IUCrData

ISSN 2414-3146

trans-Bis(2,2′-dipyridylamine-κ^2N,N')bis(1,1,3,3-tetracyano-2-ethoxypropenido-κN)copper(II)

Yaakoub Saadallah,[a] Zouaoui Setifi,[b,a] David K. Geiger,[c] Mohammed Hadi Al-Douh,[d]* Achouak Satour[a] and Fatima Setifi[a]‡

[a]Laboratoire de Chimie, Ingénierie Moléculaire et Nanostructures (LCIMN), Université Ferhat Abbas Sétif 1, Sétif 19000, Algeria, [b]Département de Technologie, Faculté de Technologie, Université 20 Août 1955-Skikda, BP 26, Route d'El-Hadaiek, Skikda 21000, Algeria, [c]Department of Chemistry, SUNY-College at Geneseo, Geneseo, NY 14454, USA, and [d]Chemistry Department, Faculty of Science, Hadhramout University, Mukalla, Hadhramout, Yemen. *Correspondence e-mail: m.aldouh@hu.edu.ye

Received 6 December 2022
Accepted 10 December 2022

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

‡ Additional correspondence author, e-mail: fatima.setifi@univ-setif.dz.

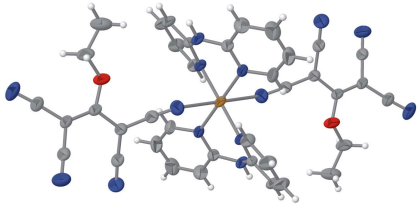
Keywords: crystal structure; copper(II); 2,2′-dipyridylamine (dpa); 1,1,3,3-tetracyano-2-ethoxypropenide (tcnoet).

CCDC reference: 2225624

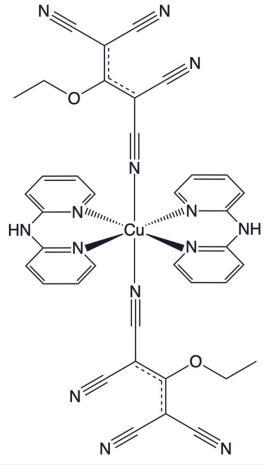
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Cu(C_9H_5N_4O)_2(C_{10}H_9N_3)_2]$, was synthesized solvothermally. The complex exhibits a distorted octahedral coordination geometry. The Cu^{II} atom is located on an inversion centre. The distorted octahedral CuN_6 coordination sphere is composed of bidentate 2,2′-dipyridylamine in the equatorial sites while the axial sites are occupied by 1,1,3,3-tetracyano-2-ethoxypropenide ligands. In the crystal, N—H···N hydrogen bonding results in chains parallel to [010].

3D view



Chemical scheme



Structure description

Anionic polynitrile ligands are of interest because of their ability to act as bridging ligands with different coordination modes to generate many different topologies by functioning alone or in combination with other neutral co-ligands (Miyazaki *et al.*, 2003; Benmansour *et al.*, 2008, 2010, 2012; Setifi *et al.*, 2013; Dmitrienko *et al.*, 2020). In view of this coordinating ability, these ligands have also been explored for their utility in developing materials capable of magnetic exchange coupling (Yuste *et al.*, 2009; Atmani *et al.*, 2008). As a part of our continuing studies of the structural and magnetic properties of Cu^{II} complexes containing both polynitrile and polypyridyl units (Setifi *et al.*, 2006, 2007, 2009, 2014; Addala *et al.*, 2015), we report here the synthesis and the crystal and molecular structure of a new mononuclear compound based on 2,2′-dipyridylamine (dpa) as co-ligand and 1,1,3,3-tetracyano-2-ethoxypropenide (tcnoet) as ligands.

The title compound exhibits a distorted octahedral coordination environment, as expected for a six-coordinate, d^9 coordination complex due to the Jahn–Teller effect (see

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.0196 (13)	Cu1—N6	2.4828 (16)
Cu1—N3	2.0196 (13)		
N1—Cu1—N3^{i}	94.54 (5)	N3—Cu1—N6	92.15 (6)
N1—Cu1—N6	91.81 (6)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N8^{ii}	0.85 (2)	2.18 (2)	3.020 (2)	171.2 (19)
C7—H7···N5^{iii}	0.93	2.43	3.234 (2)	145
C10—H10···N8^{ii}	0.93	2.62	3.385 (3)	140
C12—H12A···N5	0.97	2.64	3.404 (3)	136

Symmetry codes: (ii) $x, y+1, z$; (iii) $x, y, z-1$.

