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Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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μ-Acetato-tri-μ-ferrocenecarboxylato-bis[(*N*,*N*-dimethylformamide)copper(II)]

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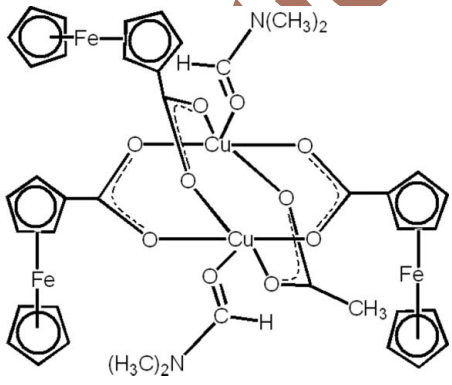
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.012 Å; R factor = 0.060; wR factor = 0.184; data-to-parameter ratio = 18.7.

The title compound, $[Cu_2Fe_3(C_5H_5)_3(C_2H_3O_2)(C_6H_4O_2)_3(C_3H_7NO)_2]$, contains a dinuclear copper(II) paddlewheel unit, where the metal ions are bridged by the O atoms of three ferrocenecarboxylate groups and one acetate group. The crystal packing is mainly determined by van der Waals interactions.

Related literature

For related literature, see: Chung & Wei (1999); Churchill *et al.* (1985); Erre *et al.* (1985); Maspoch *et al.* (2002); Porter & Doedens (1984); Viossat *et al.* (2005); Chen *et al.* (2006).



Experimental

Crystal data

$[Cu_2Fe_3(C_5H_5)_3(C_2H_3O_2)(C_6H_4O_2)_3(C_3H_7NO)_2]$
M_r = 1019.41
Triclinic, $P\overline{1}$
a = 10.948 (2) Å
b = 13.548 (3) Å
c = 15.828 (3) Å
α = 108.96 (3)°
β = 94.57 (3)°
γ = 110.33 (3)°
V = 2032.3 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.13 mm^{-1}
T = 295 K
0.22 × 0.18 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
19821 measured reflections
9106 independent reflections
6613 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.184
S = 1.05
9106 reflections
486 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −1.39 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O8	1.964 (4)	Cu2—O1	1.945 (4)
Cu1—O4	1.970 (4)	Cu2—O3	1.963 (4)
Cu1—O6	1.978 (4)	Cu2—O5	1.973 (4)
Cu1—O2	1.987 (4)	Cu2—O7	1.988 (4)
Cu1—O10	2.164 (4)	Cu2—O9	2.161 (4)
Cu1—Cu2	2.6183 (11)		

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2167).

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supplementary materials

Acta Cryst. (2007). E**63**, m3094 [**doi:10.1107/S1600536807059041**]

μ-Acetato-tri-μ-ferrocenecarboxylato-bis[(*N*,*N*-dimethylformamide)copper(II)]

D. Liu, J. Lin, Y. Xu, C. Huang and X. Li

Comment

It is well known that dicopper(II) carboxylates form a class of compounds in which a pair of copper atoms are symmetrically bridged by four carboxylates to give a paddlewheel or lantern structure (Chung & Wei, 1999; Chen *et al.*, 2006). There are few examples of this kind of complexes consisting of two different carboxylate acids, especially bulky acids (Maspoch *et al.*, 2002; Erre *et al.*, 1985). Ferrocenecarboxylic acid was used to synthesize the title compound, resulting in a complex molecule containing three ferrocenecarboxylate groups and one acetate group which, as far as we know, is the first example of a dinuclear copper(II) carboxylate of this type.

In the structure of the title compound, the copper(II) metal atoms display a square-pyramidal coordination with the oxygen atoms of three ferrocenecarboxylate groups and one acetate group occupying the basal positions (Fig. 1). The four carboxylates bridge between the copper ions, forming a paddlewheel cage with a Cu—Cu separation of 2.6182 (11) Å. This value is a little larger than that observed for the tetrakis(ferrocenecarboxylato-*O*,*O*')bis(tetrahydrofuran)dicopper(ii) complex (Churchill *et al.*, 1985). The Cu1 and Cu2 atoms are displaced 0.2143 (10) and 0.2059 (10) Å respectively from the basal plane. The Cu—O distances (Table 1) are in the range 1.946 (3)–1.9884 (4) Å, as observed in other dicopper complexes (Maspoch at al., 2002; Porter & Doedens, 1984; Viossat *et al.*, 2005). The oxygen atom of a DMF molecule occupies the apical position, with Cu1—O10 and Cu2—O9 bond lengths of 2.166 (4) and 2.161 (4) Å, respectively. The ferrocenecarboxylate groups containing Fe1 and Fe2 are *cis*-oriented with respect to the C1···C12 vector. The crystal packing is mainly determined by van der Waals interactions (Fig. 2).

Experimental

A solution of ferrocenecarboxylic acid (0.046 g 0.02 mmol) in methanol (10 ml) and $NaHCO_3$ (0.017 g 0.02 mmol) was stirred for half an hour. Then $Cu(OAc)_2{\cdot}H_2O$ (0.025 g, 0.013 mmol) was added. The mixture was stirred for 3 h at room temperature. All the volatiles were removed under vacuum and the residue was recrystallized from CCl_2H_2—DMF mixture (1:1 *v*/*v*) to give green crystal of the title compound suitable for X-ray analysis.

Refinement

All of H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for methyl H atoms.

Figures

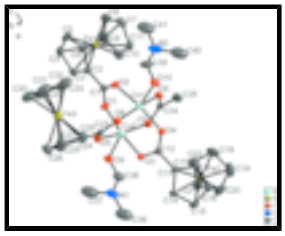

Fig. 1. The molecular structure of the title compound showing the atom-labelling scheme and 30% probability displacemene ellipsoids. H atoms are omitted for clarity.

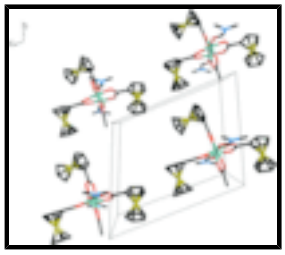

Fig. 2. Packing diagram of the title compound viewed along the *a* axis. H atoms are omitted for clarity.

