Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(diphenyl-*p*-tolylphosphane-κP)(2-hydroxy-3,5,7-bromocyclohepta-2,4,6-trienonato-$\kappa^2 O,O'$)copper(I)

Nicola I. Barnard* and Tania N. Hill

Department of Chemistry, University of the Free State, Bloemfontein, Free State. South Africa
Correspondence e-mail: 2000011219@ufs4life.ac.za

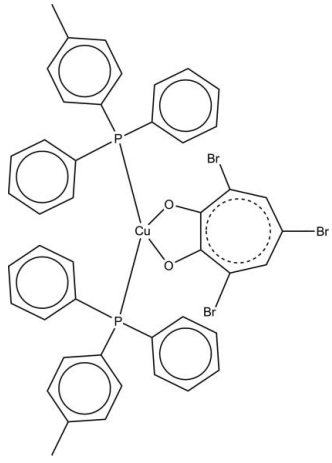
Received 8 October 2012; accepted 9 October 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.044; wR factor = 0.130; data-to-parameter ratio = 20.8.

The Cu^I atom in the title compund, $[Cu(C_7H_2Br_3O_2)(C_{19}H_{17}P)_2]$, is located on a twofold rotation axis; the 3,5,7-tribromotropolonate anion coordinates as a bidentate ligand with a bite angle of 76.42 (9)°. An intramolecular C—H···O interaction occurs. Within the crystal, extensive weak C—H···π interactions contribute to the herringbone pattern observed in the packing of the molecules.

Related literature

For background to tropolone and its derivatives, see: Dewar (1945); Hill & Steyl (2008); Crous *et al.* (2005). For bis-troplolonato–copper(II) complexes, see: Chipperfield *et al.* (1998); Hasegawa *et al.* (1997); Ho (2010); Ho *et al.* (2009). For work on the effect the troplonato ligand has on the solid state and chemical behaviour of copper(I) phosphine metal complexes, see: Roodt *et al.* (2003); Steyl (2007, 2009); Steyl & Hill (2009); Steyl & Roodt (2006).



Experimental

Crystal data

$[Cu(C_7H_2Br_3O_2)(C_{19}H_{17}P)_2]$
M_r = 973.95
Monoclinic, $C2/c$
a = 15.4522 (8) Å
b = 13.9073 (8) Å
c = 19.3269 (10) Å
β = 103.862 (3)°
V = 4032.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.63 mm^{-1}
T = 100 K
0.18 × 0.09 × 0.06 mm

Data collection

Bruker X8 APEXII 4K Kappa CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.686, T_{max} = 0.746
27602 measured reflections
5022 independent reflections
3970 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.04
5022 reflections
241 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.51 e Å^{-3}
$\Delta\rho_{min}$ = −1.57 e Å^{-3}

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

*Cg*2 and *Cg*3 are the centroids of the C121–C126 and C131–C136 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C136—H136···O2	0.95	2.52	3.365 (4)	149
C115—H115···*Cg*3^{i}	0.95	2.86	3.621 (4)	138
C137—H13*A*···*Cg*2^{ii}	0.98	3.18	4.144 (6)	168

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); 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).

Professors G. Steyland and A. Roodt, University of the Free State, and Mr Renier Koen are thanked for the data collection. Financial assistance from the University of the Free State Strategic Academic Cluster Initiative, SASOL, the South African NationalResearch Foundation (SA–NRF/THRIP) and the Inkaba yeAfrika Research Initiative is gratefully acknowledged. Part of this material is based on work supported by the SA–NRF/THRIP under grant No. GUN 2068915. Opinions, findings,conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the SA–NRF.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5299).

References

Brandenburg, K. & Putz, H. (2005). Crystal Impact GbR, Bonn, Germany.
Bruker (2004). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin. USA.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chipperfield, J. R., Clark, S., Elliott, J. & Sinn, E. (1998). *Chem. Commun.* pp. 195–196.
Crous, R., Datt, M., Foster, D., Bennie, L., Steenkamp, C., Huyser, J., Kirsten, L., Steyl, G. & Roodt, A. (2005). *Dalton Trans.* pp. 1108–1115.
Dewar, M. J. S. (1945). *Nature (London)*, **155**, 141–145.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hasegawa, M., Inomaki, Y., Inayoshi, T., Mosbi, T. & Kobayashi, M. (1997). *Inorg. Chim. Acta*, **257**, 259–264.
Hill, T. N. & Steyl, G. (2008). *Acta Cryst.* E**64**, m1580–m1581.
Ho, D. M. (2010). *Acta Cryst.* C**66**, m294–m299.
Ho, D. M., Berardini, M. E. & Arvanitis, G. M. (2009). *Acta Cryst.* C**65**, m391–m394.
Roodt, A., Otto, S. & Steyl, G. (2003). *Coord. Chem. Rev.* **245**, 121–137.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Steyl, G. (2007). *Acta Cryst.* E**63**, m2613–m2614.
Steyl, G. (2009). *Acta Cryst.* E**65**, m448.
Steyl, G. & Hill, T. N. (2009). *Acta Cryst.* E**65**, m233.
Steyl, G. & Roodt, A. (2006). *S. Afr. J. Chem.* **59**, 21–27.

