Crystal structure of *catena*-poly[[[(2-ethoxypyrazine-κN)copper(I)]-di-μ_2-cyanido] [copper(I)-μ_2-cyanido]]

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In the asymmetric unit of the title coordination compound, $\{[Cu(CN)(C_4H_3\text{-}OC_2H_5N_2)][Cu(CN)]\}_n$, there are two Cu atoms with different coordination environments. One Cu^I ion is coordinated in a triangular coordination geometry by the N atom of the 2-ethoxypyrazine molecule and by two bridging cyanide ligands, equally disordered over two sites exchanging C and N atoms, thus forming polymeric chains parallel to the *c* axis. The other Cu atom is connected to two bridging cyanide groups disordered over two sites with an occupancy of 0.5 for each C and N atom, and forming an almost linear polymeric chain parallel to the *b* axis. In the crystal, the two types of chain, which are orthogonal to each other, are connected by cuprophilic Cu···Cu interactions [2.7958 (13) Å], forming two-dimensional metal–organic coordination layers parallel to the *bc* plane. The coordination framework is further stabilized by weak long-range (electrostatic type) C—H···π interactions between cyano groups and 2-ethoxypyrazine rings.

1. Chemical context

The design and synthesis of coordination polymers has received much attention in the field of inorganic chemistry due to their structural features, as well as their potential applications in catalysis, adsorption, luminescence and as chemical sensors (Li *et al.*, 2012; Czaja *et al.*, 2009; Etaiw *et al.*, 2016; Ley *et al.*, 2010). Complexes with the cyano group, which is one of the important bridging and assembling ligands acting as a monodentate, bidentate or tridentate ligand, are the subject of much interest (Ley *et al.*, 2010). Different types of metal cyanides with building blocks from linear $M(CN)_2$ (Okabayashi *et al.*, 2009), trigonal $M(CN)_3$ (Su *et al.*, 2011), tetrahedral $M(CN)_4$ (Jószai *et al.*, 2005) to high connected $M(CN)_7$ (Qian *et al.*, 2013) and $M(CN)_8$ (Chorazy *et al.*, 2013) units have been reported with various metal ions. Among the large number of various metal cyanides, copper(I) cyanide complexes are very important in organic, organometallic and supramolecular chemistry because of both the copper centre, which possesses several coordination modes (two-, three-, four-, five- or six-coordinate) and can form diverse geometries, and the versatile cyanide ligand (Pike, 2012). In general, the crystallochemistry of Cu^ICN systems is highly complex and provides several recurrent structural motifs: (i) linear chains similar to those of pure CuCN with possible disorder in the cyanide groups; (ii) six CN ligands connected by copper dimers with stoichiometry $Cu_2(1,1,2\text{-}\mu_3\text{-}CN)_2(CN)_4$ and Cu···Cu distances typical of cuprophilic interactions; (iii) $(CuCN)_x$ rings with square, pentagonal or hexagonal geometry
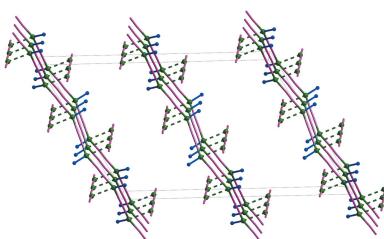
(Grifasi *et al.*, 2016; Pike, 2012). Mixed-valence Cu^{I}/Cu^{II} coordination complexes with cyanide and amine ligands having different supramolecular architectures and their luminescence properties have also been reported (Grifasi *et al.*, 2016). To improve the design of copper cyanide coordination polymers, as well as to investigate its influence on the resulting luminescence and other properties, different types of co-ligands were used, in particular, *N*-donor bridging or chelating ligands, such as 1,10-phenanthroline, 4,4′-bipyridine (Su *et al.*, 2011), pyridines with methyl, ethyl, methoxy and other substituents (Dembo *et al.*, 2010), and pyrazine (Qin *et al.*, 2012; Chesnut *et al.*, 2001) and its derivatives (Chesnut *et al.*, 2001). Here we describe the crystal structure of a new [CuCN]-based metal–organic coordination framework of the general formula $\{[Cu(CN)_2(EtOpz)][CuCN]\}_n$ (where EtOpz is 2-ethoxypyrazine).
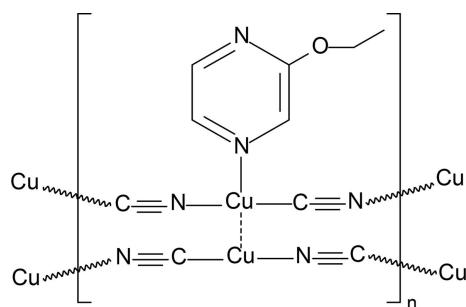
2. Structural commentary