μ-Acetato-tri-μ-ferrocenecarboxylato-bis[(*N*,*N*-dimethylformamide)copper(II)]

Crystal data

$[Cu_2Fe_3(C_5H_5)_3(C_2H_3O_2)(C_6H_4O_2)_3(C_3H_7NO)_2]$	$Z = 2$
$M_r = 1019.41$	$F_{000} = 1040$
Triclinic, $P\overline{1}$	$D_x = 1.666$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.948$ (2) Å	Cell parameters from 14862 reflections
$b = 13.548$ (3) Å	$\theta = 3.1$–27.5º
$c = 15.828$ (3) Å	$\mu = 2.14$ mm^{-1}
$\alpha = 108.96$ (3)º	$T = 295$ K
$\beta = 94.57$ (3)º	Block, green
$\gamma = 110.33$ (3)º	0.22 × 0.18 × 0.18 mm
$V = 2032.3$ (10) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	6613 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.045$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 568(2)$ K	$\theta_{min} = 3.1$º
Oscillation scans	$h = -14 \rightarrow 13$
Absorption correction: none	$k = -17 \rightarrow 17$
19821 measured reflections	$l = -20 \rightarrow 20$
9106 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.060$	H-atom parameters constrained
$wR(F^2) = 0.184$	$w = 1/[\sigma^2(F_o^2) + (0.0962P)^2 + 3.4415P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
9106 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
486 parameters	$\Delta\rho_{min} = -1.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Cu1	0.61220 (6)	0.29677 (5)	0.14850 (4)	0.02853 (16)
Cu2	0.87075 (6)	0.35953 (5)	0.16691 (4)	0.02790 (16)
Fe2	0.73811 (9)	0.15331 (7)	−0.19309 (5)	0.0366 (2)
Fe1	0.76655 (8)	0.22841 (7)	0.46343 (5)	0.0373 (2)
Fe3	0.74862 (10)	0.73109 (8)	0.36609 (7)	0.0506 (2)
O3	0.8335 (4)	0.3589 (3)	0.0433 (2)	0.0351 (8)
O7	0.8240 (4)	0.1930 (3)	0.1141 (3)	0.0381 (8)
O6	0.6555 (4)	0.4598 (3)	0.1752 (3)	0.0359 (8)
O4	0.6113 (4)	0.2705 (3)	0.0184 (2)	0.0380 (8)
O5	0.8760 (4)	0.5149 (3)	0.2192 (3)	0.0388 (9)
O2	0.6557 (4)	0.3314 (4)	0.2820 (2)	0.0420 (9)
O1	0.8682 (4)	0.3497 (4)	0.2867 (2)	0.0402 (9)
O8	0.6111 (4)	0.1451 (3)	0.1259 (3)	0.0398 (9)
O10	0.3985 (4)	0.2433 (4)	0.1349 (3)	0.0463 (10)
O9	1.0815 (4)	0.4089 (4)	0.1694 (3)	0.0443 (9)
N1	1.2437 (6)	0.4268 (6)	0.0902 (5)	0.0675 (18)
N2	0.2132 (7)	0.2176 (6)	0.1945 (6)	0.0697 (19)
C1	0.7695 (6)	0.3445 (4)	0.3222 (3)	0.0343 (11)

C2	0.7867 (6)	0.3563 (5)	0.4188 (4)	0.0395 (12)
C3	0.9086 (7)	0.3769 (5)	0.4743 (4)	0.0460 (14)
H3	0.9886	0.3847	0.4555	0.055*
C4	0.8882 (8)	0.3834 (5)	0.5624 (4)	0.0548 (17)
H4	0.9523	0.3977	0.6119	0.066*
C5	0.7540 (9)	0.3645 (6)	0.5617 (4)	0.0573 (18)
H5	0.7132	0.3626	0.6109	0.069*
C6	0.6905 (8)	0.3487 (6)	0.4738 (4)	0.0521 (16)
H6	0.6015	0.3357	0.4555	0.063*
C7	0.6141 (8)	0.0739 (7)	0.4289 (6)	0.068 (2)
H7	0.5252	0.0607	0.4304	0.082*
C8	0.7128 (10)	0.0913 (6)	0.5000 (5)	0.069 (2)
H8	0.7004	0.0921	0.5577	0.083*
C9	0.8316 (9)	0.1072 (6)	0.4718 (6)	0.069 (2)
H9	0.9123	0.1196	0.5060	0.083*
C10	0.8074 (9)	0.1012 (6)	0.3804 (6)	0.068 (2)
H10	0.8704	0.1100	0.3443	0.082*
C11	0.6745 (8)	0.0800 (6)	0.3539 (5)	0.0597 (18)
H11	0.6323	0.0712	0.2970	0.072*
C12	0.7189 (5)	0.3073 (4)	−0.0066 (3)	0.0301 (10)
C13	0.7077 (5)	0.2853 (4)	−0.1057 (3)	0.0314 (10)
C14	0.8150 (6)	0.3260 (5)	−0.1483 (4)	0.0387 (12)
H14	0.9026	0.3749	−0.1183	0.046*
C15	0.7639 (7)	0.2787 (5)	−0.2438 (4)	0.0483 (15)
H15	0.8120	0.2900	−0.2881	0.058*
C16	0.6262 (7)	0.2108 (5)	−0.2599 (4)	0.0459 (14)
H16	0.5685	0.1701	−0.3170	0.055*
C17	0.5908 (6)	0.2146 (5)	−0.1762 (4)	0.0403 (12)
H17	0.5061	0.1776	−0.1681	0.048*
C18	0.6875 (9)	0.0107 (6)	−0.1635 (7)	0.068 (2)
H18	0.6154	−0.0170	−0.1383	0.082*
C19	0.6858 (10)	−0.0179 (7)	−0.2583 (7)	0.077 (3)
H19	0.6132	−0.0672	−0.3065	0.092*
C20	0.8156 (10)	0.0431 (7)	−0.2648 (5)	0.070 (2)
H20	0.8440	0.0413	−0.3189	0.084*
C21	0.8948 (7)	0.1067 (6)	−0.1768 (5)	0.0547 (16)
H21	0.9849	0.1540	−0.1621	0.066*
C22	0.8153 (8)	0.0872 (6)	−0.1148 (5)	0.0521 (16)
H22	0.8431	0.1198	−0.0514	0.062*
C23	0.7722 (5)	0.5336 (4)	0.2103 (3)	0.0316 (10)
C24	0.7895 (6)	0.6546 (5)	0.2447 (4)	0.0390 (12)
C25	0.9056 (7)	0.7480 (6)	0.3031 (5)	0.0557 (17)
H25	0.9856	0.7444	0.3231	0.067*
C26	0.8796 (7)	0.8480 (6)	0.3260 (6)	0.064 (2)
H26	0.9389	0.9211	0.3636	0.076*
C27	0.7461 (8)	0.8160 (6)	0.2810 (5)	0.0613 (18)
H27	0.7026	0.8646	0.2835	0.074*
C28	0.6914 (7)	0.6974 (6)	0.2318 (5)	0.0517 (15)
H28	0.6050	0.6543	0.1967	0.062*