supporting information

Acta Cryst. (2012). E**68**, m1354–m1355 [doi:10.1107/S1600536812042286]

Bis(diphenyl-*p*-tolylphosphane-κP)(2-hydroxy-3,5,7-bromocyclohepta-2,4,6-trienonato-$\kappa^2 O,O'$)copper(I)

Nicola I. Barnard and Tania N. Hill

S1. Comment

Tropolone and its derivatives have been of interest ever since their first discovery in the early 1940's (Dewar, 1945); they are known to have applications in both pharmacology (Hill & Steyl, 2008) and catalysis (Crous *et al.*, 2005). Bis troplolonato copper(II) complexes are most frequently reported (Ho, 2010; Ho *et al.*, 2009; Chipperfield *et al.*, 1998; Hasegawa *et al.*, 1997). Recently, reseach in this area has been extended to include copper(I) phosphine metal complexes and the effect the troplonato ligand has on the solid state and chemical behaviour of these complexes (Steyl, 2007; Steyl & Roodt, 2006; Roodt *et al.*, 2003). In this paper, the structure of the tropolonato-bis[diphenyl(*p*-tolyl)-phosphine]copper(I) complex is reported (Fig. 1).

The Cu—O and Cu—P bond distances were found to be 2.090 (1) Å and 2.229 (1) Å respectively and are well within comparable ranges for copper(I) phosphine complexes. the bond angles about the Cu atom show significantly distorted tetrahedral coordination (Table 1). The bidentate bite angle O2—Cu—O2^{i} observed at 76.42 (9)° is close to analogous angles in previously reported structures (Steyl, 2009).

The title compound (I) displays intramolecular C—H···Br interactions with a distance of 3.4666 (5) Å as seen in Figure 2. Figure 3 illustrates the packing diagram for compound (I), a zigzag pattern is adopted with inverted repeating units creating diagonals in all directions. This intricate design is achieved though numerous C—H···π itermolecular interactions see Figure 4. These interactions occur between methyl H atoms of the *p*-tolyl and phenyl π, phenyl H to *p*-tolyl π, phenyl H to phenyl π and *p*-tolyl π to *p*-tolyl The C—H···π itermolecular interactions range from 3.1816 (1) Å - 3.7267 (2) Å.

S2. Experimental

3,5,7-Tribomotropolone (0.3 mmol) was dissolved in methanol (20 ml). To this solution was added Bis(diphenyl(*p*-tolyl)-phosphine) copper nitrate (0.3 mmol). The resulting mixture was stirred at room temperature for 30 minutes before filtering. The filtrate was then slowly evaporated yielding crystals siutable for X-ray diffraction after 48 h.

S3. Refinement

Hydroge atoms were placed in calculated positions, and were allowed to ride on their parent C atoms.

The final difference Fouier map had a peak/hole in the vicinity of Br1.

