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μ_2-Methanol-κ^2O:O-bis[(1,10-phenanthroline-κ^2N,N')bis(2,3,4,5-tetrafluorobenzoato)-$\kappa O;\kappa^2O,O'$-copper(II)]

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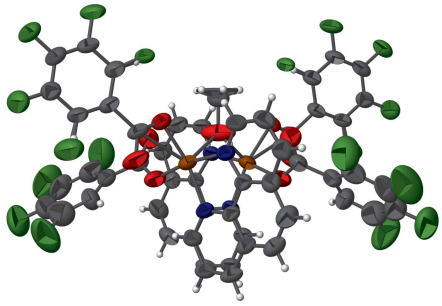
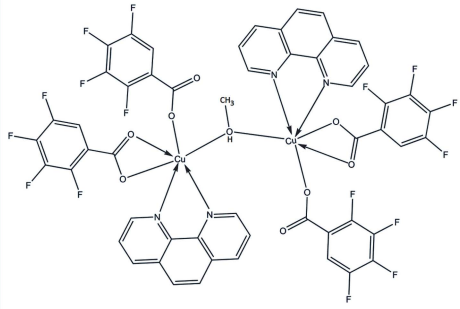
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Cu_2(C_7HF_4O_2)_4(C_{12}H_8N_2)_2(CH_3OH)]$, the molecule lies on a twofold rotation axis in space group $C2/c$. The Cu^{2+} ion exhibits a distorted octahedral sphere with two N atoms from the phenanthroline ligand, three O atoms from the 2,3,4,5-tetrafluorobenzoate ligands and one O atom from a methanol molecule. The distortion from an octahedral shape is a consequence of the Jahn–Teller effect of Cu^{II} and the small bite angle for the bidentate fluorobenzoate ligand [54.50 (11)°]. The methanol molecule bridges two symmetry-related Cu^{II} atoms to form the complete molecule. In the bidentate fluorobenzoate ligand, one F atom is disordered over two positions of equal occupancy. In the crystal structure, only weak intermolecular interactions are observed.

3D view



Chemical scheme



Structure description

The rational design and synthesis of metal–organic coordination compounds has received great interest owing to their magnetic, luminescence, gas storage/separation and catalytic properties (Wu & Lee, 2006; Han *et al.*, 2006; Noro *et al.*, 2000). The general strategy for the choice of organic building blocks and the framework of the coordination complex relies on the utilization of multidentate ligands, which can act as bridging ligands. It is well known that the spacer ligands with appropriate backbones and coordination conformations are important in regulating the final structure of coordination complexes, especially carboxylates, because of their diverse coordination modes in the construction of coordination complexes (Sun *et al.*, 2009). In this study, we selected 2,3,4,5-tetrafluorobenzoic acid as ligand, with 1,10-phenanthroline and methanol as co-ligands.

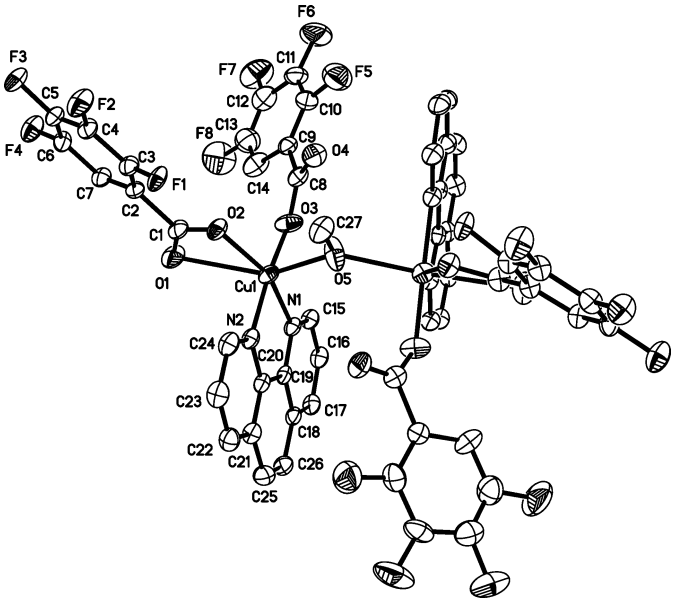


Figure 1
The molecular structure of the title compound, with atom labels for the asymmetric unit, and 20% probability displacement ellipsoids. Non-labelled atoms are generated by the symmetry operation $1-x, y, \frac{3}{2}-z$. H atoms are omitted for clarity.

