O(3)—C(6)—C(1)	113.0 (2)	O(3)—C(6)—C(5)	106.4 (2)
O(1)—C(7)—O(2)	122.2 (3)	O(1)—C(7)—C(4)	126.1 (3)
O(2)—C(7)—C(4)	111.8 (2)	O(4)—C(9)—O(5)	107.3 (2)
O(4)—C(9)—C(10)	108.4 (2)	O(5)—C(9)—C(10)	110.1 (2)
O(5)—C(13)—C(12)	111.5 (2)		

H atoms were located from difference Fourier maps, positioned geometrically and included as riding atoms with fixed isotropic displacement parameters in the structure-factor calculations.

Data collection: *R3m/V* diffractometer software. Cell refinement: *R3m/V* diffractometer software. Data reduction: *SHELXTL-Plus* (Sheldrick, 1991). Program(s) used to solve structure: *SHELXTL-Plus*. Program(s) used to refine structure: *SHELXTL-Plus*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1053). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A New Pyrethroid Insecticide, RU41414

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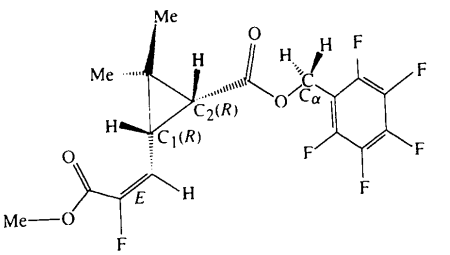
Abstract

An X-ray diffraction study of RU41414, methyl 3-[2,2-dimethyl-3-(pentafluorophenylmethyloxycarbonyl)-cyclopropyl]-2-fluoropropenoate, $C_{17}H_{14}F_6O_4$, establishes the molecular structure, the configuration (*R*) of the asymmetric C atoms C12 and C8 of the cyclopropane ring and the stereochemistry of the propenoate C5═C7 double bond.

Comment

Biological activity in pyrethroids is related to molecular structure and depends strongly on the stereochemistry at the three centres C_1, C_2 and C_α. We report here the structure of RU41414, a useful pyrethroid insecticide.



RU41414

The cyclopropane ring has a mean bond length of 1.524 (10) Å, which is in the expected range as found from earlier studies (Hamzaoui, Lamiot & Baert, 1993; Baert, Guelzim & Germain, 1991). The average C—F bond length in the pentafluorophenyl ring is 1.337 (12) Å and the C—C distances in this ring vary between 1.318 (17) and 1.384 (12) Å. Knowledge of the stereochemistry of the C4═C5 double bond allows chemists to predict precisely the activity of the insecticide concerned (Tessier, Teche & Demoute, 1982).

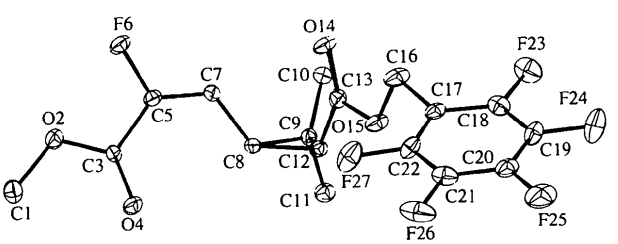


Fig. 1. An *ORTEP*II (Johnson, 1976) view of RU41414 showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 50% probability level.

Experimental

Single crystals were grown at room temperature by slow evaporation of an aqueous solution of RU41414.

Crystal data

$C_{17}H_{14}F_6O_4$
M_r = 396.29

Mo $K\alpha$ radiation
λ = 0.71073 Å

Orthorhombic
$P2_12_12_1$
a = 23.85 (2) Å
b = 6.08 (1) Å
c = 12.14 (2) Å
V = 1760 Å^3
Z = 4
D_x = 1.495 Mg m^{-3}

Cell parameters from 25 reflections
θ = 11–22°
μ = 0.15 mm^{-1}
T = 295 K
Parallelepiped
0.3 × 0.25 × 0.2 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2602 measured reflections
2602 independent reflections
1005 observed reflections [$I \geq 3\sigma(I)$]

θ_{max} = 30°
$h = 0 \rightarrow 33$
$k = 0 \rightarrow 8$
$l = 0 \rightarrow 12$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F
R = 0.05
wR = 0.05
S = 1.07
1005 reflections
224 parameters
H-atom parameters not refined
$w = 1/\sigma^2(F_o)$

