

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

{ μ -Bis(1-methylimidazol-2-yl)methane- $\kappa^2N^3:N^{3'}$ }bis{[(1-methylimidazol-2-yl)methane- $\kappa^2N^3,N^{3'}$]copper(I)} bis(trifluoromethanesulfonate)

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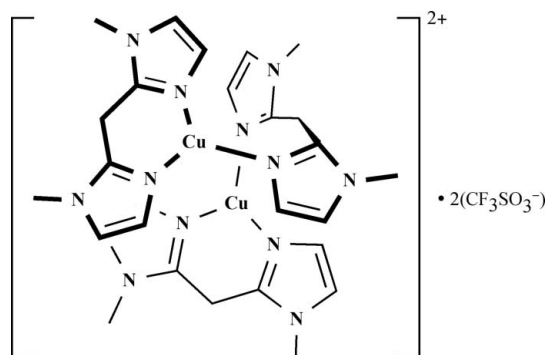
Received 10 August 2009; accepted 29 September 2009

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.055; wR factor = 0.146; data-to-parameter ratio = 17.0.

The title compound, $[Cu_2(C_9H_{12}N_4)_3](CF_3SO_3)_2$, contains two Cu^I ions, three bis(1-methylimidazol-2-yl)methane (Me_2BIM) ligands, and two trifluoromethanesulfonate anions in the asymmetric unit. Each Cu^I ion has a distorted trigonal-planar geometry and is coordinated by two N atoms from the Me_2BIM ligand and another N atom from the Me_2BIM that acts as a bridging ligand, another N atom of the bridging Me_2BIM being linked to the second Cu^I ion. The imidazole rings of Me_2BIM form intramolecular π - π stacking interactions [centroid-centroid distances = 3.445 (2) and 3.547 (2) Å].

Related literature

For the protonated ligand Me_2BIM , see: Messerle *et al.* (2003). For coordination complexes with one or two Me_2BIM ligands chelating one metal center, see: Elgafi *et al.* (1999); Abuskhuna *et al.* (2004a); Burling *et al.* (2004); Kennedy *et al.* (2007); Dabb *et al.* (2009). For Cu^{II} complexes with two BIM ligands chelating one metal center, see: Place *et al.* (1998). For Ag^I complexes with two BIM ligands bridging two metals, see: Abuskhuna *et al.* (2004b). The Me_2BIM ligand was synthesized by modified literature methods (Byers & Canty, 1990; Elgafi *et al.*, 1997).



Experimental

Crystal data

$[Cu_2(C_9H_{12}N_4)_3](CF_3SO_3)_2$
 $M_r = 953.88$
 Monoclinic, $P2_1/n$
 $a = 22.5575$ (11) Å
 $b = 7.0307$ (3) Å
 $c = 25.4982$ (16) Å
 $\beta = 109.118$ (2)°

$V = 3820.9$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.31$ mm⁻¹
 $T = 173$ K
 $0.20 \times 0.15 \times 0.15$ mm

Data collection

Rigaku Mercury diffractometer
 Absorption correction: none
 29376 measured reflections

8745 independent reflections
 6639 reflections with $I^2 > 2\sigma(I^2)$
 $R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.146$
 $S = 1.14$
 8745 reflections

515 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.58$ e Å⁻³
 $\Delta\rho_{min} = -0.72$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	2.042 (2)	Cu2—N5	2.049 (3)
Cu1—N3	1.958 (3)	Cu2—N7	1.935 (3)
Cu1—N9	1.914 (2)	Cu2—N11	1.916 (3)
N1—Cu1—N3	95.56 (12)	N5—Cu2—N7	93.66 (12)
N1—Cu1—N9	121.37 (12)	N5—Cu2—N11	115.27 (11)
N3—Cu1—N9	142.95 (12)	N7—Cu2—N11	150.78 (12)

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 2007); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

We gratefully acknowledge support of this work by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2129).

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supplementary materials

Acta Cryst. (2009). E65, m1286-m1287 [doi:10.1107/S1600536809039622]

{ μ -Bis(1-methylimidazol-2-yl)methane- $\kappa^2N^3:N^3'$ }bis{(1-methylimidazol-2-yl)methane- κ^2N^3,N^3' }copper(I)} bis(trifluoromethanesulfonate)

J. Matsumoto, Y. Kajita and H. Masuda

Comment

Ligand bis(imidazol-2-yl)methane derivative is a bidentate ligand, either chelating one metal center or bridging two metals. The crystal structures of Cu^{II} complexes with bis(imidazol-2-yl)methane (BIM) and bis(1-methylimidazol-2-yl)methane (Me₂BIM) have been reported by Place *et al.* (1998), Abuskhuna *et al.* (2004a), respectively. In addition, that of Ag^I complex with BIM has been reported by Abuskhuna *et al.* (2004b). The Cu^{II} complexes have four- or six-coordinate structure that is coordinated with two Me₂BIM ligands, and the Ag^I complex forms a two-coordinate structure bridged by BIM. The title compound, [(μ -Me₂BIM){Cu(Me₂BIM)}₂](OTf)₂, contains two Cu^I ions, three bis(1-methylimidazol-2-yl)methane (Me₂BIM) ligands, and two trifluoromethanesulfonate anions as an independent unit in the unit cell. Each Cu^I ion has a distorted trigonal planar geometry coordinated with two N atoms from Me₂BIM and one N atom from a bridging Me₂BIM ligand, and an N atom from an additional bridging Me₂BIM which is linked to another Cu^I ion. This is a novel dinuclear Cu^I complex with Me₂BIM. An intramolecular π — π stackings are formed between the imidazol rings; angles between the imidazole ring 1 containing N(1) and the ring 2 containing N(7) and between the ring 3 containing N(5) and the ring 4 containing N(9) are 4.4 (1) and 2.2 (2)°, respectively, and distances of the centroid of plane 1 to plane 2 and that of plane 3 to plane 4 are 3.445 (2) and 3.547 (2) Å, respectively.

Experimental

Ligand Me₂BIM was synthesized by modifying the literature methods of Byers *et al.* (1990) and Elgafi *et al.* (1997). Ligand Me₂BIM (1.13 mmol, 200 mg) in CH₂Cl₂ (4 ml) was added into a MeCN solution (3 ml) of [Cu(MeCN)₄](OTf) (1.15 mmol, 433 mg). The mixture was stirred for 1 h at room temperature in a glovebox ([O₂] < 1 p.p.m. and [H₂O] < 1 p.p.m.). After addition of Et₂O (7 ml), the resulting precipitates were collected by filtration and dried to give an yellow powder in a 65% yield. Single crystals suitable for X-ray crystallographic analysis were obtained by recrystallization from CH₂Cl₂/MeCN/Et₂O.

