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Bis[tris(1-pyrazolyl)methane-κ^3N,N',N'']copper(II) dichloride methanol disolvate

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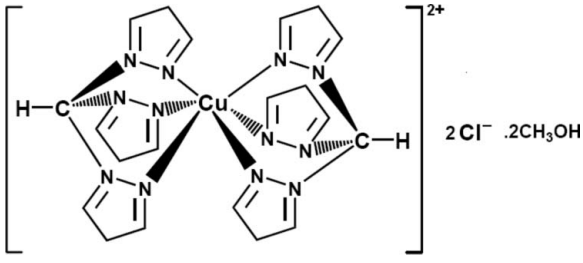
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.085; data-to-parameter ratio = 10.7.

The reaction between copper(II) chloride dihydrate and excess tris(1-pyrazolyl)methane results in the formation of the title complex, $[Cu(C_{10}H_{10}N_6)_2]Cl_2{\cdot}2CH_3OH$. The centrosymmetric complex cation is mononuclear with octahedral coordination for Cu and two tridentate ligands. Two short and one long Cu—N distances [2.002 (3), 2.011 (2) and 2.413 (2) Å] are found, as expected for Jahn–Teller distortion.

Related literature

For related literature, see: Allen *et al.* (1987); Astley *et al.* (1993); Kitajima *et al.* (1990); Martini *et al.* (2002); Orpen *et al.* (1989); Qiu *et al.* (1994).



Experimental

Crystal data

$[Cu(C_{10}H_{10}N_6)_2]Cl_2{\cdot}2CH_4O$
M_r = 627.00
Monoclinic, $P2_1/c$
a = 8.5069 (13) Å
b = 10.4307 (16) Å
c = 16.101 (3) Å
β = 91.574 (8)°
V = 1428.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 150 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.907, T_{max} = 0.943
6690 measured reflections
2497 independent reflections
1871 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.085
S = 0.97
2497 reflections
234 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2103).

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supplementary materials

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Bis[tris(1-pyrazolyl)methane-κ^3N,N',N'']copper(II) dichloride methanol disolvate

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Comment

Copper complexes of tripodal N3-donor ligands are of significance from a bioinorganic point of view since, for example, the N3–1igand coordination can mimic some spectroscopic features of blue copper proteins (Kitajima *et al.*, 1990; Qiu *et al.*, 1994). Compared with the enormous number of synthetic and structural studies of poly(1-pyrazolyl)borate Cu(II) comp1exes, only a few studies have been reported on the analogous poly(1-pyrazolyl)methane derivatives (Astley *et al.*, 1993; Martini *et al.*, 2002). We describe here a copper(II) complex containing tris(1-pyrazolyl)methane ligands, (I).

The structure of (I) (Fig. 1) consists of discrete centrosymmetric octahedral mononuclear Cu^{II} species with two tris(1-pyrazolyl)methane ligands, Cl^- counter-ions, and methanol of crystallization. The bonding parameters are similar to those of the analogous complexes $[Cu\{HC(pz)_3\}_2](NO_3)_2$ and $[Cu\{HC(pz)_3\}_2](ClO_4)_2$ (Martini *et al.*, 2002).

The Cu—N distances are close to those for $[Cu\{HC(pz)_3\}_2](ClO_4)_2$ (Martini *et al.*, 2002). Two short Cu—N distances, approximately 2.0 Å, and one long, approximately 2.4 Å, are observed in both cases, consistent with Jahn-Teller distortion. All other bond lengths are normal (Allen *et al.*, 1987; Orpen *et al.*, 1989).

