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Dibromidotetrakis(1-vinyl-1*H*-imidazole-κN^3)copper(II)

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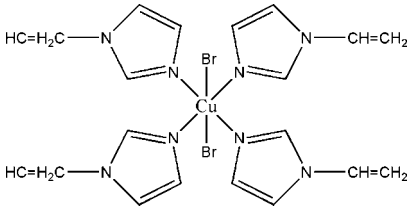
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.015 Å; R factor = 0.065; wR factor = 0.164; data-to-parameter ratio = 19.5.

In the title compound, $[CuBr_2(C_5H_6N_2)_4]$, the Cu^{II} cation is located on a crystallographic centre of symmetry and coordinated by four N atoms from four 1-vinylimidazole ligands and two *trans* coordinated Br^- anions in a distorted octahedral geometry. In the crystal structure, intra- and intermolecular C—H···Br hydrogen bonds form three-dimensional hydrogen-bond networks which stabilize the structure.

Related literature

For related literature, see: Parker & Breneman (1995).



Experimental

Crystal data

$[CuBr_2(C_5H_6N_2)_4]$
M_r = 599.82
Monoclinic, $P2_1/n$
a = 7.7280 (15) Å
b = 15.144 (3) Å
c = 11.039 (2) Å
β = 107.23 (3)°
V = 1234.0 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.15 mm^{-1}
T = 293 (2) K
0.40 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.605, T_{max} = 0.659
2568 measured reflections
2416 independent reflections
1446 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.164
S = 1.03
2416 reflections
124 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···Br^{i}	0.93	2.79	3.643 (12)	154
C3—H3A···Br^{i}	0.93	2.93	3.717 (9)	144
C8—H8A···Br^{ii}	0.93	2.87	3.772 (9)	163
C10—H10A···Br	0.93	2.88	3.480 (8)	124

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

This work was supported by the National Natural Science Foundation of China (grant No. 20601015) and the Natural Science Foundation of Shandong Province (grant No. Y2006B12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2284).

References

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Parker, O. J. & Breneman, G. L. (1995). *Acta Cryst.* C**51**, 1097–1099.
Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.

supplementary materials

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Dibromidotetrakis(1-vinyl-1*H*-imidazole-κN^3)copper(II)

F.-Q. Liu, R.-X. Li, S.-X. Li, C.-Q. Li and G.-Y. Liu

Comment

In the title compound,(I), The Cu^{II} cation is coordinated by four N atoms from four 1-vinylimidazole ligand and two *trans* coordinated Br^- anions in a distorted octahedral geometry (Fig. 1). The equatorial planes are formed by four Cu—*N*(1-vinylimadazole) bonds [Cu—N2 = 2.007 (6) Å, Cu—N4 = 2.029 (6) Å] and the axial positions are occupied by two Br^- ions [Cu—Br = 3.0340 (11) Å]. The Cu—N bond lengths agree well with those observed in [Cu(imidazole)Br_2] (Parker & Breneman, 1995), but the Cu—Br bond length is shorter than that in [Cu(imidazole)Br_2]. In the crystal, the intramolecular and intermolecular C—H···Br hydrogen bonds form three-dimensional hydrogen bond networks to stabilize the structure.

Experimental

The title compound was prepared by the reaction of 1-vinylimidazole (0.47 g, 5 mmol) with $CuBr_2$ (0.72 g, 5 mmol) by means of hydrothermal synthesis in a stainless-steel reactor with a Teflon liner at 383 K for 24 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

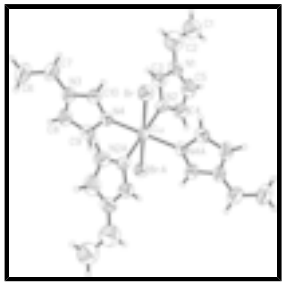

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme [symmetry code: (A):-*x* + 1,-*y* + 1,-*z* + 1].

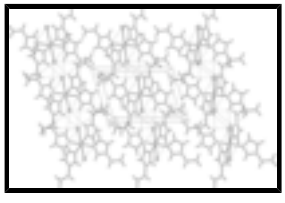

Fig. 2. The packing of (I), viewed down the *b* axis.

