Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*S*)-Diethyl {(4-fluorophenyl)[5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-ylamino]methyl}phosphonate

Rong Wan,* Feng Han, Jin-jun Zhang, Li-he Yin and Jin-tang Wang

Department of Applied Chemistry, College of Science, Nanjing University of Technology, No. 5 Xinmofan Road, Nanjing 210009, People's Republic of China
Correspondence e-mail: rwan01@jlonline.com

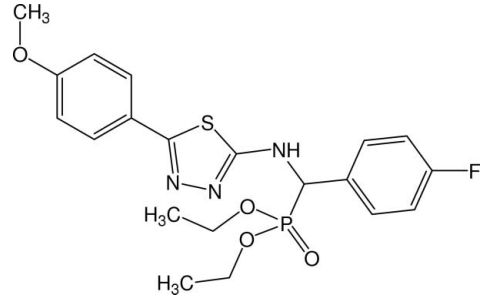
Received 27 August 2007; accepted 21 September 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.050; wR factor = 0.157; data-to-parameter ratio = 14.8.

In the molecule of the title compound, $C_{20}H_{23}FN_3O_4PS$, two methyl groups are disordered over two positions each, with site occupancy factors in the approximate ratio 2:1. The thiadiazole and benzene rings are planar; the thiadiazole ring is oriented with respect to the adjacent benzene ring at a dihedral angle of 7.54 (3)°, while the dihedral angle between the two benzene rings is 81.28 (3)°. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules, and a weak intramolecular C—H···S hydrogen bond is also present.

Related literature

For related literature, see: Nakagawa *et al.* (1996); Wang *et al.* (1999). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{23}FN_3O_4PS$
M_r = 451.44
Triclinic, $P\overline{1}$
a = 9.4140 (19) Å
b = 10.227 (2) Å
c = 12.923 (3) Å
α = 110.44 (3)°
β = 98.80 (3)°
γ = 100.58 (3)°
V = 1113.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.927, T_{max} = 0.951
4656 measured reflections
4374 independent reflections
3276 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.157
S = 0.82
4374 reflections
295 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.86	2.13	2.795 (5)	133
C19—H19A···S	0.93	2.73	3.142 (4)	108

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

The authors gratefully acknowledge Professor Hua-Qin Wang of the Analysis Center, Nanjing University, for providing the Enraf–Nonius CAD-4 diffractometer for this research project.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2321).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Nakagawa, Y., Nishimura, K., Izumi, K., Kinoshita, K., Kimura, T. & Kurihara, N. (1996). *J. Pestic. Sci.* **21**, 195–201.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, Y. G., Cao, L., Yan, J., Ye, W. F., Zhou, Q. C. & Lu, B. X. (1999). *Chem. J. Chin. Univ.* **20**, 1903–1905.

  doi:10.1107/S1600536807046521

supplementary materials

Acta Cryst. (2007). E**63**, o4158 [**doi:10.1107/S1600536807046521**]

(*S*)-Diethyl {(4-fluorophenyl)[5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-ylamino]methyl}phosphonate

R. Wan, F. Han, J. Zhang, L. Yin and J. Wang

Comment

1,3,4-Thiadiazole derivatives represent an interesting class of compounds possessing broad spectrum biological activities (Nakagawa *et al.*, 1996; Wang *et al.*, 1999). These compounds are known to exhibit diverse biological effects, such as insecticidal and fungicidal activities (Wang *et al.*, 1999). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C6—C11), B (S/N2/N3/C12/C13) and C (C14—C18) are, of course, planar and they are oriented at dihedral angles of A/B = 82.53 (3)°, A/C = 81.28 (3)° and B/C = 7.54 (3)°.

In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules (Fig. 2); a weak intramolecular C—H···S hydrogen bond (Table 1) is also present, in which they seem to be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, (I), *N*-(4-fluorobenzylidene)-5 -(4-methoxyphenyl)-1,3,4-thiadiazol-2-amine (620 mg, 2 mmol) and diethyl phosphite (690 mg, 5 mmol) were added in a flask (25 ml) and reacted in an oil bath (363 K) for 6 h. After cooling and filtering, the title compound, (I), was obtained (m.p. 465 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetone solution.

