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Structure of (*E*)-[(2-Isopropylphenyl)(phenyl)methylene](mesityl)phosphine

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Abstract. $C_{25}H_{27}P$, $M_r = 358{\cdot}46$, triclinic, $P\bar{1}$, $a = 7{\cdot}991\,(1)$, $b = 9{\cdot}155\,(1)$, $c = 14{\cdot}937\,(4)$ Å, $\alpha = 102{\cdot}98\,(1)$, $\beta = 90{\cdot}20\,(2)$, $\gamma = 100{\cdot}63\,(1)°$, $V = 1045{\cdot}4\,(3)$ Å^3, $Z = 2$, $D_x = 1{\cdot}139$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 1{\cdot}3$ cm^{-1}, $F(000) = 384$, $T = 295$ K, $R = 0{\cdot}0487$ for 4106 observed reflections with $I > 2\sigma(I)$. The central phosphaalkene part of the molecule is planar within 0·027 (5) Å. The angles between this plane and the attached phenyl rings are 47·91 (8), 66·64 (8) and 69·49 (9)° respectively. The P=C distance is 1·682 (2) Å.

Experimental. An *E*-isomer crystal was obtained by crystallization from a 2:1 *E*/*Z*-isomer mixture in pentane. Colourless rhombus-shaped crystal 0·88 × 0·63 × 0·33 mm mounted under nitrogen in a Lindemann-glass capillary. Unit-cell parameters and their e.s.d.'s derived from a least-squares treatment of 17 reflections ($15{\cdot}4 < \theta < 18{\cdot}6°$). 5033 intensity data were collected within one half of the reflection sphere ($0 \le h \le 10$; $-12 \le k \le 11$; $-19 \le l \le 19$; $1{\cdot}40 < \theta < 28{\cdot}0°$) on an Enraf–Nonius CAD-4*F* diffractometer, Zr-filtered Mo $K\alpha$ radiation, $\omega/2\theta$ scan mode with $\Delta\omega = (0{\cdot}75 + 0{\cdot}35\tan\theta)°$. Three reference reflections ($\bar{2}\bar{2}\bar{7}$, $4\bar{1}\bar{2}$, $2\bar{3}\bar{3}$) measured every hour of X-ray exposure time showed a consistent linear increase of 5% in intensity during the 114 h of X-ray exposure time. Intensity data were corrected for this effect and for Lp. No absorption correction. Standard deviations of the intensities as obtained by counting statistics were increased according to an analysis of the excess variance of the reference reflections: $\sigma^2(I) = \sigma^2_{cs}(I) + (0{\cdot}0071I)^2$ resulting in 4106 observed reflections with $I > 2\sigma(I)$ (McCandlish, Stout & Andrews, 1975). Structure solved by direct methods (*SHELXS*86; Sheldrick, 1986), the solution with the best figure of merit revealed all non-H atoms. All non-H atoms were refined with anisotropic thermal parameters by full-matrix least-squares techniques, minimizing $\sum w\Delta F^2$, using the *SHELX*76 package (Sheldrick, 1976). H atoms were introduced on calculated positions (C—H = 0·98 Å)

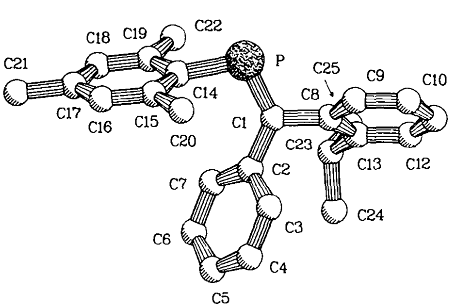

Fig. 1. *PLUTO* (*EUCLID* version) drawing of the title compound as viewed perpendicular to the phosphaalkene plane. H atoms were omitted for clarity.

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Table 1. *Positional and equivalent isotropic thermal parameters for the non*-H *atoms with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$(Å^2)
P	0·90218 (6)	0·90985 (6)	0·19183 (3)	0·0480 (2)
C(1)	0·7644 (2)	0·9011 (2)	0·2762 (1)	0·0399 (5)
C(2)	0·6298 (2)	0·9922 (2)	0·3029 (1)	0·0378 (4)
C(3)	0·6149 (2)	1·0572 (2)	0·3961 (1)	0·0465 (5)
C(4)	0·4884 (3)	1·1395 (2)	0·4236 (1)	0·0543 (6)
C(5)	0·3719 (3)	1·1553 (2)	0·3599 (1)	0·0555 (6)
C(6)	0·3839 (2)	1·0914 (2)	0·2679 (1)	0·0513 (6)
C(7)	0·5133 (2)	1·0122 (2)	0·2396 (1)	0·0432 (5)
C(8)	0·7808 (2)	0·7890 (2)	0·3336 (1)	0·0425 (5)
C(9)	0·9256 (3)	0·8122 (2)	0·3906 (1)	0·0565 (6)
C(10)	0·9415 (3)	0·7127 (3)	0·4470 (2)	0·0640 (6)
C(11)	0·8126 (3)	0·5909 (2)	0·4462 (1)	0·0639 (8)
C(12)	0·6704 (3)	0·5656 (2)	0·3892 (1)	0·0590 (6)
C(13)	0·6495 (2)	0·6623 (2)	0·3314 (1)	0·0450 (5)
C(14)	0·8558 (2)	1·0595 (2)	0·1372 (1)	0·0432 (5)
C(15)	0·8962 (2)	1·2151 (2)	0·1799 (1)	0·0469 (6)
C(16)	0·8685 (3)	1·3214 (2)	0·1305 (2)	0·0601 (6)
C(17)	0·8004 (3)	1·2773 (3)	0·0410 (2)	0·0659 (6)
C(18)	0·7629 (3)	1·1246 (3)	0·0001 (1)	0·0626 (8)
C(19)	0·7891 (2)	1·0141 (2)	0·0454 (1)	0·0517 (6)
C(20)	0·9682 (3)	1·2717 (2)	0·2771 (1)	0·0620 (6)
C(21)	0·7666 (4)	1·3940 (4)	−0·0112 (2)	0·105 (1)
C(22)	0·7437 (3)	0·8494 (3)	−0·0033 (2)	0·0699 (8)
C(23)	0·4905 (2)	0·6297 (2)	0·2682 (1)	0·0509 (6)
C(24)	0·3337 (3)	0·6598 (3)	0·3213 (2)	0·082 (1)
C(25)	0·4575 (4)	0·4685 (3)	0·2076 (2)	0·083 (1)

