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Tris(pentafluorophenyl)phosphine oxide

Brian K. Nicholson* and Susanna E. Thwaite

Chemistry Department, University of Waikato, Private Bag 3105, Hamilton, New Zealand

Correspondence e-mail: b. nicholson@waikato.ac.nz

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Key indicators

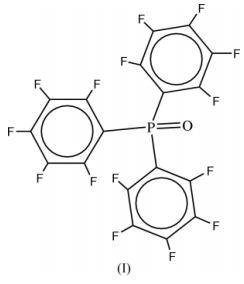
Single-crystal X-ray study
T = 83 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.096
Data-to-parameter ratio = 11.6

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

Crystals of the title compound, $(C_6F_5)_3P{=}O$ or $C_{18}H_{15}OP$, have two independent molecules in the asymmetric unit, with average P=O and P—C bond lengths of 1.467 (2) and 1.817 (2) Å, respectively, and an average O=P—C angle of 112.9 (1)°.

Comment

Crystals of the title compound, (I), contain two molecules of $(C_6F_5)_3P{=}O$ in the asymmetric unit, but these are not significantly different. Average structural features include a P=O bond length of 1.467 (2) Å, a P—C length of 1.817 (2) Å, a C—P—C angle of 103.5 (1)° and an O=P—C angle of 112.9 (1)°. These compare with results reported for $(C_6F_5)_3P$ (Karipides & Cosio, 1989), which has longer P—C bonds (1.831 Å) but essentially identical C—P—C angles (103.3°). In $(C_6H_5)_3P{=}O$ (Thomas & Hamor, 1993; Spek, 1987; Brock *et al.*, 1985), the P=O bond is longer (1.492 Å), the P—C bonds shorter (1.803 Å), and the C—P—C bonds more open (106.4°). This can be rationalized by Bent's rule (Bent, 1961*a*,*b*), the electron-withdrawing $-C_6F_5$ groups concentrating relatively more *p*-orbital character in the P—C bonds, compared with the $-C_6H_5$ ones.



(I)

Experimental

Crystals of $(C_6F_5)_3P{=}O$ were isolated in low yield from a reaction involving $(C_6F_5)_3PAuCl$ and Ag_2O. Better syntheses are available (Emeleus & Miller, 1966). Crystals were obtained from a cooled ether–pentane solution.

Crystal data

$C_{18}F_{15}OP$
M_r = 548.15
Monoclinic, $P2_1/c$
a = 9.562 (1) Å
b = 20.489 (1) Å
c = 18.303 (1) Å
β = 95.95 (1)°
V = 3566.5 (5) Å^3
Z = 8
D_x = 2.042 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7905 reflections
θ = 2–26°
μ = 0.32 mm^{-1}
T = 83 (2) K
Needle, white
0.46 × 0.18 × 0.16 mm

Data collection

Siemens SMART CCD diffractometer	7300 independent reflections
	5418 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.034$
Absorption correction: multi-scan (Blessing, 1995)	$\theta_{max} = 26.4°$
	$h = -11 \rightarrow 11$
$T_{min} = 0.867$, $T_{max} = 0.951$	$k = 0 \rightarrow 25$
14186 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 2.4099P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	
$wR(F^2) = 0.096$	
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
7300 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
631 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Version 1.64; Farrugia, 1999).

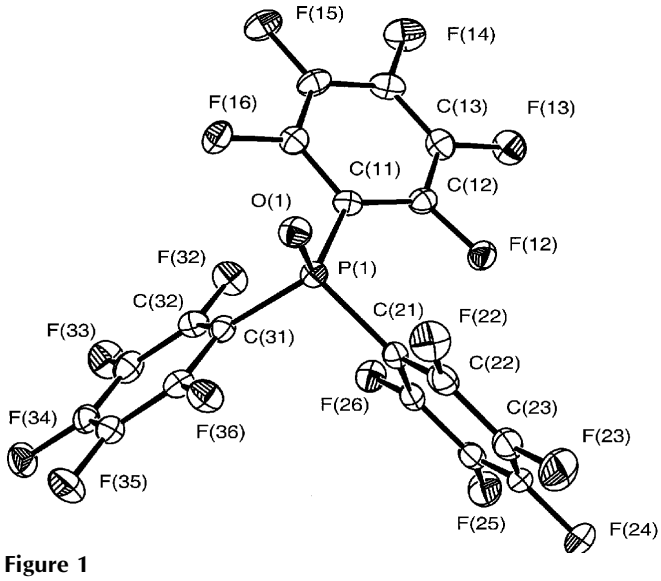


Figure 1
The structure of one of the independent molecules of (I), with displacement ellipsoids drawn at the 50% probability level (Farrugia, 1997).

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