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Tetrakis(μ-2-methylbenzoato)bis[(2-methylbenzoic acid)copper(II)]

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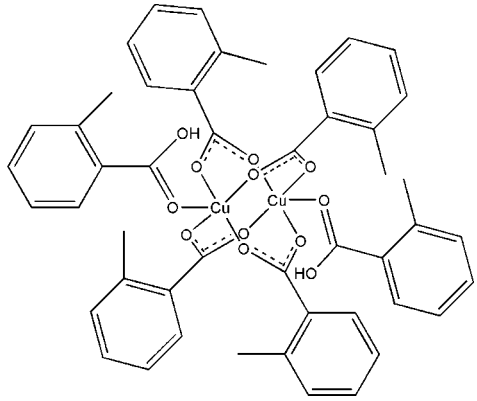
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 18.1.

In the title centrosymmetric dinuclear compound, $[Cu_2(C_8H_7O_2)_4(C_8H_8O_2)_2]$, four *o*-toluate anions form a cage around two Cu atoms in a *syn–syn* configuration. Two more *o*-toluic acid molecules are apically bonded to the Cu atoms, which show a square-pyramidal coordination geometry. The acid H atoms are hydrogen bonded to the cage carboxyl O atoms [O···O = 2.660 (2) Å]. The molecular packing forms a puckered pseudo-hexagonal close-packed layer in the (*h*00) plane, with soft intermolecular H···H contacts (2.46–2.58 Å).

Related literature

For the synthesis of aromatic carboxylic acids, see: Kaeding (1967). For tetrakis(μ_2-2-fluorobenzoato)bis(2-fluorobenzoic acid)dicopper(II), see: Valach *et al.* (2000), For tetrakis(μ_2-benzoato)bis(2-fluorobenzoic acid)dicopper(II), see: Kawata *et al.* (1992).



Experimental

Crystal data

$[Cu_2(C_8H_7O_2)_4(C_8H_8O_2)_2]$
M_r = 939.96
Triclinic, $P\overline{1}$
a = 10.530 (3) Å
b = 10.579 (3) Å
c = 10.773 (4) Å
α = 109.248 (2)°
β = 93.156 (2)°
γ = 106.287 (2)°
V = 1073.0 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 100 (2) K
0.25 × 0.08 × 0.06 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004b)
T_{min} = 0.778, T_{max} = 0.939
17497 measured reflections
5138 independent reflections
4668 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.065
S = 1.05
5138 reflections
284 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O21^{i}	1.9402 (12)	Cu1—O22^{i}	1.9900 (13)
Cu1—O11	1.9559 (12)	Cu1—O31	2.1622 (13)
Cu1—O12	1.9585 (13)	Cu1···Cu1^{i}	2.5780 (9)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O32—H32···O22^{i}	0.82	1.85	2.6604 (18)	168
C16—H16···O21	0.93	2.39	2.721 (2)	101

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2426).

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supporting information

Acta Cryst. (2008). E**64**, m553–m554 [doi:10.1107/S1600536808006661]

Tetrakis(*μ*-2-methylbenzoato)bis[(2-methylbenzoic acid)copper(II)]

Abraham C. Sunil, Barend C. B. Bezuidenhoudt and J. Marthinus Janse van Rensburg

S1. Comment

In our endeavours to produce phenols from aromatic carboxylic acids, we came across work by Kaeding (1967). In order to verify the reaction sequence as proposed by Kaeding, we prepared the copper salt of *o*-toluic acid and obtained single crystals.

The title compound, (I), $[Cu_2(C_8H_7O_2)_4(C_8H_8O_2)_2]$ crystallized with molecular symmetry -1 (Fig.1). The title compound exhibits a cage-like structure. Four *o*-toluic anionic ligands form a cage around two Cu-atoms in a *syn-syn* configuration. Two more carboxylic acid are apically bonded to the Cu-atoms. The acid protons are hydrogen bonded to the cage carboxylate O atoms, O32—H32···O22 = 167.6° and O32···O22 = 2.6604 (18) Å. Another intra-molecular H···H short contact is present at C16···O21 with C16—H16···O21 = 100.9° and C16···O21 = 2.721 (2) Å.

