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Di-μ_3-iodido-diiodidobis(μ_2-4′-phenyl-2,2′:6′,2″-terpyridine)tetracopper(I)

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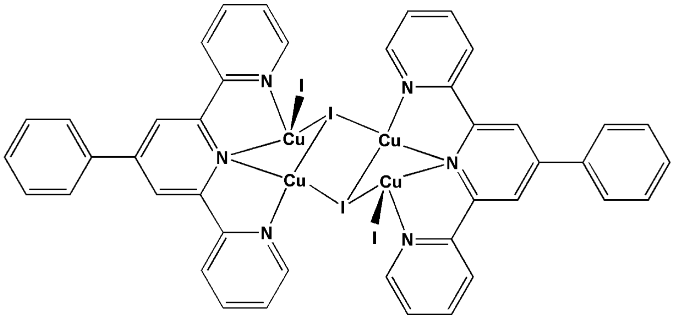
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.037; wR factor = 0.106; data-to-parameter ratio = 16.6.

The title complex, $[Cu_4I_4(C_{21}H_{15}N_3)_2]$, lies on an inversion centre located at the centroid of a four-membered ring formed by one of the crystallographically independent Cu^I ions and a triply bridging iodide ligand. The 2,2′:6′,2″-terpyridine (phterpy) ligand chelates each of the independent Cu^I centres in a bidentate fashion, with the N atom of the central pyridyl ring bridging the two Cu^I centres and those of the outer pyridyl rings binding the two independent Cu^I ions individually to form a dinuclear system. These are further linked by triply-bridging I^- anions to form the centrosymmetric tetranuclear units. One independent Cu atom binds to each of the inversion-related I^- anions while the other coordinates to one bridging and one terminal monodentate iodide ligand. The outer pyridyl rings are twisted relative to the central pyridyl ring of the phterpy ligand with dihedral angles of 18.7 (1) and 35.6 (1)°, respectively.

Related literature

For terpyridyl complexes in supramolecular frameworks and functional materials, see: Constable *et al.* (2005); Hofmeier & Schubert (2004); Thompson (1997). For common terpyridyl complexes, see: Andres & Schubert (2004). For terpyridyl Cu^I and Ag^I double helical complexes, see: Constable *et al.* (1994); Hou & Li (2005). For the preparation of the phterpy ligand, see: Constable *et al.* (1990)



Experimental

Crystal data

$[Cu_4I_4(C_{21}H_{15}N_3)_2]$
M_r = 1380.48
Monoclinic, $P2_1/c$
a = 8.8536 (6) Å
b = 9.7836 (7) Å
c = 25.4728 (18) Å
β = 102.542 (2)°
V = 2153.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.85 mm^{-1}
T = 293 (2) K
0.14 × 0.11 × 0.07 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.550, T_{max} = 0.728
11822 measured reflections
4208 independent reflections
3267 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 1.03
4208 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

I1—Cu1^i	2.5760 (8)	Cu1—N2	2.212 (4)
I1—Cu1	2.6317 (8)	Cu1—Cu1^i	2.5982 (12)
I1—Cu2	2.7212 (8)	Cu1—Cu2	2.6604 (11)
I2—Cu2	2.4674 (7)	Cu2—N3	2.014 (4)
Cu1—N1	2.029 (4)	Cu2—N2	2.449 (4)
Cu1^i—I1—Cu1	59.85 (2)	I1^i—Cu1—I1	120.15 (2)
Cu1^i—I1—Cu2	102.16 (2)	N3—Cu2—N2	75.98 (15)
Cu1—I1—Cu2	59.58 (2)	N3—Cu2—I2	137.12 (12)
N1—Cu1—N2	77.43 (15)	N2—Cu2—I2	102.33 (9)
N1—Cu1—I1^i	123.67 (13)	N3—Cu2—I1	100.63 (11)
N2—Cu1—I1^i	99.72 (10)	N2—Cu2—I1	109.59 (9)
N1—Cu1—I1	107.45 (13)	I2—Cu2—I1	119.33 (3)
N2—Cu1—I1	121.33 (11)		

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); 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: SJ2432).

