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Dibromidotetrakis(1*H*-indazole-κN^2)copper(II)

Moayad Hossaini Sadr,[a] Behzad Soltani,[a] Shan Gao[b] and Seik Weng Ng[c]*

[a]Department of Chemistry, Azarbaijan University of Tarbiat Moallem, Tabriz, Iran, [b]School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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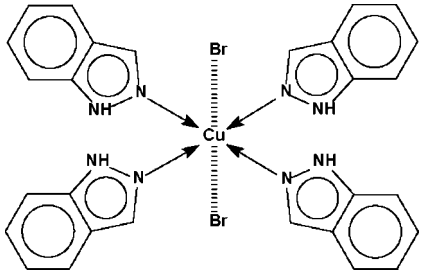
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.012 Å; R factor = 0.061; wR factor = 0.228; data-to-parameter ratio = 17.9.

The Cu atom in the title compound, $[CuBr_2(C_7H_6N_2)_4]$, is surrounded by four N-heterocycles that define an N_4 square-planar geometry. The coordination geometry is distorted towards an elongated octahedron owing to the presence of the two Br^- anions, which are located at about 3 Å above and below the square plane. There are two independent molecules in the asymmetric unit, each with their Cu atom lying on an inversion centre.

Related literature

For related structures, see Hossaini Sadr *et al.* (2004, 2005, 2006). For related literature, see: Allen (2002).



Experimental

Crystal data

$[CuBr_2(C_7H_6N_2)_4]$
M_r = 695.91
Triclinic, $P\overline{1}$
a = 10.338 (1) Å
b = 10.923 (1) Å
c = 13.730 (1) Å
α = 72.545 (3)°
β = 77.329 (3)°
γ = 73.890 (3)°
V = 1405.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.65 mm^{-1}
T = 295 (2) K
0.24 × 0.21 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.073, T_{max} = 0.668
13779 measured reflections
6389 independent reflections
2895 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.228
S = 1.13
6389 reflections
356 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	2.027 (5)	Cu2—N5	2.024 (7)
Cu1—N3	2.008 (6)	Cu2—N7	2.023 (6)
Cu1—Br1	3.033 (1)	Cu2—Br2	2.980 (1)

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2226).

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supplementary materials

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Dibromidotetrakis(1*H*-indazole-κN^2)copper(II)

M. Hossaini Sadr, B. Soltani, S. Gao and S. W. Ng

Comment

Unlike benzimidazole, which affords a number of adducts with metal salts, indazole furnishes only few complexes (Cambridge Structural Database, Version 5.28; Allen, 2002). The present study of the copper dibromide adduct (I) follows previous studies on Cu complexes of pyrazole-based N-heterocycles (Hossaini Sadr *et al.*, 2005; 2006).

Two independent $[Cu(C_7H_6N_2)_4]^{2+}2Br^-$ formula units comprise the asymmetric unit in (I), each with the Cu atom situated on a center of inversion. Complex (I) is formally a salt (Fig. 1) owing to the large distance of the Br ions (more than 3 Å) above and below the N_4 square plane defined by the four N-heterocycles. In the corresponding imidazole adduct, one Br atom is covalently bonded whereas the other is uncoordinated, so that the geometry is a square pyramid (Hossaini Sadr *et al.*, 2004).

Experimental

Copper dibromide (0.05 g, 0.25 mmol) and indazole (0.12 g, 1 mmol) were dissolved in acetone (25 ml). Slow evapoaration of the filtered solution yielded crystals.

Refinement

The C– and N-bound H atoms were placed in calculated positions and included in the refinement in the riding-model approximation with N—H = 0.86 Å and C—H = 0.93 Å, and with U_{iso}(H) 1.2U_{eq}(C,*N*). The vibrations of the Cu atoms appeared elongated in the directions of the weakly associated Br anions and, accordingly, the displacement factors were restrained to be nearly isotropic. The final difference Fourier map had a maximum and minimum residual density peaks at 1.35 Å from Br1 and Br2, respectively {AU to confirm this}.