Comparing the Van der Waals radii of copper, 2.32 Å, and the metallic Cu—Cu bond length, 2.55 Å, to the Cu—Cu separation in (I), 2.5780 (9) Å, one would expect the presence of weak orbital interaction. The Cu—O bond lengths of the cage carboxylates vary between 1.9402 (12) - 1.9900 (13) Å. The Cu—O bond distances to the adducted acid molecules show a *ca* 0.2 Å increase. Each Cu atom is displaced from the basal plane of the four caged carboxylates by 0.171 Å, towards the apical O atom. Compound (I) forms a puckered pseudo-hexagonal close packed layer in the (h 0 0) plane, with soft inter-molecular H···H contacts, 2.457–2.580 Å (Fig.2).

S2. Experimental

The complex $[Cu_2(C_8H_7O_2)_4(C_8H_8O_2)_2]$ was prepared by heating *o*-toluic acid (2.52 g, 18.5 mmol), copper carbonate (0.73 g, 3.3 mmol) and magnesium oxide (0.19 g, 4.68 mmol) under reflux, in toluene (30 ml) for 24 h. The product was extacted and crystallized from diethyl ether to yield a blue crystalline solid. (Yield: 84%)

S3. Refinement

Hydrogen atoms were placed in calculated positions, and they ride on the parent C-atoms, with U set to 1.2 to 1.5 times U_{eq}(C).

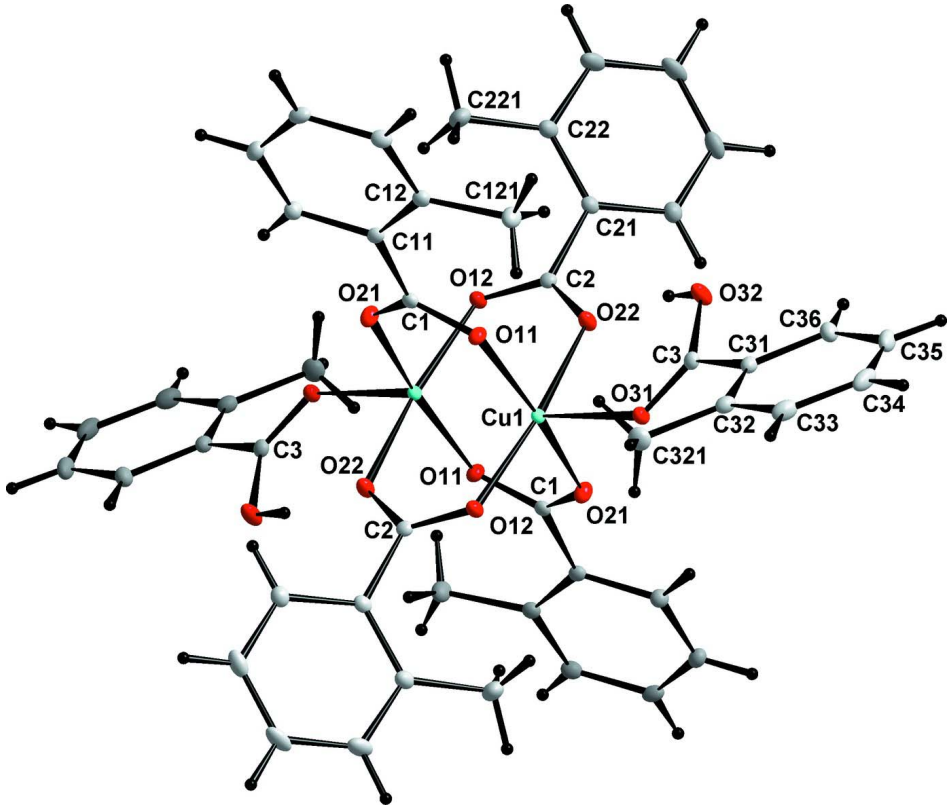

Figure 1

A view of (I) showing the atom-numbering scheme with displacement ellipsoids at the 30% probability level, non labelled atoms are symmetric equivalents. For the phenyl C-atoms, the first digit indicates ring number and the second digit the position of the atom in the ring.

