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Static Disorder in (−)-(1R,5R,9R,13S)-2′-Hydroxy-5,9-dimethyl-2-(2-methyltetrahydrofurfuryl)-6,7-benzomorphan,* C20H29NO2. Crystal Structure and MM2 Pucker Analysis of the Tetrahydrofuran Ring†

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Abstract

$M_r = 315.454$, monoclinic, $P2_1$, $a = 8.942\,(4)$, $b = 13.719\,(6)$, $c = 7.313\,(3)$ Å, $\beta = 91.80\,(3)°$, $V = 896.7\,(7)$ Å^3, $Z = 2$, $D_m = 1.15\,(2)$, $D_x = 1.168$ Mg m^{-3}, $\lambda(\text{Mo }K\alpha) = 0.71069$ Å, $\mu(\text{Mo }K\alpha) = 0.069$ mm^{-1}, $F(000) = 344$, $T = 291$ K, final $R = 0.041$ for 1010 observed reflections. The side-chain torsion angles about the exocyclic nitrogen bond are eclipsed while the N—C—C—O torsion angle is (−)-synclinal. Static disorder of the tetrahydrofuran ring is analyzed through MM2 force-field calculations of the pseudorotation pathway. Two equienergetic mirror-image puckering forms are identified as minima. A straightforward interpretation of the principles governing their selection is given. The ability of the molecular-mechanics approach to scrutinize this kind of problem in a successful way is verified through a Cambridge Structural Database search. Other cases of similar disorder are pointed out, and a warning is issued against using databases without consulting the original papers.

Introduction

Initially the structure of the title compound was determined as part of a structure–activity study on 6,7-benzomorphans. The drug is a mixed opioid

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* Chemical abstracts name: (−)-(2R,6R,11R,2′S)-1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(2-methyltetrahydrofurfuryl)-2,6-methano-3-benzazocin-8-ol.

† Structural Studies of Substituted 6,7-Benzomorphan Compounds. XIII. Part XII: Verlinde, Blaton, Peeters & De Ranter (1988).

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agonist–antagonist in vivo (Merz & Stockhaus, 1979), and is about as potent as the prototype κ-opioid agonist (±)-U-50 488 (Lahti, Von Voightlander & Barsuhn, 1982) in the rabbit vas deferens twitch inhibition test (Verlinde & De Ranter, 1988).

The main purpose of this determination was to provide insight into the conformational behaviour of the N-side chain which is believed to be essential for opioid κ activity (De Ranter, Verlinde, Blaton & Peeters, 1984). Most likely, the oxygen in β-position engages as an acceptor in a hydrogen bond with the receptor. In this respect, the conformational restriction of the oxygen in a tetrahydrofuran ring should affect the intramolecular entropy in a favourable way compared with the virtually inactive opened-ring analogues.

However, upon solving the structure a major drawback of the conformational restriction in a five-membered ring became apparent: the presence of more than one puckering mode of the tetrahydrofuran. Full crystallographic elucidation through group refinement of this phenomenon proved to be very hard, mainly because of large correlations. Accordingly a molecular-mechanics study of the puckering was undertaken, using the MM2 force field (Allinger & Flanagan, 1983). Although MM2 is widely used, and has been found to be applicable to large numbers of compounds and chemical problems (Allinger & Lii, 1987), a confrontation with a large sample of experimental data was considered to be necessary. For this purpose use was made of tetrahydrofuryl fragments obtained through a search of the Cambridge Structural Database (CSD) (Allen, Bellard, Brice, Cartwright, Doubleday, Higgs, Hummelink, Hummelink-Peters, Kennard, Motherwell, Rodgers & Watson, 1979).

$C_{20}H_{29}NO_2$

It will subsequently be shown that the *MM2* force field is capable of explaining the puckering behaviour of substituted tetrahydrofuran compounds. Furthermore, this approach leads to a straightforward scheme which can be used to predict the selection of the ring pucker. On the other hand, it will be demonstrated that whereas X-ray crystallographic data provide a means to test the quality of a force field, only half of the information is given by the CSD in its present form.