The asymmetric unit of the title complex contains two 2,3,4,5-tetrafluorobenzoate anions, one 1,10-phenanthroline, and one coordinating methanol molecule. The Cu^{II} atom exhibits a distorted octahedral sphere, which is formed by two 1,10-phenanthroline N atoms, two O atoms from one bidentate tetrafluorobenzoate ligand, one O atom from the other independent tetrafluorobenzoate ligand and one O atom from the methanol molecule. The distortion is ascribed to the Jahn–Teller effect of Cu^{II} and the small bite angle of the bidentate tetrafluorobenzoate ligand, O1—Cu1—O2 = 54.50 (11)°. The Cu—N bond lengths are 2.010 (3) and 2.014 (3) Å. The Cu—O coordination bond lengths are in the range 1.919 (3) to 2.686 (4) Å. The latter distance is very long, while the other distances are close to the literature reported distances [for example 1.942 (3) Å; Sun, 2014]. The methanol molecule is located on a twofold rotation axis of space group *C*2/*c* and bridges two metal centres, forming a dinuclear complex (Fig. 1).

Synthesis and crystallization

2,3,4,5-Tetrafluorobenzoic acid (0.194 g, 1 mmol), copper acetate (0.199 g, 1 mmol) and 1,10-phenanthroline (0.198 g, 1 mmol) were dissolved in methanol. The mixture was heated to 40°C for 3 h, resulting in a blue-coloured solution. Crystals of the title compound were obtained by slow evaporation within one week (yield: 78%). Elemental analysis: calculated for $C_{53}H_{24}Cu_2F_{16}N_4O_9$: C 49.28, H 1.87, N 4.34; found: C 49.31, H 1.49, N 4.54.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Cu_2(C_7HF_4O_2)_4(C_{12}H_8N_2)_2\cdot(CH_4O)]$
M_r	1291.84
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	295
a, *b*, *c* (Å)	14.5119 (12), 24.8953 (19), 15.2514 (17)
β (°)	115.360 (1)
V (Å^3)	4979.0 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.98
Crystal size (mm)	0.34 × 0.31 × 0.28
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.741, 0.794
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14347, 5087, 3096
R_{int}	0.083
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.183, 0.97
No. of reflections	5087
No. of parameters	389
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.93, −0.50

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2015* (Sheldrick, 2015*b*), *XP* in *SHELXTL-Plus* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. One F atom on the C2–C7 ring was found to be disordered over two chemically equivalent positions (F1 and F1′); the occupancies for these F atoms were fixed at 0.5.

Funding information

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References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Han, H., Zhang, S., Hou, H., Fan, Y. & Zhu, Y. (2006). *Eur. J. Inorg. Chem.* pp. 1594–1600.
Noro, S.-I., Kitagawa, S., Kondo, M. & Seki, K. (2000). *Angew. Chem. Int. Ed.* **39**, 2081–2084.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Sun, D., Luo, G.-G., Zhang, N., Chen, J.-H., Huang, R.-B., Lin, L.-R. & Zheng, L.-S. (2009). *Polyhedron*, **28**, 2983–2988.
Sun, J. (2014). *Acta Cryst.* E**70**, m365–m366.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wu, M.-C. & Lee, C.-S. (2006). *Inorg. Chem.* **45**, 9634–9636.

full crystallographic data

IUCrData (2019). **4**, x191583 [https://doi.org/10.1107/S2414314619015839]

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Crystal data

$[Cu_2(C_7HF_4O_2)_4(C_{12}H_8N_2)_2(CH_4O)]$
M_r = 1291.84
Monoclinic, $C2/c$
a = 14.5119 (12) Å
b = 24.8953 (19) Å
c = 15.2514 (17) Å
β = 115.360 (1)°
V = 4979.0 (8) Å^3
Z = 4
$F(000)$ = 2576.0
D_x = 1.721 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3671 reflections
θ = 2.7–22.7°
μ = 0.98 mm^{-1}
T = 295 K
Block, blue
0.34 × 0.31 × 0.28 mm