Table 1). The molecular geometry and atom-labelling scheme are represented in Fig. 1. The Cu^{II} ion is located on an inversion centre. The bidentate dpa ligands occupy equatorial sites, with coordinating tcnoet ligands in the axial sites. The Cu—N6 bond length compares well with those reported for other Cu^{II} complexes with axially coordinated tcnoet ligands (Thetiot *et al.*, 2003; Addala *et al.*, 2015).

The extended structure exhibits an N2—H2···N8 hydrogen-bonding network (Table 2), resulting in chains running parallel to [010], as seen in Fig. 2. Intra- and intermolecular C—H···N hydrogen bonds are also observed (Table 2).

Synthesis and crystallization

The title compound was synthesized solvothermally under autogenous pressure using a mixture of copper(II) sulfate pentahydrate (25 mg, 0.1 mmol), 2,2′-dipyridylamine (34 mg, 0.2 mmol) and potassium 1,1,3,3-tetracyano-2-ethoxypropenide (45 mg, 0.2 mmol) in water-methanol (3:1 *v*/*v*, 20 ml). The mixture was sealed in a Teflon-lined autoclave and held at 438 K for 2 d, and then cooled to ambient temperature at a rate of 10 K per hour (yield 42%). Green blocks of the title complex suitable for single-crystal X-ray diffraction were selected directly from the synthesized product.

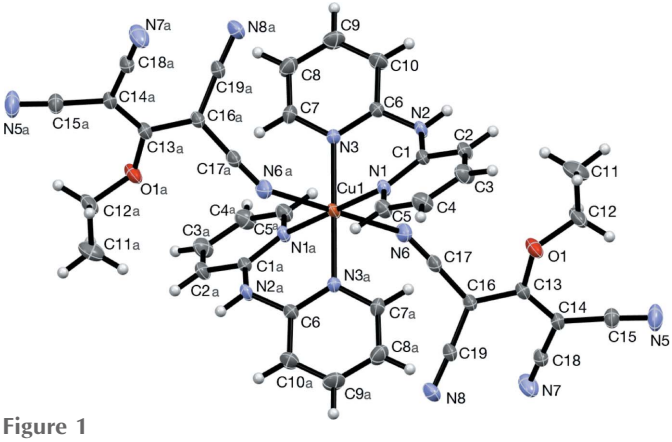


Figure 1
View of the title compound showing the atom-labelling scheme. Anisotropic displacement parameters of non-H atoms are drawn at the 30% probability level. [Symmetry code: (*a*) $-x+1, -y+1, -z+1$.]

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_9H_5N_4O)_2(C_{10}H_9N_3)_2]$
M_r	776.28
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	300
a, b, c (Å)	7.5101 (3), 9.2232 (4), 13.6405 (6)
α, β, γ (°)	99.068 (1), 98.864 (1), 93.139 (1)
V (Å^3)	918.86 (7)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.65
Crystal size (mm)	0.40 × 0.10 × 0.06
Data collection	
Diffractometer	Oxford Diffraction Xcalibur CCD
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.481, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	51758, 5649, 4388
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.094, 1.05
No. of reflections	5649
No. of parameters	255
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.44

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *PLATON* (Spek, 2020), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

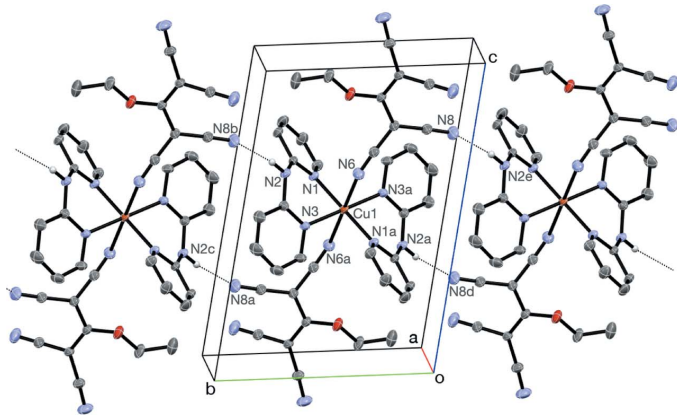


Figure 2
Partial packing diagram showing the N—H···N hydrogen-bonding interactions. Only H atoms involved in the intermolecular interactions are shown. [Symmetry codes: (*a*) $-x+1, -y+1, -z+1$; (*b*) $x, y+1, z$; (*c*) $-x+1, -y+2, -z+1$; (*d*) $-x+1, -y, -z+1$; (*e*) $x, y-1, z$.]

