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Key indicators

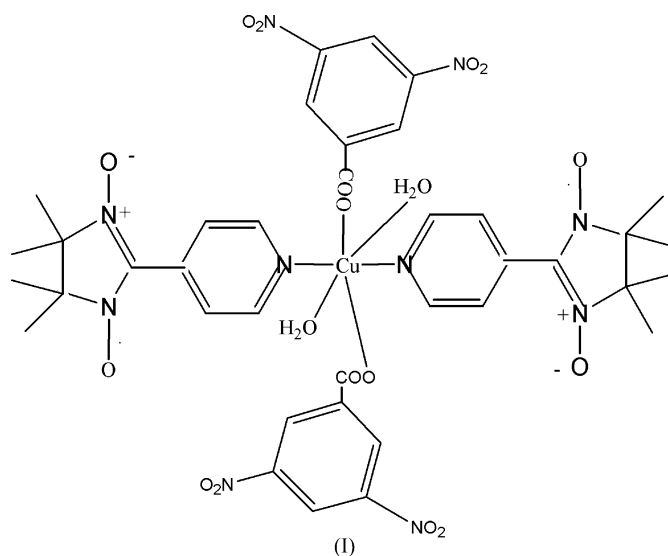
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.052
 wR factor = 0.104
Data-to-parameter ratio = 14.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaqua(3,5-dinitrobenzoato)bis[4,4,5,5-tetra-
methyl-2-(4-pyridyl)imidazolin-1-oxyl 3-oxide]-
copper(II)

The title compound, $[\text{Cu}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_3)_2(\text{H}_2\text{O})_2]$, was prepared by the reaction of 4,4,5,5-tetramethyl-2-(4-pyridyl)imidazolin-1-oxyl 3-oxide (nitronyl nitroxide), copper(II) nitrate and 3,5-dinitrobenzoic acid. The Cu^{II} ion lies on a crystallographic inversion centre and is in a distorted octahedral environment. Two N atoms from two nitronyl nitroxide and two O atoms from two 3,5-dinitrobenzoate ligands form the equatorial plane, while two O atoms from two water molecules occupy axial positions.

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Comment

Nitroxide radicals are widely used as units in the synthesis of molecule-based magnetic materials, especially since they can act as ligands in the formation of metal-radical complexes (Vostrikova *et al.*, 2000; Oshio *et al.*, 2002). 3,5-Dinitrobenzoic acid has received considerable attention in recent years because of its strong ability to coordinate to transition metals to form polymeric structural topologies (Stachovo *et al.*, 2006). By combining these two approaches, the title new copper(II) complex, (I), with 2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide (nitronyl nitroxide, NIT4py) and 3,5-dinitrobenzoate (DBA), has been prepared.



In complex (I) (Fig. 1), the Cu atom lies on an inversion centre. It is six-coordinated in a distorted octahedral environment. The equatorial plane is formed by two N atoms from two NIT4py ligands [Cu–N 2.020 (2) Å] and two O atoms from two DBA ligands [Cu–O 1.9954 (18) Å]. The axial positions are occupied by two O atoms from two water mol-

ecules [Cu—O 2.317 (2) Å]. The dihedral angle between the pyridyl ring and the O—N—C=N—O unit is 12.5(1)°.

Experimental

All reagents were purchased from ABCR GmbH Co. KG and used as received. 2-(4-Pyridyl)-4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide was prepared by the Ullman method (Ullman *et al.*, 1974). 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 2-(4-pyridyl)-4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide (0.1 mmol) and copper(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 of (I) suitable for X-ray analysis were obtained.

Crystal data

[Cu(C₇H₃N₂O₆)₂(C₁₂H₁₆N₃O₃)₂·(H₂O)₂] $\gamma = 85.374 (4)^\circ$
 $M_r = 990.36$ $V = 1088.2 (5) \text{ \AA}^3$
 Triclinic, $P\bar{1}$ $Z = 1$
 $a = 10.123 (3) \text{ \AA}$ $D_x = 1.511 \text{ Mg m}^{-3}$
 $b = 10.198 (3) \text{ \AA}$ Mo $K\alpha$ radiation $\mu = 0.59 \text{ mm}^{-1}$
 $c = 10.810 (3) \text{ \AA}$ $T = 293 (2) \text{ K}$
 $\alpha = 78.517 (4)^\circ$ Block, blue
 $\beta = 85.848 (5)^\circ$ $0.18 \times 0.14 \times 0.12 \text{ mm}$

Data collection

Bruker SMART CCD area-detector 6388 measured reflections
 diffractometer 4436 independent reflections
 φ and ω scans 3069 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan $R_{\text{int}} = 0.033$
 (SADABS; Sheldrick, 1996) $\theta_{\text{max}} = 26.5^\circ$
 $T_{\text{min}} = 0.797$, $T_{\text{max}} = 0.929$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.042P]$
 $R[F^2 > 2\sigma(F^2)] = 0.052$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.104$ $(\Delta/\sigma)_{\text{max}} = 0.001$
 $S = 1.01$ $\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
 4436 reflections $\Delta\rho_{\text{min}} = -0.47 \text{ e \AA}^{-3}$
 308 parameters
 H-atom parameters constrained

Table 1

Selected bond lengths (Å).

Cu1—O1	1.9954 (18)	Cu1—O9	2.317 (2)
Cu1—N1	2.020 (2)		

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

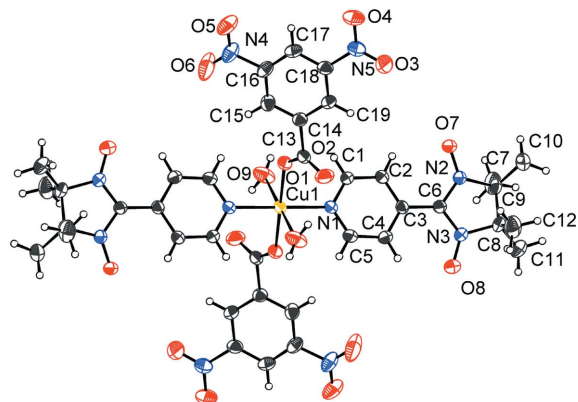


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. Symmetry-equivalent atoms are related to atoms in the asymmetric unit by the symmetry operator $(-x, -y + 2, -z + 2)$.

H atoms were included in calculated positions and refined using a riding-model approximation, with C—H(aromatic) = 0.93 Å and C—H(methyl) = 0.96 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ for aromatic H or $1.5U_{\text{eq}}(\text{C})$ for methyl H.

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPIII (Burnett & Johnson, 1996) and SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL and WinGX (Farrugia, 1999).

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