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Aqua(1,10-phenanthroline-κ*N*,*N*′)-bis(2,3,4,5-tetrafluorobenzoato-κ*O*)-copper(II) 1,2,3,4-tetrafluorobenzene solvate

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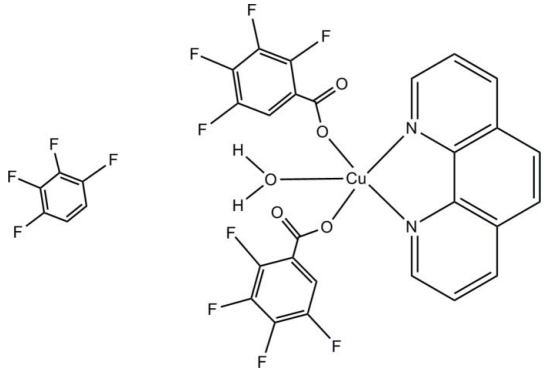
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.015 Å; disorder in main residue; R factor = 0.076; wR factor = 0.241; data-to-parameter ratio = 11.4.

In the title compound, $[Cu(C_{13}H_6F_4O_2)_2(C_{12}H_8N_2)(H_2O)]\cdot C_6H_2F_4$, each Cu^{II} ion is coordinated by two N atoms [Cu—N = 1.985 (6) and 2.052 (6) Å] from a 1,10-phenanthroline ligand, and three O atoms [Cu—O = 1.922 (6)–2.243 (5) Å] from two 2,3,4,5-tetrafluorobenzoate ligands and a water molecule, respectively, in a distorted square-pyramidal geometry. Intermolecular O—H···O hydrogen bonds link the complex molecules into chains parallel to the *a* axis. The crystal packing exhibits weak C—H···O hydrogen bonds and π–π interactions, as evidenced by a short distance of 3.717 (13) Å between the centroids of the benzene rings of neighbouring solvent molecules. One F atom is disordered over two positions; the site occupancy factors are 0.57 and 0.43.

Related literature

For the crystal structures of related organotin(IV) carboxylate complexes, see: Ma *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{13}H_6F_4O_2)_2(C_{12}H_8N_2)(H_2O)]\cdot C_6H_2F_4$
M_r = 797.99
Monoclinic, $P2_1/c$
a = 6.8150 (8) Å
b = 28.9810 (16) Å
c = 15.44800 (8) Å
β = 99.226 (2)°
V = 3011.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 298 (2) K
0.37 × 0.15 × 0.14 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.745, T_{max} = 0.891
14410 measured reflections
5137 independent reflections
2352 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.241
S = 1.03
5137 reflections
450 parameters
594 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O2^{i}	0.85	2.05	2.776 (8)	143
O5—H5B···O4^{i}	0.85	2.08	2.831 (7)	147
C25—H25···O2^{ii}	0.93	2.53	3.221 (10)	131
C26—H26···O4^{ii}	0.93	2.44	3.329 (10)	159

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+2$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2347).

References

Ma, C. L., Sun, J. S., Zhang, R. F. & Wang, D. Q. (2006). *Inorg. Chim. Acta*, **359**, 4179–4190.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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supplementary materials

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Aqua(1,10-phenanthroline-*κN*,*N*')bis(2,3,4,5-tetrafluorobenzoato-*κO*)copper(II) 1,2,3,4-tetrafluorobenzene solvate

J. Sun, C. Ma, G. He and J. Li

Comment

Metal complexes with carboxylates are among the most investigated complexes in the field of coordination chemistry. Nevertheless, the crystal structures of metal complexes with fluorated carboxylic ligands have rarely been reported. In our work, we have reported the organotin(IV) carboxylates complexes with this ligand (Ma *et al.*, 2006). In continuation of this study, we present here the crystal structure of the title compound.

In the title compound (Fig. 1), the Cu^{II} ion exhibits a five-coordinated square-pyramidal environment formed by three O atoms from two carboxylic ligands (Cu1—O1 1.922 (6) Å, Cu1—O3 1.948 (5) Å) and one water molecule (Cu1—O5 2.243 (5) Å), and two N atoms (Cu1—N1 1.985 (6) Å, Cu1—N2 2.052 (6) Å) from 1,10-phenanthroline ligand. Two N atoms and two O atoms form the basal plane and atom O5 occupies the apical site.

The intermolecular O—H···O hydrogen bonds (Table 1) link the main molecules related by translation along *a* axis into chains. The crystal packing exhibits also weak C—H···O hydrogen bonds (Table 1) and π···π interactions, proved by short distance of 3.717 (13) Å between the centroids of benzene rings of neighbouring solvent molecules.