Experimental

The title compound was prepared by the previously published procedure (Martini *et al.*, 2002) using copper(II) chloride dihydrate and tris(1-pyrazolyl)methane as starting materials and a reaction time of 24 h. Suitable crystals for X-ray study were obtained by vapour diffusion of diethyl ether into a methanol solution of (I) at 278 K. Anal. Cal. for $CuC_{22}H_{28}N_{12}Cl_2O$: C, 42.1; H, 4.5; N, 26.8. Found: C, 42.4; H, 4.0; N, 28.4%. IR (KBr pellet): 3092.0 [s, ν (C–H)], 1630.2 and 1518.4 [s, ν (C═C), ν (N═C), $HC(pz)_3$]. EPR (90 K): g = 2.0732; a_{Cu} = 168; a_N = 12.5. FAB^+—MS, m/*z*: 626 $[M]^+$, 611 $[M - O]^+$, 561 $[M - pz]^+$, 528 $[M - 2pz + Cl]^+$, 493 $[M - 2pz]^+$. FAB^-–MS, m/*z*: 35 $[Cl]^-$–.

Refinement

All H atoms were located in a difference map and refined freely, giving C—H = 0.86 (3)–0.99 (4)° and O—H = 0.76 (4) Å.

Figures

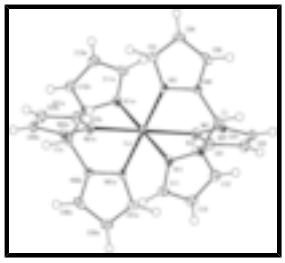


Fig. 1. The structure of the cation of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. [Symmetry code: (*a*) −*x*, −*y*, −*z*.]

Bis[tris(1-pyrazolyl)methane-κ^3*N*,*N*',*N*'']copper(II) dichloride methanol disolvate

Crystal data

$[Cu(C_{10}H_{10}N_6)_2]Cl_2·2CH_4O$	F_{000} = 646
M_r = 627.00	D_x = 1.458 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 8.5069 (13) Å	Cell parameters from 829 reflections
b = 10.4307 (16) Å	θ = 2.5–22.6º
c = 16.101 (3) Å	μ = 1.00 mm^{-1}
β = 91.574 (8)º	T = 150 (2) K
V = 1428.1 (4) Å^3	Block, blue
Z = 2	0.10 × 0.08 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2497 independent reflections
Radiation source: fine-focus sealed tube	1871 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
T = 150(2) K	θ_{max} = 25.3º
φ and ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −9→8
T_{min} = 0.907, T_{max} = 0.943	k = −12→8
6690 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	All H-atom parameters refined
$wR(F^2)$ = 0.085	$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 0.97	$(\Delta/\sigma)_{max}$ = 0.001
2497 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
234 parameters	$\Delta\rho_{min}$ = −0.34 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}
C1	0.1681 (4)	0.2505 (3)	−0.05452 (19)	0.0131 (7)
C10	−0.0476 (7)	0.3472 (4)	0.2225 (3)	0.0405 (11)
C11	0.2292 (4)	−0.0536 (3)	−0.1423 (2)	0.0181 (8)
C12	0.3208 (4)	0.1382 (3)	−0.16536 (19)	0.0173 (8)
C13	0.3323 (4)	0.0143 (3)	−0.1904 (2)	0.0198 (8)
C21	0.2827 (4)	0.1359 (3)	0.1412 (2)	0.0169 (7)
C22	0.3558 (4)	0.2975 (3)	0.0643 (2)	0.0163 (7)
C23	0.3904 (4)	0.2372 (3)	0.1373 (2)	0.0200 (8)
C31	−0.2408 (4)	0.2123 (3)	−0.0468 (2)	0.0183 (8)
C32	−0.0855 (4)	0.3708 (3)	−0.0796 (2)	0.0182 (8)
C33	−0.2401 (4)	0.3394 (3)	−0.0739 (2)	0.0209 (8)
N11	0.1550 (3)	0.0229 (2)	−0.09019 (15)	0.0142 (6)
N12	0.2121 (3)	0.1422 (2)	−0.10577 (15)	0.0135 (6)
N21	0.1868 (3)	0.1328 (2)	0.07567 (16)	0.0154 (6)
N22	0.2318 (3)	0.2345 (2)	0.02865 (16)	0.0139 (6)
N31	−0.0963 (3)	0.1681 (2)	−0.03537 (16)	0.0143 (6)
N32	0.0001 (3)	0.2665 (2)	−0.05655 (16)	0.0141 (6)
O10	−0.0946 (3)	0.3534 (2)	0.13793 (16)	0.0265 (6)
Cl1	0.38445 (10)	0.47169 (6)	−0.14522 (5)	0.0183 (2)
Cu1	0.0000	0.0000	0.0000	0.01293 (17)
H1	0.214 (3)	0.329 (3)	−0.0776 (17)	0.008 (7)*
H10	−0.170 (5)	0.390 (3)	0.132 (2)	0.031 (13)*
H10A	−0.138 (8)	0.321 (6)	0.254 (4)	0.14 (3)*
H10B	−0.018 (5)	0.434 (4)	0.243 (3)	0.050 (12)*
H10C	0.036 (7)	0.293 (5)	0.229 (3)	0.11 (2)*
H11	0.205 (4)	−0.141 (3)	−0.1439 (19)	0.021 (9)*
H12	0.366 (4)	0.207 (3)	−0.181 (2)	0.020 (9)*