Data collection

Bruker SMART APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.741, T_{max} = 0.794
14347 measured reflections
5087 independent reflections
3096 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 26.4°, θ_{min} = 1.8°
h = −18→12
k = −30→31
l = −9→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.183
S = 0.97
5087 reflections
389 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1076P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Special details

Refinement. All H atoms bonded to C atoms were placed in idealized positions, while the H atom for the hydroxy group in methanol was found in a difference map. They were refined with calculated isotropic displacement parameters, U_{iso}(H) = 1.5U_{eq}(carrier atom) for the methanol molecule, and U_{iso}(H) = 1.2U_{eq}(carrier atom) for other H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.34551 (4)	0.11688 (2)	0.66779 (4)	0.0594 (2)	
F1	0.2002 (3)	−0.04902 (16)	0.6375 (4)	0.0661 (13)	0.5
F1′	−0.0297 (6)	0.0968 (3)	0.6070 (7)	0.138 (3)	0.5
F2	0.0645 (2)	−0.11549 (9)	0.6484 (3)	0.0951 (10)	
F3	−0.1166 (2)	−0.08059 (10)	0.6335 (2)	0.0861 (8)	
F4	−0.1603 (2)	0.02528 (11)	0.6133 (2)	0.0949 (9)	
F5	0.3880 (4)	0.1024 (2)	1.0631 (3)	0.1549 (16)	
F6	0.2833 (5)	0.1509 (2)	1.1452 (3)	0.183 (2)	
F7	0.1278 (4)	0.2134 (2)	1.0437 (4)	0.174 (2)	
F8	0.0803 (4)	0.2335 (2)	0.8579 (4)	0.191 (2)	
N1	0.3711 (2)	0.19254 (11)	0.6371 (2)	0.0524 (8)	
N2	0.3552 (2)	0.10156 (12)	0.5426 (2)	0.0541 (8)	
O1	0.1410 (3)	0.11257 (12)	0.5917 (3)	0.0948 (12)	
O2	0.2644 (2)	0.05231 (11)	0.6604 (2)	0.0669 (8)	
O3	0.3402 (3)	0.14324 (12)	0.7838 (2)	0.0859 (10)	
O4	0.4020 (3)	0.07702 (14)	0.8920 (3)	0.0880 (10)	
O5	0.500000	0.06843 (17)	0.750000	0.114 (2)	
H5	0.507559	0.087454	0.718056	0.170*	0.5
C1	0.1719 (3)	0.06834 (15)	0.6248 (3)	0.0638 (11)	
C2	0.0938 (3)	0.02777 (15)	0.6269 (3)	0.0558 (10)	
C3	0.1167 (3)	−0.02735 (16)	0.6371 (3)	0.0609 (10)	
H3A	0.179641	−0.039620	0.643094	0.073*	0.5
C4	0.0439 (3)	−0.06323 (15)	0.6380 (3)	0.0618 (10)	
C5	−0.0490 (3)	−0.04519 (16)	0.6303 (3)	0.0641 (11)	
C6	−0.0700 (3)	0.00815 (16)	0.6191 (3)	0.0613 (10)	
C7	0.0008 (3)	0.04419 (15)	0.6171 (3)	0.0596 (10)	
H7A	−0.015434	0.080538	0.608791	0.072*	0.5
C8	0.3517 (4)	0.11736 (17)	0.8595 (4)	0.0669 (12)	
C9	0.2945 (3)	0.14200 (17)	0.9129 (3)	0.0640 (11)	
C10	0.3157 (5)	0.1326 (2)	1.0070 (4)	0.0913 (16)	
C11	0.2593 (6)	0.1583 (3)	1.0534 (4)	0.1020 (19)	
C12	0.1783 (6)	0.1904 (3)	0.9955 (6)	0.111 (2)	
C13	0.1601 (6)	0.1995 (3)	0.9059 (6)	0.118 (2)	
C14	0.2117 (5)	0.1761 (2)	0.8620 (5)	0.0988 (18)	
H14A	0.192403	0.182506	0.796444	0.119*	
C15	0.3733 (3)	0.23756 (15)	0.6848 (3)	0.0581 (10)	
H15A	0.369135	0.235347	0.743833	0.070*	
C16	0.3816 (3)	0.28796 (15)	0.6491 (3)	0.0630 (11)	
H16A	0.382954	0.318711	0.684241	0.076*	
C17	0.3879 (3)	0.29221 (15)	0.5628 (3)	0.0631 (11)	
H17A	0.392998	0.325803	0.538613	0.076*	
C18	0.3864 (3)	0.24496 (15)	0.5100 (3)	0.0552 (9)	
C19	0.3773 (3)	0.19618 (14)	0.5514 (3)	0.0488 (9)	
C20	0.3699 (3)	0.14693 (14)	0.4999 (3)	0.0509 (9)	
C21	0.3765 (3)	0.14670 (17)	0.4121 (3)	0.0641 (11)	