Refinement

When the crystal structure was solved,the atoms C1, H1A, H1B, H1C, C3, H3A, H3B and H3C were found to be disordered. During refinement with isotropic thermal parameters, the occupancies of disordered H atoms were refined as H1A, H1B, H1C, H3A, H3B, H3C = 0.66 (2) and H1A', H1B', H1C', H3A', H3B', H3C' = 0.34 (2). The remaining site occupancy factors were also refined as C1, C3 = 0.66 (2) and C1', C3' = 0.34 (2), during anisotropic refinement. H atoms were positioned geometrically with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

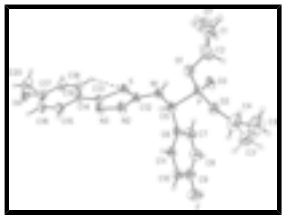


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bond is shown as dashed line.

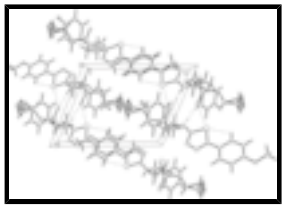


Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

(*S*)-Diethyl {(4-fluorophenyl)[5-(4-methoxyphenyl)-1,3,4-thiadiazol-2- ylamino]methyl}phosphonate

Crystal data

$C_{20}H_{23}FN_3O_4PS$	$Z = 2$
$M_r = 451.44$	$F_{000} = 472$
Triclinic, $P\overline{1}$	$D_x = 1.346$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 465 K
$a = 9.4140$ (19) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.227$ (2) Å	Cell parameters from 25 reflections
$c = 12.923$ (3) Å	$\theta = 10$–13°
$\alpha = 110.44$ (3)°	$\mu = 0.26$ mm^{-1}
$\beta = 98.80$ (3)°	$T = 298$ (2) K
$\gamma = 100.58$ (3)°	Block, colorless
$V = 1113.7$ (5) Å^3	0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.019$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0^\circ$
Monochromator: graphite	$\theta_{min} = 1.7^\circ$
$T = 298(2)$ K	$h = -11 \rightarrow 11$
$\omega/2\theta$ scans	$k = -12 \rightarrow 11$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 15$
$T_{min} = 0.927$, $T_{max} = 0.951$	3 standard reflections
4656 measured reflections	every 120 min
4374 independent reflections	intensity decay: none
3276 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.157$	$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 2.5493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.82$	$(\Delta/\sigma)_{max} < 0.001$
4374 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
295 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
P	0.43635 (9)	0.67087 (8)	−0.10499 (7)	0.0491 (2)	
S	0.87296 (9)	0.75456 (8)	0.24611 (7)	0.0517 (2)	
F	0.9354 (3)	0.4665 (3)	−0.3671 (2)	0.1057 (9)	
N1	0.6691 (3)	0.7228 (3)	0.0607 (2)	0.0522 (6)	
H1	0.6079	0.6613	0.0747	0.063*	
N2	0.8756 (3)	0.9250 (3)	0.1405 (2)	0.0606 (7)	
N3	0.9991 (3)	0.9880 (3)	0.2313 (2)	0.0616 (7)	
O1	0.3723 (3)	0.7941 (3)	−0.0351 (2)	0.0662 (6)	
O2	0.4072 (3)	0.6740 (2)	−0.22638 (19)	0.0637 (6)	
O3	0.3799 (2)	0.5289 (2)	−0.1037 (2)	0.0634 (6)	
O4	1.4759 (3)	1.0977 (3)	0.6845 (2)	0.0969 (10)	
C1	0.1394 (13)	0.7103 (15)	0.0092 (13)	0.100 (4)	0.66 (2)
H1A	0.1483	0.6129	−0.0121	0.150*	0.66 (2)
H1B	0.0362	0.7101	−0.0028	0.150*	0.66 (2)
H1C	0.1875	0.7645	0.0880	0.150*	0.66 (2)
C1'	0.146 (4)	0.794 (6)	0.024 (3)	0.102 (17)	0.34 (2)
H1A'	0.1728	0.7332	0.0620	0.153*	0.34 (2)