Experimental

Crystals obtained at room temperature from an equimolar ethyl acetate–isopropanol solution. Density measured by flotation in *n*-heptane/CCl$_4$, prism crystal with equilateral triangle at the base (length 1·4 mm) and height of 0·3 mm, Syntex $P2_1$ computer-controlled four-circle diffractometer, graphite-monochromated Mo $K\alpha$ radiation, ω-scan technique ($2\theta_{max} = 50°$, $0 \leq h \leq 10, 0 \leq k \leq 7, -8 \leq l \leq 8$ with measurement of Friedel pairs), cell dimensions by least-squares refinement of the setting angles of 24 reflections with $27 < 2\theta < 30°$, space group $P2_1$ from systematic absences $0k0$ for k odd. Three standard reflections ($103, 1\bar{1}0, 120$) monitored every 50 reflections fluctuated between 97·7 and 100·0% of their initial intensity. 2303 reflections measured resulted in 1087 independent reflections (Friedel pairs were averaged), 1010 observed reflections with $[I > 2\sigma(I)]$, Lorentz–polarization corrections, absorption corrections by the method of North, Phillips & Mathews (1968), scattering factors from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965) (for H).

The structure was solved by direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). After an unsuccessful default run of the program the following strategy was adopted. The fused three-ring benzomorphan skeleton was used to calculate a group scattering factor, the criterion for acceptance of phase relationships was raised ($\kappa = 1·0$), besides the three origin-defining reflections five general reflections were included in the starting set, and the statistically weighted tangent formula was used. The set with the third-best combined figure of merit revealed the benzomorphan nucleus and the C(12) of the *N*-side chain. The missing atoms were obtained from a Fourier synthesis. Refinement with *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) by block-diagonal least squares on F, first with isotropic temperature factors and then anisotropically; full-matrix least squares finally executed. H positions from ΔF synthesis included in refinement with fixed isotropic temperature factors of the atoms to which they are attached; final $R = 0·041$, $wR = 0·053$ and $S = 0·15$, $w = (2·0 + |F_o| + 0·005|F_o|^2)^{-1}$; $(\Delta/\sigma)_{ave} = 0·21$, $(\Delta/\sigma)_{max} = 0·73$, $-0·14 \leq$ final $\Delta\rho$ excursions $\leq 0·16$ e Å^{-3}.

Discussion

(a) Crystal structure

The atomic numbering scheme is given in Fig. 1 and parameters are listed in Table 1.* Bond lengths and angles are given in Table 2. An *ORTEP* (Johnson, 1965) stereopair is shown in Fig. 2. From a weighted least-squares plane and puckering analysis some of the usual features of the benzomorphan ring are found: a planar aromatic ring ($\chi^2 = 7·8$) with a piperidine in the chair conformation perpendicular to its plane. In contrast to Mr1526, an analogue lacking the 2-methyl substitution and possessing the opposite configuration at the 2 position on the *N*-side chain (Peeters, De Ranter & Blaton, 1982), several typical characteristics of free-base benzomorphans are absent in the title compound. It lacks the marked flattening of the piperidine at N(2) while the interconnecting ring between phenol and piperidine is not midway between

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* Lists of structure factors, anisotropic thermal parameters, torsion angles, bond lengths and angles involving H atoms, least-squares planes, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51317 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
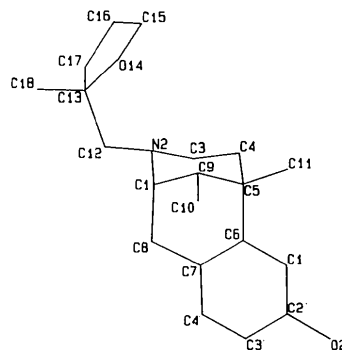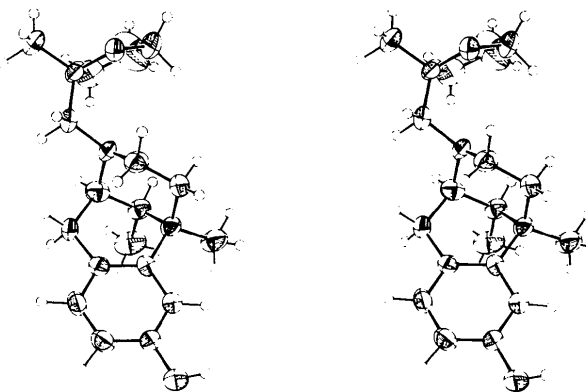

Fig. 1. Atomic numbering scheme.