C22	0.3703 (3)	0.0972 (2)	0.3674 (3)	0.0720 (12)	
H22A	0.375267	0.095025	0.308735	0.086*	
C23	0.3568 (3)	0.05181 (18)	0.4108 (4)	0.0753 (13)	
H23A	0.353094	0.018445	0.382027	0.090*	
C24	0.3485 (3)	0.05565 (17)	0.4976 (3)	0.0671 (12)	
H24A	0.337867	0.024404	0.525349	0.081*	
C25	0.3883 (4)	0.1983 (2)	0.3731 (4)	0.0784 (13)	
H25A	0.393410	0.199276	0.314372	0.094*	
C26	0.3922 (4)	0.24431 (19)	0.4199 (3)	0.0714 (12)	
H26A	0.398746	0.276591	0.392409	0.086*	
C27	0.500000	0.0126 (2)	0.750000	0.087 (2)	
H27A	0.468494	−0.000260	0.789962	0.130*	0.5
H27B	0.568936	−0.000260	0.775153	0.130*	0.5
H27C	0.462570	−0.000260	0.684885	0.130*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0700 (4)	0.0378 (3)	0.0787 (4)	−0.0107 (2)	0.0399 (3)	−0.0006 (2)
F1	0.043 (2)	0.036 (2)	0.117 (4)	0.0006 (18)	0.033 (2)	0.007 (2)
F1′	0.118 (6)	0.076 (4)	0.224 (9)	0.001 (4)	0.078 (6)	0.021 (5)
F2	0.093 (2)	0.0375 (13)	0.156 (3)	−0.0039 (12)	0.0553 (19)	0.0089 (13)
F3	0.0818 (18)	0.0639 (16)	0.123 (2)	−0.0259 (13)	0.0534 (16)	0.0013 (14)
F4	0.0665 (17)	0.0773 (19)	0.147 (3)	−0.0014 (14)	0.0520 (17)	0.0028 (17)
F5	0.134 (3)	0.199 (4)	0.132 (3)	0.030 (3)	0.057 (3)	0.038 (3)
F6	0.240 (5)	0.242 (6)	0.085 (3)	−0.063 (5)	0.086 (3)	−0.015 (3)
F7	0.207 (5)	0.180 (4)	0.206 (5)	−0.008 (4)	0.155 (4)	−0.039 (3)
F8	0.156 (4)	0.202 (5)	0.228 (5)	0.095 (4)	0.097 (4)	0.037 (4)
N1	0.0495 (18)	0.0399 (16)	0.068 (2)	−0.0079 (13)	0.0252 (16)	0.0004 (14)
N2	0.0499 (18)	0.0406 (16)	0.071 (2)	−0.0052 (14)	0.0256 (16)	−0.0031 (14)
O1	0.086 (2)	0.0580 (19)	0.131 (3)	−0.0046 (16)	0.038 (2)	0.0402 (18)
O2	0.0623 (19)	0.0488 (15)	0.093 (2)	−0.0109 (14)	0.0362 (16)	0.0031 (14)
O3	0.141 (3)	0.0483 (17)	0.098 (2)	−0.0090 (18)	0.079 (2)	0.0014 (16)
O4	0.082 (2)	0.080 (2)	0.107 (3)	0.0179 (18)	0.0459 (19)	0.0157 (19)
O5	0.088 (4)	0.050 (3)	0.130 (4)	0.000	−0.022 (3)	0.000
C1	0.070 (3)	0.042 (2)	0.079 (3)	−0.014 (2)	0.031 (2)	0.0069 (19)
C2	0.059 (2)	0.045 (2)	0.060 (2)	−0.0071 (18)	0.0223 (19)	0.0126 (17)
C3	0.060 (2)	0.047 (2)	0.072 (3)	−0.0040 (18)	0.025 (2)	0.0090 (18)
C4	0.068 (3)	0.0377 (19)	0.074 (3)	−0.0110 (18)	0.025 (2)	0.0028 (17)
C5	0.067 (3)	0.054 (2)	0.070 (3)	−0.023 (2)	0.028 (2)	−0.0004 (19)
C6	0.053 (2)	0.055 (2)	0.070 (3)	−0.0047 (19)	0.021 (2)	−0.0006 (19)
C7	0.062 (3)	0.0377 (19)	0.076 (3)	−0.0010 (18)	0.027 (2)	0.0099 (18)
C8	0.070 (3)	0.053 (2)	0.085 (3)	−0.013 (2)	0.041 (2)	−0.004 (2)
C9	0.067 (3)	0.058 (2)	0.070 (3)	−0.010 (2)	0.033 (2)	0.003 (2)
C10	0.091 (4)	0.087 (4)	0.085 (4)	0.000 (3)	0.028 (3)	0.031 (3)
C11	0.128 (5)	0.124 (5)	0.065 (3)	−0.039 (4)	0.051 (4)	−0.003 (3)
C12	0.118 (6)	0.105 (5)	0.128 (6)	−0.015 (4)	0.069 (5)	−0.020 (4)
C13	0.113 (5)	0.116 (5)	0.121 (6)	0.016 (4)	0.046 (5)	0.021 (4)