H13	0.396 (4)	−0.016 (3)	−0.2311 (19)	0.015 (9)*
H21	0.280 (4)	0.074 (3)	0.185 (2)	0.021 (9)*
H22	0.397 (4)	0.370 (3)	0.0392 (18)	0.017 (8)*
H23	0.468 (4)	0.258 (3)	0.173 (2)	0.029 (10)*
H31	−0.331 (4)	0.159 (3)	−0.038 (2)	0.029 (10)*
H32	−0.027 (4)	0.444 (3)	−0.0968 (18)	0.010 (8)*
H33	−0.334 (4)	0.391 (3)	−0.0892 (19)	0.023 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.013 (2)	0.0095 (15)	0.0171 (17)	−0.0023 (13)	0.0011 (14)	0.0012 (13)
C10	0.041 (3)	0.040 (2)	0.040 (3)	0.008 (2)	−0.015 (2)	−0.006 (2)
C11	0.018 (2)	0.0151 (16)	0.0214 (19)	0.0027 (14)	0.0051 (15)	−0.0027 (14)
C12	0.018 (2)	0.0179 (17)	0.0165 (18)	0.0002 (14)	0.0068 (15)	0.0042 (13)
C13	0.020 (2)	0.0203 (17)	0.0194 (18)	0.0031 (15)	0.0116 (16)	−0.0001 (15)
C21	0.018 (2)	0.0168 (16)	0.0159 (18)	−0.0037 (14)	0.0023 (15)	0.0014 (13)
C22	0.015 (2)	0.0128 (16)	0.0215 (18)	−0.0038 (14)	0.0059 (15)	−0.0021 (13)
C23	0.017 (2)	0.0245 (17)	0.0189 (19)	−0.0029 (15)	−0.0024 (16)	−0.0042 (15)
C31	0.014 (2)	0.0191 (16)	0.0220 (19)	0.0024 (15)	0.0014 (15)	−0.0013 (14)
C32	0.028 (2)	0.0092 (15)	0.0175 (17)	0.0017 (14)	0.0008 (15)	0.0029 (13)
C33	0.016 (2)	0.0179 (16)	0.029 (2)	0.0073 (15)	0.0013 (16)	0.0046 (15)
N11	0.0165 (17)	0.0097 (12)	0.0166 (14)	−0.0024 (11)	0.0029 (12)	0.0037 (10)
N12	0.0163 (17)	0.0104 (12)	0.0140 (14)	−0.0027 (11)	0.0043 (12)	0.0015 (10)
N21	0.0144 (17)	0.0157 (13)	0.0160 (14)	−0.0033 (11)	0.0015 (12)	0.0017 (11)
N22	0.0144 (16)	0.0096 (12)	0.0180 (15)	−0.0020 (11)	0.0035 (12)	0.0028 (11)
N31	0.0098 (17)	0.0117 (12)	0.0216 (15)	−0.0038 (11)	0.0041 (12)	0.0020 (11)
N32	0.0119 (17)	0.0114 (12)	0.0191 (15)	0.0014 (11)	0.0029 (12)	0.0013 (11)
O10	0.0262 (18)	0.0226 (13)	0.0306 (15)	0.0054 (12)	−0.0027 (13)	−0.0015 (11)
Cl1	0.0164 (5)	0.0161 (4)	0.0225 (4)	−0.0028 (3)	0.0027 (4)	0.0023 (3)
Cu1	0.0121 (3)	0.0095 (3)	0.0174 (3)	0.0000 (2)	0.0042 (2)	0.0027 (2)