Fig. 1 shows a fragment of the title compound, which is a polymeric copper complex with different coordination envir-

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

Cg is the centroid of the C1/N1–C1^{i}/N1^{i} cyano group [symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$]

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
C8—H8⋯*Cg*	0.93	2.93	3.558 (6)	126

onments of the two crystallographically independent Cu^{I} ions. The Cu1 atom is coordinated to the N atom of a 2-ethoxy-pyrazine molecule [Cu1—N5 = 2.090 (4) Å]. Two other coordination positions are occupied by bridging cyanide groups, which are equally disordered over two sites, exchanging C and N atoms [Cu1—C1/N1 = 1.905 (4) Å and Cu1—C2/N2 = 1.888 (4) Å], thus forming an irregular triangular coordination geometry where the copper ion is displaced from the centre [C2/N2—Cu1—N5 = 108.9 (2)°, C1/N1—Cu1—N5 = 103.2 (2)° and C2/N2—Cu1—C1/N1 = 147.7 (2)°]. The Cu2 atom is coordinated by two cyanide ligands, which are also disordered over two sites with an occupancy of 0.5 for each C and N atom [Cu2—C3/N3 = 1.859 (5) Å and Cu2—C4/N4^{iii} = 1.841 (4) Å; symmetry codes: (i) $-x + 1, y, -z + \frac{1}{2}$; (ii) $-x + 1, -y, -z + 1$; (iii) $x, y - 1, z$] to form an almost linear chain [C4/N4^{iii}—Cu2—C3/N3 = 170.5 (2)°]. The two Cu^{I} centres are connected through a Cu⋯Cu interaction [Cu1—Cu2 = 2.7958 (13) Å] that could be interpreted as a cuprophilic contact (Hermann *et al.*, 2001).

3. Supramolecular features

The crystal packing of the title compound (Fig. 2) consists of two types of orthogonal polymeric chains (the first involving the Cu1 atoms and parallel to the *c* axis and the second involving the Cu2 atoms and parallel to the *b* axis) interconnected by Cu⋯Cu contacts and forming two-dimensional layers parallel to (100). The Cu⋯Cu contacts are almost perpendicular to the [Cu2(CN)] chains [C3/N3—Cu2—Cu1 =


Figure 1
A fragment of the crystal structure of the title compound, with displacement ellipsoids drawn at the 65% probability level [symmetry codes: (i) $-x + 1, y, -z + \frac{1}{2}$; (ii) $-x + 1, -y, -z + 1$; (iii) $x, y - 1, z$]. Four of the cyanide ligands (C1/N1—C1/N1^{i}, C2/N2—C2/N2^{ii}, C3/N3—C4/N4 and C4/N4^{iii}—C3/N3^{iii}) are disordered over two sites with occupancies of 0.5. The Cu⋯Cu contact is shown as a dashed line.
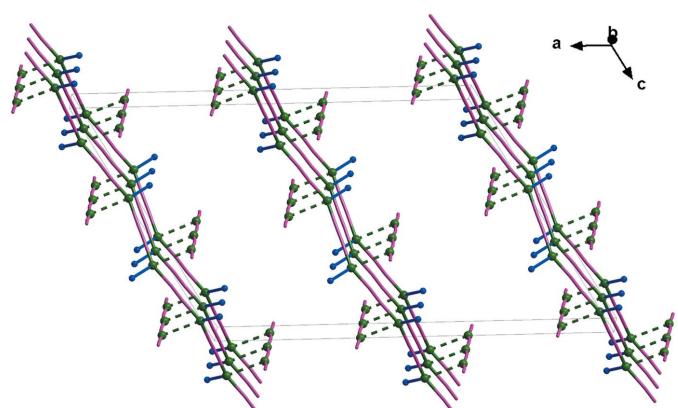
Figure 2
A view normal to the *ac* plane of the crystal structure of the title compound, showing the Cu⋯Cu contacts as dashed lines. 2-Ethoxy-pyrazine rings (except for the N atoms connected to Cu1) and H atoms have been omitted for clarity. Colour code: Cu green, N blue and CN group magenta.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(CN)(C_6H_8N_2O)][Cu(CN)]$
M_r	303.26
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	293
a, b, c (Å)	26.840 (5), 4.830 (1), 18.620 (4)
β (°)	119.91 (3)
V (Å³)	2092.3 (9)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.04
Crystal size (mm)	$0.09 \times 0.04 \times 0.01$
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.630, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12437, 2498, 1396
R_{int}	0.113
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.091, 0.84
No. of reflections	2498
No. of parameters	137
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.72, −0.73

Computer programs: *SAINT* (Bruker, 2013), *APEX2* (Bruker, 2013), *SHELXT* (Sheldrick, 2015a), *SHELXL2017* (Sheldrick, 2015b) and *OLEX2* (Dolomanov et al., 2009).