Experimental

The reaction was carried out by the solvothermal method. 2,3,4,5-tetrafluorobenzoic acid(0.386 g,2 mmol) and cupric acetate(0.199 g, 1 mmol) and 1,10-phenanthroline(0.180 g, 1 mmol) were added to the airtight vessel with 20 ml water. The resulting green solution was filtered. The filtrate was placed for sevaral days yielding green block-shaped crystals.

The yield is 81% and elemental analysis: calc. for $C_{32}H_{14}CuF_{12}N_2O_5$: C 48.16, H 1.77, N 3.51; found: C 48.45, H 3.39, N 3.22. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

Refinement

All H atoms were geometrically positioned (C—H 0.93 Å, O—H 0.82 Å) and refined as riding, with U_{iso}(H)=1.2Ueq of the parent atom. Atom F1 was treated as statistically disordered bwteen two positions with the refined occupancies of 0.572 (7) and 0.428 (7), respectively.

Figures

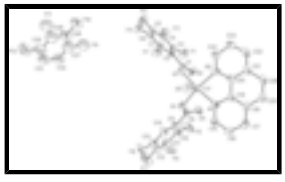


Fig. 1. View of the title compound with the atomic numbering and 30% probability displacement ellipsoids. H atoms omitted for clarity.

Aqua(1,10-phenanthroline-κ*N*,*N*')bis(2,3,4,5-tetrafluorobenzoato-κ*O*)copper(II) 1,2,3,4-tetrafluorobenzene solvate

Crystal data

$[Cu(C_{13}H_6F_4O_2)_2(C_{12}H_8N_2)(H_2O)]\cdot C_6H_2F_4$	F_{000} = 1588
M_r = 797.99	D_x = 1.760 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.8150 (8) Å	Cell parameters from 2282 reflections
b = 28.9810 (16) Å	θ = 2.7–25.3º
c = 15.44800 (8) Å	μ = 0.85 mm^{-1}
β = 99.226 (2)º	T = 298 (2) K
V = 3011.6 (4) Å^3	Block, green
Z = 4	0.37 × 0.15 × 0.14 mm

Data collection

CCD area detector diffractometer	5137 independent reflections
Radiation source: fine-focus sealed tube	2352 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.067
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→6
T_{min} = 0.745, T_{max} = 0.891	k = −26→34
14410 measured reflections	l = −18→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.076	H-atom parameters constrained
$wR(F^2)$ = 0.241	$w = 1/[\sigma^2(F_o^2) + (0.1138P)^2 + 2.0328P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
5137 reflections	$\Delta\rho_{max}$ = 0.77 e Å^{-3}
450 parameters	$\Delta\rho_{min}$ = −0.68 e Å^{-3}
594 restraints	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0025 (8)

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}	Occ. (<1)
Cu1	0.78922 (12)	0.40017 (3)	0.82641 (6)	0.0500 (4)	
F1	1.3110 (12)	0.4545 (3)	0.6146 (6)	0.092 (2)	0.572 (7)
F1'	0.6297 (16)	0.4035 (4)	0.5423 (8)	0.092 (2)	0.428 (7)
F2	1.3111 (7)	0.46696 (19)	0.4451 (3)	0.0910 (16)	
F3	0.9875 (8)	0.45009 (19)	0.3259 (3)	0.0962 (17)	
F4	0.6523 (8)	0.4203 (2)	0.3754 (3)	0.0969 (17)	
F5	1.4666 (8)	0.2934 (2)	0.9151 (5)	0.136 (3)	
F6	1.5600 (9)	0.2049 (2)	0.9159 (6)	0.160 (3)	
F7	1.2794 (10)	0.14033 (18)	0.8663 (5)	0.146 (3)	
F8	0.8983 (9)	0.16610 (18)	0.8170 (5)	0.129 (2)	
F9	0.5918 (14)	0.2803 (3)	0.2011 (7)	0.188 (2)	
F10	0.2495 (13)	0.3180 (2)	0.1405 (6)	0.173 (3)	
F11	−0.0500 (14)	0.2650 (3)	0.0694 (7)	0.188 (2)	
F12	−0.0109 (15)	0.1768 (3)	0.0570 (8)	0.225 (5)	
N1	0.7820 (8)	0.40042 (19)	0.9543 (4)	0.0516 (15)	
N2	0.7463 (8)	0.4693 (2)	0.8454 (4)	0.0520 (16)	
O1	0.7985 (8)	0.40807 (18)	0.7036 (4)	0.0688 (15)	
O2	1.1109 (8)	0.4300 (2)	0.7359 (4)	0.0768 (17)	
O3	0.8838 (8)	0.33670 (17)	0.8284 (3)	0.0617 (14)	
O4	1.1788 (8)	0.35633 (18)	0.9038 (4)	0.0701 (16)	
O5	0.4629 (7)	0.38446 (19)	0.7994 (4)	0.0707 (16)	
H5A	0.3958	0.4073	0.7765	0.085*	
H5B	0.4205	0.3765	0.8460	0.085*	
C1	0.9584 (12)	0.4212 (3)	0.6839 (5)	0.0525 (17)	
C2	0.9670 (11)	0.4291 (2)	0.5874 (5)	0.0507 (17)	
C3	1.1382 (11)	0.4449 (2)	0.5596 (5)	0.0561 (18)	
H3	1.2503	0.4513	0.6006	0.067*	0.428 (7)
C4	1.1439 (12)	0.4510 (3)	0.4727 (6)	0.0600 (19)	
C5	0.9808 (13)	0.4434 (3)	0.4121 (5)	0.063 (2)	
C6	0.8114 (12)	0.4276 (3)	0.4375 (6)	0.0628 (19)	
C7	0.8020 (11)	0.4210 (3)	0.5250 (5)	0.0573 (18)	
H7	0.6841	0.4111	0.5421	0.069*	0.572 (7)
C8	1.0611 (12)	0.3282 (3)	0.8664 (6)	0.0578 (19)	