$(\Delta/\sigma)_{max}$ = 0.018
$\Delta\rho_{max}$ = 0.018 e Å^{-3}
$\Delta\rho_{min}$ = −0.222 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
C1	0.4590 (3)	0.7622 (15)	0.2145 (8)	0.072 (14)
O2	0.4302 (2)	0.5600 (9)	0.2408 (5)	0.070 (8)
C3	0.3777 (3)	0.5480 (14)	0.2054 (6)	0.050 (11)
O4	0.3552 (2)	0.6874 (10)	0.1541 (5)	0.076 (11)
F6	0.3834 (2)	0.2147 (8)	0.3062 (4)	0.084 (7)
C5	0.3516 (3)	0.3350 (14)	0.2342 (6)	0.062 (11)
C7	0.3036 (3)	0.2498 (12)	0.2014 (6)	0.056 (11)
C8	0.2659 (3)	0.3555 (12)	0.1195 (6)	0.059 (10)
C9	0.2297 (3)	0.2204 (12)	0.0434 (6)	0.051 (10)
C10	0.2201 (3)	0.3221 (16)	−0.0696 (6)	0.078 (13)
C11	0.2340 (3)	−0.0277 (13)	0.0411 (7)	0.066 (12)
C12	0.2011 (3)	0.3396 (13)	0.1362 (6)	0.060 (10)
C13	0.1792 (3)	0.2204 (15)	0.2337 (7)	0.064 (12)
O14	0.1978 (2)	0.0627 (11)	0.2786 (5)	0.104 (9)
O15	0.1307 (2)	0.3174 (11)	0.2661 (4)	0.109 (9)
C17	0.0563 (3)	0.3486 (17)	0.3960 (7)	0.081 (13)
C16	0.1070 (4)	0.2156 (17)	0.3639 (7)	0.130 (16)
C18	0.0024 (4)	0.2725 (16)	0.3780 (7)	0.066 (14)
C19	−0.0437 (4)	0.3890 (21)	0.4125 (8)	0.083 (16)
C20	−0.0371 (4)	0.5797 (21)	0.4623 (9)	0.107 (17)
C21	0.0147 (6)	0.6630 (17)	0.4797 (8)	0.085 (17)
C22	0.0609 (4)	0.5476 (18)	0.4449 (7)	0.068 (15)
F23	−0.0062 (3)	0.0770 (11)	0.3292 (4)	0.100 (10)
F24	−0.0947 (2)	0.3073 (14)	0.3958 (5)	0.137 (14)
F25	−0.0817 (3)	0.6946 (13)	0.4946 (6)	0.202 (14)
F26	0.0213 (3)	0.8594 (11)	0.5296 (5)	0.141 (13)
F27	0.1114 (2)	0.6336 (11)	0.4618 (5)	0.107 (11)

Table 2. *Selected geometric parameters (Å, °)*

C1—O2	1.444 (9)	C13—O15	1.356 (11)
O2—C3	1.327 (9)	O15—C16	1.456 (11)
C3—O4	1.181 (10)	C17—C16	1.506 (13)
C3—C5	1.480 (12)	C17—C18	1.384 (12)
C5—C7	1.318 (10)	C17—C22	1.354 (15)
F6—C5	1.369 (10)	C18—C19	1.373 (14)
C7—C8	1.489 (10)	C18—F23	1.345 (11)
C8—C12	1.560 (10)	C19—C20	1.318 (17)
C9—C10	1.523 (11)	C19—F24	1.331 (11)
C9—C11	1.514 (11)	C20—C21	1.351 (17)
C9—C8	1.508 (10)	C20—F25	1.332 (13)
C9—C12	1.504 (10)	C21—C22	1.374 (16)
C12—C13	1.484 (11)	C21—F26	1.350 (12)
C13—O14	1.189 (11)	C22—F27	1.329 (11)
O4—C3—C5	124.3 (7)	C18—C17—C22	116.4 (8)
C3—C5—C7	129.6 (7)	C12—C13—O14	129.0 (8)
C10—C9—C11	113.5 (6)	C17—C18—C19	121.5 (9)
C10—C9—C12	114.3 (6)	C16—C17—C18	121.6 (8)
C11—C9—C12	121.7 (6)	C17—C18—F23	120.5 (8)
O2—C3—O4	124.0 (7)	C19—C18—F23	118.0 (9)
C7—C8—C9	121.3 (6)	C18—C19—C20	120.0 (10)
C7—C8—C12	119.0 (6)	C18—C19—F24	119.5 (9)
C9—C12—C8	59.0 (5)	C20—C19—F24	120.5 (10)
C8—C12—C13	118.9 (6)	C19—C20—C21	120.7 (11)
O2—C3—C5	111.6 (6)	C19—C20—F25	120.2 (10)
C5—C7—C8	123.9 (7)	C21—C20—F25	119.1 (10)
C10—C9—C8	114.6 (6)	C20—C21—C22	119.6 (11)
C11—C9—C8	121.1 (6)	C20—C21—F26	120.7 (10)
C8—C9—C12	62.4 (5)	C22—C21—F26	119.7 (10)
C9—C8—C12	58.7 (5)	C17—C22—C21	121.8 (9)
C16—C17—C22	122.0 (8)	C17—C22—F27	119.6 (8)
C9—C12—C13	121.4 (7)	C21—C22—F27	118.6 (9)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELX76* (Sheldrick, 1976). Molecular graphics: *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: PA1209). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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