C14	0.101 (4)	0.083 (4)	0.144 (5)	0.010 (3)	0.082 (4)	−0.005 (3)
C15	0.059 (2)	0.043 (2)	0.072 (3)	−0.0046 (17)	0.028 (2)	−0.0050 (18)
C16	0.062 (3)	0.039 (2)	0.084 (3)	−0.0066 (18)	0.027 (2)	−0.0075 (19)
C17	0.060 (3)	0.038 (2)	0.079 (3)	−0.0079 (17)	0.018 (2)	0.0084 (18)
C18	0.046 (2)	0.050 (2)	0.063 (2)	−0.0105 (17)	0.0171 (18)	0.0065 (18)
C19	0.0370 (19)	0.0411 (18)	0.064 (2)	−0.0056 (15)	0.0171 (17)	0.0031 (16)
C20	0.041 (2)	0.045 (2)	0.065 (2)	−0.0044 (15)	0.0209 (18)	0.0004 (17)
C21	0.055 (2)	0.066 (3)	0.072 (3)	−0.005 (2)	0.028 (2)	−0.003 (2)
C22	0.068 (3)	0.071 (3)	0.077 (3)	−0.004 (2)	0.031 (2)	−0.013 (2)
C23	0.074 (3)	0.056 (3)	0.096 (4)	0.000 (2)	0.036 (3)	−0.020 (2)
C24	0.066 (3)	0.044 (2)	0.092 (3)	−0.0065 (19)	0.035 (2)	−0.009 (2)
C25	0.086 (3)	0.081 (3)	0.071 (3)	−0.014 (3)	0.035 (3)	0.004 (2)
C26	0.071 (3)	0.064 (3)	0.076 (3)	−0.016 (2)	0.028 (2)	0.011 (2)
C27	0.083 (5)	0.054 (4)	0.129 (6)	0.000	0.050 (4)	0.000

Geometric parameters (Å, º)