Figures

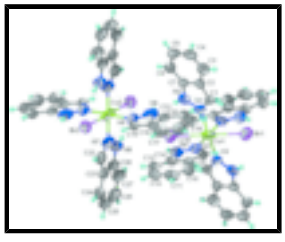


Fig. 1. Molecular structures of the two independent molecules of $[Cu(C_7H_6N_2)_4]^{2+}$ $2Br^-$ (I) showing displacement ellipsoids at the 50% probability level and H atoms as spheres of arbitrary radius. Each of the Cu atoms is located on a crystallographic center of inversion. The Cu···Br interactions are denoted by dashed lines.

Dibromidotetrakis(1*H*-indazole-κN^2)copper(II)

Crystal data

$[CuBr_2(C_7H_6N_2)_4]$	$Z = 2$
$M_r = 695.91$	$F_{000} = 694$
Triclinic, $P\overline{1}$	$D_x = 1.645$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.338$ (1) Å	Cell parameters from 7166 reflections
$b = 10.923$ (1) Å	$\theta = 3.2$–27.5º
$c = 13.730$ (1) Å	$\mu = 3.65$ mm^{-1}
$\alpha = 72.545$ (3)º	$T = 295$ (2) K
$\beta = 77.329$ (3)º	Prism, blue
$\gamma = 73.890$ (3)º	0.24 × 0.21 × 0.12 mm
$V = 1405.3$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	6389 independent reflections
Radiation source: fine-focus sealed tube	2895 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.046$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295$(2) K	$\theta_{min} = 3.2$º
ω scans	$h = -13 \rightarrow 13$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -11 \rightarrow 14$
$T_{min} = 0.073$, $T_{max} = 0.668$	$l = -17 \rightarrow 17$
13779 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.228$	$w = 1/[\sigma^2(F_o^2) + (0.1018P)^2 + 0.0608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} = 0.001$
6389 reflections	$\Delta\rho_{max} = 0.65$ e Å^{-3}
356 parameters	$\Delta\rho_{min} = -1.00$ e Å^{-3}
12 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.008 (2)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.62566 (10)	0.25866 (8)	0.41676 (7)	0.1011 (4)
Br2	−0.25176 (8)	0.40169 (7)	1.09777 (6)	0.0840 (3)
Cu1	0.5000	0.5000	0.5000	0.0843 (5)
Cu2	0.0000	0.5000	1.0000	0.1230 (8)
N1	0.5411 (5)	0.3924 (6)	0.6427 (4)	0.0636 (14)
N2	0.5199 (6)	0.4347 (6)	0.7267 (5)	0.0774 (16)
H2N	0.4877	0.5155	0.7291	0.093*
N3	0.3196 (6)	0.4493 (7)	0.5367 (4)	0.0748 (17)
N4	0.2108 (6)	0.5102 (6)	0.5891 (5)	0.0803 (17)
H4N	0.2071	0.5797	0.6078	0.096*
N5	0.0567 (9)	0.3532 (6)	0.9272 (5)	0.093 (2)
N6	0.1763 (9)	0.3169 (7)	0.8743 (6)	0.100 (2)
H6N	0.2408	0.3579	0.8604	0.120*
N7	−0.0951 (9)	0.6246 (6)	0.8816 (5)	0.090 (2)
N8	−0.0317 (7)	0.7102 (6)	0.8075 (5)	0.0885 (19)
H8N	0.0514	0.7141	0.8031	0.106*
C1	0.5920 (6)	0.2639 (6)	0.6683 (4)	0.0569 (15)
H1	0.6170	0.2106	0.6226	0.068*
C2	0.6029 (6)	0.2195 (6)	0.7719 (5)	0.0591 (15)
C3	0.6478 (8)	0.0951 (8)	0.8374 (6)	0.084 (2)
H3	0.6801	0.0206	0.8120	0.101*
C4	0.6428 (7)	0.0863 (9)	0.9382 (6)	0.090 (3)
H4	0.6683	0.0038	0.9828	0.108*
C5	0.6006 (8)	0.1974 (10)	0.9777 (6)	0.091 (3)
H5	0.6017	0.1881	1.0471	0.109*
C6	0.5577 (7)	0.3201 (9)	0.9148 (6)	0.086 (2)
H6	0.5296	0.3945	0.9404	0.103*
C7	0.5573 (6)	0.3298 (6)	0.8111 (4)	0.0592 (15)
C8	0.2874 (6)	0.3499 (7)	0.5225 (5)	0.0630 (16)
H8	0.3460	0.2906	0.4871	0.076*
C9	0.1562 (6)	0.3431 (7)	0.5663 (4)	0.0604 (16)
C10	0.0743 (8)	0.2577 (8)	0.5751 (6)	0.086 (2)
H10	0.1071	0.1862	0.5461	0.104*
C11	−0.0530 (8)	0.2800 (9)	0.6261 (7)	0.091 (2)
H11	−0.1082	0.2229	0.6327	0.109*
C12	−0.1034 (7)	0.3866 (9)	0.6692 (6)	0.084 (2)
H12	−0.1923	0.4004	0.7035	0.101*
C13	−0.0257 (7)	0.4712 (8)	0.6621 (6)	0.0763 (19)
H13	−0.0599	0.5420	0.6919	0.092*
C14	0.1048 (6)	0.4501 (6)	0.6102 (5)	0.0581 (15)
C15	−0.0112 (7)	0.2676 (7)	0.9321 (5)	0.0622 (16)
H15	−0.1001	0.2704	0.9658	0.075*
C16	0.0607 (6)	0.1736 (6)	0.8832 (5)	0.0578 (15)
C17	0.0283 (10)	0.0657 (9)	0.8687 (7)	0.096 (3)
H17	−0.0571	0.0472	0.8945	0.116*