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supporting information

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Di-μ_3-iodido-diiodidobis(μ_2-4′-phenyl-2,2′:6′,2′′-terpyridine)tetracopper(I)

Han-Yuan Xie, Lei Zhang and Wen-Juan Shi

S1. Comment

2,2′:6′,2"-Terpyridine (terpy) is well known for its applications in the synthesis of supramolecular frameworks and functional materials because of its strong affinity for transition metal ions and the ability to freely functionalize the central pyridyl ring (Constable *et al.*, 2005; Hofmeier & Schubert, 2004; Thompson, 1997). For many reported terpyridyl complexes, the ligand often chelates to a single metal ion to form stable complexes (Andres & Schubert, 2004). Additionally, partitioning of terpy into one monodentate and bidentate domains on coordination to a Cu^I or Ag^I center may lead to the formation of polynuclear double helical cations (Constable *et al.*, 1994; Hou & Li, 2005). We report here a new tetranuclear complex, incorporating the 4′-phenyl-2,2′:6′,2"-terpyridine (phterpy) ligand.

The asymmetric unit of the title complex contains two crystallographically independent Cu^I ions with distorted tetrahedral geometry, Table 1, defined by the N1 and N2 atoms from the phterpy ligand and two triply briging I1$^-$ ions for Cu1 and the N2 and N3 atoms from the phterpy ligand, one triply bridging I1$^-$ anion and one monodentate, terminal I2$^-$ ion, for Cu2, Fig. 1. The phterpy ligand chelates each of the independent Cu^I centres in a bidentate fashion, with the N2 atom of the central pyridyl ring bridging the two Cu^I centres and N1 and N3 of the outer pyridyl rings binding to Cu1 and Cu2 respectively to form a dinuclear system [Cu1···Cu2 distance of 2.6604 (11) Å]. These are further bridged by two symmetry-related I1 and I1A (symmetry code, A: -*x*, 1 - *y*, -*z*) ions to form a centrosymmetric tetranuclear unit. The Cu1···Cu1A distance is 2.5982 (12) Å. The I1$^-$ anion bridges three Cu^I cations and a monodentate I2$^-$ anion completes the coordination sphere of the Cu2 cation. The N1 and N3 pyridyl rings are twisted about central N2 pyridyl ring with dihedral angles of 18.7 and 35.6 °, respectively. The values of the bite angles of the terpyridyl unit are 77.43 (15) and 75.98 (15) °, respectively.

S2. Experimental

4′-Phenyl-2,2′:6′,2"-terpyridine was synthesized using a reported procedure (Constable *et al.*, 1990). The ligand (0.030 g, 0.1 mmol), copper(I) iodide (0.019, 0.1 mmol) and ethanol (8 ml) were mixed in a 12-ml Telfon-lined, stainless-steel Parr bomb. The bomb was heated at 418 K for 72 h and then cooled to room temperature at a rate of 5 K h^{-1}. Black block-shaped crystals were obtained in about 40% yield (0.028 g).

S3. Refinement

The carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and refined as riding, with U(H) = 1.2U_{eq}(C).