C9	1.1242 (11)	0.2780 (3)	0.8655 (6)	0.065 (2)
C10	1.3182 (13)	0.2639 (3)	0.8900 (7)	0.076 (2)
C11	1.3644 (14)	0.2171 (3)	0.8885 (7)	0.088 (3)
C12	1.2302 (15)	0.1857 (3)	0.8678 (7)	0.084 (2)
C13	1.0365 (15)	0.1984 (3)	0.8409 (7)	0.086 (2)
C14	0.9808 (14)	0.2456 (3)	0.8398 (6)	0.077 (2)
H14	0.8493	0.2544	0.8218	0.093*
C15	0.7900 (11)	0.3644 (3)	1.0091 (5)	0.0626 (19)
H15	0.7997	0.3347	0.9872	0.075*
C16	0.7840 (12)	0.3702 (3)	1.0981 (6)	0.072 (2)
H16	0.7858	0.3441	1.1334	0.086*
C17	0.7758 (12)	0.4119 (3)	1.1349 (6)	0.068 (2)
H17	0.7750	0.4151	1.1947	0.082*
C18	0.7686 (10)	0.4502 (3)	1.0802 (5)	0.0543 (17)
C19	0.7699 (10)	0.4428 (3)	0.9901 (5)	0.0529 (17)
C20	0.7507 (10)	0.4802 (3)	0.9295 (6)	0.0531 (17)
C21	0.7379 (10)	0.5253 (3)	0.9603 (6)	0.0590 (18)
C22	0.7192 (11)	0.5600 (3)	0.8973 (7)	0.067 (2)
H22	0.7150	0.5907	0.9142	0.081*
C23	0.7073 (12)	0.5493 (3)	0.8130 (7)	0.071 (2)
H23	0.6892	0.5724	0.7708	0.086*
C24	0.7222 (11)	0.5028 (3)	0.7875 (6)	0.064 (2)
H24	0.7148	0.4957	0.7284	0.077*
C25	0.7577 (11)	0.4964 (3)	1.1095 (6)	0.066 (2)
H25	0.7590	0.5020	1.1689	0.079*
C26	0.7457 (10)	0.5319 (3)	1.0539 (6)	0.0634 (19)
H26	0.7423	0.5617	1.0758	0.076*
C27	0.451 (3)	0.2499 (7)	0.1628 (13)	0.188 (2)
C28	0.278 (3)	0.2712 (5)	0.1346 (12)	0.173 (3)
C29	0.132 (3)	0.2465 (7)	0.1038 (13)	0.188 (2)
C30	0.151 (3)	0.1996 (5)	0.0959 (11)	0.163 (4)
C31	0.328 (3)	0.1800 (5)	0.1200 (11)	0.165 (4)
H31	0.3432	0.1487	0.1101	0.198*
C32	0.486 (2)	0.2046 (5)	0.1583 (11)	0.162 (4)
H32	0.6083	0.1913	0.1796	0.195*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0465 (6)	0.0506 (6)	0.0529 (6)	0.0004 (4)	0.0082 (4)	−0.0032 (4)
F1	0.061 (4)	0.131 (6)	0.082 (5)	−0.011 (4)	0.007 (4)	0.000 (5)
F1'	0.061 (4)	0.131 (6)	0.082 (5)	−0.011 (4)	0.007 (4)	0.000 (5)
F2	0.085 (3)	0.111 (4)	0.086 (4)	−0.003 (3)	0.040 (3)	0.016 (3)
F3	0.109 (4)	0.128 (5)	0.057 (3)	0.007 (3)	0.028 (3)	0.008 (3)
F4	0.085 (4)	0.138 (5)	0.059 (3)	−0.011 (3)	−0.014 (3)	−0.002 (3)
F5	0.062 (3)	0.079 (4)	0.264 (9)	−0.010 (3)	0.015 (4)	0.010 (4)
F6	0.082 (4)	0.106 (5)	0.293 (10)	0.041 (4)	0.035 (5)	0.038 (5)
F7	0.157 (6)	0.056 (3)	0.238 (9)	0.043 (4)	0.070 (6)	0.008 (4)

