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O,O-Bis(2-*tert*-butyl-4-methoxyphenyl) chlorothiophosphonate. Corrigendum.

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.028
wR factor = 0.073
Data-to-parameter ratio = 12.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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In the original report by Odabaşoğlu, Büyükgüngör & Albayrak [*Acta Cryst.* (2005), E**61**, o2528–o2530], the structure was reported in the incorrect space group *Cc*. The structure is now reported as disordered in the correct space group *C*2/*c*. The P atom lies on a twofold rotation axis.A revised description of the hydrogen bonding is also given.

Comment

An *ORTEP-3* (Farrugia, 1997) view of (I) and a packing diagram are shown in Figs. 1 and 2, respectively. The P atom lies on a twofold rotation axis, eading to disorder of the Cl and S atoms. Compound (I) has no classical hydrogen bonds, but there are two C—H$\cdots\pi$ interactions: H8*A*$\cdots$*Cg*1= 3.12 (2) Å and C8—H8*A*$\cdots$*Cg*1 = 122.8 (2)° (*Cg*1 is the centroid of the C1^{ii}–C6^{ii} ring), and H11*A*$\cdots$*Cg*2 = 2.71 (2) Å and C11—H11*A*$\cdots$*Cg*2 = 142.7 (1)° (*Cg*2 is the centroid of the C1^{iii}–C6^{iii}

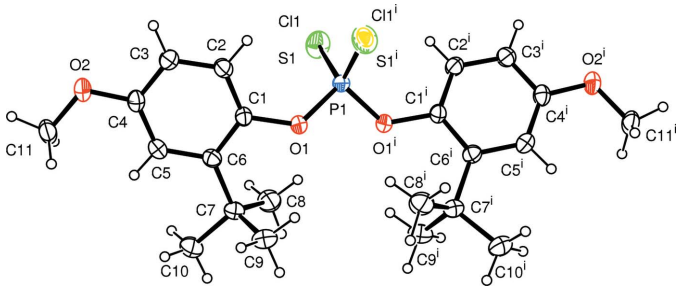

Figure 1
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids·[Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$]

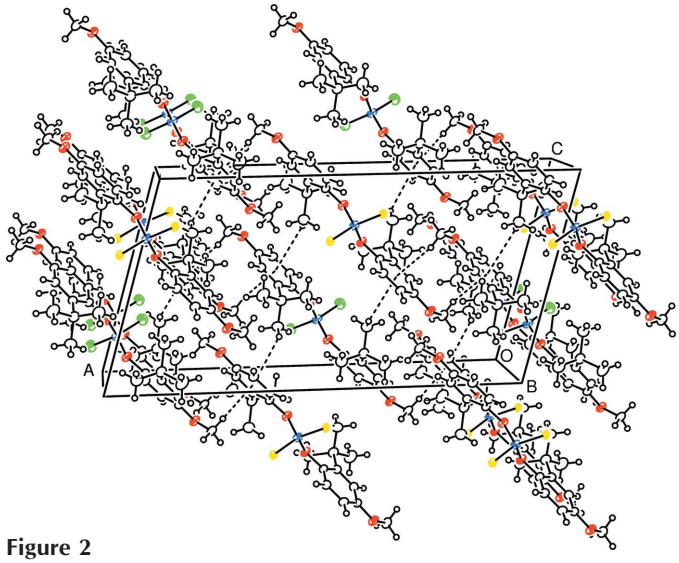

Figure 2
A view of the packing of (I); C—H$\cdots\pi$ interactions are drawn as dashed lines.

ring) [symmetry codes: (ii) $x, 1-y, \frac{1}{2}+z$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, -z$]. The dihedral angle between the symmetry-related benzene rings is 41.2 (2)°. Selected bond distances and angles are given in Table 1.

Experimental

Crystal data

$C_{22}H_{30}ClO_4PS$
M_r = 456.94
Monoclinic, $C2/c$
a = 23.592 (3) Å
b = 8.3111 (6) Å
c = 12.5067 (14) Å
β = 105.740 (9)°
V = 2360.3 (4) Å^3
Z = 4
D_x = 1.286 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16485 reflections
θ = 1.7–26.7°
μ = 0.34 mm^{-1}
T = 150 K
Prism, colorless
0.64 × 0.59 × 0.55 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.824, T_{max} = 0.869
16485 measured reflections
2327 independent reflections
2146 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°
$h = -28 \rightarrow 28$
$k = -10 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
S = 1.08
2327 reflections
192 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 1.6163P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.3946 (18)	C4—C5	1.4017 (19)
C1—C6	1.4086 (17)	C5—C6	1.4088 (18)
C1—O1	1.4226 (14)	O1—P1	1.5750 (9)
C2—C3	1.3860 (18)	P1—S1^{i}	1.9791 (4)
C3—C4	1.3979 (18)	P1—Cl1	1.9791 (4)
C2—C1—C6	123.25 (11)	C4—C5—C6	121.99 (12)
C2—C1—O1	119.13 (11)	C1—C6—C5	115.48 (11)
C6—C1—O1	117.58 (11)	O1—P1—O1^{i}	97.08 (7)
C3—C2—C1	119.77 (12)	O1—P1—S1^{i}	111.27 (4)
C2—C3—C4	119.11 (12)	O1—P1—Cl1	111.44 (3)
C3—C4—C5	120.39 (11)	S1^{i}—P1—Cl1	113.26 (3)

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

All H atoms were refined freely. Atoms S1 and Cl1 were assigned to the same atomic site and refined freely with the same atomic coordinates and with fixed site-occupancy factors of 0.5.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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