Fig. 2. Stereoscopic view of the title compound with 50% probability anisotropic displacement ellipsoids for the non-H atoms.

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters with e.s.d.'s of the refined parameters in parentheses*

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j.$$

	x	y	z	$B_{eq}(\text{Å}^2)$
C(1')	−1656 (3)	3961 (5)	3188 (4)	3·4 (2)
C(2')	−3040 (3)	3743 (5)	3873 (5)	3·1 (2)
O(2')	−4211 (2)	4394*	3697 (3)	4·5 (1)
C(3')	−3262 (4)	2905 (5)	4783 (5)	3·8 (2)
C(4')	−2086 (4)	2256 (5)	5027 (5)	3·7 (2)
C(1)	2060 (4)	1993 (7)	3848 (4)	3·8 (2)
N(2)	2259 (3)	1610 (5)	2004 (4)	3·2 (2)
C(3)	1111 (4)	1992 (8)	717 (4)	3·7 (2)
C(4)	1126 (4)	3075 (7)	691 (4)	3·8 (2)
C(5)	1045 (4)	3544 (6)	2593 (5)	3·4 (2)
C(6)	−472 (3)	3302 (5)	3402 (4)	3·1 (2)
C(7)	−683 (3)	2444 (5)	4344 (4)	3·2 (2)
C(8)	563 (4)	1719 (5)	4704 (4)	3·6 (2)
C(9)	2290 (4)	3075 (6)	3836 (5)	3·6 (2)
C(10)	2372 (5)	3494 (6)	5753 (7)	5·6 (2)
C(11)	1318 (5)	4617 (7)	2425 (8)	5·5 (3)
C(12)	2512 (4)	576 (7)	1897 (5)	3·8 (2)
C(13)	3984 (4)	311 (7)	1007 (5)	3·5 (2)
O(14)	3909 (3)	681 (4)	−878 (3)	3·8 (1)
C(15)	4955 (7)	1459 (6)	−1072 (7)	5·4 (2)
C(16)	5985 (8)	1409 (8)	490 (10)	9·9 (4)
C(17)	5308 (5)	849 (6)	1892 (6)	5·4 (2)
C(18)	4184 (6)	−755 (8)	951 (6)	4·9 (2)

* Parameter kept fixed for origin fixation.

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

C(1')−C(2')	1·382 (5)	C(5)−C(6)	1·534 (5)
C(1')−C(6)	1·398 (7)	C(5)−C(9)	1·554 (7)
C(2')−O(2')	1·380 (5)	C(5)−C(11)	1·497 (13)
C(2')−C(3')	1·346 (9)	C(6)−C(7)	1·379 (9)
C(3')−C(4')	1·386 (7)	C(7)−C(8)	1·512 (8)
C(4')−C(7)	1·389 (5)	C(9)−C(10)	1·516 (7)
C(1)−N(2)	1·463 (6)	C(12)−C(13)	1·531 (6)
C(1)−C(8)	1·542 (6)	C(13)−O(14)	1·469 (5)
C(1)−C(9)	1·499 (13)	C(13)−C(17)	1·522 (8)
N(2)−C(3)	1·468 (6)	C(13)−C(18)	1·474 (15)
N(2)−C(12)	1·439 (13)	O(14)−C(15)	1·429 (9)
C(3)−C(4)	1·486 (15)	C(15)−C(16)	1·447 (9)
C(4)−C(5)	1·536 (7)	C(16)−C(17)	1·430 (11)