H1B'	0.0400	0.7665	−0.0049	0.153*	0.34 (2)
H1C'	0.1771	0.8926	0.0761	0.153*	0.34 (2)
C2	0.2111 (4)	0.7775 (5)	−0.0612 (4)	0.0870 (13)	
H2A	0.1692	0.7176	−0.1410	0.104*	
H2B	0.1914	0.8713	−0.0466	0.104*	
C3	0.287 (3)	0.5362 (15)	−0.4207 (9)	0.121 (8)	0.66 (2)
H3A	0.1913	0.5461	−0.4063	0.160*	0.66 (2)
H3B	0.2747	0.4448	−0.4812	0.160*	0.66 (2)
H3C	0.3300	0.6126	−0.4421	0.160*	0.66 (2)
C3'	0.3900 (4)	0.5599 (19)	−0.4201 (13)	0.100 (8)	0.34 (2)
H3A'	0.3191	0.4835	−0.4836	0.150*	0.34 (2)
H3B'	0.4887	0.5582	−0.4299	0.150*	0.34 (2)
H3C'	0.3724	0.6510	−0.4156	0.150*	0.34 (2)
C4	0.3732 (8)	0.5430 (6)	−0.3294 (4)	0.098 (2)	
H4A	0.4667	0.5280	−0.3475	0.118*	
H4B	0.3287	0.4625	−0.3116	0.118*	
C5	0.6343 (3)	0.7417 (3)	−0.0464 (3)	0.0478 (7)	
H5A	0.6603	0.8452	−0.0307	0.057*	
C6	0.7176 (3)	0.6676 (3)	−0.1318 (3)	0.0508 (7)	
C7	0.7093 (4)	0.5201 (4)	−0.1631 (3)	0.0686 (10)	
H7A	0.6543	0.4677	−0.1300	0.082*	
C8	0.7820 (5)	0.4521 (4)	−0.2427 (4)	0.0788 (11)	
H8A	0.7770	0.3543	−0.2638	0.095*	
C9	0.8619 (4)	0.5325 (4)	−0.2896 (3)	0.0707 (10)	
C10	0.8720 (4)	0.6766 (4)	−0.2615 (3)	0.0625 (9)	
H10A	0.9266	0.7281	−0.2954	0.075*	
C11	0.7994 (3)	0.7430 (3)	−0.1818 (3)	0.0530 (8)	
H11A	0.8057	0.8410	−0.1613	0.064*	
C12	0.7997 (3)	0.8036 (3)	0.1388 (3)	0.0476 (7)	
C13	1.0132 (3)	0.9141 (3)	0.2943 (3)	0.0495 (7)	
C14	1.1326 (3)	0.9586 (3)	0.3959 (3)	0.0520 (7)	
C15	1.2501 (4)	1.0796 (4)	0.4250 (3)	0.0669 (9)	
H15A	1.2531	1.1326	0.3794	0.080*	
C16	1.3619 (4)	1.1212 (4)	0.5212 (3)	0.0740 (11)	
H16A	1.4403	1.2015	0.5391	0.089*	
C17	1.3596 (4)	1.0462 (4)	0.5914 (3)	0.0668 (10)	
C18	1.2444 (4)	0.9278 (4)	0.5645 (3)	0.0672 (9)	
H18A	1.2419	0.8754	0.6105	0.081*	
C19	1.1308 (4)	0.8862 (4)	0.4678 (3)	0.0598 (8)	
H19A	1.0515	0.8072	0.4513	0.072*	
C20	1.4839 (6)	1.0152 (6)	0.7528 (4)	0.1139 (18)	
H20A	1.5718	1.0605	0.8136	0.171*	
H20B	1.4877	0.9196	0.7071	0.171*	
H20C	1.3977	1.0099	0.7839	0.171*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