Dibromidotetrakis(1-vinyl-1*H*-imidazole-κN^3)copper(II)

Crystal data

$[CuBr_2(C_5H_6N_2)_4]$	F_{000} = 598
M_r = 599.82	D_x = 1.614 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2268 reflections
a = 7.7280 (15) Å	θ = 4–15º
b = 15.144 (3) Å	μ = 4.15 mm^{-1}
c = 11.039 (2) Å	T = 293 (2) K
β = 107.23 (3)º	Block, blue
V = 1234.0 (5) Å^3	0.40 × 0.10 × 0.10 mm
Z = 2	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2416 independent reflections
Radiation source: fine-focus sealed tube	1446 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.013
T = 293(2) K	θ_{max} = 26.0º
Thin–slice ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −9→9
T_{min} = 0.605, T_{max} = 0.659	k = 0→18
2568 measured reflections	l = 0→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.065	H-atom parameters constrained
$wR(F^2)$ = 0.164	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
2416 reflections	$\Delta\rho_{max}$ = 0.82 e Å^{-3}
124 parameters	$\Delta\rho_{min}$ = −0.84 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Br	0.17188 (11)	0.38082 (6)	0.45787 (8)	0.054
Cu	0.5000	0.5000	0.5000	0.0477 (4)
N1	0.3333 (10)	0.5776 (5)	0.8077 (7)	0.0598 (19)
N2	0.4621 (8)	0.5408 (4)	0.6632 (6)	0.0460 (16)
N3	0.0973 (9)	0.6672 (4)	0.2833 (7)	0.0514 (17)
N4	0.3382 (8)	0.5963 (4)	0.3984 (6)	0.0452 (16)
C1	0.1989 (17)	0.6136 (7)	0.9774 (11)	0.100
H1A	0.3135	0.6120	1.0361	0.120*
H1B	0.0980	0.6262	1.0039	0.120*
C2	0.1776 (18)	0.5966 (8)	0.8455 (11)	0.104
H2A	0.0635	0.5981	0.7861	0.125*
C3	0.3085 (11)	0.5535 (5)	0.6875 (8)	0.053 (2)
H3A	0.1954	0.5466	0.6282	0.064*
C4	0.5950 (13)	0.5582 (7)	0.7757 (9)	0.066 (3)
H4A	0.7193	0.5556	0.7880	0.079*
C5	0.5153 (15)	0.5795 (7)	0.8639 (9)	0.076 (3)
H5A	0.5738	0.5931	0.9483	0.091*
C6	−0.1584 (14)	0.7383 (7)	0.1260 (10)	0.089 (3)
H6A	−0.0796	0.7619	0.0851	0.106*
H6B	−0.2820	0.7497	0.0952	0.106*
C7	−0.0897 (13)	0.6847 (6)	0.2360 (8)	0.072 (3)
H7A	−0.1687	0.6612	0.2767	0.086*
C8	0.2447 (13)	0.7082 (6)	0.2648 (8)	0.060 (2)
H8A	0.2434	0.7573	0.2140	0.072*
C9	0.3952 (12)	0.6632 (6)	0.3353 (8)	0.059 (2)
H9A	0.5147	0.6758	0.3396	0.071*
C10	0.1625 (11)	0.6012 (5)	0.3668 (8)	0.052 (2)
H10A	0.0902	0.5638	0.3980	0.062*

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Br	0.054	0.054	0.054	0.000	0.016	0.000
Cu	0.0553 (8)	0.0510 (8)	0.0381 (8)	0.0152 (7)	0.0157 (6)	0.0062 (7)
N1	0.071 (5)	0.066 (5)	0.050 (5)	0.006 (4)	0.029 (4)	−0.002 (4)
N2	0.039 (3)	0.052 (4)	0.046 (4)	0.009 (3)	0.012 (3)	0.003 (3)
N3	0.060 (4)	0.041 (4)	0.052 (4)	0.008 (3)	0.014 (3)	0.009 (3)
N4	0.050 (4)	0.047 (4)	0.040 (4)	0.007 (3)	0.015 (3)	0.010 (3)
C1	0.100	0.100	0.100	0.000	0.030	0.000
C2	0.104	0.104	0.104	0.000	0.031	0.000
C3	0.056 (5)	0.049 (5)	0.056 (6)	0.001 (4)	0.018 (4)	−0.002 (4)
C4	0.063 (6)	0.086 (7)	0.049 (6)	0.007 (5)	0.018 (5)	−0.010 (5)
C5	0.093 (8)	0.076 (7)	0.048 (6)	0.007 (6)	0.007 (6)	−0.004 (5)
C6	0.076 (7)	0.085 (8)	0.090 (8)	0.018 (6)	0.002 (6)	0.024 (7)
C7	0.068 (6)	0.074 (7)	0.065 (7)	0.019 (5)	0.008 (5)	0.000 (5)
C8	0.083 (6)	0.043 (5)	0.056 (6)	0.016 (5)	0.021 (5)	0.011 (4)
C9	0.063 (5)	0.061 (6)	0.060 (6)	0.005 (5)	0.027 (5)	0.013 (5)
C10	0.055 (5)	0.036 (5)	0.068 (6)	0.007 (4)	0.024 (4)	0.008 (4)