C(2')−C(1')−C(6)	120·2 (5)	C(1')−C(6)−C(7)	119·5 (3)
C(1')−C(2')−O(2')	120·7 (5)	C(5)−C(6)−C(7)	120·9 (4)
C(1')−C(2')−C(3')	120·8 (4)	C(4')−C(7)−C(6)	118·5 (4)
O(2')−C(2')−C(3')	118·4 (3)	C(4')−C(7)−C(8)	119·0 (5)
C(2')−C(3')−C(4')	119·3 (3)	C(6)−C(7)−C(8)	122·5 (3)
C(3')−C(4')−C(7)	121·7 (5)	C(1)−C(8)−C(7)	114·5 (5)
N(2)−C(1)−C(8)	114·8 (4)	C(1)−C(9)−C(5)	108·5 (4)
N(2)−C(1)−C(9)	109·2 (5)	C(1)−C(9)−C(10)	111·9 (5)
C(8)−C(1)−C(9)	111·4 (5)	C(5)−C(9)−C(10)	113·4 (5)
C(1)−N(2)−C(3)	111·1 (5)	N(2)−C(12)−C(13)	113·3 (6)
C(1)−N(2)−C(12)	115·3 (5)	C(12)−C(13)−O(14)	107·6 (4)
C(3)−N(2)−C(12)	115·1 (5)	C(12)−C(13)−C(17)	111·8 (5)
N(2)−C(3)−C(4)	111·0 (5)	C(12)−C(13)−C(18)	110·7 (6)
C(3)−C(4)−C(5)	114·0 (5)	O(14)−C(13)−C(17)	104·1 (5)
C(4)−C(5)−C(6)	109·0 (4)	O(14)−C(13)−C(18)	108·6 (4)
C(4)−C(5)−C(9)	107·6 (5)	C(17)−C(13)−C(18)	113·6 (5)
C(4)−C(5)−C(11)	109·0 (5)	C(13)−O(14)−C(15)	109·9 (4)
C(6)−C(5)−C(9)	108·1 (4)	O(14)−C(15)−C(16)	106·8 (6)
C(6)−C(5)−C(11)	113·1 (5)	C(15)−C(16)−C(17)	108·6 (6)
C(9)−C(5)−C(11)	109·8 (5)	C(13)−C(17)−C(16)	107·2 (4)
C(1')−C(6)−C(5)	119·5 (5)		

Table 3. *Mean-square displacement amplitude normal to the mean plane of the tetrahydrofuran ring ($\times 10^4$ Å^2), and out-of-plane displacement from the puckering plane (Å)*

C(13)	315	0·004 (5)
O(14)	451	−0·066 (5)
C(15)	580	0·103 (6)
C(16)	1932	−0·100 (6)
C(17)	673	0·059 (6)

half-boat and half-chair. Instead, the half-boat usually found with protonated benzomorphans is present [puckering parameters according to Cremer & Pople (1975a): $Q = 0.541$ (6) Å, $\theta_2 = 128.3$ (4)°, $\varphi_2 = 120.9$ (6)° for the sequence C(1)−C(8)−C(7)−C(6)−C(5)−C(9)].

The mediocre ability of the oxygen O(2') for fixing the origin in the y direction is reflected in the higher e.s.d.'s of the y parameters of other atoms (inspection of the correlation matrix reveals rather large correlations between the y parameters). Some abnormally short distances can easily be understood from an anisotropic displacement-factor analysis of the atoms involved. In particular, the tetrahydrofuran ring seems to be badly affected. Puckering analysis (Cremer & Pople, 1975a) calculates a puckering amplitude of 0·169 (9) Å, which is far out of range of the normal value of 0·37 Å (Cremer & Pople, 1975b). From an analysis of the out-of-plane components of the mean-square vibrational amplitude of all atoms in the ring (Table 3), a major displacement of C(16) is observed together with still large but smaller displacements of C(15) and C(17), while those of the remaining atoms are fairly normal. It should be realized that these amplitudes correspond to displacements of 0·18 to 0·44 Å. From comparison with the out-of-plane distances of the atomic positions (values up to 0·1 Å) it becomes rather obvious that the common practice of using the positions to describe the pucker is at least questionable.

Subsequent to the final refinement, a difference Fourier synthesis without the oxolane ring was there-fore performed. A section perpendicular to the ring was scrutinized, especially about C(16) in view of its large mean-square displacement in this direction (Fig. 3). The highest zero-flux electrondensity curve consists of two straight lines connected through a curvilinear part. From this presence of two rather than one main axes, two C(16) positions should be suspected. On these grounds there is little doubt that the apparently odd geometry of the ring is a result of static disorder.

Consequently, a few rather short bond lengths in other parts of the molecule [e.g. C(2')−C(3'), C(6)−C(7), C(1)−C(9) and C(3)−C(4)] are probably refinement artefacts resulting from the poor model of the disorder. However, bond angles about these atoms are fairly normal.