Geometric parameters (Å, °)

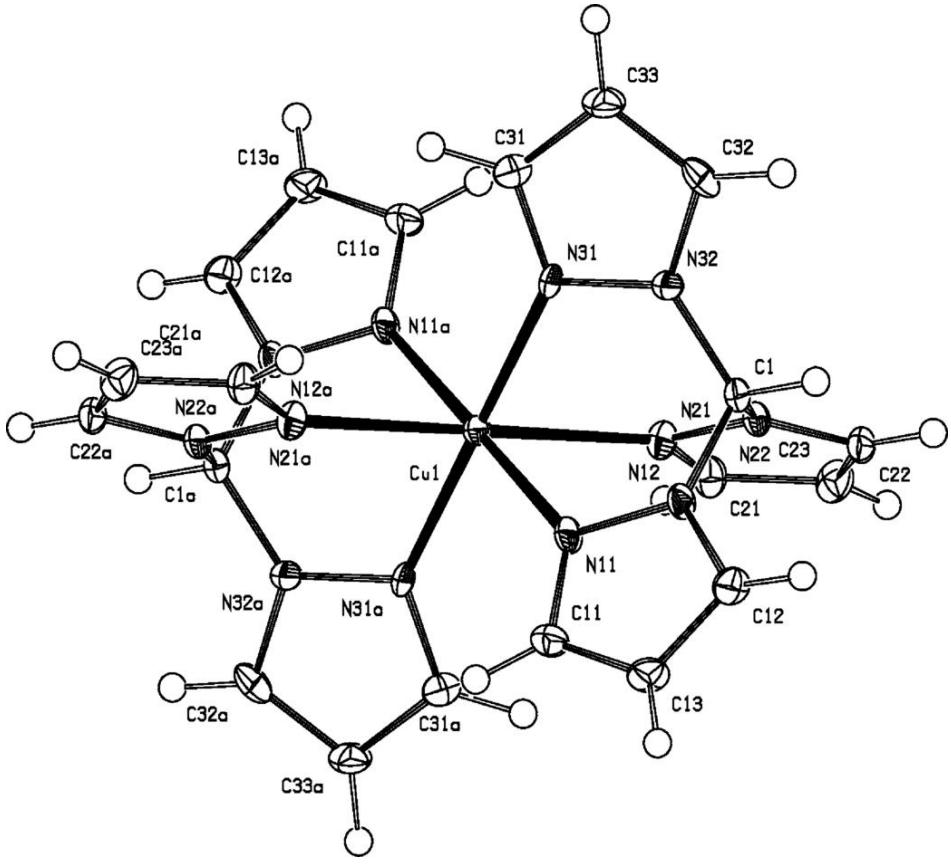
C1—N32	1.438 (4)	C22—H22	0.93 (3)
C1—N22	1.440 (4)	C23—H23	0.89 (4)
C1—N12	1.454 (4)	C31—N31	1.321 (4)
C1—H1	0.99 (3)	C31—C33	1.396 (4)
C10—O10	1.411 (5)	C31—H31	0.96 (3)
C10—H10A	0.98 (7)	C32—N32	1.355 (4)
C10—H10B	0.99 (4)	C32—C33	1.361 (5)
C10—H10C	0.91 (6)	C32—H32	0.96 (3)
C11—N11	1.329 (4)	C33—H33	0.98 (3)
C11—C13	1.382 (5)	N11—N12	1.362 (3)
C11—H11	0.93 (3)	N11—Cu1	2.002 (3)
C12—N12	1.352 (4)	N21—N22	1.364 (3)
C12—C13	1.358 (4)	N21—Cu1	2.413 (2)
C12—H12	0.86 (3)	N31—N32	1.363 (3)
C13—H13	0.92 (3)	N31—Cu1	2.011 (2)

