Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bromido(3,5-dimethylpyrazole-κN)-[hydrotris(3,5-dimethylpyrazolyl)-borato-$\kappa^3 N,N',N''$]copper(II)

Xing-Jing Zhang, Jing Han, Chun-Guang Wang and Yong-Heng Xing*

College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China
Correspondence e-mail: xingyongheng2000@163.com

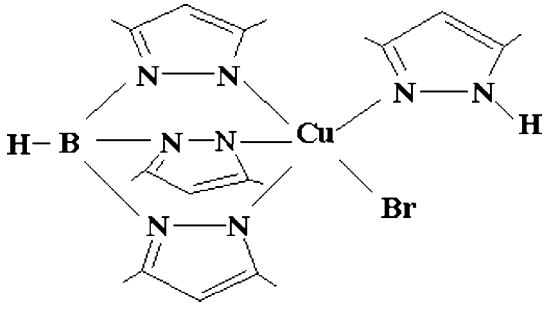
Received 6 September 2007; accepted 21 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.050; wR factor = 0.136; data-to-parameter ratio = 17.6.

In the title copper complex, $[CuBr(C_{15}H_{22}BN_6)(C_5H_8N_2)]$, the Cu^{II} atom is coordinated by one Br atom, three N atoms from the hydrotris(3,5-dimethylpyrazolyl)borate ligand and one N atom from the 3,5-dimethylpyrazole ligand, forming a distorted trigonal–bipyramidal geometry. The equatorial positions are occupied by the Br atom and the N atoms of the hydrotris(3,5-dimethylpyrazolyl)borate ligand.

Related literature

For related literature, see: Badura & Vahrenkamp (2002); Blosch *et al.* (1991); Fernandez *et al.* (1989); Fujisawa *et al.* (2004); Ghosh *et al.* (1988); Kitajima *et al.* (1988); Puerta & Cohen (2002); Trofimenko (1972, 1993, 2004).



Experimental

Crystal data

$[CuBr(C_{15}H_{22}BN_6)(C_5H_8N_2)]$
M_r = 536.78
Monoclinic, $P2_1/c$
a = 17.223 (4) Å
b = 7.9231 (18) Å
c = 19.236 (4) Å
β = 107.618 (3)°
V = 2501.7 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.49 mm^{-1}
T = 293 (2) K
0.21 × 0.16 × 0.13 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.626, T_{max} = 0.723
4917 measured reflections
4917 independent reflections
3349 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.03
4917 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N2	2.019 (3)	Cu—N6	2.176 (3)
Cu—N4	2.035 (3)	Cu—Br1	2.4607 (8)
Cu—N8	2.067 (4)		
N2—Cu—N4	85.28 (13)	N8—Cu—N6	92.99 (14)
N2—Cu—N8	88.77 (14)	N2—Cu—Br1	152.93 (10)
N4—Cu—N8	174.01 (14)	N4—Cu—Br1	96.65 (9)
N2—Cu—N6	95.06 (13)	N8—Cu—Br1	88.31 (10)
N4—Cu—N6	88.27 (13)	N6—Cu—Br1	111.97 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7A···Br1	0.86	2.51	3.045 (4)	121

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the National Natural Science Foundation of China (grant No. 20771051), the Education Foundation of Liaoning Province (grant No. 05 L212) and the Scientific Research Foundation for the Returned Overseas Chinese Scholars, State Education Ministry, for financial assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2205).

References

Badura, D. & Vahrenkamp, H. (2002). *Inorg. Chem.* **41**, 6013–6019.
Blosch, L. L., Abboud, K. & Boncella, J. M. (1991). *J. Am. Chem. Soc.* **113**, 7066–7068.
Bruker (2005). *APEX2*. Version 1.27. Bruker AXS Inc., Madison, Wisconsin, USA.
Fernandez, M. J., Rodriguez, M. J., Oro, L. A. & Lahoz, F. J. (1989). *Dalton Trans.* **10**, 2073–2076.
Fujisawa, K., Tada, N., Ishikawa, Y., Higashimura, H., Miyashita, Y. & Okamoto, K. (2004). *Inorg. Chem. Commun.* **7**, 209–212.
Ghosh, C. K., Rodgers, D. P. S. & Graham, W. A. G. (1988). *Chem. Commun.* **15**, 1511–1512.
Kitajima, N., Moro-oka, Y., Uchida, A., Sasada, Y. & Ohashi, Y. (1988). *Acta Cryst.* C**44**, 1876–1878.