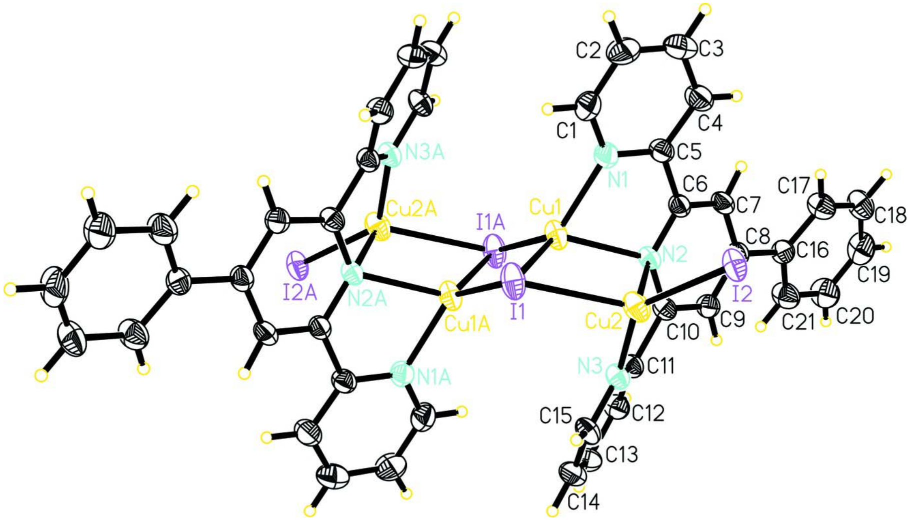

Figure 1

The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level, and H atoms as spheres of arbitrary radius; symmetry code, A: -*x*, 1 - *y*, -*z*.

Di-μ_3-iodido-diiodidobis(μ_2-4′-phenyl-2,2′:6′,2″- terpyridine)tetracopper(I)

Crystal data

$[Cu_4I_4(C_{21}H_{15}N_3)_2]$
$M_r = 1380.48$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.8536$ (6) Å
$b = 9.7836$ (7) Å
$c = 25.4728$ (18) Å
$\beta = 102.542$ (2)°
$V = 2153.8$ (3) Å^3
$Z = 2$

$F(000) = 1304$
$D_x = 2.129$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1992 reflections
$\theta = 2.4$–24.8°
$\mu = 4.85$ mm^{-1}
$T = 293$ K
Block, black
0.14 × 0.11 × 0.07 mm

Data collection

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.550$, $T_{max} = 0.728$

11822 measured reflections
4208 independent reflections
3267 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.6°$
$h = -10 \rightarrow 8$
$k = -12 \rightarrow 10$
$l = -30 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.106$
$S = 1.03$
4208 reflections
253 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.14$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

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}
I1	−0.20412 (4)	0.35622 (4)	−0.017321 (14)	0.06204 (15)
I2	−0.15633 (4)	0.14399 (4)	0.141286 (13)	0.05679 (14)
Cu1	0.00247 (8)	0.49793 (8)	0.05117 (2)	0.0555 (2)
Cu2	−0.02931 (8)	0.23388 (8)	0.07129 (3)	0.0582 (2)
N1	−0.0966 (5)	0.5543 (4)	0.11258 (16)	0.0514 (11)
N2	0.1542 (4)	0.3995 (4)	0.12147 (15)	0.0417 (9)
N3	0.1674 (5)	0.1989 (4)	0.04594 (15)	0.0455 (10)
C1	−0.2391 (7)	0.6083 (7)	0.1069 (3)	0.0680 (17)
H1	−0.2978	0.6209	0.0723	0.082*
C2	−0.3018 (8)	0.6453 (7)	0.1488 (3)	0.078 (2)
H2	−0.4016	0.6805	0.1431	0.093*
C3	−0.2136 (9)	0.6293 (7)	0.2001 (3)	0.081 (2)
H3	−0.2515	0.6570	0.2297	0.097*
C4	−0.0680 (7)	0.5715 (6)	0.2070 (2)	0.0640 (16)
H4	−0.0082	0.5575	0.2414	0.077*
C5	−0.0124 (6)	0.5350 (5)	0.1625 (2)	0.0481 (12)
C6	0.1388 (6)	0.4662 (5)	0.16612 (18)	0.0423 (11)
C7	0.2558 (6)	0.4698 (5)	0.21210 (18)	0.0475 (12)
H7	0.2418	0.5190	0.2419	0.057*
C8	0.3941 (6)	0.4006 (5)	0.21402 (18)	0.0448 (12)
C9	0.4080 (6)	0.3321 (5)	0.1678 (2)	0.0475 (12)
H9	0.4989	0.2850	0.1671	0.057*
C10	0.2884 (6)	0.3325 (5)	0.12245 (19)	0.0428 (11)
C11	0.2994 (6)	0.2570 (5)	0.07320 (18)	0.0418 (11)
C12	0.4370 (6)	0.2468 (5)	0.0554 (2)	0.0511 (13)
H12	0.5261	0.2903	0.0740	0.061*
C13	0.4395 (7)	0.1722 (5)	0.0102 (2)	0.0539 (14)
H13	0.5310	0.1627	−0.0017	0.065*
C14	0.3049 (7)	0.1111 (6)	−0.0177 (2)	0.0569 (15)
H14	0.3039	0.0599	−0.0486	0.068*
C15	0.1743 (6)	0.1281 (5)	0.00135 (19)	0.0490 (13)
H15	0.0836	0.0881	−0.0177	0.059*