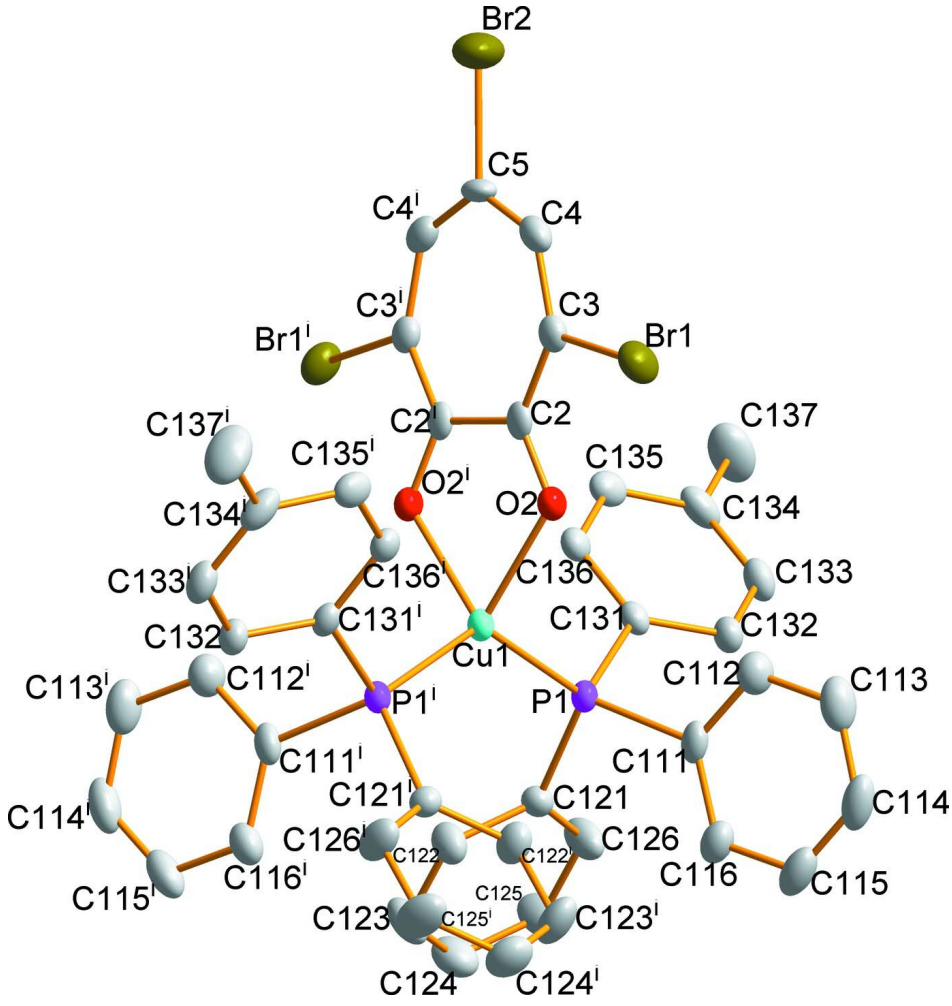


Figure 1

A view of (I). Displacement ellipsoids are drawn at 50% proabiity level. Hydrogen atoms have been ommited.

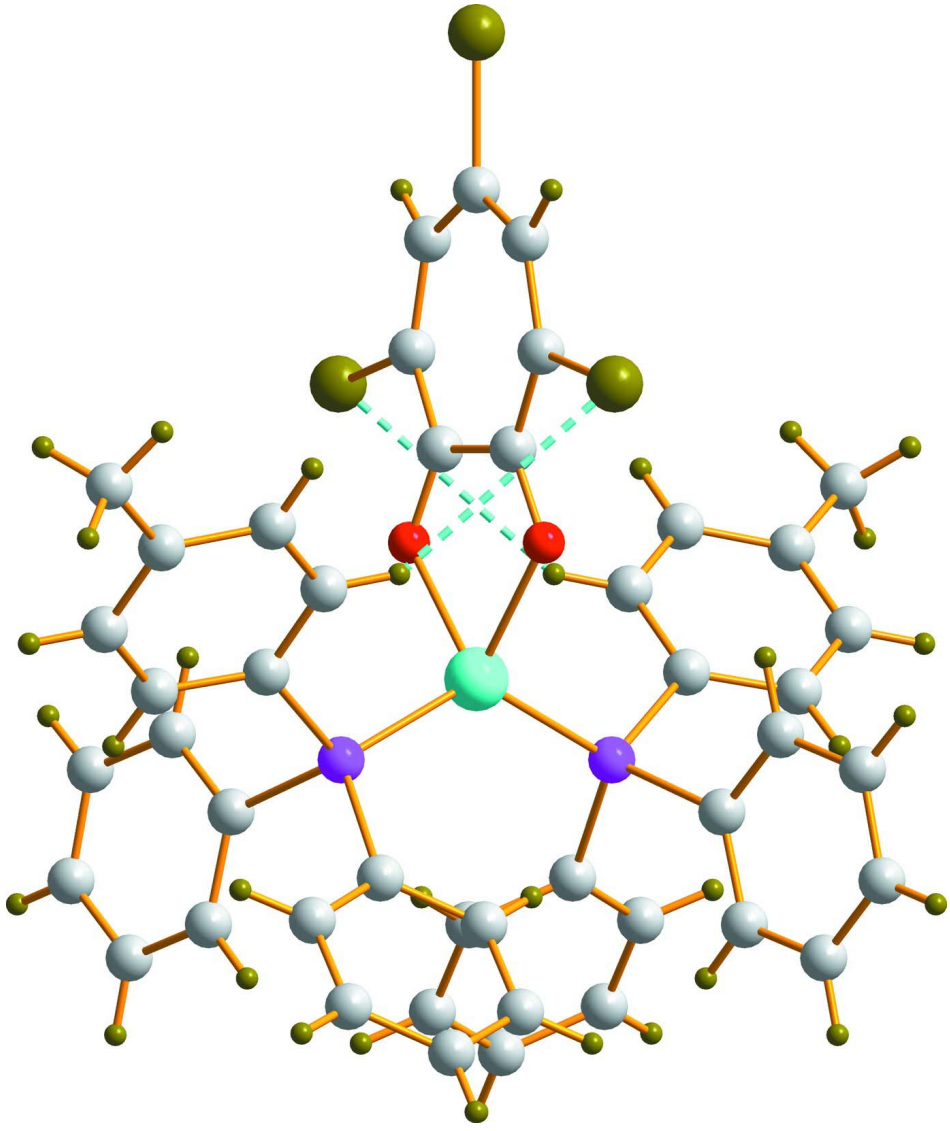


Figure 2

Intramolecular H···Br interactions (dashed bonds) for the title compound.

