

Poly[(2,2'-bipyridyl)- μ_3 -cyanido-di- μ_2 -cyanido-dicopper(I,II)]

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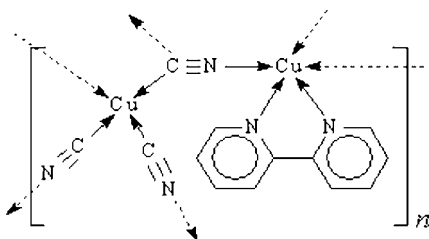
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.031; wR factor = 0.081; data-to-parameter ratio = 15.9.

The title compound, $[\text{Cu}_2(\text{CN})_3(\text{C}_{10}\text{H}_8\text{N}_2)]_n$, crystallizes as a cyanido-bridged three-dimensional polymeric structure, where there coexist Cu^{I} and Cu^{II} ions along with μ_3 - and μ_2 -bridging cyanide groups. Each Cu^{I} ion is coordinated by four C atoms [$\text{Cu}-\text{C} = 1.956(3)$ – $2.147(3)$ Å] from two μ_3 - and two μ_2 -cyanide groups in a tetrahedral environment. The Cu^{II} ion is coordinated by two N atoms from the 2,2'-bipyridyl ligand and three N atoms from one μ_3 - and two μ_2 -cyanide groups in a square-pyramidal geometry [$\text{Cu}-\text{N} = 1.967(3)$ – $2.183(3)$ Å]. The Cu^{I} ions are paired by two C atoms from two cyanide groups into a dinuclear unit with a short $\text{Cu}^{\text{I}} \cdots \text{Cu}^{\text{I}}$ distance of $2.5398(8)$ Å. Each dinuclear unit links six Cu^{II} ions by four μ_2 - and two μ_3 -cyanide groups to form a 4,6-connected framework, with $\text{Cu}^{\text{I}} \cdots \text{Cu}^{\text{II}}$ separations ranging from $4.864(4)$ to $5.252(4)$ Å.

Related literature

For related crystal structures, see: Chesnut & Zubieta (1998); He *et al.* (2005); Mao *et al.* (2005); Yan *et al.* (2006).



Experimental

Crystal data

$[\text{Cu}_2(\text{CN})_3(\text{C}_{10}\text{H}_8\text{N}_2)]$
 $M_r = 361.32$
 Monoclinic, $P2_1/n$
 $a = 8.3009(17)$ Å
 $b = 13.972(3)$ Å
 $c = 10.814(2)$ Å
 $\beta = 90.27(3)^\circ$

$V = 1254.2(4)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 3.39$ mm⁻¹
 $T = 293(2)$ K
 $0.10 \times 0.08 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\text{min}} = 0.948$, $T_{\text{max}} = 1.000$
 (expected range = 0.723–0.763)

12108 measured reflections
 2869 independent reflections
 2458 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.081$
 $S = 1.09$
 2869 reflections

181 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.50$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.60$ e Å⁻³

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); 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: CV2355).

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supplementary materials

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Poly[(2,2'-bipyridyl)- μ_3 -cyanido-di- μ_2 -cyanido-dicopper(I,II)]

Y. Rui and M. Lu

Comment

The crystal structures of some cyano-bridged Cu^I or Cu^{II} complexes with 2,2'-bipyridyl as co-ligand have been reported, such as catena-[(μ_2 -cyano)-bis(2,2'-bipyridyl)-copper(I)] hexakis[(μ_2 -cyano)-penta-copper(I)] (Chesnut & Zubietta, 1998); catena-[(μ_2 -cyano)-(2,2'-bipyridyl)-copper(I)] (He et al., 2005, Mao et al., 2005) and catena-[(μ_2 -cyano)-bis(2,2'-bipyridyl)-cyano-copper(II)] (Yan et al., 2006). In such complexes, one type of Cu ion either Cu^I or Cu^{II} appeared, and the cyano groups adopted only μ_2 bridging mode. Herein, we report a new three-dimensional polymeric Cu complex, C₁₃H₈Cu₂N₅ (I), in which there exist both Cu^I and Cu^{II} ions, and μ_3 - and μ_2 - coordination cyano groups.