C16	0.5203 (6)	0.3988 (5)	0.26341 (19)	0.0480 (12)
C17	0.4964 (7)	0.4382 (6)	0.3127 (2)	0.0629 (15)
H17	0.3981	0.4665	0.3154	0.075*
C18	0.6128 (8)	0.4373 (7)	0.3581 (2)	0.0728 (18)
H18	0.5923	0.4628	0.3911	0.087*
C19	0.7590 (8)	0.3989 (7)	0.3548 (3)	0.078 (2)
H19	0.8384	0.3997	0.3855	0.093*
C20	0.7890 (8)	0.3592 (7)	0.3067 (3)	0.079 (2)
H20	0.8882	0.3324	0.3045	0.094*
C21	0.6691 (7)	0.3593 (6)	0.2610 (2)	0.0686 (17)
H21	0.6894	0.3322	0.2283	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0509 (2)	0.0852 (3)	0.0451 (2)	−0.01917 (18)	−0.00047 (17)	0.01160 (18)
I2	0.0519 (2)	0.0800 (3)	0.0395 (2)	−0.00421 (17)	0.01224 (16)	0.01046 (16)
Cu1	0.0535 (4)	0.0751 (5)	0.0373 (3)	−0.0026 (3)	0.0088 (3)	0.0060 (3)
Cu2	0.0506 (4)	0.0782 (5)	0.0497 (4)	−0.0087 (3)	0.0191 (3)	0.0008 (3)
N1	0.048 (3)	0.060 (3)	0.047 (2)	0.006 (2)	0.012 (2)	0.005 (2)
N2	0.038 (2)	0.054 (2)	0.033 (2)	−0.0018 (19)	0.0069 (17)	−0.0023 (18)
N3	0.043 (2)	0.056 (3)	0.037 (2)	−0.003 (2)	0.0071 (18)	−0.0025 (19)
C1	0.065 (4)	0.078 (4)	0.058 (4)	0.022 (3)	0.008 (3)	0.013 (3)
C2	0.055 (4)	0.093 (5)	0.085 (5)	0.031 (3)	0.015 (4)	0.001 (4)
C3	0.085 (5)	0.088 (5)	0.078 (5)	0.024 (4)	0.033 (4)	−0.011 (4)
C4	0.062 (4)	0.082 (4)	0.047 (3)	0.011 (3)	0.011 (3)	−0.008 (3)
C5	0.044 (3)	0.058 (3)	0.043 (3)	0.004 (2)	0.011 (2)	−0.003 (2)
C6	0.044 (3)	0.049 (3)	0.034 (2)	0.002 (2)	0.007 (2)	−0.001 (2)
C7	0.055 (3)	0.055 (3)	0.032 (2)	0.001 (2)	0.008 (2)	−0.009 (2)
C8	0.045 (3)	0.051 (3)	0.036 (2)	0.000 (2)	0.004 (2)	−0.002 (2)
C9	0.044 (3)	0.054 (3)	0.042 (3)	0.005 (2)	0.003 (2)	−0.003 (2)
C10	0.038 (3)	0.051 (3)	0.039 (3)	−0.004 (2)	0.008 (2)	−0.006 (2)
C11	0.040 (3)	0.048 (3)	0.035 (2)	0.000 (2)	0.004 (2)	−0.003 (2)
C12	0.041 (3)	0.063 (4)	0.047 (3)	0.002 (2)	0.004 (2)	−0.006 (2)
C13	0.048 (3)	0.059 (3)	0.058 (3)	0.006 (3)	0.021 (3)	−0.005 (3)
C14	0.067 (4)	0.059 (4)	0.049 (3)	−0.002 (3)	0.021 (3)	−0.010 (3)
C15	0.050 (3)	0.062 (3)	0.034 (3)	−0.011 (2)	0.006 (2)	−0.009 (2)
C16	0.048 (3)	0.051 (3)	0.040 (3)	0.000 (2)	−0.002 (2)	−0.005 (2)
C17	0.053 (3)	0.080 (4)	0.052 (3)	−0.003 (3)	0.003 (3)	−0.013 (3)
C18	0.077 (5)	0.092 (5)	0.043 (3)	−0.006 (4)	−0.002 (3)	−0.009 (3)
C19	0.071 (5)	0.088 (5)	0.058 (4)	−0.008 (4)	−0.023 (3)	−0.001 (3)
C20	0.060 (4)	0.103 (6)	0.062 (4)	0.008 (4)	−0.010 (3)	−0.007 (4)
C21	0.060 (4)	0.090 (5)	0.050 (3)	0.008 (3)	0.000 (3)	−0.012 (3)

Geometric parameters (Å, º)

I1—Cu1^{i}	2.5760 (8)	C7—C8	1.391 (7)
I1—Cu1	2.6317 (8)	C7—H7	0.9300

I1—Cu2	2.7212 (8)	C8—C9	1.384 (7)
I2—Cu2	2.4674 (7)	C8—C16	1.490 (6)
Cu1—N1	2.029 (4)	C9—C10	1.387 (7)
Cu1—N2	2.212 (4)	C9—H9	0.9300
Cu1—I1^{i}	2.5760 (8)	C10—C11	1.478 (6)
Cu1—Cu1^{i}	2.5982 (12)	C11—C12	1.393 (7)
Cu1—Cu2	2.6604 (11)	C12—C13	1.367 (7)
Cu2—N3	2.014 (4)	C12—H12	0.9300
Cu2—N2	2.449 (4)	C13—C14	1.384 (8)
N1—C5	1.340 (6)	C13—H13	0.9300
N1—C1	1.346 (7)	C14—C15	1.358 (7)
N2—C6	1.343 (6)	C14—H14	0.9300
N2—C10	1.352 (6)	C15—H15	0.9300
N3—C15	1.343 (6)	C16—C17	1.373 (7)
N3—C11	1.349 (6)	C16—C21	1.387 (8)
C1—C2	1.356 (9)	C17—C18	1.373 (8)
C1—H1	0.9300	C17—H17	0.9300
C2—C3	1.377 (10)	C18—C19	1.369 (9)
C2—H2	0.9300	C18—H18	0.9300
C3—C4	1.383 (9)	C19—C20	1.365 (9)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.377 (7)	C20—C21	1.395 (8)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.484 (7)	C21—H21	0.9300
C6—C7	1.385 (7)		