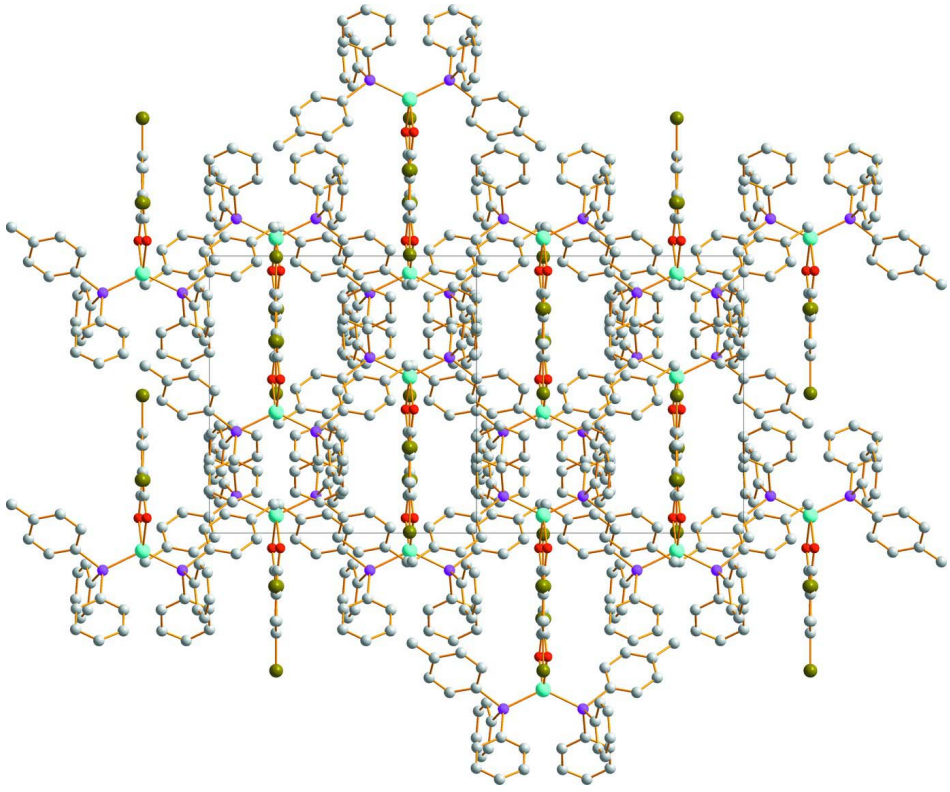


Figure 3

A packing diagram of the title compound, illustrating the herringbone patturnation as viewed along the [1,0,1] axis. Hydrogen atoms have been ommited.