Geometric parameters (Å, °)

Cu—Br	3.0340 (11)	C1—H1A	0.9300
Cu—N2	2.007 (6)	C1—H1B	0.9300
Cu—N2^{i}	2.007 (6)	C2—H2A	0.9300
Cu—N4^{i}	2.029 (6)	C3—H3A	0.9300
Cu—N4	2.029 (6)	C4—C5	1.336 (13)
N1—C3	1.334 (10)	C4—H4A	0.9300
N1—C5	1.359 (12)	C5—H5A	0.9300
N1—C2	1.414 (13)	C6—C7	1.427 (8)
N2—C3	1.306 (9)	C6—H6A	0.9300
N2—C4	1.383 (11)	C6—H6B	0.9300
N3—C10	1.351 (10)	C7—H7A	0.9300
N3—C8	1.365 (11)	C8—C9	1.374 (12)
N3—C7	1.408 (10)	C8—H8A	0.9300
N4—C10	1.301 (10)	C9—H9A	0.9300
N4—C9	1.373 (10)	C10—H10A	0.9300
C1—C2	1.439 (9)		
N2—Cu—N2^{i}	180.000 (1)	N2—C3—N1	111.9 (8)
N2—Cu—N4^{i}	87.4 (2)	N2—C3—H3A	124.0
N2^{i}—Cu—N4^{i}	92.6 (2)	N1—C3—H3A	124.0
N2—Cu—N4	92.6 (2)	C5—C4—N2	108.6 (9)
N2^{i}—Cu—N4	87.4 (2)	C5—C4—H4A	125.7
N4^{i}—Cu—N4	180.000 (1)	N2—C4—H4A	125.7
C3—N1—C5	106.5 (8)	C4—C5—N1	107.5 (9)
C3—N1—C2	117.7 (9)	C4—C5—H5A	126.2
C5—N1—C2	135.8 (9)	N1—C5—H5A	126.2
C3—N2—C4	105.4 (7)	C7—C6—H6A	120.0
C3—N2—Cu	127.8 (6)	C7—C6—H6B	120.0
C4—N2—Cu	126.7 (5)	H6A—C6—H6B	120.0

C10—N3—C8	106.2 (7)	N3—C7—C6	120.3 (9)
C10—N3—C7	121.8 (7)	N3—C7—H7A	119.8
C8—N3—C7	132.0 (7)	C6—C7—H7A	119.8
C10—N4—C9	106.7 (7)	N3—C8—C9	107.1 (7)
C10—N4—Cu	127.8 (5)	N3—C8—H8A	126.5
C9—N4—Cu	124.9 (5)	C9—C8—H8A	126.5
C2—C1—H1A	120.0	N4—C9—C8	108.0 (8)
C2—C1—H1B	120.0	N4—C9—H9A	126.0
H1A—C1—H1B	120.0	C8—C9—H9A	126.0
N1—C2—C1	118.8 (11)	N4—C10—N3	112.0 (7)
N1—C2—H2A	120.6	N4—C10—H10A	124.0
C1—C2—H2A	120.6	N3—C10—H10A	124.0
$N4^{i}$—Cu—N2—C3	−126.5 (7)	Cu—N2—C4—C5	−176.9 (6)
N4—Cu—N2—C3	53.5 (7)	N2—C4—C5—N1	−1.3 (12)
$N4^{i}$—Cu—N2—C4	51.0 (7)	C3—N1—C5—C4	1.2 (11)
N4—Cu—N2—C4	−129.0 (7)	C2—N1—C5—C4	−176.8 (11)
N2—Cu—N4—C10	−73.6 (7)	C10—N3—C7—C6	−164.0 (9)
$N2^{i}$—Cu—N4—C10	106.4 (7)	C8—N3—C7—C6	18.7 (15)
N2—Cu—N4—C9	115.8 (7)	C10—N3—C8—C9	2.0 (10)
$N2^{i}$—Cu—N4—C9	−64.2 (7)	C7—N3—C8—C9	179.6 (9)
C3—N1—C2—C1	173.5 (10)	C10—N4—C9—C8	0.0 (10)
C5—N1—C2—C1	−8.7 (19)	Cu—N4—C9—C8	172.3 (6)
C4—N2—C3—N1	−0.2 (10)	N3—C8—C9—N4	−1.3 (10)
Cu—N2—C3—N1	177.6 (5)	C9—N4—C10—N3	1.3 (10)
C5—N1—C3—N2	−0.6 (10)	Cu—N4—C10—N3	−170.7 (5)
C2—N1—C3—N2	177.8 (8)	C8—N3—C10—N4	−2.1 (10)
C3—N2—C4—C5	1.0 (11)	C7—N3—C10—N4	−180.0 (7)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···Br^{ii}	0.93	2.79	3.643 (12)	154
C3—H3A···Br^{ii}	0.93	2.93	3.717 (9)	144
C8—H8A···Br^{iii}	0.93	2.87	3.772 (9)	163
C10—H10A···Br	0.93	2.88	3.480 (8)	124

