conditions (Ghosh, Ray, Saha & Kolay, 1984). CNDO/2 results, as discussed earlier, also support such a decrease in reductive power. Such a substitution thus decreases the reductive capacity as well as the hydrophilic character of the molecule and these two factors probably act together, leading to a slight decrease of its antibacterial activity.

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Structure of Ethyl 4-Acetyl-5-methyl-3-trifluoromethylpyrrole-2-carboxylate

BY NORIKO YAMAMOTO, KATSUNOSUKE MACHIDA AND TOORU TAGA*

Faculty of Pharmaceutical Sciences, Kyoto University, Sakyo-ku, Kyoto 606, Japan

AND HISANOBU OGOSHI

Department of Materials Science and Technology, Technological University of Nagaoka, Kamitomioka, Nagaoka 949–54, Japan

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Abstract. $C_{11}H_{12}F_3NO_3$, $M_r = 263{\cdot}22$, triclinic, $P\bar{1}$, $a = 13{\cdot}584\,(2)$, $b = 11{\cdot}696\,(2)$, $c = 10{\cdot}268\,(3)$ Å, $\alpha = 64{\cdot}29\,(2)$, $\beta = 70{\cdot}40\,(2)$, $\gamma = 57{\cdot}45\,(1)°$, $V = 1227{\cdot}6$ Å^3, $Z = 4$, $D_x = 1{\cdot}424$ Mg m^{-3}, λ(Cu $K\alpha$) = $1{\cdot}54178$ Å, $\mu = 0{\cdot}743$ mm^{-1}, $F(000) = 544$, $T = 293$ K. $R(F) = 0{\cdot}064$ for 3026 observed reflections with $F_o > 3\sigma(F_o)$. The two independent molecules are in a similar conformation and form a hydrogen-bonded dimer; they are stacked along the $[1\bar{1}\bar{1}]$ direction. Short intermolecular F···CH_3 contacts are 3·279 (7) Å for F(3′)···C(10′) and 3·302 (6) Å for F(2′)···C(10).

* To whom correspondence should be addressed.

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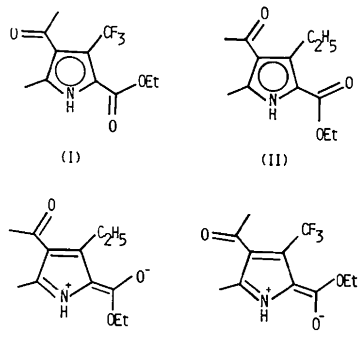
Introduction. 2-Ethoxycarbonyl pyrrole derivatives are chemically and biologically important compounds in the synthesis of phthalocyanines and porphyrins. The title compound (I) has a trifluoromethyl substituent at the 3-position of the pyrrole ring. The structure of compound (II) has already been studied, and a large distortion has been observed in the bonds of the pyrrole ring (Bonnett, Hursthouse & Neidle, 1972). One point of interest in structure (I) was, therefore, the effect of the trifluoromethyl group on the bond distortion of the pyrrole ring. Another point of interest was the intermolecular contacts of the F atoms with other atoms, especially the CH_3 group, since short contacts between the F atom and CH_3 group have been reported for several crystals so far (Kim & Rich, 1967; Valente, Pohl & Trager, 1980; Dahl, 1971, *etc.*).



(I) (II) (III) (IV)

Experimental. Transparent prism-like crystal 0·2 × 0·2 × 0·2 mm from *n*-hexane–methylene chloride mixed solvent, mounted on a Rigaku AFC-5RU diffractometer; graphite-monochromated Cu $K\alpha$ radiation; cell parameters refined by least squares with 24 2θ values, $19.74 < 2\theta < 45.89°$; intensities were measured using 2θ–ω scan; scan width $\Delta(\omega) = 0.8° + 0.5° \tan\theta$; 3880 unique reflections with $2\theta < 120°$; h −15→15, k −13→13, l 0→11; 3026 independent reflections with $F_o > 3\sigma(F_o)$ used; no significant intensity variation for three standard reflections; no absorption correction. Structure solved by direct methods with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); block-diagonal least squares, $\sum w|F_o - kF_c|^2$ minimized with $w^{-1} = \sigma^2(F_o) + (0.023F_o)^2$; reflection 110 is omitted because of large extinction effect; C(7′) in disordered state (occupies two positions with equal probability); non-H atoms except for C(7′) anisotropic; H atoms except for the disordered group determined from the difference Fourier map; H atoms and C(7′) isotropic; $R = 0.064$, $wR = 0.104$, $(\Delta/\sigma)_{max} = 0.71$; scattering factors from *International Tables for X-ray Crystallography* (1974). All computations were performed on a FACOM M382 computer at the Data Processing Center of Kyoto University, using *KPPXRAY* programs (Taga, Higashi & Iizuka, 1985).