Cu1^{i}—I1—Cu1	59.85 (2)	N1—C5—C4	121.3 (5)
Cu1^{i}—I1—Cu2	102.16 (2)	N1—C5—C6	115.6 (4)
Cu1—I1—Cu2	59.58 (2)	C4—C5—C6	123.1 (5)
N1—Cu1—N2	77.43 (15)	N2—C6—C7	122.3 (4)
N1—Cu1—I1^{i}	123.67 (13)	N2—C6—C5	115.1 (4)
N2—Cu1—I1^{i}	99.72 (10)	C7—C6—C5	122.7 (4)
N1—Cu1—Cu1^{i}	148.60 (13)	C6—C7—C8	120.5 (4)
N2—Cu1—Cu1^{i}	133.94 (11)	C6—C7—H7	119.7
I1^{i}—Cu1—Cu1^{i}	61.14 (3)	C8—C7—H7	119.7
N1—Cu1—I1	107.45 (13)	C9—C8—C7	116.5 (4)
N2—Cu1—I1	121.33 (11)	C9—C8—C16	121.6 (5)
I1^{i}—Cu1—I1	120.15 (2)	C7—C8—C16	121.9 (4)
Cu1^{i}—Cu1—I1	59.01 (3)	C8—C9—C10	120.9 (5)
N1—Cu1—Cu2	91.95 (12)	C8—C9—H9	119.5
N2—Cu1—Cu2	59.51 (10)	C10—C9—H9	119.5
I1^{i}—Cu1—Cu2	135.42 (3)	N2—C10—C9	121.7 (5)
Cu1^{i}—Cu1—Cu2	103.24 (4)	N2—C10—C11	116.5 (4)
I1—Cu1—Cu2	61.89 (2)	C9—C10—C11	121.7 (5)
N3—Cu2—N2	75.98 (15)	N3—C11—C12	121.6 (4)
N3—Cu2—I2	137.12 (12)	N3—C11—C10	116.0 (4)
N2—Cu2—I2	102.33 (9)	C12—C11—C10	122.4 (4)
N3—Cu2—Cu1	88.18 (13)	C13—C12—C11	119.2 (5)

N2—Cu2—Cu1	51.10 (9)	C13—C12—H12	120.4
I2—Cu2—Cu1	124.69 (3)	C11—C12—H12	120.4
N3—Cu2—I1	100.63 (11)	C12—C13—C14	119.6 (5)
N2—Cu2—I1	109.59 (9)	C12—C13—H13	120.2
I2—Cu2—I1	119.33 (3)	C14—C13—H13	120.2
Cu1—Cu2—I1	58.54 (2)	C15—C14—C13	117.9 (5)
C5—N1—C1	118.2 (5)	C15—C14—H14	121.0
C5—N1—Cu1	116.7 (3)	C13—C14—H14	121.0
C1—N1—Cu1	125.1 (4)	N3—C15—C14	124.4 (5)
C6—N2—C10	118.0 (4)	N3—C15—H15	117.8
C6—N2—Cu1	108.6 (3)	C14—C15—H15	117.8
C10—N2—Cu1	127.1 (3)	C17—C16—C21	117.0 (5)
C6—N2—Cu2	125.8 (3)	C17—C16—C8	122.2 (5)
C10—N2—Cu2	99.8 (3)	C21—C16—C8	120.8 (5)
Cu1—N2—Cu2	69.39 (11)	C16—C17—C18	122.2 (6)
C15—N3—C11	117.3 (4)	C16—C17—H17	118.9
C15—N3—Cu2	124.1 (3)	C18—C17—H17	118.9
C11—N3—Cu2	118.5 (3)	C19—C18—C17	119.8 (6)
N1—C1—C2	123.7 (6)	C19—C18—H18	120.1
N1—C1—H1	118.1	C17—C18—H18	120.1
C2—C1—H1	118.1	C20—C19—C18	120.3 (6)
C1—C2—C3	118.2 (6)	C20—C19—H19	119.8
C1—C2—H2	120.9	C18—C19—H19	119.8
C3—C2—H2	120.9	C19—C20—C21	119.2 (7)
C2—C3—C4	119.2 (6)	C19—C20—H20	120.4
C2—C3—H3	120.4	C21—C20—H20	120.4
C4—C3—H3	120.4	C16—C21—C20	121.5 (6)
C5—C4—C3	119.5 (6)	C16—C21—H21	119.3
C5—C4—H4	120.3	C20—C21—H21	119.3
C3—C4—H4	120.3		