C18	0.1251 (14)	−0.0105 (9)	0.8162 (8)	0.108 (3)
H18	0.1061	−0.0843	0.8069	0.130*
C19	0.2487 (11)	0.0154 (10)	0.7764 (7)	0.104 (3)
H19	0.3122	−0.0410	0.7408	0.124*
C20	0.2836 (7)	0.1224 (9)	0.7868 (6)	0.088 (2)
H20	0.3684	0.1409	0.7577	0.105*
C21	0.1863 (6)	0.2026 (6)	0.8430 (4)	0.0564 (14)
C22	−0.2200 (10)	0.6462 (7)	0.8630 (6)	0.086 (2)
H22	−0.2851	0.5999	0.9022	0.103*
C23	−0.2393 (9)	0.7522 (7)	0.7731 (6)	0.080 (2)
C24	−0.3451 (10)	0.8178 (9)	0.7148 (8)	0.103 (3)
H24	−0.4286	0.7942	0.7328	0.124*
C25	−0.3207 (13)	0.9197 (9)	0.6288 (7)	0.112 (3)
H25	−0.3900	0.9653	0.5893	0.135*
C26	−0.1982 (13)	0.9552 (10)	0.6004 (7)	0.113 (3)
H26	−0.1866	1.0240	0.5423	0.135*
C27	−0.0951 (11)	0.8941 (8)	0.6536 (6)	0.104 (3)
H27	−0.0121	0.9187	0.6346	0.124*
C28	−0.1185 (9)	0.7895 (7)	0.7408 (6)	0.080 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1416 (8)	0.0637 (6)	0.0882 (6)	0.0001 (5)	−0.0230 (5)	−0.0221 (4)
Br2	0.0917 (6)	0.0649 (5)	0.0874 (6)	−0.0117 (4)	−0.0083 (4)	−0.0166 (4)
Cu1	0.0608 (7)	0.1132 (11)	0.0637 (7)	−0.0366 (7)	−0.0251 (6)	0.0265 (7)
Cu2	0.232 (2)	0.0513 (8)	0.0766 (8)	0.0341 (10)	−0.0776 (11)	−0.0246 (6)
N1	0.054 (3)	0.085 (4)	0.051 (3)	−0.021 (3)	−0.012 (2)	−0.007 (3)
N2	0.070 (3)	0.069 (4)	0.083 (4)	−0.011 (3)	−0.020 (3)	−0.003 (3)
N3	0.064 (3)	0.086 (5)	0.057 (3)	−0.012 (3)	−0.015 (3)	0.007 (3)
N4	0.087 (4)	0.073 (4)	0.080 (4)	−0.021 (3)	−0.021 (3)	−0.011 (3)
N5	0.134 (6)	0.056 (4)	0.067 (4)	0.023 (4)	−0.027 (4)	−0.016 (3)
N6	0.151 (7)	0.067 (4)	0.097 (5)	−0.041 (5)	−0.055 (5)	−0.002 (4)
N7	0.151 (6)	0.042 (3)	0.072 (4)	0.002 (4)	−0.044 (4)	−0.010 (3)
N8	0.122 (5)	0.058 (4)	0.089 (4)	−0.008 (4)	−0.050 (4)	−0.011 (3)
C1	0.064 (3)	0.054 (4)	0.045 (3)	−0.007 (3)	−0.014 (3)	−0.004 (3)
C2	0.058 (3)	0.056 (4)	0.058 (3)	−0.009 (3)	−0.009 (3)	−0.011 (3)
C3	0.097 (5)	0.059 (4)	0.084 (5)	−0.008 (4)	−0.021 (4)	−0.005 (4)
C4	0.077 (5)	0.095 (6)	0.070 (5)	−0.010 (4)	−0.021 (4)	0.018 (4)
C5	0.083 (5)	0.121 (8)	0.055 (4)	−0.018 (5)	−0.016 (4)	−0.005 (5)
C6	0.078 (5)	0.100 (6)	0.072 (5)	−0.009 (4)	−0.011 (4)	−0.023 (4)
C7	0.055 (3)	0.069 (4)	0.047 (3)	−0.013 (3)	−0.009 (3)	−0.004 (3)
C8	0.051 (3)	0.066 (4)	0.063 (4)	−0.004 (3)	−0.003 (3)	−0.017 (3)
C9	0.051 (3)	0.073 (4)	0.053 (3)	−0.018 (3)	−0.009 (3)	−0.006 (3)
C10	0.084 (5)	0.081 (5)	0.103 (6)	−0.026 (4)	−0.009 (4)	−0.034 (4)
C11	0.076 (5)	0.098 (7)	0.106 (6)	−0.042 (5)	−0.028 (5)	−0.005 (5)
C12	0.059 (4)	0.092 (6)	0.079 (5)	−0.015 (4)	−0.001 (4)	0.002 (4)
C13	0.068 (4)	0.070 (5)	0.082 (5)	−0.005 (4)	−0.006 (4)	−0.020 (4)

