cally refined. Atomic scattering factors as stored in the *NRCVAX* program were those of Cromer & Waber (1974). Function minimized: $\Sigma w(|F_o| - |F_c|)^2$, $w = 1/\sigma^2(F)$.

Discussion. The atomic parameters x, y, z and B_{eq} are listed in Table 1.* Intramolecular distances and angles are given in Table 2. The numbering scheme is shown along with an *ORTEP* view of the molecules in Fig. 1.

The tricyclic carbon backbone is identical in the four compounds. The crystal structure determinations of the two pairs of Diels–Alder adducts show that the compounds have the convenient stereochemistry at C(5) to permit a possible connection between C(17) and C(1) (Fig. 1). The reasons for the failure of the cyclization reaction *via* aldol condensation are still to be clarified.

---

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, torsion angles and spectroscopic data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53595 (84 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Interestingly, the separations of pairs of diastereomers (4*a*)/(5*a*) and (4*b*)/(5*b*) by thin-layer chromatography was made possible by the differences in polarities generated by different orientations of the lactone moiety, as revealed by the present study.

No abnormal intermolecular contacts were observed.

References

CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

DESLONGCHAMPS, P., BÉLANGER A., BERNEY, D. J. F., BORSCH-BERG, H.-J., BROUSSEAU, R., DOUTHEAU, A., DURAND, R., KATAYAMA, H., LAPALME, R., LETURC, D. M., LIAO, C.-C., MACLACHLAN, F. N., MAFFRAND, J.-P., MARAZZA, F., MARTINO, R., MOREAU, C., RUEST, L., ST-LAURENT, L., SAINTONGE, R. & SOUCY, P. (1990). *Can. J. Chem.* **68**, 115–126.

GABE, E. J., LEE, F. L. & LE PAGE, Y. (1985). *The NRCVAX Crystal Structure System.* In *Crystallographic Computing 3: Data Collection, Structure Determination, Proteins and Databases*, edited by G. M. SHELDRICK, C. KRÜGER & R. GODDARD, pp. 167–174. Oxford: Clarendon Press.

JOHNSON, C. K. (1976). *ORTEPII.* Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

LARSON, A. C. (1967). *Acta Cryst.* **23**, 664–665.

ZACHARIASEN, W. H. (1963). *Acta Cryst.* **16**, 1139–1144.

Structure of Two Pyrethroid Insecticides: Acrynathryn (RU 38702) and a Derivative (RU 38181)*

BY F. BAERT AND A. GUELZIM

Laboratoire de Dynamique des Cristaux Moléculaires associé au CNRS UA 801,
Université des Sciences et Techniques de Lille Flandres Artois, 59655 Villeneuve d'Ascq CEDEX, France

AND G. GERMAIN

Laboratoire de Chimie Quantique, Bâtiment Lavoisier, Place Louis Pasteur 1, B-1348 Louvain-la-Neuve, Belgium

Abstract. The crystal structures of two crystalline pyrethroid insecticides have been determined at 293 K from three-dimensional X-ray diffraction data. (I), α-cyano-3-phenoxybenzyl 2-(*tert*-butoxycarbonylvinyl)-3,3-dimethylcyclopropanecarboxylate (RU 38181), $C_{27}H_{29}NO_5$, monoclinic, $P2_1$, $M_r = 447.5$, $a = 17.740$ (9), $b = 6.133$ (3), $c = 11.064$ (7) Å, $\beta = 98.96$ (0.5)°, $Z = 2$, $V = 1189.1$ Å^3, $D_x = 1.25$ Mg m^{-3}, Mo $K\bar\alpha$, $\lambda = 0.7107$ Å, $\mu = 0.50$ mm^{-1}, $F(000) = 476$. (II), α-cyano-3-phenoxybenzyl 2-(1,1,1,3,3,3-hexafluoro-2-propoxy-carbonylvinyl)-3,3-dimethylcyclopropanecarboxylate (RU 38702), $C_{26}H_{21}F_6NO_5$, orthorhombic, $P2_12_12_1$, $M_r = 541.4$, $a = 9.400$ (7), $b = 37.323$ (13), $c = 7.535$ (4) Å, $Z = 4$, $V = 2643.6$ Å^3, $D_x = 1.36$ Mg m^{-3}, Mo $K\bar\alpha$, $\lambda = 0.7107$ Å, $\mu = 0.81$ mm^{-1}, $F(000) = 1112$. The residual R factors are 0.054 and 0.084 respectively for the observed structure factors with $I > 3\sigma(I)$. The most significant