Refinement

Hydrogen atoms attached to carbon atoms were positioned geometrically and treated as riding with aromatic C—H = 0.95 Å, methyl C—H = 0.98 Å, and methylenic C—H = 0.99 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

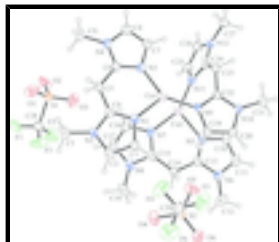


Fig. 1. The molecular view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

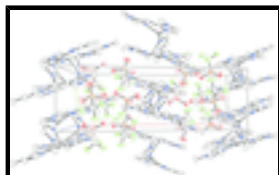


Fig. 2. The crystal packing of the title compound viewed along the *c* axis. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms that are not involved in hydrogen bonding are omitted for clarity.

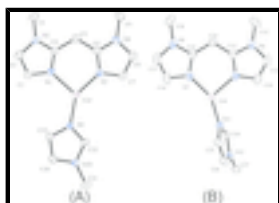


Fig. 3. The structures of (A) and (B) show the circumferences of the copper centers, Cu(1) and Cu(2), respectively. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms that are not involved in hydrogen bonding have been omitted for clarity.

{ μ -Bis(1-methylimidazol-2-yl)methane- $\kappa^2N^3:N^3$ }bis{[(1-methylimidazol-2-yl)methane- κ^2N^3,N^3]copper(I)} bis(trifluoromethanesulfonate)

Crystal data

[Cu₂(C₉H₁₂N₄)₃](CF₃SO₃)₂

M_r = 953.88

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2yn

a = 22.5575 (11) Å

b = 7.0307 (3) Å

c = 25.4982 (16) Å

β = 109.118 (2)°

V = 3820.9 (3) Å³

Z = 4

*F*₀₀₀ = 1944.00

D_x = 1.658 Mg m⁻³

Mo *K*α radiation, λ = 0.71070 Å

Cell parameters from 10516 reflections

θ = 3.0–27.5°

μ = 1.31 mm⁻¹

T = 173 K

Block, yellow

0.20 × 0.15 × 0.15 mm

Data collection

Rigaku Mercury diffractometer

Detector resolution: 7.31 pixels mm⁻¹

T = 173 K

ω scans

Absorption correction: none

29376 measured reflections

6639 reflections with *F*² > 2σ(*F*²)

*R*_{int} = 0.039

θ_{max} = 27.5°

h = -29→23

k = -9→9

l = -27→33

8745 independent reflections

Refinement

Refinement on F^2

$$R[F^2 > 2\sigma(F^2)] = 0.055$$

$$wR(F^2) = 0.146$$

$$S = 1.14$$

8745 reflections

515 parameters

All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 1.5952P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.72 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

Refinement. Refinement was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu(1)	0.525378 (19)	0.21542 (6)	0.763364 (17)	0.03927 (13)
Cu(2)	0.52080 (2)	0.61525 (6)	0.716419 (19)	0.04633 (14)
S(1)	0.81822 (4)	0.46106 (15)	0.93194 (4)	0.0487 (2)
S(2)	0.34890 (4)	0.48802 (15)	0.89323 (4)	0.0475 (2)
F(1)	0.87401 (14)	0.6587 (6)	1.02074 (11)	0.1071 (12)
F(2)	0.8022 (2)	0.8084 (4)	0.96078 (14)	0.1107 (12)
F(3)	0.77953 (15)	0.5968 (4)	1.01045 (15)	0.1008 (11)
F(4)	0.38615 (13)	0.1387 (4)	0.91831 (15)	0.0937 (9)
F(5)	0.28917 (13)	0.1643 (4)	0.87220 (15)	0.0935 (10)
F(6)	0.32319 (18)	0.2407 (5)	0.95855 (15)	0.1125 (12)
O(1)	0.83456 (19)	0.2915 (5)	0.96391 (16)	0.0920 (12)
O(2)	0.86351 (15)	0.5278 (5)	0.90881 (12)	0.0753 (9)
O(3)	0.75529 (14)	0.4666 (5)	0.89437 (15)	0.0845 (10)
O(4)	0.40376 (14)	0.5429 (5)	0.93745 (14)	0.0859 (11)
O(5)	0.35806 (17)	0.4652 (4)	0.84099 (12)	0.0761 (9)
O(6)	0.29232 (13)	0.5838 (4)	0.89142 (13)	0.0627 (7)
N(1)	0.54920 (13)	0.1991 (3)	0.84769 (11)	0.0379 (6)
N(2)	0.61408 (14)	0.2013 (4)	0.93364 (11)	0.0406 (6)
N(3)	0.60648 (13)	0.1266 (4)	0.76032 (12)	0.0416 (6)
N(4)	0.70290 (13)	0.0161 (4)	0.78893 (13)	0.0461 (7)
N(5)	0.44244 (14)	0.7760 (4)	0.70788 (12)	0.0413 (6)
N(6)	0.36224 (14)	0.8792 (4)	0.73090 (14)	0.0474 (7)
N(7)	0.55491 (14)	0.6557 (4)	0.79575 (13)	0.0449 (7)
N(8)	0.55692 (15)	0.7111 (4)	0.88142 (13)	0.0489 (7)
N(9)	0.44262 (12)	0.2866 (3)	0.71791 (11)	0.0342 (5)
N(10)	0.36179 (12)	0.3562 (3)	0.64410 (11)	0.0359 (6)
N(11)	0.52866 (13)	0.5210 (4)	0.64851 (12)	0.0409 (6)