As shown in Fig. 1, the Cu^I ion [Cu1] is coordinated to four C atoms from two μ_3 - and two μ_2 -cyano groups, respectively, in a tetrahedral environment. The Cu^{II} ion [Cu2] coordinates with two N atoms of one 2,2'-bipyridyl ligand, one μ_3 - and two μ_2 -cyano N atoms in a square-pyramidal geometry. In the structure, each two Cu^I atoms [Cu1 and Cu1A] are bridged by two μ_2 -C atoms of μ_3 - cyano groups to form a dinuclear unit with a Cu—Cu distance of 2.5398 (8) Å. Each such dinuclear unit is further linked to six Cu^{II} ions by four μ_2 - and two μ_3 -cyano groups, to give a 4,6-connected framework, with the Cu^I—Cu^{II} separations of 4.864 (4) Å for Cu1—Cu2, 4.963 (4) Å for Cu1B—Cu2, 5.010 (4) Å for Cu1C—Cu2 and 5.252 (4) Å for Cu1A—Cu2, corresponding to Fig. 1.

Experimental

CuCl₂·2H₂O (34 mg, 0.2 mmol), 2,2'-bipyridine (31 mg, 0.2 mmol) and cyanoacetic acid (51 mg, 0.6 mmol) were dissolved in ammonium hydroxide (20%, 10 ml). The solution was filtered and the filtrate was allowed to stand for about 30 days. Black crystals of (I) were isolated in about 20% yield with respect to Cu. The cyano groups and Cu^I ions in the product come from the in situ decomposition of cyanoacetic acid and the reduction of Cu^{II} ions, respectively.

Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Figures

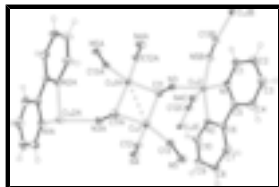


Fig. 1. A portion of the polymeric network in (I), showing the atomic numbering and 30% probability displacement ellipsoids [symmetry codes: (A) $-x, 1 - y, 1 - z$; (B) $1/2 - x, 1/2 + y, 3/2 - z$; (C) $1 - x, 1 - y, 1 - z$].

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Crystal data

[Cu₂(CN)₃(C₁₀H₈N₂)]

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Hall symbol: $-P\ 2_1n$

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$b = 13.972$ (3) Å

$c = 10.814$ (2) Å

$\beta = 90.27$ (3)°

$V = 1254.2$ (4) Å³

$Z = 4$

$F_{000} = 716$

$D_x = 1.914$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 10053 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 3.39$ mm⁻¹

$T = 293$ (2) K

Block, black

$0.10 \times 0.08 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

φ and ω scan

Absorption correction: multi-scan (SADABS; Bruker, 1998)

$T_{\min} = 0.948$, $T_{\max} = 1.000$

12108 measured reflections

2869 independent reflections

2458 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 3.1$ °

$h = -10 \rightarrow 10$

$k = -17 \rightarrow 18$

$l = -13 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.081$

$S = 1.09$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 1.8789P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

2869 reflections $\Delta\rho_{\max} = 0.50 \text{ e } \text{\AA}^{-3}$
 181 parameters $\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$
 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.07091 (5)	0.42052 (3)	0.51708 (3)	0.02646 (11)
Cu2	0.44880 (5)	0.61074 (3)	0.75886 (3)	0.02377 (11)
N1	0.3200 (3)	0.57131 (19)	0.9116 (2)	0.0273 (6)
N2	0.4729 (3)	0.46640 (18)	0.7511 (2)	0.0272 (6)
N3	0.2456 (4)	0.59756 (19)	0.6310 (3)	0.0322 (6)
C12	0.2496 (4)	0.3838 (2)	0.4065 (3)	0.0282 (7)
C13	0.0437 (4)	0.3177 (2)	0.6380 (3)	0.0293 (7)
C1	0.2443 (4)	0.6312 (3)	0.9891 (3)	0.0356 (8)
H1A	0.2484	0.6967	0.9738	0.043*
C2	0.1606 (4)	0.5987 (3)	1.0907 (3)	0.0402 (9)
H2A	0.1075	0.6415	1.1423	0.048*
C3	0.1570 (5)	0.5032 (3)	1.1144 (3)	0.0431 (9)
H3A	0.1024	0.4801	1.1830	0.052*
C4	0.2352 (5)	0.4403 (3)	1.0356 (3)	0.0401 (8)
H4A	0.2345	0.3749	1.0511	0.048*
C5	0.3145 (4)	0.4766 (2)	0.9334 (3)	0.0282 (7)
C6	0.3988 (4)	0.4166 (2)	0.8423 (3)	0.0269 (6)
C7	0.4030 (5)	0.3175 (2)	0.8446 (3)	0.0374 (8)
H7A	0.3535	0.2841	0.9083	0.045*
C8	0.4813 (5)	0.2692 (2)	0.7519 (4)	0.0428 (9)
H8A	0.4853	0.2027	0.7525	0.051*
C9	0.5534 (5)	0.3196 (3)	0.6583 (4)	0.0422 (9)
H9A	0.6056	0.2880	0.5944	0.051*
C10	0.5469 (5)	0.4182 (2)	0.6612 (3)	0.0382 (8)
H10A	0.5960	0.4525	0.5980	0.046*
C11	0.1443 (4)	0.5593 (2)	0.5813 (3)	0.0313 (7)
N4	0.3625 (4)	0.37243 (19)	0.3484 (3)	0.0338 (6)
N5	0.0438 (4)	0.2456 (2)	0.6877 (3)	0.0350 (7)

