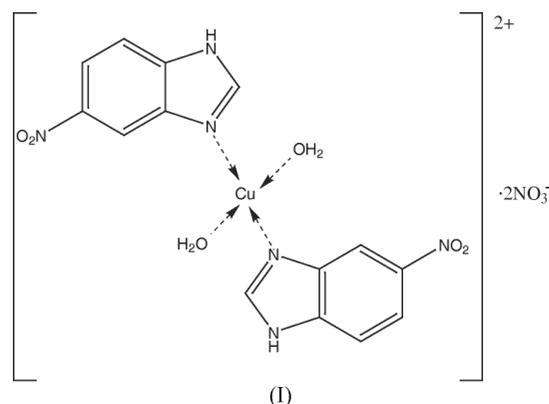


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zhangshush@public.qd.sd.cn**Key indicators**Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.030
 wR factor = 0.083
Data-to-parameter ratio = 12.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**Diaquabis(5-nitro-1*H*-benzimidazole- κN^3)-copper(II) dinitrate**

In the title compound, $[\text{Cu}(\text{C}_7\text{H}_5\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$, the Cu atom, located on an inversion centre, is four-coordinated by the two O atoms from two water molecules and two N atoms from two benzimidazole ligands. The geometry around the Cu atom is nearly perfect square planar. The crystal packing is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Received 6 December 2004
Accepted 23 December 2004
Online 8 January 2005**Comment**

Benzimidazole derivatives and their coordination complexes are widely used for medicaments due to their biological activities (Ozbey *et al.*, 1998; David *et al.*, 1993). In this paper, we report the crystal structure of the title complex, (I).



In (I), the Cu^{II} atom, which is located on a crystallographic inversion centre, is four-coordinated by the two O atoms from two water molecules and two N atoms from two benzimidazole ligands (Fig. 1). The geometry around the Cu atom is nearly perfect square planar, with $\text{N}-\text{Cu}-\text{O}$ bond angles of $90.11(6)$ and $89.89(6)^\circ$. The bond lengths in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987). The two 6-nitro-3*H*-benzimidazole ligands are each planar, with a dihedral angle of $0.44(11)^\circ$ between the benzene ring and the fused five-membered ring.

The crystal packing is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2). The hydrogen-bonded cations form ribbons along the b axis (Fig. 2).

Experimental

To a solution of 6-nitro-3*H*-benzimidazole (0.32 g, 1 mmol) in ethanol (10 ml) was added cupric nitrate (0.18 g, 1 mmol) in 10 ml distilled water. The mixture was stirred and refluxed for 1 h, then filtered. The filtrate was left to stand undisturbed at room temperature. Blue crystals appeared after 7 d.

Crystal data

[Cu(C₇H₅N₃O₂)₂(H₂O)₂](NO₃)₂
M_r = 549.87
 Triclinic, *P*1̄
a = 7.2372 (8) Å
b = 8.1279 (9) Å
c = 9.1779 (10) Å
 α = 69.491 (2)°
 β = 78.012 (2)°
 γ = 84.999 (2)°
V = 494.57 (9) Å³

Z = 1
D_x = 1.846 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2166 reflections
 θ = 2.4–27.5°
 μ = 1.19 mm⁻¹
T = 293 (2) K
 Plate, blue
 0.35 × 0.32 × 0.06 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.680, *T_{max}* = 0.932
 3050 measured reflections

2155 independent reflections
 2051 reflections with *I* > 2σ(*I*)
R_{int} = 0.011
 θ_{max} = 27.5°
h = -9 → 7
k = -10 → 10
l = -11 → 11

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.030
wR(*F*²) = 0.083
S = 1.04
 2155 reflections
 168 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.2519P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.36 e Å⁻³
 Δρ_{min} = -0.26 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1–N2	1.9931 (15)	N1–C7	1.336 (2)
Cu1–O1W	2.0036 (14)	N1–C1	1.367 (2)
O1–N3	1.223 (2)	N2–C7	1.320 (2)
O2–N3	1.223 (2)	N2–C6	1.400 (2)
N2–Cu1–N2 ⁱ	180	N2–Cu1–O1W	90.11 (6)
N2–Cu1–O1W ⁱ	89.89 (6)	O1W ⁱ –Cu1–O1W	180

Symmetry code: (i) 1 - *x*, -*y*, -*z*.