Cu1—O1	2.686 (4)	C8—C9	1.519 (6)
Cu1—O2	1.967 (3)	C9—C10	1.354 (7)
Cu1—O3	1.919 (3)	C9—C14	1.403 (7)
Cu1—O5	2.376 (2)	C10—C11	1.440 (9)
Cu1—N1	2.014 (3)	C11—C12	1.383 (9)
Cu1—N2	2.010 (3)	C12—C13	1.297 (9)
F1—C3	1.324 (6)	C13—C14	1.332 (9)
F1′—C7	1.370 (8)	C14—H14A	0.9300
F2—C4	1.329 (4)	C15—C16	1.393 (5)
F3—C5	1.336 (4)	C15—H15A	0.9300
F4—C6	1.345 (5)	C16—C17	1.361 (6)
F5—C10	1.277 (6)	C16—H16A	0.9300
F6—C11	1.303 (6)	C17—C18	1.421 (6)
F7—C12	1.366 (8)	C17—H17A	0.9300
F8—C13	1.366 (8)	C18—C19	1.401 (5)
N1—C15	1.329 (5)	C18—C26	1.413 (6)
N1—C19	1.350 (5)	C19—C20	1.435 (5)
N2—C24	1.316 (5)	C20—C21	1.383 (6)
N2—C20	1.366 (5)	C21—C22	1.393 (6)
O1—C1	1.214 (5)	C21—C25	1.456 (6)
O2—C1	1.278 (5)	C22—C23	1.364 (6)
O3—C8	1.270 (5)	C22—H22A	0.9300
O4—C8	1.216 (5)	C23—C24	1.383 (6)
O5—C27	1.390 (7)	C23—H23A	0.9300
O5—H5	0.7207	C24—H24A	0.9300
O5—H5^{i}	0.7207	C25—C26	1.338 (7)
C1—C2	1.528 (5)	C25—H25A	0.9300
C2—C7	1.356 (6)	C26—H26A	0.9300
C2—C3	1.405 (5)	C27—H27A	0.9600
C3—C4	1.388 (6)	C27—H27B	0.9600
C3—H3A	0.9300	C27—H27C	0.9600

C4—C5	1.377 (6)	C27—H27A^{i}	0.9600
C5—C6	1.357 (6)	C27—H27B^{i}	0.9600
C6—C7	1.374 (6)	C27—H27C^{i}	0.9600
C7—H7A	0.9300		

O3—Cu1—O2	94.16 (13)	F6—C11—C10	121.2 (7)
O3—Cu1—N2	170.84 (12)	C12—C11—C10	116.8 (5)
O2—Cu1—N2	94.25 (12)	C13—C12—F7	125.5 (8)
O3—Cu1—N1	88.80 (13)	C13—C12—C11	120.4 (7)
O2—Cu1—N1	156.46 (13)	F7—C12—C11	113.9 (7)
N2—Cu1—N1	82.04 (13)	C12—C13—C14	123.3 (7)
O3—Cu1—O5	95.09 (12)	C12—C13—F8	114.5 (7)
O2—Cu1—O5	91.23 (12)	C14—C13—F8	122.1 (7)
N2—Cu1—O5	88.34 (9)	C13—C14—C9	121.3 (6)
N1—Cu1—O5	111.79 (12)	C13—C14—H14A	119.4
O3—Cu1—O1	86.47 (15)	C9—C14—H14A	119.4
O2—Cu1—O1	54.50 (11)	N1—C15—C16	122.1 (4)
N2—Cu1—O1	95.49 (13)	N1—C15—H15A	119.0
N1—Cu1—O1	102.52 (11)	C16—C15—H15A	119.0
O5—Cu1—O1	145.68 (10)	C17—C16—C15	120.0 (4)
C15—N1—C19	118.5 (3)	C17—C16—H16A	120.0
C15—N1—Cu1	128.7 (3)	C15—C16—H16A	120.0
C19—N1—Cu1	112.5 (2)	C16—C17—C18	119.5 (4)
C24—N2—C20	117.4 (4)	C16—C17—H17A	120.2
C24—N2—Cu1	129.9 (3)	C18—C17—H17A	120.2
C20—N2—Cu1	112.7 (3)	C19—C18—C26	119.0 (4)
C1—O2—Cu1	105.3 (2)	C19—C18—C17	116.4 (4)
C8—O3—Cu1	128.6 (3)	C26—C18—C17	124.7 (4)
C27—O5—Cu1	120.51 (9)	N1—C19—C18	123.5 (3)
C27—O5—Cu1^{i}	120.51 (9)	N1—C19—C20	116.9 (3)
Cu1—O5—Cu1^{i}	118.98 (18)	C18—C19—C20	119.6 (4)
C27—O5—H5	131.1	N2—C20—C21	123.3 (4)
Cu1—O5—H5	72.1	N2—C20—C19	115.8 (4)
Cu1^{i}—O5—H5	68.9	C21—C20—C19	120.9 (3)
C27—O5—H5^{i}	131.077 (4)	C20—C21—C22	117.4 (4)
Cu1—O5—H5^{i}	68.94 (5)	C20—C21—C25	117.4 (4)
Cu1^{i}—O5—H5^{i}	72.07 (6)	C22—C21—C25	125.1 (5)
H5—O5—H5^{i}	97.8	C23—C22—C21	119.2 (4)
O1—C1—O2	126.4 (4)	C23—C22—H22A	120.4
O1—C1—C2	117.6 (4)	C21—C22—H22A	120.4
O2—C1—C2	116.0 (3)	C22—C23—C24	119.7 (4)
C7—C2—C3	118.9 (4)	C22—C23—H23A	120.1
C7—C2—C1	120.7 (4)	C24—C23—H23A	120.1
C3—C2—C1	120.4 (4)	N2—C24—C23	122.9 (4)
F1—C3—C4	115.9 (4)	N2—C24—H24A	118.5
F1—C3—C2	124.8 (4)	C23—C24—H24A	118.5
C4—C3—C2	119.0 (4)	C26—C25—C21	121.5 (5)
C4—C3—H3A	120.5	C26—C25—H25A	119.2