P	0.0473 (4)	0.0461 (4)	0.0491 (4)	0.0022 (3)	0.0015 (3)	0.0215 (4)
S	0.0508 (4)	0.0441 (4)	0.0535 (4)	−0.0007 (3)	0.0014 (3)	0.0218 (3)
F	0.123 (2)	0.0909 (18)	0.122 (2)	0.0464 (16)	0.0713 (18)	0.0367 (16)
N1	0.0445 (14)	0.0525 (15)	0.0548 (15)	−0.0055 (11)	0.0002 (11)	0.0289 (12)
N2	0.0568 (16)	0.0501 (15)	0.0670 (18)	−0.0068 (12)	−0.0027 (13)	0.0308 (14)
N3	0.0562 (16)	0.0511 (15)	0.0636 (17)	−0.0086 (12)	−0.0024 (13)	0.0239 (14)
O1	0.0536 (13)	0.0646 (15)	0.0669 (15)	0.0127 (11)	0.0055 (11)	0.0145 (12)
O2	0.0720 (15)	0.0640 (14)	0.0497 (13)	0.0073 (12)	0.0020 (11)	0.0256 (11)
O3	0.0551 (13)	0.0545 (13)	0.0754 (16)	−0.0040 (10)	−0.0006 (11)	0.0347 (12)
O4	0.091 (2)	0.091 (2)	0.0657 (17)	0.0096 (16)	−0.0207 (15)	0.0022 (15)
C1	0.055 (5)	0.146 (10)	0.117 (8)	0.029 (5)	0.035 (5)	0.064 (8)
C1'	0.081 (19)	0.142 (5)	0.073 (13)	0.014 (3)	0.035 (12)	0.034 (2)
C2	0.060 (2)	0.101 (3)	0.104 (4)	0.031 (2)	0.007 (2)	0.044 (3)
C3	0.156 (18)	0.125 (11)	0.084 (6)	0.076 (12)	−0.050 (8)	−0.003 (6)
C3'	0.131 (18)	0.108 (12)	0.047 (8)	0.014 (11)	0.016 (9)	0.025 (7)
C4	0.148 (7)	0.085 (4)	0.054 (3)	−0.011 (4)	0.004 (4)	0.015 (3)
C5	0.0490 (16)	0.0401 (15)	0.0526 (17)	0.0018 (12)	0.0042 (13)	0.0241 (13)
C6	0.0454 (16)	0.0452 (16)	0.0588 (19)	0.0020 (13)	0.0072 (14)	0.0237 (14)
C7	0.072 (2)	0.056 (2)	0.093 (3)	0.0159 (17)	0.030 (2)	0.043 (2)
C8	0.089 (3)	0.053 (2)	0.104 (3)	0.023 (2)	0.035 (2)	0.034 (2)
C9	0.073 (2)	0.068 (2)	0.073 (2)	0.0220 (19)	0.025 (2)	0.025 (2)
C10	0.060 (2)	0.062 (2)	0.066 (2)	0.0053 (16)	0.0163 (17)	0.0299 (18)
C11	0.0545 (18)	0.0470 (17)	0.0529 (18)	0.0030 (14)	0.0046 (14)	0.0222 (14)
C12	0.0454 (16)	0.0430 (16)	0.0502 (17)	0.0039 (12)	0.0086 (13)	0.0182 (13)
C13	0.0479 (17)	0.0423 (16)	0.0495 (17)	0.0039 (13)	0.0095 (13)	0.0123 (13)
C14	0.0497 (17)	0.0442 (16)	0.0496 (17)	0.0072 (13)	0.0085 (14)	0.0072 (14)
C15	0.057 (2)	0.060 (2)	0.067 (2)	−0.0039 (16)	0.0013 (17)	0.0204 (17)
C16	0.061 (2)	0.060 (2)	0.073 (2)	−0.0026 (17)	−0.0052 (18)	0.0110 (19)
C17	0.068 (2)	0.062 (2)	0.0485 (19)	0.0188 (18)	−0.0030 (16)	0.0008 (16)
C18	0.074 (2)	0.065 (2)	0.055 (2)	0.0168 (18)	0.0063 (17)	0.0177 (17)
C19	0.060 (2)	0.0509 (18)	0.058 (2)	0.0088 (15)	0.0048 (16)	0.0160 (16)
C20	0.128 (4)	0.126 (4)	0.063 (3)	0.043 (3)	−0.020 (3)	0.020 (3)