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0284 (2)	0.0192 (2)	0.0318 (2)	0.00216 (15)	0.00388 (15)	0.00332 (14)
Cu2	0.0269 (2)	0.01838 (19)	0.02610 (19)	-0.00175 (14)	0.00628 (14)	-0.00388 (13)
N1	0.0273 (14)	0.0282 (14)	0.0262 (13)	-0.0015 (11)	0.0030 (10)	-0.0018 (10)
N2	0.0318 (15)	0.0206 (13)	0.0292 (13)	-0.0009 (11)	0.0045 (11)	-0.0020 (10)
N3	0.0315 (15)	0.0267 (14)	0.0383 (15)	0.0014 (12)	-0.0078 (12)	-0.0078 (11)
C12	0.0302 (17)	0.0217 (15)	0.0329 (16)	-0.0012 (13)	0.0062 (13)	-0.0025 (12)
C13	0.0328 (18)	0.0245 (16)	0.0308 (16)	0.0033 (13)	0.0085 (13)	0.0019 (13)
C1	0.0350 (19)	0.0338 (19)	0.0380 (18)	0.0014 (15)	0.0076 (14)	-0.0052 (14)
C2	0.0316 (19)	0.058 (2)	0.0308 (17)	0.0021 (17)	0.0095 (14)	-0.0071 (16)
C3	0.037 (2)	0.062 (3)	0.0303 (18)	-0.0030 (18)	0.0115 (15)	0.0063 (16)
C4	0.041 (2)	0.042 (2)	0.0374 (19)	-0.0071 (16)	0.0013 (15)	0.0112 (15)
C5	0.0250 (16)	0.0316 (17)	0.0281 (16)	-0.0021 (13)	-0.0007 (12)	-0.0004 (12)
C6	0.0262 (16)	0.0259 (16)	0.0286 (15)	-0.0036 (12)	-0.0019 (12)	0.0006 (12)
C7	0.045 (2)	0.0251 (18)	0.0423 (19)	-0.0033 (15)	0.0011 (16)	0.0067 (14)
C8	0.055 (2)	0.0163 (16)	0.057 (2)	0.0014 (15)	-0.0017 (18)	-0.0020 (15)
C9	0.051 (2)	0.0264 (18)	0.049 (2)	0.0051 (16)	0.0104 (17)	-0.0089 (15)
C10	0.048 (2)	0.0252 (17)	0.0418 (19)	-0.0012 (15)	0.0150 (16)	-0.0041 (14)
C11	0.0291 (17)	0.0346 (18)	0.0302 (16)	-0.0008 (14)	0.0058 (13)	-0.0047 (13)
N4	0.0359 (16)	0.0244 (14)	0.0411 (16)	-0.0030 (12)	0.0109 (13)	-0.0021 (11)
N5	0.0423 (17)	0.0266 (15)	0.0361 (15)	0.0041 (12)	0.0131 (12)	0.0059 (11)

Geometric parameters (\AA , $^\circ$)