---

discrepancies between the two molecules are in the conformations of the 3-phenoxybenzyl groups.

Introduction. Biological activity in pyrethroids is related to molecular structure and strongly dependent on the stereochemistry at the three asymmetric centres: C_1, C_3 and C_α (Tessier, 1985).

An extra geometric isomerism appears in 'nor pyrethric' structures. In these products, strong insecticidal and miticidal properties are only found with Z geometry in the olefinic side chain (Tessier, Teche & Demoute, 1983). We are concerned here with compounds of the general formula depicted below.
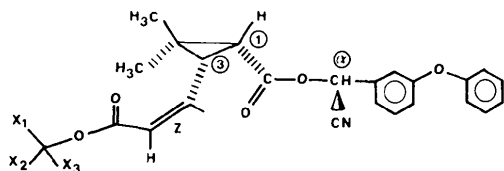
(I) RU 38181 $X_1 = X_2 = X_3 = CH_3$

(II) RU 38702 $X_1 = X_2 = CF_3$, $X_3 = H$

The conformations of the two compounds, RU 38181 and RU 38702 (acrynathrin), are compared with each other.

Experimental. Both crystals had a prismatic shape, $0.6 \times 0.4 \times 0.2$ mm for (I) and $0.3 \times 0.15 \times 0.4$ mm for (II). Philips PW1100 four-circle diffractometer, room temperature, Mo $K\alpha$ radiation, lattice parameters from 25 reflections $(20 < \theta < 27°)$; $\omega{-}2\theta$ scan, scan width $= 1.3°$, scan speed $= 0.010°$ s^{-1} for both crystals, $-24 < h < 24$, $0 < k < 8$, $0 < l < 15$
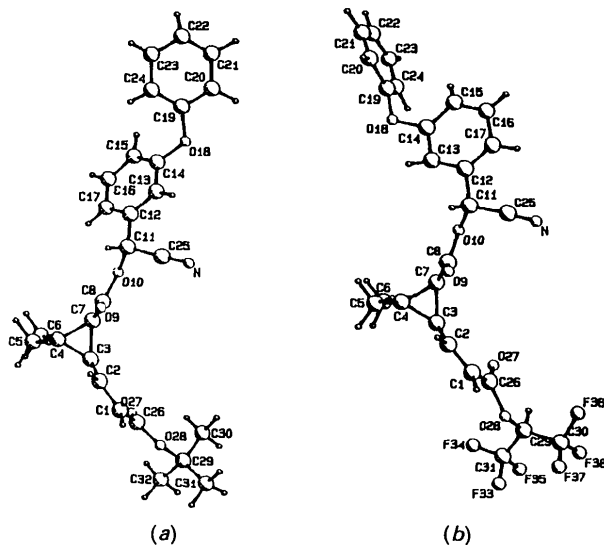

(a)   (b)

Fig. 1. Perspective view of the molecule and key to the numbering system used. (a) RU 38181 and (b) RU 38702.

