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catena-Poly[[[(3,5-dimethyl-1*H*-pyrazole-κN^2)copper(II)]-μ-[(3,5-dimethyl-1*H*-pyrazol-1-yl)-methylamino]acetato] nitrate monohydrate]

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.098
Data-to-parameter ratio = 13.2

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

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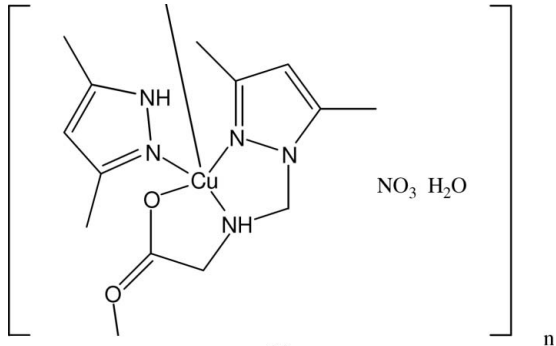
In the title complex, $\{[Cu(C_8H_{12}N_3O_2)(C_5H_8N)]NO_3\cdot H_2O\}_n$, the Cu atom is coordinated by two [(3,5-dimethyl-1*H*-pyrazol-1-yl)methylamino]acetate anions and one 3,5-dimethyl-1*H*-pyrazole ligand. There is one nitrate anion and one water molecule in the asymmetric unit. The crystal packing is stabilized by N—H···O and O—H···O hydrogen bonds.

Comment

An perspective view of the asymmetric unit of the title complex, (I), is shown in Fig. 1.



(I)

The Cu atom is coordinated by two [(3,5-dimethyl-1*H*-pyrazol-1-yl)methylamino]acetate anions and one 3,5-dimethyl-1*H*-pyrazole ligand. The coordination around copper is square pyramidal, with two N atoms and one O atom of [(3,5-dimethyl-1*H*-pyrazol-1-yl)methylamino]acetate and one N atom of 3,5-dimethyl-1*H*-pyrazole forming the basal plane (r.m.s. deviation = 0.187 Å). The Cu atom is displaced by 0.353 (1) Å from this plane. The coordination is completed by an O atom of another acetate anion, which is 2.487 (2) Å above the basal plane. The resulting structure is polymeric and the chains run along the *b* axis. The crystal structure is completed by nitrate ions and water molecules, with the nitrate ions acting as hydrogen-bond acceptors for the amino N atom of the [(3,5-dimethyl-1*H*-pyrazol-1-yl)methylamino]acetate anion and water, and the water O atom acting as acceptor for the NH group of the heterocycle. Details of the hydrogen bonds are listed in Table 2.

Experimental

The title complex was prepared by reacting equimolar quantities (10 mmol of each) of copper nitrate dihydrate, [(3,5-dimethyl-1*H*-pyrazol-1-yl)methylamino]acetic acid and 3,5-dimethyl-1*H*-pyrazole in water. This complex is stable under ambient conditions.

Crystal data

$[Cu(C_8H_{12}N_3O_2)(C_5H_8N)]NO_3\cdot H_2O$
$M_r = 421.91$
Monoclinic, $C2/c$
$a = 24.440$ (2) Å
$b = 6.9711$ (6) Å
$c = 23.924$ (2) Å
$\beta = 119.728$ (6)°
$V = 3539.6$ (6) Å^3
$Z = 8$
$D_x = 1.583$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 18154 reflections
$\theta = 1.9$–25.2°
$\mu = 1.28$ mm^{-1}
$T = 173$ (2) K
Block, blue
0.29 × 0.24 × 0.16 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{min} = 0.708$, $T_{max} = 0.822$
18327 measured reflections
3228 independent reflections
2695 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 25.4°$
$h = -29 \rightarrow 29$
$k = -8 \rightarrow 8$
$l = -28 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.098$
$S = 0.97$
3228 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9767 (17)	Cu1—N21	2.021 (2)
Cu1—N11	1.978 (2)	Cu1—O2^{i}	2.1476 (18)
Cu1—N1	2.016 (2)		
O1—Cu1—N11	92.06 (8)	N1—Cu1—N21	81.53 (8)
O1—Cu1—N1	83.81 (8)	O1—Cu1—O2^{i}	105.47 (8)
N11—Cu1—N1	170.30 (9)	N11—Cu1—O2^{i}	89.03 (8)
O1—Cu1—N21	146.20 (8)	N1—Cu1—O2^{i}	100.52 (8)
N11—Cu1—N21	97.40 (9)	N21—Cu1—O2^{i}	107.06 (8)