C29	0.7967 (13)	0.7074 (11)	0.4817 (7)	0.1035 (17)
H29	0.8765	0.7039	0.5022	0.124*
C30	0.7749 (13)	0.8055 (11)	0.5033 (7)	0.1035 (17)
H30	0.8348	0.8789	0.5398	0.124*
C31	0.6402 (13)	0.7706 (11)	0.4575 (7)	0.1035 (17)
H31	0.5955	0.8181	0.4589	0.124*
C32	0.5877 (13)	0.6540 (11)	0.4106 (7)	0.1035 (17)
H32	0.5019	0.6094	0.3749	0.124*
C33	0.6860 (13)	0.6156 (12)	0.4263 (7)	0.1035 (17)
H33	0.6779	0.5406	0.4032	0.124*
C35	0.6934 (8)	−0.0006 (5)	0.0838 (5)	0.0558 (17)
H35A	0.7419	−0.0080	0.1331	0.084*
H35B	0.7273	−0.0232	0.0298	0.084*
H35C	0.6005	−0.0483	0.0720	0.084*
C36	1.1219 (7)	0.3952 (6)	0.0992 (6)	0.0590 (18)
H36	1.0569	0.3571	0.0452	0.071*
C37	1.3472 (11)	0.4908 (11)	0.1742 (10)	0.112 (2)
H37A	1.3168	0.4657	0.2218	0.168*
H37B	1.3659	0.5703	0.1923	0.168*
H37C	1.4268	0.4784	0.1638	0.168*
C38	1.2905 (11)	0.4134 (11)	0.0096 (9)	0.112 (2)
H38A	1.2170	0.3662	−0.0420	0.168*
H38B	1.3532	0.3784	0.0093	0.168*
H38C	1.3336	0.4865	0.0060	0.168*
C34	0.7101 (6)	0.1220 (5)	0.1097 (4)	0.0373 (12)
C40	0.1239 (11)	0.1510 (11)	0.1034 (10)	0.112 (2)
H40A	0.1700	0.1690	0.0579	0.168*
H40B	0.0466	0.1691	0.1017	0.168*
H40C	0.0967	0.0714	0.0913	0.168*
C41	0.1499 (11)	0.2274 (10)	0.2676 (9)	0.112 (2)
H41A	0.2151	0.2753	0.3237	0.168*
H41B	0.1043	0.1535	0.2691	0.168*
H41C	0.0867	0.2601	0.2606	0.168*
C39	0.3427 (8)	0.2540 (7)	0.1983 (6)	0.062 (2)
H39	0.3977	0.2924	0.2565	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0279 (3)	0.0294 (3)	0.0301 (3)	0.0118 (2)	0.0105 (2)	0.0119 (2)
Cu2	0.0276 (3)	0.0293 (3)	0.0285 (3)	0.0122 (3)	0.0081 (2)	0.0116 (2)
Fe2	0.0524 (5)	0.0332 (4)	0.0312 (4)	0.0214 (4)	0.0126 (3)	0.0154 (3)
Fe1	0.0448 (5)	0.0330 (4)	0.0328 (4)	0.0120 (4)	0.0073 (3)	0.0149 (3)
Fe3	0.0512 (5)	0.0473 (5)	0.0511 (5)	0.0241 (4)	0.0134 (4)	0.0103 (4)
O3	0.035 (2)	0.040 (2)	0.0288 (17)	0.0120 (17)	0.0066 (16)	0.0147 (16)
O7	0.041 (2)	0.0286 (18)	0.047 (2)	0.0154 (17)	0.0158 (18)	0.0137 (16)
O6	0.036 (2)	0.0304 (18)	0.0402 (19)	0.0146 (17)	0.0078 (17)	0.0113 (16)
O4	0.040 (2)	0.043 (2)	0.0296 (17)	0.0147 (18)	0.0102 (16)	0.0132 (16)