  doi:10.1107/S1600536807046491

Puerta, D. T. & Cohen, S. M. (2002). *Inorg. Chem.* **41**, 5075–5082.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Trofimenko, S. (1972). *Chem. Rev.* **72**, 497–509.
Trofimenko, S. (1993). *Chem. Rev.* **93**, 943–980.
Trofimenko, S. (2004). *Polyhedron*, **23**, 197–203.

supplementary materials

Acta Cryst. (2007). E**63**, m2620-m2621 [**doi:10.1107/S1600536807046491**]

Bromido(3,5-dimethylpyrazole-*κN*)[hydrotris(3,5-dimethylpyrazolyl)borato-κ^3*N*,*N*',*N*'']copper(II)

X.-J. Zhang, J. Han, C.-G. Wang and Y.-H. Xing

Comment

Since Trofimenko discovered poly(pyrazolyl)borate (Trofimenko, 1972), these ligands have been proven to be extremely popular for coordination chemists in a wide range of applications because of their ease of synthesis, ease of functionalization, and the steric protection which they afford to transition metal centers. So poly(pyrazolyl)borate ligands have been used for a number of different purposes, including modeling of metalloprotein active site (Trofimenko, 1993, 2004), mimicking metalloenzyme systems in bioinorganic chemistry (Puerta & Cohen, 2002), polymerization catalysts (Blosch *et al.*, 1991) and C—H activation (Ghosh *et al.*, 1988; Fernandez *et al.*, 1989). The donor N atoms of pyrazole (or modified pyrazole) and poly(pyrazolyl)borate can coordinate to metal atoms together to form half sandwich structure. Based on these findings, we attempted to determine the structure of the title complex, (I).

The structure of (I) shows a distorting trigonal bipyramidal geometry of Cu^{II}, which is coordinated to one Br atom and four N atoms: three from tris(3,5-dimethylpyrazolyl)borate ligand [Cu—N(N2, N4, N6)] with bond lengths of 2.019 (3), 2.035 (3), 2.176 (3) Å and one from 3,5-dimethylpyrazole ligand (Cu—N8) with the bond distance of 2.067 (4) Å. In the structure, the atoms Br, N2 and N6 are in the triangle plane, and N4 and N8 are at the axial positions. The copper atom is in the center of the triangle double pyramide geometry (Fig. 1). Selected bond lengths and angles are listed in Table 1. It can be found that the Cu—N distances (from tris(pyrazolyl)borate ligand) are shorter than those of bis(hydrotris(3,5-dimethylpyrazolyl) borato-κ^3*N*,*N*',*N*'')copper(II) (Kitajima *et al.*, 1988) [2.034 (13), 2.085 (12), 2.296 (12) Å], longer than those of chloro(hydrotris(3-adamantyl-5-isopropyl-1-pyrazolyl) borato-κ^3*N*,*N*',*N*'')copper(II) (Fujisawa *et al.*, 2004) [2.125 (3), 2.005 (2), 1.961 (2) Å]. For the bond angles, the range of N—Cu—N (from tris(pyrazolyl)borate ligand) in the title complex is from 85.28 (13) to 95.06 (13)°, but in bis(hydrotris(3,5-dimethylpyrazolyl)borato-κ^3*N*,*N*',*N*'')copper(II) (Kitajima *et al.*, 1988) complex, the range of N—Cu—N (from tris(pyrazolyl)borate ligand) is from 86.7 (4) to 88.1 (4)°.

Experimental

All chemicals purchased were of reagent grade or better and were used without further purification. A methanol solution of $K[HB(C_5H_7N_2)_3]$ (2 mmol) and 3,5-dimethylpyrazole (1 mmol) was added to an methanol solution of CuBr (1 mmol). The mixture was stirred for 4 h at room temperature, yielding a blue solution. This was set aside to crystallize, yielding analytically pure (I) as single crystals suitable for X-ray structure determination. Yield: 0.494 g, *ca* 72% (based on Cu). Anal. Calcd for $C_{20}H_{30}N_8BBrCu$ (FW: 536.78): C 44.69, H 5.63, N 20.86%. Found: C 44.71, H 5.59, N 20.87. IR (KBr, μ, cm^{-1}): 3190, 2979, 2507, 2364, 1567, 1541, 1448, 1414, 1383, 1348, 1269, 1195, 1183, 1127, 1067, 1047, 1022, 984, 944, 911, 852, 808, 787, 693, 664, 644, 611, 593, 465, 436, 352, 303.