Cu1—C11 ⁱ	2.094 (4)	C2—C3	1.359 (6)
Cu1—C11	2.147 (3)	C2—H2A	0.9300
Cu1—C12	1.977 (3)	C3—C4	1.387 (5)
Cu1—C13	1.956 (3)	C3—H3A	0.9300
Cu1—Cu1 ⁱ	2.5398 (8)	C4—C5	1.385 (5)
Cu2—N1	2.047 (3)	C4—H4A	0.9300
Cu2—N2	2.028 (3)	C5—C6	1.473 (4)
Cu2—N3	2.183 (3)	C6—C7	1.385 (5)
Cu2—N4 ⁱⁱ	1.967 (3)	C7—C8	1.375 (5)
Cu2—N5 ⁱⁱⁱ	1.972 (3)	C7—H7A	0.9300
N1—C1	1.343 (4)	C8—C9	1.373 (5)
N1—C5	1.344 (4)	C8—H8A	0.9300
N2—C10	1.335 (4)	C9—C10	1.379 (5)
N2—C6	1.357 (4)	C9—H9A	0.9300
N3—C11	1.131 (4)	C10—H10A	0.9300
C12—N4	1.143 (4)	C11—Cu1 ⁱ	2.094 (4)
C13—N5	1.142 (4)	N4—Cu2 ⁱⁱ	1.967 (3)
C1—C2	1.380 (5)	N5—Cu2 ^{iv}	1.972 (3)
C1—H1A	0.9300		
C13—Cu1—C12	107.62 (13)	C2—C1—H1A	119.0

C13—Cu1—C11 ⁱ	109.73 (14)	C3—C2—C1	119.0 (3)
C12—Cu1—C11 ⁱ	111.61 (13)	C3—C2—H2A	120.5
C13—Cu1—C11	118.70 (13)	C1—C2—H2A	120.5
C12—Cu1—C11	102.58 (13)	C2—C3—C4	119.7 (3)
C11 ⁱ —Cu1—C11	106.44 (11)	C2—C3—H3A	120.2
C13—Cu1—Cu1 ⁱ	133.18 (10)	C4—C3—H3A	120.2
C12—Cu1—Cu1 ⁱ	119.19 (9)	C5—C4—C3	118.9 (3)
C11 ⁱ —Cu1—Cu1 ⁱ	54.18 (9)	C5—C4—H4A	120.5
C11—Cu1—Cu1 ⁱ	52.25 (10)	C3—C4—H4A	120.5
N4 ⁱⁱ —Cu2—N5 ⁱⁱⁱ	92.00 (11)	N1—C5—C4	121.1 (3)
N4 ⁱⁱ —Cu2—N2	90.89 (11)	N1—C5—C6	115.2 (3)
N5 ⁱⁱⁱ —Cu2—N2	163.61 (12)	C4—C5—C6	123.6 (3)
N4 ⁱⁱ —Cu2—N1	158.12 (12)	N2—C6—C7	121.0 (3)
N5 ⁱⁱⁱ —Cu2—N1	92.08 (11)	N2—C6—C5	114.4 (3)
N2—Cu2—N1	79.50 (10)	C7—C6—C5	124.7 (3)
N4 ⁱⁱ —Cu2—N3	104.58 (12)	C8—C7—C6	119.3 (3)
N5 ⁱⁱⁱ —Cu2—N3	106.79 (12)	C8—C7—H7A	120.3
N2—Cu2—N3	88.05 (11)	C6—C7—H7A	120.3
N1—Cu2—N3	94.78 (11)	C9—C8—C7	119.6 (3)
Cu1 ⁱ —C11—Cu1	73.56 (11)	C9—C8—H8A	120.2
C1—N1—C5	119.2 (3)	C7—C8—H8A	120.2
C1—N1—Cu2	125.7 (2)	C8—C9—C10	118.6 (3)
C5—N1—Cu2	115.1 (2)	C8—C9—H9A	120.7
C10—N2—C6	118.9 (3)	C10—C9—H9A	120.7
C10—N2—Cu2	125.3 (2)	N2—C10—C9	122.6 (3)
C6—N2—Cu2	115.8 (2)	N2—C10—H10A	118.7
C11—N3—Cu2	155.8 (3)	C9—C10—H10A	118.7
N4—C12—Cu1	171.4 (3)	N3—C11—Cu1 ⁱ	144.0 (3)
N5—C13—Cu1	164.3 (3)	N3—C11—Cu1	142.2 (3)
N1—C1—C2	122.0 (3)	C12—N4—Cu2 ⁱⁱ	164.9 (3)
N1—C1—H1A	119.0	C13—N5—Cu2 ^{iv}	168.8 (3)
N4 ⁱⁱ —Cu2—N1—C1	115.0 (4)	Cu2—N1—C5—C4	178.2 (3)
N5 ⁱⁱⁱ —Cu2—N1—C1	14.4 (3)	C1—N1—C5—C6	179.1 (3)
N2—Cu2—N1—C1	-179.7 (3)	Cu2—N1—C5—C6	-1.4 (4)
N3—Cu2—N1—C1	-92.6 (3)	C3—C4—C5—N1	1.7 (5)
N4 ⁱⁱ —Cu2—N1—C5	-64.5 (4)	C3—C4—C5—C6	-178.8 (3)
N5 ⁱⁱⁱ —Cu2—N1—C5	-165.1 (2)	C10—N2—C6—C7	1.7 (5)
N2—Cu2—N1—C5	0.7 (2)	Cu2—N2—C6—C7	178.2 (3)
N3—Cu2—N1—C5	87.8 (2)	C10—N2—C6—C5	-177.3 (3)
N4 ⁱⁱ —Cu2—N2—C10	-23.5 (3)	Cu2—N2—C6—C5	-0.8 (3)
N5 ⁱⁱⁱ —Cu2—N2—C10	-123.7 (4)	N1—C5—C6—N2	1.4 (4)
N1—Cu2—N2—C10	176.3 (3)	C4—C5—C6—N2	-178.1 (3)
N3—Cu2—N2—C10	81.0 (3)	N1—C5—C6—C7	-177.5 (3)
N4 ⁱⁱ —Cu2—N2—C6	160.3 (2)	C4—C5—C6—C7	3.0 (5)