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N(12)	0.52401 (13)	0.3560 (4)	0.57365 (12)	0.0449 (7)
C(1)	0.51766 (17)	0.2603 (4)	0.88285 (15)	0.0418 (7)
C(2)	0.55684 (17)	0.2619 (5)	0.93589 (15)	0.0441 (8)
C(3)	0.67175 (18)	0.1869 (6)	0.98115 (15)	0.0542 (10)
C(4)	0.60759 (15)	0.1658 (4)	0.87997 (13)	0.0362 (7)
C(5)	0.66238 (16)	0.1017 (5)	0.86426 (14)	0.0410 (7)
C(6)	0.65498 (16)	0.0818 (4)	0.80423 (15)	0.0395 (7)
C(7)	0.62501 (18)	0.0857 (5)	0.71475 (15)	0.0500 (9)
C(8)	0.68394 (18)	0.0176 (6)	0.73197 (16)	0.0536 (9)
C(9)	0.76404 (18)	-0.0461 (7)	0.82589 (18)	0.0656 (12)
C(10)	0.39374 (18)	0.8252 (5)	0.66014 (17)	0.0507 (9)
C(11)	0.34477 (18)	0.8879 (5)	0.67389 (17)	0.0528 (10)
C(12)	0.3231 (2)	0.9282 (6)	0.7644 (2)	0.0670 (12)
C(13)	0.42209 (15)	0.8108 (4)	0.74969 (14)	0.0373 (7)
C(14)	0.45525 (16)	0.7850 (5)	0.81032 (14)	0.0429 (8)
C(15)	0.52150 (16)	0.7159 (4)	0.82688 (14)	0.0401 (7)
C(16)	0.61394 (17)	0.6113 (5)	0.83269 (18)	0.0539 (10)
C(17)	0.61495 (19)	0.6439 (5)	0.88480 (18)	0.0565 (10)
C(18)	0.5355 (2)	0.7561 (6)	0.92820 (17)	0.0621 (11)
C(19)	0.39341 (15)	0.3483 (4)	0.73479 (14)	0.0373 (7)
C(20)	0.34333 (16)	0.3899 (4)	0.68955 (15)	0.0404 (7)
C(21)	0.32136 (18)	0.3793 (5)	0.58651 (15)	0.0524 (9)
C(22)	0.42150 (15)	0.2945 (4)	0.66262 (13)	0.0339 (6)
C(23)	0.45787 (16)	0.2303 (5)	0.62668 (15)	0.0414 (7)
C(24)	0.50238 (15)	0.3732 (5)	0.61708 (14)	0.0377 (7)
C(25)	0.56876 (17)	0.6003 (5)	0.62356 (17)	0.0502 (9)
C(26)	0.56674 (18)	0.4982 (6)	0.57821 (18)	0.0586 (10)
C(27)	0.50716 (19)	0.2054 (6)	0.53201 (17)	0.0612 (11)
C(28)	0.8175 (2)	0.6401 (6)	0.98281 (17)	0.0580 (10)
C(29)	0.3366 (2)	0.2461 (7)	0.9112 (2)	0.0617 (11)
H(3A)	0.6629	0.2203	1.0152	0.065*
H(3B)	0.7032	0.2745	0.9761	0.065*
H(3C)	0.6877	0.0564	0.9841	0.065*
H(9A)	0.7932	-0.0578	0.8048	0.079*
H(9B)	0.7597	-0.1698	0.8420	0.079*
H(9C)	0.7803	0.0474	0.8557	0.079*
H(12A)	0.2814	0.9670	0.7400	0.080*
H(12B)	0.3424	1.0333	0.7894	0.080*
H(12C)	0.3190	0.8174	0.7863	0.080*
H(18A)	0.5687	0.7257	0.9630	0.074*
H(18B)	0.4980	0.6811	0.9254	0.074*
H(18C)	0.5254	0.8919	0.9275	0.074*
H(21A)	0.3013	0.5046	0.5818	0.063*
H(21B)	0.2891	0.2800	0.5772	0.063*
H(21C)	0.3466	0.3688	0.5619	0.063*
H(27A)	0.5262	0.2318	0.5033	0.073*
H(27B)	0.4614	0.2002	0.5151	0.073*
H(27C)	0.5226	0.0832	0.5497	0.073*
H(5A)	0.6759	-0.0232	0.8821	0.049*

H(5B)	0.6971	0.1923	0.8807	0.049*
H(14A)	0.4308	0.6940	0.8247	0.051*
H(14B)	0.4550	0.9084	0.8289	0.051*
H(23A)	0.4279	0.1925	0.5902	0.050*
H(23B)	0.4820	0.1155	0.6436	0.050*
H(1)	0.4747	0.2960	0.8714	0.050*
H(2)	0.5470	0.2973	0.9680	0.053*
H(7)	0.5998	0.1031	0.6771	0.060*
H(8)	0.7077	-0.0216	0.7093	0.064*
H(10)	0.3950	0.8157	0.6234	0.061*
H(11)	0.3056	0.9303	0.6491	0.063*
H(16)	0.6482	0.5650	0.8226	0.065*
H(17)	0.6494	0.6240	0.9178	0.068*
H(19)	0.3946	0.3597	0.7722	0.045*
H(20)	0.3034	0.4337	0.6893	0.049*
H(25)	0.5939	0.7100	0.6364	0.060*
H(26)	0.5904	0.5207	0.5541	0.070*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu(1)	0.0346 (2)	0.0410 (2)	0.0372 (2)	-0.00196 (17)	0.00483 (17)	0.00048 (18)
Cu(2)	0.0499 (2)	0.0403 (2)	0.0498 (2)	-0.00973 (19)	0.0176 (2)	-0.0088 (2)
S(1)	0.0388 (4)	0.0551 (5)	0.0516 (5)	0.0004 (4)	0.0142 (4)	0.0076 (4)
S(2)	0.0425 (5)	0.0587 (5)	0.0429 (5)	-0.0080 (4)	0.0163 (4)	-0.0085 (4)
F(1)	0.0700 (18)	0.202 (3)	0.0457 (15)	-0.017 (2)	0.0142 (13)	-0.0382 (19)
F(2)	0.188 (3)	0.0547 (17)	0.085 (2)	0.000 (2)	0.039 (2)	-0.0057 (16)
F(3)	0.103 (2)	0.100 (2)	0.140 (2)	-0.0088 (18)	0.095 (2)	-0.017 (2)
F(4)	0.0673 (18)	0.079 (2)	0.135 (2)	0.0213 (15)	0.0337 (18)	0.0262 (19)
F(5)	0.0582 (16)	0.0613 (16)	0.148 (2)	-0.0143 (13)	0.0164 (17)	-0.0128 (18)
F(6)	0.129 (2)	0.132 (3)	0.104 (2)	0.016 (2)	0.076 (2)	0.050 (2)
O(1)	0.127 (3)	0.072 (2)	0.095 (2)	0.047 (2)	0.061 (2)	0.038 (2)
O(2)	0.077 (2)	0.111 (2)	0.0459 (16)	-0.0351 (19)	0.0308 (14)	-0.0173 (17)
O(3)	0.0433 (16)	0.079 (2)	0.109 (2)	-0.0067 (15)	-0.0063 (16)	-0.019 (2)
O(4)	0.0546 (19)	0.105 (2)	0.084 (2)	-0.0264 (18)	0.0035 (16)	-0.033 (2)
O(5)	0.107 (2)	0.084 (2)	0.0552 (17)	0.0041 (19)	0.0506 (18)	0.0037 (16)
O(6)	0.0498 (16)	0.0592 (17)	0.078 (2)	-0.0022 (13)	0.0193 (14)	-0.0176 (15)
N(1)	0.0391 (15)	0.0367 (14)	0.0355 (14)	-0.0044 (11)	0.0091 (12)	-0.0003 (12)
N(2)	0.0475 (16)	0.0373 (15)	0.0316 (14)	-0.0037 (12)	0.0055 (12)	0.0020 (12)
N(3)	0.0387 (15)	0.0454 (16)	0.0394 (15)	0.0008 (12)	0.0109 (12)	0.0008 (13)
N(4)	0.0367 (15)	0.0469 (17)	0.0494 (17)	0.0066 (13)	0.0071 (13)	0.0001 (14)
N(5)	0.0436 (16)	0.0340 (14)	0.0393 (16)	-0.0042 (12)	0.0039 (12)	-0.0025 (12)
N(6)	0.0399 (16)	0.0362 (15)	0.063 (2)	-0.0016 (12)	0.0133 (14)	0.0012 (14)
N(7)	0.0379 (15)	0.0330 (14)	0.0543 (18)	-0.0078 (12)	0.0023 (13)	-0.0037 (13)
N(8)	0.0566 (19)	0.0388 (16)	0.0391 (16)	-0.0131 (14)	-0.0010 (14)	0.0003 (13)
N(9)	0.0340 (13)	0.0348 (14)	0.0314 (13)	-0.0053 (11)	0.0075 (11)	-0.0033 (11)
N(10)	0.0323 (13)	0.0367 (14)	0.0350 (14)	-0.0013 (11)	0.0057 (11)	-0.0002 (11)
N(11)	0.0336 (14)	0.0384 (15)	0.0484 (16)	-0.0036 (11)	0.0104 (12)	0.0030 (13)

