

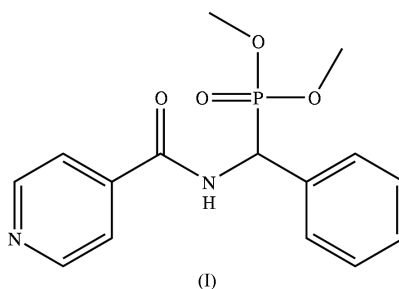
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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.060  
 $wR$  factor = 0.139  
Data-to-parameter ratio = 13.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Dimethyl [phenyl(pyridine-4-carboxamido)-  
methyl]phosphonateIn the crystal structure, the title compound,  $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_4\text{P}$ , exists as a centrosymmetric dimer containing  $\text{N}-\text{H}\cdots\text{O}=\text{P}$  hydrogen bonds. The amino N atom interacts with the doubly bonded phosphoryl O atom.Received 5 January 2005  
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## Comment

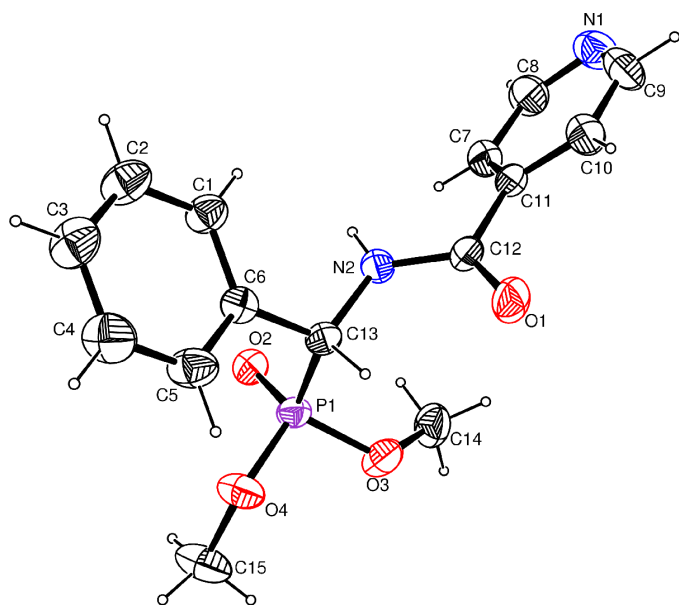
The title compound, (I), was synthesized in order to study its cytotoxicity against the KB cancer cell line. The amidophosphonic acid derivative was found to be moderately cytotoxic with an  $\text{IC}_{50}$  value of  $114 \mu\text{g ml}^{-1}$ . The adjacent bonds  $\text{P1}-\text{O3}$  and  $\text{P1}-\text{O4}$  [mean  $1.560(2)$  Å] are similar to that in ammonium dimethylphosphate [ $1.559(7)$  Å; Giarda *et al.*, 1973]. The amide unit is involved in hydrogen-bonding interactions with the phosphoryl O atom [ $\text{N}\cdots\text{O} = 2.949(3)$  Å] to give centrosymmetric dimers (Fig. 2).

## Experimental

The hydrochloride of dialkyl  $\alpha$ -aminobenzylphosphonate was prepared according to the literature procedure of Takahashi *et al.* (1994). Triphenylphosphine (3.93 g, 15 mmol) and hexachloroethane (3.58 g, 15 mmol) in dried 1,2-dichloroethane (15 ml) were reacted for 1 h in an ice bath. The resulting solution was added dropwise to a mixture of the hydrochloride of dialkyl  $\alpha$ -aminobenzylphosphonate (2.79 g, 10 mmol) and isonicotinic acid (1.23 g, 10 mmol) in 1,2-dichloroethane (90 ml) and triethylamine (4 ml). After completion of the reaction, the solvent was removed to give the crude product, which was purified by recrystallization from hot ethanol. Analysis calculated for  $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_4\text{P}$ : C 53.26, H 5.66, N 8.28%; found C 53.55, H 5.54, N 8.09%.