Considering the N-side-chain conformation, the C(1)−N(2)−C(12)−C(13) and C(3)−N(2)−C(12)−C(13) torsion angles are found to be −121·9 (6) and

106·6 (6)° respectively. This eclipsing about N(2)—C(12) has not been observed previously in 6,7-benzomorphan crystal structures and can only be attributed to the requirements for hydrogen bonding of O(14). Indeed, the N(2)—C(12)—C(13)—O(14) torsion angle at −61·9 (6)° then allows for hydrogen bonding between the ether oxygen of one molecule and the phenolic hydrogen of a neighbouring molecule, thus forming endless chains along **b** [O(14)···O(2′)ⁱ 2·734 (5), O(14)···H(2′)ⁱ 1·91 (5) Å, ∠O(14)···H(2′)ⁱ—O(2′)ⁱ 168 (4)°, symmetry operator: (i) $-x, y-\frac{1}{2}, -z$] (Fig. 4). Further elements for understanding the ability of the crystal to accommodate disorder of the tetrahydrofuran ring can be found in the packing. With the program *OPEC* (Gavezzotti, 1983) a packing coefficient of 0·66 was calculated, which is rather low especially for the space group present (Kitaigorodsky, 1973).
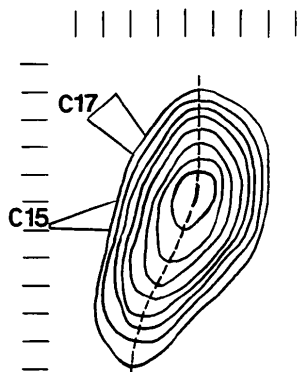

Fig. 3. *ΔF* section perpendicular to the tetrahydrofuran ring at C(16) (contour spacing of $0\cdot1 \text{ e Å}^{-3}$, maximum at the central contour $1\cdot5 \text{ e Å}^{-3}$, grid resolution 0·18 Å), with zero-flux electron density curve (dashed line).

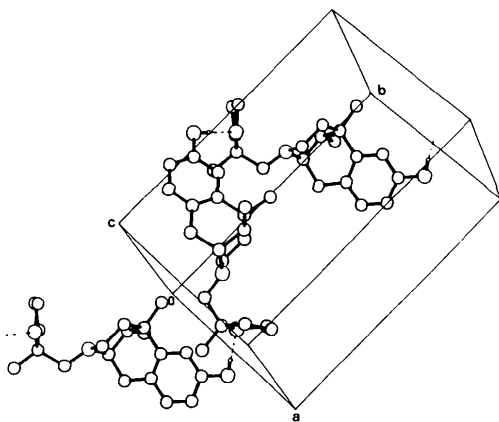### (b) Molecular-mechanics calculations

The soundness of the static disorder interpretation was further assessed in a molecular-mechanics puckering analysis of the tetrahydrofuryl group. Direct use of the existing computational and experimental puckering studies on furanoses in nucleic acids (for a review, see Saenger, 1984) appeared questionable because of the different substitution pattern of the ring. Furthermore, the through-conjugation between purine or pyrimidine base and furanose ether oxygen which causes a serious shortening of the C—O bond, is absent in the present study. Out of several puckering formalisms (for an excellent review, see Harvey & Prabhakaran, 1986) the one by Cremer & Pople (1975*a*) has been adopted. Here the amplitude-phase pair (Q, φ_2) describes the out-of-plane displacement of each atom of the five-membered ring. In order to retain the existing furanose-ring nomenclature, atoms 0 through 4 were taken to be O(14), C(13), C(17), C(16), C(15), and the Cremer & Pople phase angle was increased by $\pi/2$; in this way the ^3_2T pucker corresponds to a phase angle of 0° (Fig. 5).

Molecular-mechanics calculations were performed with the program *MM2* (Allinger & Flanagan, 1983), updated with the 1985 parameters including electro-negativity corrections (Allinger, 1985). The existence of regions in the domain of the pseudorotation function where the phase angle is almost linearly dependent on one of the torsion angles was exploited together with the torsion-angle driver in the program to construct the full pseudorotational pathway of the tetrahydrofuryl group. Because of overlap of these linear-dependence regions it was possible to check that the constructed pathway was indeed a lowest energy one. As the anisotropic displacement factors of C(13) and O(14) were fairly low the exocyclic dihedral angle N(2)—C(12)—C(13)—O(14) was kept fixed at its observed (−)-synclinal value.

