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2-Phenylisophosphindoline-1,3-dione

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The title compound, $C_{14}H_9O_2P$, displays a near-planar isophosphindoline-1,3-dione skeleton with slightly displaced P and O atoms. Weak C—H···O hydrogen bonding in the crystal structure results in a three-dimensional network.

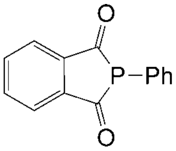
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.091
Data-to-parameter ratio = 10.4

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

Comment

The title compound, (I), is a rare example of a crystallographically characterized dicarbonylphosphine. The only related compound whose crystal structure has been reported is bis(2,2-dimethylpropionyl)phenylphosphine, $[{}^t\text{BuC(O)}]_2$P–Ph, (II) (Becker *et al.*, 1985).



(I)

The isophosphindoline-1,3-dione skeleton in (I) is almost planar, in contrast to compound (II), where rotation around the P—C bonds results in an almost orthogonal orientation of the two carbonyl groups with an O—C···C—O angle of 73.49° [no standard uncertainty available (Becker *et al.*, 1985)]. In compound (I), the P and O atoms deviate by −0.388 (2), 0.209 (3) and 0.204 (2) Å from the C1/C3/C3*A*/C7*A* plane, most likely because of the steric demand of the phenyl group. In the absence of the phenyl group, as is the case in the isophosphindolyl-1,3-dione anion (Liotta *et al.*, 1984), planarity of the same molecular fragment is observed. The geometry at the P atom is trigonal–pyramidal in compound (I), indicating a stereochemically active electron pair. This is in contrast to the nitrogen analogue of (I) (Magomedova *et al.*, 1981), where the N atom is in a trigonal–planar environment. In the crystal lattice, 2-phenylisophosphindoline-1,3-dione

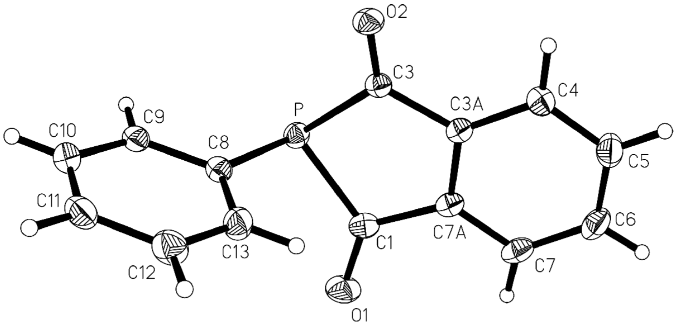


Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level.

employs both carbonyl O atoms for C—H···O hydrogen bonding (see Table 1), resulting in a three-dimensional network.

Experimental

The title compound was prepared according to a published procedure (Fenske *et al.*, 1976).

Crystal data

$C_{14}H_9O_2P$
$M_r = 240.18$
Monoclinic, $P2_1/n$
$a = 9.4273\ (15)$ Å
$b = 14.479\ (2)$ Å
$c = 9.4762\ (15)$ Å
$\beta = 117.662\ (2)°$
$V = 1145.7\ (3)$ Å^3
$Z = 4$
$D_x = 1.393$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3469 reflections
$\theta = 2.5$–$25.9°$
$\mu = 0.22$ mm^{-1}
$T = 173\ (2)$ K
Plate, yellow
0.40 × 0.30 × 0.05 mm

Data collection

Bruker SMART 1000/*P*4 diffractometer
ω and φ scans
Absorption correction: none
5722 measured reflections
1970 independent reflections
1736 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 25.0°$
$h = -11 \rightarrow 10$
$k = -16 \rightarrow 17$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.091$
$S = 1.07$
1970 reflections
190 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.297P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2$^{\rm i}$	0.96 (2)	2.59 (2)	3.517 (2)	163.5 (14)
C7—H7···O2$^{\rm ii}$	0.91 (2)	2.37 (2)	3.201 (2)	150.5 (17)
C10—H10···O1$^{\rm iii}$	0.90 (2)	2.53 (2)	3.368 (2)	155.5 (16)

Symmetry codes: (i) $1 - x, -y, -z$; (ii) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iii) $\frac{5}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$.

H atoms were found in difference Fourier maps and refined with isotropic displacement parameters. The final C—H distances are in the range 0.91 (2)–0.96 (2) Å.

Data collection: *SMART* (Bruker, 1997–1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997–1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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