Geometric parameters (Å, °)

C1—C2	1.487 (13)	C9—F	1.359 (4)
C1—H1A	0.9600	C9—C10	1.369 (5)
C1—H1B	0.9600	C10—C11	1.373 (5)
C1—H1C	0.9600	C10—H10A	0.9300
C1'—C2	1.31 (3)	C11—H11A	0.9300
C1'—H1A'	0.9600	C12—N2	1.305 (4)
C1'—H1B'	0.9600	C12—N1	1.371 (4)
C1'—H1C'	0.9600	C12—S	1.723 (3)
C2—O1	1.468 (4)	C13—N3	1.299 (4)
C2—H2A	0.9700	C13—C14	1.462 (4)
C2—H2B	0.9700	C13—S	1.743 (3)
C3—C4	1.299 (10)	C14—C19	1.376 (5)
C3—H3A	0.9600	C14—C15	1.393 (4)
C3—H3B	0.9600	C15—C16	1.378 (5)

C3—H3C	0.9600	C15—H15A	0.9300
C3'—C4	1.269 (14)	C16—C17	1.377 (5)
C3'—H3A'	0.9600	C16—H16A	0.9300
C3'—H3B'	0.9600	C17—O4	1.366 (4)
C3'—H3C'	0.9600	C17—C18	1.368 (5)
C4—O2	1.462 (5)	C18—C19	1.392 (5)
C4—H4A	0.9700	C18—H18A	0.9300
C4—H4B	0.9700	C19—H19A	0.9300
C5—N1	1.460 (4)	C20—O4	1.421 (6)
C5—C6	1.518 (4)	C20—H20A	0.9600
C5—P	1.806 (3)	C20—H20B	0.9600
C5—H5A	0.9800	C20—H20C	0.9600
C6—C11	1.375 (4)	N1—H1	0.8600
C6—C7	1.402 (4)	N2—N3	1.387 (4)
C7—C8	1.378 (5)	O1—P	1.555 (3)
C7—H7A	0.9300	O2—P	1.563 (2)
C8—C9	1.368 (5)	O3—P	1.459 (2)
C8—H8A	0.9300		
C2—C1—H1A	109.5	C10—C9—C8	122.9 (4)
C2—C1—H1B	109.5	C9—C10—C11	118.3 (3)
C2—C1—H1C	109.5	C9—C10—H10A	120.9
C2—C1'—H1A'	109.5	C11—C10—H10A	120.9
C2—C1'—H1B'	109.5	C10—C11—C6	121.3 (3)
H1A'—C1'—H1B'	109.5	C10—C11—H11A	119.4
C2—C1'—H1C'	109.5	C6—C11—H11A	119.4
H1A'—C1'—H1C'	109.5	N2—C12—N1	123.2 (3)
H1B'—C1'—H1C'	109.5	N2—C12—S	114.8 (2)
C1'—C2—O1	116.8 (13)	N1—C12—S	122.0 (2)
O1—C2—C1	110.7 (6)	N3—C13—C14	124.2 (3)
C1'—C2—H2A	128.0	N3—C13—S	113.0 (2)
O1—C2—H2A	109.5	C14—C13—S	122.8 (2)
C1—C2—H2A	109.5	C19—C14—C15	117.7 (3)
C1'—C2—H2B	78.1	C19—C14—C13	121.5 (3)
O1—C2—H2B	109.5	C15—C14—C13	120.7 (3)
C1—C2—H2B	109.5	C16—C15—C14	120.3 (4)
H2A—C2—H2B	108.1	C16—C15—H15A	119.9
C4—C3—H3A	109.5	C14—C15—H15A	119.9
C4—C3—H3B	109.5	C15—C16—C17	121.3 (3)
C4—C3—H3C	109.5	C15—C16—H16A	119.4
C4—C3'—H3A'	109.5	C17—C16—H16A	119.4
C4—C3'—H3B'	111.0	O4—C17—C18	124.7 (4)
H3A'—C3'—H3B'	109.5	O4—C17—C16	116.1 (4)
C4—C3'—H3C'	109.5	C18—C17—C16	119.2 (3)
H3A'—C3'—H3C'	109.5	C17—C18—C19	119.7 (4)
H3B'—C3'—H3C'	109.5	C17—C18—H18A	120.2
C3'—C4—O2	116.7 (10)	C19—C18—H18A	120.2
C3—C4—O2	118.7 (7)	C14—C19—C18	121.8 (3)
C3'—C4—H4A	67.0	C14—C19—H19A	119.1
C3—C4—H4A	107.6	C18—C19—H19A	119.1