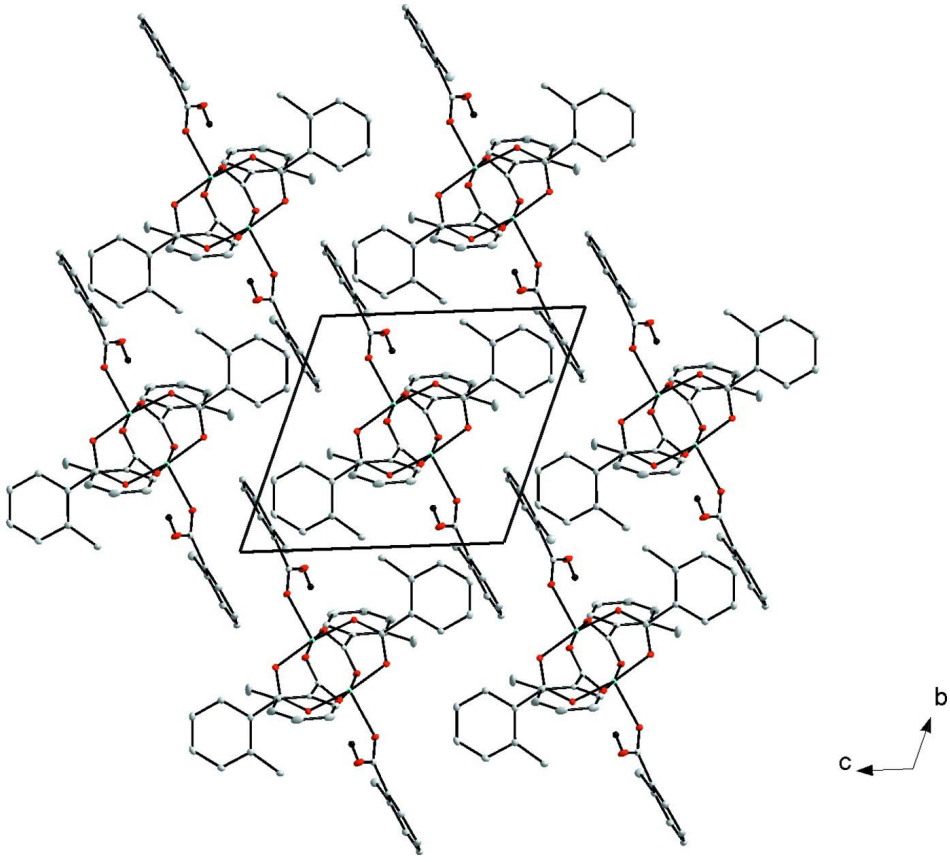

Figure 2

Indication of pseudo-hexagonal close packing along the *b* axis.

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Crystal data

$[Cu_2(C_8H_7O_2)_4(C_8H_8O_2)_2]$
M_r = 939.96
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 10.530 (3) Å
b = 10.579 (3) Å
c = 10.773 (4) Å
α = 109.248 (2)°
β = 93.156 (2)°
γ = 106.287 (2)°
V = 1073.0 (6) Å^3
Z = 1
$F(000)$ = 486
D_x = 1.455 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 8974 reflections
θ = 2.6–28.3°
μ = 1.06 mm^{-1}
T = 100 K
Needle, blue
0.25 × 0.08 × 0.06 mm