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N(12)	0.0333 (14)	0.0611 (19)	0.0413 (16)	0.0005 (13)	0.0135 (12)	-0.0041 (14)
C(1)	0.0435 (19)	0.0390 (18)	0.0415 (19)	-0.0008 (14)	0.0119 (15)	-0.0008 (15)
C(2)	0.053 (2)	0.0401 (18)	0.0392 (19)	-0.0049 (15)	0.0150 (16)	0.0008 (15)
C(3)	0.054 (2)	0.063 (2)	0.0341 (19)	-0.0035 (19)	-0.0005 (16)	0.0042 (18)
C(4)	0.0431 (18)	0.0308 (15)	0.0318 (16)	-0.0065 (13)	0.0082 (13)	0.0010 (13)
C(5)	0.0374 (17)	0.0411 (18)	0.0385 (18)	-0.0034 (14)	0.0045 (14)	0.0005 (15)
C(6)	0.0364 (17)	0.0347 (16)	0.0433 (18)	-0.0033 (13)	0.0074 (14)	-0.0026 (14)
C(7)	0.047 (2)	0.063 (2)	0.0380 (19)	0.0073 (18)	0.0116 (16)	0.0002 (17)
C(8)	0.048 (2)	0.066 (2)	0.048 (2)	0.0044 (19)	0.0182 (17)	-0.0013 (19)
C(9)	0.042 (2)	0.085 (3)	0.063 (2)	0.019 (2)	0.0084 (19)	0.000 (2)
C(10)	0.053 (2)	0.0403 (19)	0.046 (2)	-0.0089 (16)	-0.0012 (17)	0.0015 (16)
C(11)	0.044 (2)	0.0393 (19)	0.058 (2)	-0.0037 (16)	-0.0056 (17)	0.0087 (18)
C(12)	0.052 (2)	0.056 (2)	0.100 (3)	0.0067 (19)	0.035 (2)	0.013 (2)
C(13)	0.0368 (17)	0.0288 (15)	0.0432 (18)	-0.0054 (12)	0.0091 (14)	0.0008 (14)
C(14)	0.0447 (19)	0.0423 (19)	0.0395 (18)	-0.0092 (15)	0.0109 (15)	-0.0065 (15)
C(15)	0.0422 (18)	0.0312 (16)	0.0391 (18)	-0.0103 (13)	0.0027 (14)	-0.0001 (14)
C(16)	0.0362 (19)	0.0389 (19)	0.072 (2)	-0.0077 (15)	-0.0022 (18)	0.0017 (19)
C(17)	0.049 (2)	0.043 (2)	0.056 (2)	-0.0084 (17)	-0.0129 (18)	0.0064 (18)
C(18)	0.081 (3)	0.055 (2)	0.040 (2)	-0.018 (2)	0.006 (2)	-0.0049 (18)
C(19)	0.0357 (17)	0.0369 (17)	0.0399 (17)	-0.0049 (13)	0.0130 (14)	-0.0053 (14)
C(20)	0.0369 (17)	0.0372 (18)	0.048 (2)	-0.0017 (14)	0.0150 (15)	-0.0017 (15)
C(21)	0.049 (2)	0.057 (2)	0.042 (2)	-0.0015 (18)	0.0023 (16)	0.0024 (18)
C(22)	0.0351 (16)	0.0311 (15)	0.0331 (16)	-0.0044 (12)	0.0078 (13)	-0.0045 (13)
C(23)	0.0411 (18)	0.0405 (18)	0.0440 (19)	-0.0058 (14)	0.0159 (15)	-0.0092 (15)
C(24)	0.0314 (16)	0.0441 (19)	0.0356 (17)	0.0008 (13)	0.0083 (13)	-0.0019 (14)
C(25)	0.0355 (18)	0.054 (2)	0.064 (2)	-0.0065 (16)	0.0199 (17)	-0.0021 (19)
C(26)	0.042 (2)	0.080 (3)	0.061 (2)	-0.007 (2)	0.0266 (19)	0.000 (2)
C(27)	0.047 (2)	0.089 (3)	0.051 (2)	-0.002 (2)	0.0214 (18)	-0.022 (2)
C(28)	0.059 (2)	0.068 (2)	0.048 (2)	-0.003 (2)	0.0191 (19)	0.001 (2)
C(29)	0.048 (2)	0.071 (2)	0.066 (2)	0.001 (2)	0.018 (2)	0.009 (2)

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

Cu(1)—N(1)	2.042 (2)	N(12)—C(27)	1.459 (5)
Cu(1)—N(3)	1.958 (3)	C(1)—C(2)	1.352 (4)
Cu(1)—N(9)	1.914 (2)	C(4)—C(5)	1.488 (5)
Cu(2)—N(5)	2.049 (3)	C(5)—C(6)	1.491 (5)
Cu(2)—N(7)	1.935 (3)	C(7)—C(8)	1.344 (5)
Cu(2)—N(11)	1.916 (3)	C(10)—C(11)	1.338 (6)
S(1)—O(1)	1.423 (3)	C(13)—C(14)	1.492 (4)
S(1)—O(2)	1.416 (3)	C(14)—C(15)	1.495 (4)
S(1)—O(3)	1.430 (2)	C(16)—C(17)	1.341 (6)
S(1)—C(28)	1.811 (4)	C(19)—C(20)	1.356 (4)
S(2)—O(4)	1.427 (2)	C(22)—C(23)	1.486 (5)
S(2)—O(5)	1.422 (3)	C(23)—C(24)	1.496 (5)
S(2)—O(6)	1.430 (3)	C(25)—C(26)	1.349 (6)
S(2)—C(29)	1.807 (5)	C(1)—H(1)	0.950
F(1)—C(28)	1.331 (4)	C(2)—H(2)	0.950
F(2)—C(28)	1.307 (5)	C(3)—H(3A)	0.980