## Crystal data

 $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_4\text{P}$   
 $M_r = 320.28$   
Monoclinic,  $P2_1/n$   
 $a = 10.748(3)$  Å  
 $b = 14.417(4)$  Å  
 $c = 10.920(3)$  Å  
 $\beta = 111.280(4)^\circ$   
 $V = 1576.7(8)$  Å<sup>3</sup>  
 $Z = 4$  $D_x = 1.349$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 3217  
reflections  
 $\theta = 2.5-27.3^\circ$   
 $\mu = 0.19$  mm<sup>-1</sup>  
 $T = 293(2)$  K  
Chunk, colorless  
 $0.21 \times 0.19 \times 0.15$  mm



**Figure 1**  
ORTEP-3 plot (Farrugia, 1997) of (1), with displacement ellipsoids drawn at the 30% probability level. H atoms are drawn as spheres of arbitrary radii.

#### Data collection

Bruker SMART APEX area-detector diffractometer	2753 independent reflections
$\varphi$ and $\omega$ scans	2514 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$R_{\text{int}} = 0.023$
$T_{\text{min}} = 0.93$ , $T_{\text{max}} = 0.97$	$\theta_{\text{max}} = 25.0^\circ$
7824 measured reflections	$h = -11 \rightarrow 12$
	$k = -17 \rightarrow 16$
	$l = -12 \rightarrow 12$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.963P]$
$R[F^2 > 2\sigma(F^2)] = 0.060$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.139$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{\AA}^{-3}$
2753 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$
201 parameters	
H-atom parameters constrained	

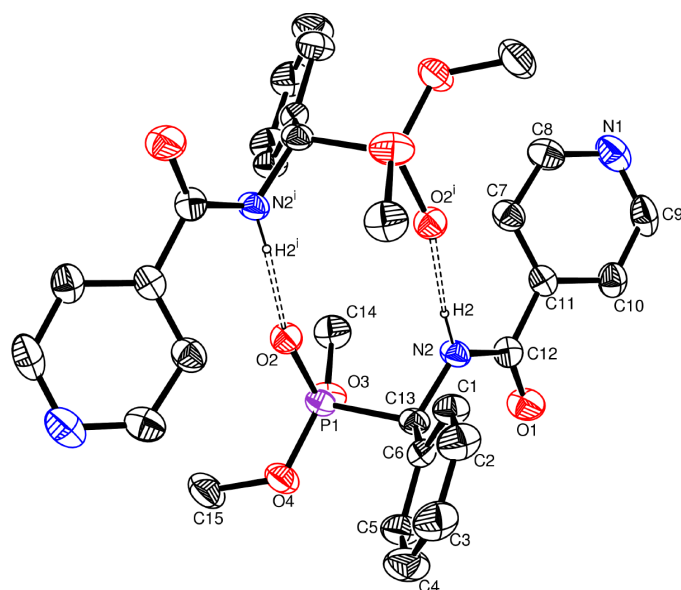
**Table 1**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2\cdots O2^i$	0.86	2.10	2.949 (3)	167

Symmetry code: (i)  $1 - x, -y, 1 - z$ .

The H atoms were positioned geometrically ( $C-H = 0.93, 0.98$  or  $0.96 \text{ \AA}$  for phenyl, tertiary or methyl H atoms, respectively, and  $N-$



**Figure 2**  
ORTEP-3 plot (Farrugia, 1997) showing the formation of a dimer through  $N-H\cdots O$  hydrogen-bonding interactions (dashed lines). [Symmetry code: (i)  $1 - x, -y, 1 - z$ .]

$H = 0.86 \text{ \AA}$ ) and were included in the refinement in the riding-model approximation. The displacement parameters of the methyl H atoms were set at  $1.5U_{\text{eq}}$  of their parent atoms, while those of the other H atoms were set at  $1.2U_{\text{eq}}(C,N)$ .

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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