Acknowledgements

Author contributions are as follows. Conceptualization, ZS and MHAD; methodology, ZS and MHAD; investigation, YS and AS; writing (original draft), DKG and ZS; writing (review and editing of the manuscript), DKG, FS and ZS; visualization, ZS and DKG; funding acquisition, ZS and MHAD; resources, FS; supervision, FS.

Funding information

Funding for this research was provided by: the Algerian MESRS (Ministère de l'Enseignement Supérieur et de la Recherche Scientifique); the Algerian DGRSDT (Direction Générale de la Recherche Scientifique et du Développement Technologique; PRFU project (grant No. B00L01UN190120230003).

References

Addala, A., Setifi, F., Kottrup, K. G., Glidewell, C., Setifi, Z., Smith, G. & Reedijk, J. (2015). *Polyhedron*, **87**, 307–310.

Atmani, C., Setifi, F., Benmansour, S., Triki, S., Marchivie, M., Salaün, J.-Y. & Gómez-García, C. J. (2008). *Inorg. Chem. Commun.* **11**, 921–924.

Benmansour, S., Atmani, C., Setifi, F., Triki, S., Marchivie, M. & Gómez-García, C. J. (2010). *Coord. Chem. Rev.* **254**, 1468–1478.

Benmansour, S., Setifi, F., Gómez-García, C. J., Triki, S. & Coronado, E. (2008). *Inorg. Chim. Acta*, **361**, 3856–3862.

Benmansour, S., Setifi, F., Triki, S. & Gómez-García, C. J. (2012). *Inorg. Chem.* **51**, 2359–2365.

Dmitrienko, A. O., Buzin, M. I., Setifi, Z., Setifi, F., Alexandrov, E. V., Voronova, E. D. & Vologzhanina, A. V. (2020). *Dalton Trans.* **49**, 7084–7092.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Miyazaki, A., Okabe, K., Enoki, T., Setifi, F., Golhen, S., Ouahab, L., Toita, T. & Yamada, J. (2003). *Synth. Met.* **137**, 1195–1196.

Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.

Setifi, F., Benmansour, S., Marchivie, M., Dupouy, G., Triki, S., Sala-Pala, J., Salaün, J.-Y., Gómez-García, C. J., Pillet, S., Lecomte, C. & Ruiz, E. (2009). *Inorg. Chem.* **48**, 1269–1271.

Setifi, F., Benmansour, S., Triki, S., Gómez-García, C. J., Marchivie, M., Salaün, J.-Y. & Mustapha, M. (2007). *Inorg. Chim. Acta*, **360**, 3879–3886.

Setifi, F., Bouchama, A., Sala-Pala, J., Salaün, J.-Y. & Triki, S. (2006). *Inorg. Chim. Acta*, **359**, 3269–3274.

Setifi, F., Charles, C., Houille, S., Thétiot, F., Triki, S., Gómez-García, C. J. & Pillet, S. (2013). *Polyhedron*, **61**, 242–247.

Setifi, Z., Setifi, F., El Ammari, L., El-Ghozzi, M., Sopková-de Oliveira Santos, J., Merazig, H. & Glidewell, C. (2014). *Acta Cryst.* C**70**, 19–22.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Thétiot, F., Triki, S. & Sala Pala, J. (2003). *Polyhedron*, **22**, 1837–1843.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Yuste, C., Bentama, A., Marino, N., Armentano, D., Setifi, F., Triki, S., Lloret, F. & Julve, M. (2009). *Polyhedron*, **28**, 1287–1294.

full crystallographic data

IUCrData (2022). **7**, x221180 [https://doi.org/10.1107/S2414314622011804]

trans-Bis(2,2′-dipyridylamine-κ^2N,N')bis(1,1,3,3-tetracyano-2-ethoxypropenido-κN)copper(II)