F(3)—C(28)	1.310 (6)	C(3)—H(3B)	0.980
F(4)—C(29)	1.312 (5)	C(3)—H(3C)	0.980
F(5)—C(29)	1.329 (4)	C(5)—H(5A)	0.990
F(6)—C(29)	1.337 (6)	C(5)—H(5B)	0.990
N(1)—C(1)	1.383 (5)	C(7)—H(7)	0.950
N(1)—C(4)	1.326 (3)	C(8)—H(8)	0.950
N(2)—C(2)	1.378 (5)	C(9)—H(9A)	0.980
N(2)—C(3)	1.462 (4)	C(9)—H(9B)	0.980
N(2)—C(4)	1.351 (4)	C(9)—H(9C)	0.980
N(3)—C(6)	1.322 (3)	C(10)—H(10)	0.950
N(3)—C(7)	1.388 (5)	C(11)—H(11)	0.950
N(4)—C(6)	1.346 (5)	C(12)—H(12A)	0.980
N(4)—C(8)	1.373 (5)	C(12)—H(12B)	0.980
N(4)—C(9)	1.459 (4)	C(12)—H(12C)	0.980
N(5)—C(10)	1.390 (4)	C(14)—H(14A)	0.990
N(5)—C(13)	1.314 (5)	C(14)—H(14B)	0.990
N(6)—C(11)	1.377 (5)	C(16)—H(16)	0.950
N(6)—C(12)	1.458 (6)	C(17)—H(17)	0.950
N(6)—C(13)	1.364 (4)	C(18)—H(18A)	0.980
N(7)—C(15)	1.330 (5)	C(18)—H(18B)	0.980
N(7)—C(16)	1.392 (4)	C(18)—H(18C)	0.980
N(8)—C(15)	1.359 (4)	C(19)—H(19)	0.950
N(8)—C(17)	1.368 (5)	C(20)—H(20)	0.950
N(8)—C(18)	1.461 (6)	C(21)—H(21A)	0.980
N(9)—C(19)	1.385 (4)	C(21)—H(21B)	0.980
N(9)—C(22)	1.333 (4)	C(21)—H(21C)	0.980
N(10)—C(20)	1.374 (5)	C(23)—H(23A)	0.990
N(10)—C(21)	1.462 (4)	C(23)—H(23B)	0.990
N(10)—C(22)	1.345 (4)	C(25)—H(25)	0.950
N(11)—C(24)	1.327 (4)	C(26)—H(26)	0.950
N(11)—C(25)	1.382 (5)	C(27)—H(27A)	0.980
N(12)—C(24)	1.354 (5)	C(27)—H(27B)	0.980
N(12)—C(26)	1.367 (5)	C(27)—H(27C)	0.980
N(1)—Cu(1)—N(3)	95.56 (12)	S(1)—C(28)—F(1)	110.9 (3)
N(1)—Cu(1)—N(9)	121.37 (12)	S(1)—C(28)—F(2)	112.6 (3)
N(3)—Cu(1)—N(9)	142.95 (12)	S(1)—C(28)—F(3)	112.6 (3)
N(5)—Cu(2)—N(7)	93.66 (12)	F(1)—C(28)—F(2)	106.2 (3)
N(5)—Cu(2)—N(11)	115.27 (11)	F(1)—C(28)—F(3)	105.7 (3)
N(7)—Cu(2)—N(11)	150.78 (12)	F(2)—C(28)—F(3)	108.3 (4)
O(1)—S(1)—O(2)	115.4 (2)	S(2)—C(29)—F(4)	112.4 (3)
O(1)—S(1)—O(3)	114.9 (2)	S(2)—C(29)—F(5)	111.7 (3)
O(1)—S(1)—C(28)	103.5 (2)	S(2)—C(29)—F(6)	110.8 (3)
O(2)—S(1)—O(3)	113.9 (2)	F(4)—C(29)—F(5)	107.1 (3)
O(2)—S(1)—C(28)	104.2 (2)	F(4)—C(29)—F(6)	107.1 (3)
O(3)—S(1)—C(28)	102.8 (2)	F(5)—C(29)—F(6)	107.4 (4)
O(4)—S(2)—O(5)	114.6 (2)	N(1)—C(1)—H(1)	124.9
O(4)—S(2)—O(6)	115.6 (2)	C(2)—C(1)—H(1)	124.9
O(4)—S(2)—C(29)	102.7 (2)	N(2)—C(2)—H(2)	127.2
O(5)—S(2)—O(6)	115.13 (19)	C(1)—C(2)—H(2)	127.2