Table 1. *Atomic coordinates* $(\times 10^4)$ *and* U_{eq} *values* $(\mathring{A}^2 \times 10^3)$

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

	x	y	z	U_{eq}
(I)				
C(1)	9280 (4)	5119 (16)	5078 (6)	35 (8)
C(2)	8955 (4)	6460 (15)	4135 (7)	33 (8)
C(3)	8235 (3)	7658 (16)	4068 (6)	30 (8)
C(4)	8113 (3)	9726 (15)	3322 (6)	30 (8)
C(5)	8750 (4)	10588 (15)	2682 (7)	40 (9)
C(6)	7636 (4)	11474 (15)	3811 (6)	37 (9)
C(7)	7654 (3)	7679 (15)	2870 (6)	29 (8)
C(8)	7768 (4)	6536 (14)	1748 (6)	34 (8)
O(9)	8336 (2)	6105 (12)	1349 (4)	42 (6)
O(10)	7049 (2)	5934 (1)	1166 (4)	29 (5)
C(11)	7019 (4)	5006 (15)	−30 (6)	29 (8)
C(25)	7232 (4)	2640 (17)	89 (7)	36 (9)
N	7367 (4)	843 (16)	175 (6)	51 (9)
C(12)	6213 (4)	5281 (15)	−694 (6)	30 (8)
C(13)	5855 (4)	3662 (15)	−1440 (6)	38 (8)
C(14)	5117 (4)	3973 (15)	−2040 (6)	31 (8)
C(15)	4719 (4)	5879 (16)	−1875 (6)	39 (9)
C(16)	5096 (4)	7519 (16)	−1156 (7)	48 (10)
C(17)	5841 (4)	7226 (15)	−563 (7)	34 (9)
O(18)	4771 (3)	2227 (12)	−2672 (5)	40 (7)
C(19)	4364 (4)	2474 (17)	−3836 (6)	37 (9)
C(20)	3884 (3)	736 (18)	−4240 (7)	42 (9)
C(21)	3461 (4)	795 (20)	−5399 (8)	47 (11)
C(22)	3532 (5)	2549 (22)	3859 (7)	54 (13)
C(23)	4000 (5)	4264 (19)	−5753 (7)	63 (12)
C(24)	4431 (4)	4250 (17)	−4576 (7)	41 (10)
C(26)	8922 (4)	4558 (16)	6162 (6)	33 (9)
O(27)	8388 (3)	5437 (13)	6494 (4)	64 (7)
O(28)	9298 (2)	2846 (12)	6713 (4)	46 (6)
C(29)	9049 (4)	1784 (16)	7810 (6)	47 (9)
C(30)	8232 (4)	957 (19)	7460 (7)	52 (12)
C(31)	9615 (5)	−70 (18)	8078 (8)	80 (13)
C(32)	9138 (5)	3439 (19)	8846 (7)	53 (13)
(II)				
C(19)	8042 (25)	776 (4)	3774 (19)	54 (27)
C(20)	8913 (19)	487 (6)	3274 (23)	97 (29)
C(21)	8224 (27)	221 (4)	2459 (25)	89 (31)
C(22)	6751 (26)	221 (5)	2237 (25)	72 (33)
C(23)	5933 (19)	473 (5)	2843 (25)	88 (28)
C(24)	6594 (23)	766 (3)	3565 (24)	87 (27)
O(18)	8648 (18)	1097 (3)	4451 (13)	94 (23)
C(13)	9191 (18)	1478 (4)	6831 (18)	63 (21)
C(14)	8681 (19)	1153 (4)	6278 (19)	60 (22)
C(15)	8185 (17)	890 (3)	7466 (18)	46 (18)
C(16)	8324 (15)	955 (4)	9219 (18)	55 (19)
C(17)	8872 (17)	1288 (4)	9823 (16)	47 (18)
C(12)	9311 (13)	1539 (3)	8621 (17)	40 (15)
C(11)	9923 (16)	1897 (3)	9172 (17)	50 (17)
C(25)	9903 (19)	1950 (3)	11140 (22)	71 (22)
N	9918 (19)	2007 (4)	12593 (21)	95 (25)
O(10)	9117 (9)	2179 (2)	8317 (12)	47 (11)
C(8)	9832 (15)	2493 (3)	8144 (21)	58 (20)
O(9)	10984 (10)	2543 (2)	8666 (17)	71 (17)
C(7)	8830 (15)	2743 (3)	7130 (19)	58 (19)
C(4)	9353 (17)	2953 (4)	5560 (24)	76 (25)
C(5)	10993 (19)	2924 (5)	4964 (26)	123 (32)
C(6)	8230 (22)	3008 (4)	4086 (23)	92 (30)
C(3)	8991 (15)	3153 (3)	7274 (21)	64 (20)
C(2)	10141 (15)	3309 (2)	8428 (22)	65 (21)
C(1)	9967 (14)	3572 (3)	9618 (23)	57 (22)
C(26)	8584 (17)	3717 (3)	10024 (21)	59 (21)
C(31)	7369 (26)	4546 (6)	10379 (34)	117 (39)
O(27)	7409 (11)	3610 (3)	9736 (17)	66 (18)
O(28)	8756 (9)	4044 (2)	10952 (15)	57 (13)
C(29)	7548 (17)	4234 (4)	11513 (22)	61 (24)
C(30)	7687 (29)	4309 (5)	13480 (31)	95 (38)
F(33)	8458 (14)	4774 (3)	10643 (21)	139 (24)
F(36)	7747 (20)	3982 (3)	14309 (17)	192 (30)
F(34)	7280 (17)	4470 (4)	8731 (17)	152 (25)
F(38)	6570 (14)	4461 (3)	14124 (19)	136 (25)
F(35)	6181 (13)	4739 (3)	10871 (24)	199 (28)
F(37)	8841 (14)	4484 (4)	13825 (18)	106 (24)