Yaakoub Saadallah, Zouaoui Setifi, David K. Geiger, Mohammed Hadi Al-Douh, Achouak Satour and Fatima Setifi

***trans*-Bis(2,2′-dipyridylamine-κ^2N,N')bis(1,1,3,3-tetracyano-2-ethoxypropenido-κN)copper(II)**

Crystal data

$[Cu(C_9H_5N_4O)_2(C_{10}H_9N_3)_2]$
$M_r = 776.28$
Triclinic, $P\overline{1}$
$a = 7.5101$ (3) Å
$b = 9.2232$ (4) Å
$c = 13.6405$ (6) Å
$\alpha = 99.068$ (1)°
$\beta = 98.864$ (1)°
$\gamma = 93.139$ (1)°
$V = 918.86$ (7) Å^3
$Z = 1$
$F(000) = 399$
$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 937 reflections
$\theta = 2.6$–$28.1°$
$\mu = 0.65$ mm^{-1}
$T = 300$ K
Block, blue
0.40 × 0.10 × 0.06 mm

Data collection

Oxford Diffraction X calibur CCD diffractometer
Radiation source: Enhance (Mo) X-ray source
ω scans
Absorption correction: multi-scan (CrysalisRed; Oxford Diffraction, 2009)
$T_{min} = 0.481$, $T_{max} = 1.000$
51758 measured reflections
5649 independent reflections
4388 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 30.6°$, $\theta_{min} = 2.5°$
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.094$
$S = 1.05$
5649 reflections
255 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 0.4397P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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.

Refinement. All hydrogen atoms bonded to C atoms were positioned geometrically and treated as riding atoms, using C—H = 0.93 Å (aromatic), 0.96 Å (CH_3) or 0.97 Å (CH_2), and with $U_{iso}(H) = kU_{eq}(C)$, where k = 1.5 for the methyl groups and 1.2 for all other H atoms bonded to C atoms. The H atom bonded to the amine N atom was refined freely, including its isotropic displacement parameter.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5	0.5	0.5	0.03141 (9)
N1	0.67538 (19)	0.64977 (14)	0.59690 (10)	0.0313 (3)
N2	0.4406 (2)	0.79956 (16)	0.62884 (10)	0.0345 (3)
H2	0.413 (3)	0.872 (2)	0.6688 (16)	0.042 (5)*
N3	0.37389 (19)	0.67548 (15)	0.46127 (10)	0.0313 (3)
O1	0.33800 (19)	0.57177 (13)	0.88700 (10)	0.0459 (3)
N5	0.2377 (3)	0.4862 (2)	1.13970 (13)	0.0691 (6)
N6	0.3087 (3)	0.47360 (18)	0.63022 (12)	0.0506 (4)
N7	0.0144 (3)	0.1256 (2)	0.91228 (16)	0.0691 (6)
N8	0.3262 (3)	0.07139 (19)	0.75000 (14)	0.0630 (5)
C1	0.6156 (2)	0.76147 (16)	0.65471 (11)	0.0301 (3)
C2	0.7266 (3)	0.84429 (19)	0.73900 (13)	0.0416 (4)
H2A	0.68	0.9168	0.781	0.05*
C3	0.9045 (3)	0.8172 (2)	0.75871 (16)	0.0511 (5)
H3	0.98	0.8703	0.8148	0.061*
C4	0.9713 (3)	0.7099 (2)	0.69434 (16)	0.0487 (5)
H4	1.0934	0.6934	0.7044	0.058*
C5	0.8543 (2)	0.6287 (2)	0.61567 (14)	0.0394 (4)
H5	0.8991	0.5557	0.5731	0.047*
C6	0.3509 (2)	0.78931 (17)	0.53097 (12)	0.0318 (3)
C7	0.2986 (3)	0.6766 (2)	0.36427 (13)	0.0403 (4)
H7	0.3195	0.6006	0.315	0.048*
C8	0.1940 (3)	0.7837 (2)	0.33556 (15)	0.0506 (5)
H8	0.1454	0.7811	0.2683	0.061*
C9	0.1619 (3)	0.8964 (3)	0.40891 (17)	0.0568 (6)
H9	0.0872	0.9688	0.3918	0.068*
C10	0.2409 (3)	0.9008 (2)	0.50707 (15)	0.0482 (5)
H10	0.2217	0.9766	0.557	0.058*
C11	0.3586 (4)	0.8295 (2)	0.9359 (2)	0.0680 (7)
H11A	0.4881	0.8317	0.9499	0.102*
H11B	0.3188	0.9096	0.979	0.102*
H11C	0.321	0.839	0.8669	0.102*
C12	0.2784 (4)	0.6878 (2)	0.95455 (17)	0.0560 (6)
H12A	0.3177	0.676	1.0238	0.067*
H12B	0.1475	0.6855	0.9424	0.067*

