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Diazidobis(2,2′-biimidazole)copper(II)

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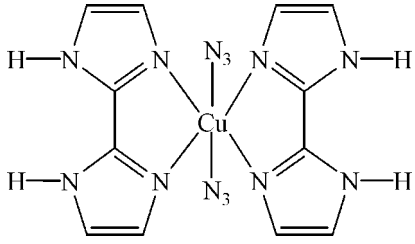
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.128; data-to-parameter ratio = 11.9.

In the title compound, $[Cu(N_3)_2(C_6H_6N_4)_2]$, the Cu atom (site symmetry $\bar{1}$) is bonded to two azide ions and two bidentate biimidizole ligands, resulting in a slightly distorted octahedral CuN_6 geometry for the metal. In the crystal structure, N—H···N hydrogen bonds help to consolidate the packing.

Related literature

For related literature, see: Scapin *et al.* (1997); Okabe & Oya (2000); Serre *et al.* (2005).



Experimental

Crystal data

$[Cu(N_3)_2(C_6H_6N_4)_2]$
M_r = 415.90
Monoclinic, $C2/c$
a = 12.457 (1) Å
b = 9.0112 (5) Å
c = 14.081 (1) Å
β = 91.84 (1)°
V = 1579.80 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 293 (2) K
0.43 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.581, T_{max} = 0.746
1929 measured reflections
1479 independent reflections
1233 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.128
S = 1.00
1479 reflections
124 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N7	2.092 (2)	Cu1—N1	2.122 (3)
Cu1—N4	2.107 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···N3^{i}	0.86	2.01	2.831 (4)	158
N6—H6A···N1^{ii}	0.86	2.53	3.029 (4)	118
N6—H6A···N3^{i}	0.86	2.26	3.032 (4)	150

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2565).

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supplementary materials

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Diazidobis(2,2'-biimidazole)copper(II)

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Comment

In recent years, N-heterocycle ligands have been widely used as polydentate ligands which show various metal chelation reactions (Scapin *et al.*, 1997; Okabe & Oya, 2000; Serre *et al.*, 2005). In this paper, we report the structure of the title compound, (I).

In compound (I), the Cu ion occupies an inversion centre, and is hexacoordinated by six N atoms from two chelating ligands of H_2bim (biimidizole; $C_6H_6N_4$) and two azide ions, showing a slightly distorted octahedral geometry (Table 1). The four N atoms from the chelating H_2bim consist of the base and the other two N atoms from two azide ions ocupy the axial positions. In the crystal of (I), N—H···N hydrogen bonds, one of which is bifurcated (Table 2), help to consolidate the packing.

Experimental

A mixture of $CuCl_{2.2}(H_2O)$ (1 mmoL), 2,2'-biimidazoline (2 mmoL) and Na_3N_3 (2 mmoL) in 20 ml me thanol was reflued for two hours. The above cooled solution was filterated and the filtrate was evaporated naturally at room temperature. Two day later, blue blocks of (I) were obtained with a yield of 31%. Anal. Calc. for $C_{12}H_{12}CuN_{14}$: C 40.39, H 3.37, N 47.13%; Found: C 40.32, H 3.42, N 47.08%.

Refinement

All H atoms were placed in calculated positions with C—H = 0.93Å and N—H = 0.86Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

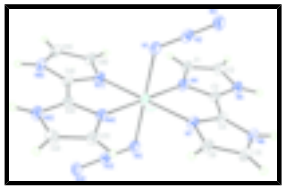


Fig. 1. The molecular structure of (I), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms. Atoms with suffix I are at the symmetry position (−*x* + 1/2, −*y* − 1/2, −*z* + 1).

Diazidobis(2,2'-biimidazole)copper(II)

