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Diaquatetrakis(2,3,5-triiodobenzoato-κ^2O:O')dicopper(II)(*Cu–Cu*) bis(methanol-κO)tetrakis(2,3,5-triiodobenzoato-κ^2O:O')dicopper(II)(*Cu–Cu*) methanol disolvate

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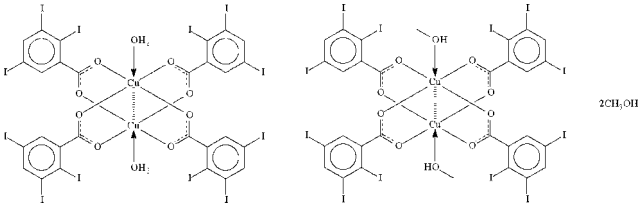
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; R factor = 0.051; wR factor = 0.146; data-to-parameter ratio = 25.0.

The title cocrystal, $[Cu_2(C_7H_2I_3O_2)_4(H_2O)_2][Cu_2(C_7H_2I_3O_2)_4(CH_4O)_2]\cdot 2CH_4O$, contains two dinuclear complexes. In both centrosymmetric molecules, four triiodobenzoates bridge a pair of Cu atoms. The Cu atoms show square-pyramidal coordination; for one, the apical position is occupied by a water molecule, and for the other, this site is occupied by a methanol molecule.

Related literature

There are many examples of such di(ligand)tetra(carboxylato)dicopper compounds in which the carboxylate group bridges two Cu atoms that are separated by a distance less than the sum of the van der Waals radius of copper. The Cambridge Structural Database (Version 5.28, November 2006; Allen, 2002) lists more than 500 entries.



Experimental

Crystal data

$[Cu_2(C_7H_2I_3O_2)_4(H_2O)_2]$-$[Cu_2(C_7H_2I_3O_2)_4$-$(CH_4O)_2]\cdot 2CH_4O$
M_r = 4408.65
Triclinic, $P\overline{1}$
a = 11.9321 (6) Å
b = 11.9345 (6) Å
c = 17.921 (1) Å
α = 96.799 (1)°
β = 103.136 (1)°
γ = 91.532 (1)°
V = 2464.0 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 8.43 mm^{-1}
T = 295 (2) K
0.24 × 0.19 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.084, T_{max} = 1.00
(expected range = 0.026–0.307)
24361 measured reflections
11203 independent reflections
9161 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.146
S = 1.06
11203 reflections
449 parameters
14 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.37 e Å^{-3}
$\Delta\rho_{min}$ = −1.51 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2517).

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supplementary materials

Acta Cryst. (2007). E**63**, m2617 [**doi:10.1107/S1600536807046430**]

Diaquatetrakis(2,3,5-triiodobenzoato-κ^2O:O')dicopper(II)(*Cu-Cu*) bis(methanol-κO)tetrakis(2,3,5-triiodobenzoato-κ^2O:O')dicopper(II)(*Cu-Cu*) methanol disolvate

P.-G. Chen, S. Gao and S. W. Ng

Comment

There are many examples of di(ligand)tetra(carboxylato)dicopper compounds in which the carboxylate group bridges two copper atoms that are separated by a distance less than the sum of the van der Waals radius of copper. The Cambridge Structural Database (Version 5.28, Nov. 2006) lists more than 500 entries.

Experimental

In a long 0.8 cm diameter tube was placed an aqueous (5 ml) solution of copper(II) acetate monohydrate (0.5 mmol). A methanol solution (5 ml) of 2,4,5-triiodobenzoic acid (1 mmol) was layered over this. After several days, blue prisms separated from solution. The C&H elemental percentages were C 16.43 and H 0.58% (*versus* calculated values of C 16.35 and H 0.82%).

Refinement

The aromatic rings were refined as rigid hexagons of 1.39 Å sides. The anisotropic temperature factors of the free methanol molecule were restrained to be nearly isotropic. Carbon-bound H atoms were generated geometrically (C–H 0.93 – 0.96 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C). The water and methanolic H atoms were placed in chemically sensible positions on the basis of hydrogen bonding interactions but they were not refined; U(H) was set to 1.5U_{eq}(O). The final difference Fourier map had peaks/holes in the vicinity of the iodine atoms.

Figures

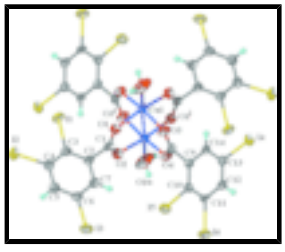


Fig. 1. Thermal ellipsoid plot of the water-coordinated complex. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. Symmetry code $i = 2 - x, 2 - y, 1 - z$.

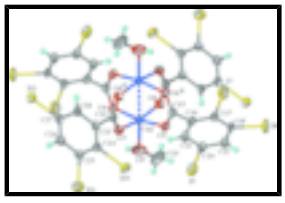


Fig. 2. Thermal ellipsoid plot of the methanol-coordinated complex. Displacement lelipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. Symmetry code $ii = 2 - x, 2 - y, 2 - z$.