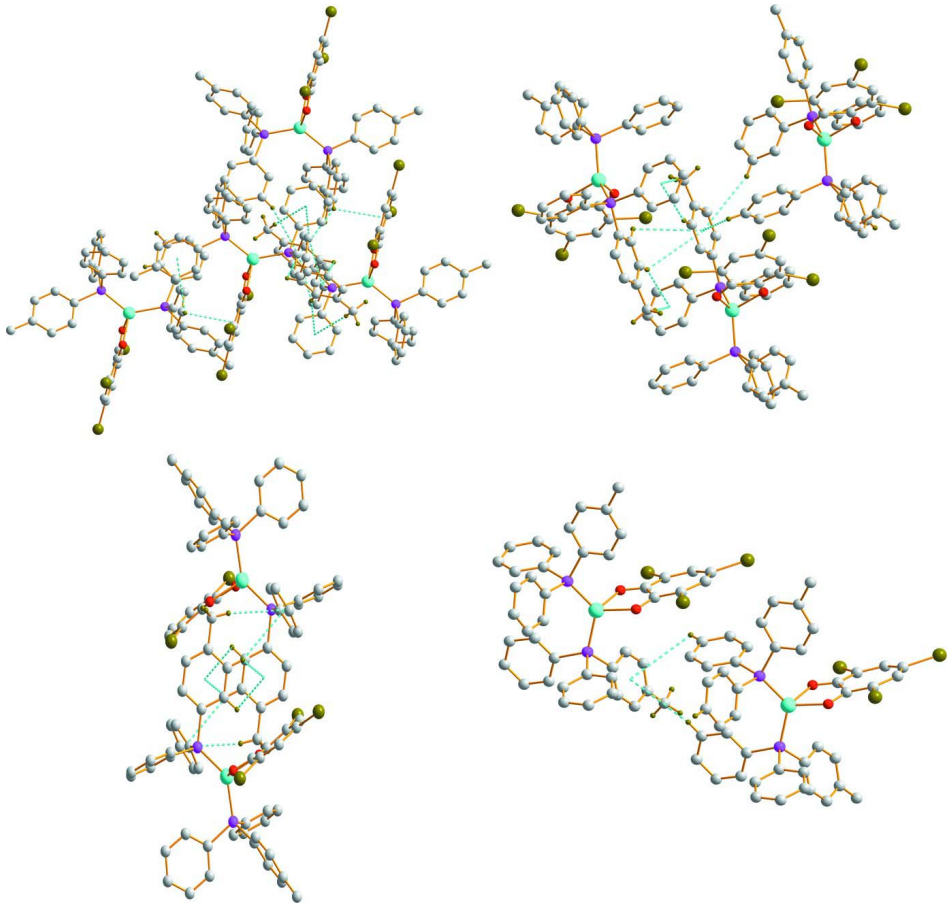


Figure 4

Four differing views highlighting elaborate web of H···π intermolecular interactions (dashed bonds) creating the three dimentional herringbone design, non-relevant hydrogen atoms have been ommited for clarity.

Bis(diphenyl-*p*-tolylphosphane-κP)(2-hydroxy-3,5,7-bromocyclohepta-2,4,6-trienonato-$\kappa^2 O,O'$)copper(I)

Crystal data

$[Cu(C_7H_2Br_3O_2)(C_{19}H_{17}P)_2]$
$M_r = 973.95$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 15.4522$ (8) Å
$b = 13.9073$ (8) Å
$c = 19.3269$ (10) Å
$\beta = 103.862$ (3)°
$V = 4032.4$ (4) Å^3
$Z = 4$
$F(000) = 1944$
$D_x = 1.604$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8436 reflections
$\theta = 2.3$–$28.4°$
$\mu = 3.63$ mm^{-1}
$T = 100$ K
Cuboid, green
0.18 × 0.09 × 0.06 mm

Data collection

Bruker X8 APEXII 4K Kappa CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 512 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.686$, $T_{max} = 0.746$
27602 measured reflections
5022 independent reflections
3970 reflections with $I > 2\sigma(I)$

R_{int} = 0.053
θ_{max} = 28.4°, θ_{min} = 2°
h = −19→20
k = −15→18
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.04
5022 reflections
241 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 16.6643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.51 e Å^{-3}
$\Delta\rho_{min}$ = −1.57 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C2	0.5382 (2)	0.6353 (3)	0.28258 (18)	0.0213 (7)
C3	0.5717 (2)	0.7199 (3)	0.32159 (19)	0.0230 (7)
C4	0.5556 (2)	0.8171 (3)	0.3086 (2)	0.0294 (8)
H4	0.5867	0.8596	0.3446	0.035*
C5	0.5	0.8599 (3)	0.25	0.0295 (12)
C111	0.3102 (2)	0.3211 (3)	0.25441 (19)	0.0242 (7)
C112	0.2526 (2)	0.3880 (3)	0.2148 (2)	0.0309 (8)
H112	0.2662	0.4546	0.2202	0.037*
C113	0.1744 (3)	0.3578 (4)	0.1667 (2)	0.0373 (10)
H113	0.1339	0.4041	0.1411	0.045*
C114	0.1562 (3)	0.2615 (4)	0.1565 (2)	0.0375 (10)
H114	0.1041	0.2411	0.1227	0.045*
C115	0.2132 (3)	0.1946 (3)	0.1954 (2)	0.0384 (10)
H115	0.2003	0.128	0.1883	0.046*
C116	0.2898 (2)	0.2235 (3)	0.2451 (2)	0.0310 (8)
H116	0.3281	0.1769	0.2725	0.037*
C121	0.4606 (2)	0.2639 (2)	0.36831 (19)	0.0221 (7)
C122	0.5385 (3)	0.2234 (3)	0.3588 (2)	0.0317 (8)
H122	0.5645	0.2472	0.3223	0.038*
C123	0.5799 (3)	0.1478 (3)	0.4021 (3)	0.0432 (11)
H123	0.6334	0.1205	0.3949	0.052*
C124	0.5423 (3)	0.1126 (3)	0.4559 (2)	0.0412 (10)