supplementary materials

N5 ⁱⁱⁱ —Cu2—N2—C6	60.2 (5)	N2—C6—C7—C8	-1.1 (5)
N1—Cu2—N2—C6	0.1 (2)	C5—C6—C7—C8	177.8 (3)
N3—Cu2—N2—C6	-95.1 (2)	C6—C7—C8—C9	-0.2 (6)
N4 ⁱⁱ —Cu2—N3—C11	110.5 (7)	C7—C8—C9—C10	0.8 (6)
N5 ⁱⁱⁱ —Cu2—N3—C11	-152.8 (7)	C6—N2—C10—C9	-1.1 (6)
N2—Cu2—N3—C11	20.1 (7)	Cu2—N2—C10—C9	-177.1 (3)
N1—Cu2—N3—C11	-59.2 (7)	C8—C9—C10—N2	-0.2 (6)
C12—Cu1—C13—N5	-24.5 (12)	Cu2—N3—C11—Cu1 ⁱ	160.3 (4)
C11 ⁱ —Cu1—C13—N5	97.1 (12)	Cu2—N3—C11—Cu1	-28.0 (10)
C11—Cu1—C13—N5	-140.2 (12)	C13—Cu1—C11—N3	60.8 (5)
Cu1 ⁱ —Cu1—C13—N5	156.1 (11)	C12—Cu1—C11—N3	-57.6 (5)
C5—N1—C1—C2	-0.1 (5)	C11 ⁱ —Cu1—C11—N3	-175.0 (5)
Cu2—N1—C1—C2	-179.6 (3)	Cu1 ⁱ —Cu1—C11—N3	-175.0 (5)
N1—C1—C2—C3	1.2 (6)	C13—Cu1—C11—Cu1 ⁱ	-124.25 (13)
C1—C2—C3—C4	-0.8 (6)	C12—Cu1—C11—Cu1 ⁱ	117.34 (12)
C2—C3—C4—C5	-0.6 (6)	C11 ⁱ —Cu1—C11—Cu1 ⁱ	0.0
C1—N1—C5—C4	-1.4 (5)	Cu1—C13—N5—Cu2 ^{iv}	-16 (3)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1/2, y+1/2, -z+3/2$; (iv) $-x+1/2, y-1/2, -z+3/2$.