Two equienergetic minima that are almost each other's mirror image are calculated at ^3E and ^4_3T (Fig. 6). The activation barrier between these minima is substantial and amounts to 5·6 and 8·1 kJ mol⁻¹ *via* the O-*exo* and O-*endo* routes respectively. Scrutinizing the energies along the pseudorotational pathway reveals only major fluctuations in torsional strain and to a
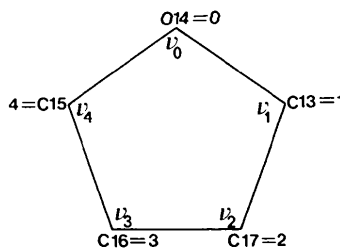

Fig. 4. Packing of the crystal. Hydrogen bonds are indicated by dashed lines.

Fig. 5. Puckering nomenclature with atoms 0 through 4 and corresponding endocyclic valence angles v_i.

lesser extent in bending strain. This identification of internal energy contributions is in excellent agreement with the study by Harvey & Prabhakaran (1986) in which ribose puckering dynamics in Phe-t-RNA were simulated with another force field. Thus, the warning against interpreting strain partitioning because of force-field dependence (Burkert & Allinger, 1982) should not be considered too serious in the present study.

A straightforward interpretation in this light seems possible. In Fig. 7 the torsional strain for the hypothetical flat five-membered ring is divided over the different contributions from each central bond, and for each bond the torsional relief for a 30° endocyclic dihedral-angle deviation is given. Analogous to unsubstituted tetrahydrofuran (Luger & Buschmann, 1983) maximal relief is possible in ^2_3T and ^3_2T, but the C(17)-endo or -exo puckering gives rise to unfavourable contacts with the exocyclic C(13) substituents. Hence, the minimum is shifted in the direction of the C(16)-endo or -exo puckering. Owing to the rather symmetrical substitution of the plane of the ring at C(13) no clear preference for endo or exo puckering in C(16) is present in contrast to its C(13)-demethylated analogue where the exocyclic torsion angles clearly select one form, in this case the $_2E$ one (Peeters, De Ranter & Blaton, 1982).
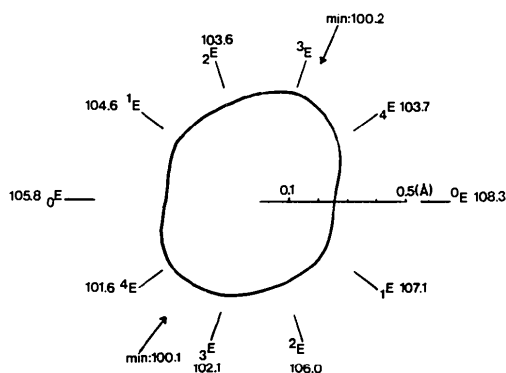

Fig. 6. Polar plot of the puckering pathway of the title compound. Amplitude in Å, energy in kJ mol⁻¹.
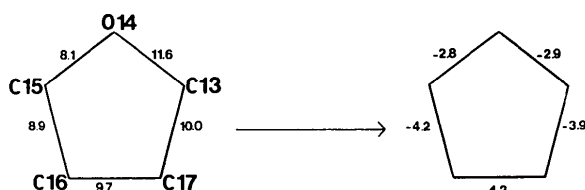

Fig. 7. Torsional strain in the flat tetrahydrofuran ring (left), and strain relief for a 30° endocyclic dihedral-angle deviation (right). Energies are in kJ mol⁻¹.

Fluctuations of the endocyclic valence angles along the pseudorotational pathway (Fig. 8) are very similar to the ones found experimentally in furanoses (Bartenev, Kameneva & Lipanov, 1987). As a consequence of the increasing bending force constants C—C—C < C—C—O < C—O—C, they are largest for v_2 and v_3 and smallest for v_0. Each endocyclic valence angle reaches a minimum whenever its central atom is at the apex of an envelope conformation. The total bending energy reaches a minimum in the O-endo and O-exo conformation since the concomitant decrease of the oxygen valence angle is in fact a relaxation (natural valence angle = 106·8°). Alternatively, in other puckering forms the valence-angle decrease at the apex involves an increase in bending strain (the valence angle decreases from the natural value).