F8	0.123 (5)	0.053 (3)	0.201 (7)	−0.014 (3)	−0.005 (5)	−0.028 (4)
F9	0.184 (5)	0.148 (4)	0.213 (5)	−0.018 (4)	−0.025 (4)	0.040 (4)
F10	0.218 (6)	0.085 (4)	0.200 (6)	0.006 (4)	−0.014 (5)	0.017 (4)
F11	0.184 (5)	0.148 (4)	0.213 (5)	−0.018 (4)	−0.025 (4)	0.040 (4)
F12	0.206 (9)	0.136 (7)	0.302 (14)	−0.052 (6)	−0.055 (9)	0.038 (7)
N1	0.040 (3)	0.035 (3)	0.079 (5)	0.006 (3)	0.007 (3)	0.001 (3)
N2	0.037 (3)	0.059 (4)	0.061 (4)	−0.002 (3)	0.012 (3)	0.017 (3)
O1	0.053 (3)	0.082 (4)	0.075 (4)	−0.005 (3)	0.020 (3)	−0.007 (3)
O2	0.066 (4)	0.108 (5)	0.052 (4)	0.007 (3)	−0.006 (3)	−0.005 (3)
O3	0.059 (3)	0.062 (3)	0.065 (4)	−0.001 (3)	0.013 (3)	−0.005 (3)
O4	0.060 (3)	0.053 (3)	0.097 (5)	−0.008 (3)	0.011 (3)	−0.009 (3)
O5	0.044 (3)	0.084 (4)	0.086 (4)	−0.004 (3)	0.014 (3)	0.001 (3)
C1	0.052 (4)	0.058 (4)	0.047 (4)	0.011 (3)	0.006 (4)	0.002 (3)
C2	0.051 (4)	0.056 (4)	0.047 (4)	0.003 (3)	0.011 (3)	0.000 (3)
C3	0.050 (4)	0.058 (4)	0.059 (4)	0.005 (3)	0.006 (4)	−0.001 (4)
C4	0.056 (4)	0.064 (4)	0.063 (5)	0.001 (4)	0.020 (4)	0.002 (4)
C5	0.073 (5)	0.076 (5)	0.042 (4)	0.000 (4)	0.014 (4)	0.000 (4)
C6	0.063 (4)	0.071 (5)	0.054 (4)	−0.005 (4)	0.008 (4)	−0.001 (4)
C7	0.053 (4)	0.070 (4)	0.051 (4)	−0.007 (4)	0.016 (4)	−0.001 (4)
C8	0.055 (4)	0.048 (4)	0.075 (5)	−0.007 (4)	0.021 (4)	0.001 (4)
C9	0.050 (4)	0.051 (4)	0.097 (6)	−0.001 (3)	0.023 (4)	0.000 (4)
C10	0.059 (5)	0.058 (4)	0.112 (6)	0.001 (4)	0.016 (4)	0.001 (4)
C11	0.070 (5)	0.076 (5)	0.120 (7)	0.014 (5)	0.021 (5)	0.009 (5)
C12	0.083 (5)	0.049 (5)	0.121 (6)	0.006 (4)	0.025 (5)	0.004 (5)
C13	0.084 (5)	0.059 (5)	0.113 (6)	−0.002 (5)	0.008 (5)	−0.004 (5)
C14	0.075 (5)	0.053 (4)	0.104 (6)	−0.004 (4)	0.012 (4)	−0.012 (4)
C15	0.056 (4)	0.062 (4)	0.070 (5)	0.006 (4)	0.012 (4)	−0.004 (4)
C16	0.062 (4)	0.089 (5)	0.063 (5)	0.001 (4)	0.010 (4)	0.017 (4)
C17	0.058 (4)	0.086 (5)	0.059 (4)	−0.004 (4)	0.001 (4)	−0.007 (4)
C18	0.033 (3)	0.068 (4)	0.061 (4)	−0.004 (3)	0.007 (3)	−0.012 (4)
C19	0.032 (3)	0.061 (4)	0.065 (4)	−0.005 (3)	0.005 (3)	−0.008 (3)
C20	0.033 (3)	0.055 (4)	0.074 (4)	−0.003 (3)	0.017 (3)	−0.013 (3)
C21	0.033 (3)	0.061 (4)	0.084 (5)	−0.008 (3)	0.013 (3)	−0.015 (4)
C22	0.048 (4)	0.055 (4)	0.100 (5)	0.002 (3)	0.015 (4)	−0.001 (4)
C23	0.055 (4)	0.061 (5)	0.101 (6)	−0.001 (4)	0.021 (4)	0.012 (4)
C24	0.056 (4)	0.063 (4)	0.076 (5)	0.001 (4)	0.019 (4)	0.008 (4)
C25	0.042 (4)	0.081 (5)	0.073 (5)	−0.003 (4)	0.007 (4)	−0.020 (4)
C26	0.039 (4)	0.065 (4)	0.085 (5)	−0.004 (3)	0.008 (4)	−0.027 (4)
C27	0.184 (5)	0.148 (4)	0.213 (5)	−0.018 (4)	−0.025 (4)	0.040 (4)
C28	0.218 (6)	0.085 (4)	0.200 (6)	0.006 (4)	−0.014 (5)	0.017 (4)
C29	0.184 (5)	0.148 (4)	0.213 (5)	−0.018 (4)	−0.025 (4)	0.040 (4)
C30	0.174 (9)	0.105 (7)	0.195 (9)	−0.017 (7)	−0.017 (8)	0.043 (7)
C31	0.179 (9)	0.105 (7)	0.195 (9)	0.000 (7)	−0.021 (8)	0.040 (7)
C32	0.170 (8)	0.110 (7)	0.191 (9)	0.004 (7)	−0.021 (8)	0.043 (7)