(I), $0 < h < 13$, $0 < k < 49$, $0 < l < 9$ (II), $2\theta_{max} = 60°$ for (I) and (II), 1709 reflections (I) and 1643 (II) with $I > 3\sigma(I)$ used for structure

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

	(I)	(II)
C(1)—C(2)	1·383 (11)	1·342 (20)
C(1)—C(26)	1·482 (10)	1·449 (20)
C(2)—C(3)	1·464 (11)	1·505 (20)
C(3)—C(4)	1·510 (12)	1·530 (22)
C(3)—C(7)	1·547 (9)	1·539 (15)
C(4)—C(5)	1·519 (10)	1·609 (25)
C(4)—C(6)	1·517 (11)	1·547 (26)
C(4)—C(7)	1·538 (12)	1·501 (22)
C(7)—C(8)	1·468 (10)	1·531 (18)
C(8)—O(9)	1·190 (8)	1·168 (17)
C(8)—O(10)	1·387 (8)	1·358 (13)
O(10)—C(11)	1·433 (8)	1·446 (14)
C(11)—C(25)	1·500 (14)	1·495 (21)
C(11)—C(12)	1·512 (9)	1·513 (15)
C(25)—N	1·129 (14)	1·114 (23)
C(12)—C(13)	1·382 (11)	1·373 (19)
C(12)—C(17)	1·382 (12)	1·368 (17)
C(13)—C(14)	1·385 (10)	1·369 (20)
C(14)—C(15)	1·393 (12)	1·406 (19)
C(14)—O(18)	1·371 (10)	1·392 (17)
C(15)—C(16)	1·387 (12)	1·349 (19)
C(16)—C(17)	1·393 (11)	1·421 (19)
O(18)—C(19)	1·383 (8)	1·422 (21)
C(19)—C(20)	1·394 (13)	1·405 (27)
C(19)—C(24)	1·379 (13)	1·371 (31)
C(21)—C(22)	1·373 (13)	1·395 (35)
C(23)—C(22)	1·370 (13)	1·298 (28)
C(20)—C(21)	1·382 (11)	1·336 (27)
C(23)—C(24)	1·404 (11)	1·371 (21)
C(26)—O(27)	1·196 (9)	1·195 (18)
C(26)—O(28)	1·338 (11)	1·421 (18)
O(28)—C(29)	1·503 (9)	1·404 (18)
C(29)—C(30)	1·530 (13)	1·514 (29)
C(29)—C(31)	1·516 (13)	1·452 (28)
C(29)—C(32)	1·520 (13)	
C(31)—F(33)		1·347 (26)
C(31)—F(34)		1·276 (28)
C(31)—F(35)		1·379 (27)
C(30)—F(36)		1·370 (24)
C(30)—F(37)		1·293 (29)
C(30)—F(38)		1·290 (29)
C(2)—C(1)—C(26)	124·6 (7)	121·8 (13)
