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(2-Methoxyphenyl)phenylphosphine oxide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.122
Data-to-parameter ratio = 16.3

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

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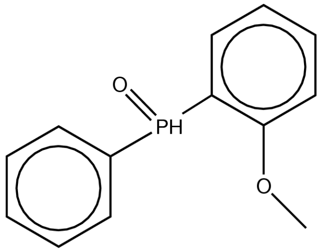
All interatomic distances in the title compound, $C_{13}H_{13}O_2P$, can be considered normal. The phosphorus tetrahedron exhibits its usual deformation. The (2-methoxyphenyl)-phosphine section is almost planar. The structure is assembled *via* intermolecular C—H···O hydrogen bonds, to form of one-dimensional chains.

Comment

Secondary phosphine oxides are important synthetic intermediates in organophosphorus chemistry and their high reactivity is typically connected with the presence of a relatively acidic hydrogen in their structure (Engel, 1988). They exist in two tautomeric forms: R_2P(═O)H and R_2POH, the former being predominant in the equilibrium (Bailey & Fox, 1963, 1964). There are, however, cases in transition-metal complexes, where the latter form is seen exclusively (Parkins, 1996; Han *et al.*, 1996). It was, therefore, deemed interesting to study the crystal structure of some model secondary phosphine oxides in order to reveal their tautomeric preferences in the solid state, and to study the character of the expected hydrogen bonding implied by their acidic functionality. The selected models include one alkylarylphosphine oxide, *i.e.* benzylphenylphosphine oxide (Kruszynski *et al.*, 2002), and one diarylphosphine oxide, *viz.* (2-methoxyphenyl)phenylphosphine oxide, (I).



(I)

A perspective view of (I), together with the atom-numbering scheme, is shown in Fig. 1. All interatomic distances can be considered normal and the phenyl rings are planar within experimental error. The overall molecular geometry of (I) is similar to that in (2-methoxyphenyl)-(phenyl)vinylphosphine oxide, (II) (Wieczorek, 1995). The weighted r.m.s. deviation for all non-H atoms in (I) and the respective atoms of (II) is 0.156 (4) Å. The superposition of the two molecules (I) and (II) is shown in Fig. 2. The phosphorus tetrahedron exhibits its usual deformation, with C—P—C and C—P—H angles smaller than tetrahedral, and O—P—C and O—P—H angles greater than tetrahedral

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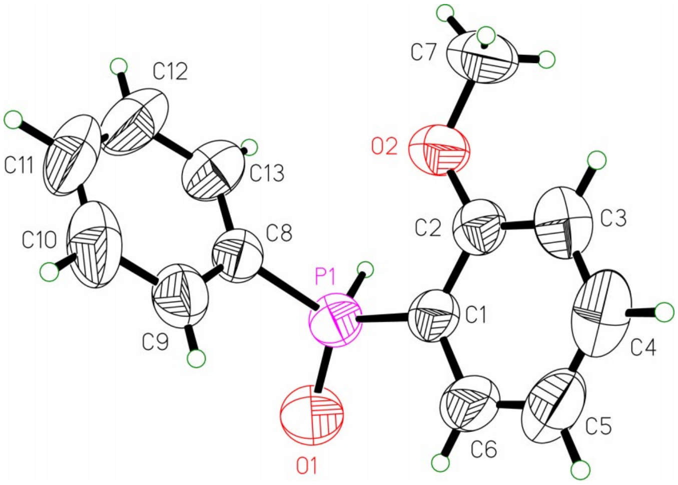

Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

(Table 1). The P═O bond makes angles of 7.6 (2) and 46.56 (2)° with the phenyl rings containing atoms C1 and C8, respectively. Analogous angles in (II) are 1.7 (1) and 52.0 (1)°. The (2-methoxyphenyl)phosphine section is almost planar, with a maximum deviation of 0.0181 (17) Å for atom C6. The adjacent C atom deviates by −1.551 (2) Å from this plane, and the O atom deviates by 0.190 (2) Å. The dihedral angle between the weighted least-squares planes of the phenyl rings is 82.53 (7)°. In the structure there is one short C—H···O short intermolecular interaction (Table 2), which can be considered as a weak intermolecular hydrogen bond (Taylor & Kennard, 1982; Desiraju & Steiner, 1999). In this way, a one-dimensional hydrogen-bond chain is created (Fig. 3). There are no unusual intermolecular short contacts except for the hydrogen bond described in Table 2.