Geometric parameters (Å, °)

Cu1—O1	1.922 (6)	C8—C9	1.517 (10)
Cu1—O3	1.948 (5)	C9—C14	1.367 (11)

Cu1—N1	1.985 (6)	C9—C10	1.378 (11)
Cu1—N2	2.052 (6)	C10—C11	1.393 (12)
Cu1—O5	2.243 (5)	C11—C12	1.294 (12)
F1—C3	1.366 (11)	C12—C13	1.369 (12)
F1'—C7	1.345 (13)	C13—C14	1.421 (11)
F2—C4	1.360 (8)	C14—H14	0.9300
F3—C5	1.354 (8)	C15—C16	1.391 (11)
F4—C6	1.345 (9)	C15—H15	0.9300
F5—C10	1.332 (9)	C16—C17	1.341 (11)
F6—C11	1.379 (10)	C16—H16	0.9300
F7—C12	1.358 (9)	C17—C18	1.391 (11)
F8—C13	1.336 (10)	C17—H17	0.9300
F9—C27	1.368 (17)	C18—C19	1.410 (10)
F10—C28	1.373 (15)	C18—C25	1.418 (10)
F11—C29	1.378 (18)	C19—C20	1.425 (10)
F12—C30	1.343 (17)	C20—C21	1.399 (10)
N1—C15	1.340 (9)	C21—C22	1.390 (11)
N1—C19	1.354 (9)	C21—C26	1.450 (11)
N2—C24	1.312 (9)	C22—C23	1.329 (11)
N2—C20	1.333 (9)	C22—H22	0.9300
O1—C1	1.238 (9)	C23—C24	1.412 (11)
O2—C1	1.234 (9)	C23—H23	0.9300
O3—C8	1.280 (9)	C24—H24	0.9300
O4—C8	1.222 (9)	C25—C26	1.335 (11)
O5—H5A	0.8501	C25—H25	0.9300
O5—H5B	0.8499	C26—H26	0.9300
C1—C2	1.520 (10)	C27—C32	1.34 (2)
C2—C7	1.378 (10)	C27—C28	1.34 (2)
C2—C3	1.384 (10)	C28—C29	1.25 (2)
C3—C4	1.361 (10)	C29—C30	1.37 (2)
C3—H3	0.9300	C30—C31	1.334 (19)
C4—C5	1.352 (11)	C31—C32	1.344 (18)
C5—C6	1.357 (11)	C31—H31	0.9300
C6—C7	1.377 (10)	C32—H32	0.9300
C7—H7	0.9300		
O1—Cu1—O3	93.7 (2)	F7—C12—C13	118.9 (9)
O1—Cu1—N1	172.9 (2)	F8—C13—C12	119.9 (8)
O3—Cu1—N1	92.8 (2)	F8—C13—C14	119.7 (8)
O1—Cu1—N2	93.0 (2)	C12—C13—C14	120.3 (9)
O3—Cu1—N2	166.9 (2)	C9—C14—C13	118.8 (9)
N1—Cu1—N2	80.0 (2)	C9—C14—H14	120.6
O1—Cu1—O5	91.7 (2)	C13—C14—H14	120.6
O3—Cu1—O5	97.3 (2)	N1—C15—C16	121.6 (8)
N1—Cu1—O5	90.2 (2)	N1—C15—H15	119.2
N2—Cu1—O5	93.7 (2)	C16—C15—H15	119.2
C15—N1—C19	116.6 (7)	C17—C16—C15	122.5 (8)
C15—N1—Cu1	128.4 (5)	C17—C16—H16	118.7
C19—N1—Cu1	115.0 (5)	C15—C16—H16	118.7
C24—N2—C20	117.9 (7)	C16—C17—C18	117.5 (8)

