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## Key indicators

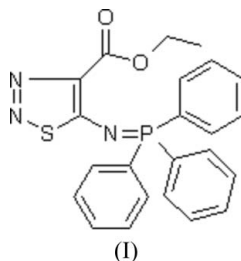
Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
Disorder in main residue  
 $R$  factor = 0.048  
 $wR$  factor = 0.128  
Data-to-parameter ratio = 17.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Ethyl 5-(triphenylphosphoranylidene)-1,2,3-thiadiazole-4-carboxylate

In the title compound,  $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_2\text{PS}$ , the molecules form a supramolecular structure *via* intermolecular  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds.Received 14 June 2006  
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## Comment

Synthetic heterocycles attract widespread interest as herbicides, insecticides, dyes, organic conductors, and drugs (Ding *et al.*, 2004). Over the past 20 years, aza-Wittig reactions of iminophosphoranes have received increased attention as the materials are obtained easily, the conditions are moderate and there is good selectivity in the synthesis of nitrogen heterocyclic compounds (Kurosawa *et al.*, 2003). We have recently focused on the synthesis of fused heterocyclic systems containing the pyrimidine ring using aza-Wittig reactions (Liu *et al.*, 2006). Iminophosphoranes are key intermediates, which with various isocyanates, involving subsequent reaction with secondary amines, can be converted into a wide range of pyrimidines at room temperature.

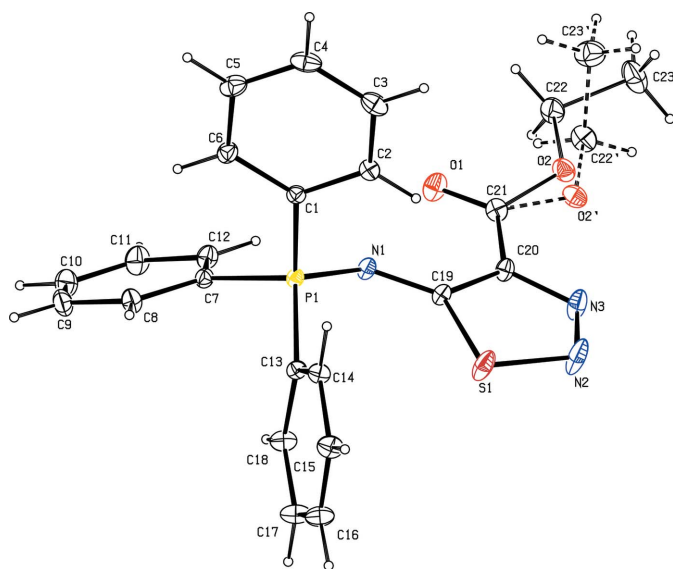


In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (atoms C1–C6), *B* (C7–C12), *C* (C13–C18) and *D* (S1/N2/N3/C19/C20) are, of course, planar and the dihedral angles between them are  $A/B = 69.53$  (4)°,  $A/C = 69.25$  (3)°,  $A/D = 86.34$  (3)°,  $B/C = 76.10$  (4)°,  $B/D = 36.87$  (5)° and  $C/D = 87.70$  (3)°. Ring *D* has a pseudo-mirror plane passing through atom C20 and the mid-point of the S1–N2 bond, as can be deduced from the torsion angles (Table 1).

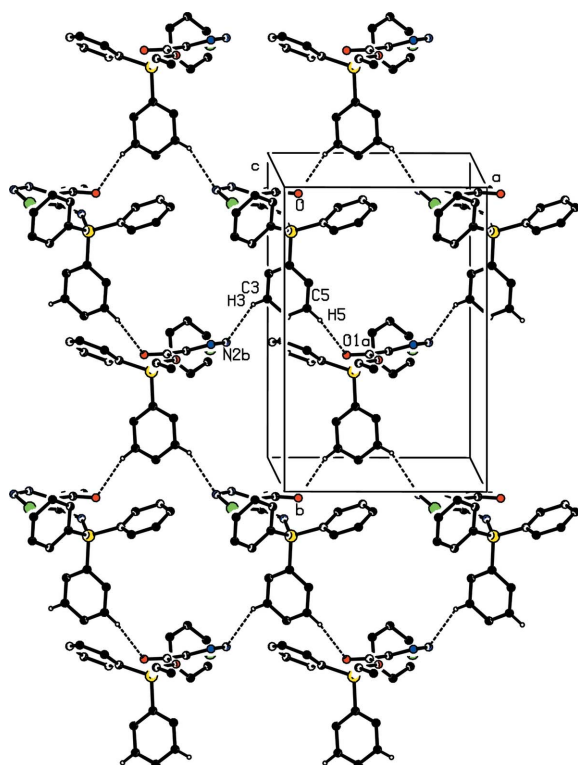
As can be seen from the packing diagram (Fig. 2), intermolecular  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds (Table 2) link the molecules, helping to stabilize the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

## Experimental

Triphenylphosphine (15 mmol), hexachloroethane (15 mmol) and triethylamine (30 mmol) were added to a solution of ethyl 5-amino-1,2,3-thiadiazole-4-carboxylate (5 mmol) in anhydrous acetonitrile



**Figure 1**  
The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Both disorder components are shown.



**Figure 2**  
A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted. The minor disorder component has been omitted. [Symmetry codes: (a)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (b)  $-x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ]

(15 ml). After the reaction mixture was allowed to stand for 5 h at room temperature, the solution was concentrated under reduced pressure and the residue was recrystallized from ethanol to give the title compound, (I). The product was recrystallized from ethanol-dichloromethane (1:2) at room temperature to give crystals suitable for X-ray analysis.

### Crystal data

$C_{23}H_{20}N_3O_2PS$   
 $M_r = 433.45$   
Monoclinic,  $P2_1/n$   
 $a = 10.4544$  (7) Å  
 $b = 15.8511$  (10) Å  
 $c = 13.2195$  (9) Å  
 $\beta = 94.377$  (1)°  
 $V = 2184.3$  (2) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.318$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.25$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
Block, colorless  
0.30 × 0.30 × 0.30 mm

### Data collection

Bruker SMART 4K CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.930$ ,  $T_{\max} = 0.930$

18972 measured reflections  
5188 independent reflections  
3901 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.045$   
 $\theta_{\max} = 28.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.128$   
 $S = 1.00$   
5188 reflections  
301 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0769P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.30$  e Å<sup>-3</sup>

**Table 1**

Selected torsion angles (°).

S1–C19–C20–N3	−0.7 (2)	N3–N2–S1–C19	0.1 (2)
S1–N2–N3–C20	−0.5 (3)	C20–C19–S1–N2	0.32 (16)
C19–C20–N3–N2	0.8 (3)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5–H5 <sup>i</sup> ⋯O1 <sup>i</sup>	0.93	2.53	3.285 (2)	138
C3–H3 <sup>ii</sup> ⋯N2 <sup>ii</sup>	0.93	2.61	3.441 (3)	149

Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $-x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$

When the crystal structure was solved, the ethoxy (O2–C22–C23) group was found to be disordered. During refinement the occupancies of disordered atoms were refined over two sites as 0.497 (11) and 0.503 (11). H atoms were positioned geometrically, with C–H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$ , where  $x = 1.5$  for methyl H and  $x = 1.2$  for other H atoms.

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: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Bruker, 2001).

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