Table 2. *Bond distances* (Å) *and bond angles* (°) *for the non*-H *atoms with e.s.d.'s in parentheses*

P—C(1)	1·682 (2)	C(11)—C(12)	1·370 (3)
P—C(14)	1·835 (2)	C(12)—C(13)	1·398 (2)
C(1)—C(2)	1·482 (2)	C(13)—C(23)	1·523 (2)
C(1)—C(8)	1·500 (2)	C(14)—C(15)	1·400 (3)
C(2)—C(3)	1·401 (2)	C(14)—C(19)	1·412 (2)
C(2)—C(7)	1·389 (2)	C(15)—C(16)	1·393 (3)
C(3)—C(4)	1·380 (3)	C(15)—C(20)	1·501 (2)
C(4)—C(5)	1·378 (3)	C(16)—C(17)	1·385 (4)
C(5)—C(6)	1·379 (2)	C(17)—C(18)	1·370 (4)
C(6)—C(7)	1·384 (2)	C(17)—C(21)	1·517 (4)
C(8)—C(9)	1·389 (3)	C(18)—C(19)	1·382 (3)
C(8)—C(13)	1·407 (3)	C(19)—C(22)	1·496 (3)
C(9)—C(10)	1·394 (3)	C(23)—C(24)	1·520 (3)
C(10)—C(11)	1·369 (3)	C(23)—C(25)	1·524 (3)
C(1)—P—C(14)	106·20 (8)	C(8)—C(13)—C(23)	121·8 (2)
P—C(1)—C(2)	128·5 (1)	C(12)—C(13)—C(23)	120·7 (2)
P—C(1)—C(8)	116·4 (1)	P—C(14)—C(15)	122·8 (1)
C(2)—C(1)—C(8)	115·1 (1)	P—C(14)—C(19)	117·5 (1)
C(1)—C(2)—C(3)	119·0 (1)	C(15)—C(14)—C(19)	119·5 (2)
C(1)—C(2)—C(7)	122·8 (1)	C(14)—C(15)—C(16)	118·9 (2)
C(3)—C(2)—C(7)	118·1 (2)	C(14)—C(15)—C(20)	122·4 (2)
C(2)—C(3)—C(4)	120·6 (1)	C(16)—C(15)—C(20)	118·7 (2)
C(3)—C(4)—C(5)	120·4 (1)	C(15)—C(16)—C(17)	121·8 (2)
C(4)—C(5)—C(6)	119·9 (2)	C(16)—C(17)—C(18)	118·4 (2)
C(5)—C(6)—C(7)	120·0 (2)	C(16)—C(17)—C(21)	121·3 (2)
C(2)—C(7)—C(6)	121·0 (1)	C(18)—C(17)—C(21)	120·2 (2)
C(1)—C(8)—C(9)	119·6 (2)	C(17)—C(18)—C(19)	122·3 (2)
C(1)—C(8)—C(13)	120·6 (1)	C(14)—C(19)—C(18)	119·1 (2)
C(9)—C(8)—C(13)	119·8 (2)	C(14)—C(19)—C(22)	121·6 (2)
C(8)—C(9)—C(10)	120·8 (2)	C(18)—C(19)—C(22)	119·3 (2)
C(9)—C(10)—C(11)	119·5 (2)	C(13)—C(23)—C(24)	112·0 (2)
C(10)—C(11)—C(12)	120·2 (2)	C(13)—C(23)—C(25)	112·6 (2)
C(11)—C(12)—C(13)	122·1 (2)	C(24)—C(23)—C(25)	110·4 (2)
C(8)—C(13)—C(12)	117·5 (2)		

and refined riding on their corresponding C atoms, with one common isotropic thermal parameter. At the final stage of the refinement, weights were introduced resulting in $R = 0{\cdot}0487$, $wR = 0{\cdot}0697$, $S = 0{\cdot}40$, $w = 1/[\sigma^2(F) + 0{\cdot}00037F^2]$, $(\Delta/\sigma)_{\rm av} = 0{\cdot}0915$, $(\Delta/\sigma)_{\rm max} = 0{\cdot}38$ for 4106 reflections and 251 parameters. A final difference Fourier synthesis revealed residual densities between 0·31 and −0·26 e Å^{-3}.

Scattering factors were taken from Cromer & Mann (1968). All calculations were carried out on a MicroVAX II with the programs mentioned above and with the *EUCLID* package (Spek, 1982; molecular geometry and illustrations). A view of the molecule with the adopted atom numbering is shown in Fig. 1. Final atomic parameters are given in Table 1,* bond distances and angles in Table 2.

Related literature. For the preparation of the title compound, a discussion of the results and a comparison with two similar compounds see van der Does, Bickelhaupt, Smeets & Spek (1987). The structures of the related non-isopropyl compound and its nitrogen equivalent are discussed in van der Knaap, Klebach, Visser, Bickelhaupt, Ros, Baerends, Stam & Konijn (1984) and Bokkers, Kroon & Spek (1979) respectively.

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and geometrical data involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44019 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.