Refinement

Hydrogen atoms were placed at calculated positions (C—H = 0.93–0.96, N—H = 0.86 and B—H = 0.98 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C, B, N) or 1.5U_{eq}(methyl C).

Figures

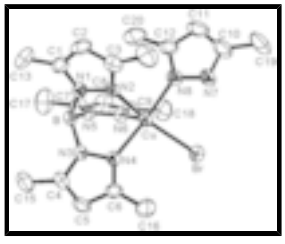


Fig. 1. The molecular structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted.

Bromido(3,5-dimethylpyrazole-κ*N*)[hydrotris(3,5-dimethylpyrazolyl)\ borato-κ^3*N*,*N*',*N*'']copper(II)

Crystal data

$[CuBr(C_{15}H_{22}BN_6)(C_5H_8N_2)]$	F_{000} = 1100
M_r = 536.78	D_x = 1.425 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -p 2ybc	Cell parameters from 4917 reflections
a = 17.223 (4) Å	θ = 2.2–26.0º
b = 7.9231 (18) Å	μ = 2.49 mm^{-1}
c = 19.236 (4) Å	T = 293 (2) K
β = 107.618 (3)º	Plate, green
V = 2501.7 (10) Å^3	0.21 × 0.16 × 0.13 mm
Z = 4	

Data collection

Bruker P4 diffractometer	4917 independent reflections
Radiation source: fine-focus sealed tube	3349 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 293(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	h = −13→21
T_{min} = 0.626, T_{max} = 0.723	k = −9→9
4917 measured reflections	l = −23→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
4917 reflections	$\Delta\rho_{max} = 0.75$ e Å^{-3}
280 parameters	$\Delta\rho_{min} = -0.65$ 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 $F^2 > \sigma(F^2)$ 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}
Cu	0.23841 (3)	0.86990 (6)	0.30904 (3)	0.03100 (17)
Br1	0.26691 (3)	1.02181 (7)	0.20786 (3)	0.0571 (2)
C1	0.1549 (3)	0.5592 (6)	0.4415 (2)	0.0433 (11)
C2	0.1719 (3)	0.4300 (6)	0.4000 (3)	0.0491 (13)
H2A	0.1681	0.3149	0.4079	0.059*
C3	0.1953 (3)	0.5040 (6)	0.3447 (2)	0.0424 (11)
C4	0.0315 (3)	1.0552 (6)	0.3462 (2)	0.0410 (11)
C5	0.0068 (3)	1.1021 (6)	0.2754 (3)	0.0460 (12)
H5A	−0.0412	1.1581	0.2513	0.055*
C6	0.0667 (3)	1.0510 (6)	0.2457 (2)	0.0390 (11)
C7	0.2787 (3)	1.0521 (6)	0.5238 (2)	0.0469 (12)
C8	0.3505 (3)	1.1191 (7)	0.5189 (3)	0.0557 (14)
H8A	0.3902	1.1745	0.5555	0.067*
C9	0.3520 (3)	1.0874 (6)	0.4479 (3)	0.0454 (12)
C10	0.4449 (3)	0.6283 (8)	0.2855 (4)	0.0704 (17)
C11	0.4591 (3)	0.5844 (7)	0.3563 (4)	0.0702 (17)
H11A	0.5026	0.5204	0.3844	0.084*
C12	0.3964 (3)	0.6531 (6)	0.3791 (3)	0.0490 (12)