Diaquatetrakis(2,3,5-triiodobenzoato- κ^2O:O')dicopper(II)(*Cu–Cu*) bis(methanol-κ*O*)tetrakis(2,3,5-triiodobenzoato- κ^2O:O')dicopper(II)(*Cu–Cu*) methanol disolvate

Crystal data

$[Cu_2(C_7H_2I_3O_2)_4(H_2O)_2][Cu_2(C_7H_2I_3O_2)_4(CH_4O)_2]\cdot 2CH_4O$	
$M_r = 4408.65$	$F_{000} = 1960$
Triclinic, $P\overline{1}$	$D_x = 2.971$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.9321$ (6) Å	Cell parameters from 18920 reflections
$b = 11.9345$ (6) Å	$\theta = 3.0$–27.5º
$c = 17.921$ (1) Å	$\mu = 8.43$ mm^{-1}
$\alpha = 96.799$ (1)º	$T = 295$ (2) K
$\beta = 103.136$ (1)º	Prism, blue
$\gamma = 91.532$ (1)º	0.24 × 0.19 × 0.14 mm
$V = 2464.0$ (2) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	11203 independent reflections
Radiation source: fine-focus sealed tube	9161 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.050$
$T = 295$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -14\rightarrow15$
$T_{min} = 0.084$, $T_{max} = 1.00$	$k = -15\rightarrow14$
24361 measured reflections	$l = -23\rightarrow23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.146$	$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 3.5241P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
11203 reflections	$\Delta\rho_{max} = 2.37$ e Å^{-3}
449 parameters	$\Delta\rho_{min} = -1.51$ e Å^{-3}
14 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	1.21746 (5)	1.31313 (5)	0.68454 (3)	0.05455 (15)
I2	1.16902 (5)	1.60545 (5)	0.74506 (4)	0.05628 (16)
I3	0.72402 (5)	1.56610 (5)	0.50800 (4)	0.05953 (17)
I4	0.41538 (4)	0.71789 (4)	0.45628 (3)	0.04599 (14)
I5	0.66311 (5)	1.18239 (5)	0.33814 (3)	0.05117 (15)
I6	0.35562 (5)	1.14333 (5)	0.31042 (4)	0.05908 (17)
I7	1.38248 (5)	0.89448 (5)	1.14510 (4)	0.06038 (17)
I8	1.55290 (4)	0.64621 (5)	1.12823 (4)	0.06330 (18)
I9	1.13581 (5)	0.38570 (4)	0.93389 (4)	0.05658 (16)
I10	0.88626 (5)	0.63810 (5)	0.81397 (4)	0.06055 (17)
I11	0.61385 (5)	0.49247 (5)	0.71699 (4)	0.05900 (16)
I12	0.37236 (4)	0.80116 (5)	0.90462 (3)	0.05159 (15)
Cu1	0.98855 (7)	0.97560 (7)	0.56782 (5)	0.03541 (19)
Cu2	1.02862 (6)	1.00342 (6)	0.93345 (4)	0.02765 (16)
O1	0.9864 (5)	1.1416 (4)	0.5920 (3)	0.0445 (12)
O2	1.0072 (5)	1.1823 (4)	0.4774 (3)	0.0487 (13)
O3	0.8236 (4)	0.9712 (5)	0.5188 (3)	0.0488 (13)
O4	0.8441 (4)	1.0097 (5)	0.4027 (3)	0.0443 (12)
O5	1.1244 (4)	0.8783 (4)	0.9646 (3)	0.0408 (11)
O6	1.0761 (4)	0.8700 (4)	1.0779 (3)	0.0440 (12)
O7	0.8965 (4)	0.8963 (4)	0.8912 (3)	0.0427 (11)
O8	0.8489 (4)	0.8904 (4)	1.0042 (3)	0.0380 (11)
O9	1.0766 (6)	1.0293 (7)	0.8275 (4)	0.077 (2)
H9o	1.0351	1.0832	0.8096	0.115*
O10	0.9491 (14)	1.1794 (14)	0.7471 (9)	0.181 (6)
H10o	1.0010	1.2137	0.7270	0.272*
O1w	0.9549 (6)	0.9362 (10)	0.6753 (4)	0.097 (3)
H1w1	1.0140	0.9077	0.7008	0.145*
H1w2	0.9426	0.9975	0.7015	0.145*
C1	0.9970 (6)	1.2078 (6)	0.5447 (4)	0.0386 (15)
C2	0.9899 (4)	1.3311 (3)	0.5709 (3)	0.0394 (15)
C3	1.0703 (3)	1.3925 (4)	0.6314 (3)	0.0384 (15)
C4	1.0540 (4)	1.5050 (4)	0.6545 (2)	0.0447 (17)
C5	0.9575 (4)	1.5562 (3)	0.6172 (3)	0.0449 (17)
H5	0.9466	1.6315	0.6327	0.054*
C6	0.8771 (3)	1.4948 (4)	0.5568 (3)	0.0416 (16)
C7	0.8933 (3)	1.3823 (4)	0.5336 (2)	0.0426 (16)
H7	0.8396	1.3412	0.4932	0.051*
C8	0.7861 (6)	0.9872 (6)	0.4502 (4)	0.0392 (15)
C9	0.6566 (2)	0.9741 (3)	0.4221 (3)	0.0340 (14)
C10	0.5875 (3)	1.0486 (3)	0.3809 (3)	0.0350 (14)
C11	0.4683 (3)	1.0310 (3)	0.3632 (3)	0.0346 (14)
C12	0.4181 (2)	0.9388 (4)	0.3866 (3)	0.0408 (16)
H12	0.3383	0.9270	0.3748	0.049*
C13	0.4872 (3)	0.8643 (3)	0.4278 (3)	0.0374 (14)