O2—C4—H4A	107.6	O4—C20—H20A	109.5
C3'—C4—H4B	135.0	O4—C20—H20B	109.5
C3—C4—H4B	107.6	H20A—C20—H20B	109.5
O2—C4—H4B	107.6	O4—C20—H20C	109.5
H4A—C4—H4B	107.1	H20A—C20—H20C	109.5
N1—C5—C6	113.1 (2)	H20B—C20—H20C	109.5
N1—C5—P	107.85 (19)	C12—N1—C5	119.7 (2)
C6—C5—P	109.9 (2)	C12—N1—H1	120.1
N1—C5—H5A	108.6	C5—N1—H1	120.1
C6—C5—H5A	108.6	C12—N2—N3	111.4 (3)
P—C5—H5A	108.6	C13—N3—N2	113.8 (2)
C11—C6—C7	118.8 (3)	C2—O1—P	119.1 (3)
C11—C6—C5	120.6 (3)	C4—O2—P	122.2 (3)
C7—C6—C5	120.6 (3)	C17—O4—C20	117.4 (4)
C8—C7—C6	120.5 (3)	O3—P—O1	116.31 (15)
C8—C7—H7A	119.7	O3—P—O2	113.80 (14)
C6—C7—H7A	119.7	O1—P—O2	103.59 (14)
C9—C8—C7	118.1 (3)	O3—P—C5	112.94 (14)
C9—C8—H8A	120.9	O1—P—C5	102.91 (14)
C7—C8—H8A	120.9	O2—P—C5	106.07 (14)
F—C9—C10	118.7 (3)	C12—S—C13	87.04 (15)
F—C9—C8	118.4 (4)		
N1—C5—C6—C11	−127.1 (3)	C6—C5—N1—C12	77.7 (3)
P—C5—C6—C11	112.3 (3)	P—C5—N1—C12	−160.5 (2)
N1—C5—C6—C7	54.6 (4)	N1—C12—N2—N3	177.1 (3)
P—C5—C6—C7	−66.0 (3)	S—C12—N2—N3	−0.7 (4)
C11—C6—C7—C8	0.0 (5)	C14—C13—N3—N2	−179.0 (3)
C5—C6—C7—C8	178.4 (3)	S—C13—N3—N2	0.6 (4)
C6—C7—C8—C9	0.0 (6)	C12—N2—N3—C13	0.1 (4)
C7—C8—C9—F	179.2 (4)	C1'—C2—O1—P	126 (3)
C7—C8—C9—C10	−0.3 (7)	C1—C2—O1—P	91.2 (8)
F—C9—C10—C11	−179.0 (3)	C3'—C4—O2—P	−162.0 (5)
C8—C9—C10—C11	0.5 (6)	C3—C4—O2—P	148.3 (14)
C9—C10—C11—C6	−0.5 (5)	C18—C17—O4—C20	5.6 (6)
C7—C6—C11—C10	0.2 (5)	C16—C17—O4—C20	−174.4 (4)
C5—C6—C11—C10	−178.2 (3)	C2—O1—P—O3	−57.8 (3)
N3—C13—C14—C19	171.1 (3)	C2—O1—P—O2	67.8 (3)
S—C13—C14—C19	−8.4 (4)	C2—O1—P—C5	178.2 (3)
N3—C13—C14—C15	−6.7 (5)	C4—O2—P—O3	−19.2 (4)
S—C13—C14—C15	173.7 (3)	C4—O2—P—O1	−146.4 (4)
C19—C14—C15—C16	1.8 (5)	C4—O2—P—C5	105.6 (4)
C13—C14—C15—C16	179.7 (3)	N1—C5—P—O3	−47.2 (3)
C14—C15—C16—C17	−0.8 (6)	C6—C5—P—O3	76.5 (2)
C15—C16—C17—O4	−179.7 (4)	N1—C5—P—O1	79.0 (2)
C15—C16—C17—C18	0.3 (6)	C6—C5—P—O1	−157.3 (2)
O4—C17—C18—C19	179.3 (3)	N1—C5—P—O2	−172.5 (2)
C16—C17—C18—C19	−0.7 (6)	C6—C5—P—O2	−48.8 (2)
C15—C14—C19—C18	−2.3 (5)	N2—C12—S—C13	0.9 (3)
C13—C14—C19—C18	179.8 (3)	N1—C12—S—C13	−177.0 (3)