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O(5)—S(2)—C(29)	102.3 (2)	N(2)—C(3)—H(3A)	109.5
O(6)—S(2)—C(29)	103.9 (2)	N(2)—C(3)—H(3B)	109.5
Cu(1)—N(1)—C(1)	130.7 (2)	N(2)—C(3)—H(3C)	109.5
Cu(1)—N(1)—C(4)	121.9 (2)	H(3A)—C(3)—H(3B)	109.5
C(1)—N(1)—C(4)	105.7 (2)	H(3A)—C(3)—H(3C)	109.5
C(2)—N(2)—C(3)	125.3 (3)	H(3B)—C(3)—H(3C)	109.5
C(2)—N(2)—C(4)	107.9 (2)	C(4)—C(5)—H(5A)	107.6
C(3)—N(2)—C(4)	126.7 (3)	C(4)—C(5)—H(5B)	107.6
Cu(1)—N(3)—C(6)	124.5 (2)	C(6)—C(5)—H(5A)	107.6
Cu(1)—N(3)—C(7)	129.8 (2)	C(6)—C(5)—H(5B)	107.6
C(6)—N(3)—C(7)	105.5 (3)	H(5A)—C(5)—H(5B)	107.1
C(6)—N(4)—C(8)	107.6 (2)	N(3)—C(7)—H(7)	125.1
C(6)—N(4)—C(9)	126.5 (3)	C(8)—C(7)—H(7)	125.1
C(8)—N(4)—C(9)	125.9 (3)	N(4)—C(8)—H(8)	126.9
Cu(2)—N(5)—C(10)	129.6 (2)	C(7)—C(8)—H(8)	126.8
Cu(2)—N(5)—C(13)	122.3 (2)	N(4)—C(9)—H(9A)	109.5
C(10)—N(5)—C(13)	106.2 (3)	N(4)—C(9)—H(9B)	109.5
C(11)—N(6)—C(12)	126.1 (3)	N(4)—C(9)—H(9C)	109.5
C(11)—N(6)—C(13)	107.1 (3)	H(9A)—C(9)—H(9B)	109.5
C(12)—N(6)—C(13)	126.7 (3)	H(9A)—C(9)—H(9C)	109.5
Cu(2)—N(7)—C(15)	124.2 (2)	H(9B)—C(9)—H(9C)	109.5
Cu(2)—N(7)—C(16)	129.7 (3)	N(5)—C(10)—H(10)	125.2
C(15)—N(7)—C(16)	105.7 (3)	C(11)—C(10)—H(10)	125.2
C(15)—N(8)—C(17)	107.6 (3)	N(6)—C(11)—H(11)	126.7
C(15)—N(8)—C(18)	126.1 (3)	C(10)—C(11)—H(11)	126.7
C(17)—N(8)—C(18)	126.1 (3)	N(6)—C(12)—H(12A)	109.5
Cu(1)—N(9)—C(19)	128.0 (2)	N(6)—C(12)—H(12B)	109.5
Cu(1)—N(9)—C(22)	126.2 (2)	N(6)—C(12)—H(12C)	109.5
C(19)—N(9)—C(22)	105.7 (2)	H(12A)—C(12)—H(12B)	109.5
C(20)—N(10)—C(21)	124.5 (2)	H(12A)—C(12)—H(12C)	109.5
C(20)—N(10)—C(22)	107.7 (2)	H(12B)—C(12)—H(12C)	109.5
C(21)—N(10)—C(22)	127.7 (3)	C(13)—C(14)—H(14A)	108.1
Cu(2)—N(11)—C(24)	131.4 (2)	C(13)—C(14)—H(14B)	108.1
Cu(2)—N(11)—C(25)	123.0 (2)	C(15)—C(14)—H(14A)	108.1
C(24)—N(11)—C(25)	105.5 (3)	C(15)—C(14)—H(14B)	108.2
C(24)—N(12)—C(26)	107.3 (3)	H(14A)—C(14)—H(14B)	107.3
C(24)—N(12)—C(27)	125.6 (3)	N(7)—C(16)—H(16)	125.2
C(26)—N(12)—C(27)	126.9 (3)	C(17)—C(16)—H(16)	125.2
N(1)—C(1)—C(2)	110.2 (3)	N(8)—C(17)—H(17)	126.5
N(2)—C(2)—C(1)	105.7 (3)	C(16)—C(17)—H(17)	126.5
N(1)—C(4)—N(2)	110.6 (3)	N(8)—C(18)—H(18A)	109.5
N(1)—C(4)—C(5)	129.1 (3)	N(8)—C(18)—H(18B)	109.5
N(2)—C(4)—C(5)	120.3 (2)	N(8)—C(18)—H(18C)	109.5
C(4)—C(5)—C(6)	118.8 (2)	H(18A)—C(18)—H(18B)	109.5
N(3)—C(6)—N(4)	110.9 (3)	H(18A)—C(18)—H(18C)	109.5
N(3)—C(6)—C(5)	129.1 (3)	H(18B)—C(18)—H(18C)	109.5
N(4)—C(6)—C(5)	120.0 (2)	N(9)—C(19)—H(19)	125.3
N(3)—C(7)—C(8)	109.7 (3)	C(20)—C(19)—H(19)	125.3
N(4)—C(8)—C(7)	106.3 (3)	N(10)—C(20)—H(20)	126.8