89.8 (2)° and C4/N4^{iii}—Cu2—Cu1 = 99.7 (2)°]. At the same time, the Cu2 atom occupies an axial position with respect to the triangular $[N(CN)_2]$ coordination environment of Cu1 [C1/N1—Cu1—Cu2 = 70.6 (2)° and C2/N2—Cu1—Cu2 = 87.6 (2)°]. The resulting metal–organic coordination framework is additionally stabilized by weak long-range (electrostatic-type) C—H···π interactions between cyanide groups and 2-ethoxypyrazine rings (Aliev et al., 2015; Table 1). Short Cu2···O1^{iv} contacts of 3.060 (3) Å are also observed [symmetry code: (iv) −x + 1, −y + 1, −z + 1].

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.39, last update November 2017; Groom et al., 2016) confirmed that the structure of the title complex has not been reported previously and revealed for the fragment –C≡N—Cu—C≡N– and an azine ligand attached to Cu (unsubstituted, substituted and fused azines) 128 structures, which are polymeric copper cyanide chains decorated with various co-ligands. Most of these co-ligands are derivatives of pyridine, piperidine, methylenetetramine and piperazine. In particular, the structure of catena-[pentakis(μ_2-cyano)tris(1-phenylpiperazine)pentacopper] (refcode VIYPOK; Pike et al., 2014) contains five independent Cu atoms and five non-symmetrically disordered cyanides, and forms two independent one-dimensional chain sublattices, i.e. (CuCN)(PhPip) and (CuCN)₃(PhPip), associated by Cu···Cu pairwise cupro-

philic interactions, with distances of 2.5586 (10) and 2.6441 (10) Å. A search of the CSD for two C—N—Cu—C—N fragments with a defined Cu···Cu distance less than 2.8 Å gave 80 hits, among which is an example close to the title structure, i.e. catena-[(μ_2-N-benzylpiperazine-N,N′)tetrakis(μ_2-cyano)tetracopper(I)] (refcode LOGWIO; Lim et al., 2008), where the resulting network is composed of planar rows of undulating CuCN chains running roughly parallel to the a axis and crosslinked by bridging benzylpiperazine ligands in the c direction, forming two-dimensional double sheets capped by nonbridging ligands. Two Cu···Cu interactions are present in the mentioned coordination polymer, with distances of 2.6650 (6) and 2.9644 (6) Å.

5. Synthesis and crystallization

Crystals of the title compound were obtained by slow diffusion within three layers in a 3 ml glass tube. The first layer was a solution of K[Cu(CN)₂] (7.7 mg, 0.05 mmol) in 1 ml of H₂O, the second layer was a H₂O/EtOH mixture (1:1 v/v, 1 ml) and the third layer was a solution of 2-ethoxypyrazine (3.1 mg, 0.025 mmol) in 0.5 ml of EtOH. After two weeks, colourless block-shaped crystals had formed in the middle layer. The crystals were kept under the mother solution prior to measurement.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic hydrogens, C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for the CH₂ group, and C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for the CH₃ group. A rotating model was used for the methyl group. All cyano ligands are disordered over two sites with occupancies of 0.5. The coordinates of C and N atoms sharing the same sites and their displacement ellipsoids were constrained to be the same.

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Crystal structure of *catena*-poly[[[(2-ethoxypyrazine-*κN*)copper(I)]-di-*μ₂*-cyanido] [copper(I)-*μ₂*-cyanido]]

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Computing details

Data collection: *SAINT* (Bruker, 2013); cell refinement: *APEX2* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

catena-**Poly[[[(2-ethoxypyrazine-*κN*)copper(I)]-di-*μ₂*-cyanido] [copper(I)-*μ₂*-cyanido]]**

Crystal data

[Cu(CN)(C₆H₈N₂O)][Cu(CN)]	$F(000) = 1200$
$M_r = 303.26$	$D_x = 1.925$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 26.840$ (5) Å	Cell parameters from 1229 reflections
$b = 4.830$ (1) Å	$\theta = 3.1–22.8°$
$c = 18.620$ (4) Å	$\mu = 4.04$ mm^{-1}
$\beta = 119.91$ (3)°	$T = 293$ K
$V = 2092.3$ (9) Å^3	Block, colourless
$Z = 8$	$0.09 × 0.04 × 0.01$ mm