C14	0.6064 (3)	0.8819 (3)	0.4455 (3)	0.0355 (14)
H14	0.6526	0.8321	0.4730	0.043*
C15	1.1284 (6)	0.8369 (5)	1.0268 (4)	0.0339 (14)
C16	1.1994 (3)	0.7351 (3)	1.0369 (3)	0.0368 (14)
C17	1.3128 (3)	0.7405 (3)	1.0795 (3)	0.0354 (14)
C18	1.3761 (3)	0.6444 (3)	1.0802 (3)	0.0394 (15)
C19	1.3261 (3)	0.5429 (3)	1.0382 (3)	0.0397 (15)
H19	1.3685	0.4786	1.0386	0.048*
C20	1.2127 (3)	0.5375 (3)	0.9956 (3)	0.0385 (15)
C21	1.1493 (3)	0.6335 (3)	0.9950 (3)	0.0365 (15)
H21	1.0735	0.6299	0.9665	0.044*
C22	0.8351 (6)	0.8618 (5)	0.9338 (4)	0.0337 (14)
C23	0.7314 (3)	0.7821 (3)	0.8958 (2)	0.0351 (14)
C24	0.7315 (3)	0.6902 (3)	0.8404 (3)	0.0358 (14)
C25	0.6289 (4)	0.6292 (3)	0.8038 (2)	0.0357 (14)
C26	0.5263 (3)	0.6601 (3)	0.8228 (3)	0.0402 (16)
H26	0.4577	0.6192	0.7983	0.048*
C27	0.5263 (3)	0.7520 (4)	0.8782 (3)	0.0364 (14)
C28	0.6289 (3)	0.8130 (3)	0.9147 (2)	0.0379 (15)
H28	0.6288	0.8745	0.9518	0.045*
C29	1.1933 (8)	1.0578 (10)	0.8206 (7)	0.083 (4)
H29A	1.1922	1.0662	0.7679	0.125*
H29B	1.2425	0.9985	0.8366	0.125*
H29C	1.2219	1.1274	0.8529	0.125*
C30	0.8630 (11)	1.2632 (11)	0.7502 (8)	0.087 (3)
H30A	0.8062	1.2359	0.7750	0.131*
H30B	0.8264	1.2762	0.6987	0.131*
H30C	0.8997	1.3326	0.7790	0.131*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0427 (3)	0.0641 (3)	0.0515 (3)	0.0108 (2)	−0.0035 (2)	0.0118 (2)
I2	0.0454 (3)	0.0580 (3)	0.0587 (3)	−0.0114 (3)	0.0063 (2)	−0.0049 (2)
I3	0.0456 (3)	0.0604 (3)	0.0766 (4)	0.0172 (3)	0.0102 (3)	0.0293 (3)
I4	0.0468 (3)	0.0389 (2)	0.0528 (3)	−0.0049 (2)	0.0148 (2)	0.0034 (2)
I5	0.0510 (3)	0.0535 (3)	0.0531 (3)	0.0009 (2)	0.0138 (2)	0.0205 (2)
I6	0.0471 (3)	0.0586 (3)	0.0710 (4)	0.0181 (3)	0.0022 (3)	0.0256 (3)
I7	0.0575 (3)	0.0460 (3)	0.0636 (4)	0.0062 (3)	−0.0065 (3)	−0.0103 (2)
I8	0.0321 (2)	0.0648 (3)	0.0835 (4)	0.0146 (2)	−0.0063 (3)	0.0067 (3)
I9	0.0474 (3)	0.0323 (2)	0.0854 (4)	0.0019 (2)	0.0109 (3)	−0.0023 (2)
I10	0.0411 (3)	0.0685 (3)	0.0666 (4)	0.0092 (3)	0.0138 (2)	−0.0174 (3)
I11	0.0632 (3)	0.0478 (3)	0.0585 (3)	−0.0039 (3)	0.0112 (3)	−0.0166 (2)
I12	0.0370 (2)	0.0694 (3)	0.0492 (3)	0.0042 (2)	0.0141 (2)	0.0025 (2)
Cu1	0.0273 (4)	0.0489 (5)	0.0301 (4)	0.0029 (3)	0.0070 (3)	0.0044 (3)
Cu2	0.0285 (3)	0.0262 (3)	0.0290 (4)	0.0054 (3)	0.0078 (3)	0.0037 (3)
O1	0.047 (3)	0.045 (3)	0.042 (3)	0.007 (2)	0.012 (2)	0.005 (2)
O2	0.059 (3)	0.047 (3)	0.042 (3)	0.002 (3)	0.016 (2)	0.003 (2)