C13	0.1268 (4)	0.5499 (7)	0.5069 (3)	0.0633 (16)
H13A	0.1204	0.6619	0.5233	0.095*
H13B	0.1662	0.4897	0.5448	0.095*
H13C	0.0754	0.4919	0.4948	0.095*
C14	0.2180 (3)	0.4232 (7)	0.2831 (3)	0.0636 (15)
H14A	0.2313	0.5092	0.2534	0.095*
H14B	0.1729	0.3578	0.2540	0.095*
H14C	0.2642	0.3510	0.3024	0.095*
C15	−0.0100 (3)	1.0777 (8)	0.4035 (3)	0.0680 (16)
H15A	0.0231	1.0301	0.4486	0.102*
H15B	−0.0618	1.0217	0.3886	0.102*
H15C	−0.0180	1.1959	0.4101	0.102*
C16	0.0640 (3)	1.0668 (8)	0.1676 (2)	0.0608 (15)
H16A	0.1129	1.0205	0.1613	0.091*
H16B	0.0596	1.1837	0.1538	0.091*
H16C	0.0177	1.0063	0.1374	0.091*
C17	0.2459 (4)	1.0483 (8)	0.5871 (3)	0.0795 (19)
H17A	0.1942	0.9919	0.5733	0.119*
H17B	0.2392	1.1617	0.6020	0.119*
H17C	0.2832	0.9889	0.6269	0.119*
C18	0.4151 (3)	1.1289 (8)	0.4123 (3)	0.0637 (16)
H18A	0.3977	1.0894	0.3628	0.096*
H18B	0.4654	1.0751	0.4383	0.096*
H18C	0.4228	1.2489	0.4128	0.096*
C19	0.4902 (4)	0.5946 (10)	0.2306 (5)	0.121 (3)
H19A	0.4610	0.6447	0.1847	0.181*
H19B	0.4944	0.4751	0.2245	0.181*
H19C	0.5438	0.6428	0.2478	0.181*
C20	0.3829 (3)	0.6372 (7)	0.4518 (3)	0.0665 (16)
H20A	0.3345	0.6978	0.4515	0.100*
H20B	0.4288	0.6834	0.4886	0.100*
H20C	0.3767	0.5203	0.4621	0.100*
N1	0.1701 (2)	0.7062 (4)	0.41197 (17)	0.0336 (8)
N2	0.1952 (2)	0.6716 (4)	0.35195 (17)	0.0331 (8)
N3	0.1048 (2)	0.9768 (4)	0.35979 (17)	0.0322 (8)
N4	0.1276 (2)	0.9762 (4)	0.29746 (17)	0.0329 (8)
N5	0.2399 (2)	0.9827 (4)	0.45886 (17)	0.0352 (9)
N6	0.2847 (2)	1.0044 (4)	0.41192 (17)	0.0356 (9)
N7	0.3765 (2)	0.7205 (5)	0.2677 (2)	0.0506 (10)
H7A	0.3544	0.7628	0.2251	0.061*
N8	0.3461 (2)	0.7391 (5)	0.32409 (19)	0.0407 (9)
B1	0.1575 (3)	0.8903 (6)	0.4308 (3)	0.0339 (11)
H1	0.1291	0.8942	0.4679	0.041*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0280 (3)	0.0343 (3)	0.0322 (3)	0.0016 (2)	0.0114 (2)	0.0010 (2)