H124	0.57	0.0613	0.4856	0.049*
C125	0.4650 (3)	0.1526 (3)	0.4655 (3)	0.0470 (12)
H125	0.4394	0.1292	0.5023	0.056*
C126	0.4237 (3)	0.2272 (3)	0.4219 (3)	0.0391 (10)
H126	0.3697	0.2535	0.4288	0.047*
C131	0.3738 (2)	0.4421 (2)	0.37497 (17)	0.0202 (7)
C132	0.2920 (2)	0.4256 (3)	0.39248 (19)	0.0236 (7)
H132	0.2525	0.3778	0.3677	0.028*
C133	0.2690 (2)	0.4791 (3)	0.4460 (2)	0.0277 (8)
H133	0.2138	0.4667	0.4579	0.033*
C134	0.3244 (3)	0.5498 (3)	0.4823 (2)	0.0303 (8)
C135	0.4049 (2)	0.5684 (3)	0.46311 (19)	0.0263 (7)
H135	0.443	0.6183	0.4864	0.032*
C136	0.4292 (2)	0.5143 (3)	0.41023 (18)	0.0222 (7)
H136	0.4841	0.527	0.3981	0.027*
C137	0.3016 (3)	0.6032 (4)	0.5422 (3)	0.0512 (13)
H13A	0.3485	0.6502	0.5612	0.077*
H13B	0.2964	0.5579	0.5798	0.077*
H13C	0.2447	0.6368	0.5249	0.077*
O2	0.56859 (15)	0.55420 (17)	0.30362 (13)	0.0227 (5)
P1	0.41329 (5)	0.36611 (6)	0.31230 (5)	0.01920 (18)
Cu1	0.5	0.43613 (4)	0.25	0.01987 (15)
Br1	0.65536 (3)	0.69166 (3)	0.40942 (2)	0.03295 (13)
Br2	0.5	0.99600 (5)	0.25	0.0638 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0140 (14)	0.0293 (18)	0.0231 (17)	−0.0008 (13)	0.0096 (13)	0.0021 (14)
C3	0.0171 (14)	0.0279 (18)	0.0259 (17)	−0.0019 (13)	0.0090 (13)	−0.0002 (14)
C4	0.0225 (17)	0.0277 (19)	0.041 (2)	−0.0066 (14)	0.0132 (15)	−0.0078 (16)
C5	0.027 (2)	0.011 (2)	0.054 (3)	0	0.016 (2)	0
C111	0.0150 (14)	0.036 (2)	0.0230 (17)	−0.0030 (14)	0.0071 (12)	−0.0048 (15)
C112	0.0273 (18)	0.037 (2)	0.0276 (19)	−0.0005 (16)	0.0047 (15)	−0.0003 (16)
C113	0.0256 (19)	0.061 (3)	0.0243 (19)	0.0036 (18)	0.0034 (15)	0.0005 (18)
C114	0.0222 (17)	0.062 (3)	0.030 (2)	−0.0106 (18)	0.0086 (15)	−0.015 (2)
C115	0.030 (2)	0.047 (3)	0.041 (2)	−0.0167 (18)	0.0150 (18)	−0.017 (2)
C116	0.0234 (17)	0.036 (2)	0.036 (2)	−0.0069 (15)	0.0102 (15)	−0.0061 (17)
C121	0.0212 (15)	0.0196 (17)	0.0260 (17)	0.0014 (13)	0.0070 (13)	−0.0005 (13)
C122	0.0262 (18)	0.036 (2)	0.036 (2)	0.0055 (16)	0.0138 (16)	0.0070 (17)
C123	0.034 (2)	0.044 (3)	0.055 (3)	0.0189 (19)	0.018 (2)	0.018 (2)
C124	0.045 (2)	0.034 (2)	0.047 (2)	0.0110 (19)	0.015 (2)	0.0116 (19)
C125	0.054 (3)	0.040 (2)	0.057 (3)	0.013 (2)	0.034 (2)	0.021 (2)
C126	0.035 (2)	0.036 (2)	0.055 (3)	0.0110 (17)	0.027 (2)	0.015 (2)
C131	0.0173 (14)	0.0229 (17)	0.0209 (16)	0.0055 (13)	0.0057 (12)	0.0038 (13)
C132	0.0178 (15)	0.0269 (17)	0.0273 (18)	0.0018 (13)	0.0076 (13)	0.0003 (14)
C133	0.0203 (16)	0.037 (2)	0.0273 (18)	0.0075 (15)	0.0077 (14)	0.0022 (15)
C134	0.0307 (18)	0.036 (2)	0.0238 (18)	0.0155 (16)	0.0051 (14)	−0.0003 (16)

C135	0.0262 (17)	0.0257 (18)	0.0227 (17)	0.0044 (14)	−0.0026 (13)	0.0007 (14)
C136	0.0176 (14)	0.0236 (17)	0.0239 (17)	0.0037 (13)	0.0021 (12)	0.0024 (13)
C137	0.045 (3)	0.070 (3)	0.039 (2)	0.012 (2)	0.010 (2)	−0.018 (2)
O2	0.0171 (11)	0.0233 (13)	0.0272 (12)	−0.0008 (9)	0.0041 (9)	0.0014 (10)
P1	0.0145 (4)	0.0208 (4)	0.0234 (4)	−0.0004 (3)	0.0068 (3)	−0.0008 (3)
Cu1	0.0149 (3)	0.0214 (3)	0.0249 (3)	0	0.0078 (2)	0
Br1	0.0317 (2)	0.0367 (2)	0.0276 (2)	−0.00878 (16)	0.00144 (15)	−0.00242 (16)
Br2	0.0539 (4)	0.0268 (3)	0.1064 (7)	0	0.0112 (4)	0