O5	0.043 (2)	0.0306 (19)	0.043 (2)	0.0169 (17)	0.0132 (18)	0.0111 (16)
O2	0.049 (2)	0.050 (2)	0.0316 (18)	0.021 (2)	0.0152 (18)	0.0183 (17)
O1	0.045 (2)	0.048 (2)	0.0312 (18)	0.0200 (19)	0.0103 (17)	0.0179 (17)
O8	0.039 (2)	0.0298 (19)	0.053 (2)	0.0129 (17)	0.0192 (19)	0.0176 (17)
O10	0.032 (2)	0.046 (2)	0.066 (3)	0.0177 (18)	0.020 (2)	0.023 (2)
O9	0.033 (2)	0.051 (2)	0.052 (2)	0.0152 (19)	0.0143 (19)	0.023 (2)
N1	0.044 (3)	0.069 (4)	0.108 (5)	0.027 (3)	0.039 (4)	0.047 (4)
N2	0.058 (4)	0.091 (5)	0.111 (6)	0.050 (4)	0.050 (4)	0.073 (5)
C1	0.045 (3)	0.031 (3)	0.030 (2)	0.016 (2)	0.007 (2)	0.014 (2)
C2	0.053 (3)	0.039 (3)	0.029 (2)	0.018 (3)	0.009 (2)	0.016 (2)
C3	0.053 (4)	0.029 (3)	0.046 (3)	0.003 (3)	0.000 (3)	0.019 (2)
C4	0.075 (5)	0.036 (3)	0.039 (3)	0.012 (3)	−0.006 (3)	0.011 (3)
C5	0.099 (6)	0.057 (4)	0.032 (3)	0.043 (4)	0.020 (3)	0.022 (3)
C6	0.073 (5)	0.066 (4)	0.041 (3)	0.045 (4)	0.024 (3)	0.028 (3)
C7	0.054 (4)	0.054 (4)	0.080 (5)	0.003 (4)	0.010 (4)	0.024 (4)
C8	0.102 (7)	0.045 (4)	0.059 (4)	0.018 (4)	0.015 (4)	0.029 (3)
C9	0.086 (6)	0.043 (4)	0.078 (5)	0.032 (4)	−0.001 (5)	0.019 (4)
C10	0.077 (5)	0.044 (4)	0.078 (5)	0.022 (4)	0.038 (4)	0.013 (4)
C11	0.071 (5)	0.043 (4)	0.042 (3)	0.009 (3)	−0.001 (3)	0.006 (3)
C12	0.040 (3)	0.024 (2)	0.031 (2)	0.017 (2)	0.010 (2)	0.0118 (19)
C13	0.041 (3)	0.033 (3)	0.028 (2)	0.018 (2)	0.009 (2)	0.016 (2)
C14	0.051 (3)	0.033 (3)	0.041 (3)	0.017 (3)	0.017 (3)	0.022 (2)
C15	0.080 (5)	0.048 (3)	0.040 (3)	0.036 (4)	0.029 (3)	0.030 (3)
C16	0.063 (4)	0.045 (3)	0.032 (3)	0.022 (3)	0.004 (3)	0.017 (2)
C17	0.044 (3)	0.040 (3)	0.041 (3)	0.018 (3)	0.008 (3)	0.019 (2)
C18	0.079 (5)	0.048 (4)	0.110 (7)	0.035 (4)	0.041 (5)	0.055 (4)
C19	0.090 (6)	0.042 (4)	0.088 (6)	0.036 (4)	−0.012 (5)	0.009 (4)
C20	0.123 (8)	0.074 (5)	0.049 (4)	0.071 (6)	0.038 (5)	0.026 (4)
C21	0.056 (4)	0.053 (4)	0.068 (4)	0.032 (3)	0.017 (3)	0.028 (3)
C22	0.078 (5)	0.056 (4)	0.051 (3)	0.045 (4)	0.024 (3)	0.034 (3)
C23	0.040 (3)	0.031 (3)	0.028 (2)	0.017 (2)	0.013 (2)	0.012 (2)
C24	0.046 (3)	0.027 (3)	0.044 (3)	0.016 (2)	0.015 (3)	0.010 (2)
C25	0.046 (4)	0.044 (4)	0.075 (5)	0.020 (3)	0.020 (3)	0.016 (3)
C26	0.055 (4)	0.036 (3)	0.092 (5)	0.013 (3)	0.021 (4)	0.017 (4)
C27	0.072 (5)	0.045 (4)	0.077 (5)	0.031 (4)	0.019 (4)	0.025 (4)
C28	0.056 (4)	0.048 (4)	0.053 (4)	0.026 (3)	0.009 (3)	0.017 (3)
C29	0.129 (4)	0.127 (4)	0.081 (3)	0.069 (4)	0.058 (3)	0.044 (3)
C30	0.129 (4)	0.127 (4)	0.081 (3)	0.069 (4)	0.058 (3)	0.044 (3)
C31	0.129 (4)	0.127 (4)	0.081 (3)	0.069 (4)	0.058 (3)	0.044 (3)
C32	0.129 (4)	0.127 (4)	0.081 (3)	0.069 (4)	0.058 (3)	0.044 (3)
C33	0.129 (4)	0.127 (4)	0.081 (3)	0.069 (4)	0.058 (3)	0.044 (3)
C35	0.072 (5)	0.034 (3)	0.072 (4)	0.026 (3)	0.029 (4)	0.024 (3)
C36	0.046 (4)	0.061 (4)	0.081 (5)	0.025 (3)	0.024 (4)	0.034 (4)
C37	0.088 (4)	0.122 (5)	0.184 (6)	0.067 (4)	0.074 (4)	0.091 (5)
C38	0.088 (4)	0.122 (5)	0.184 (6)	0.067 (4)	0.074 (4)	0.091 (5)
C34	0.052 (3)	0.028 (3)	0.032 (2)	0.014 (2)	0.014 (2)	0.014 (2)
C40	0.088 (4)	0.122 (5)	0.184 (6)	0.067 (4)	0.074 (4)	0.091 (5)
C41	0.088 (4)	0.122 (5)	0.184 (6)	0.067 (4)	0.074 (4)	0.091 (5)
C39	0.067 (4)	0.077 (5)	0.085 (5)	0.047 (4)	0.048 (4)	0.057 (4)

Geometric parameters (Å, °)

Cu1—O8	1.964 (4)	C7—C11	1.416 (11)
Cu1—O4	1.970 (4)	C7—H7	0.9300
Cu1—O6	1.978 (4)	C8—C9	1.377 (12)
Cu1—O2	1.987 (4)	C8—H8	0.9300
Cu1—O10	2.164 (4)	C9—C10	1.420 (12)
Cu1—Cu2	2.6183 (11)	C9—H9	0.9300
Cu2—O1	1.945 (4)	C10—C11	1.381 (11)
Cu2—O3	1.963 (4)	C10—H10	0.9300
Cu2—O5	1.973 (4)	C11—H11	0.9300
Cu2—O7	1.988 (4)	C12—C13	1.485 (7)
Cu2—O9	2.161 (4)	C13—C17	1.424 (8)
Fe2—C13	2.025 (5)	C13—C14	1.434 (7)
Fe2—C22	2.034 (6)	C14—C15	1.413 (8)
Fe2—C14	2.036 (6)	C14—H14	0.9300
Fe2—C18	2.036 (7)	C15—C16	1.416 (10)
Fe2—C20	2.042 (7)	C15—H15	0.9300
Fe2—C21	2.048 (7)	C16—C17	1.399 (8)
Fe2—C15	2.049 (6)	C16—H16	0.9300
Fe2—C19	2.049 (7)	C17—H17	0.9300
Fe2—C16	2.053 (6)	C18—C22	1.388 (11)
Fe2—C17	2.054 (6)	C18—C19	1.420 (12)
Fe1—C3	2.013 (6)	C18—H18	0.9300
Fe1—C10	2.014 (7)	C19—C20	1.405 (13)
Fe1—C2	2.025 (6)	C19—H19	0.9300
Fe1—C11	2.028 (7)	C20—C21	1.394 (11)
Fe1—C8	2.031 (7)	C20—H20	0.9300
Fe1—C7	2.037 (8)	C21—C22	1.391 (9)
Fe1—C9	2.039 (7)	C21—H21	0.9300
Fe1—C6	2.042 (7)	C22—H22	0.9300
Fe1—C5	2.046 (6)	C23—C24	1.486 (7)
Fe1—C4	2.055 (6)	C24—C28	1.416 (9)
Fe3—C31	2.000 (9)	C24—C25	1.416 (9)
Fe3—C29	2.018 (12)	C25—C26	1.419 (9)
Fe3—C28	2.019 (7)	C25—H25	0.9300
Fe3—C32	2.022 (11)	C26—C27	1.423 (11)
Fe3—C30	2.023 (10)	C26—H26	0.9300
Fe3—C24	2.033 (5)	C27—C28	1.411 (9)
Fe3—C25	2.037 (6)	C27—H27	0.9300
Fe3—C33	2.038 (12)	C28—H28	0.9300
Fe3—C27	2.040 (8)	C29—C33	1.364 (16)
Fe3—C26	2.046 (8)	C29—C30	1.371 (16)
O3—C12	1.249 (6)	C29—H29	0.9300
O7—C34	1.264 (7)	C30—C31	1.431 (16)
O6—C23	1.257 (6)	C30—H30	0.9300
O4—C12	1.261 (6)	C31—C32	1.384 (16)
O5—C23	1.255 (6)	C31—H31	0.9300

O2—C1	1.279 (7)	C32—C33	1.386 (15)
O1—C1	1.249 (6)	C32—H32	0.9300
O8—C34	1.250 (7)	C33—H33	0.9300
O10—C39	1.211 (7)	C35—C34	1.515 (8)
O9—C36	1.210 (8)	C35—H35A	0.9600
N1—C36	1.287 (8)	C35—H35B	0.9600
N1—C38	1.393 (12)	C35—H35C	0.9600
N1—C37	1.460 (15)	C36—H36	0.9300
N2—C39	1.319 (9)	C37—H37A	0.9600
N2—C41	1.389 (12)	C37—H37B	0.9600
N2—C40	1.472 (15)	C37—H37C	0.9600
C1—C2	1.474 (7)	C38—H38A	0.9600
C2—C6	1.416 (8)	C38—H38B	0.9600
C2—C3	1.423 (9)	C38—H38C	0.9600
C3—C4	1.408 (9)	C40—H40A	0.9600
C3—H3	0.9300	C40—H40B	0.9600
C4—C5	1.399 (11)	C40—H40C	0.9600
C4—H4	0.9300	C41—H41A	0.9600
C5—C6	1.420 (9)	C41—H41B	0.9600
C5—H5	0.9300	C41—H41C	0.9600
C6—H6	0.9300	C39—H39	0.9300
C7—C8	1.396 (12)		
O8—Cu1—O4	89.37 (17)	C4—C5—H5	125.6
O8—Cu1—O6	167.62 (15)	C6—C5—H5	125.6
O4—Cu1—O6	89.89 (16)	Fe1—C5—H5	126.1
O8—Cu1—O2	88.57 (18)	C2—C6—C5	107.8 (6)
O4—Cu1—O2	167.40 (16)	C2—C6—Fe1	69.0 (3)
O6—Cu1—O2	89.46 (17)	C5—C6—Fe1	69.8 (4)
O8—Cu1—O10	95.06 (16)	C2—C6—H6	126.1
O4—Cu1—O10	96.20 (17)	C5—C6—H6	126.1
O6—Cu1—O10	97.31 (16)	Fe1—C6—H6	126.6
O2—Cu1—O10	96.36 (17)	C8—C7—C11	107.2 (7)
O8—Cu1—Cu2	84.26 (12)	C8—C7—Fe1	69.7 (4)
O4—Cu1—Cu2	84.55 (12)	C11—C7—Fe1	69.3 (4)
O6—Cu1—Cu2	83.36 (11)	C8—C7—H7	126.4
O2—Cu1—Cu2	82.87 (12)	C11—C7—H7	126.4
O10—Cu1—Cu2	178.98 (12)	Fe1—C7—H7	126.2
O1—Cu2—O3	168.23 (16)	C9—C8—C7	109.5 (7)
O1—Cu2—O5	89.34 (17)	C9—C8—Fe1	70.5 (4)
O3—Cu2—O5	89.81 (17)	C7—C8—Fe1	70.2 (4)
O1—Cu2—O7	88.32 (17)	C9—C8—H8	125.2
O3—Cu2—O7	90.03 (17)	C7—C8—H8	125.2
O5—Cu2—O7	167.72 (16)	Fe1—C8—H8	125.6
O1—Cu2—O9	99.92 (17)	C8—C9—C10	107.0 (8)
O3—Cu2—O9	91.85 (16)	C8—C9—Fe1	69.9 (4)
O5—Cu2—O9	96.55 (17)	C10—C9—Fe1	68.5 (4)
O7—Cu2—O9	95.72 (16)	C8—C9—H9	126.5
O1—Cu2—Cu1	85.06 (12)	C10—C9—H9	126.5
O3—Cu2—Cu1	83.17 (11)	Fe1—C9—H9	126.6

O5—Cu2—Cu1	84.36 (12)	C11—C10—C9	108.6 (7)
O7—Cu2—Cu1	83.44 (12)	C11—C10—Fe1	70.6 (4)
O9—Cu2—Cu1	174.93 (11)	C9—C10—Fe1	70.4 (4)
C13—Fe2—C22	106.6 (2)	C11—C10—H10	125.7
C13—Fe2—C14	41.3 (2)	C9—C10—H10	125.7
C22—Fe2—C14	115.7 (3)	Fe1—C10—H10	124.9
C13—Fe2—C18	116.4 (3)	C10—C11—C7	107.8 (7)
C22—Fe2—C18	39.9 (3)	C10—C11—Fe1	69.5 (4)
C14—Fe2—C18	148.9 (3)	C7—C11—Fe1	70.0 (4)
C13—Fe2—C20	166.1 (3)	C10—C11—H11	126.1
C22—Fe2—C20	67.1 (3)	C7—C11—H11	126.1
C14—Fe2—C20	128.8 (3)	Fe1—C11—H11	126.0
C18—Fe2—C20	67.4 (3)	O3—C12—O4	126.5 (5)
C13—Fe2—C21	127.6 (3)	O3—C12—C13	117.1 (4)
C22—Fe2—C21	39.8 (3)	O4—C12—C13	116.4 (5)
C14—Fe2—C21	107.1 (3)	C17—C13—C14	107.6 (5)
C18—Fe2—C21	67.1 (3)	C17—C13—C12	126.3 (5)
C20—Fe2—C21	39.9 (3)	C14—C13—C12	126.0 (5)
C13—Fe2—C15	68.7 (2)	C17—C13—Fe2	70.6 (3)
C22—Fe2—C15	149.3 (3)	C14—C13—Fe2	69.7 (3)
C14—Fe2—C15	40.5 (2)	C12—C13—Fe2	122.2 (3)
C18—Fe2—C15	169.9 (3)	C15—C14—C13	107.8 (5)
C20—Fe2—C15	109.9 (3)	C15—C14—Fe2	70.2 (3)
C21—Fe2—C15	117.7 (3)	C13—C14—Fe2	68.9 (3)
C13—Fe2—C19	150.7 (3)	C15—C14—H14	126.1
C22—Fe2—C19	67.7 (3)	C13—C14—H14	126.1
C14—Fe2—C19	167.7 (3)	Fe2—C14—H14	126.3
C18—Fe2—C19	40.7 (4)	C14—C15—C16	107.6 (5)
C20—Fe2—C19	40.2 (4)	C14—C15—Fe2	69.3 (3)
C21—Fe2—C19	67.5 (3)	C16—C15—Fe2	70.0 (3)
C15—Fe2—C19	131.0 (3)	C14—C15—H15	126.2
C13—Fe2—C16	68.0 (2)	C16—C15—H15	126.2
C22—Fe2—C16	167.9 (3)	Fe2—C15—H15	126.1
C14—Fe2—C16	67.9 (3)	C17—C16—C15	109.3 (5)
C18—Fe2—C16	131.6 (3)	C17—C16—Fe2	70.1 (3)
C20—Fe2—C16	120.6 (3)	C15—C16—Fe2	69.6 (4)
C21—Fe2—C16	151.9 (3)	C17—C16—H16	125.3
C15—Fe2—C16	40.4 (3)	C15—C16—H16	125.3
C19—Fe2—C16	111.4 (3)	Fe2—C16—H16	126.5
C13—Fe2—C17	40.9 (2)	C16—C17—C13	107.7 (5)
C22—Fe2—C17	129.2 (2)	C16—C17—Fe2	70.1 (3)
C14—Fe2—C17	68.7 (2)	C13—C17—Fe2	68.5 (3)
C18—Fe2—C17	109.5 (3)	C16—C17—H17	126.2
C20—Fe2—C17	152.5 (3)	C13—C17—H17	126.2
C21—Fe2—C17	166.4 (3)	Fe2—C17—H17	126.8
C15—Fe2—C17	68.1 (2)	C22—C18—C19	108.3 (7)
C19—Fe2—C17	119.2 (3)	C22—C18—Fe2	70.0 (4)
C16—Fe2—C17	39.8 (2)	C19—C18—Fe2	70.2 (4)
C3—Fe1—C10	108.2 (3)	C22—C18—H18	125.9