C(1)—C(2)—C(3)	126·5 (7)	125·6 (13)
C(2)—C(3)—C(4)	119·9 (6)	121·1 (12)
C(2)—C(3)—C(7)	120·5 (6)	119·7 (11)
C(4)—C(3)—C(7)	60·4 (5)	58·6 (9)
C(3)—C(4)—C(5)	119·6 (6)	118·8 (13)
C(3)—C(4)—C(6)	116·0 (6)	112·9 (13)
C(3)—C(4)—C(7)	61·0 (5)	61·0 (9)
C(5)—C(4)—C(6)	114·7 (6)	117·5 (14)
C(5)—C(4)—C(7)	121·9 (6)	120·0 (13)
C(6)—C(4)—C(7)	113·3 (6)	114·3 (13)
C(3)—C(7)—C(4)	58·6 (5)	60·4 (9)
C(3)—C(7)—C(8)	124·0 (6)	120·7 (11)
C(4)—C(7)—C(8)	121·9 (6)	120·7 (12)
C(7)—C(8)—O(9)	131·0 (7)	130·0 (13)
C(7)—C(8)—O(10)	106·4 (6)	105·7 (10)
O(9)—C(8)—O(10)	122·6 (6)	124·3 (12)
C(8)—O(10)—C(11)	115·7 (5)	114·2 (9)
O(10)—C(11)—C(25)	109·3 (6)	109·8 (10)
O(10)—C(11)—C(12)	107·5 (6)	108·6 (10)
C(25)—C(11)—C(12)	110·9 (6)	112·6 (11)
C(11)—C(25)—N	177·7 (9)	176·2 (17)
C(11)—C(12)—C(13)	121·5 (7)	116·7 (11)
C(11)—C(12)—C(17)	118·5 (7)	122·6 (11)
C(13)—C(12)—C(17)	120·0 (7)	120·7 (12)
C(12)—C(13)—C(14)	120·0 (7)	118·5 (13)
C(13)—C(14)—C(15)	120·9 (7)	122·6 (14)
C(15)—C(14)—O(18)	121·7 (7)	121·2 (13)
C(14)—C(15)—C(16)	118·3 (7)	117·9 (13)
C(15)—C(16)—C(17)	120·9 (8)	120·3 (13)
C(12)—C(17)—C(16)	119·7 (7)	119·8 (12)
C(14)—O(18)—C(19)	121·1 (6)	119·3 (11)
O(18)—C(19)—C(20)	114·8 (7)	120·8 (16)
O(18)—C(19)—C(24)	·124·0 (7)	117·5 (16)
C(20)—C(19)—C(24)	121·2 (8)	121·8 (17)
C(21)—C(22)—C(23)	121·6 (9)	123·1 (19)
C(19)—C(20)—C(21)	119·6 (8)	114·3 (18)
C(19)—C(24)—C(23)	118·1 (8)	121·1 (17)
C(1)—C(26)—O(27)	127·1 (7)	132·0 (14)
C(1)—C(26)—O(28)	107·8 (6)	109·0 (12)
O(27)—C(26)—O(28)	125·1 (7)	119·0 (13)
C(26)—O(28)—C(29)	121·3 (6)	119·5 (11)

