

Diazido[*N,N*-bis(2-pyridylmethyl- κ N)glycine- κ^2 N,O]copper(II) monohydrateYun-Cheng Cui, Guang-Bo Che,*
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
H-atom completeness 83%
 R factor = 0.027
 wR factor = 0.088
Data-to-parameter ratio = 11.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the structure of the title complex, $[\text{Cu}(\text{N}_3)_2(\text{C}_{14}\text{H}_{15}\text{N}_3\text{O}_2)] \cdot \text{H}_2\text{O}$, the Cu atom exhibits a CuN_5O coordination environment formed by five N atoms, three from the *N,N*-bis(2-pyridylmethyl)glycine (bpg) ligand and two from azide anions, and one O atom belonging to bpg. The Cu–N distances range from 1.931 (3) to 1.960 (3) Å, with an average of 1.945 (3) Å, and the Cu–O distance is 1.900 (2) Å. The azide ligands are almost linear, with both N–N–N angles being 174.7 (4)°.

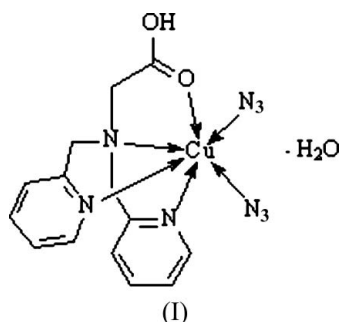
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Comment

N,N-Bis(2-pyridylmethyl)glycine (bpg) is a multifunctional ligand with N and O donors. Some crystal structures of metal complexes with this ligand have been reported. For example, $[\text{Cu}(\text{bpg})](\text{ClO}_4) \cdot \text{H}_2\text{O}$ (Choi *et al.*, 2004) has a one-dimensional structure formed by *syn-anti* carboxylate group bridging Cu atoms, $[\text{Fe}_2(\text{O})(\text{bpg})_2(\text{H}_2\text{O})_2](\text{ClO}_4)_2$ (Mortensen *et al.*, 2004) exhibited an oxo-bridged dinuclear structure, and $\text{Zn}(\text{bpg})\text{Br}_2$ (Abufarag & Vahrenkamp, 1995) is a mononuclear complex. In these complexes, bpg shows several coordination modes. We report here the structure of a mononuclear complex $[\text{Cu}(\text{bpg})(\text{N}_3)_2] \cdot \text{H}_2\text{O}$, (I), containing this ligand, in which two azide ligands act as anions and the carboxylic acid group of the bpg ligand is undissociated.



As shown in Fig. 1, complex (I) consists of a mononuclear neutral $[\text{Cu}(\text{bpg})(\text{N}_3)_2]$ and water molecules. The geometry around the copper centre is approximately octahedral. Selected bond distances and angles are listed in Table 1. The Cu–N distances range from 1.931 (3) to 1.960 (3) Å, with an average of 1.945 (3) Å, and the Cu–O distance is 1.900 (2) Å. The azide ligands are almost linear, with both N–N–N angles equal to 174.7 (4)°, and coordinate with the Cu atom in the *cis* configuration. Both five-membered picolylamine chelate rings, Cu1/N7/C10/C24/N8 and Cu1/N7/C1/C26/N9, adopt the common envelope motif, with atom N7 slightly out of the plane of the other four atoms.

Experimental

N,N-Bis(2-pyridymethyl)glycine (bpg) was synthesized by a literature method (Choi *et al.*, 2004). Complex (I) was hydrothermally synthesized under autogenous pressure; a mixture of bpg, Cu(NO₃)₂·6H₂O, NaN₃ and water in a molar ratio of 1:2:2:5000 was sealed in a Teflon-lined autoclave and heated to 413 K for 3 d. Blue crystals were obtained in *ca* 30% yield based on copper.