C21—N21	1.316 (4)	O10—H10	0.76 (4)
C21—C23	1.401 (4)	Cu1—N11^{i}	2.002 (3)
C21—H21	0.95 (3)	Cu1—N31^{i}	2.011 (2)
C22—N22	1.357 (4)	Cu1—N21^{i}	2.413 (2)
C22—C23	1.357 (5)		
N32—C1—N22	112.5 (3)	C32—C33—H33	128.9 (18)
N32—C1—N12	110.4 (2)	C31—C33—H33	125.7 (18)
N22—C1—N12	110.0 (2)	C11—N11—N12	104.7 (2)
N32—C1—H1	107.5 (17)	C11—N11—Cu1	136.0 (2)
N22—C1—H1	107.7 (16)	N12—N11—Cu1	119.17 (18)
N12—C1—H1	108.6 (16)	C12—N12—N11	110.9 (2)
O10—C10—H10A	108 (4)	C12—N12—C1	128.2 (2)
O10—C10—H10B	110 (2)	N11—N12—C1	120.5 (2)
H10A—C10—H10B	106 (4)	C21—N21—N22	104.4 (2)
O10—C10—H10C	110 (4)	C21—N21—Cu1	143.5 (2)
H10A—C10—H10C	113 (5)	N22—N21—Cu1	110.92 (18)
H10B—C10—H10C	109 (4)	C22—N22—N21	111.6 (3)
N11—C11—C13	111.5 (3)	C22—N22—C1	127.3 (3)
N11—C11—H11	120 (2)	N21—N22—C1	120.1 (2)
C13—C11—H11	129 (2)	C31—N31—N32	105.5 (2)
N12—C12—C13	107.3 (3)	C31—N31—Cu1	135.5 (2)
N12—C12—H12	121 (2)	N32—N31—Cu1	118.98 (19)
C13—C12—H12	132 (2)	C32—N32—N31	110.5 (3)
C12—C13—C11	105.6 (3)	C32—N32—C1	128.8 (3)
C12—C13—H13	126.0 (19)	N31—N32—C1	120.7 (2)
C11—C13—H13	128.4 (19)	C10—O10—H10	112 (3)
N21—C21—C23	111.9 (3)	N11—Cu1—N11^{i}	180.00 (14)
N21—C21—H21	123 (2)	N11—Cu1—N31	87.82 (10)
C23—C21—H21	125 (2)	N11^{i}—Cu1—N31	92.18 (10)
N22—C22—C23	106.8 (3)	N11—Cu1—N31^{i}	92.18 (10)
N22—C22—H22	120.5 (19)	N11^{i}—Cu1—N31^{i}	87.82 (10)
C23—C22—H22	132.6 (19)	N31—Cu1—N31^{i}	180.00 (15)
C22—C23—C21	105.2 (3)	N11—Cu1—N21	81.95 (9)
C22—C23—H23	126 (2)	N11^{i}—Cu1—N21	98.05 (9)
C21—C23—H23	129 (2)	N31—Cu1—N21	84.24 (9)
N31—C31—C33	111.3 (3)	N31^{i}—Cu1—N21	95.76 (9)
N31—C31—H31	121 (2)	N11—Cu1—N21^{i}	98.05 (9)
C33—C31—H31	127 (2)	N11^{i}—Cu1—N21^{i}	81.95 (9)
N32—C32—C33	107.6 (3)	N31—Cu1—N21^{i}	95.76 (9)
N32—C32—H32	116.0 (18)	N31^{i}—Cu1—N21^{i}	84.24 (9)
C33—C32—H32	136.4 (18)	N21—Cu1—N21^{i}	180.00 (14)
C32—C33—C31	105.2 (3)		
N12—C12—C13—C11	−1.2 (4)	C31—N31—N32—C1	−177.7 (3)
N11—C11—C13—C12	0.6 (4)	Cu1—N31—N32—C1	0.6 (3)
N22—C22—C23—C21	1.0 (4)	N22—C1—N32—C32	114.0 (3)