Table 2 (*cont.*)

	(I)	(II)
O(28)—C(29)—C(30)	109·0 (6)	108·5 (14)
O(28)—C(29)—C(31)	102·4 (6)	108·8 (15)
C(30)—C(20)—C(31)	112·0 (7)	116·1 (17)
O(28)—C(29)—C(32)	108·0 (6)	
C(30)—C(29)—C(32)	113·4 (7)	
C(31)—C(29)—C(32)	111·4 (7)	
C(29)—C(31)—F(33)		109·3 (18)
C(29)—C(31)—F(34)		113·7 (19)
C(29)—C(31)—F(35)		110·7 (18)
F(33)—C(31)—F(34)		109·5 (19)
F(33)—C(31)—F(35)		104·2 (18)
F(34)—C(31)—F(35)		108·9 (19)
C(29)—C(30)—F(36)		106·7 (17)
C(29)—C(30)—F(38)		112·3 (18)
C(29)—C(30)—F(37)		111·2 (18)
F(36)—C(30)—F(38)		104·8 (18)
F(36)—C(30)—F(37)		108·9 (19)
F(38)—C(30)—F(37)		112·6 (19)

refinement, three standard reflections and no intensity variation. Lp correction applied, absorption and extinction ignored.

Direct methods using 499 reflections with $E > 1·43$ (I), $E > 1·48$ (II) in *MULTAN* (Germain, Main & Woolfson, 1971) and Fourier methods, anisotropic full-matrix refinement on F (Sheldrick, 1976), H from $\Delta\rho$ synthesis and theoretically adjusted, isotropically refined; atomic scattering factors from *International Tables for X-ray Crystallography* (1974), and for H atoms from Stewart, Davidson & Simpson (1965); final $R = 0·054$ (I) and 0·084 (II), unit weights; $\Delta\rho$ in final map $= 0·27$, $-0·26$ e Å^{-3} (I), 0·23, $-0·26$ e Å^{-3} (II); $(\Delta/\sigma)_{max} = 0·035$ (I), 0·65 (II).

Discussion. Fractional coordinates and equivalent isotropic thermal parameters for non-H atoms are given in Table 1, selected interatomic distances and angles in Table 2.* The conformation of the molecules and the atomic numbering are depicted in Fig. 1.

The mean C—C distance in the phenyl rings is 1·383 (3) Å, except for the terminal ring of the 3-phenoxybenzyl group in (II) where we observe a shortening of two distances which reduced the mean value to 1·362 (5) Å. The cyclopropane rings have mean bond lengths of 1·531 (4) for (I) and 1·523 (5) Å for (II).

The two molecules are almost identical, except at the end of the molecule the 3-phenoxybenzyl group has slightly changed its conformation [C(14)—O(18)—C(19)—C(24) = -14 (0·7)° (I), and 83 (2)° (II)], while the whole group has rotated around the C(11)—C(12) bond [O(10)—C(11)—C(12)—(13) =

$-140\ (0\cdot8)^\circ$ (I), 54 (1)° (II)]. It seems that there is a certain degree of flexibility at each end of the molecule with the cyclopropane carboxylic linkage in the middle forming a fairly rigid entity. No intermolecular distances are less than the sum of the van der Waals radii of the atoms involved, except that between C(7)—C(20) = 3·52 Å (x, y, $1+z$). The lack of close intermolecular contacts (no hydrogen bonds) in the crystal structures so far determined is certainly related to the great solubility of those compounds in water.

References

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A27, 368–376.
SHELDRICK, G. M. (1976). *SHELX76.* Program for crystal structure determination. Univ. of Cambridge, England.
STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *Chem. Phys.* 42, 3175–3187.
TESSIER, J. (1985). *Recent Advances in the Chemistry of Insect Control,* edited by N. F. JANES, pp. 26–52.
TESSIER, J., TECHE, A. & DEMOUTE, J. P. (1983). *Pesticide Chemistry, Human Welfare and the Environment,* Vol. I, edited by J. MYAMOTO & P. C. KEARNEY, pp. 95–100. Oxford: Pergamon Press.