Geometric parameters (Å, º)

C2—O2	1.252 (4)	C123—C124	1.396 (6)
C2—C3	1.426 (5)	C123—H123	0.95
C2—C2^{i}	1.506 (6)	C124—C125	1.370 (6)
C3—C4	1.387 (5)	C124—H124	0.95
C3—Br1	1.911 (4)	C125—C126	1.391 (6)
C4—C5	1.382 (5)	C125—H125	0.95
C4—H4	0.95	C126—H126	0.95
C5—C4^{i}	1.382 (5)	C131—C136	1.388 (5)
C5—Br2	1.893 (5)	C131—C132	1.403 (4)
C111—C112	1.384 (5)	C131—P1	1.820 (3)
C111—C116	1.395 (5)	C132—C133	1.387 (5)
C111—P1	1.824 (3)	C132—H132	0.95
C112—C113	1.400 (5)	C133—C134	1.381 (6)
C112—H112	0.95	C133—H133	0.95
C113—C114	1.375 (7)	C134—C135	1.405 (5)
C113—H113	0.95	C134—C137	1.486 (6)
C114—C115	1.374 (7)	C135—C136	1.391 (5)
C114—H114	0.95	C135—H135	0.95
C115—C116	1.392 (6)	C136—H136	0.95
C115—H115	0.95	C137—H13A	0.98
C116—H116	0.95	C137—H13B	0.98
C121—C122	1.381 (5)	C137—H13C	0.98
C121—C126	1.393 (5)	O2—Cu1	2.090 (2)
C121—P1	1.830 (4)	P1—Cu1	2.2284 (9)
C122—C123	1.398 (6)	Cu1—O2^{i}	2.090 (2)
C122—H122	0.95	Cu1—P1^{i}	2.2284 (9)
O2—C2—C3	120.7 (3)	C124—C125—H125	119.7
O2—C2—C2^{i}	115.45 (19)	C126—C125—H125	119.7
C3—C2—C2^{i}	123.7 (2)	C125—C126—C121	120.9 (4)
C4—C3—C2	133.0 (3)	C125—C126—H126	119.5
C4—C3—Br1	114.5 (3)	C121—C126—H126	119.5
C2—C3—Br1	112.5 (3)	C136—C131—C132	119.0 (3)
C5—C4—C3	128.1 (4)	C136—C131—P1	118.8 (2)
C5—C4—H4	115.9	C132—C131—P1	122.0 (3)
C3—C4—H4	115.9	C133—C132—C131	119.9 (3)
C4^{i}—C5—C4	129.0 (5)	C133—C132—H132	120.1

C4^{i}—C5—Br2	115.5 (2)	C131—C132—H132	120.1
C4—C5—Br2	115.5 (2)	C134—C133—C132	121.5 (3)
C112—C111—C116	119.1 (3)	C134—C133—H133	119.2
C112—C111—P1	117.4 (3)	C132—C133—H133	119.2
C116—C111—P1	123.4 (3)	C133—C134—C135	118.5 (3)
C111—C112—C113	120.2 (4)	C133—C134—C137	121.2 (4)
C111—C112—H112	119.9	C135—C134—C137	120.3 (4)
C113—C112—H112	119.9	C136—C135—C134	120.4 (3)
C114—C113—C112	120.2 (4)	C136—C135—H135	119.8
C114—C113—H113	119.9	C134—C135—H135	119.8
C112—C113—H113	119.9	C131—C136—C135	120.6 (3)
C113—C114—C115	119.9 (4)	C131—C136—H136	119.7
C113—C114—H114	120.1	C135—C136—H136	119.7
C115—C114—H114	120.1	C134—C137—H13A	109.5
C114—C115—C116	120.6 (4)	C134—C137—H13B	109.5
C114—C115—H115	119.7	H13A—C137—H13B	109.5
C116—C115—H115	119.7	C134—C137—H13C	109.5
C115—C116—C111	119.9 (4)	H13A—C137—H13C	109.5
C115—C116—H116	120.1	H13B—C137—H13C	109.5
C111—C116—H116	120.1	C2—O2—Cu1	116.1 (2)
C122—C121—C126	118.3 (3)	C131—P1—C111	102.98 (15)
C122—C121—P1	118.4 (3)	C131—P1—C121	101.98 (16)
C126—C121—P1	123.2 (3)	C111—P1—C121	105.21 (17)
C121—C122—C123	121.0 (4)	C131—P1—Cu1	116.55 (12)
C121—C122—H122	119.5	C111—P1—Cu1	111.62 (12)
C123—C122—H122	119.5	C121—P1—Cu1	116.91 (11)
C122—C123—C124	119.9 (4)	O2—Cu1—O2^{i}	76.42 (13)
C122—C123—H123	120.1	O2—Cu1—P1	112.00 (7)
C124—C123—H123	120.1	O2^{i}—Cu1—P1	108.19 (7)
C125—C124—C123	119.3 (4)	O2—Cu1—P1^{i}	108.19 (7)
C125—C124—H124	120.3	O2^{i}—Cu1—P1^{i}	112.00 (7)
C123—C124—H124	120.3	P1—Cu1—P1^{i}	128.18 (5)
C124—C125—C126	120.6 (4)		