C24—N2—Cu1	129.0 (6)	C16—C17—H17	121.3
C20—N2—Cu1	113.0 (5)	C18—C17—H17	121.3
C1—O1—Cu1	116.7 (5)	C17—C18—C19	118.2 (7)
C8—O3—Cu1	118.3 (5)	C17—C18—C25	123.8 (8)
Cu1—O5—H5A	111.7	C19—C18—C25	117.9 (8)
Cu1—O5—H5B	111.0	N1—C19—C18	123.5 (7)
H5A—O5—H5B	109.3	N1—C19—C20	115.3 (7)
O2—C1—O1	125.9 (8)	C18—C19—C20	121.2 (7)
O2—C1—C2	116.5 (7)	N2—C20—C21	124.2 (8)
O1—C1—C2	117.5 (7)	N2—C20—C19	116.4 (7)
C7—C2—C3	118.2 (7)	C21—C20—C19	119.5 (8)
C7—C2—C1	120.3 (7)	C22—C21—C20	116.1 (8)
C3—C2—C1	121.4 (7)	C22—C21—C26	126.0 (8)
C4—C3—F1	115.4 (8)	C20—C21—C26	117.9 (8)
C4—C3—C2	120.5 (8)	C23—C22—C21	120.1 (8)
F1—C3—C2	124.0 (8)	C23—C22—H22	119.9
C4—C3—H3	119.7	C21—C22—H22	119.9
F1—C3—H3	4.4	C22—C23—C24	120.0 (9)
C2—C3—H3	119.7	C22—C23—H23	120.0
C5—C4—F2	118.4 (7)	C24—C23—H23	120.0
C5—C4—C3	120.8 (7)	N2—C24—C23	121.5 (9)
F2—C4—C3	120.8 (8)	N2—C24—H24	119.2
C4—C5—F3	120.3 (7)	C23—C24—H24	119.2
C4—C5—C6	119.8 (8)	C26—C25—C18	121.5 (8)
F3—C5—C6	119.8 (8)	C26—C25—H25	119.3
F4—C6—C5	118.3 (8)	C18—C25—H25	119.3
F4—C6—C7	121.2 (7)	C25—C26—C21	121.9 (8)
C5—C6—C7	120.5 (8)	C25—C26—H26	119.0
F1'—C7—C6	115.2 (9)	C21—C26—H26	119.0
F1'—C7—C2	124.5 (8)	C32—C27—C28	126.3 (19)
C6—C7—C2	120.1 (7)	C32—C27—F9	122.4 (18)
F1'—C7—H7	6.2	C28—C27—F9	111.3 (19)
C6—C7—H7	120.0	C29—C28—C27	117.3 (18)
C2—C7—H7	120.0	C29—C28—F10	119 (2)
O4—C8—O3	126.1 (7)	C27—C28—F10	124.0 (19)
O4—C8—C9	118.6 (8)	C28—C29—C30	121 (2)
O3—C8—C9	115.4 (7)	C28—C29—F11	122.2 (19)
C14—C9—C10	119.1 (8)	C30—C29—F11	116.1 (17)
C14—C9—C8	118.1 (7)	C31—C30—F12	123.8 (16)
C10—C9—C8	122.8 (7)	C31—C30—C29	119.3 (18)
F5—C10—C9	122.7 (7)	F12—C30—C29	116.6 (17)
F5—C10—C11	117.7 (8)	C30—C31—C32	121.4 (17)
C9—C10—C11	119.5 (8)	C30—C31—H31	119.3
C12—C11—F6	120.3 (9)	C32—C31—H31	119.3
C12—C11—C10	122.5 (9)	C27—C32—C31	113.9 (17)
F6—C11—C10	117.1 (9)	C27—C32—H32	123.1
C11—C12—F7	121.3 (9)	C31—C32—H32	123.1
C11—C12—C13	119.7 (9)		
O1—Cu1—N1—C15	−172.2 (16)	C9—C10—C11—F6	−178.3 (9)