Data collection

Bruker X8 APEXII 4K KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004b)
T_{min} = 0.778, T_{max} = 0.939
17497 measured reflections
5138 independent reflections
4668 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 28°, θ_{min} = 2.2°
h = −13→13
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.065$
$S = 1.05$
5138 reflections
284 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.024P)^2 + 0.7431P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Experimental. The intensity data was collected on a Bruker X8 Apex II 4 K Kappa CCD diffractometer using an exposure time of 30 s/frame. The 1757 frames were collected with a frame width of 0.5° covering up to $\theta = 28°$ with 99.3% completeness accomplished.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.444832 (17)	0.389154 (17)	0.395103 (17)	0.01027 (6)
O32	0.51055 (11)	0.07974 (12)	0.26534 (12)	0.0217 (2)
H32	0.5525	0.1594	0.3175	0.033*
O31	0.36065 (11)	0.18596 (11)	0.23619 (10)	0.0154 (2)
O21	0.47477 (11)	0.50089 (11)	0.70973 (10)	0.0175 (2)
O22	0.38457 (10)	0.65099 (11)	0.57571 (11)	0.0168 (2)
O11	0.38005 (11)	0.30802 (11)	0.52758 (10)	0.0157 (2)
O12	0.29312 (10)	0.46128 (11)	0.39073 (10)	0.0150 (2)
C16	0.36586 (15)	0.36861 (16)	0.87485 (15)	0.0161 (3)
H16	0.3999	0.4666	0.9049	0.019*
C31	0.31192 (15)	−0.05882 (15)	0.11267 (14)	0.0142 (3)
C11	0.35899 (14)	0.29021 (15)	0.74017 (14)	0.0126 (3)
C36	0.37677 (17)	−0.14773 (16)	0.03537 (16)	0.0189 (3)
H36	0.4698	−0.1226	0.0517	0.023*
C25	0.00903 (16)	0.72093 (17)	0.56202 (18)	0.0235 (3)
H25	−0.0326	0.7479	0.6358	0.028*
C321	0.09555 (16)	−0.00753 (18)	0.17572 (17)	0.0229 (3)
H32A	0.0954	0.0674	0.1443	0.034*
H32B	0.138	0.0318	0.2672	0.034*
H32C	0.0049	−0.065	0.1684	0.034*
C1	0.40786 (14)	0.37152 (15)	0.65233 (14)	0.0127 (3)
C12	0.30930 (15)	0.14154 (15)	0.69355 (15)	0.0143 (3)
C15	0.32315 (16)	0.30349 (17)	0.96407 (16)	0.0183 (3)
H15	0.3285	0.3569	1.0533	0.022*
C2	0.29274 (14)	0.57566 (15)	0.47500 (14)	0.0119 (3)
C13	0.26600 (15)	0.07881 (16)	0.78583 (16)	0.0166 (3)
H13	0.2318	−0.0191	0.7571	0.02*
C32	0.17142 (16)	−0.09665 (16)	0.09292 (15)	0.0168 (3)
C21	0.17807 (14)	0.62904 (14)	0.45946 (15)	0.0131 (3)

