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)

Jun Matsumoto, Yuji Kajita and Hideki Masuda*

Department of Applied Chemistry, Nagoya Institute of Technology, Showa-ku, Nagoya 466-8555, Japan
Correspondence e-mail: masuda.hideki@nitech.ac.jp

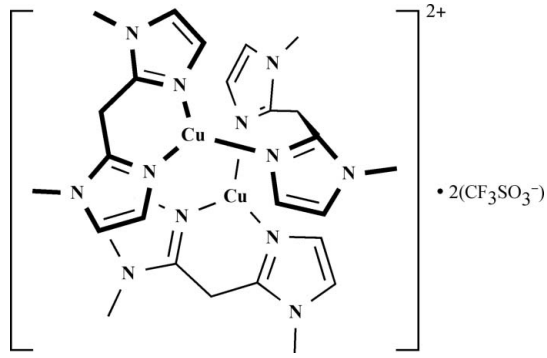
Received 10 August 2009; accepted 29 September 2009

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(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.* (2004*a*); 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.* (2004*b*). 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
β = 109.118 (2)°
V = 3820.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.31 mm^{-1}
T = 173 K
0.20 × 0.15 × 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).

References

Abuskhuna, S., Briody, J., McCann, M., Devereux, M., Kavanagh, K., Fontecha, J. B. & McKee, V. (2004*b*). *Polyhedron*, **23**, 1249–1255.

Abuskhuna, S., McCann, M., Briody, J., Devereux, M. & McKee, V. (2004*a*). *Polyhedron*, **23**, 1731–1737.

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.

Burling, S., Field, L. D., Messerle, B. A. & Turner, P. (2004). *Organometallics*, **23**, 1714–1721.

Byers, P. K. & Canty, A. J. (1990). *Organometallics*, **9**, 210–220.

Dabb, S. L., Ho, J. H. H., Hodgson, R., Messerle, B. A. & Wagler, J. (2009). *Dalton Trans.* pp. 634–642.

Elgafi, S., Field, L. D., Messerle, B. A., Hambley, T. W. & Turner, P. (1997). *J. Chem. Soc. Dalton Trans.* pp. 2341–2345.

Elgafi, S., Field, L. D., Messerle, B. A., Turner, P. & Hambley, T. W. (1999). *J. Organomet. Chem.* **588**, 69–77.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Kennedy, D. F., Messerle, B. A. & Smith, M. K. (2007). *Eur. J. Inorg. Chem.* pp. 80–89.

Messerle, B. A., Tolhurst, V. & Turner, P. (2003). *Eur. J. Inorg. Chem.* pp. 293–300.

Place, C., Zimmermann, J., Mulliez, E., Guillot, G., Bois, C. & Chottard, J. (1998). *Inorg. Chem.* **37**, 4030–4039.

Rigaku (2007). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.

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

supplementary materials

Acta Cryst. (2009). E**65**, m1286-m1287 [**doi:10.1107/S1600536809039622**]

{μ-Bis(1-methylimidazol-2-yl)methane-κ^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 (Me_2BIM) have been reported by Place *et al.* (1998), Abuskhuna *et al.* (2004*a*), respectively. In addition, that of Ag^{I} complex with BIM has been reported by Abuskhuna *et al.* (2004*b*). The Cu^{II} complexes have four- or six-coordinate structure that is coordinated with two Me_2BIM ligands, and the Ag^{I} complex forms a two-coordinate structure bridged by BIM. The title compound, [(μ-Me_2BIM){Cu(Me_2BIM)}$_2$](OTf)$_2$, contains two Cu^{I} ions, three bis(1-methylimidazol-2-yl)methane (Me_2BIM) 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 Me_2BIM and one N atom from a bridging Me_2BIM ligand, and an N atom from an additional bridging Me_2BIM which is linked to another Cu^{I} ion. This is a novel dinuclear Cu^{I} complex with Me_2BIM. 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 Me_2BIM was synthesized by modifying the literature methods of Byers *et al.* (1990) and Elgafi *et al.* (1997). Ligand Me_2BIM (1.13 mmol, 200 mg) in CH_2Cl_2 (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 ([O_2] < 1 p.p.m. and [H_2O] < 1 p.p.m.). After addition of Et_2O (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 CH_2Cl_2/MeCN/Et_2O.