Data collection

Bruker SMART CCD diffractometer	2498 independent reflections
ω scan	1396 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$R_{int} = 0.113$
	$\theta_{max} = 27.9°$, $\theta_{min} = 1.8°$
$T_{min} = 0.630$, $T_{max} = 0.746$	$h = -34→31$
12437 measured reflections	$k = -6→6$
	$l = -24→24$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2]$
$wR(F^2) = 0.091$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.84$	$(\Delta/\sigma)_{max} = 0.001$
2498 reflections	$\Delta\rho_{max} = 1.72$ e Å^{-3}
137 parameters	$\Delta\rho_{min} = -0.73$ e Å^{-3}
0 restraints	
Primary atom site location: dual	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Cu1	0.48390 (3)	0.21483 (12)	0.37001 (4)	0.02665 (19)	
Cu2	0.60202 (3)	0.16869 (12)	0.43005 (4)	0.0350 (2)	
O1	0.31627 (15)	0.7706 (7)	0.3834 (2)	0.0307 (8)	
N5	0.42154 (19)	0.5236 (7)	0.3357 (2)	0.0242 (10)	
N6	0.3369 (2)	0.9360 (8)	0.2842 (3)	0.0303 (11)	
C4	0.6090 (2)	0.7890 (9)	0.4339 (3)	0.0284 (11)	0.5
C5	0.3898 (2)	0.5558 (10)	0.3714 (3)	0.0230 (12)	
H5	0.395884	0.440570	0.415076	0.028*	
C3	0.6081 (2)	0.5524 (10)	0.4335 (3)	0.0313 (12)	0.5
C8	0.4114 (2)	0.7025 (10)	0.2737 (3)	0.0256 (11)	
H8	0.432622	0.687906	0.246866	0.031*	
C6	0.3472 (2)	0.7606 (10)	0.3445 (3)	0.0269 (12)	
C7	0.3710 (3)	0.9009 (10)	0.2504 (3)	0.0320 (14)	
H7	0.366143	1.021425	0.208471	0.038*	
C9	0.2705 (2)	0.9697 (11)	0.3541 (4)	0.0355 (14)	
H9A	0.242718	0.935695	0.296265	0.043*	
H9B	0.285567	1.155698	0.359242	0.043*	
C10	0.2431 (3)	0.9374 (13)	0.4063 (4)	0.0437 (16)	
H10A	0.210384	1.058036	0.386082	0.066*	
H10B	0.270287	0.984284	0.462610	0.066*	
H10C	0.230857	0.749007	0.403666	0.066*	
N3	0.6081 (2)	0.5524 (10)	0.4335 (3)	0.0313 (12)	0.5
N4	0.6090 (2)	0.7890 (9)	0.4339 (3)	0.0284 (11)	0.5
C2	0.4969 (2)	0.0527 (9)	0.4702 (3)	0.0274 (12)	0.5
C1	0.4978 (2)	0.2054 (8)	0.2793 (3)	0.0254 (11)	0.5
N1	0.4978 (2)	0.2054 (8)	0.2793 (3)	0.0254 (11)	0.5
N2	0.4969 (2)	0.0527 (9)	0.4702 (3)	0.0274 (12)	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0346 (4)	0.0309 (4)	0.0197 (3)	0.0007 (3)	0.0175 (3)	0.0022 (3)
Cu2	0.0518 (5)	0.0196 (3)	0.0408 (5)	0.0005 (3)	0.0285 (4)	−0.0002 (3)
O1	0.030 (2)	0.041 (2)	0.0252 (19)	0.0082 (18)	0.0169 (17)	0.0077 (17)
N5	0.035 (3)	0.017 (2)	0.022 (2)	−0.0055 (19)	0.016 (2)	−0.0010 (18)
N6	0.035 (3)	0.022 (2)	0.031 (3)	−0.002 (2)	0.015 (3)	0.003 (2)
C4	0.035 (3)	0.026 (2)	0.024 (3)	0.000 (2)	0.015 (2)	−0.001 (2)
C5	0.033 (3)	0.022 (3)	0.017 (3)	0.000 (2)	0.015 (3)	0.002 (2)
C3	0.038 (3)	0.032 (3)	0.021 (3)	0.001 (3)	0.013 (3)	−0.003 (2)