Br1	0.0572 (4)	0.0688 (4)	0.0551 (3)	0.0191 (3)	0.0319 (3)	0.0230 (3)
C1	0.040 (3)	0.041 (3)	0.048 (3)	−0.003 (2)	0.012 (2)	0.010 (2)
C2	0.054 (3)	0.027 (3)	0.062 (3)	−0.006 (2)	0.011 (3)	0.014 (2)
C3	0.034 (3)	0.038 (3)	0.051 (3)	−0.003 (2)	0.006 (2)	−0.005 (2)
C4	0.030 (2)	0.045 (3)	0.050 (3)	0.003 (2)	0.015 (2)	−0.006 (2)
C5	0.028 (2)	0.050 (3)	0.056 (3)	0.012 (2)	0.007 (2)	0.006 (2)
C6	0.030 (2)	0.043 (3)	0.040 (2)	0.002 (2)	0.003 (2)	0.006 (2)
C7	0.055 (3)	0.049 (3)	0.033 (2)	−0.003 (3)	0.007 (2)	−0.011 (2)
C8	0.052 (3)	0.060 (4)	0.045 (3)	−0.020 (3)	0.001 (2)	−0.019 (2)
C9	0.041 (3)	0.038 (3)	0.053 (3)	−0.010 (2)	0.009 (2)	−0.002 (2)
C10	0.049 (3)	0.061 (4)	0.115 (5)	0.016 (3)	0.047 (4)	0.016 (4)
C11	0.037 (3)	0.060 (4)	0.112 (5)	0.017 (3)	0.021 (3)	0.025 (4)
C12	0.032 (3)	0.045 (3)	0.065 (3)	0.003 (2)	0.008 (2)	0.014 (2)
C13	0.078 (4)	0.061 (4)	0.056 (3)	−0.016 (3)	0.028 (3)	0.017 (3)
C14	0.069 (4)	0.043 (3)	0.082 (4)	−0.005 (3)	0.028 (3)	−0.024 (3)
C15	0.057 (4)	0.086 (5)	0.071 (4)	0.024 (3)	0.035 (3)	0.002 (3)
C16	0.045 (3)	0.089 (4)	0.041 (3)	0.006 (3)	0.002 (2)	0.014 (3)
C17	0.090 (5)	0.109 (5)	0.040 (3)	−0.020 (4)	0.021 (3)	−0.028 (3)
C18	0.041 (3)	0.078 (4)	0.070 (3)	−0.021 (3)	0.014 (3)	−0.002 (3)
C19	0.104 (6)	0.118 (7)	0.179 (8)	0.062 (5)	0.101 (6)	0.037 (6)
C20	0.048 (3)	0.074 (4)	0.061 (3)	0.005 (3)	−0.009 (3)	0.014 (3)
N1	0.0305 (19)	0.035 (2)	0.0337 (18)	−0.0037 (16)	0.0079 (15)	0.0022 (16)
N2	0.033 (2)	0.033 (2)	0.0360 (18)	−0.0016 (16)	0.0138 (16)	−0.0001 (15)
N3	0.030 (2)	0.035 (2)	0.0342 (18)	0.0026 (16)	0.0135 (16)	−0.0002 (15)
N4	0.030 (2)	0.037 (2)	0.0340 (18)	0.0004 (16)	0.0130 (16)	0.0008 (15)
N5	0.039 (2)	0.038 (2)	0.0291 (18)	−0.0030 (17)	0.0106 (16)	−0.0055 (15)
N6	0.034 (2)	0.037 (2)	0.0339 (19)	−0.0065 (16)	0.0083 (16)	−0.0034 (16)
N7	0.040 (2)	0.050 (3)	0.071 (3)	0.010 (2)	0.030 (2)	0.007 (2)
N8	0.032 (2)	0.043 (2)	0.048 (2)	0.0019 (18)	0.0134 (18)	0.0019 (18)
B1	0.032 (3)	0.041 (3)	0.032 (2)	−0.001 (2)	0.014 (2)	−0.002 (2)

Geometric parameters (Å, °)

Cu—N2	2.019 (3)	C13—H13A	0.9600
Cu—N4	2.035 (3)	C13—H13B	0.9600
Cu—N8	2.067 (4)	C13—H13C	0.9600
Cu—N6	2.176 (3)	C14—H14A	0.9600
Cu—Br1	2.4607 (8)	C14—H14B	0.9600
C1—N1	1.355 (5)	C14—H14C	0.9600
C1—C2	1.383 (7)	C15—H15A	0.9600
C1—C13	1.480 (6)	C15—H15B	0.9600
C2—C3	1.378 (7)	C15—H15C	0.9600
C2—H2A	0.9300	C16—H16A	0.9600
C3—N2	1.335 (5)	C16—H16B	0.9600
C3—C14	1.499 (7)	C16—H16C	0.9600
C4—C5	1.350 (6)	C17—H17A	0.9600
C4—N3	1.360 (5)	C17—H17B	0.9600
C4—C15	1.495 (6)	C17—H17C	0.9600
C5—C6	1.382 (6)	C18—H18A	0.9600