Crystal data

[Cu(N₃)₂(C₁₄H₁₅N₃O₂)]·H₂O
M_r = 422.91
 Monoclinic, *Cc*
a = 13.5526 (6) Å
b = 9.5725 (5) Å
c = 14.3309 (7) Å
 β = 114.072 (2)°
V = 1697.49 (14) Å³
Z = 4

D_x = 1.655 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 6914 reflections
 θ = 2.7–31.1°
 μ = 1.33 mm⁻¹
T = 293 (2) K
 Block, blue
 0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.589, *T_{max}* = 0.767
 6245 measured reflections

2734 independent reflections
 2702 reflections with *I* > 2σ(*I*)
R_{int} = 0.016
 θ_{max} = 25.5°
h = -16 → 16
k = -7 → 11
l = -17 → 17

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.028
wR(*F*²) = 0.083
S = 1.13
 2734 reflections
 245 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.3792P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 ($\Delta\sigma$)_{max} = 0.001
 $\Delta\rho_{max}$ = 0.34 e Å⁻³
 $\Delta\rho_{min}$ = -0.35 e Å⁻³
 Absolute structure: Flack (1983),
 2647 Friedel pairs
 Flack parameter: 0.06 (1)

Table 1

Selected geometric parameters (Å, °).

Cu1–N3	1.940 (3)	Cu1–N7	1.957 (2)
Cu1–N6	1.960 (3)	Cu1–N8	1.937 (4)
Cu1–O1	1.900 (2)	Cu1–N9	1.931 (3)
O1–Cu1–N3	92.11 (10)	N8–Cu1–N3	94.22 (12)
O1–Cu1–N6	176.47 (11)	N8–Cu1–N6	87.07 (12)
O1–Cu1–N7	87.39 (10)	N8–Cu1–N7	84.77 (12)
O1–Cu1–N8	91.42 (9)	N9–Cu1–N3	96.10 (13)
O1–Cu1–N9	90.87 (11)	N9–Cu1–N6	90.04 (12)
N3–Cu1–N6	91.19 (12)	N9–Cu1–N7	84.93 (11)
N3–Cu1–N7	178.87 (12)	N9–Cu1–N8	169.34 (13)
N7–Cu1–N6	89.29 (11)		

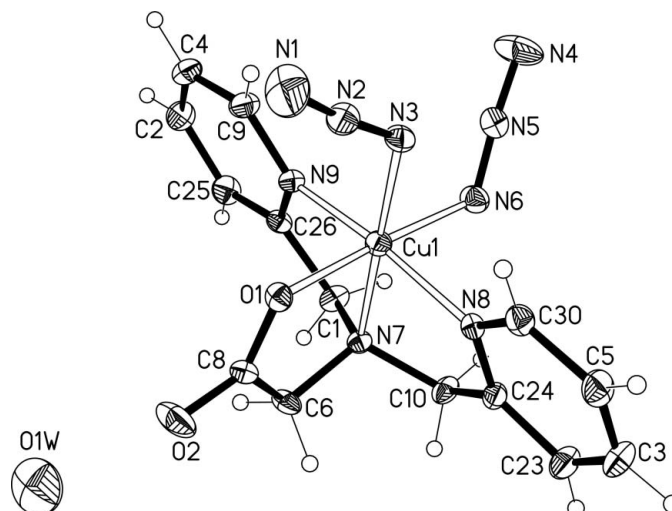


Figure 1

The structure of (I), showing displacement ellipsoids at the 30% probability level.

The H atoms of the organic ligand were included in calculated positions and treated in the subsequent refinement as riding atoms, with C–H = 0.93 or 0.97 Å and *U*_{iso}(H) = 1.2*U*_{eq}(carrier atom). The H atoms of the water molecule were not included because they could not be located from difference maps.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998; data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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References

Abufarag, A. & Vahrenkamp, H. (1995). *Inorg. Chem.* **34**, 2207–2216.
 Bruker (1998). SMART (Version 5.051), SAINT (Version 5.01), SADABS (Version 2.03) and SHELXTL (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
 Choi, K.-Y., Jeon, Y.-M., Ryu, H., Oh, J.-J., Lim, H.-H. & Kim, M.-W. (2004). *Polyhedron*, **23**, 903–911.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Mortensen, M. N., Jensen, B., Hazell, A., Bond, A. D. & McKenzie, C. J. (2004). *Dalton Trans.* pp. 3396–3402.
 Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.