N(5)—C(10)—C(11)	109.6 (3)	C(19)—C(20)—H(20)	126.8
N(6)—C(11)—C(10)	106.6 (3)	N(10)—C(21)—H(21A)	109.5
N(5)—C(13)—N(6)	110.4 (2)	N(10)—C(21)—H(21B)	109.5
N(5)—C(13)—C(14)	128.9 (3)	N(10)—C(21)—H(21C)	109.5
N(6)—C(13)—C(14)	120.6 (3)	H(21A)—C(21)—H(21B)	109.5
C(13)—C(14)—C(15)	116.6 (3)	H(21A)—C(21)—H(21C)	109.5
N(7)—C(15)—N(8)	110.2 (3)	H(21B)—C(21)—H(21C)	109.5
N(7)—C(15)—C(14)	130.1 (2)	C(22)—C(23)—H(23A)	108.4
N(8)—C(15)—C(14)	119.7 (3)	C(22)—C(23)—H(23B)	108.4
N(7)—C(16)—C(17)	109.5 (3)	C(24)—C(23)—H(23A)	108.4
N(8)—C(17)—C(16)	106.9 (3)	C(24)—C(23)—H(23B)	108.4
N(9)—C(19)—C(20)	109.4 (3)	H(23A)—C(23)—H(23B)	107.4
N(10)—C(20)—C(19)	106.4 (3)	N(11)—C(25)—H(25)	125.2
N(9)—C(22)—N(10)	110.8 (3)	C(26)—C(25)—H(25)	125.2
N(9)—C(22)—C(23)	124.1 (2)	N(12)—C(26)—H(26)	126.7
N(10)—C(22)—C(23)	125.0 (2)	C(25)—C(26)—H(26)	126.7
C(22)—C(23)—C(24)	115.6 (2)	N(12)—C(27)—H(27A)	109.5
N(11)—C(24)—N(12)	110.8 (3)	N(12)—C(27)—H(27B)	109.5
N(11)—C(24)—C(23)	128.2 (3)	N(12)—C(27)—H(27C)	109.5
N(12)—C(24)—C(23)	121.0 (3)	H(27A)—C(27)—H(27B)	109.5
N(11)—C(25)—C(26)	109.7 (3)	H(27A)—C(27)—H(27C)	109.5
N(12)—C(26)—C(25)	106.7 (4)	H(27B)—C(27)—H(27C)	109.5
N(1)—Cu(1)—N(3)—C(6)	-1.1 (2)	Cu(2)—N(5)—C(10)—C(11)	163.8 (2)
N(1)—Cu(1)—N(3)—C(7)	174.5 (3)	Cu(2)—N(5)—C(13)—N(6)	-165.2 (2)
N(3)—Cu(1)—N(1)—C(1)	171.7 (2)	Cu(2)—N(5)—C(13)—C(14)	14.8 (4)
N(3)—Cu(1)—N(1)—C(4)	9.0 (2)	C(10)—N(5)—C(13)—N(6)	0.4 (3)
N(1)—Cu(1)—N(9)—C(19)	5.9 (3)	C(10)—N(5)—C(13)—C(14)	-179.6 (3)
N(1)—Cu(1)—N(9)—C(22)	-177.2 (2)	C(13)—N(5)—C(10)—C(11)	-0.3 (4)
N(9)—Cu(1)—N(1)—C(1)	-11.5 (3)	C(12)—N(6)—C(11)—C(10)	-178.1 (3)
N(9)—Cu(1)—N(1)—C(4)	-174.2 (2)	C(11)—N(6)—C(13)—N(5)	-0.3 (3)
N(3)—Cu(1)—N(9)—C(19)	-179.4 (2)	C(11)—N(6)—C(13)—C(14)	179.7 (3)
N(3)—Cu(1)—N(9)—C(22)	-2.5 (3)	C(13)—N(6)—C(11)—C(10)	0.1 (3)
N(9)—Cu(1)—N(3)—C(6)	-176.5 (2)	C(12)—N(6)—C(13)—N(5)	177.9 (3)
N(9)—Cu(1)—N(3)—C(7)	-1.0 (4)	C(12)—N(6)—C(13)—C(14)	-2.2 (5)
N(5)—Cu(2)—N(7)—C(15)	17.9 (2)	Cu(2)—N(7)—C(15)—N(8)	173.6 (2)
N(5)—Cu(2)—N(7)—C(16)	-170.1 (3)	Cu(2)—N(7)—C(15)—C(14)	-7.2 (5)
N(7)—Cu(2)—N(5)—C(10)	176.6 (3)	Cu(2)—N(7)—C(16)—C(17)	-172.7 (2)
N(7)—Cu(2)—N(5)—C(13)	-21.6 (2)	C(15)—N(7)—C(16)—C(17)	0.4 (4)
N(5)—Cu(2)—N(11)—C(24)	-80.3 (3)	C(16)—N(7)—C(15)—N(8)	0.0 (3)
N(5)—Cu(2)—N(11)—C(25)	102.8 (2)	C(16)—N(7)—C(15)—C(14)	179.2 (3)
N(11)—Cu(2)—N(5)—C(10)	0.8 (3)	C(15)—N(8)—C(17)—C(16)	0.6 (4)
N(11)—Cu(2)—N(5)—C(13)	162.7 (2)	C(17)—N(8)—C(15)—N(7)	-0.4 (4)
N(7)—Cu(2)—N(11)—C(24)	108.3 (3)	C(17)—N(8)—C(15)—C(14)	-179.7 (3)
N(7)—Cu(2)—N(11)—C(25)	-68.6 (3)	C(18)—N(8)—C(15)—N(7)	-176.3 (3)
N(11)—Cu(2)—N(7)—C(15)	-169.9 (2)	C(18)—N(8)—C(15)—C(14)	4.4 (5)
N(11)—Cu(2)—N(7)—C(16)	2.1 (4)	C(18)—N(8)—C(17)—C(16)	176.5 (3)
O(1)—S(1)—C(28)—F(1)	62.2 (3)	Cu(1)—N(9)—C(19)—C(20)	178.1 (2)
O(1)—S(1)—C(28)—F(2)	-179.0 (3)	Cu(1)—N(9)—C(22)—N(10)	-177.9 (2)
O(1)—S(1)—C(28)—F(3)	-56.2 (3)	Cu(1)—N(9)—C(22)—C(23)	6.2 (4)

supplementary materials

O(2)—S(1)—C(28)—F(1)	-58.9 (3)	C(19)—N(9)—C(22)—N(10)	-0.5 (3)
O(2)—S(1)—C(28)—F(2)	59.9 (3)	C(19)—N(9)—C(22)—C(23)	-176.4 (3)
O(2)—S(1)—C(28)—F(3)	-177.2 (2)	C(22)—N(9)—C(19)—C(20)	0.8 (3)
O(3)—S(1)—C(28)—F(1)	-178.0 (3)	C(21)—N(10)—C(20)—C(19)	178.7 (3)
O(3)—S(1)—C(28)—F(2)	-59.1 (4)	C(20)—N(10)—C(22)—N(9)	0.0 (3)
O(3)—S(1)—C(28)—F(3)	63.7 (3)	C(20)—N(10)—C(22)—C(23)	175.9 (3)
O(4)—S(2)—C(29)—F(4)	-55.1 (3)	C(22)—N(10)—C(20)—C(19)	0.5 (3)
O(4)—S(2)—C(29)—F(5)	-175.5 (3)	C(21)—N(10)—C(22)—N(9)	-178.1 (3)
O(4)—S(2)—C(29)—F(6)	64.7 (3)	C(21)—N(10)—C(22)—C(23)	-2.2 (5)
O(5)—S(2)—C(29)—F(4)	64.0 (3)	Cu(2)—N(11)—C(24)—N(12)	-177.3 (2)
O(5)—S(2)—C(29)—F(5)	-56.5 (4)	Cu(2)—N(11)—C(24)—C(23)	-1.0 (5)
O(5)—S(2)—C(29)—F(6)	-176.3 (2)	Cu(2)—N(11)—C(25)—C(26)	176.7 (2)
O(6)—S(2)—C(29)—F(4)	-175.9 (3)	C(24)—N(11)—C(25)—C(26)	-0.9 (3)
O(6)—S(2)—C(29)—F(5)	63.7 (4)	C(25)—N(11)—C(24)—N(12)	-0.0 (3)
O(6)—S(2)—C(29)—F(6)	-56.1 (3)	C(25)—N(11)—C(24)—C(23)	176.2 (3)
Cu(1)—N(1)—C(1)—C(2)	-165.4 (2)	C(24)—N(12)—C(26)—C(25)	-1.4 (4)
Cu(1)—N(1)—C(4)—N(2)	167.0 (2)	C(26)—N(12)—C(24)—N(11)	0.9 (3)
Cu(1)—N(1)—C(4)—C(5)	-11.9 (4)	C(26)—N(12)—C(24)—C(23)	-175.7 (2)
C(1)—N(1)—C(4)—N(2)	0.6 (3)	C(27)—N(12)—C(24)—N(11)	177.4 (3)
C(1)—N(1)—C(4)—C(5)	-178.4 (3)	C(27)—N(12)—C(24)—C(23)	0.9 (4)
C(4)—N(1)—C(1)—C(2)	-0.5 (3)	C(27)—N(12)—C(26)—C(25)	-177.9 (3)
C(3)—N(2)—C(2)—C(1)	177.6 (3)	N(1)—C(1)—C(2)—N(2)	0.3 (4)
C(2)—N(2)—C(4)—N(1)	-0.4 (3)	N(1)—C(4)—C(5)—C(6)	4.6 (5)
C(2)—N(2)—C(4)—C(5)	178.7 (3)	N(2)—C(4)—C(5)—C(6)	-174.2 (3)
C(4)—N(2)—C(2)—C(1)	0.0 (3)	C(4)—C(5)—C(6)—N(3)	5.5 (5)
C(3)—N(2)—C(4)—N(1)	-178.0 (3)	C(4)—C(5)—C(6)—N(4)	-177.0 (3)
C(3)—N(2)—C(4)—C(5)	1.1 (5)	N(3)—C(7)—C(8)—N(4)	-0.2 (3)
Cu(1)—N(3)—C(6)—N(4)	176.7 (2)	N(5)—C(10)—C(11)—N(6)	0.1 (3)
Cu(1)—N(3)—C(6)—C(5)	-5.6 (5)	N(5)—C(13)—C(14)—C(15)	2.1 (5)
Cu(1)—N(3)—C(7)—C(8)	-176.2 (2)	N(6)—C(13)—C(14)—C(15)	-177.9 (2)
C(6)—N(3)—C(7)—C(8)	-0.0 (3)	C(13)—C(14)—C(15)—N(7)	-7.0 (5)
C(7)—N(3)—C(6)—N(4)	0.3 (4)	C(13)—C(14)—C(15)—N(8)	172.1 (3)
C(7)—N(3)—C(6)—C(5)	178.0 (3)	N(7)—C(16)—C(17)—N(8)	-0.6 (4)
C(6)—N(4)—C(8)—C(7)	0.4 (4)	N(9)—C(19)—C(20)—N(10)	-0.8 (3)
C(8)—N(4)—C(6)—N(3)	-0.4 (4)	N(9)—C(22)—C(23)—C(24)	-84.8 (3)
C(8)—N(4)—C(6)—C(5)	-178.3 (3)	N(10)—C(22)—C(23)—C(24)	99.9 (3)
C(9)—N(4)—C(6)—N(3)	179.7 (3)	C(22)—C(23)—C(24)—N(11)	23.6 (4)
C(9)—N(4)—C(6)—C(5)	1.8 (5)	C(22)—C(23)—C(24)—N(12)	-160.4 (2)
C(9)—N(4)—C(8)—C(7)	-179.7 (3)	N(11)—C(25)—C(26)—N(12)	1.4 (4)