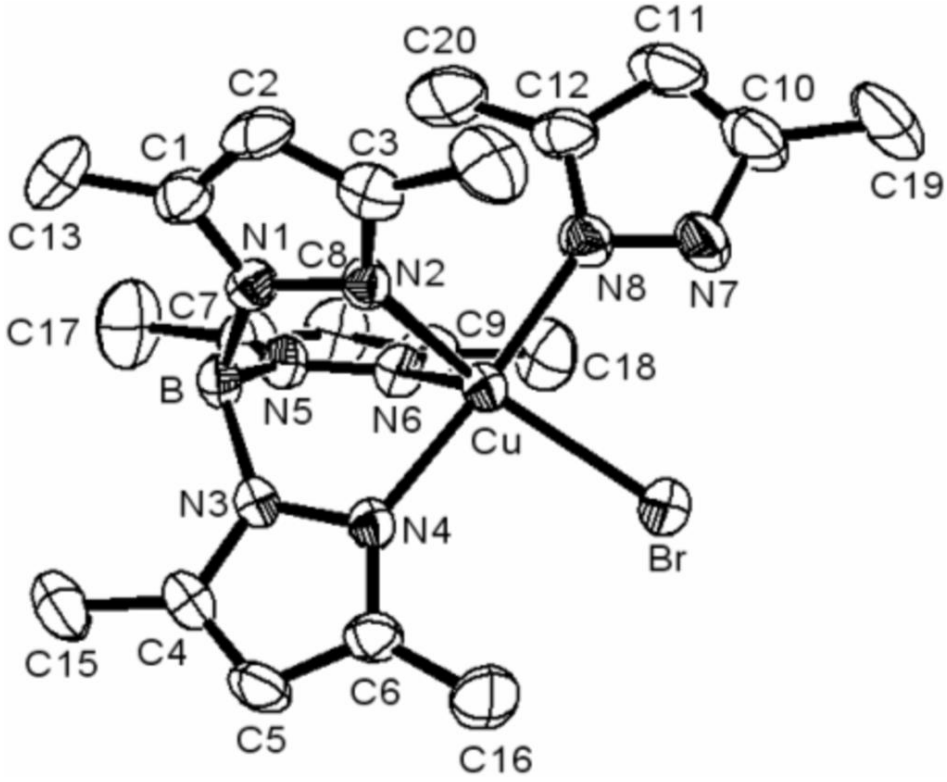
C5—H5A	0.9300	C18—H18B	0.9600
C6—N4	1.346 (5)	C18—H18C	0.9600
C6—C16	1.494 (6)	C19—H19A	0.9600
C7—N5	1.343 (5)	C19—H19B	0.9600
C7—C8	1.374 (7)	C19—H19C	0.9600
C7—C17	1.491 (6)	C20—H20A	0.9600
C8—C9	1.396 (6)	C20—H20B	0.9600
C8—H8A	0.9300	C20—H20C	0.9600
C9—N6	1.331 (5)	N1—N2	1.378 (4)
C9—C18	1.485 (6)	N1—B1	1.534 (6)
C10—N7	1.340 (6)	N3—N4	1.370 (4)
C10—C11	1.353 (8)	N3—B1	1.552 (6)
C10—C19	1.514 (8)	N5—N6	1.364 (4)
C11—C12	1.394 (7)	N5—B1	1.542 (6)
C11—H11A	0.9300	N7—N8	1.348 (5)
C12—N8	1.333 (5)	N7—H7A	0.8600
C12—C20	1.491 (7)	B1—H1	0.9800
N2—Cu—N4	85.28 (13)	H15A—C15—H15C	109.5
N2—Cu—N8	88.77 (14)	H15B—C15—H15C	109.5
N4—Cu—N8	174.01 (14)	C6—C16—H16A	109.5
N2—Cu—N6	95.06 (13)	C6—C16—H16B	109.5
N4—Cu—N6	88.27 (13)	H16A—C16—H16B	109.5
N8—Cu—N6	92.99 (14)	C6—C16—H16C	109.5
N2—Cu—Br1	152.93 (10)	H16A—C16—H16C	109.5
N4—Cu—Br1	96.65 (9)	H16B—C16—H16C	109.5
N8—Cu—Br1	88.31 (10)	C7—C17—H17A	109.5
N6—Cu—Br1	111.97 (10)	C7—C17—H17B	109.5
N1—C1—C2	107.1 (4)	H17A—C17—H17B	109.5
N1—C1—C13	123.6 (4)	C7—C17—H17C	109.5
C2—C1—C13	129.3 (5)	H17A—C17—H17C	109.5
C3—C2—C1	107.0 (4)	H17B—C17—H17C	109.5
C3—C2—H2A	126.5	C9—C18—H18A	109.5
C1—C2—H2A	126.5	C9—C18—H18B	109.5
N2—C3—C2	109.4 (4)	H18A—C18—H18B	109.5
N2—C3—C14	121.1 (4)	C9—C18—H18C	109.5
C2—C3—C14	129.5 (5)	H18A—C18—H18C	109.5
C5—C4—N3	108.0 (4)	H18B—C18—H18C	109.5
C5—C4—C15	129.5 (4)	C10—C19—H19A	109.5
N3—C4—C15	122.5 (4)	C10—C19—H19B	109.5
C4—C5—C6	106.9 (4)	H19A—C19—H19B	109.5
C4—C5—H5A	126.5	C10—C19—H19C	109.5
C6—C5—H5A	126.5	H19A—C19—H19C	109.5
N4—C6—C5	109.5 (4)	H19B—C19—H19C	109.5
N4—C6—C16	124.1 (4)	C12—C20—H20A	109.5
C5—C6—C16	126.3 (4)	C12—C20—H20B	109.5
N5—C7—C8	107.5 (4)	H20A—C20—H20B	109.5
N5—C7—C17	123.1 (5)	C12—C20—H20C	109.5
C8—C7—C17	129.4 (4)	H20A—C20—H20C	109.5
C7—C8—C9	106.3 (4)	H20B—C20—H20C	109.5

