Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

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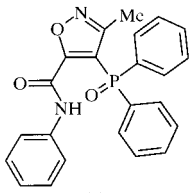
Received 11 January 2000
Accepted 18 January 2000

Data validation number: IUC0000020

The title compound, $C_{23}H_{19}N_2O_3P$, was prepared by the reaction of ethynyldiphenylphosphine oxide with phenyl isocyanate, triethylamine and nitoethane in benzene. The molecular structure is stabilized by an intramolecular N—H···O hydrogen bond.

Comment

Ethynyldiphenylphosphine oxide (Charrier *et al.*, 1966) was treated by the method of Mukaiyama & Hoshino (1960) with phenyl isocyanate, triethylamine and nitroethane in benzene to give 4-(diphenylphosphinoyl)-3-methylisoxazole and 5-(diphenylphosphinoyl)-3-methylisoxazole in a 1:1 ratio. The title compound, (I), was formed as a by-product in 16% yield.



(I)

Experimental

The title compound was obtained in 16% yield from the reaction of ethynyldiphenylphosphine oxide with phenyl isocyanate, triethylamine and nitroethane in benzene (Charrier *et al.*, 1966; Mukaiyama & Hoshino, 1960). The solvent was removed and the residue chromatographed on a silica-gel column with ethyl acetate as eluent. Colourless crystals were grown by slow evaporation from the ethyl acetate solution at room temperature, m.p. 467–468 K.

Crystal data

$C_{23}H_{19}N_2O_3P$	$Z = 2$
$M_r = 402.37$	$D_x = 1.328$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.4055$ (2) Å	Cell parameters from 11324 reflections
$b = 10.3008$ (4) Å	$\theta = 3.43$–$25.02°$
$c = 13.6543$ (5) Å	$\mu = 0.164$ mm^{-1}
$\alpha = 79.896$ (1)°	$T = 291$ (1) K
$\beta = 79.283$ (2)°	Block, colourless
$\gamma = 85.338$ (2)°	0.30 × 0.20 × 0.20 mm
$V = 1006.27$ (6) Å^3	

Data collection

Nonius KappaCCD diffractometer	2477 reflections with $I > 2\sigma(I)$
360 frames *via* ω-rotation ($\Delta\omega = 1°$) at different θ values and two times 20 s per frame	$R_{int} = 0.017$
	$\theta_{max} = 25.02°$
	$h = -7 \rightarrow 7$
Absorption correction: none	$k = -12 \rightarrow 12$
11 324 measured reflections	$l = -15 \rightarrow 16$
3308 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.998$	$\Delta\rho_{max} = 0.180$ e Å^{-3}
3308 reflections	$\Delta\rho_{min} = -0.247$ e Å^{-3}
263 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H6···O2	0.86	1.87	2.726 (2)	172

Crystal decay was monitored by repeating the initial frames at the end of data collection. Analysing the duplicate reflections there were no indications for any decay. H atoms were placed geometrically and refined with a riding model (including free rotation about C—C) with U_{iso} constrained to be $1.5U_{eq}$ of the carrier atom.

Data collection: Nonius KappaCCD software; cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997) and *PARST*95 (Nardelli, 1995).

We thank the Fonds der Chemischen Industrie for financial support.

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