Crystal data

$[Cu(N_3)_2(C_6H_6N_4)_2]$	F_{000} = 844
M_r = 415.90	D_x = 1.749 Mg m^{-3}

Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 1479 reflections
$a = 12.457$ (1) Å	$\theta = 2.8–25.6°$
$b = 9.0112$ (5) Å	$\mu = 1.42$ mm^{-1}
$c = 14.081$ (1) Å	$T = 293$ (2) K
$\beta = 91.84$ (1)°	Block, blue
$V = 1579.80$ (19) Å^3	0.43 × 0.28 × 0.22 mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	1479 independent reflections
Radiation source: fine-focus sealed tube	1233 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 293(2)$ K	$\theta_{max} = 25.6°$
φ and ω scans	$\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -1\rightarrow15$
$T_{min} = 0.581$, $T_{max} = 0.746$	$k = -1\rightarrow10$
1929 measured reflections	$l = -17\rightarrow17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.128$	$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 1.7026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
1479 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
124 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.2500	−0.2500	0.5000	0.0416 (2)
C1	0.3231 (3)	−0.0321 (4)	0.6784 (2)	0.0474 (8)
H1	0.3724	−0.0908	0.7122	0.057*
C2	0.2945 (3)	0.1098 (4)	0.7029 (2)	0.0491 (8)
H2	0.3203	0.1633	0.7553	0.059*
C3	0.2097 (2)	0.0439 (3)	0.5743 (2)	0.0374 (6)
C4	0.1460 (2)	0.0370 (3)	0.4894 (2)	0.0378 (7)
C5	0.0370 (3)	0.0753 (4)	0.3717 (2)	0.0462 (8)
H5	−0.0130	0.1180	0.3296	0.055*
C6	0.0846 (3)	−0.0622 (4)	0.3624 (2)	0.0462 (8)
H6	0.0715	−0.1281	0.3126	0.055*
N1	0.3825 (2)	−0.1638 (3)	0.42674 (19)	0.0447 (6)
N2	0.3960 (2)	−0.0324 (3)	0.42134 (18)	0.0443 (7)
N3	0.4102 (3)	0.0983 (3)	0.4146 (2)	0.0578 (8)
N4	0.2686 (2)	−0.0741 (3)	0.59778 (17)	0.0408 (6)
N5	0.2220 (2)	0.1569 (3)	0.63632 (19)	0.0439 (6)
H5A	0.1901	0.2416	0.6340	0.053*
N6	0.0766 (2)	0.1363 (3)	0.45316 (18)	0.0413 (6)
H6A	0.0605	0.2212	0.4767	0.050*
N7	0.1528 (2)	−0.0858 (3)	0.43695 (17)	0.0394 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0427 (4)	0.0416 (4)	0.0399 (4)	0.0115 (2)	−0.0075 (2)	−0.0051 (2)
C1	0.0473 (17)	0.053 (2)	0.0409 (16)	0.0051 (15)	−0.0089 (13)	−0.0010 (14)
C2	0.0541 (19)	0.054 (2)	0.0386 (16)	−0.0005 (16)	−0.0074 (14)	−0.0082 (14)
C3	0.0370 (14)	0.0393 (16)	0.0360 (14)	0.0045 (12)	0.0027 (12)	−0.0025 (12)
C4	0.0337 (14)	0.0409 (17)	0.0388 (15)	0.0068 (12)	0.0020 (11)	0.0010 (12)
C5	0.0424 (16)	0.056 (2)	0.0403 (16)	0.0164 (15)	−0.0036 (13)	0.0046 (14)
C6	0.0423 (16)	0.058 (2)	0.0382 (15)	0.0133 (15)	−0.0063 (13)	−0.0035 (14)
N1	0.0440 (14)	0.0404 (16)	0.0495 (15)	0.0094 (12)	−0.0012 (12)	−0.0033 (12)
N2	0.0385 (14)	0.0527 (19)	0.0412 (14)	0.0130 (13)	−0.0071 (11)	−0.0069 (12)
N3	0.0591 (18)	0.0401 (17)	0.073 (2)	0.0079 (14)	−0.0097 (15)	−0.0072 (15)
N4	0.0421 (14)	0.0420 (15)	0.0380 (13)	0.0069 (12)	−0.0054 (11)	−0.0054 (11)
N5	0.0477 (15)	0.0408 (15)	0.0431 (13)	0.0075 (12)	−0.0005 (11)	−0.0058 (12)
N6	0.0423 (14)	0.0414 (14)	0.0401 (13)	0.0134 (12)	0.0011 (11)	0.0013 (11)
N7	0.0369 (13)	0.0442 (15)	0.0368 (13)	0.0107 (11)	−0.0041 (10)	−0.0038 (11)

Geometric parameters (Å, °)

Cu1—N7^{i}	2.092 (2)	C3—C4	1.415 (4)
Cu1—N7	2.092 (2)	C4—N7	1.335 (4)
Cu1—N4^{i}	2.107 (2)	C4—N6	1.334 (4)

