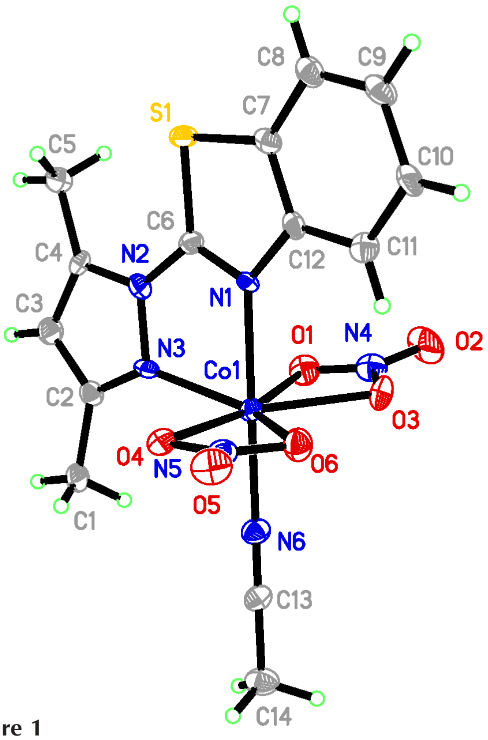


Figure 1
A molecular view of complex A, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

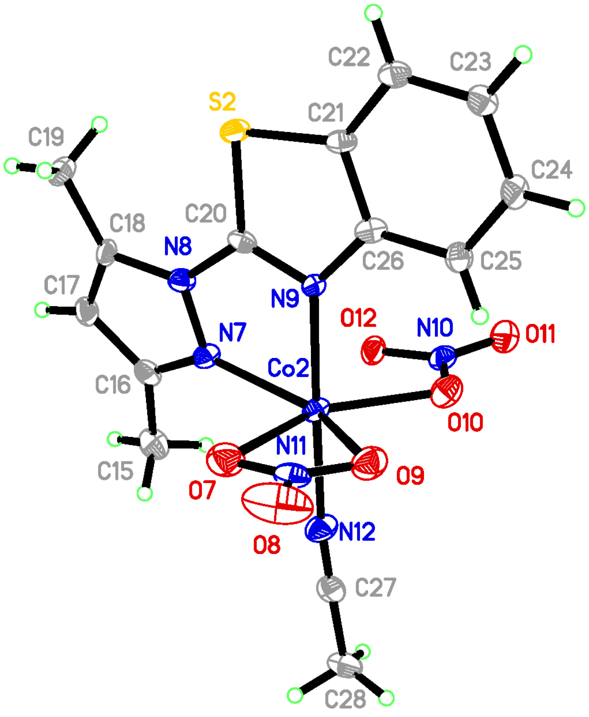


Figure 2
A molecular view of complex B, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

consider that the geometry of the Co^{II} ions is better described as being intermediate between distorted pentagonal bipyramidal, in which the two NO_3 groups behave as bidentate ligands (molecule A, Fig. 1), and distorted octahedral, in which one of the nitrate groups behaves as a monodentate ligand (molecule B, Fig. 2).

Experimental

All chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China. 2-(3,5-Dimethylpyrazol-1-yl)benzothiazole was first prepared by published procedures (Arali *et al.*, 1993). 2-(3,5-Dimethylpyrazol-1-yl)benzothiazole (15 ml, 0.001 mol) and $Co(NO_3)_2\cdot 6H_2O$ (5 ml, 0.001 mol) were each dissolved in hot acetonitrile, and then mixed together and refluxed for 4 h. The reaction mixture was then filtered and the filtrate was allowed to stand at room temperature for several days, affording red crystals of (I).

Crystal data

$[Co(NO_3)_2(C_2H_3N)(C_{12}H_{11}N_3S)]$
$M_r = 453.30$
Triclinic, $P\overline{1}$
$a = 9.407$ (4) Å
$b = 10.776$ (4) Å
$c = 18.174$ (7) Å
$\alpha = 84.279$ (5)°
$\beta = 86.952$ (5)°
$\gamma = 84.890$ (5)°
$V = 1824.1$ (12) Å^3

$Z = 4$
$D_x = 1.651$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3897 reflections
$\theta = 2.3$–27.0°
$\mu = 1.10$ mm^{-1}
$T = 293$ (2) K
Block, red
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.733$, $T_{max} = 0.810$
7293 measured reflections

6103 independent reflections
5806 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$
$h = -11 \rightarrow 11$
$k = -8 \rightarrow 12$
$l = -20 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.098$
$wR(F^2) = 0.208$
$S = 1.20$
6103 reflections
511 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 16.6816P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.20$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}

H atoms attached to C atoms were placed in geometrically idealized positions, with Csp^3—H = 0.96 Å and Csp^2—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}$(methyl C) or $1.2U_{eq}$(other C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

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References

Arali, V. H., Revankar, V. K. & Mahale, V. B. (1993). *Transition Met. Chem.* **18**, 158–162.

Bruker (2000). *SMART* (Version 5.0) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.

Cotton, F. A., Goodgame, D. M. L. & Sonderberg, R. H. (1963). *Inorg. Chem.* **2**, 1162–1165.

Locher, K., Blonk, H. L., Driessen, W. L. & Reedijk, J. (1987). *Acta Cryst.* C**43**, 651–653.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.

Sorrell, T. N., Malachowski, M. R. & Jameson, D. L. (1982). *Inorg. Chem.* **21**, 3250–3252.

Acta Cryst. (2005). E**61**, m1307–m1309 Zhang *et al.* • $[Co(NO_3)_2(C_2H_3N)(C_{12}H_{11}N_3S)]$ **m1309**