Cu1^{i}—I1—Cu1—N1	148.74 (13)	I2—Cu2—N3—C15	103.2 (4)
Cu2—I1—Cu1—N1	−82.68 (13)	Cu1—Cu2—N3—C15	−113.5 (4)
Cu1^{i}—I1—Cu1—N2	−125.60 (13)	I1—Cu2—N3—C15	−56.0 (4)
Cu2—I1—Cu1—N2	2.98 (12)	N2—Cu2—N3—C11	11.9 (3)
Cu1^{i}—I1—Cu1—I1^{i}	0.0	I2—Cu2—N3—C11	−81.2 (4)
Cu2—I1—Cu1—I1^{i}	128.58 (4)	Cu1—Cu2—N3—C11	62.1 (3)
Cu2—I1—Cu1—Cu1^{i}	128.58 (4)	I1—Cu2—N3—C11	119.6 (3)
Cu1^{i}—I1—Cu1—Cu2	−128.58 (4)	C5—N1—C1—C2	0.6 (10)
N1—Cu1—Cu2—N3	−147.57 (16)	Cu1—N1—C1—C2	−179.8 (5)
N2—Cu1—Cu2—N3	−73.40 (16)	N1—C1—C2—C3	1.3 (11)
I1^{i}—Cu1—Cu2—N3	−1.98 (12)	C1—C2—C3—C4	−2.5 (11)
Cu1^{i}—Cu1—Cu2—N3	60.13 (11)	C2—C3—C4—C5	1.9 (10)
I1—Cu1—Cu2—N3	103.64 (11)	C1—N1—C5—C4	−1.2 (8)
N1—Cu1—Cu2—N2	−74.17 (17)	Cu1—N1—C5—C4	179.1 (4)
I1^{i}—Cu1—Cu2—N2	71.42 (12)	C1—N1—C5—C6	175.8 (5)
Cu1^{i}—Cu1—Cu2—N2	133.53 (12)	Cu1—N1—C5—C6	−3.8 (6)
I1—Cu1—Cu2—N2	177.04 (12)	C3—C4—C5—N1	0.0 (9)