O3—Cu1—N1—C15	−15.0 (6)	F6—C11—C12—F7	−4.8 (17)
N2—Cu1—N1—C15	176.1 (6)	C10—C11—C12—F7	179.6 (10)
O5—Cu1—N1—C15	82.3 (6)	F6—C11—C12—C13	179.8 (10)
O1—Cu1—N1—C19	7(2)	C10—C11—C12—C13	4.2 (17)
O3—Cu1—N1—C19	164.1 (5)	C11—C12—C13—F8	178.0 (10)
N2—Cu1—N1—C19	−4.8 (4)	F7—C12—C13—F8	2.5 (16)
O5—Cu1—N1—C19	−98.6 (5)	C11—C12—C13—C14	−3.1 (17)
O1—Cu1—N2—C24	4.0 (6)	F7—C12—C13—C14	−178.6 (9)
O3—Cu1—N2—C24	124.9 (10)	C10—C9—C14—C13	1.3 (14)
N1—Cu1—N2—C24	−177.4 (6)	C8—C9—C14—C13	−178.3 (8)
O5—Cu1—N2—C24	−87.8 (6)	F8—C13—C14—C9	179.2 (9)
O1—Cu1—N2—C20	−173.7 (5)	C12—C13—C14—C9	0.3 (15)
O3—Cu1—N2—C20	−52.8 (11)	C19—N1—C15—C16	0.6 (10)
N1—Cu1—N2—C20	4.9 (4)	Cu1—N1—C15—C16	179.7 (5)
O5—Cu1—N2—C20	94.4 (5)	N1—C15—C16—C17	−2.0 (12)
O3—Cu1—O1—C1	−87.6 (5)	C15—C16—C17—C18	1.5 (12)
N1—Cu1—O1—C1	70 (2)	C16—C17—C18—C19	0.1 (11)
N2—Cu1—O1—C1	81.1 (5)	C16—C17—C18—C25	179.4 (7)
O5—Cu1—O1—C1	174.9 (5)	C15—N1—C19—C18	1.0 (10)
O1—Cu1—O3—C8	107.7 (5)	Cu1—N1—C19—C18	−178.2 (5)
N1—Cu1—O3—C8	−69.6 (6)	C15—N1—C19—C20	−176.7 (6)
N2—Cu1—O3—C8	−13.1 (13)	Cu1—N1—C19—C20	4.1 (7)
O5—Cu1—O3—C8	−160.1 (5)	C17—C18—C19—N1	−1.4 (10)
Cu1—O1—C1—O2	−0.6 (10)	C25—C18—C19—N1	179.2 (6)
Cu1—O1—C1—C2	−178.2 (5)	C17—C18—C19—C20	176.2 (6)
O2—C1—C2—C7	−178.7 (7)	C25—C18—C19—C20	−3.1 (10)
O1—C1—C2—C7	−0.9 (11)	C24—N2—C20—C21	−2.2 (10)
O2—C1—C2—C3	0.6 (10)	Cu1—N2—C20—C21	175.8 (5)
O1—C1—C2—C3	178.4 (7)	C24—N2—C20—C19	177.8 (6)
C7—C2—C3—C4	−1.7 (11)	Cu1—N2—C20—C19	−4.2 (7)
C1—C2—C3—C4	179.0 (7)	N1—C19—C20—N2	0.2 (9)
C7—C2—C3—F1	179.5 (8)	C18—C19—C20—N2	−177.6 (6)
C1—C2—C3—F1	0.2 (12)	N1—C19—C20—C21	−179.8 (6)
F1—C3—C4—C5	−178.8 (8)	C18—C19—C20—C21	2.4 (10)
C2—C3—C4—C5	2.3 (12)	N2—C20—C21—C22	0.1 (10)
F1—C3—C4—F2	−1.8 (11)	C19—C20—C21—C22	−179.9 (6)
C2—C3—C4—F2	179.4 (7)	N2—C20—C21—C26	−179.7 (6)
F2—C4—C5—F3	2.2 (12)	C19—C20—C21—C26	0.3 (9)
C3—C4—C5—F3	179.3 (7)	C20—C21—C22—C23	2.4 (11)
F2—C4—C5—C6	−179.8 (7)	C26—C21—C22—C23	−177.8 (7)
C3—C4—C5—C6	−2.7 (12)	C21—C22—C23—C24	−2.7 (12)
C4—C5—C6—F4	−179.7 (7)	C20—N2—C24—C23	1.9 (10)
F3—C5—C6—F4	−1.7 (12)	Cu1—N2—C24—C23	−175.8 (5)
C4—C5—C6—C7	2.5 (13)	C22—C23—C24—N2	0.5 (12)
F3—C5—C6—C7	−179.5 (7)	C17—C18—C25—C26	−178.2 (7)
F4—C6—C7—F1'	5.0 (13)	C19—C18—C25—C26	1.1 (11)
C5—C6—C7—F1'	−177.3 (9)	C18—C25—C26—C21	1.6 (11)
F4—C6—C7—C2	−179.7 (7)	C22—C21—C26—C25	177.9 (7)
C5—C6—C7—C2	−2.0 (12)	C20—C21—C26—C25	−2.3 (10)