C13	0.2780 (2)	0.43072 (17)	0.87862 (12)	0.0315 (3)
C14	0.2105 (2)	0.37033 (18)	0.95387 (12)	0.0335 (3)
C15	0.2291 (3)	0.4382 (2)	1.05654 (13)	0.0417 (4)
C16	0.2916 (2)	0.34824 (18)	0.78366 (12)	0.0344 (4)
C17	0.3030 (3)	0.42011 (19)	0.70040 (13)	0.0377 (4)
C18	0.1052 (3)	0.2327 (2)	0.92985 (13)	0.0415 (4)
C19	0.3079 (3)	0.1948 (2)	0.76699 (13)	0.0407 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.04112 (17)	0.02558 (14)	0.02394 (14)	0.00860 (11)	0.00108 (11)	−0.00461 (10)
N1	0.0365 (7)	0.0290 (6)	0.0257 (6)	0.0051 (5)	0.0044 (5)	−0.0037 (5)
N2	0.0445 (8)	0.0299 (7)	0.0270 (7)	0.0121 (6)	0.0069 (6)	−0.0056 (5)
N3	0.0402 (7)	0.0299 (6)	0.0231 (6)	0.0083 (6)	0.0039 (5)	0.0018 (5)
O1	0.0580 (8)	0.0292 (6)	0.0501 (8)	−0.0050 (6)	0.0255 (6)	−0.0082 (5)
N5	0.0958 (16)	0.0746 (14)	0.0308 (9)	−0.0078 (12)	0.0136 (9)	−0.0077 (9)
N6	0.0751 (12)	0.0427 (9)	0.0402 (9)	0.0118 (8)	0.0270 (8)	0.0065 (7)
N7	0.1046 (17)	0.0401 (10)	0.0621 (12)	−0.0155 (10)	0.0345 (12)	−0.0062 (9)
N8	0.1070 (16)	0.0381 (9)	0.0497 (10)	0.0243 (10)	0.0317 (11)	0.0004 (8)
C1	0.0411 (9)	0.0237 (7)	0.0246 (7)	0.0038 (6)	0.0062 (6)	0.0004 (6)
C2	0.0569 (11)	0.0287 (8)	0.0331 (9)	0.0042 (8)	0.0005 (8)	−0.0069 (7)
C3	0.0535 (12)	0.0390 (10)	0.0490 (11)	−0.0008 (9)	−0.0125 (9)	−0.0061 (8)
C4	0.0383 (10)	0.0434 (10)	0.0579 (12)	0.0025 (8)	−0.0034 (9)	0.0004 (9)
C5	0.0378 (9)	0.0376 (9)	0.0411 (9)	0.0069 (7)	0.0072 (7)	−0.0004 (7)
C6	0.0370 (8)	0.0295 (8)	0.0297 (8)	0.0084 (6)	0.0080 (6)	0.0029 (6)
C7	0.0500 (10)	0.0451 (10)	0.0246 (8)	0.0065 (8)	0.0035 (7)	0.0037 (7)
C8	0.0548 (12)	0.0627 (13)	0.0359 (10)	0.0155 (10)	0.0006 (9)	0.0162 (9)
C9	0.0601 (13)	0.0600 (13)	0.0559 (13)	0.0299 (11)	0.0059 (10)	0.0221 (10)
C10	0.0575 (12)	0.0427 (10)	0.0474 (11)	0.0248 (9)	0.0119 (9)	0.0064 (8)
C11	0.0748 (16)	0.0323 (10)	0.0917 (19)	−0.0020 (10)	0.0112 (14)	−0.0005 (11)
C12	0.0835 (16)	0.0299 (9)	0.0549 (12)	0.0032 (9)	0.0289 (11)	−0.0086 (8)
C13	0.0350 (8)	0.0281 (7)	0.0295 (8)	0.0034 (6)	0.0076 (6)	−0.0030 (6)
C14	0.0420 (9)	0.0317 (8)	0.0255 (7)	0.0056 (7)	0.0072 (7)	−0.0017 (6)
C15	0.0478 (10)	0.0447 (10)	0.0307 (9)	0.0008 (8)	0.0082 (8)	0.0005 (7)
C16	0.0458 (10)	0.0290 (8)	0.0298 (8)	0.0060 (7)	0.0140 (7)	0.0003 (6)
C17	0.0495 (10)	0.0309 (8)	0.0349 (9)	0.0077 (7)	0.0183 (8)	−0.0010 (7)
C18	0.0612 (12)	0.0335 (9)	0.0317 (9)	0.0058 (8)	0.0172 (8)	0.0009 (7)
C19	0.0586 (11)	0.0349 (9)	0.0308 (8)	0.0107 (8)	0.0166 (8)	0.0004 (7)