C3—Fe1—C2	41.3 (2)	C19—C18—H18	125.9
C10—Fe1—C2	114.7 (3)	Fe2—C18—H18	125.6
C3—Fe1—C11	130.4 (3)	C20—C19—C18	106.4 (8)
C10—Fe1—C11	40.0 (3)	C20—C19—Fe2	69.6 (4)
C2—Fe1—C11	107.5 (3)	C18—C19—Fe2	69.2 (4)
C3—Fe1—C8	148.2 (3)	C20—C19—H19	126.8
C10—Fe1—C8	67.6 (3)	C18—C19—H19	126.8
C2—Fe1—C8	170.3 (3)	Fe2—C19—H19	126.0
C11—Fe1—C8	67.7 (3)	C21—C20—C19	108.8 (7)
C3—Fe1—C7	169.9 (3)	C21—C20—Fe2	70.3 (4)
C10—Fe1—C7	67.8 (3)	C19—C20—Fe2	70.2 (4)
C2—Fe1—C7	130.9 (3)	C21—C20—H20	125.6
C11—Fe1—C7	40.8 (3)	C19—C20—H20	125.6
C8—Fe1—C7	40.1 (3)	Fe2—C20—H20	125.5
C3—Fe1—C9	116.1 (3)	C22—C21—C20	108.0 (7)
C10—Fe1—C9	41.0 (3)	C22—C21—Fe2	69.5 (4)
C2—Fe1—C9	147.8 (3)	C20—C21—Fe2	69.8 (4)
C11—Fe1—C9	68.0 (3)	C22—C21—H21	126.0
C8—Fe1—C9	39.6 (4)	C20—C21—H21	126.0
C7—Fe1—C9	67.5 (4)	Fe2—C21—H21	126.2
C3—Fe1—C6	68.5 (3)	C18—C22—C21	108.5 (7)
C10—Fe1—C6	147.1 (3)	C18—C22—Fe2	70.2 (4)
C2—Fe1—C6	40.8 (2)	C21—C22—Fe2	70.6 (4)
C11—Fe1—C6	115.9 (3)	C18—C22—H22	125.7
C8—Fe1—C6	132.6 (3)	C21—C22—H22	125.7
C7—Fe1—C6	109.5 (3)	Fe2—C22—H22	125.1
C9—Fe1—C6	170.7 (3)	O5—C23—O6	126.1 (5)
C3—Fe1—C5	67.9 (3)	O5—C23—C24	116.6 (5)
C10—Fe1—C5	170.6 (4)	O6—C23—C24	117.2 (5)
C2—Fe1—C5	68.5 (2)	C28—C24—C25	107.3 (5)
C11—Fe1—C5	149.0 (3)	C28—C24—C23	126.9 (5)
C8—Fe1—C5	110.9 (3)	C25—C24—C23	125.6 (5)
C7—Fe1—C5	117.5 (3)	C28—C24—Fe3	69.0 (3)
C9—Fe1—C5	132.0 (3)	C25—C24—Fe3	69.8 (3)
C6—Fe1—C5	40.7 (3)	C23—C24—Fe3	122.7 (4)
C3—Fe1—C4	40.5 (3)	C24—C25—C26	108.6 (6)
C10—Fe1—C4	131.7 (3)	C24—C25—Fe3	69.5 (3)
C2—Fe1—C4	68.7 (2)	C26—C25—Fe3	70.0 (4)
C11—Fe1—C4	169.5 (3)	C24—C25—H25	125.7
C8—Fe1—C4	117.5 (3)	C26—C25—H25	125.7
C7—Fe1—C4	148.9 (3)	Fe3—C25—H25	126.4
C9—Fe1—C4	109.7 (3)	C25—C26—C27	107.5 (6)
C6—Fe1—C4	68.0 (3)	C25—C26—Fe3	69.3 (4)
C5—Fe1—C4	39.9 (3)	C27—C26—Fe3	69.4 (4)
C31—Fe3—C29	67.2 (5)	C25—C26—H26	126.3
C31—Fe3—C28	122.9 (4)	C27—C26—H26	126.3
C29—Fe3—C28	159.9 (4)	Fe3—C26—H26	126.6
C31—Fe3—C32	40.2 (4)	C28—C27—C26	107.8 (6)
C29—Fe3—C32	66.7 (5)	C28—C27—Fe3	68.9 (4)

C28—Fe3—C32	108.6 (4)	C26—C27—Fe3	69.9 (4)
C31—Fe3—C30	41.7 (4)	C28—C27—H27	126.1
C29—Fe3—C30	39.7 (4)	C26—C27—H27	126.1
C28—Fe3—C30	159.1 (4)	Fe3—C27—H27	126.7
C32—Fe3—C30	68.7 (5)	C27—C28—C24	108.8 (6)
C31—Fe3—C24	158.7 (4)	C27—C28—Fe3	70.4 (4)
C29—Fe3—C24	123.7 (4)	C24—C28—Fe3	70.1 (4)
C28—Fe3—C24	40.9 (2)	C27—C28—H28	125.6
C32—Fe3—C24	123.1 (4)	C24—C28—H28	125.6
C30—Fe3—C24	158.1 (4)	Fe3—C28—H28	125.5
C31—Fe3—C25	159.4 (4)	C33—C29—C30	111.1 (13)
C29—Fe3—C25	108.3 (4)	C33—C29—Fe3	71.1 (7)
C28—Fe3—C25	68.4 (3)	C30—C29—Fe3	70.3 (7)
C32—Fe3—C25	158.6 (4)	C33—C29—H29	124.4
C30—Fe3—C25	121.8 (4)	C30—C29—H29	124.4
C24—Fe3—C25	40.7 (3)	Fe3—C29—H29	125.7
C31—Fe3—C33	67.2 (5)	C29—C30—C31	105.0 (12)
C29—Fe3—C33	39.3 (5)	C29—C30—Fe3	70.0 (6)
C28—Fe3—C33	124.6 (4)	C31—C30—Fe3	68.3 (6)
C32—Fe3—C33	39.9 (4)	C29—C30—H30	127.5
C30—Fe3—C33	67.5 (5)	C31—C30—H30	127.5
C24—Fe3—C33	108.5 (4)	Fe3—C30—H30	125.8
C25—Fe3—C33	123.0 (4)	C32—C31—C30	108.3 (12)
C31—Fe3—C27	107.9 (4)	C32—C31—Fe3	70.7 (6)
C29—Fe3—C27	158.3 (4)	C30—C31—Fe3	70.0 (6)
C28—Fe3—C27	40.7 (3)	C32—C31—H31	125.8
C32—Fe3—C27	124.1 (4)	C30—C31—H31	125.8
C30—Fe3—C27	122.4 (4)	Fe3—C31—H31	125.0
C24—Fe3—C27	68.7 (3)	C31—C32—C33	107.7 (13)
C25—Fe3—C27	68.4 (3)	C31—C32—Fe3	69.0 (7)
C33—Fe3—C27	160.4 (4)	C33—C32—Fe3	70.7 (7)
C31—Fe3—C26	123.3 (4)	C31—C32—H32	126.2
C29—Fe3—C26	122.8 (5)	C33—C32—H32	126.2
C28—Fe3—C26	68.6 (3)	Fe3—C32—H32	125.7
C32—Fe3—C26	159.9 (4)	C29—C33—C32	107.8 (12)
C30—Fe3—C26	106.4 (4)	C29—C33—Fe3	69.6 (7)
C24—Fe3—C26	68.7 (3)	C32—C33—Fe3	69.4 (7)
C25—Fe3—C26	40.7 (3)	C29—C33—H33	126.1
C33—Fe3—C26	158.0 (4)	C32—C33—H33	126.1
C27—Fe3—C26	40.8 (3)	Fe3—C33—H33	126.5
C12—O3—Cu2	121.8 (3)	C34—C35—H35A	109.5
C34—O7—Cu2	121.7 (3)	C34—C35—H35B	109.5
C23—O6—Cu1	121.6 (3)	H35A—C35—H35B	109.5
C12—O4—Cu1	120.3 (3)	C34—C35—H35C	109.5
C23—O5—Cu2	121.2 (4)	H35A—C35—H35C	109.5
C1—O2—Cu1	121.8 (3)	H35B—C35—H35C	109.5
C1—O1—Cu2	122.0 (4)	O9—C36—N1	128.0 (8)
C34—O8—Cu1	122.4 (3)	O9—C36—H36	116.0
C39—O10—Cu1	124.8 (5)	N1—C36—H36	116.0