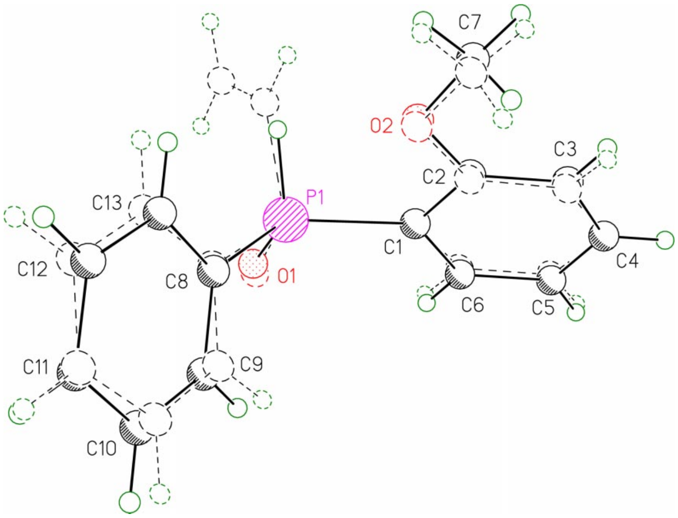

Figure 2
Superposition of molecules (I) and (II). Molecule (II) is indicated by dashed lines.

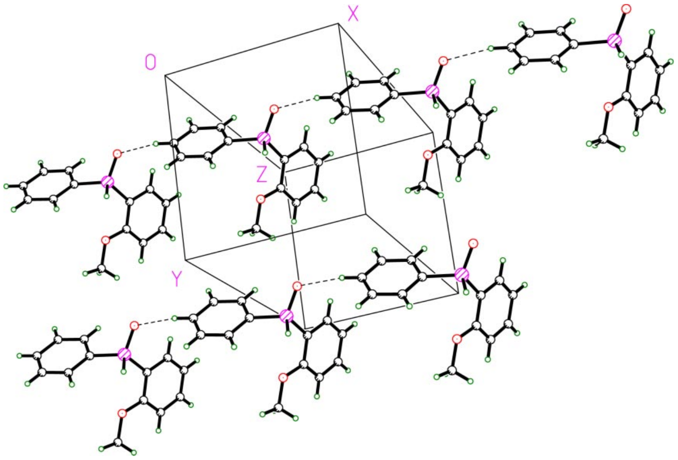

Figure 3
Part of the molecular packing of the title compound, showing the intermolecular hydrogen bonds creating a chain structure along the *a* axis. Hydrogen bonds are indicated by dashed lines.

Experimental

The title compound was synthesized according to previously published procedures and its physical and spectral properties were in full agreement with the literature data (Maffei & Buono, 1988; Emmick & Letsinger, 1968). Crystals were obtained by crystallization from benzene.

Crystal data

$C_{13}H_{13}O_2P$
$M_r = 232.20$
Monoclinic, $P2_1/c$
$a = 8.576$ (3) Å
$b = 8.804$ (4) Å
$c = 15.921$ (6) Å
$\beta = 94.69$ (3)°
$V = 1198.1$ (8) Å^3
$Z = 4$

$D_x = 1.287$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 99 reflections
$\theta = 18.7$–$28.9°$
$\mu = 1.89$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.55 × 0.23 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1999)
$T_{min} = 0.421$, $T_{max} = 0.809$
5076 measured reflections
2465 independent reflections
2175 reflections with $I > 2\sigma(I)$

$R_{int} = 0.029$
$\theta_{max} = 75.1°$
$h = 0 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$
3 standard reflections frequency: 60 min intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.122$
$S = 1.09$
2465 reflections
151 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.2516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0052 (7)

Table 1
Selected geometric parameters (Å, °).

P1—O1	1.4787 (16)	P1—C8	1.7895 (18)
P1—C1	1.789 (2)	P1—H1P	1.330 (18)
O1—P1—C1	112.06 (9)	O1—P1—H1P	115.0 (7)
O1—P1—C8	113.17 (9)	C1—P1—H1P	102.9 (8)
C1—P1—C8	107.72 (8)	C8—P1—H1P	105.2 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.93	2.48	3.371 (3)	160

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

All H atoms, except that bonded to the P atom, were placed in calculated positions and treated as riding on the adjacent C atom. The H atom bonded to the P atom was located in a difference Fourier synthesis and refined isotropically. The methyl group was allowed to rotate about its local threefold axis.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/*PC (Sheldrick, 1990*b*) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 1990).

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