Cu1—N4	2.107 (2)	C5—N6	1.350 (4)
Cu1—N1	2.122 (3)	C5—C6	1.381 (5)
Cu1—N1^{i}	2.122 (3)	C5—H5	0.9300
C1—N4	1.358 (4)	C6—N7	1.346 (4)
C1—C2	1.374 (5)	C6—H6	0.9300
C1—H1	0.9300	N1—N2	1.199 (4)
C2—N5	1.349 (4)	N2—N3	1.196 (4)
C2—H2	0.9300	N5—H5A	0.8600
C3—N4	1.327 (4)	N6—H6A	0.8600
C3—N5	1.346 (4)		
N7^{i}—Cu1—N7	180.0	N7—C4—N6	113.3 (3)
N7^{i}—Cu1—N4^{i}	78.17 (10)	N7—C4—C3	117.4 (3)
N7—Cu1—N4^{i}	101.83 (10)	N6—C4—C3	129.3 (3)
N7^{i}—Cu1—N4	101.83 (10)	N6—C5—C6	107.4 (3)
N7—Cu1—N4	78.17 (10)	N6—C5—H5	126.3
N4^{i}—Cu1—N4	180.0	C6—C5—H5	126.3
N7^{i}—Cu1—N1	90.95 (10)	N7—C6—C5	109.2 (3)
N7—Cu1—N1	89.05 (10)	N7—C6—H6	125.4
N4^{i}—Cu1—N1	91.62 (10)	C5—C6—H6	125.4
N4—Cu1—N1	88.38 (10)	N2—N1—Cu1	120.3 (2)
N7^{i}—Cu1—N1^{i}	89.05 (10)	N3—N2—N1	178.9 (4)
N7—Cu1—N1^{i}	90.95 (10)	C3—N4—C1	104.0 (3)
N4^{i}—Cu1—N1^{i}	88.38 (10)	C3—N4—Cu1	113.09 (19)
N4—Cu1—N1^{i}	91.62 (10)	C1—N4—Cu1	142.9 (2)
N1—Cu1—N1^{i}	180.0	C3—N5—C2	105.8 (3)
N4—C1—C2	110.0 (3)	C3—N5—H5A	127.1
N4—C1—H1	125.0	C2—N5—H5A	127.1
C2—C1—H1	125.0	C4—N6—C5	105.5 (3)
N5—C2—C1	107.0 (3)	C4—N6—H6A	127.3
N5—C2—H2	126.5	C5—N6—H6A	127.3
C1—C2—H2	126.5	C4—N7—C6	104.6 (3)
N4—C3—N5	113.2 (3)	C4—N7—Cu1	113.43 (19)
N4—C3—C4	117.7 (3)	C6—N7—Cu1	141.7 (2)
N5—C3—C4	129.0 (3)		

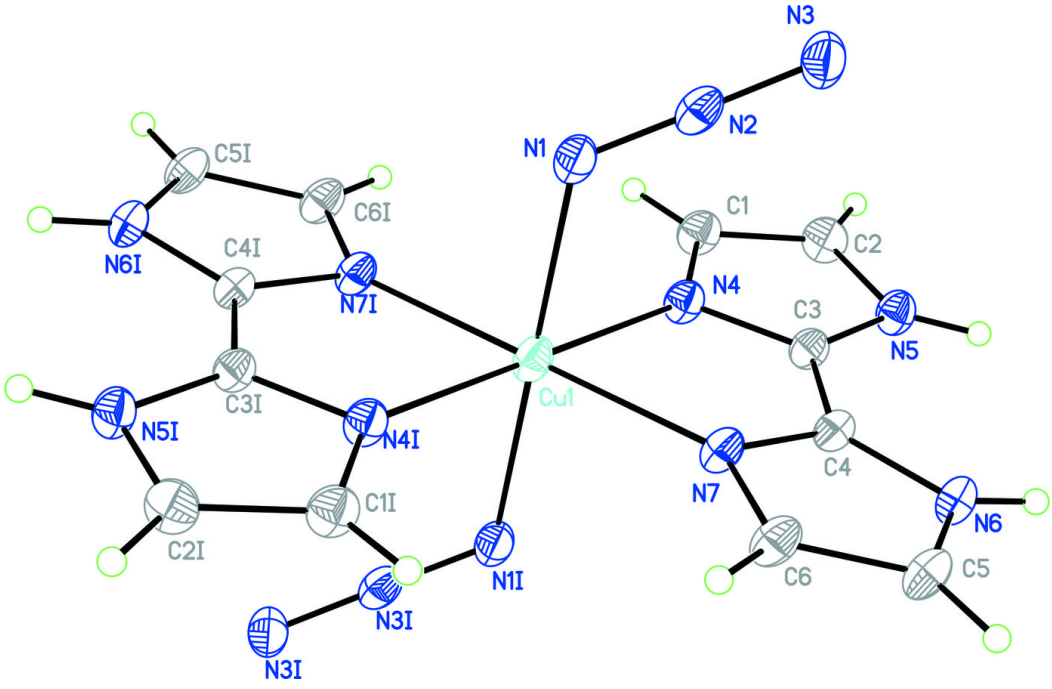
Symmetry codes: (i) −*x*+1/2, −*y*−1/2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5A···N3^{ii}	0.86	2.01	2.831 (4)	158
N6—H6A···N1^{iii}	0.86	2.53	3.029 (4)	118
N6—H6A···N3^{ii}	0.86	2.26	3.032 (4)	150

Symmetry codes: (ii) −*x*+1/2, −*y*+1/2, −*z*+1; (iii) *x*−1/2, *y*+1/2, *z*.

Fig. 1


N3
N2
N1
C5I
C6I
C1
C2
N6I
C4I
N7I
N4
C3
N5
C3I
Cu1
N5I
N4I
C4
N7
C1I
N6
C2I
N1I
C6
C5
N3I
N3I