C14	0.049 (3)	0.063 (4)	0.060 (3)	−0.025 (3)	−0.007 (3)	0.000 (3)
C15	0.062 (4)	0.061 (4)	0.056 (3)	0.000 (3)	−0.006 (3)	−0.017 (3)
C16	0.059 (3)	0.052 (4)	0.057 (3)	−0.010 (3)	−0.013 (3)	−0.006 (3)
C17	0.118 (6)	0.086 (6)	0.096 (6)	−0.060 (6)	−0.028 (5)	0.001 (5)
C18	0.166 (10)	0.056 (5)	0.117 (8)	−0.011 (6)	−0.058 (8)	−0.029 (5)
C19	0.123 (8)	0.086 (7)	0.094 (6)	0.031 (6)	−0.044 (6)	−0.042 (5)
C20	0.065 (4)	0.117 (7)	0.077 (5)	−0.011 (4)	−0.011 (4)	−0.026 (5)
C21	0.072 (4)	0.044 (3)	0.054 (3)	−0.011 (3)	−0.016 (3)	−0.012 (3)
C22	0.120 (7)	0.055 (5)	0.073 (5)	0.004 (4)	−0.014 (5)	−0.023 (4)
C23	0.112 (6)	0.055 (4)	0.068 (4)	0.009 (4)	−0.030 (4)	−0.022 (3)
C24	0.106 (6)	0.098 (7)	0.104 (6)	0.011 (5)	−0.028 (5)	−0.045 (5)
C25	0.153 (9)	0.082 (7)	0.087 (6)	0.032 (6)	−0.064 (7)	−0.020 (5)
C26	0.161 (10)	0.084 (7)	0.074 (5)	0.010 (7)	−0.030 (7)	−0.020 (5)
C27	0.156 (8)	0.059 (5)	0.087 (5)	−0.005 (5)	−0.038 (6)	−0.009 (4)
C28	0.118 (6)	0.050 (4)	0.069 (4)	−0.003 (4)	−0.035 (4)	−0.012 (3)

Geometric parameters (Å, °)