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

Fig. 1

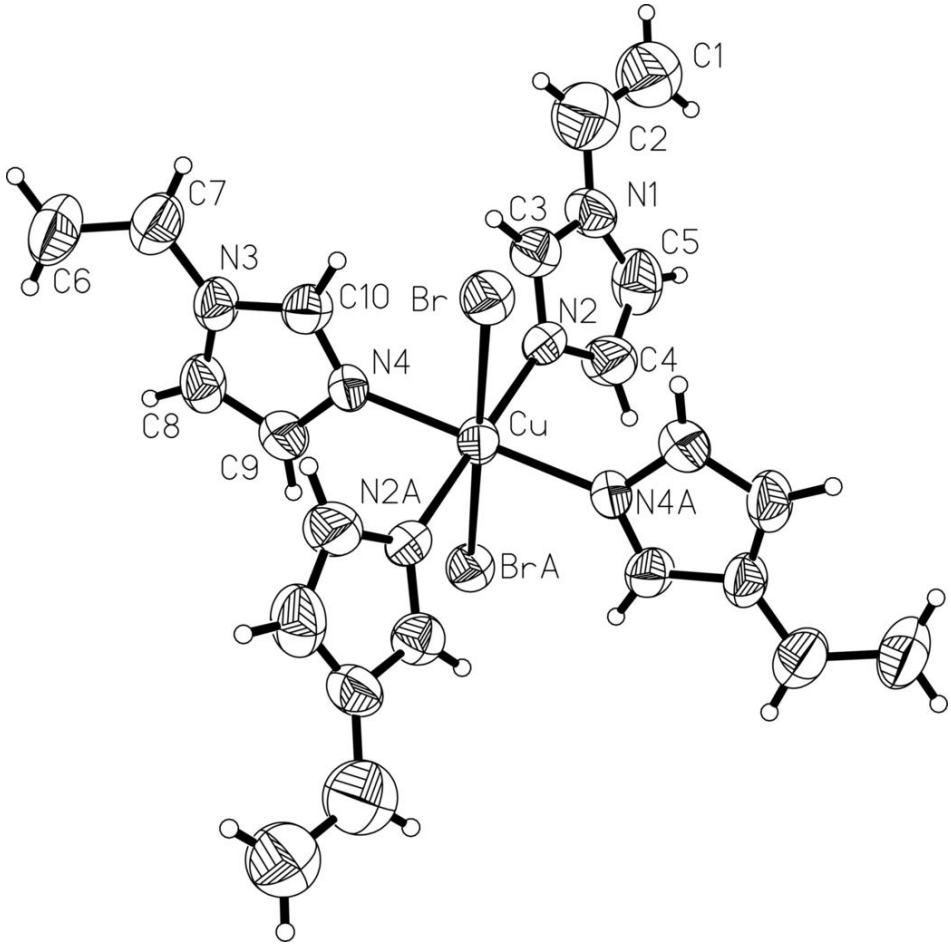

Fig. 2