C8	0.036 (3)	0.026 (3)	0.020 (3)	−0.004 (3)	0.018 (3)	0.000 (2)
C6	0.036 (3)	0.020 (2)	0.024 (3)	−0.006 (2)	0.015 (3)	−0.002 (2)
C7	0.043 (4)	0.026 (3)	0.030 (3)	−0.006 (3)	0.020 (3)	0.007 (2)
C9	0.030 (4)	0.043 (3)	0.031 (3)	0.007 (3)	0.013 (3)	0.004 (3)
C10	0.030 (4)	0.063 (4)	0.045 (4)	0.013 (3)	0.024 (3)	0.009 (3)
N3	0.038 (3)	0.032 (3)	0.021 (3)	0.001 (3)	0.013 (3)	−0.003 (2)
N4	0.035 (3)	0.026 (2)	0.024 (3)	0.000 (2)	0.015 (2)	−0.001 (2)
C2	0.033 (3)	0.029 (3)	0.021 (3)	0.000 (2)	0.014 (3)	0.000 (2)
C1	0.023 (3)	0.025 (2)	0.030 (3)	0.002 (2)	0.015 (2)	0.003 (2)
N1	0.023 (3)	0.025 (2)	0.030 (3)	0.002 (2)	0.015 (2)	0.003 (2)
N2	0.033 (3)	0.029 (3)	0.021 (3)	0.000 (2)	0.014 (3)	0.000 (2)

Geometric parameters (Å, º)

Cu1—Cu2	2.7958 (13)	C5—H5	0.9300
Cu1—N5	2.090 (4)	C5—C6	1.402 (7)
Cu1—C2	1.888 (4)	C3—N4	1.143 (6)
Cu1—C1	1.905 (4)	C8—H8	0.9300
Cu1—N1	1.905 (4)	C8—C7	1.347 (7)
Cu1—N2	1.888 (4)	C7—H7	0.9300
Cu2—C3	1.859 (5)	C9—H9A	0.9700
Cu2—N3	1.859 (5)	C9—H9B	0.9700
O1—C6	1.347 (5)	C9—C10	1.492 (7)
O1—C9	1.436 (6)	C10—H10A	0.9600
N5—C5	1.325 (6)	C10—H10B	0.9600
N5—C8	1.357 (6)	C10—H10C	0.9600
N6—C6	1.322 (6)	C2—C2[i]	1.155 (8)
N6—C7	1.354 (6)	C1—C1[ii]	1.152 (8)
C4—N3	1.143 (6)		
N5—Cu1—Cu2	139.01 (11)	C7—C8—H8	119.5
C2—Cu1—Cu2	87.55 (16)	O1—C6—C5	116.4 (4)
C2—Cu1—N5	108.86 (18)	N6—C6—O1	120.7 (5)
C1—Cu1—Cu2	70.59 (14)	N6—C6—C5	122.9 (5)
C1—Cu1—N5	103.17 (17)	N6—C7—H7	117.9
N1—Cu1—Cu2	70.59 (14)	C8—C7—N6	124.2 (5)
N1—Cu1—N5	103.17 (17)	C8—C7—H7	117.9
N2—Cu1—Cu2	87.55 (16)	O1—C9—H9A	110.4
N2—Cu1—N5	108.86 (18)	O1—C9—H9B	110.4
C3—Cu2—Cu1	89.85 (17)	O1—C9—C10	106.7 (4)
N3—Cu2—Cu1	89.85 (17)	H9A—C9—H9B	108.6
C6—O1—C9	117.2 (4)	C10—C9—H9A	110.4
C5—N5—Cu1	123.2 (3)	C10—C9—H9B	110.4
C5—N5—C8	116.4 (4)	C9—C10—H10A	109.5
C8—N5—Cu1	120.3 (3)	C9—C10—H10B	109.5
C6—N6—C7	114.3 (4)	C9—C10—H10C	109.5
N5—C5—H5	119.4	H10A—C10—H10B	109.5
N5—C5—C6	121.2 (4)	H10A—C10—H10C	109.5

C6—C5—H5	119.4	H10B—C10—H10C	109.5
N4—C3—Cu2	176.6 (5)	C4—N3—Cu2	176.6 (5)
N5—C8—H8	119.5	C2^i—C2—Cu1	177.4 (7)
C7—C8—N5	121.0 (5)	C1^{ii}—C1—Cu1	175.0 (6)

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

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1/N1–C1^i/N1^i cyano group (symmetry code: (i) 1-x, y, 1/2-z)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···*Cg*	0.93	2.93	3.558 (6)	126