Geometric parameters (Å, º)

Cu1—N1	2.0196 (13)	C4—C5	1.367 (3)
Cu1—N1^{i}	2.0196 (13)	C4—H4	0.93
Cu1—N3^{i}	2.0196 (13)	C5—H5	0.93
Cu1—N3	2.0196 (13)	C6—C10	1.400 (2)
Cu1—N6^{i}	2.4828 (16)	C7—C8	1.363 (3)
Cu1—N6	2.4828 (16)	C7—H7	0.93

N1—C1	1.3374 (19)	C8—C9	1.383 (3)
N1—C5	1.359 (2)	C8—H8	0.93
N2—C6	1.386 (2)	C9—C10	1.372 (3)
N2—C1	1.386 (2)	C9—H9	0.93
N2—H2	0.85 (2)	C10—H10	0.93
N3—C6	1.339 (2)	C11—C12	1.484 (3)
N3—C7	1.358 (2)	C11—H11A	0.96
O1—C13	1.335 (2)	C11—H11B	0.96
O1—C12	1.436 (2)	C11—H11C	0.96
N5—C15	1.142 (2)	C12—H12A	0.97
N6—C17	1.149 (2)	C12—H12B	0.97
N7—C18	1.140 (3)	C13—C14	1.389 (2)
N8—C19	1.145 (2)	C13—C16	1.416 (2)
C1—C2	1.400 (2)	C14—C18	1.422 (2)
C2—C3	1.366 (3)	C14—C15	1.423 (2)
C2—H2A	0.93	C16—C19	1.413 (2)
C3—C4	1.385 (3)	C16—C17	1.413 (2)
C3—H3	0.93		

N1—Cu1—N1^{i}	180.0	N3—C6—N2	119.59 (14)
N1—Cu1—N3^{i}	94.54 (5)	N3—C6—C10	121.57 (16)
N1^{i}—Cu1—N3^{i}	85.46 (5)	N2—C6—C10	118.82 (15)
N1—Cu1—N3	85.46 (5)	N3—C7—C8	123.29 (17)
N1^{i}—Cu1—N3	94.54 (5)	N3—C7—H7	118.4
N3^{i}—Cu1—N3	180.00 (7)	C8—C7—H7	118.4
N1—Cu1—N6^{i}	88.19 (6)	C7—C8—C9	118.40 (18)
N1^{i}—Cu1—N6^{i}	91.82 (6)	C7—C8—H8	120.8
N3^{i}—Cu1—N6^{i}	92.15 (6)	C9—C8—H8	120.8
N3—Cu1—N6^{i}	87.85 (6)	C10—C9—C8	119.61 (18)
N1—Cu1—N6	91.81 (6)	C10—C9—H9	120.2
N1^{i}—Cu1—N6	88.18 (6)	C8—C9—H9	120.2
N3^{i}—Cu1—N6	87.85 (6)	C9—C10—C6	119.00 (18)
N3—Cu1—N6	92.15 (6)	C9—C10—H10	120.5
N6^{i}—Cu1—N6	180.0	C6—C10—H10	120.5
C1—N1—C5	117.73 (14)	C12—C11—H11A	109.5
C1—N1—Cu1	120.69 (11)	C12—C11—H11B	109.5
C5—N1—Cu1	120.93 (11)	H11A—C11—H11B	109.5
C6—N2—C1	124.60 (14)	C12—C11—H11C	109.5
C6—N2—H2	113.2 (14)	H11A—C11—H11C	109.5
C1—N2—H2	113.6 (14)	H11B—C11—H11C	109.5
C6—N3—C7	117.92 (14)	O1—C12—C11	107.53 (18)
C6—N3—Cu1	121.18 (11)	O1—C12—H12A	110.2
C7—N3—Cu1	120.73 (11)	C11—C12—H12A	110.2
C13—O1—C12	122.75 (14)	O1—C12—H12B	110.2
C17—N6—Cu1	141.76 (15)	C11—C12—H12B	110.2
N1—C1—N2	119.24 (14)	H12A—C12—H12B	108.5
N1—C1—C2	121.84 (16)	O1—C13—C14	124.44 (14)
N2—C1—C2	118.89 (14)	O1—C13—C16	112.14 (15)