Cu1—N1	2.027 (5)	C6—H6	0.9300
Cu1—N3	2.008 (6)	C8—C9	1.370 (8)
Cu1—Br1	3.033 (1)	C8—H8	0.9300
Cu2—N5	2.024 (7)	C9—C10	1.389 (10)
Cu2—N7	2.023 (6)	C9—C14	1.395 (9)
Cu2—Br2	2.980 (1)	C10—C11	1.342 (11)
Cu1—N3^{i}	2.008 (6)	C10—H10	0.9300
Cu1—N1^{i}	2.027 (5)	C11—C12	1.385 (12)
Cu2—N7^{ii}	2.023 (6)	C11—H11	0.9300
Cu2—N5^{ii}	2.024 (7)	C12—C13	1.354 (12)
N1—N2	1.320 (8)	C12—H12	0.9300
N1—C1	1.321 (8)	C13—C14	1.374 (8)
N2—C7	1.400 (8)	C13—H13	0.9300
N2—H2N	0.8600	C15—C16	1.352 (9)
N3—C8	1.298 (9)	C15—H15	0.9300
N3—N4	1.320 (8)	C16—C21	1.378 (8)
N4—C14	1.364 (8)	C16—C17	1.389 (10)
N4—H4N	0.8600	C17—C18	1.340 (13)
N5—C15	1.295 (10)	C17—H17	0.9300
N5—N6	1.312 (9)	C18—C19	1.347 (13)
N6—C21	1.409 (9)	C18—H18	0.9300
N6—H6N	0.8600	C19—C20	1.368 (13)
N7—C22	1.315 (10)	C19—H19	0.9300
N7—N8	1.347 (9)	C20—C21	1.397 (10)
N8—C28	1.359 (9)	C20—H20	0.9300
N8—H8N	0.8600	C22—C23	1.424 (10)
C1—C2	1.377 (8)	C22—H22	0.9300
C1—H1	0.9300	C23—C28	1.362 (11)
C2—C7	1.388 (9)	C23—C24	1.399 (12)
C2—C3	1.404 (9)	C24—C25	1.391 (13)