N1—Cu1—Cu2—I2	2.84 (13)	C3—C4—C5—C6	−176.8 (6)
N2—Cu1—Cu2—I2	77.01 (12)	C10—N2—C6—C7	1.0 (7)
I1^{i}—Cu1—Cu2—I2	148.43 (3)	Cu1—N2—C6—C7	−153.0 (4)
Cu1^{i}—Cu1—Cu2—I2	−149.46 (4)	Cu2—N2—C6—C7	129.4 (4)
I1—Cu1—Cu2—I2	−105.95 (4)	C10—N2—C6—C5	−178.8 (4)
N1—Cu1—Cu2—I1	108.79 (12)	Cu1—N2—C6—C5	27.1 (5)
N2—Cu1—Cu2—I1	−177.04 (12)	Cu2—N2—C6—C5	−50.4 (6)
I1^{i}—Cu1—Cu2—I1	−105.62 (4)	N1—C5—C6—N2	−17.4 (7)
Cu1^{i}—Cu1—Cu2—I1	−43.51 (3)	C4—C5—C6—N2	159.6 (5)
Cu1^{i}—I1—Cu2—N3	−37.47 (13)	N1—C5—C6—C7	162.7 (5)
Cu1—I1—Cu2—N3	−81.21 (13)	C4—C5—C6—C7	−20.3 (8)
Cu1^{i}—I1—Cu2—N2	41.30 (10)	N2—C6—C7—C8	−1.6 (8)
Cu1—I1—Cu2—N2	−2.44 (10)	C5—C6—C7—C8	178.3 (5)
Cu1^{i}—I1—Cu2—I2	158.68 (3)	C6—C7—C8—C9	1.3 (8)
Cu1—I1—Cu2—I2	114.93 (4)	C6—C7—C8—C16	−178.0 (5)
Cu1^{i}—I1—Cu2—Cu1	43.74 (3)	C7—C8—C9—C10	−0.6 (8)
N2—Cu1—N1—C5	13.9 (4)	C16—C8—C9—C10	178.8 (5)
I1^{i}—Cu1—N1—C5	−79.5 (4)	C6—N2—C10—C9	−0.3 (7)
Cu1^{i}—Cu1—N1—C5	−168.2 (3)	Cu1—N2—C10—C9	148.4 (4)
I1—Cu1—N1—C5	133.2 (4)	Cu2—N2—C10—C9	−140.1 (4)
Cu2—Cu1—N1—C5	72.1 (4)	C6—N2—C10—C11	178.2 (4)
N2—Cu1—N1—C1	−165.7 (5)	Cu1—N2—C10—C11	−33.1 (6)
I1^{i}—Cu1—N1—C1	100.9 (5)	Cu2—N2—C10—C11	38.4 (5)
Cu1^{i}—Cu1—N1—C1	12.2 (6)	C8—C9—C10—N2	0.1 (8)
I1—Cu1—N1—C1	−46.4 (5)	C8—C9—C10—C11	−178.4 (5)
Cu2—Cu1—N1—C1	−107.5 (5)	C15—N3—C11—C12	1.4 (7)
N1—Cu1—N2—C6	−22.3 (3)	Cu2—N3—C11—C12	−174.5 (4)
I1^{i}—Cu1—N2—C6	100.2 (3)	C15—N3—C11—C10	−179.2 (4)
Cu1^{i}—Cu1—N2—C6	159.2 (3)	Cu2—N3—C11—C10	4.9 (6)
I1—Cu1—N2—C6	−125.3 (3)	N2—C10—C11—N3	−34.7 (6)
Cu2—Cu1—N2—C6	−122.2 (3)	C9—C10—C11—N3	143.8 (5)
N1—Cu1—N2—C10	−173.4 (4)	N2—C10—C11—C12	144.6 (5)
I1^{i}—Cu1—N2—C10	−50.8 (4)	C9—C10—C11—C12	−36.8 (7)
Cu1^{i}—Cu1—N2—C10	8.2 (5)	N3—C11—C12—C13	−2.3 (8)
I1—Cu1—N2—C10	83.7 (4)	C10—C11—C12—C13	178.3 (5)
Cu2—Cu1—N2—C10	86.7 (4)	C11—C12—C13—C14	1.6 (8)
N1—Cu1—N2—Cu2	99.89 (14)	C12—C13—C14—C15	0.0 (8)
I1^{i}—Cu1—N2—Cu2	−137.55 (6)	C11—N3—C15—C14	0.3 (8)
Cu1^{i}—Cu1—N2—Cu2	−78.55 (14)	Cu2—N3—C15—C14	175.9 (4)
I1—Cu1—N2—Cu2	−3.05 (12)	C13—C14—C15—N3	−0.9 (9)
N3—Cu2—N2—C6	−162.3 (4)	C9—C8—C16—C17	−164.7 (5)
I2—Cu2—N2—C6	−26.4 (4)	C7—C8—C16—C17	14.7 (8)
Cu1—Cu2—N2—C6	98.5 (4)	C9—C8—C16—C21	16.6 (8)
I1—Cu2—N2—C6	101.2 (4)	C7—C8—C16—C21	−164.0 (5)
N3—Cu2—N2—C10	−26.9 (3)	C21—C16—C17—C18	−0.9 (9)
I2—Cu2—N2—C10	109.0 (3)	C8—C16—C17—C18	−179.6 (6)
Cu1—Cu2—N2—C10	−126.1 (3)	C16—C17—C18—C19	1.4 (10)
I1—Cu2—N2—C10	−123.4 (3)	C17—C18—C19—C20	−1.1 (11)

N3—Cu2—N2—Cu1	99.16 (15)	C18—C19—C20—C21	0.4 (11)
I2—Cu2—N2—Cu1	−124.90 (7)	C17—C16—C21—C20	0.2 (9)
I1—Cu2—N2—Cu1	2.68 (11)	C8—C16—C21—C20	178.9 (6)
N2—Cu2—N3—C15	−163.7 (4)	C19—C20—C21—C16	0.0 (11)

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