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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.036

wR factor = 0.088

Data-to-parameter ratio = 14.3

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

Diaquabis(3,5-dinitrobenzoato)bis[4,4,5,5-tetramethyl-2-(4-pyridyl)-4,5-dihydro-1H-imidazole-1-oxyl-3-oxide]cobalt(II)

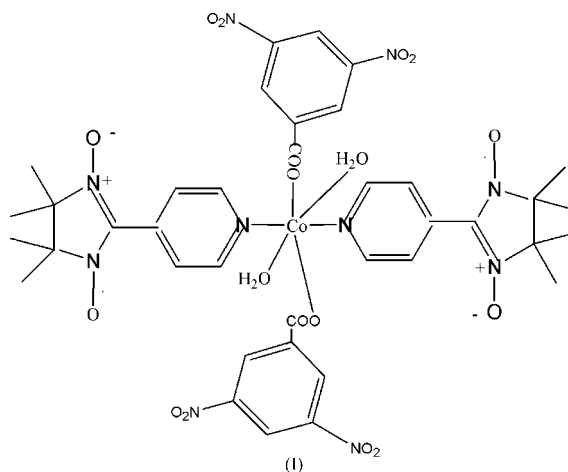
The title compound, $[\text{Co}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})_2]$, was prepared by reacting the ligand 4,4,5,5-tetramethyl-2-(4-pyridyl)imidazolin-1-oxyl-3-oxide (nitronyl nitroxide) with cobalt(II) nitrate and 3,5-dinitrobenzoic acid (DBA). The cobalt(II) ion lies on a crystallographic centre of symmetry. The central cobalt(II) ion is in a distorted octahedral geometry, and is coordinated by two N atoms from two different nitronyl nitroxide ligands, two O atoms from two different 3,5-dinitrobenzoate ligands and the two O atoms of two water molecules in a *trans* arrangement.

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Comment

Nitronyl nitroxides are widely used as units in the synthesis of molecule-based magnetic materials, especially as they can act as ligands in the formation of metal–nitroxide complexes (Vostrikova *et al.*, 2000; Oshio *et al.*, 2002). 3,5-Dinitrobenzoic acid has attracted considerable attention in recent years because of its strong ability to coordinate transition metals, forming a polymeric structural topology (Stachovo *et al.*, 2006). By combining the two approaches, a new cobalt(II) complex, (I), with 4,4,5,5-tetramethyl-2-(4-pyridyl)imidazolin-1-oxyl-3-oxide (nitronyl nitroxide) and 3,5-dinitrobenzoate (DBA) has been prepared.



The cobalt(II) ion lies on a crystallographic centre of symmetry. The centrosymmetric molecule is illustrated in Fig. 1. The central cobalt(II) ion is in a distorted octahedral CoN_2O_4 environment, coordinated by two N atoms from two nitronyl nitroxide ligands, two O atoms from two 3,5-dinitrobenzoate ligands and two O atoms of two water molecules in a *trans* arrangement. The dihedral angle between the pyridyl ring and the O–N–C–N–O group is $6.7(3)^\circ$.

Experimental

The title compound was prepared by adding an aqueous solution (10 ml) of 3,5-dinitrobenzoic acid (0.1 mmol) to a methanol solution (10 ml) of nitronyl nitroxide (0.1 mmol) and cobalt(II) nitrate (0.1 mmol). The mixture was stirred for 1 h and then filtered. The filtrate was slowly evaporated at room temperature, and blue crystals suitable for X-ray analysis were obtained.

Crystal data

[Co(C₇H₃N₂O₆)₂(C₁₂H₁₆N₃O₂)₂·(H₂O)₂] $\gamma = 85.999 (6)^\circ$
 $M_r = 985.75$ $V = 1085.1 (6) \text{ \AA}^3$
 Triclinic, $P\bar{1}$ $Z = 1$
 $a = 10.110 (4) \text{ \AA}$ $D_x = 1.508 \text{ Mg m}^{-3}$
 $b = 10.290 (3) \text{ \AA}$ Mo $K\alpha$ radiation $\mu = 0.48 \text{ mm}^{-1}$
 $c = 10.656 (4) \text{ \AA}$ $T = 293 (2) \text{ K}$
 $\alpha = 79.004 (5)^\circ$ Block, blue
 $\beta = 87.806 (5)^\circ$ $0.35 \times 0.25 \times 0.20 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer 6324 measured reflections
 4406 independent reflections
 φ and ω scans 3654 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan $R_{int} = 0.017$
 (SADABS; Sheldrick, 1996) $\theta_{max} = 26.4^\circ$
 $T_{min} = 0.841, T_{max} = 0.929$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.4378P]$
 $R[F^2 > 2\sigma(F^2)] = 0.036$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.088$ $(\Delta/\sigma)_{max} < 0.001$
 $S = 1.02$ $\Delta\rho_{max} = 0.27 \text{ e \AA}^{-3}$
 4406 reflections $\Delta\rho_{min} = -0.33 \text{ e \AA}^{-3}$
 308 parameters
 H-atom parameters constrained

Table 1 Selected bond lengths (Å).

Co1—O3	2.0785 (14)	Co1—N1	2.1456 (16)
Co1—O9	2.0945 (15)		

C-bound H atoms were included in calculated positions and refined using a riding-model approximation, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms. The water H atoms were located in a difference Fourier map and then refined as riding, with O—H = 0.85 Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: SMART (Bruker, 1999); cell refinement: SMART; data reduction: SAINT (Bruker, 1999); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine

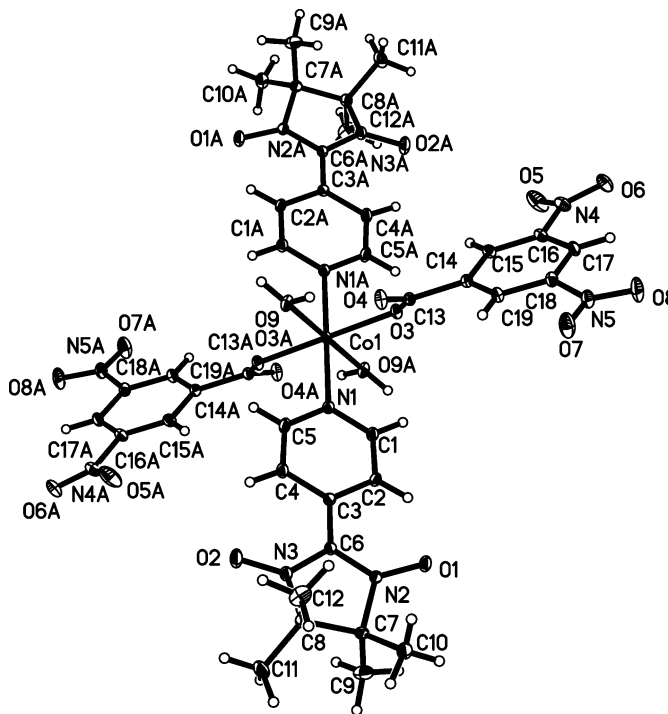


Figure 1 The molecular structure of (I), with displacement ellipsoids drawn at the 15% probability level. [Symmetry code: (A) $-x + 1, -y + 1, -z + 1$.]

structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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