C17—C18—C19—C14	1.8 (5)	N3—C13—S—C12	−0.8 (3)
N2—C12—N1—C5	21.0 (5)	C14—C13—S—C12	178.8 (3)
S—C12—N1—C5	−161.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.86	2.13	2.795 (5)	133
C19—H19A···S	0.93	2.73	3.142 (4)	108

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Fig. 1

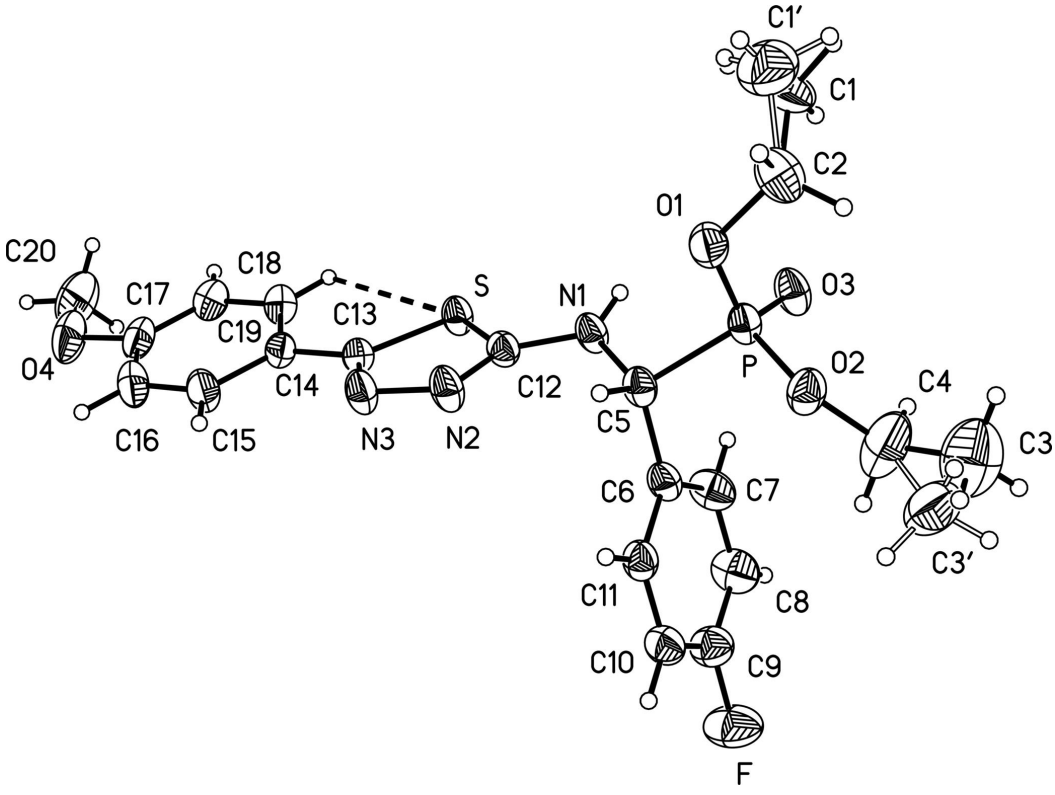

C1′
C1
C2
O1
C20
C18
C17
S
N1
O3
C19
C13
O4
C14
C12
P
O2
C4
C16
C15
N3
N2
C5
C3
C6
C7
C3′
C11
C8
C10
C9
F

Fig. 2