O3	0.028 (2)	0.077 (4)	0.041 (3)	0.004 (2)	0.004 (2)	0.018 (3)
O4	0.033 (2)	0.061 (3)	0.041 (3)	0.007 (2)	0.010 (2)	0.013 (2)
O5	0.041 (3)	0.037 (2)	0.047 (3)	0.016 (2)	0.012 (2)	0.007 (2)
O6	0.044 (3)	0.043 (3)	0.049 (3)	0.020 (2)	0.014 (2)	0.013 (2)
O7	0.036 (2)	0.047 (3)	0.042 (3)	−0.007 (2)	0.008 (2)	−0.002 (2)
O8	0.040 (2)	0.038 (2)	0.035 (3)	−0.005 (2)	0.009 (2)	0.0035 (19)
O9	0.091 (5)	0.101 (5)	0.049 (4)	−0.007 (4)	0.040 (4)	0.010 (4)
O10	0.214 (10)	0.183 (9)	0.150 (9)	0.073 (8)	0.039 (7)	0.030 (7)
O1w	0.062 (4)	0.191 (10)	0.040 (4)	0.009 (5)	0.013 (3)	0.025 (5)
C1	0.032 (3)	0.047 (4)	0.034 (4)	0.007 (3)	0.003 (3)	0.006 (3)
C2	0.032 (3)	0.047 (4)	0.038 (4)	0.003 (3)	0.006 (3)	0.007 (3)
C3	0.028 (3)	0.051 (4)	0.039 (4)	0.006 (3)	0.009 (3)	0.010 (3)
C4	0.038 (4)	0.044 (4)	0.052 (4)	−0.003 (3)	0.009 (3)	0.006 (3)
C5	0.047 (4)	0.041 (4)	0.047 (4)	0.004 (3)	0.013 (3)	0.004 (3)
C6	0.032 (3)	0.047 (4)	0.049 (4)	0.010 (3)	0.010 (3)	0.017 (3)
C7	0.037 (3)	0.047 (4)	0.042 (4)	0.004 (3)	0.005 (3)	0.005 (3)
C8	0.026 (3)	0.042 (3)	0.044 (4)	−0.001 (3)	0.005 (3)	−0.005 (3)
C9	0.025 (3)	0.036 (3)	0.040 (4)	0.005 (3)	0.008 (3)	−0.001 (3)
C10	0.042 (3)	0.032 (3)	0.031 (3)	0.000 (3)	0.010 (3)	0.002 (2)
C11	0.030 (3)	0.039 (3)	0.035 (3)	0.011 (3)	0.004 (3)	0.011 (3)
C12	0.027 (3)	0.044 (4)	0.046 (4)	0.004 (3)	−0.001 (3)	0.002 (3)
C13	0.036 (3)	0.037 (3)	0.037 (4)	0.003 (3)	0.006 (3)	0.000 (3)
C14	0.029 (3)	0.037 (3)	0.036 (3)	0.000 (3)	0.001 (3)	0.003 (3)
C15	0.035 (3)	0.025 (3)	0.040 (4)	0.009 (3)	0.004 (3)	0.003 (2)
C16	0.037 (3)	0.033 (3)	0.044 (4)	0.015 (3)	0.013 (3)	0.008 (3)
C17	0.036 (3)	0.034 (3)	0.036 (3)	0.008 (3)	0.005 (3)	0.006 (3)
C18	0.031 (3)	0.046 (4)	0.040 (4)	0.018 (3)	0.001 (3)	0.009 (3)
C19	0.038 (3)	0.032 (3)	0.049 (4)	0.014 (3)	0.005 (3)	0.012 (3)
C20	0.036 (3)	0.029 (3)	0.051 (4)	0.008 (3)	0.008 (3)	0.008 (3)
C21	0.030 (3)	0.028 (3)	0.050 (4)	0.004 (3)	0.005 (3)	0.008 (3)
C22	0.035 (3)	0.028 (3)	0.038 (4)	0.001 (3)	0.006 (3)	0.009 (3)
C23	0.033 (3)	0.032 (3)	0.040 (4)	0.005 (3)	0.007 (3)	0.007 (3)
C24	0.036 (3)	0.030 (3)	0.039 (4)	0.006 (3)	0.006 (3)	0.001 (3)
C25	0.043 (3)	0.029 (3)	0.035 (3)	0.007 (3)	0.008 (3)	0.004 (3)
C26	0.039 (3)	0.035 (3)	0.041 (4)	−0.003 (3)	0.002 (3)	0.001 (3)
C27	0.032 (3)	0.041 (3)	0.038 (4)	0.000 (3)	0.009 (3)	0.012 (3)
C28	0.034 (3)	0.040 (3)	0.039 (4)	0.004 (3)	0.008 (3)	0.003 (3)
C29	0.095 (8)	0.093 (8)	0.095 (9)	0.039 (6)	0.067 (7)	0.053 (7)
C30	0.086 (6)	0.098 (7)	0.084 (7)	0.017 (6)	0.026 (5)	0.023 (6)

Geometric parameters (Å, °)