C33	0.10027 (17)	−0.22517 (17)	−0.00704 (16)	0.0229 (3)
H33	0.0071	−0.2536	−0.0213	0.027*
C22	0.13237 (16)	0.63473 (16)	0.33772 (16)	0.0182 (3)
C121	0.30291 (18)	0.04573 (16)	0.55228 (16)	0.0211 (3)
H12A	0.278	−0.0505	0.5475	0.032*
H12B	0.3892	0.0707	0.5256	0.032*
H12C	0.2375	0.0561	0.4939	0.032*
C26	0.11778 (16)	0.67358 (16)	0.57076 (16)	0.0175 (3)
H26	0.151	0.6714	0.6516	0.021*
C34	0.16490 (19)	−0.31154 (17)	−0.08566 (16)	0.0254 (4)
H34	0.1149	−0.396	−0.1525	0.03*
C3	0.39545 (15)	0.08020 (15)	0.21105 (14)	0.0137 (3)
C35	0.30350 (19)	−0.27297 (17)	−0.06539 (16)	0.0238 (4)
H35	0.3469	−0.3305	−0.1189	0.029*
C14	0.27235 (15)	0.15762 (17)	0.91873 (16)	0.0177 (3)
H14	0.2425	0.1125	0.9775	0.021*
C24	−0.03711 (16)	0.72774 (17)	0.44262 (19)	0.0261 (4)
H24	−0.11	0.7598	0.436	0.031*
C221	0.1966 (2)	0.5912 (2)	0.21626 (17)	0.0314 (4)
H22A	0.2917	0.6378	0.2388	0.047*
H22B	0.1603	0.6173	0.1481	0.047*
H22C	0.1789	0.4909	0.1842	0.047*
C23	0.02467 (17)	0.68697 (17)	0.33293 (18)	0.0250 (4)
H23	−0.0062	0.6945	0.2539	0.03*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01089 (9)	0.00896 (9)	0.01017 (9)	0.00293 (6)	0.00121 (6)	0.00270 (6)
O32	0.0162 (5)	0.0158 (5)	0.0258 (6)	0.0068 (4)	−0.0053 (5)	−0.0019 (5)
O31	0.0165 (5)	0.0124 (5)	0.0150 (5)	0.0054 (4)	−0.0001 (4)	0.0019 (4)
O21	0.0211 (6)	0.0135 (5)	0.0143 (5)	0.0004 (4)	0.0038 (4)	0.0047 (4)
O22	0.0126 (5)	0.0159 (5)	0.0178 (5)	0.0056 (4)	−0.0018 (4)	0.0006 (4)
O11	0.0205 (5)	0.0135 (5)	0.0122 (5)	0.0031 (4)	0.0019 (4)	0.0053 (4)
O12	0.0145 (5)	0.0132 (5)	0.0157 (5)	0.0058 (4)	−0.0003 (4)	0.0025 (4)
C16	0.0170 (7)	0.0144 (7)	0.0160 (7)	0.0042 (6)	0.0020 (6)	0.0052 (6)
C31	0.0177 (7)	0.0117 (6)	0.0126 (7)	0.0041 (6)	0.0018 (6)	0.0043 (5)
C11	0.0099 (6)	0.0153 (7)	0.0139 (7)	0.0045 (5)	0.0023 (5)	0.0066 (6)
C36	0.0235 (8)	0.0156 (7)	0.0187 (8)	0.0083 (6)	0.0057 (6)	0.0057 (6)
C25	0.0163 (8)	0.0180 (8)	0.0319 (9)	0.0058 (6)	0.0088 (7)	0.0026 (7)
C321	0.0146 (7)	0.0262 (8)	0.0265 (9)	0.0060 (6)	0.0035 (6)	0.0082 (7)
C1	0.0115 (7)	0.0141 (7)	0.0142 (7)	0.0061 (5)	0.0027 (5)	0.0055 (5)
C12	0.0121 (7)	0.0154 (7)	0.0158 (7)	0.0048 (6)	0.0011 (5)	0.0057 (6)
C15	0.0197 (8)	0.0227 (8)	0.0139 (7)	0.0081 (6)	0.0042 (6)	0.0067 (6)
C2	0.0121 (7)	0.0116 (6)	0.0131 (7)	0.0026 (5)	0.0035 (5)	0.0066 (5)
C13	0.0134 (7)	0.0149 (7)	0.0216 (8)	0.0028 (6)	0.0021 (6)	0.0083 (6)
C32	0.0190 (7)	0.0156 (7)	0.0152 (7)	0.0028 (6)	0.0008 (6)	0.0073 (6)
C21	0.0109 (6)	0.0093 (6)	0.0169 (7)	0.0015 (5)	0.0013 (5)	0.0038 (5)

