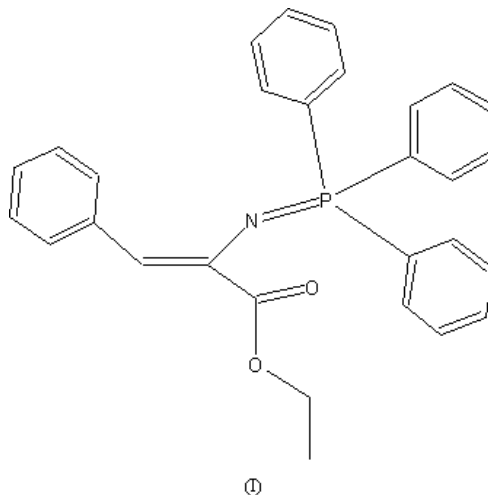


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xiaobhuang@hotmail.com**Key indicators**Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.054
 wR factor = 0.131
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(Z)-Ethyl 3-phenyl-2-[(triphenylphosphoranyl-
idene)amino]prop-2-enoate**

The title compound, $\text{C}_{29}\text{H}_{26}\text{N}_2\text{OP}$, containing four planar ring systems, exists in the *Z* form. The short $\text{C}\cdots\text{O}$ [2.711 (3) Å] and $\text{C}\cdots\text{N}$ [2.961 (3) and 2.997 (3) Å] intramolecular contacts may indicate the presence of weak intramolecular hydrogen bonds.

Comment

Recently, iminophosphoranes have received increased attention as useful building blocks for the synthesis of nitrogen-containing heterocycles (Molina *et al.*, 1994). The title compound, (I), is an intermediate in the preparation of imidazolinone, which exhibits various biological properties, for example, fungicidal and herbicidal activities (Yang *et al.*, 2004). Some interesting crystal structures involving iminophosphorane groups have been published (Batsanov *et al.*, 1997).



Compound (I) exists in the *Z*-isomeric form, as two groups of higher priority are on the same side of the exocyclic $\text{C}=\text{C}$ double bond. The molecule of (I) contains four essentially planar phenyl rings, three of which, C1–C6 (A), C7–C12 (B) and C13–C18 (C), belong to the triphenylphosphine group. The dihedral angles *A/B*, *A/C* and *B/C* are 79.7 (1), 89.7 (1) and 54.7 (1)°, respectively.

The short $\text{C}\cdots\text{O}$ and $\text{C}\cdots\text{N}$ intramolecular contacts (Table 1) may indicate the presence of weak intramolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds.

Experimental

The title compound was readily synthesized in 82% yield by the Staudinger reaction of ethyl β -azidoacetate with triphenylphosphine at room temperature (Molina *et al.*, 1993). Single crystals of (I) suitable

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for X-ray data collection were obtained by slow evaporation of a solution in ethanol (m.p. 435–436 K). Spectroscopic analysis: IR (KBr, ν , cm^{-1}): 2923, 1668, 1587, 1410, 1232; ^1H NMR (chloroform-*d*, δ , p.p.m.): 8.15–7.25 (*m*, 20H), 6.72 (*d*, 2H, $J = 7.0$ Hz), 3.85 (*q*, 2H, s , $J = 7.1$ Hz), 0.99 (*t*, 3H, $J = 7.1$ Hz); ^{13}C NMR (chloroform-*d*, δ , p.p.m.): 167.87, 138.23, 136.41, 133.65, 132.46, 132.33, 130.89, 129.34, 128.00, 127.67, 125.62, 116.41, 116.15, 77.96, 76.53, 60.65, 13.99; ^{31}P NMR (chloroform-*d*, δ , p.p.m.): 7.44 (*s*).

Crystal data

$\text{C}_{29}\text{H}_{26}\text{NO}_2\text{P}$	$D_x = 1.220 \text{ Mg m}^{-3}$
$M_r = 451.48$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3745 reflections
$a = 10.1918$ (9) Å	$\theta = 2.4\text{--}24.8^\circ$
$b = 17.7185$ (16) Å	$\mu = 0.14 \text{ mm}^{-1}$
$c = 14.1563$ (13) Å	$T = 298$ (2) K
$\beta = 106.000$ (2)°	Block, colourless
$V = 2457.4$ (4) Å ³	$0.35 \times 0.28 \times 0.21 \text{ mm}$
$Z = 4$	

Data collection

Bruker APEX area-detector diffractometer	4440 independent reflections
φ and ω scans	3764 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.025$
$T_{\text{min}} = 0.944$, $T_{\text{max}} = 0.972$	$\theta_{\text{max}} = 25.3^\circ$
12 947 measured reflections	$h = -12 \rightarrow 9$
	$k = -17 \rightarrow 21$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.6164P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
4440 reflections	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$
299 parameters	Extinction correction: none
H-atom parameters constrained	

Table 1

Intramolecular contacts (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
C1–H1 \cdots N1	0.93	2.61	2.997 (3)	106
C23–H23 \cdots O2	0.93	2.29	2.711 (3)	107
C29–H29 \cdots N1	0.93	2.34	2.961 (3)	124

H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of $Csp^2\text{--}H = 0.93$ Å, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$, or $Csp^3\text{--}H = 0.96$ Å, with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve

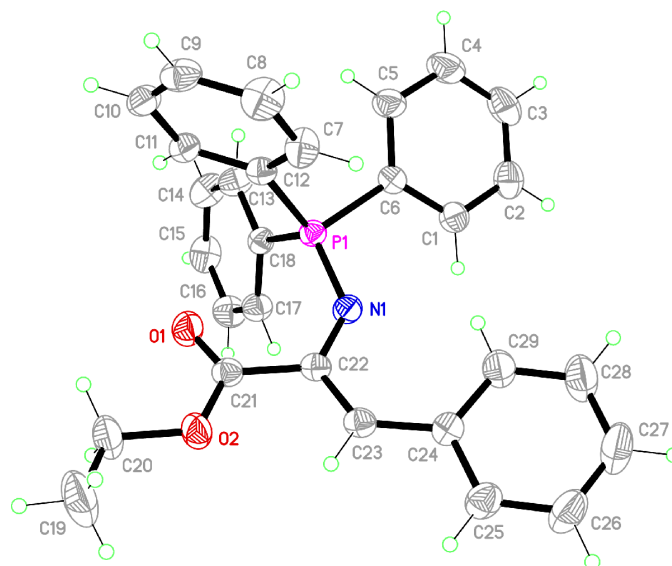


Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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