O2—C2—C3—C4	174.7 (4)	C134—C135—C136—C131	0.9 (5)
C2^{i}—C2—C3—C4	−9.2 (7)	C3—C2—O2—Cu1	171.0 (2)
O2—C2—C3—Br1	−5.6 (4)	C2^{i}—C2—O2—Cu1	−5.4 (4)
C2^{i}—C2—C3—Br1	170.5 (3)	C136—C131—P1—C111	−157.1 (3)
C2—C3—C4—C5	−1.1 (6)	C132—C131—P1—C111	27.6 (3)
Br1—C3—C4—C5	179.2 (2)	C136—C131—P1—C121	94.0 (3)
C3—C4—C5—C4^{i}	2.7 (3)	C132—C131—P1—C121	−81.3 (3)
C3—C4—C5—Br2	−177.3 (3)	C136—C131—P1—Cu1	−34.5 (3)
C116—C111—C112—C113	0.9 (5)	C132—C131—P1—Cu1	150.1 (2)
P1—C111—C112—C113	176.9 (3)	C112—C111—P1—C131	62.6 (3)
C111—C112—C113—C114	−2.6 (6)	C116—C111—P1—C131	−121.6 (3)
C112—C113—C114—C115	2.2 (6)	C112—C111—P1—C121	169.0 (3)
C113—C114—C115—C116	−0.1 (6)	C116—C111—P1—C121	−15.1 (3)
C114—C115—C116—C111	−1.6 (6)	C112—C111—P1—Cu1	−63.2 (3)

C112—C111—C116—C115	1.2 (5)	C116—C111—P1—Cu1	112.6 (3)
P1—C111—C116—C115	−174.6 (3)	C122—C121—P1—C131	−141.0 (3)
C126—C121—C122—C123	−0.4 (6)	C126—C121—P1—C131	36.4 (4)
P1—C121—C122—C123	177.2 (4)	C122—C121—P1—C111	111.8 (3)
C121—C122—C123—C124	−0.2 (7)	C126—C121—P1—C111	−70.8 (4)
C122—C123—C124—C125	0.1 (8)	C122—C121—P1—Cu1	−12.7 (3)
C123—C124—C125—C126	0.4 (8)	C126—C121—P1—Cu1	164.8 (3)
C124—C125—C126—C121	−1.0 (8)	C2—O2—Cu1—O2^{i}	2.14 (18)
C122—C121—C126—C125	0.9 (7)	C2—O2—Cu1—P1	−102.3 (2)
P1—C121—C126—C125	−176.5 (4)	C2—O2—Cu1—P1^{i}	111.2 (2)
C136—C131—C132—C133	−2.1 (5)	C131—P1—Cu1—O2	26.45 (14)
P1—C131—C132—C133	173.3 (3)	C111—P1—Cu1—O2	144.35 (15)
C131—C132—C133—C134	0.8 (6)	C121—P1—Cu1—O2	−94.47 (15)
C132—C133—C134—C135	1.3 (6)	C131—P1—Cu1—O2^{i}	−55.86 (14)
C132—C133—C134—C137	−176.7 (4)	C111—P1—Cu1—O2^{i}	62.04 (15)
C133—C134—C135—C136	−2.1 (5)	C121—P1—Cu1—O2^{i}	−176.78 (14)
C137—C134—C135—C136	175.8 (4)	C131—P1—Cu1—P1^{i}	164.68 (12)
C132—C131—C136—C135	1.2 (5)	C111—P1—Cu1—P1^{i}	−77.41 (13)
P1—C131—C136—C135	−174.3 (3)	C121—P1—Cu1—P1^{i}	43.76 (13)

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

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C121–C126 and C131–C136 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C136—H136···O2	0.95	2.52	3.365 (4)	149
C115—H115···*Cg*3^{ii}	0.95	2.86	3.621 (4)	138
C137—H13*A*···*Cg*2^{iii}	0.98	3.18	4.144 (6)	168

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