C33	0.0232 (8)	0.0182 (8)	0.0211 (8)	−0.0025 (6)	−0.0041 (7)	0.0082 (6)
C22	0.0196 (8)	0.0158 (7)	0.0181 (8)	0.0072 (6)	−0.0005 (6)	0.0038 (6)
C121	0.0297 (9)	0.0130 (7)	0.0189 (8)	0.0054 (6)	0.0039 (7)	0.0048 (6)
C26	0.0165 (7)	0.0151 (7)	0.0191 (7)	0.0040 (6)	0.0038 (6)	0.0044 (6)
C34	0.0394 (10)	0.0137 (7)	0.0149 (8)	−0.0004 (7)	−0.0029 (7)	0.0034 (6)
C3	0.0138 (7)	0.0146 (7)	0.0120 (7)	0.0041 (6)	0.0036 (5)	0.0043 (5)
C35	0.0401 (10)	0.0146 (7)	0.0167 (8)	0.0110 (7)	0.0069 (7)	0.0034 (6)
C14	0.0147 (7)	0.0242 (8)	0.0194 (8)	0.0063 (6)	0.0046 (6)	0.0141 (6)
C24	0.0141 (7)	0.0183 (8)	0.0399 (10)	0.0076 (6)	−0.0033 (7)	0.0022 (7)
C221	0.0442 (11)	0.0427 (11)	0.0175 (8)	0.0258 (9)	0.0062 (8)	0.0134 (8)
C23	0.0246 (9)	0.0205 (8)	0.0264 (9)	0.0094 (7)	−0.0085 (7)	0.0041 (7)

Geometric parameters (Å, º)

Cu1—O21^{i}	1.9402 (12)	C321—H32B	0.96
Cu1—O11	1.9559 (12)	C321—H32C	0.96
Cu1—O12	1.9585 (13)	C12—C13	1.397 (2)
Cu1—O22^{i}	1.9900 (13)	C12—C121	1.510 (2)
Cu1—O31	2.1622 (13)	C15—C14	1.385 (2)
Cu1—Cu1^{i}	2.5780 (9)	C15—H15	0.93
O32—C3	1.3184 (19)	C2—C21	1.492 (2)
O32—H32	0.82	C13—C14	1.386 (2)
O31—C3	1.2250 (18)	C13—H13	0.93
O21—C1	1.2670 (18)	C32—C33	1.394 (2)
O21—Cu1^{i}	1.9402 (12)	C21—C26	1.394 (2)
O22—C2	1.2764 (18)	C21—C22	1.398 (2)
O22—Cu1^{i}	1.9900 (13)	C33—C34	1.385 (3)
O11—C1	1.2626 (18)	C33—H33	0.93
O12—C2	1.2518 (18)	C22—C23	1.399 (2)
C16—C15	1.382 (2)	C22—C221	1.502 (2)
C16—C11	1.400 (2)	C121—H12A	0.96
C16—H16	0.93	C121—H12B	0.96
C31—C36	1.397 (2)	C121—H12C	0.96
C31—C32	1.404 (2)	C26—H26	0.93
C31—C3	1.485 (2)	C34—C35	1.384 (3)
C11—C12	1.410 (2)	C34—H34	0.93
C11—C1	1.497 (2)	C35—H35	0.93
C36—C35	1.384 (2)	C14—H14	0.93
C36—H36	0.93	C24—C23	1.383 (3)
C25—C24	1.381 (3)	C24—H24	0.93
C25—C26	1.383 (2)	C221—H22A	0.96
C25—H25	0.93	C221—H22B	0.96
C321—C32	1.506 (2)	C221—H22C	0.96
C321—H32A	0.96	C23—H23	0.93
O21^{i}—Cu1—O11	170.01 (4)	O12—C2—O22	124.23 (14)
O21^{i}—Cu1—O12	87.99 (5)	O12—C2—C21	118.96 (13)
O11—Cu1—O12	91.79 (5)	O22—C2—C21	116.81 (13)