Fig. 1

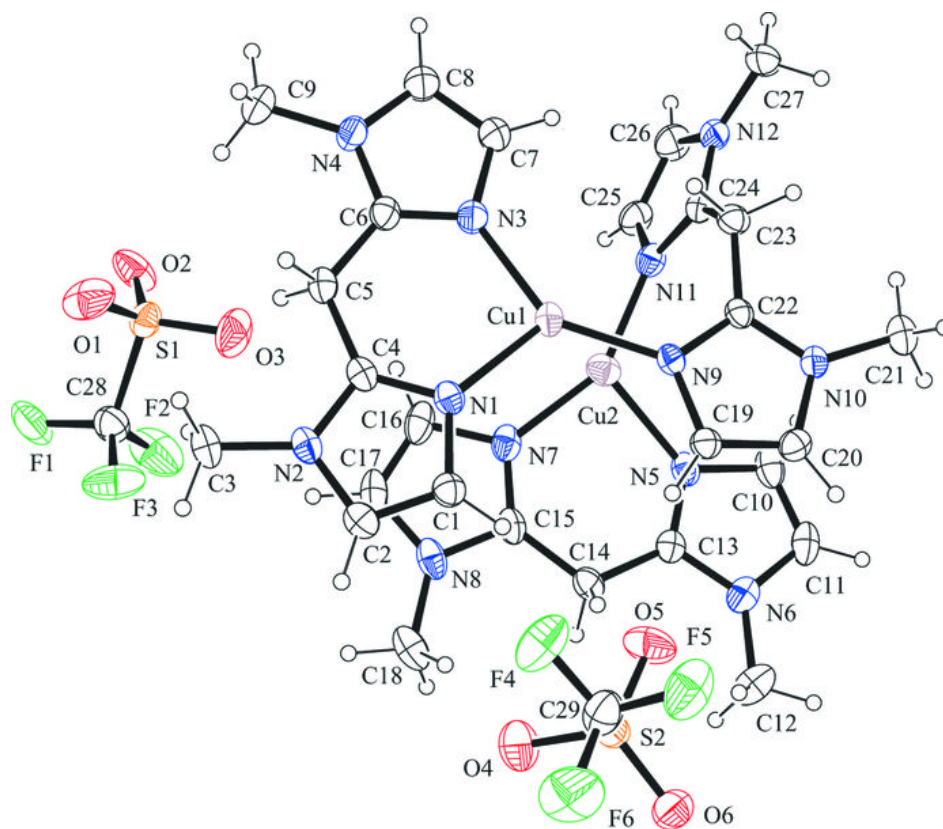


Fig. 2

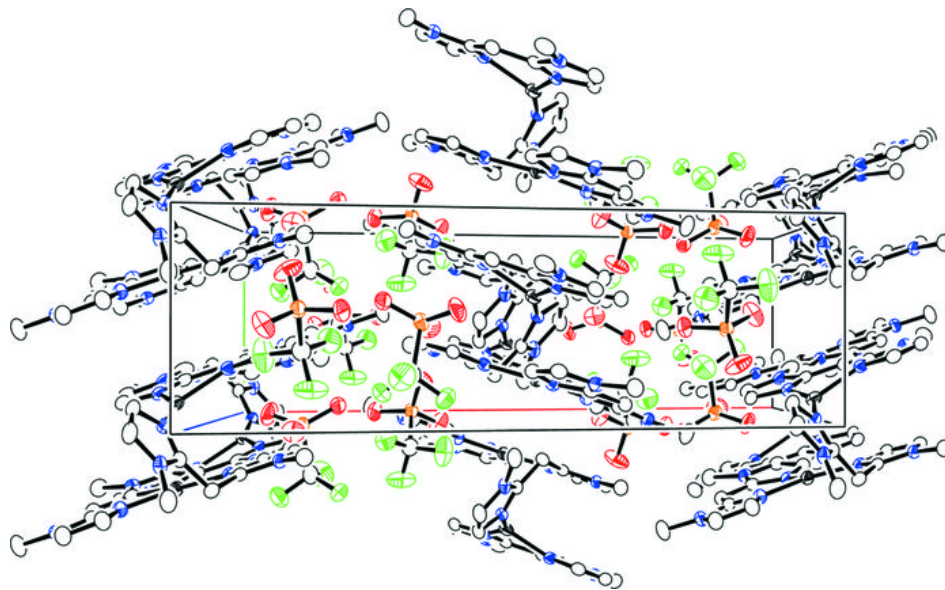


Fig. 3