Table 1. *Atomic parameters and their e.s.d.'s*

B_{eq} is the isotropic equivalent of the anisotropic thermal parameter in Å^2: $B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
F(1)	0·2779 (2)	0·5156 (3)	−0·0124 (3)	7·80 (35)
F(2)	0·2382 (2)	0·7185 (3)	−0·1724 (2)	8·38 (34)
F(3)	0·1356 (2)	0·7022 (3)	0·0354 (3)	8·39 (35)
C(1)	0·3869 (3)	0·5779 (3)	0·1386 (3)	4·57 (33)
C(2)	0·3263 (2)	0·6683 (3)	0·0183 (3)	4·61 (31)
C(3)	0·3622 (3)	0·7769 (4)	−0·0567 (3)	5·12 (35)
C(4)	0·4452 (3)	0·7483 (3)	0·0190 (3)	4·99 (35)
C(5)	0·3896 (3)	0·4518 (3)	0·2607 (3)	4·83 (35)
C(6)	0·3120 (4)	0·2876 (4)	0·3862 (4)	6·85 (47)
C(7)	0·2089 (4)	0·2780 (5)	0·3829 (6)	9·14 (68)
C(8)	0·2453 (3)	0·6515 (4)	−0·0310 (4)	5·68 (38)
C(9)	0·3181 (3)	0·9097 (4)	−0·1813 (4)	6·64 (46)
C(10)	0·1884 (4)	1·0003 (5)	−0·1834 (6)	9·98 (66)
C(11)	0·5118 (3)	0·8248 (4)	−0·0080 (4)	6·46 (47)
N(1)	0·4561 (2)	0·6310 (3)	0·1342 (3)	4·74 (26)
O(1)	0·4515 (2)	0·3948 (3)	0·3546 (3)	6·46 (33)
O(2)	0·3164 (2)	0·4098 (2)	0·2630 (2)	5·77 (26)
O(3)	0·3856 (3)	0·9510 (4)	−0·2727 (3)	9·56 (42)
F(1′)	0·1279 (2)	0·6479 (3)	0·3870 (3)	8·20 (36)
F(2′)	0·0876 (2)	0·8549 (2)	0·2336 (2)	7·17 (28)
F(3′)	0·0022 (2)	0·8342 (3)	0·4515 (3)	8·62 (35)
C(1′)	0·2791 (3)	0·6711 (3)	0·5087 (3)	4·80 (35)
C(2′)	0·2026 (3)	0·7797 (3)	0·4076 (3)	4·78 (31)
C(3′)	0·2412 (3)	0·8857 (3)	0·3322 (3)	5·11 (35)
C(4′)	0·3409 (3)	0·8385 (3)	0·3901 (3)	5·04 (35)
C(5′)	0·2894 (3)	0·5369 (3)	0·6219 (3)	5·16 (35)
C(6′)	0·1987 (4)	0·3889 (5)	0·7765 (5)	8·74 (62)
C(7′)	0·0848 (8)	0·3906 (10)	0·7865 (9)	7·85 (19)
C(7A′)	0·0718 (10)	0·4217 (13)	0·8406 (12)	10·46 (28)
C(8′)	0·1059 (3)	0·7776 (4)	0·3732 (4)	5·85 (40)
C(9′)	0·1894 (3)	1·0273 (4)	0·2200 (4)	6·02 (40)
C(10′)	0·0589 (4)	1·1197 (4)	0·2321 (5)	7·25 (47)
C(11′)	0·4176 (4)	0·9040 (4)	0·3604 (4)	6·73 (47)
N(1′)	0·3610 (2)	0·7119 (3)	0·4925 (3)	5·03 (29)
O(1′)	0·3764 (2)	0·4508 (2)	0·6823 (2)	5·74 (24)
O(2′)	0·1938 (2)	0·5211 (3)	0·6564 (3)	7·22 (33)
O(3′)	0·2531 (3)	1·0723 (3)	0·1230 (3)	9·03 (40)

Discussion. The atomic parameters are listed in Table 1.* Bond lengths and bond angles are given in Table 2. The atomic numbering and thermal ellipsoids of the non-H atoms are shown in Fig. 1. The two independent molecules have similar conformations. The ethoxycarbonyl group bonds to the pyrrole ring in an *anti* conformation with values of −178·3 (3) [169·3 (4)]° for the O(1)—C(5)—C(1)—C(2) torsion angle. The acetyl group also bonds to the pyrrole ring in an *anti* conformation with values of −143·8 (5) [−145·4 (5)]° for the O(3)—C(9)—C(3)—C(2) torsion angle. These conformations about the two exocyclic bonds differ from those of compound (II), which has a *syn* conformation for the corresponding bonds. The *anti* conformation of the present compound, (I), may be caused by electrostatic repulsion between the electronegative O and F atoms. As a result, the bulky

* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43118 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

trifluoromethyl groups have short intramolecular contacts, 2·658 (4) [2·708 (4)] Å for F(1)···O(2) and 2·943 (7) [2·900 (6)] Å for F(2)···C(10). Such an arrangement of the side-chain groups seems to affect the structure of the pyrrole ring. However, the pyrrole rings are planar within experimental error and the ring distortion from C_{2v} symmetry is small. Although the large distortion of the pyrrole ring observed in compound (II) was explained as a result of the contribution of a mesomeric dipolar structure (III) (Bonnett *et al.*, 1972), the electron-withdrawing effect of the trifluoromethyl group of (I) may have a fairly large influence on the ring distortion in addition to the contribution of the mesomeric dipolar structure (IV).

The molecular packing projected along [010] is shown in Fig. 2. The two independent molecules are bonded by N(1)···O(1′)(1−*x*, 1−*y*, 1−*z*) and N(1′)···O(1)(1−*x*, 1−*y*, 1−*z*) intermolecular hydrogen bonds with N···O distances of 2·937 (5) and 2·844 (5) Å, respectively. The hydrogen-bonded dimers are stacked with van der Waals contacts along the [1$\bar{1}\bar{1}$] direction. Short F···CH_3 intermolecular distances, 3·279 (7) and 3·302 (6) Å, are observed between F(3′)···C(10′)H_3(−*x*, 2−*y*, 1−*z*), and F(2′)···C(10)H_3(−*x*, 2−*y*, −*z*), respectively. These non-bonding distances seem to be shorter than the sum of the van der Waals radii, 1·35 Å for F and 2·0 Å for CH_3. However, the F atoms have reasonable contacts with the CH_3 groups. That is, the F(3′)···C(10′)H_3 contact has a bent form with an F(3′)···C(10′)—C(9′) angle of 102·2 (3)°, and two H atoms bonded to C(10′) come in contact with F(3′), exhibiting F···H distances of 2·805 (4) and 2·966 (3) Å.

The F(2′)···C(10)H_3 contact has a linear F(2′)···C(10)—C(9) arrangement [164·7 (5)°] and the three H atoms bonded to C(10) have F(2′)···H distances of 2·912 (2), 3·133 (3) and 3·318 (3) Å. Similar short F···CH_3 contacts have been reported for the bent F···CH_3—C form in a 5-fluorouracil-9-ethylhypoxanthine complex (Kim & Rich, 1967) and the amine derivative of pentafluorophenyl acetic acid (Valente *et al.*, 1980), and for the linear F···CH_3—C form in hexafluorobenzene complexes (Dahl, 1971, 1975, 1977).

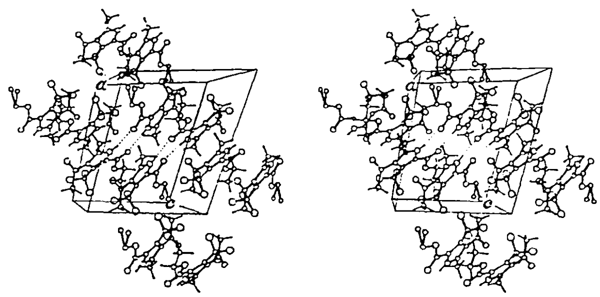


Fig. 2. Stereoview of the molecular packing projected along the [010] direction.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

F(1)–C(8)	1·340 (6)	F(1′)–C(8′)	1·328 (6)
F(2)–C(8)	1·326 (4)	F(2′)–C(8′)	1·345 (4)
F(3)–C(8)	1·324 (4)	F(3′)–C(8′)	1·328 (4)
C(1)–C(2)	1·392 (4)	C(1′)–C(2′)	1·391 (4)
C(1)–C(5)	1·455 (4)	C(1′)–C(5′)	1·458 (4)
C(1)–N(1)	1·359 (6)	C(1′)–N(1′)	1·368 (6)
C(2)–C(3)	1·417 (6)	C(2′)–C(3′)	1·416 (6)
C(2)–C(8)	1·483 (7)	C(2′)–C(8′)	1·485 (7)
C(3)–C(4)	1·395 (6)	C(3′)–C(4′)	1·395 (6)
C(3)–C(9)	1·483 (4)	C(3′)–C(9′)	1·484 (4)
C(4)–C(11)	1·477 (7)	C(4′)–C(11′)	1·486 (8)
C(4)–N(1)	1·340 (4)	C(4′)–N(1′)	1·334 (4)
C(5)–O(1)	1·211 (5)	C(5′)–O(1′)	1·211 (4)
C(5)–O(2)	1·315 (6)	C(5′)–O(2′)	1·318 (6)
C(6)–C(7)	1·476 (9)	C(6′)–C(7′)	1·505 (14)
		C(6′)–C(7A′)	1·515 (13)
C(6)–O(2)	1·456 (4)	C(6′)–O(2′)	1·485 (5)
C(9)–C(10)	1·491 (6)	C(9′)–C(10′)	1·494 (5)
C(9)–O(3)	1·207 (5)	C(9′)–O(3′)	1·213 (5)
C(2)–C(1)–C(5)	136·2 (4)	C(2′)–C(1′)–C(5′)	137·0 (4)
C(2)–C(1)–N(1)	106·4 (3)	C(2′)–C(1′)–N(1′)	105·9 (3)
C(5)–C(1)–N(1)	117·3 (3)	C(5′)–C(1′)–N(1′)	117·1 (3)
C(1)–C(2)–C(3)	107·2 (4)	C(1′)–C(2′)–C(3′)	107·8 (4)
C(1)–C(2)–C(8)	127·5 (3)	C(1′)–C(2′)–C(8′)	126·1 (4)
C(3)–C(2)–C(8)	125·2 (3)	C(3′)–C(2′)–C(8′)	125·8 (3)
C(2)–C(3)–C(4)	107·2 (3)	C(2′)–C(3′)–C(4′)	106·8 (3)
C(2)–C(3)–C(9)	131·2 (4)	C(2′)–C(3′)–C(9′)	131·0 (4)
C(4)–C(3)–C(9)	121·2 (4)	C(4′)–C(3′)–C(9′)	122·1 (4)
C(3)–C(4)–C(11)	131·2 (3)	C(3′)–C(4′)–C(11′)	132·3 (3)
C(3)–C(4)–N(1)	106·8 (4)	C(3′)–C(4′)–N(1′)	107·3 (4)
C(11)–C(4)–N(1)	121·9 (4)	C(11′)–C(4′)–N(1′)	120·3 (3)
C(1)–C(5)–O(1)	121·9 (4)	C(1′)–C(5′)–O(1′)	122·8 (4)
C(1)–C(5)–O(2)	114·5 (3)	C(1′)–C(5′)–O(2′)	113·8 (3)
O(1)–C(5)–O(2)	123·5 (3)	O(1′)–C(5′)–O(2′)	123·4 (3)
C(7)–C(6)–O(2)	107·5 (3)	C(7′)–C(6′)–O(2′)	105·1 (4)
		C(7A′)–C(6′)–O(2′)	105·8 (5)
F(1)–C(8)–F(2)	104·8 (4)	F(1′)–C(8′)–F(2′)	104·9 (4)
F(1)–C(8)–F(3)	105·4 (4)	F(1′)–C(8′)–F(3′)	107·5 (4)
F(1)–C(8)–C(2)	114·0 (3)	F(1′)–C(8′)–C(2′)	113·8 (3)
F(2)–C(8)–F(3)	105·7 (3)	F(2′)–C(8′)–F(3′)	104·9 (3)
F(2)–C(8)–C(2)	112·1 (4)	F(2′)–C(8′)–C(2′)	111·0 (3)
F(3)–C(8)–C(2)	114·0 (4)	F(3′)–C(8′)–C(2′)	114·0 (4)
C(3)–C(9)–C(10)	119·1 (3)	C(3′)–C(9′)–C(10′)	120·2 (3)
C(3)–C(9)–O(3)	120·4 (3)	C(3′)–C(9′)–O(3′)	120·1 (3)
C(10)–C(9)–O(3)	120·1 (3)	C(10′)–C(9′)–O(3′)	119·6 (3)
C(1)–N(1)–C(4)	112·4 (3)	C(1′)–N(1′)–C(4′)	112·2 (3)
C(5)–O(2)–C(6)	116·8 (3)	C(5′)–O(2′)–C(6′)	115·4 (3)

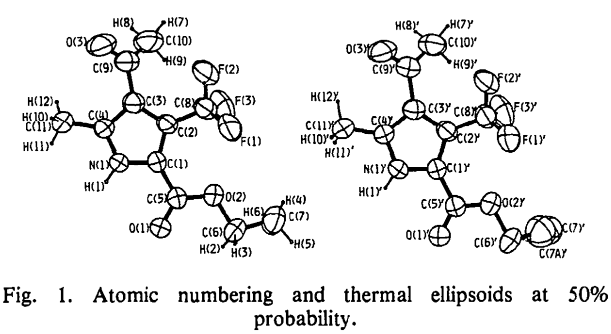


Fig. 1. Atomic numbering and thermal ellipsoids at 50% probability.

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Structure of 2-(1,5-Dimethyl-4-hexenyl)-3,6-dihydroxy-5-methyl-1,4-benzoquinone (Hydroxyperezone), a Sesquiterpene*

BY M. SORIANO-GARCÍA† AND R. A. TOSCANO

Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Coyoacán 04510, *Mexico DF*

E. FLORES-VALVERDE AND F. MONTOYA-VEGA

Departamento de Química, Escuela Nacional de Ciencias Biológicas del Instituto Politécnico Nacional, Mexico DF

AND I. LÓPEZ-CELIS

Departamento de Biotecnología, Area de Productos Naturales, UAM-Iztapalapa, Iztapalapa 09340, *Mexico DF*

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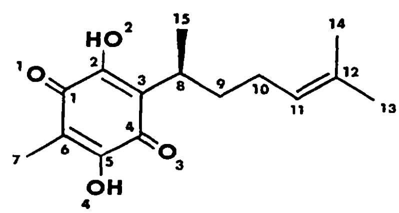
Abstract. $C_{15}H_{20}O_4$, $M_r = 264\cdot3$, orthorhombic, $P2_12_12_1$, $a = 6\cdot449$ (2), $b = 7\cdot361$ (1), $c = 31\cdot089$ (9) Å, $V = 1476$ (1) Å^3, $Z = 4$, $D_x = 1\cdot19$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1\cdot54178$ Å, $\mu = 0\cdot663$ mm^{-1}, $F(000) = 568$, $T = 300$ K, $R = 0\cdot060$ for 1031 observed reflections. The structural features determined from chemical and spectroscopic studies are confirmed and extended. The atoms of the quinone ring form a planar system. The quinone ring shows normal geometry. The angle between the quinone ring and the 1,5-dimethyl-4-hexenyl side chain is 32·1 (7)°. The molecules in the crystal are connected by intermolecular O—H···O hydrogen bonds forming continuous parallel ribbons along **b** and intramolecular O—H···O and C—H···O hydrogen bonds lend conformational stability to the molecules.

Introduction. Hydroxyperezone (1) is a sesquiterpene which was isolated from the dried and ground roots of *Perezia adnata* Gr., a member of the Compositae family found in Mexico. Chemical and spectroscopic studies led to the chemical structure (1) (Joseph-Nathan, González & Rodríguez, 1972; Joseph-Nathan, González, García, Barrios & Walls, 1974). The X-ray crystallographic structural determination of (1) was undertaken in order to understand the detailed geometry of this molecule as well as its intra- and intermolecular interactions.



(1)

Experimental. Red crystal 0·04 × 0·34 × 0·58 mm. Nicolet $R3$ four-circle diffractometer, Ni-filtered Cu $K\alpha$ radiation. Lattice parameters from 25 machine-centred reflections with $5\cdot7 < 2\theta < 51\cdot0°$. 1140 reflections with $3 < 2\theta < 110°$ for one octant, 1031 independent with $I > 2\cdot5\sigma(I)$, index range h 0→6, k 0→7, l 0→32, ω-scan mode, variable scan speed, scan width $1\cdot0°(\theta)$, two standard reflections ($00\bar{2}$; 102) monitored every 50 measurements, Lp correction, absorption ignored, $R_{int} = 0\cdot020$. Structure solved by combination of direct methods and partial structure expansion by an iterative E–Fourier procedure using *SHELXTL* (Sheldrick, 1981). Least-squares refinement of all non-H atoms treated anisotropically; C(12), C(13) and C(14) show

* Contribution No. 797 of the Instituto de Química, UNAM.
† To whom correspondence should be addressed.

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