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N12—H12···O4^{ii}	0.88	2.23	3.014 (5)	148
O4—H4*B*···O33	0.840 (10)	2.11 (3)	2.891 (4)	155 (5)
O4—H4*A*···O33^{iii}	0.845 (10)	2.13 (2)	2.957 (5)	165 (6)
N1—H1···O1^{i}	0.93	2.38	2.910 (3)	116
N1—H1···O31^{iv}	0.93	2.56	3.095 (3)	117
N1—H1···O32^{iv}	0.93	2.48	3.230 (4)	138

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+1, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (iv) $x, y-1, z$.

H atoms were located in a difference electron-density map, but those bonded to C and N were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5 U_{eq}(methyl C)] using a riding model, with N—H = 0.93 Å and C—H = 0.95–0.99 Å. The water H atoms were refined isotropically with distance restraints of 0.82 (1) Å for O—H and 1.4 (1) Å for H···H. The methyl groups were allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

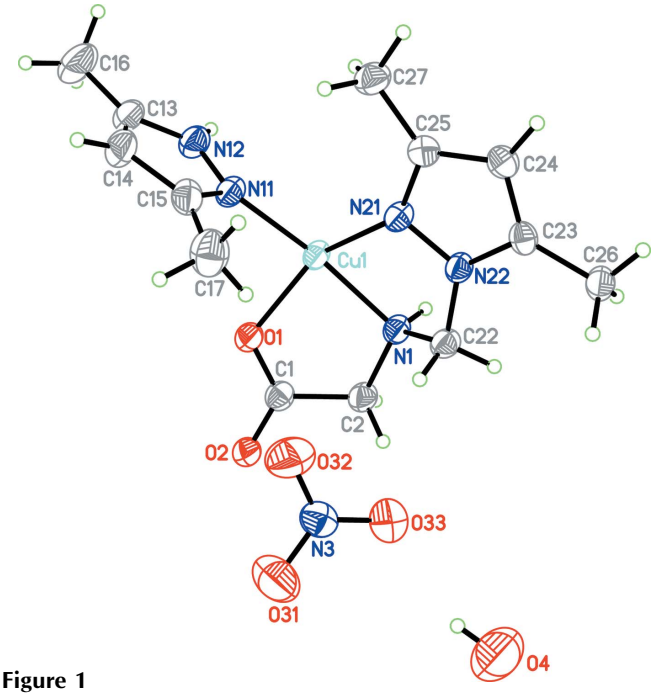


Figure 1
Perspective view of the asymmetric unit of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

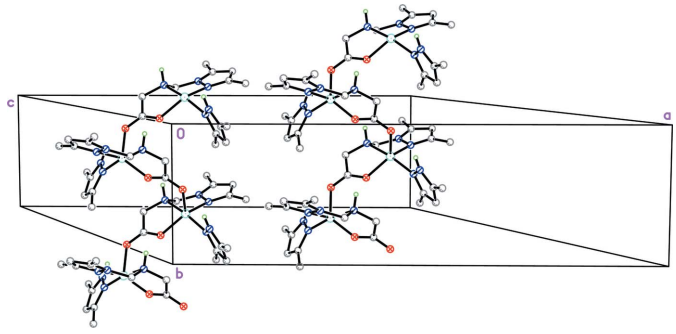


Figure 2
Partial packing diagram of the title compound, showing its polymeric structure; H atoms, nitrate counter-ions and water solvent molecules have been omitted.

References

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