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

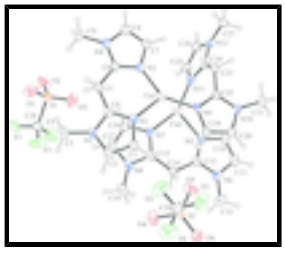


Fig. 1. The molecular view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

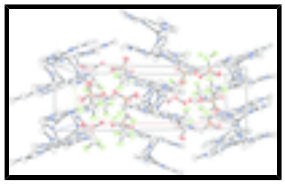


Fig. 2. The crystal packing of the title compound viewed along the *c* axis. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms that are not involved in hydrogen bonding are omitted for clarity.

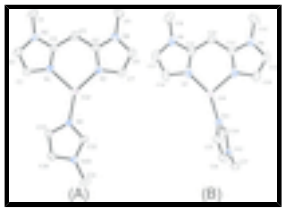


Fig. 3. The structures of (A) and (B) show the circumferences of the coppers center, Cu(1) and Cu(2), respectively. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms that are not involved in hydrogen bonding have been omitted for clarity.

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

Crystal data

$[Cu_2(C_9H_{12}N_4)_3](CF_3SO_3)_2$	F_{000} = 1944.00
M_r = 953.88	D_x = 1.658 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71070 Å
Hall symbol: -P 2yn	Cell parameters from 10516 reflections
a = 22.5575 (11) Å	θ = 3.0–27.5º
b = 7.0307 (3) Å	μ = 1.31 mm^{-1}
c = 25.4982 (16) Å	T = 173 K
β = 109.118 (2)º	Block, yellow
V = 3820.9 (3) Å^3	0.20 × 0.15 × 0.15 mm
Z = 4	

Data collection

Rigaku Mercury diffractometer	6639 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 7.31 pixels mm^{-1}	R_{int} = 0.039
T = 173 K	θ_{max} = 27.5º
ω scans	h = −29→23
Absorption correction: none	k = −9→9
29376 measured reflections	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

$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 1.5952P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.58$ e Å^{-3}

$\Delta\rho_{min} = -0.72$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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)

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 (Å^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)

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 (Å, °)

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

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)

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

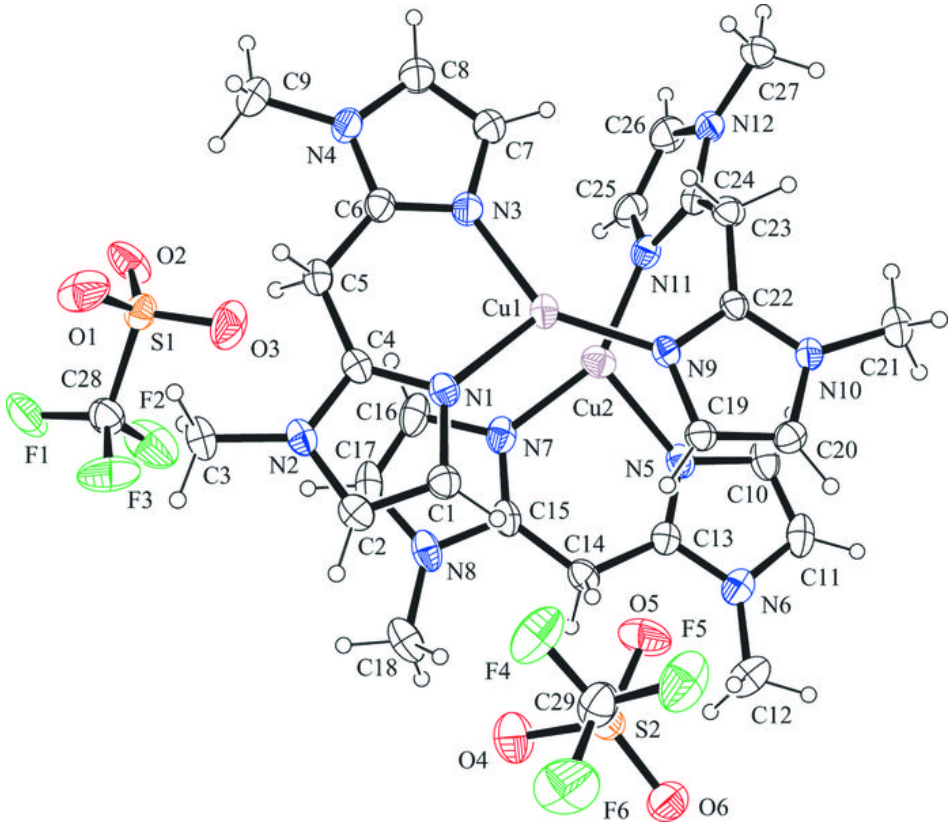

C9
C8
C27
C26
N12
N4
C7
C25
C24
C6
N3
C23
O2
C5
N11
C22
O1
S1
O3
Cu1
C4
N9
C21
C28
F2
N1
Cu2
C19
N10
C16
F1
N7
N5
C20
C3
N2
C17
C10
F3
C1
C15
C13
C2
C14
C11
N8
O5
N6
F5
C18
F4
C29
C12
S2
O4
F6
O6