(c) Cambridge Structural Database search

As an additional check on the reliability of the calculations a CSD search of 2,2-disubstituted tetrahydrofuran structures was executed. Only five well refined entries ($R < 6.5\%$, mean e.s.d. of C—C bond lengths < 0.005 Å) were retrieved, all being part of spiro-fused ring systems. They are situated on a polar pucker plot in Fig. 9 and will be referred to by their CSD code in the further discussion: BENYUO and BENZAV (Shibaeva, Rozenberg, Shapiro & Pavarov, 1981), BUCJIS (McKague, Rettig, Trotter, Douglas & Nestmann, 1983), BEXSUS (McKague, Rettig, Trotter & Douglas, 1981), TASANF (Terzis & Faught, 1978). Four out of the five structures are centrosymmetric and thus give rise to two observations on the plot with a phase-angle difference of 180°. From inspection of the anisotropic displacement factors, bond lengths, bond angles and puckering amplitudes, static disorder should be suspected for BENYUO, BENZAV and BUCJIS. Only for the latter compound is the phenomenon mentioned in the original paper. The suspected disorder in BENYUO and BENZAV is further substantiated as in both structures an H atom of the
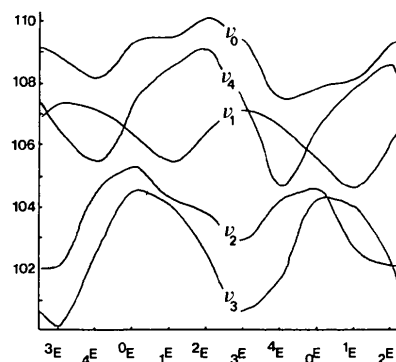

Fig. 8. Curves depicting the changing valence angles of the tetrahydrofuran ring on the pseudorotation pathway.

tetrahydrofuran ring makes a close contact with an H of the spiro-fused ring system (contact distances of 1·8 and 1·9 Å respectively). In BEXSUS disorder is probably prevented through sterical hindrance by a chlorine substituent on the adjacent ring. Owing to the very low number of retrieved structures, it is at present not possible to construct the pseudorotational pathway for this particular substitution of the tetrahydrofuran ring. In fact, the above analysis points out how easily such statistics could be void of physical meaning because of neglect of static disorder.

Concluding remarks

The static disorder in the title compound is clearly not an isolated case as can be seen from the CSD search. It appears to be due to the particular substitution pattern of the tetrahydrofuran ring. However, the statistical arguments providing this conclusion are not directly available. Although the CSD is excellent for retrieving relevant structures, it does not contain the thermal parameters indispensable for analyzing the particular nature of the puckering. On the other hand, the information obtained from thermal parameters in itself is insufficient to distinguish between static disorder and atomic vibrations, sometimes considered as dynamic disorder. In this respect, the molecular-mechanics approach provides a clear picture. It provides both the energetics of the puckering process, including the position of minima and the relative heights of activation barriers between them, and the coupled geometrical changes.

As stated in the *Introduction*, the purpose of including the oxygen in a tetrahydrofuran ring was conformational restriction of its lone pairs. Since the *exo-* and *endo*-puckering at C(16) hardly affect the direction of the lone-pair orientation at O(14), this design seems to be successful. However, a full appreciation of this aspect will only be possible after studying the dependence of the pseudorotational pathway on the exocyclic torsion angle about C(12)—C(13).
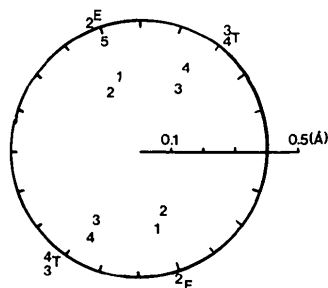

Fig. 9. Polar scatter plot of Cambridge Structural Database retrieval. 1 = BENYUO, 2 = BENZAV, 3 = BUCJIS, 4 = BEXSUS, 5 = TASANF. Amplitude in Å.

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