O21^{i}—Cu1—O22^{i}	89.93 (5)	C14—C13—C12	122.17 (14)
O11—Cu1—O22^{i}	88.55 (5)	C14—C13—H13	118.9
O12—Cu1—O22^{i}	169.88 (4)	C12—C13—H13	118.9
O21^{i}—Cu1—O31	98.74 (6)	C33—C32—C31	117.35 (15)
O11—Cu1—O31	91.16 (6)	C33—C32—C321	119.26 (15)
O12—Cu1—O31	99.14 (5)	C31—C32—C321	123.37 (14)
O22^{i}—Cu1—O31	90.97 (5)	C26—C21—C22	120.83 (14)
O21^{i}—Cu1—Cu1^{i}	87.75 (5)	C26—C21—C2	117.76 (13)
O11—Cu1—Cu1^{i}	82.27 (5)	C22—C21—C2	121.41 (13)
O12—Cu1—Cu1^{i}	86.61 (4)	C34—C33—C32	121.67 (16)
O22^{i}—Cu1—Cu1^{i}	83.41 (4)	C34—C33—H33	119.2
O31—Cu1—Cu1^{i}	171.44 (3)	C32—C33—H33	119.2
C3—O32—H32	109.5	C21—C22—C23	117.30 (15)
C3—O31—Cu1	129.50 (10)	C21—C22—C221	122.57 (15)
C1—O21—Cu1^{i}	119.83 (10)	C23—C22—C221	120.12 (15)
C2—O22—Cu1^{i}	123.41 (10)	C12—C121—H12A	109.5
C1—O11—Cu1	125.45 (10)	C12—C121—H12B	109.5
C2—O12—Cu1	122.02 (10)	H12A—C121—H12B	109.5
C15—C16—C11	121.39 (14)	C12—C121—H12C	109.5
C15—C16—H16	119.3	H12A—C121—H12C	109.5
C11—C16—H16	119.3	H12B—C121—H12C	109.5
C36—C31—C32	120.86 (14)	C25—C26—C21	120.55 (15)
C36—C31—C3	118.27 (14)	C25—C26—H26	119.7
C32—C31—C3	120.78 (13)	C21—C26—H26	119.7
C16—C11—C12	119.90 (13)	C35—C34—C33	120.44 (15)
C16—C11—C1	116.94 (13)	C35—C34—H34	119.8
C12—C11—C1	123.16 (13)	C33—C34—H34	119.8
C35—C36—C31	120.42 (16)	O31—C3—O32	123.59 (13)
C35—C36—H36	119.8	O31—C3—C31	122.29 (14)
C31—C36—H36	119.8	O32—C3—C31	114.10 (13)
C24—C25—C26	119.35 (16)	C36—C35—C34	119.22 (16)
C24—C25—H25	120.3	C36—C35—H35	120.4
C26—C25—H25	120.3	C34—C35—H35	120.4
C32—C321—H32A	109.5	C15—C14—C13	120.05 (14)
C32—C321—H32B	109.5	C15—C14—H14	120
H32A—C321—H32B	109.5	C13—C14—H14	120
C32—C321—H32C	109.5	C25—C24—C23	120.20 (16)
H32A—C321—H32C	109.5	C25—C24—H24	119.9
H32B—C321—H32C	109.5	C23—C24—H24	119.9
O11—C1—O21	124.51 (13)	C22—C221—H22A	109.5
O11—C1—C11	118.61 (13)	C22—C221—H22B	109.5
O21—C1—C11	116.88 (13)	H22A—C221—H22B	109.5
C13—C12—C11	117.39 (14)	C22—C221—H22C	109.5
C13—C12—C121	117.89 (14)	H22A—C221—H22C	109.5
C11—C12—C121	124.70 (13)	H22B—C221—H22C	109.5
C16—C15—C14	119.09 (15)	C24—C23—C22	121.72 (16)
C16—C15—H15	120.5	C24—C23—H23	119.1
C14—C15—H15	120.5	C22—C23—H23	119.1