C3—C2—C1	119.08 (17)	C14—C13—C16	123.42 (15)
C3—C2—H2A	120.5	C13—C14—C18	120.00 (15)
C1—C2—H2A	120.5	C13—C14—C15	125.50 (16)
C2—C3—C4	119.39 (17)	C18—C14—C15	114.42 (16)
C2—C3—H3	120.3	N5—C15—C14	176.1 (2)
C4—C3—H3	120.3	C19—C16—C17	115.91 (14)
C5—C4—C3	118.66 (18)	C19—C16—C13	123.65 (16)
C5—C4—H4	120.7	C17—C16—C13	120.29 (15)
C3—C4—H4	120.7	N6—C17—C16	177.3 (2)
N1—C5—C4	122.93 (17)	N7—C18—C14	176.8 (2)
N1—C5—H5	118.5	N8—C19—C16	176.7 (2)
C4—C5—H5	118.5		

C5—N1—C1—N2	170.75 (15)	C6—N3—C7—C8	−3.4 (3)
Cu1—N1—C1—N2	−18.4 (2)	Cu1—N3—C7—C8	172.08 (16)
C5—N1—C1—C2	−7.2 (2)	N3—C7—C8—C9	−0.4 (3)
Cu1—N1—C1—C2	163.65 (13)	C7—C8—C9—C10	2.5 (4)
C6—N2—C1—N1	−33.7 (2)	C8—C9—C10—C6	−0.8 (3)
C6—N2—C1—C2	144.31 (17)	N3—C6—C10—C9	−3.1 (3)
N1—C1—C2—C3	4.7 (3)	N2—C6—C10—C9	175.5 (2)
N2—C1—C2—C3	−173.20 (18)	C13—O1—C12—C11	−174.33 (19)
C1—C2—C3—C4	0.8 (3)	C12—O1—C13—C14	−25.1 (3)
C2—C3—C4—C5	−3.5 (3)	C12—O1—C13—C16	155.17 (18)
C1—N1—C5—C4	4.4 (3)	O1—C13—C14—C18	162.61 (17)
Cu1—N1—C5—C4	−166.43 (16)	C16—C13—C14—C18	−17.7 (3)
C3—C4—C5—N1	0.9 (3)	O1—C13—C14—C15	−14.0 (3)
C7—N3—C6—N2	−173.51 (16)	C16—C13—C14—C15	165.63 (18)
Cu1—N3—C6—N2	11.1 (2)	O1—C13—C16—C19	153.95 (18)
C7—N3—C6—C10	5.1 (3)	C14—C13—C16—C19	−25.7 (3)
Cu1—N3—C6—C10	−170.32 (15)	O1—C13—C16—C17	−21.4 (2)
C1—N2—C6—N3	37.9 (2)	C14—C13—C16—C17	158.95 (18)
C1—N2—C6—C10	−140.78 (18)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N8^{ii}	0.85 (2)	2.18 (2)	3.020 (2)	171.2 (19)
C7—H7···N5^{iii}	0.93	2.43	3.234 (2)	145
C10—H10···N8^{ii}	0.93	2.62	3.385 (3)	140
C12—H12*A*···N5	0.97	2.64	3.404 (3)	136

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