I1—C3	2.105 (3)	C1—C2	1.501 (8)
I2—C4	2.095 (3)	C2—C3	1.3900
I3—C6	2.088 (3)	C2—C7	1.3900
I4—C13	2.092 (3)	C3—C4	1.3900
I5—C10	2.116 (3)	C4—C5	1.3900
I6—C11	2.078 (3)	C5—C6	1.3900
I7—C17	2.100 (3)	C5—H5	0.9300

I8—C18	2.088 (3)	C6—C7	1.3900
I9—C20	2.079 (3)	C7—H7	0.9300
I10—C24	2.100 (3)	C8—C9	1.511 (7)
I11—C25	2.091 (3)	C9—C10	1.3900
I12—C27	2.081 (3)	C9—C14	1.3900
Cu1—O4^{i}	1.944 (5)	C10—C11	1.3900
Cu1—O3	1.961 (5)	C11—C12	1.3900
Cu1—O2^{i}	1.968 (5)	C12—C13	1.3900
Cu1—O1	1.979 (5)	C12—H12	0.9300
Cu1—O1w	2.156 (7)	C13—C14	1.3900
Cu1—Cu1^{i}	2.6365 (17)	C14—H14	0.9300
Cu2—O8^{ii}	1.952 (4)	C15—C16	1.505 (7)
Cu2—O7	1.953 (5)	C16—C17	1.3900
Cu2—O5	1.961 (5)	C16—C21	1.3900
Cu2—O6^{ii}	1.986 (5)	C17—C18	1.3900
Cu2—O9	2.156 (6)	C18—C19	1.3900
Cu2—Cu2^{ii}	2.6355 (15)	C19—C20	1.3900
O1—C1	1.249 (9)	C19—H19	0.9300
O2—C1	1.244 (9)	C20—C21	1.3900
O2—Cu1^{i}	1.968 (5)	C21—H21	0.9300
O3—C8	1.248 (9)	C22—C23	1.516 (7)
O4—C8	1.259 (9)	C23—C24	1.3900
O4—Cu1^{i}	1.944 (5)	C23—C28	1.3900
O5—C15	1.263 (9)	C24—C25	1.3900
O6—C15	1.254 (9)	C25—C26	1.3900
O6—Cu2^{ii}	1.986 (5)	C26—C27	1.3900
O7—C22	1.265 (8)	C26—H26	0.9300
O8—C22	1.240 (8)	C27—C28	1.3900
O8—Cu2^{ii}	1.952 (4)	C28—H28	0.9300
O9—C29	1.460 (8)	C29—H29A	0.9600
O9—H9o	0.87	C29—H29B	0.9600
O10—C30	1.457 (9)	C29—H29C	0.9600
O10—H10o	0.90	C30—H30A	0.9600
O1w—H1w1	0.85	C30—H30B	0.9600
O1w—H1w2	0.86	C30—H30C	0.9600
O4^{i}—Cu1—O3	168.5 (2)	C14—C9—C8	114.2 (4)
O4^{i}—Cu1—O2^{i}	90.9 (2)	C9—C10—C11	120.0
O3—Cu1—O2^{i}	89.1 (3)	C9—C10—I5	120.3 (2)
O4^{i}—Cu1—O1	88.6 (2)	C11—C10—I5	119.6 (2)
O3—Cu1—O1	89.0 (2)	C12—C11—C10	120.0
O2^{i}—Cu1—O1	168.2 (2)	C12—C11—I6	116.2 (2)
O4^{i}—Cu1—O1w	99.3 (3)	C10—C11—I6	123.6 (2)
O3—Cu1—O1w	92.2 (3)	C13—C12—C11	120.0
O2^{i}—Cu1—O1w	95.8 (3)	C13—C12—H12	120.0
O1—Cu1—O1w	95.9 (3)	C11—C12—H12	120.0

O4^{i}—Cu1—Cu1^{i}	85.34 (16)	C12—C13—C14	120.0
O3—Cu1—Cu1^{i}	83.20 (16)	C12—C13—I4	121.0 (2)
O2^{i}—Cu1—Cu1^{i}	84.59 (17)	C14—C13—I4	118.9 (2)
O1—Cu1—Cu1^{i}	83.64 (16)	C13—C14—C9	120.0
O1w—Cu1—Cu1^{i}	175.3 (2)	C13—C14—H14	120.0
O8^{ii}—Cu2—O7	168.1 (2)	C9—C14—H14	120.0
O8^{ii}—Cu2—O5	89.1 (2)	O6—C15—O5	126.3 (6)
O7—Cu2—O5	89.9 (2)	O6—C15—C16	118.4 (6)
O8^{ii}—Cu2—O6^{ii}	89.1 (2)	O5—C15—C16	115.2 (6)
O7—Cu2—O6^{ii}	89.6 (2)	C17—C16—C21	120.0
O5—Cu2—O6^{ii}	168.7 (2)	C17—C16—C15	123.5 (3)
O8^{ii}—Cu2—O9	92.7 (2)	C21—C16—C15	116.2 (3)
O7—Cu2—O9	99.1 (3)	C16—C17—C18	120.0
O5—Cu2—O9	100.8 (3)	C16—C17—I7	118.5 (2)
O6^{ii}—Cu2—O9	90.5 (3)	C18—C17—I7	121.5 (2)
O8^{ii}—Cu2—Cu2^{ii}	83.02 (15)	C19—C18—C17	120.0
O7—Cu2—Cu2^{ii}	85.12 (16)	C19—C18—I8	115.8 (2)
O5—Cu2—Cu2^{ii}	83.98 (16)	C17—C18—I8	123.6 (2)
O6^{ii}—Cu2—Cu2^{ii}	84.68 (17)	C18—C19—C20	120.0
O9—Cu2—Cu2^{ii}	173.6 (2)	C18—C19—H19	120.0
C1—O1—Cu1	122.6 (5)	C20—C19—H19	120.0
C1—O2—Cu1^{i}	122.1 (5)	C19—C20—C21	120.0
C8—O3—Cu1	123.0 (5)	C19—C20—I9	120.5 (2)
C8—O4—Cu1^{i}	121.1 (4)	C21—C20—I9	119.5 (2)
C15—O5—Cu2	123.4 (5)	C20—C21—C16	120.0
C15—O6—Cu2^{ii}	121.6 (4)	C20—C21—H21	120.0
C22—O7—Cu2	121.4 (4)	C16—C21—H21	120.0
C22—O8—Cu2^{ii}	124.5 (4)	O8—C22—O7	126.0 (6)
C29—O9—Cu2	125.2 (6)	O8—C22—C23	116.0 (6)
C29—O9—H9o	105.5	O7—C22—C23	118.0 (6)
Cu2—O9—H9o	105.7	C24—C23—C28	120.0
C30—O10—H10o	103.6	C24—C23—C22	124.8 (4)
Cu1—O1w—H1w1	109.0	C28—C23—C22	114.9 (4)
Cu1—O1w—H1w2	108.7	C25—C24—C23	120.0
H1w1—O1w—H1w2	108.7	C25—C24—I10	119.3 (2)
O2—C1—O1	127.1 (7)	C23—C24—I10	120.7 (2)
O2—C1—C2	116.7 (6)	C26—C25—C24	120.0
O1—C1—C2	116.1 (6)	C26—C25—I11	115.4 (2)
C3—C2—C7	120.0	C24—C25—I11	124.6 (2)
C3—C2—C1	123.7 (4)	C25—C26—C27	120.0
C7—C2—C1	116.2 (4)	C25—C26—H26	120.0
C4—C3—C2	120.0	C27—C26—H26	120.0
C4—C3—I1	121.1 (2)	C26—C27—C28	120.0
C2—C3—I1	118.8 (2)	C26—C27—I12	120.2 (2)
C3—C4—C5	120.0	C28—C27—I12	119.8 (2)

C3—C4—I2	123.3 (2)	C27—C28—C23	120.0
C5—C4—I2	116.7 (2)	C27—C28—H28	120.0
C6—C5—C4	120.0	C23—C28—H28	120.0
C6—C5—H5	120.0	O9—C29—H29A	109.5
C4—C5—H5	120.0	O9—C29—H29B	109.5
C7—C6—C5	120.0	H29A—C29—H29B	109.5
C7—C6—I3	119.6 (2)	O9—C29—H29C	109.5
C5—C6—I3	120.1 (2)	H29A—C29—H29C	109.5
C6—C7—C2	120.0	H29B—C29—H29C	109.5
C6—C7—H7	120.0	O10—C30—H30A	109.5
C2—C7—H7	120.0	O10—C30—H30B	109.5
O3—C8—O4	127.3 (6)	H30A—C30—H30B	109.5
O3—C8—C9	114.9 (6)	O10—C30—H30C	109.5
O4—C8—C9	117.8 (6)	H30A—C30—H30C	109.5
C10—C9—C14	120.0	H30B—C30—H30C	109.5
C10—C9—C8	125.7 (4)		
$O4^{i}$—Cu1—O1—C1	84.2 (6)	C9—C10—C11—C12	0.0
O3—Cu1—O1—C1	−84.5 (6)	I5—C10—C11—C12	175.7 (3)
$O2^{i}$—Cu1—O1—C1	−3.5 (14)	C9—C10—C11—I6	174.6 (4)
O1w—Cu1—O1—C1	−176.6 (6)	I5—C10—C11—I6	−9.7 (3)
$Cu1^{i}$—Cu1—O1—C1	−1.2 (5)	C10—C11—C12—C13	0.0
$O4^{i}$—Cu1—O3—C8	7.2 (17)	I6—C11—C12—C13	−175.0 (3)
$O2^{i}$—Cu1—O3—C8	−83.1 (6)	C11—C12—C13—C14	0.0
O1—Cu1—O3—C8	85.2 (6)	C11—C12—C13—I4	−175.1 (3)
O1w—Cu1—O3—C8	−178.9 (7)	C12—C13—C14—C9	0.0
$Cu1^{i}$—Cu1—O3—C8	1.5 (6)	I4—C13—C14—C9	175.2 (3)
$O8^{ii}$—Cu2—O5—C15	84.4 (5)	C10—C9—C14—C13	0.0
O7—Cu2—O5—C15	−83.8 (5)	C8—C9—C14—C13	175.9 (5)
$O6^{ii}$—Cu2—O5—C15	3.2 (14)	$Cu2^{ii}$—O6—C15—O5	1.5 (9)
O9—Cu2—O5—C15	176.9 (5)	$Cu2^{ii}$—O6—C15—C16	−175.6 (4)
$Cu2^{ii}$—Cu2—O5—C15	1.3 (5)	Cu2—O5—C15—O6	−2.1 (9)
$O8^{ii}$—Cu2—O7—C22	−1.6 (14)	Cu2—O5—C15—C16	175.1 (3)
O5—Cu2—O7—C22	83.5 (5)	O6—C15—C16—C17	−85.1 (6)
$O6^{ii}$—Cu2—O7—C22	−85.2 (5)	O5—C15—C16—C17	97.5 (6)
O9—Cu2—O7—C22	−175.7 (6)	O6—C15—C16—C21	100.8 (6)
$Cu2^{ii}$—Cu2—O7—C22	−0.5 (5)	O5—C15—C16—C21	−76.6 (6)
$O8^{ii}$—Cu2—O9—C29	30.5 (9)	C21—C16—C17—C18	0.0
O7—Cu2—O9—C29	−150.7 (8)	C15—C16—C17—C18	−173.9 (5)
O5—Cu2—O9—C29	−59.1 (9)	C21—C16—C17—I7	−177.8 (3)
$O6^{ii}$—Cu2—O9—C29	119.7 (9)	C15—C16—C17—I7	8.3 (5)
$Cu1^{i}$—O2—C1—O1	−1.2 (11)	C16—C17—C18—C19	0.0
$Cu1^{i}$—O2—C1—C2	−177.5 (4)	I7—C17—C18—C19	177.8 (4)
Cu1—O1—C1—O2	1.9 (10)	C16—C17—C18—I8	170.8 (4)
Cu1—O1—C1—C2	178.2 (4)	I7—C17—C18—I8	−11.4 (4)
O2—C1—C2—C3	−117.9 (6)	C17—C18—C19—C20	0.0