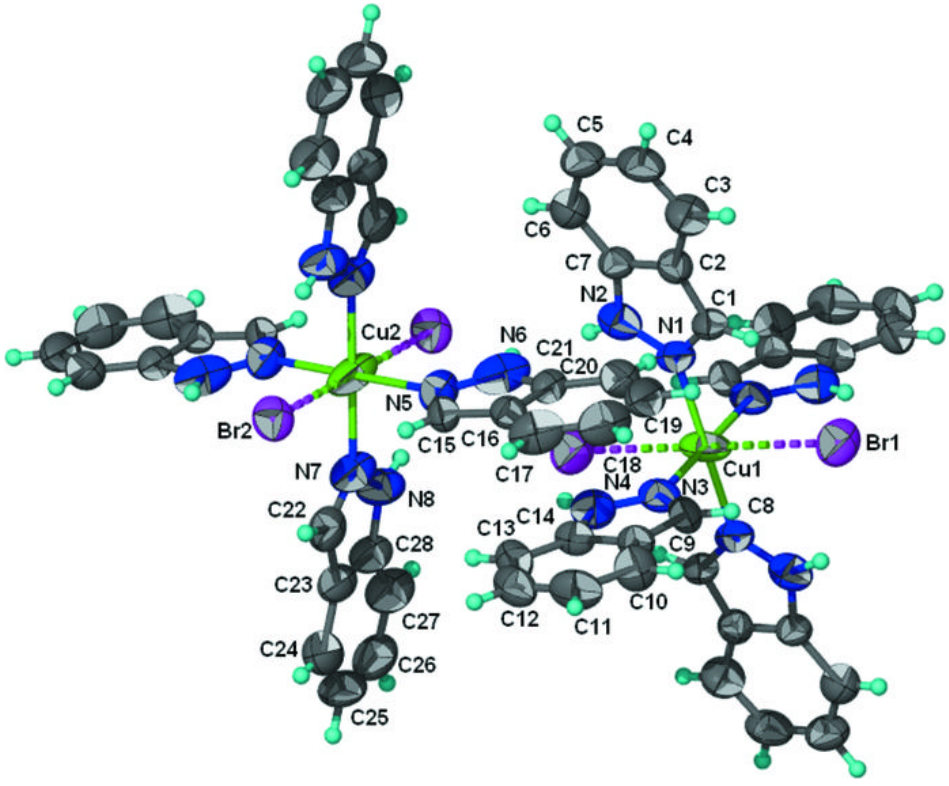
C3—C4	1.348 (11)	C24—H24	0.9300
C3—H3	0.9300	C25—C26	1.368 (14)
C4—C5	1.398 (12)	C25—H25	0.9300
C4—H4	0.9300	C26—C27	1.330 (13)
C5—C6	1.372 (11)	C26—H26	0.9300
C5—H5	0.9300	C27—C28	1.415 (11)
C6—C7	1.396 (9)	C27—H27	0.9300
N3—Cu1—N3^{i}	180.0 (4)	C5—C6—C7	118.0 (8)
N3—Cu1—N1	88.2 (2)	C5—C6—H6	121.0
N3^{i}—Cu1—N1	91.8 (2)	C7—C6—H6	121.0
N3—Cu1—N1^{i}	91.8 (2)	C2—C7—C6	121.1 (6)
N3^{i}—Cu1—N1^{i}	88.2 (2)	C2—C7—N2	104.9 (6)
N1—Cu1—N1^{i}	180.00 (16)	C6—C7—N2	133.9 (7)
N3—Cu1—Br1^{i}	90.3 (2)	N3—C8—C9	111.5 (6)
N3^{i}—Cu1—Br1^{i}	89.7 (2)	N3—C8—H8	124.2
N1—Cu1—Br1^{i}	89.84 (18)	C9—C8—H8	124.2
N1^{i}—Cu1—Br1^{i}	90.16 (18)	C8—C9—C10	134.8 (7)
N3—Cu1—Br1	89.7 (2)	C8—C9—C14	105.7 (6)
N3^{i}—Cu1—Br1	90.3 (2)	C10—C9—C14	119.6 (6)
N1—Cu1—Br1	90.16 (18)	C11—C10—C9	119.0 (8)
N1^{i}—Cu1—Br1	89.84 (18)	C11—C10—H10	120.5
Br1^{i}—Cu1—Br1	180.00 (3)	C9—C10—H10	120.5
N7^{ii}—Cu2—N7	180.000 (2)	C10—C11—C12	121.1 (7)
N7^{ii}—Cu2—N5^{ii}	91.3 (2)	C10—C11—H11	119.5
N7—Cu2—N5^{ii}	88.7 (2)	C12—C11—H11	119.5
N7^{ii}—Cu2—N5	88.7 (2)	C13—C12—C11	121.2 (7)
N7—Cu2—N5	91.3 (2)	C13—C12—H12	119.4
N5^{ii}—Cu2—N5	180.000 (2)	C11—C12—H12	119.4
N7^{ii}—Cu2—Br2	89.4 (2)	C12—C13—C14	118.6 (8)
N7—Cu2—Br2	90.6 (2)	C12—C13—H13	120.7
N5^{ii}—Cu2—Br2	92.4 (3)	C14—C13—H13	120.7
N5—Cu2—Br2	87.6 (3)	N4—C14—C13	135.3 (7)
N7^{ii}—Cu2—Br2^{ii}	90.6 (2)	N4—C14—C9	104.2 (5)
N7—Cu2—Br2^{ii}	89.4 (2)	C13—C14—C9	120.6 (6)
N5^{ii}—Cu2—Br2^{ii}	87.6 (3)	N5—C15—C16	112.9 (6)
N5—Cu2—Br2^{ii}	92.4 (3)	N5—C15—H15	123.6
Br2—Cu2—Br2^{ii}	180.00 (3)	C16—C15—H15	123.6
N2—N1—C1	107.6 (5)	C15—C16—C21	106.6 (6)
N2—N1—Cu1	127.4 (5)	C15—C16—C17	132.2 (7)
C1—N1—Cu1	125.0 (5)	C21—C16—C17	121.2 (7)
N1—N2—C7	110.5 (6)	C18—C17—C16	117.3 (8)
N1—N2—H2N	124.8	C18—C17—H17	121.3
C7—N2—H2N	124.8	C16—C17—H17	121.3
C8—N3—N4	106.6 (6)	C17—C18—C19	122.6 (9)