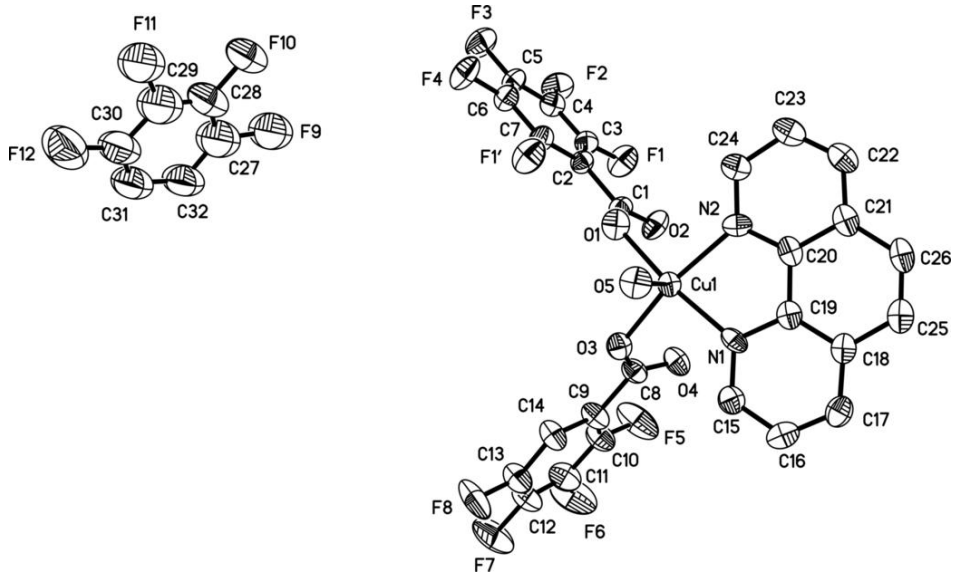
C3—C2—C7—F1'	176.5 (9)	C32—C27—C28—C29	3(4)
C1—C2—C7—F1'	−4.2 (13)	F9—C27—C28—C29	−175.1 (18)
C3—C2—C7—C6	1.5 (11)	C32—C27—C28—F10	−179.7 (16)
C1—C2—C7—C6	−179.2 (7)	F9—C27—C28—F10	2(3)
Cu1—O3—C8—O4	1.4 (11)	C27—C28—C29—C30	−3(3)
Cu1—O3—C8—C9	179.8 (5)	F10—C28—C29—C30	179.8 (16)
O4—C8—C9—C14	166.9 (8)	C27—C28—C29—F11	−177.1 (17)
O3—C8—C9—C14	−11.6 (12)	F10—C28—C29—F11	5(3)
O4—C8—C9—C10	−12.7 (13)	C28—C29—C30—C31	−1(3)
O3—C8—C9—C10	168.8 (8)	F11—C29—C30—C31	173.7 (17)
C14—C9—C10—F5	179.3 (9)	C28—C29—C30—F12	−176 (2)
C8—C9—C10—F5	−1.1 (15)	F11—C29—C30—F12	−1(3)
C14—C9—C10—C11	−0.4 (15)	F12—C30—C31—C32	179.6 (16)
C8—C9—C10—C11	179.2 (9)	C29—C30—C31—C32	5(3)
F5—C10—C11—C12	177.8 (10)	C28—C27—C32—C31	1(3)
C9—C10—C11—C12	−2.5 (17)	F9—C27—C32—C31	178.7 (17)
F5—C10—C11—F6	2.1 (14)	C30—C31—C32—C27	−5(3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O2^{i}	0.85	2.05	2.776 (8)	143
O5—H5B···O4^{i}	0.85	2.08	2.831 (7)	147
C25—H25···O2^{ii}	0.93	2.53	3.221 (10)	131
C26—H26···O4^{ii}	0.93	2.44	3.329 (10)	159

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+2, −*y*+1, −*z*+2.

Fig. 1


F11
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