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N1–H1...O4 ⁱⁱ	0.86	1.98	2.799 (2)	158
O1W–H1W1...O5 ⁱⁱⁱ	0.73 (3)	2.12 (3)	2.814 (2)	161 (3)
O1W–H1W1...O5 ⁱ	0.73 (3)	2.39 (3)	2.882 (2)	127 (3)
O1W–H2W1...O2 ^{iv}	0.74 (3)	2.13 (3)	2.857 (2)	167 (3)
C7–H7...O1 ^{iv}	0.93	2.47	3.301 (2)	149
C7–H7...O3	0.93	2.56	3.050 (2)	114

Symmetry codes: (i) 1 - *x*, -*y*, -*z*; (ii) 1 - *x*, 1 - *y*, -*z*; (iii) *x* - 1, *y*, *z*; (iv) *x*, 1 + *y*, *z* - 1.

All H atoms were located in difference Fourier maps. The water H atoms were refined freely, while the remaining H atoms were refined using a riding model, with C–H distances of 0.93 Å and with *U*_{iso}(H) = 1.2*U*_{eq}(C). A short intermolecular distance of 2.63 (1) Å between the O atoms of the NO₃⁻ anions was observed in the crystal structure.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve

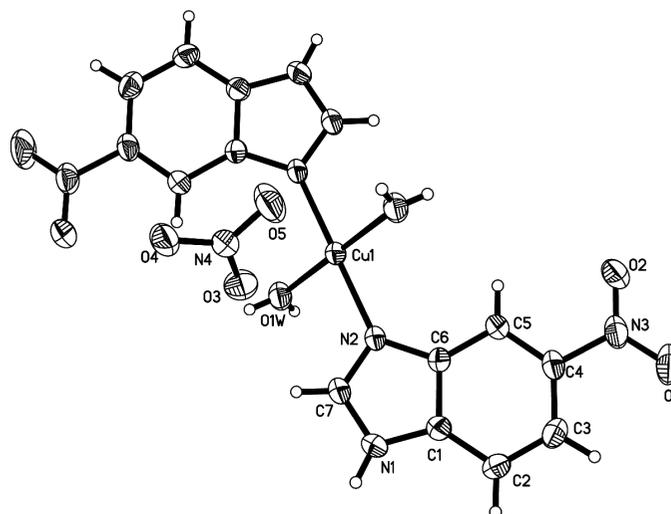


Figure 1

View of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operation (i) in Table 1; the inversion-related second nitrate anion is not shown.

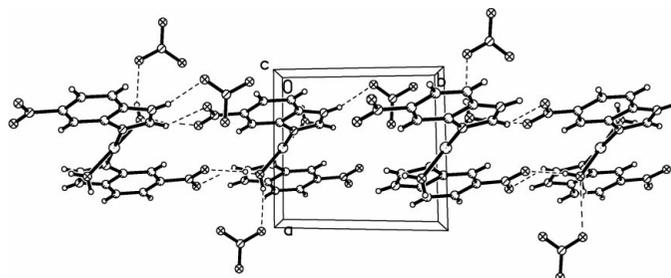


Figure 2

Packing diagram of (I), showing the ribbons along the *b* axis. Dashed lines indicate hydrogen bonds.

structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

This project was supported by the National Natural Science Foundation of China (No. 20275020 and 20475030) and the Outstanding Adult–Young Scientific Research Encouraging Foundation of Shandong Province (No. 03BS081).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- David, S. S., Abhijit, M. & David, M. P. (1993). *Chem. Rev.* **93**, 2295–2316.
- Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
- Ozbey, S., Ide, S. & Kendi, E. (1998). *J. Mol. Struct.* **442**, 23–30.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Systems, Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.