C8—N3—Cu1	129.2 (5)	C17—C18—H18	118.7
N4—N3—Cu1	124.0 (6)	C19—C18—H18	118.7
N3—N4—C14	112.1 (6)	C18—C19—C20	121.9 (8)
N3—N4—H4N	124.0	C18—C19—H19	119.1
C14—N4—H4N	124.0	C20—C19—H19	119.1
C15—N5—N6	105.9 (6)	C19—C20—C21	117.1 (7)
C15—N5—Cu2	127.4 (6)	C19—C20—H20	121.5
N6—N5—Cu2	126.4 (7)	C21—C20—H20	121.5
N5—N6—C21	111.7 (7)	C16—C21—C20	119.8 (6)
N5—N6—H6N	124.1	C16—C21—N6	102.9 (6)
C21—N6—H6N	124.1	C20—C21—N6	137.2 (7)
C22—N7—N8	108.1 (6)	N7—C22—C23	108.8 (8)
C22—N7—Cu2	131.1 (6)	N7—C22—H22	125.6
N8—N7—Cu2	120.6 (6)	C23—C22—H22	125.6
N7—N8—C28	110.0 (7)	C28—C23—C24	118.2 (8)
N7—N8—H8N	125.0	C28—C23—C22	105.7 (7)
C28—N8—H8N	125.0	C24—C23—C22	136.1 (10)
N1—C1—C2	110.9 (6)	C25—C24—C23	117.5 (10)
N1—C1—H1	124.6	C25—C24—H24	121.2
C2—C1—H1	124.6	C23—C24—H24	121.2
C1—C2—C7	106.1 (5)	C26—C25—C24	122.1 (9)
C1—C2—C3	134.0 (7)	C26—C25—H25	119.0
C7—C2—C3	119.9 (6)	C24—C25—H25	119.0
C4—C3—C2	118.4 (8)	C27—C26—C25	121.9 (10)
C4—C3—H3	120.8	C27—C26—H26	119.0
C2—C3—H3	120.8	C25—C26—H26	119.0
C3—C4—C5	122.1 (7)	C26—C27—C28	116.4 (10)
C3—C4—H4	119.0	C26—C27—H27	121.8
C5—C4—H4	119.0	C28—C27—H27	121.8
C6—C5—C4	120.4 (7)	N8—C28—C23	107.4 (7)
C6—C5—H5	119.8	N8—C28—C27	128.8 (9)
C4—C5—H5	119.8	C23—C28—C27	123.8 (8)
N3—Cu1—N1—N2	−93.9 (5)	C5—C6—C7—N2	179.1 (7)
$N3^{i}$—Cu1—N1—N2	86.1 (5)	N1—N2—C7—C2	−0.1 (7)
$Br1^{i}$—Cu1—N1—N2	−3.6 (5)	N1—N2—C7—C6	178.9 (7)
Br1—Cu1—N1—N2	176.4 (5)	N4—N3—C8—C9	−0.4 (8)
N3—Cu1—N1—C1	84.4 (5)	Cu1—N3—C8—C9	174.8 (4)
$N3^{i}$—Cu1—N1—C1	−95.6 (5)	N3—C8—C9—C10	−178.6 (8)
$Br1^{i}$—Cu1—N1—C1	174.6 (5)	N3—C8—C9—C14	0.5 (7)
Br1—Cu1—N1—C1	−5.4 (5)	C8—C9—C10—C11	178.9 (7)
C1—N1—N2—C7	−0.5 (7)	C14—C9—C10—C11	−0.2 (11)
Cu1—N1—N2—C7	178.0 (4)	C9—C10—C11—C12	0.4 (13)
N1—Cu1—N3—C8	−91.4 (6)	C10—C11—C12—C13	−0.7 (13)
$N1^{i}$—Cu1—N3—C8	88.6 (6)	C11—C12—C13—C14	0.7 (12)
$Br1^{i}$—Cu1—N3—C8	178.8 (6)	N3—N4—C14—C13	178.6 (7)
Br1—Cu1—N3—C8	−1.2 (6)	N3—N4—C14—C9	0.3 (7)
N1—Cu1—N3—N4	83.0 (5)	C12—C13—C14—N4	−178.6 (7)