O1—C1—C2—C3	65.4 (7)	I8—C18—C19—C20	−171.5 (3)
O2—C1—C2—C7	65.3 (7)	C18—C19—C20—C21	0.0
O1—C1—C2—C7	−111.4 (6)	C18—C19—C20—I9	−179.1 (4)
C7—C2—C3—C4	0.0	C19—C20—C21—C16	0.0
C1—C2—C3—C4	−176.7 (6)	I9—C20—C21—C16	179.1 (4)
C7—C2—C3—I1	−178.4 (4)	C17—C16—C21—C20	0.0
C1—C2—C3—I1	4.9 (5)	C15—C16—C21—C20	174.3 (5)
C2—C3—C4—C5	0.0	Cu2^{ii}—O8—C22—O7	−0.4 (10)
I1—C3—C4—C5	178.4 (4)	Cu2^{ii}—O8—C22—C23	−177.5 (4)
C2—C3—C4—I2	179.8 (4)	Cu2—O7—C22—O8	0.7 (10)
I1—C3—C4—I2	−1.8 (4)	Cu2—O7—C22—C23	177.7 (4)
C3—C4—C5—C6	0.0	O8—C22—C23—C24	−138.5 (5)
I2—C4—C5—C6	−179.8 (4)	O7—C22—C23—C24	44.2 (7)
C4—C5—C6—C7	0.0	O8—C22—C23—C28	47.5 (6)
C4—C5—C6—I3	173.8 (4)	O7—C22—C23—C28	−129.8 (5)
C5—C6—C7—C2	0.0	C28—C23—C24—C25	0.0
I3—C6—C7—C2	−173.8 (4)	C22—C23—C24—C25	−173.7 (5)
C3—C2—C7—C6	0.0	C28—C23—C24—I10	−177.6 (3)
C1—C2—C7—C6	176.9 (5)	C22—C23—C24—I10	8.7 (5)
Cu1—O3—C8—O4	−1.1 (11)	C23—C24—C25—C26	0.0
Cu1—O3—C8—C9	176.9 (4)	I10—C24—C25—C26	177.6 (3)
Cu1^{i}—O4—C8—O3	−0.4 (11)	C23—C24—C25—I11	178.0 (3)
Cu1^{i}—O4—C8—C9	−178.4 (4)	I10—C24—C25—I11	−4.4 (3)
O3—C8—C9—C10	133.2 (6)	C24—C25—C26—C27	0.0
O4—C8—C9—C10	−48.6 (8)	I11—C25—C26—C27	−178.1 (3)
O3—C8—C9—C14	−42.4 (7)	C25—C26—C27—C28	0.0
O4—C8—C9—C14	135.8 (6)	C25—C26—C27—I12	178.4 (3)
C14—C9—C10—C11	0.0	C26—C27—C28—C23	0.0
C8—C9—C10—C11	−175.4 (5)	I12—C27—C28—C23	−178.4 (3)
C14—C9—C10—I5	−175.6 (3)	C24—C23—C28—C27	0.0
C8—C9—C10—I5	9.0 (5)	C22—C23—C28—C27	174.3 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w2···O9	0.86	2.43	2.86 (1)	112
O1w—H1w2···O10	0.86	2.22	3.04 (2)	161
O9—H9o···O10	0.87	1.86	2.71 (2)	165
O10—H10o···I1	0.90	3.10	3.98 (2)	168