C2—C3—H3A	120.5	C21—C25—H25A	119.2
F2—C4—C5	119.4 (4)	C25—C26—C18	121.5 (4)
F2—C4—C3	119.9 (4)	C25—C26—H26A	119.3
C5—C4—C3	120.7 (4)	C18—C26—H26A	119.3
F3—C5—C6	121.4 (4)	O5—C27—H27A	109.5
F3—C5—C4	119.3 (4)	O5—C27—H27B	109.5
C6—C5—C4	119.3 (4)	H27A—C27—H27B	109.5
F4—C6—C5	118.6 (4)	O5—C27—H27C	109.5
F4—C6—C7	120.6 (4)	H27A—C27—H27C	109.5
C5—C6—C7	120.8 (4)	H27B—C27—H27C	109.5
C2—C7—F1′	124.0 (4)	O5—C27—H27A^{i}	109.470 (2)
C2—C7—C6	121.3 (4)	H27A—C27—H27A^{i}	141.1
F1′—C7—C6	114.7 (5)	H27B—C27—H27A^{i}	56.3
C2—C7—H7A	119.4	H27C—C27—H27A^{i}	56.3
C6—C7—H7A	119.4	O5—C27—H27B^{i}	109.470 (3)
O4—C8—O3	127.7 (5)	H27A—C27—H27B^{i}	56.3
O4—C8—C9	119.1 (4)	H27B—C27—H27B^{i}	141.1
O3—C8—C9	113.2 (4)	H27C—C27—H27B^{i}	56.3
C10—C9—C14	116.3 (5)	H27A^{i}—C27—H27B^{i}	109.5
C10—C9—C8	124.8 (5)	O5—C27—H27C^{i}	109.470 (3)
C14—C9—C8	118.9 (4)	H27A—C27—H27C^{i}	56.3
F5—C10—C9	124.1 (6)	H27B—C27—H27C^{i}	56.3
F5—C10—C11	114.2 (6)	H27C—C27—H27C^{i}	141.1
C9—C10—C11	121.6 (5)	H27A^{i}—C27—H27C^{i}	109.5
F6—C11—C12	122.0 (7)	H27B^{i}—C27—H27C^{i}	109.5