N1^{i}—Cu1—N3—N4	−97.0 (5)	C12—C13—C14—C9	−0.5 (10)
Br1^{i}—Cu1—N3—N4	−6.8 (5)	C8—C9—C14—N4	−0.5 (7)
Br1—Cu1—N3—N4	173.2 (5)	C10—C9—C14—N4	178.9 (6)
C8—N3—N4—C14	0.1 (7)	C8—C9—C14—C13	−179.1 (6)
Cu1—N3—N4—C14	−175.4 (4)	C10—C9—C14—C13	0.2 (10)
N7^{ii}—Cu2—N5—C15	91.4 (7)	N6—N5—C15—C16	−0.1 (8)
N7—Cu2—N5—C15	−88.6 (7)	Cu2—N5—C15—C16	−173.3 (4)
Br2—Cu2—N5—C15	2.0 (6)	N5—C15—C16—C21	−0.2 (8)
Br2^{ii}—Cu2—N5—C15	−178.0 (6)	N5—C15—C16—C17	−179.4 (7)
N7^{ii}—Cu2—N5—N6	−80.5 (6)	C15—C16—C17—C18	−179.4 (8)
N7—Cu2—N5—N6	99.5 (6)	C21—C16—C17—C18	1.5 (11)
Br2—Cu2—N5—N6	−170.0 (6)	C16—C17—C18—C19	−1.3 (14)
Br2^{ii}—Cu2—N5—N6	10.0 (6)	C17—C18—C19—C20	−0.2 (15)
C15—N5—N6—C21	0.3 (8)	C18—C19—C20—C21	1.5 (13)
Cu2—N5—N6—C21	173.7 (4)	C15—C16—C21—C20	−179.5 (6)
N5^{ii}—Cu2—N7—C22	−92.2 (7)	C17—C16—C21—C20	−0.2 (10)
N5—Cu2—N7—C22	87.8 (7)	C15—C16—C21—N6	0.4 (7)
Br2—Cu2—N7—C22	0.3 (7)	C17—C16—C21—N6	179.7 (6)
Br2^{ii}—Cu2—N7—C22	−179.7 (7)	C19—C20—C21—C16	−1.3 (11)
N5^{ii}—Cu2—N7—N8	83.4 (6)	C19—C20—C21—N6	178.9 (7)
N5—Cu2—N7—N8	−96.6 (6)	N5—N6—C21—C16	−0.4 (7)
Br2—Cu2—N7—N8	175.8 (5)	N5—N6—C21—C20	179.4 (8)
Br2^{ii}—Cu2—N7—N8	−4.2 (5)	N8—N7—C22—C23	−0.7 (8)
C22—N7—N8—C28	0.8 (8)	Cu2—N7—C22—C23	175.2 (5)
Cu2—N7—N8—C28	−175.7 (5)	N7—C22—C23—C28	0.4 (8)
N2—N1—C1—C2	0.9 (7)	N7—C22—C23—C24	178.5 (8)
Cu1—N1—C1—C2	−177.6 (4)	C28—C23—C24—C25	−1.7 (11)
N1—C1—C2—C7	−1.0 (7)	C22—C23—C24—C25	−179.7 (8)
N1—C1—C2—C3	179.1 (7)	C23—C24—C25—C26	0.6 (14)
C1—C2—C3—C4	−179.0 (7)	C24—C25—C26—C27	0.0 (15)
C7—C2—C3—C4	1.1 (11)	C25—C26—C27—C28	0.5 (14)
C2—C3—C4—C5	−3.0 (12)	N7—N8—C28—C23	−0.5 (8)
C3—C4—C5—C6	2.4 (12)	N7—N8—C28—C27	178.6 (7)
C4—C5—C6—C7	0.2 (11)	C24—C23—C28—N8	−178.4 (7)
C1—C2—C7—C6	−178.5 (6)	C22—C23—C28—N8	0.1 (8)
C3—C2—C7—C6	1.4 (10)	C24—C23—C28—C27	2.4 (11)
C1—C2—C7—N2	0.6 (7)	C22—C23—C28—C27	−179.1 (7)
C3—C2—C7—N2	−179.4 (6)	C26—C27—C28—N8	179.2 (8)
C5—C6—C7—C2	−2.0 (10)	C26—C27—C28—C23	−1.7 (13)

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

Fig. 1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