Fig. 1

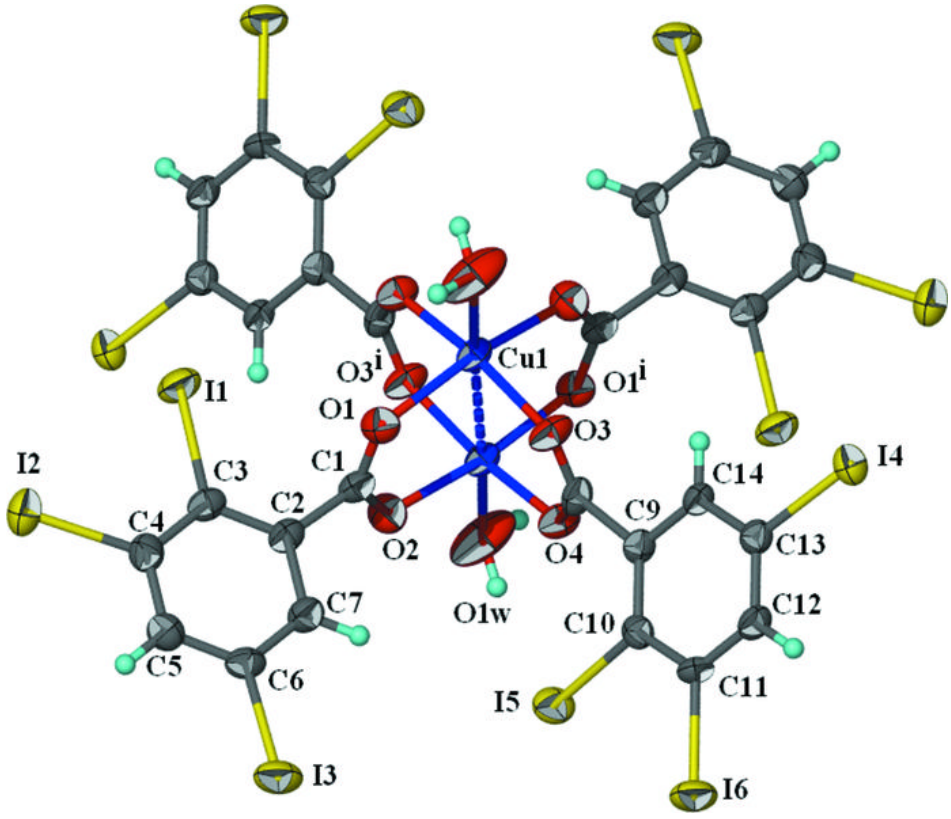
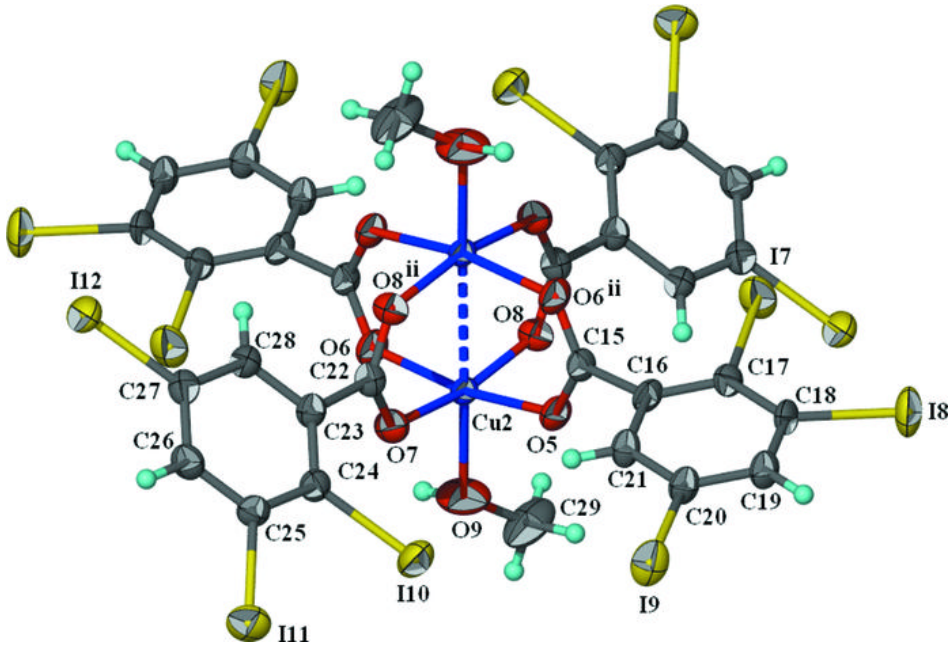

Cu1
O3i
O1i
O1
O3
I1
I2
C3
C1
C2
C4
O2
O4
C9
C14
I4
C13
C12
C7
O1w
C10
C5
C6
C11
I5
I3
I6

Fig. 2


I12
O8ii
O6ii
I7
O8
C28
O6
C15
C22
C16
C17
C27
C18
I8
Cu2
C23
O5
C26
O7
C21
C24
C29
C19
C20
O9
C25
I10
I9
I11