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1,3-Bis(5,5-dimethyl-2-oxo-1,3,2-dioxaphosphinan-2-yloxy)benzene

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Key indicators

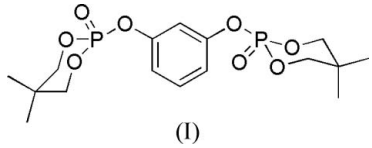
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.090
Data-to-parameter ratio = 14.1

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

In the title compound, $C_{16}H_{24}O_8P_2$, the P atoms adopt slightly distorted tetrahedral geometries as components of six-membered rings adopting chair conformations.

Comment

The title compound, (I), is a phosphorus-containing flame retardant (Horst, 1998). As part of our studies of these materials, compound (I) was synthesized and its crystal structure is reported here.



(I)

In the molecular structure of (I) (Fig. 1) the heterocyclic rings adopt chair conformations. The P atoms adopt slightly distorted tetrahedral configurations, with O—P—O bond angles ranging between 101.11 (12) and 115.28 (14)°.

Experimental

The title compound was prepared according to a previously published method (Horst, 1998) from resorcinol; crystals of (I) were obtained from methanol.

Crystal data

$C_{16}H_{24}O_8P_2$
M_r = 406.29
Monoclinic, $C2$
a = 22.646 (7) Å
b = 6.3642 (19) Å
c = 13.795 (4) Å
β = 97.960 (5)°
V = 1969.0 (10) Å^3
Z = 4
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 294 (2) K
Block, colorless
0.30 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.926, T_{max} = 0.955
5559 measured reflections
3370 independent reflections
2440 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.090
S = 1.04
3370 reflections
239 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.0335P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1154 Friedel pairs
Flack parameter: 0.05 (10)

The H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

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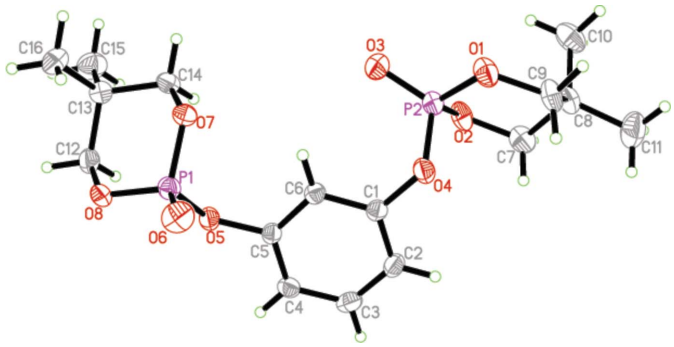

Figure 1
View of the molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms).