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α,α-Bis(1-methyl-4-trifluoromethyl-5-pyrazolyl)benzyl Benzoate and α-(1-Methyl-4-trifluoromethyl-3-pyrazolyl)-α-(1-methyl-4-trifluoromethyl-5-pyrazolyl)benzyl Benzoate: an Investigation into the Direction of Diazomethane Addition to α,α-Bis(3,3,3-trifluoropropynyl)benzyl Benzoate

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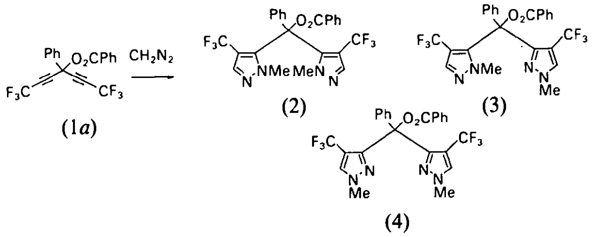
Abstract

The structures of the title compounds, two isomers of $C_{24}H_{18}F_6N_4O_2$, may be compared by considering the geometry about the tetrahedral benzyl C atoms. In each compound the planar phenyl and benzoate systems are aligned approximately parallel to the ester C—O bond with the latter substituent projecting between the phenyl and 1-methyl-4-trifluoromethylpyrazolyl rings. However, while both CF_3 substituents in the first molecule project away from the ester C—O bond [O—C—C—C(CF_3) −138.5 (5), −122.2 (6)°], removal of a methyl group to an outer N atom has reversed the situation in the second compound [O—C—C—C(CF_3) −63 (1), −41 (1) and 65 (1), 34 (1)° for the two molecules in the asymmetric unit, respectively].

Comment

The structure determinations reported herein form part of a general investigation of the reaction of 1,4-diynyl esters of type $(CF_3C{\equiv}C)_2C\mathit{R}O_2C\mathit{R}$ (1) with dienes and 1,3-dipolar reagents (Tajammal 1991; Barlow, Tajammal & Tipping 1992). The structures of the two crystalline bis(methylpyrazoles) (2) and (3) were required to determine the direction of addition of diazomethane to the 1,4-diynyl ester [(1*a*), *R* = Ph] and to establish the identity of the third isolated bis(methylpyrazole) (4).



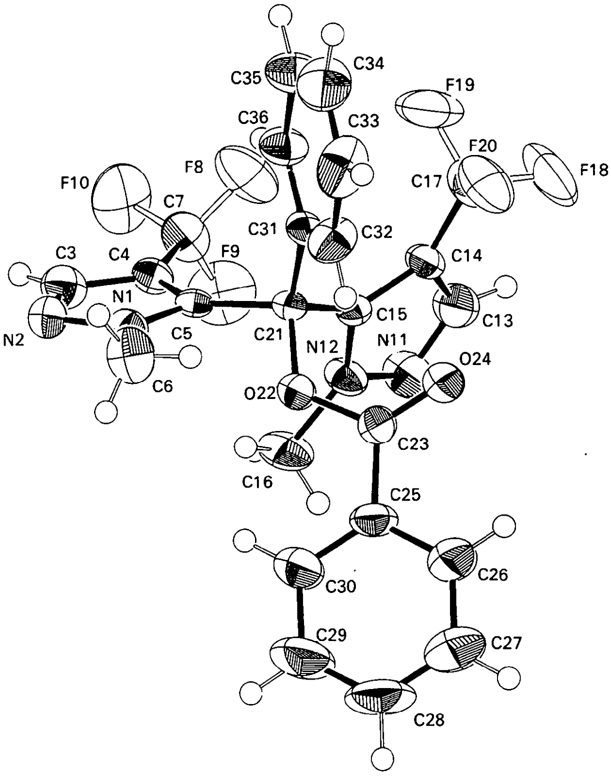


Fig. 1. α,α-Bis(1-methyl-4-trifluoromethylpyrazol-5-yl)benzyl benzoate, including atomic numbering scheme, drawn using *ORTEP*II (Johnson, 1976). Displacement ellipsoids are plotted at the 50% probability level.

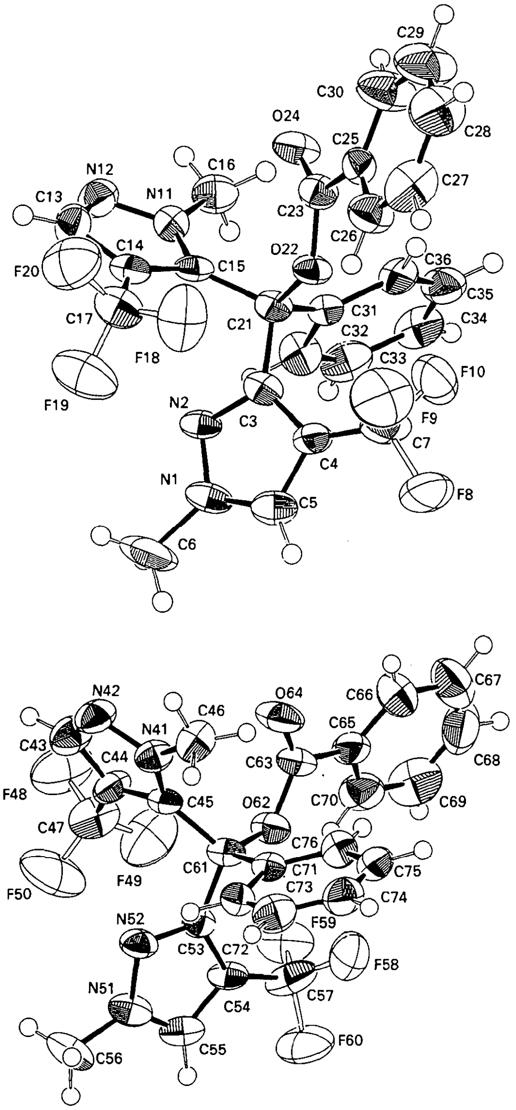


Fig. 2. The two molecules which comprise an asymmetric unit of α-(1-methyl-4-trifluoromethylpyrazol-3-yl)-α-(1-methyl-4-trifluoromethylpyrazol-5-yl)benzyl benzoate, including atomic numbering scheme, drawn using *ORTEP*II (Johnson, 1976). Displacement ellipsoids are plotted at the 50% probability level.

Experimental

A solution of diazomethane (1.91 g, 45.5 mmol) in diethyl ether (100 ml) was added to a stirred solution of α,α-bis(3,3,3-trifluoropropynyl)benzyl benzoate (1*a*) (4.50 g, 11.4 mmol) in diethyl ether (60 ml) at 273 K and stirring was continued at this temperature for 1 h. After warming to room temperature the solvent was removed *in vacuo* to give a solid residue (6.01 g) which was shown by TLC (eluant CH_2Cl_2/MeOH 98:2 *v*/*v*) to contain three major (R_F 0.75, 0.68 and 0.63) and several minor components. The major components were separated by repeated dry column flash chromatography (Merck Kieselgel 60_{GF254}; same eluant) then dissolved in diethyl ether, dried (P_2O_5) and the ether removed *in vacuo* to afford α,α-bis(1-methyl-4-trifluoromethylpyrazol-5-yl)benzyl benzoate (2) (1.15 g, 2.31 mmol, 23%; calculated for $C_{24}H_{18}F_6N_4O_2$ C 56.7, H 3.5, F 22.4, N 11.0%, *M* 508; found C 56.4, H 3.4, F 22.6, N 10.8%, M^+ 508; m.p. 418 K), α-(1-methyl-4-trifluoromethylpyrazol-3-yl)-α-(1-methyl-4-trifluoromethylpyrazol-5-yl)benzyl benzoate (3) (2.25 g, 4.40 mmol, 39%; found C 56.4, H 3.7, F 22.4, N 11.0%, M^+ 508; m.p. 421 K) and α,α-bis(1-methyl-4-trifluoromethylpyrazol-3-yl)benzyl benzoate (4) (1.04 g, 2.05 mmol, 18%; found C 56.5, H 3.5, F 22.4, N 11.1%, M^+ 508; m.p. 502 K). Compounds (2) and (3) were recrystallized from CH_2Cl_2.

Compound (2)

Crystal data

$C_{24}H_{18}F_6N_4O_2$
$M_r = 508.42$
Monoclinic
$P2_1/c$
$a = 10.503$ (3) Å
$b = 10.268$ (3) Å
$c = 21.750$ (4) Å
$\beta = 97.03$ (2)°
$V = 2328$ (1) Å^3
$Z = 4$
$D_x = 1.450$ Mg m^{-3}

Mo *K*α radiation
$\lambda = 0.71069$ Å
Cell parameters from 24 reflections
$\theta = 12.37$–$17.64°$
$\mu = 0.1205$ mm^{-1}
$T = 296$ K
Needle
0.40 × 0.20 × 0.20 mm
Colourless

Data collection

AFC-6*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: refined from Δ*F* (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.87$, $T_{\max} = 1.12$
4624 measured reflections
4370 independent reflections
1975 observed reflections [$I > 3\sigma(I)$]

$R_{\text{int}} = 0.031$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 11$
$l = -24 \rightarrow 24$
3 standard reflections monitored every 150 reflections intensity variation: none

Refinement

Refinement on *F*
$R = 0.055$
$wR = 0.036$
$S = 2.55$
1975 reflections
325 parameters
H-atom parameters not refined
Weighting scheme based on measured e.s.d.'s

$(\Delta/\sigma)_{\max} = 0.0054$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}
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) *for* (2)

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

	x	*y*	*z*	U_{eq}
N1	0.7022 (3)	0.8593 (4)	0.6723 (2)	0.035 (2)
N2	0.6185 (4)	0.9439 (4)	0.6414 (2)	0.045 (2)
C3	0.5431 (5)	0.8694 (6)	0.6042 (2)	0.049 (3)
C4	0.5759 (4)	0.7389 (5)	0.6096 (2)	0.035 (2)
C5	0.6805 (4)	0.7336 (4)	0.6547 (2)	0.027 (2)
C6	0.8051 (5)	0.9162 (5)	0.7152 (2)	0.059 (3)
C7	0.5110 (5)	0.6395 (6)	0.5695 (3)	0.055 (3)

F8	0.5902 (3)	0.5570 (3)	0.5449 (1)	0.081 (2)
F9	0.4290 (3)	0.5624 (3)	0.5953 (2)	0.087 (2)
F10	0.4379 (3)	0.6926 (3)	0.5210 (1)	0.094 (2)
N11	0.5904 (4)	0.4734 (4)	0.7005 (2)	0.042 (2)
N12	0.5461 (4)	0.3511 (4)	0.6938 (2)	0.061 (3)
C13	0.6303 (5)	0.2899 (5)	0.6641 (3)	0.058 (3)
C14	0.7292 (5)	0.3713 (5)	0.6513 (2)	0.040 (3)
C15	0.7017 (4)	0.4909 (4)	0.6755 (2)	0.031 (2)
C16	0.5171 (4)	0.5624 (5)	0.7353 (2)	0.058 (3)
C17	0.8375 (6)	0.3230 (6)	0.6201 (3)	0.063 (3)
F18	0.8365 (3)	0.1921 (3)	0.6193 (2)	0.111 (2)
F19	0.8343 (3)	0.3596 (3)	0.5616 (2)	0.089 (2)
F20	0.9544 (3)	0.3561 (3)	0.6471 (2)	0.084 (2)
C21	0.7676 (4)	0.6239 (4)	0.6820 (2)	0.031 (2)
O22	0.7849 (3)	0.6540 (3)	0.7494 (1)	0.037 (2)
C23	0.8350 (4)	0.5615 (5)	0.7905 (2)	0.043 (3)
O24	0.8885 (3)	0.4655 (3)	0.7753 (2)	0.056 (2)
C25	0.8089 (5)	0.5905 (5)	0.8553 (2)	0.047 (3)
C26	0.8583 (5)	0.5048 (6)	0.9007 (3)	0.065 (3)
C27	0.8304 (6)	0.5213 (7)	0.9608 (3)	0.086 (4)
C28	0.7577 (7)	0.6228 (8)	0.9746 (3)	0.090 (5)
C29	0.7092 (6)	0.7094 (7)	0.9304 (3)	0.096 (4)
C30	0.7362 (5)	0.6940 (6)	0.8698 (3)	0.069 (3)
C31	0.8943 (4)	0.6339 (4)	0.6542 (2)	0.035 (2)
C32	1.0107 (4)	0.6504 (5)	0.6894 (2)	0.052 (3)
C33	1.1210 (5)	0.6617 (6)	0.6600 (3)	0.075 (4)
C34	1.1134 (6)	0.6567 (7)	0.5965 (3)	0.080 (4)
C35	0.9974 (5)	0.6440 (6)	0.5613 (3)	0.067 (3)
C36	0.8890 (4)	0.6340 (5)	0.5904 (2)	0.049 (3)

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

C5—C21	1.525 (6)	C21—C31	1.531 (5)
C15—C21	1.530 (6)	O22—C23	1.365 (5)
C21—O22	1.487 (5)		
C5—C21—C15	112.3 (4)	C15—C21—O22	106.1 (3)
C5—C21—O22	103.0 (3)	C15—C21—C31	115.4 (4)
C5—C21—C31	107.8 (4)	O22—C21—C31	111.6 (4)

Compound (3)

Crystal data

$C_{24}H_{18}F_6N_4O_2$
$M_r = 508.42$
Triclinic
$P\bar{1}$
$a = 9.701$ (3) Å
$b = 26.934$ (7) Å
$c = 8.832$ (2) Å
$\alpha = 94.18$ (2)°
$\beta = 93.37$ (2)°
$\gamma = 85.44$ (2)°
$V = 2291$ (2) Å^3
$Z = 4$
$D_x = 1.474$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 23 reflections
$\theta = 12.23$–18.38°
$\mu = 0.1224$ mm^{-1}
$T = 296$ K
Needle
0.40 × 0.30 × 0.20 mm
Colourless

Data collection

AFC-6*S* diffractometer
ω scans with profile analysis
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.85$, $T_{\max} = 1.03$
8611 measured reflections
8072 independent reflections
2953 observed reflections [$I > 3\sigma(I)$]

$R_{\rm int} = 0.0295$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 11$
$k = -30 \rightarrow 30$
$l = -10 \rightarrow 10$
3 standard reflections monitored every 150 reflections intensity variation: −1.50%

Refinement

Refinement on F
$R = 0.069$
$wR = 0.061$
$S = 3.27$
2953 reflections
661 parameters
H-atom parameters not refined
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{\max} = 0.0262$

$\Delta\rho_{\max} = 0.34$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}
Extinction correction: Zachariasen (1967) Type II, Gaussian, isotropic
Extinction coefficient: 1.51×10^{-7}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (3)

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

	x	y	z	$U_{\rm eq}$
N1	0.3265 (9)	0.3534 (3)	0.712 (1)	0.047 (5)
N2	0.4636 (8)	0.3440 (3)	0.6908 (9)	0.039 (4)
C3	0.525 (1)	0.3560 (3)	0.825 (1)	0.036 (5)
C4	0.427 (1)	0.3723 (4)	0.934 (1)	0.045 (6)
C5	0.301 (1)	0.3696 (4)	0.853 (1)	0.048 (6)
C6	0.227 (1)	0.3450 (5)	0.584 (1)	0.099 (8)
C7	0.441 (1)	0.3902 (6)	1.093 (1)	0.072 (8)
F8	0.3266 (6)	0.3853 (3)	1.1681 (7)	0.091 (4)
F9	0.4673 (8)	0.4363 (3)	1.1185 (8)	0.105 (5)
F10	0.5432 (7)	0.3649 (3)	1.1730 (7)	0.089 (4)
N11	0.8419 (8)	0.3191 (3)	0.6211 (10)	0.042 (5)
N12	0.8762 (8)	0.3323 (3)	0.487 (1)	0.052 (5)
C13	0.801 (1)	0.3765 (4)	0.467 (1)	0.055 (6)
C14	0.716 (1)	0.3897 (4)	0.589 (1)	0.050 (6)
C15	0.7431 (9)	0.3496 (4)	0.687 (1)	0.036 (5)
C16	0.922 (1)	0.2747 (4)	0.676 (1)	0.054 (6)
C17	0.621 (1)	0.4336 (5)	0.596 (2)	0.067 (8)
F18	0.5933 (8)	0.4522 (3)	0.7353 (8)	0.095 (5)
F19	0.4993 (7)	0.4291 (2)	0.5230 (8)	0.100 (5)
F20	0.6764 (7)	0.4715 (3)	0.5314 (8)	0.097 (5)
C21	0.6812 (10)	0.3450 (3)	0.840 (1)	0.035 (5)
O22	0.7251 (6)	0.3860 (2)	0.9485 (7)	0.039 (3)
C23	0.861 (1)	0.3941 (4)	0.969 (1)	0.042 (6)
O24	0.9531 (7)	0.3679 (3)	0.9080 (8)	0.052 (4)
C25	0.884 (1)	0.4366 (4)	1.082 (1)	0.043 (6)
C26	0.780 (1)	0.4711 (4)	1.129 (1)	0.058 (6)
C27	0.809 (1)	0.5086 (4)	1.237 (1)	0.070 (7)
C28	0.941 (2)	0.5136 (5)	1.294 (1)	0.09 (1)
C29	1.045 (1)	0.4803 (6)	1.248 (2)	0.10 (1)
C30	1.017 (1)	0.4409 (5)	1.142 (1)	0.081 (8)
C31	0.7057 (9)	0.2940 (4)	0.908 (1)	0.040 (5)
C32	0.648 (1)	0.2543 (4)	0.826 (1)	0.050 (6)
C33	0.663 (1)	0.2078 (4)	0.884 (1)	0.061 (7)
C34	0.732 (1)	0.2004 (4)	1.025 (1)	0.061 (7)
C35	0.786 (1)	0.2422 (4)	1.105 (1)	0.057 (6)
C36	0.774 (1)	0.2880 (3)	1.049 (1)	0.050 (6)
N41	0.6006 (9)	0.2013 (3)	0.3925 (9)	0.046 (5)
N42	0.7343 (10)	0.1941 (3)	0.4477 (10)	0.058 (5)
C43	0.760 (1)	0.1461 (5)	0.449 (1)	0.064 (7)
C44	0.645 (1)	0.1209 (4)	0.398 (1)	0.052 (6)
C45	0.543 (1)	0.1566 (4)	0.359 (1)	0.043 (6)
C46	0.541 (1)	0.2532 (4)	0.389 (1)	0.056 (7)
C47	0.648 (2)	0.0664 (4)	0.389 (2)	0.068 (8)
F48	0.7339 (8)	0.0472 (3)	0.4987 (8)	0.112 (5)
F49	0.5274 (8)	0.0479 (3)	0.4111 (9)	0.112 (5)
F50	0.6898 (9)	0.0434 (3)	0.2609 (9)	0.125 (6)
N51	0.4650 (10)	0.0740 (3)	−0.0377 (10)	0.049 (5)
N52	0.4973 (9)	0.1100 (3)	0.0743 (9)	0.049 (5)
C53	0.395 (1)	0.1096 (4)	0.171 (1)	0.043 (5)
C54	0.298 (1)	0.0760 (3)	0.116 (1)	0.048 (6)
C55	0.348 (1)	0.0537 (4)	−0.018 (1)	0.063 (7)
C56	0.553 (1)	0.0647 (5)	−0.167 (1)	0.087 (8)
C57	0.172 (1)	0.0620 (5)	0.179 (1)	0.070 (8)

F58	0.0835 (7)	0.0979 (3)	0.2279 (8)	0.089 (5)
F59	0.1992 (7)	0.0321 (2)	0.2988 (7)	0.085 (4)
F60	0.0996 (7)	0.0327 (3)	0.0763 (7)	0.102 (5)
C61	0.393 (1)	0.1494 (3)	0.302 (1)	0.038 (5)
O62	0.3176 (6)	0.1301 (2)	0.4174 (7)	0.048 (4)
C63	0.313 (1)	0.1549 (4)	0.555 (1)	0.051 (6)
O64	0.3790 (8)	0.1892 (3)	0.5978 (7)	0.071 (5)
C65	0.212 (1)	0.1364 (5)	0.653 (1)	0.058 (5)
C66	0.163 (1)	0.1661 (4)	0.771 (1)	0.072 (7)
C67	0.060 (2)	0.1519 (6)	0.860 (1)	0.09 (1)
C68	0.008 (1)	0.1081 (7)	0.826 (2)	0.09 (1)
C69	0.055 (1)	0.0743 (5)	0.711 (2)	0.083 (8)
C70	0.157 (1)	0.0920 (5)	0.622 (1)	0.069 (7)
C71	0.313 (1)	0.1964 (3)	0.239 (1)	0.035 (5)
C72	0.358 (1)	0.2158 (4)	0.113 (1)	0.052 (6)
C73	0.288 (1)	0.2576 (5)	0.053 (1)	0.064 (7)
C74	0.171 (1)	0.2787 (4)	0.118 (2)	0.070 (8)
C75	0.125 (1)	0.2604 (5)	0.243 (1)	0.066 (7)
C76	0.193 (1)	0.2188 (4)	0.303 (1)	0.048 (6)

Table 4. *Selected geometric parameters* (Å, °) *for* (3)

C3—C21	1.52 (1)	C45—C61	1.53 (1)
C15—C21	1.53 (1)	C53—C61	1.52 (1)
C21—O22	1.48 (1)	C61—O62	1.44 (1)
C21—C31	1.53 (1)	C61—C71	1.55 (1)
C3—C21—C15	109.5 (8)	C45—C61—C53	108.6 (8)
C3—C21—O22	102.6 (7)	C45—C61—O62	110.7 (7)
C3—C21—C31	106.2 (8)	C45—C61—C71	114.8 (8)
C15—C21—O22	109.3 (7)	C53—C61—O62	105.5 (8)
C15—C21—C31	116.4 (7)	C53—C61—C71	106.0 (7)
O22—C21—C31	112.0 (7)	O62—C61—C71	110.6 (8)

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1989). Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *TEXSAN*; *MITHRIL* (Gilmore, 1984). Program(s) used to refine structure: *TEXSAN LS*. Molecular graphics: *TEXSAN*; *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *TEXSAN FINISH*. Literature survey: *CSSR* (1984).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: LI1106). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure Analysis of a Reversible Monoamine Oxidase A Inhibitor: 3-{4-[(*R*)-3-Hydroxybutoxy]phenyl}-(*R*)-5-methoxymethyl-1,3-oxazolidin-2-one

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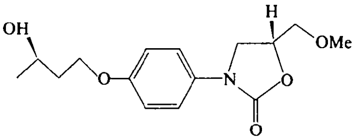
Abstract

The structure of a new reversible type-A MAO inhibitor and analogue of befloxatone is reported. Within experimental deviations, the oxazolidinone moiety of the title compound is planar and quasi coplanar with the adjacent phenyl ring [12.2 (5)°]. The sum of the angles at the N atom is 359.8°, indicating sp^2 hybridization of this atom. This is consistent with electron delocalization between the N atom and the carbonyl group [N—(C=O) 1.365 (4) Å] in the oxazolidinone ring. The lateral butoxy chain is all *trans*. As a result, the molecule is very flat with only the (*R*)-5-methoxymethyl chain and the terminal hydroxyl group out of the plane. The hydroxyl group is involved in the hydrogen bonding responsible for crystal cohesion.

Comment

In the course of our study of monoamine oxidase (MAO) inhibitors (Moureau *et al.*, 1992; Wouters, Perpete, Norberg, Evrard & Durant, 1994), we report here the X-ray structure of the title compound (I), a new reversible type-A MAO inhibitor and analogue of befloxatone (Koenig *et al.*, 1992).



(I)

Original inhibitors of monoamine oxidase (MAO) have been developed by Delalande Research (Groupe Synthelabo) in the aryloxazolidinone series. They belong to the (*R*)-5-methoxymethyl-3-aryloxazolidin-2-one family, are selective for the A form of the enzyme, are reversible and competitive against tyramine (Koenig *et al.*, 1992). Structure–activity results clearly revealed the crucial role that a hydroxybutoxy lateral chain has

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