C36—O9—Cu2	121.0 (5)	N1—C37—H37A	109.5
C36—N1—C38	128.2 (9)	N1—C37—H37B	109.5
C36—N1—C37	116.8 (8)	H37A—C37—H37B	109.5
C38—N1—C37	114.9 (8)	N1—C37—H37C	109.5
C39—N2—C41	127.3 (9)	H37A—C37—H37C	109.5
C39—N2—C40	117.3 (7)	H37B—C37—H37C	109.5
C41—N2—C40	115.2 (8)	N1—C38—H38A	109.5
O1—C1—O2	125.2 (5)	N1—C38—H38B	109.5
O1—C1—C2	117.1 (5)	H38A—C38—H38B	109.5
O2—C1—C2	117.6 (5)	N1—C38—H38C	109.5
C6—C2—C3	107.0 (5)	H38A—C38—H38C	109.5
C6—C2—C1	128.6 (6)	H38B—C38—H38C	109.5
C3—C2—C1	124.4 (5)	O8—C34—O7	125.3 (5)
C6—C2—Fe1	70.2 (3)	O8—C34—C35	117.8 (5)
C3—C2—Fe1	68.9 (3)	O7—C34—C35	116.9 (5)
C1—C2—Fe1	125.3 (4)	N2—C40—H40A	109.5
C4—C3—C2	108.8 (6)	N2—C40—H40B	109.5
C4—C3—Fe1	71.4 (4)	H40A—C40—H40B	109.5
C2—C3—Fe1	69.8 (3)	N2—C40—H40C	109.5
C4—C3—H3	125.6	H40A—C40—H40C	109.5
C2—C3—H3	125.6	H40B—C40—H40C	109.5
Fe1—C3—H3	124.8	N2—C41—H41A	109.5
C5—C4—C3	107.6 (6)	N2—C41—H41B	109.5
C5—C4—Fe1	69.7 (4)	H41A—C41—H41B	109.5
C3—C4—Fe1	68.2 (3)	N2—C41—H41C	109.5
C5—C4—H4	126.2	H41A—C41—H41C	109.5
C3—C4—H4	126.2	H41B—C41—H41C	109.5
Fe1—C4—H4	127.5	O10—C39—N2	127.7 (9)
C4—C5—C6	108.8 (6)	O10—C39—H39	116.2
C4—C5—Fe1	70.4 (4)	N2—C39—H39	116.2
C6—C5—Fe1	69.5 (4)		

Fig. 1

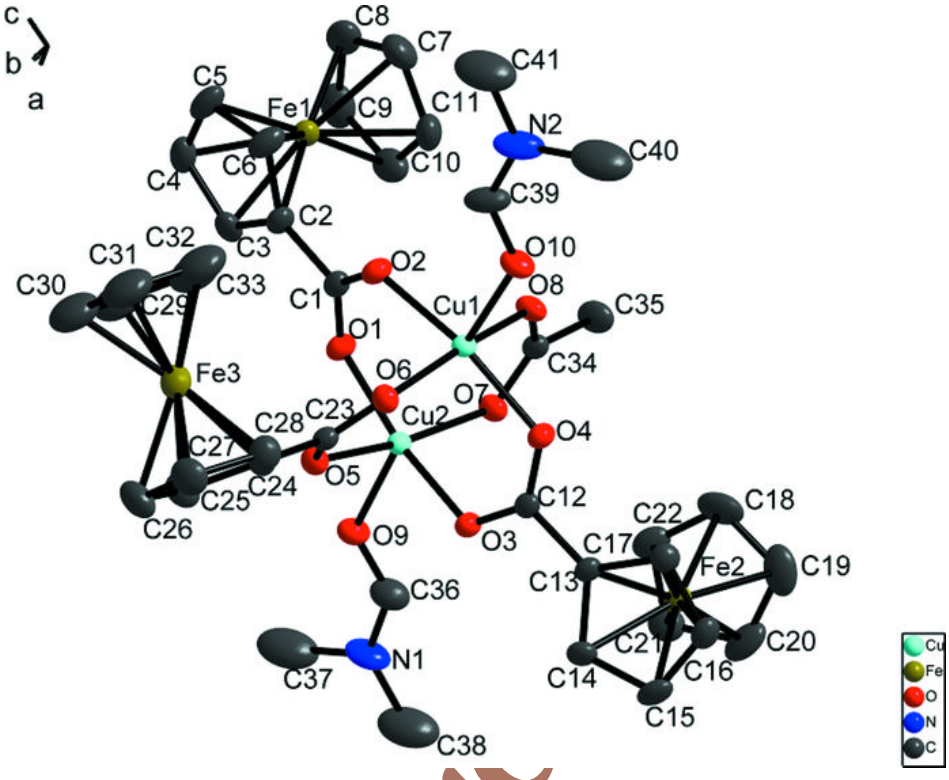

Fig. 2