N21—C21—C23—C22	−0.2 (4)	N12—C1—N32—C32	−122.7 (3)
N32—C32—C33—C31	−0.2 (4)	N22—C1—N32—N31	−67.7 (3)
N31—C31—C33—C32	0.8 (4)	N12—C1—N32—N31	55.6 (3)
C13—C11—N11—N12	0.2 (4)	C11—N11—Cu1—N11^{i}	22 (5)
C13—C11—N11—Cu1	−177.0 (2)	N12—N11—Cu1—N11^{i}	−155 (5)
C13—C12—N12—N11	1.4 (4)	C11—N11—Cu1—N31	−145.0 (3)
C13—C12—N12—C1	174.0 (3)	N12—N11—Cu1—N31	38.1 (2)
C11—N11—N12—C12	−1.0 (3)	C11—N11—Cu1—N31^{i}	35.0 (3)
Cu1—N11—N12—C12	176.8 (2)	N12—N11—Cu1—N31^{i}	−141.9 (2)
C11—N11—N12—C1	−174.2 (3)	C11—N11—Cu1—N21	130.5 (3)
Cu1—N11—N12—C1	3.5 (4)	N12—N11—Cu1—N21	−46.4 (2)
N32—C1—N12—C12	129.8 (3)	C11—N11—Cu1—N21^{i}	−49.5 (3)
N22—C1—N12—C12	−105.5 (3)	N12—N11—Cu1—N21^{i}	133.6 (2)
N32—C1—N12—N11	−58.3 (3)	C31—N31—Cu1—N11	137.2 (3)
N22—C1—N12—N11	66.4 (3)	N32—N31—Cu1—N11	−40.4 (2)
C23—C21—N21—N22	−0.6 (3)	C31—N31—Cu1—N11^{i}	−42.8 (3)
C23—C21—N21—Cu1	164.7 (3)	N32—N31—Cu1—N11^{i}	139.6 (2)
C23—C22—N22—N21	−1.4 (4)	C31—N31—Cu1—N31^{i}	−14 (25)
C23—C22—N22—C1	−169.9 (3)	N32—N31—Cu1—N31^{i}	169 (25)
C21—N21—N22—C22	1.2 (3)	C31—N31—Cu1—N21	−140.7 (3)
Cu1—N21—N22—C22	−169.5 (2)	N32—N31—Cu1—N21	41.7 (2)
C21—N21—N22—C1	170.6 (3)	C31—N31—Cu1—N21^{i}	39.3 (3)
Cu1—N21—N22—C1	0.0 (3)	N32—N31—Cu1—N21^{i}	−138.3 (2)
N32—C1—N22—C22	−131.0 (3)	C21—N21—Cu1—N11	−118.9 (4)
N12—C1—N22—C22	105.5 (3)	N22—N21—Cu1—N11	45.76 (19)
N32—C1—N22—N21	61.4 (3)	C21—N21—Cu1—N11^{i}	61.1 (4)
N12—C1—N22—N21	−62.1 (4)	N22—N21—Cu1—N11^{i}	−134.24 (19)
C33—C31—N31—N32	−1.0 (4)	C21—N21—Cu1—N31	152.5 (4)
C33—C31—N31—Cu1	−178.9 (2)	N22—N21—Cu1—N31	−42.85 (19)
C33—C32—N32—N31	−0.5 (4)	C21—N21—Cu1—N31^{i}	−27.5 (4)
C33—C32—N32—C1	178.0 (3)	N22—N21—Cu1—N31^{i}	137.15 (19)
C31—N31—N32—C32	0.9 (3)	C21—N21—Cu1—N21^{i}	−1.5 (4)
Cu1—N31—N32—C32	179.2 (2)	N22—N21—Cu1—N21^{i}	163.16 (15)

Symmetry codes: (i) −*x*, −*y*, −*z*.

Fig. 1


C33
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N21
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N31a
C11
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