Cu1—O2—C1—O1	8.2 (6)	C10—C11—C12—F7	179.7 (5)
Cu1—O2—C1—C2	−170.2 (3)	F7—C12—C13—C14	179.9 (7)
O1—C1—C2—C7	−17.2 (7)	C11—C12—C13—C14	5.1 (12)
O2—C1—C2—C7	161.4 (4)	F7—C12—C13—F8	−2.8 (11)
O1—C1—C2—C3	161.6 (4)	C11—C12—C13—F8	−177.6 (6)
O2—C1—C2—C3	−19.9 (6)	C12—C13—C14—C9	−4.0 (11)
C7—C2—C3—F1	173.0 (5)	F8—C13—C14—C9	178.9 (6)
C1—C2—C3—F1	−5.8 (7)	C10—C9—C14—C13	2.8 (8)
C7—C2—C3—C4	−0.8 (6)	C8—C9—C14—C13	−178.8 (6)
C1—C2—C3—C4	−179.6 (4)	C19—N1—C15—C16	0.0 (6)
F1—C3—C4—F2	6.3 (6)	Cu1—N1—C15—C16	−173.2 (3)
C2—C3—C4—F2	−179.4 (4)	N1—C15—C16—C17	0.0 (6)
F1—C3—C4—C5	−175.1 (4)	C15—C16—C17—C18	−0.4 (6)
C2—C3—C4—C5	−0.8 (6)	C16—C17—C18—C19	0.7 (6)
F2—C4—C5—F3	0.1 (6)	C16—C17—C18—C26	179.9 (4)
C3—C4—C5—F3	−178.5 (4)	C15—N1—C19—C18	0.4 (5)
F2—C4—C5—C6	−179.7 (4)	Cu1—N1—C19—C18	174.7 (3)
C3—C4—C5—C6	1.7 (7)	C15—N1—C19—C20	−177.2 (3)
F3—C5—C6—F4	1.3 (6)	Cu1—N1—C19—C20	−2.9 (4)
C4—C5—C6—F4	−178.9 (4)	C26—C18—C19—N1	−179.9 (3)
F3—C5—C6—C7	179.2 (4)	C17—C18—C19—N1	−0.7 (5)
C4—C5—C6—C7	−1.0 (7)	C26—C18—C19—C20	−2.4 (5)

C3—C2—C7—F1′	179.7 (6)	C17—C18—C19—C20	176.7 (3)
C1—C2—C7—F1′	−1.5 (8)	C24—N2—C20—C21	1.0 (6)
C3—C2—C7—C6	1.5 (6)	Cu1—N2—C20—C21	−178.4 (3)
C1—C2—C7—C6	−179.8 (4)	C24—N2—C20—C19	−179.7 (3)
F4—C6—C7—C2	177.3 (4)	Cu1—N2—C20—C19	0.9 (4)
C5—C6—C7—C2	−0.6 (7)	N1—C19—C20—N2	1.3 (5)
F4—C6—C7—F1′	−1.2 (7)	C18—C19—C20—N2	−176.3 (3)
C5—C6—C7—F1′	−179.0 (6)	N1—C19—C20—C21	−179.3 (3)
Cu1—O3—C8—O4	28.6 (7)	C18—C19—C20—C21	3.0 (5)
Cu1—O3—C8—C9	−151.9 (3)	N2—C20—C21—C22	−1.7 (6)
O4—C8—C9—C10	19.5 (7)	C19—C20—C21—C22	179.0 (4)
O3—C8—C9—C10	−160.1 (5)	N2—C20—C21—C25	177.7 (4)
O4—C8—C9—C14	−158.8 (5)	C19—C20—C21—C25	−1.6 (6)
O3—C8—C9—C14	21.6 (6)	C20—C21—C22—C23	0.9 (6)
C14—C9—C10—F5	179.7 (6)	C25—C21—C22—C23	−178.5 (4)
C8—C9—C10—F5	1.4 (9)	C21—C22—C23—C24	0.6 (7)
C14—C9—C10—C11	−3.0 (8)	C20—N2—C24—C23	0.6 (6)
C8—C9—C10—C11	178.7 (5)	Cu1—N2—C24—C23	179.9 (3)
F5—C10—C11—F6	0.8 (9)	C22—C23—C24—N2	−1.4 (7)
C9—C10—C11—F6	−176.8 (5)	C20—C21—C25—C26	−0.4 (7)
F5—C10—C11—C12	−178.3 (6)	C22—C21—C25—C26	179.0 (5)
C9—C10—C11—C12	4.1 (9)	C21—C25—C26—C18	1.0 (7)
F6—C11—C12—C13	175.9 (6)	C19—C18—C26—C25	0.5 (6)
C10—C11—C12—C13	−5.0 (10)	C17—C18—C26—C25	−178.6 (4)
F6—C11—C12—F7	0.6 (9)		

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···N2	0.72	2.67	3.067 (3)	118
O5—H5···O3^{i}	0.72	2.62	3.184 (4)	137
O5—H5···O4^{i}	0.72	2.55	3.065 (4)	130

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.