Structures of Two Conformationally Defined Phenylethanolamines: *exo*-1,4-Epoxy-2-formamido-1,2,3,4-tetrahydro-8-trifluoromethylnaphthalene and *exo*-1,4-Epoxy-2-formamido-1,2,3,4-tetrahydro-6-trifluoromethylnaphthalene

BY GARY L. GRUNEWALD* AND MOORTHY S. S. PALANKI

Department of Medicinal Chemistry, The University of Kansas, Lawrence, KS 66045, USA

AND FUSAO TAKUSAGAWA

*Department of Chemistry, The University of Kansas, Lawrence, KS 66045, USA*

Abstract. ($\pm$)-*exo*-1,4-Epoxy-2-formamido-1,2,3,4-tetrahydro-8-trifluoromethylnaphthalene (1), $C_{12}H_{10}F_3NO_2$, $M_r = 257\cdot21$, $Pccn$, $a = 8\cdot895$ (1), $b = 19\cdot968$ (5), $c = 12\cdot656$ (3) Å, $V = 2247\cdot9$ (8) Å^3, $Z = 8$, $D_x = 1\cdot520$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1\cdot49$ cm^{-1}, $F(000) = 1056$, $T = 297$ K, $R = 0\cdot0466$ for 1481 independent reflections collected. The torsion angle for N(10)—C(2)—C(1)—C(8*a*) is 167·4 (2)°. ($\pm$)-*exo*-1,4-Epoxy-2-formamido-1,2,3,4-tetrahydro-6-trifluoromethylnaphthalene, (2), $C_{12}H_{10}F_3NO_2$, $M_r = 257\cdot21$, $P2_12_12_1$, $a = 8\cdot52$ (2), $b = 26\cdot15$ (2), $c = 5\cdot06$ (5) Å, $V = 1127$ (11) Å^3, $Z = 4$, $D_x = 1\cdot516$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1\cdot29$ cm^{-1}, $F(000) = 528$, $T = 297$ K, $R = 0\cdot108$ for 932 independent reflections collected. The torsion angle N(10)—C(2)—C(1)—C(8a) is 172·5 (6)°; the formamido group in both (1) and (2) is *exo*. X-ray studies on (1) suggest a hydrogen bond between N(10) and O(12) and similarly for (2).

Introduction. As part of our studies to understand the relationship between conformations of biogenic amines and their affinities for the active site of phenylethanolamine *N*-methyltransferase (PNMT)

(Grunewald, Arrington, Bartlett, Reitz & Sall, 1986; Grunewald, Ye & Takusagawa, 1987; Ye & Grunewald, 1989), we have prepared ($\pm$)-*exo*-1,4-epoxy-2-formamido-1,2,3,4-tetrahydro-8-trifluoromethylnaphthalene (1) and ($\pm$)-*exo*-1,4-epoxy-2-formamide-1,2,3,4-tetrahydro-6-trifluoromethylnaphthalene (2). These are conformationally defined analogs of trifluoromethyl-substituted β-phenylethanolamine, in which the ethanolamine side chain has been fixed.

(1)

(2)
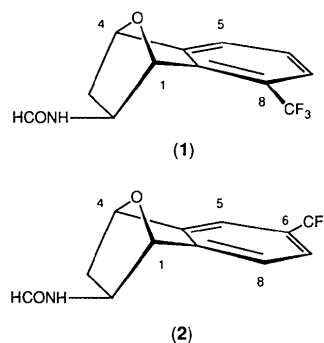
In the case of the analogous compounds with a methylene bridge replacing the oxo bridge

---

* To whom correspondence should be addressed.