Fig. 2

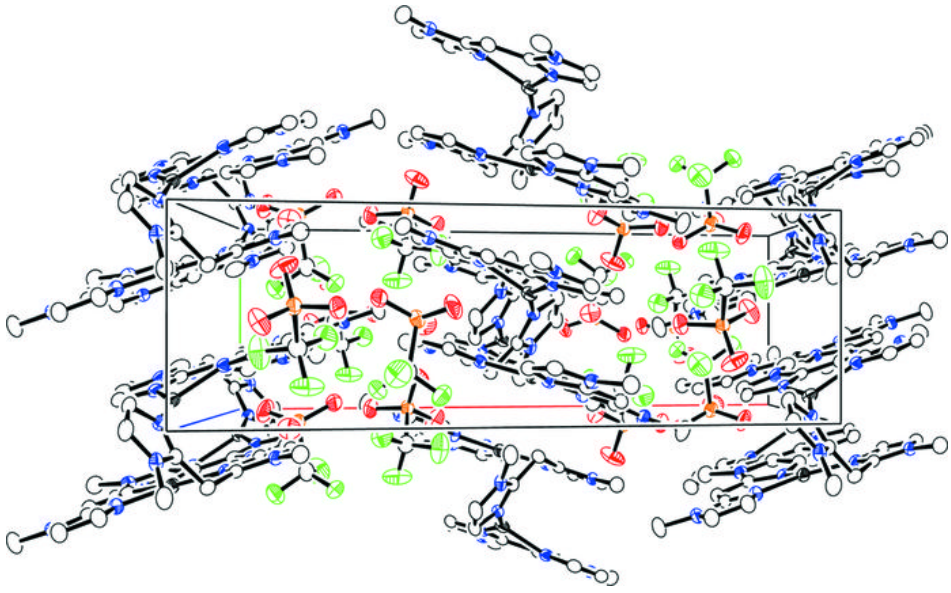
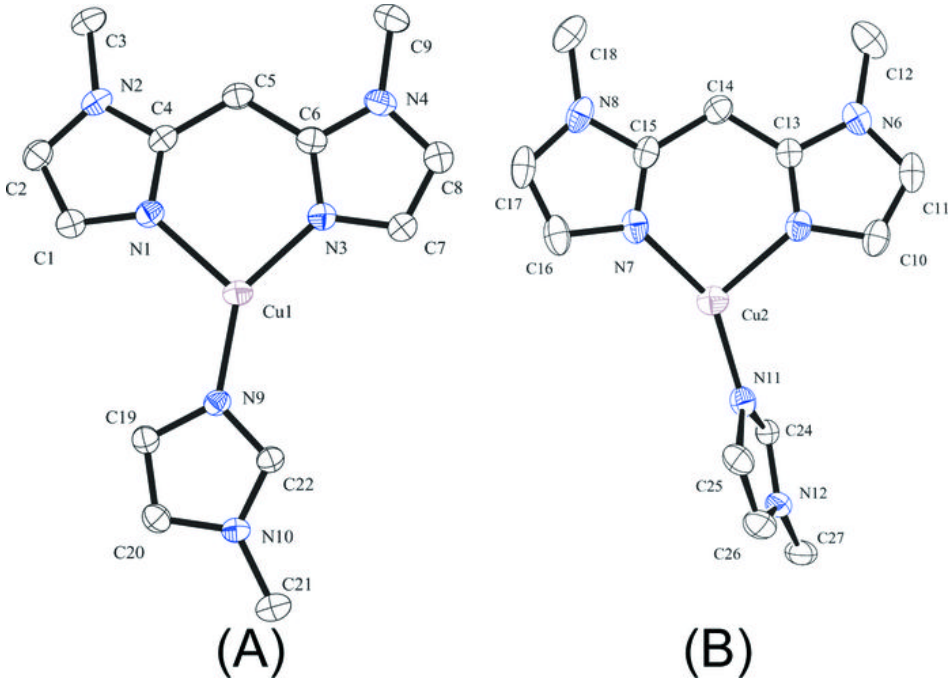


Fig. 3


C3
N2
C4
C5
C6
N4
C9
C2
C8
C1
N1
N3
C7
Cu1
N9
C19
C22
N10
C20
C21
(A)
C18
N8
C14
C15
C13
N6
C12
C17
C11
C16
N7
C10
Cu2
N11
C24
C25
N12
C27
C26
(B)