C7—C8—H8A	126.8	C1—N1—N2	109.2 (3)
C9—C8—H8A	126.8	C1—N1—B1	131.2 (4)
N6—C9—C8	109.0 (4)	N2—N1—B1	119.3 (3)
N6—C9—C18	120.9 (4)	C3—N2—N1	107.2 (3)
C8—C9—C18	130.1 (4)	C3—N2—Cu	136.0 (3)
N7—C10—C11	106.0 (5)	N1—N2—Cu	115.8 (2)
N7—C10—C19	121.1 (6)	C4—N3—N4	109.2 (3)
C11—C10—C19	133.0 (6)	C4—N3—B1	129.2 (4)
C10—C11—C12	107.1 (5)	N4—N3—B1	121.5 (3)
C10—C11—H11A	126.4	C6—N4—N3	106.3 (3)
C12—C11—H11A	126.4	C6—N4—Cu	139.3 (3)
N8—C12—C11	109.2 (5)	N3—N4—Cu	114.4 (2)
N8—C12—C20	122.6 (4)	C7—N5—N6	109.9 (4)
C11—C12—C20	128.2 (5)	C7—N5—B1	131.8 (4)
C1—C13—H13A	109.5	N6—N5—B1	118.2 (3)
C1—C13—H13B	109.5	C9—N6—N5	107.3 (3)
H13A—C13—H13B	109.5	C9—N6—Cu	137.4 (3)
C1—C13—H13C	109.5	N5—N6—Cu	114.6 (2)
H13A—C13—H13C	109.5	C10—N7—N8	112.3 (4)
H13B—C13—H13C	109.5	C10—N7—H7A	123.9
C3—C14—H14A	109.5	N8—N7—H7A	123.9
C3—C14—H14B	109.5	C12—N8—N7	105.4 (4)
H14A—C14—H14B	109.5	C12—N8—Cu	135.0 (3)
C3—C14—H14C	109.5	N7—N8—Cu	119.5 (3)
H14A—C14—H14C	109.5	N1—B1—N5	110.7 (4)
H14B—C14—H14C	109.5	N1—B1—N3	107.4 (3)
C4—C15—H15A	109.5	N5—B1—N3	109.2 (4)
C4—C15—H15B	109.5	N1—B1—H1	109.8
H15A—C15—H15B	109.5	N5—B1—H1	109.8
C4—C15—H15C	109.5	N3—B1—H1	109.8

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7A···Br1	0.86	2.51	3.045 (4)	121

Fig. 1


C11
C20
C12
C10
C2
C1
C3
C19
C13
N1
C8
N2
N8
N7
C7
C17
C9
C18
B
N5
N6
Cu
N3
N4
Br
C15
C4
C6
C5
C16