O21^{i}—Cu1—O31—C3	108.89 (13)	C11—C12—C13—C14	−0.8 (2)
O11—Cu1—O31—C3	−69.75 (13)	C121—C12—C13—C14	177.70 (14)
O12—Cu1—O31—C3	−161.75 (13)	C36—C31—C32—C33	−0.5 (2)
O22^{i}—Cu1—O31—C3	18.81 (13)	C3—C31—C32—C33	176.08 (14)
O12—Cu1—O11—C1	−88.41 (12)	C36—C31—C32—C321	178.06 (14)
O22^{i}—Cu1—O11—C1	81.47 (12)	C3—C31—C32—C321	−5.4 (2)
O31—Cu1—O11—C1	172.41 (12)	O12—C2—C21—C26	131.59 (15)
Cu1^{i}—Cu1—O11—C1	−2.08 (11)	O22—C2—C21—C26	−47.95 (19)
O21^{i}—Cu1—O12—C2	−87.01 (12)	O12—C2—C21—C22	−48.5 (2)
O11—Cu1—O12—C2	83.00 (12)	O22—C2—C21—C22	131.91 (15)
O22^{i}—Cu1—O12—C2	−8.8 (3)	C31—C32—C33—C34	−1.1 (2)
O31—Cu1—O12—C2	174.46 (11)	C321—C32—C33—C34	−179.70 (15)
Cu1^{i}—Cu1—O12—C2	0.85 (11)	C26—C21—C22—C23	0.1 (2)
C15—C16—C11—C12	−0.8 (2)	C2—C21—C22—C23	−179.71 (14)
C15—C16—C11—C1	179.95 (14)	C26—C21—C22—C221	178.43 (16)
C32—C31—C36—C35	2.2 (2)	C2—C21—C22—C221	−1.4 (2)
C3—C31—C36—C35	−174.48 (14)	C24—C25—C26—C21	−1.9 (2)
Cu1—O11—C1—O21	5.1 (2)	C22—C21—C26—C25	1.7 (2)
Cu1—O11—C1—C11	−175.02 (9)	C2—C21—C26—C25	−178.42 (14)
Cu1^{i}—O21—C1—O11	−5.4 (2)	C32—C33—C34—C35	1.0 (2)
Cu1^{i}—O21—C1—C11	174.78 (9)	Cu1—O31—C3—O32	−13.1 (2)
C16—C11—C1—O11	−166.58 (13)	Cu1—O31—C3—C31	168.70 (10)
C12—C11—C1—O11	14.2 (2)	C36—C31—C3—O31	144.89 (15)
C16—C11—C1—O21	13.27 (19)	C32—C31—C3—O31	−31.8 (2)
C12—C11—C1—O21	−165.91 (14)	C36—C31—C3—O32	−33.43 (19)
C16—C11—C12—C13	1.3 (2)	C32—C31—C3—O32	149.91 (14)
C1—C11—C12—C13	−179.57 (13)	C31—C36—C35—C34	−2.2 (2)
C16—C11—C12—C121	−177.11 (14)	C33—C34—C35—C36	0.7 (2)
C1—C11—C12—C121	2.1 (2)	C16—C15—C14—C13	0.6 (2)
C11—C16—C15—C14	−0.1 (2)	C12—C13—C14—C15	−0.2 (2)
Cu1—O12—C2—O22	−5.0 (2)	C26—C25—C24—C23	0.3 (2)
Cu1—O12—C2—C21	175.52 (9)	C25—C24—C23—C22	1.6 (3)
Cu1^{i}—O22—C2—O12	7.4 (2)	C21—C22—C23—C24	−1.8 (2)
Cu1^{i}—O22—C2—C21	−173.12 (9)	C221—C22—C23—C24	179.87 (17)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O32—H32···O22^{i}	0.82	1.85	2.6604 (18)	168
C16—H16···O21	0.93	2.39	2.721 (2)	101

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