between envelope and half chair with the puckering parameters $Q = 0{\cdot}382\,(5)$ Å, $\varphi = 263{\cdot}2\,(6)°$ and lowest asymmetry factors $\mathscr{f}C_2(\mathrm{C}17) = 0{\cdot}035\,(5)$ and $\mathscr{f}C_s(\mathrm{O}16) = 0{\cdot}074\,(6)$ Å. The general features of the molecule resemble those of molecule (I) of spirosta-5,25(27)-diene-1β,3β,11α-triol monohydrate (Kálmán, Argay, Ribár, Živanov-Stakić & Vladimirov, 1985). However, there is one difference, namely the *B* ring of molecule (I) has a pronounced envelope conformation.

There is one hydrogen bond between symmetrically related molecules [O(11)—H···O(16)($-x$, $0{\cdot}5 + y$, $0{\cdot}5 - z$): O(11)···O(16) 2·956 (6), H···O(16) 2·18 (5) Å, ∠O(11)—H···O(16) 173 (4)°], which forms a helix about the twofold screw *b* axis.

References

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Kálmán, A., Argay, Gy., Ribár, B., Živanov-Stakić, D. & Vladimirov, S. (1985). *Acta Cryst.* C**41**, 1645–1647.

Kálmán, A., Czugler, M. & Simon, K. (1982). *Molecular Structure and Biological Activity*, edited by J. F. Griffin & W. L. Duax, pp. 367–376. New York: Elsevier Biomedical.

Sheldrick, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

Acta Cryst. (1986). C**42**, 1782–1785

The Structure of 9α-Acetoxy-8β-[2′-(*N*-morpholino)ethyl]-10β-methyl-*trans*-2-decalone[*]

By Kay D. Onan[†]

Department of Chemistry, Northeastern University, Boston, MA 02115, *USA*

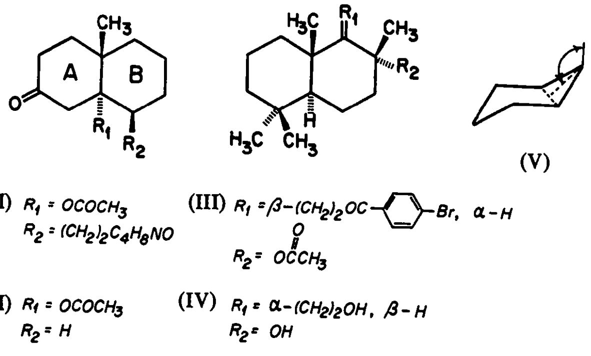
and James A. Nelson and Thomas A. Spencer

Department of Chemistry, Dartmouth College, Hanover, NH 03755, *USA*

(*Received* 21 *January* 1986; *accepted* 25 *June* 1986)

Abstract. $C_{19}H_{31}NO_4$, $M_r = 337{\cdot}5$, monoclinic, $P2_1/c$, $a = 8{\cdot}289\,(8)$, $b = 10{\cdot}631\,(1)$, $c = 21{\cdot}500\,(2)$ Å, $\beta = 94{\cdot}25\,(1)°$, $U = 1889{\cdot}1\,(4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}186$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu(\mathrm{Cu}\,K\alpha) = 6{\cdot}6$ cm^{-1}, $F(000) = 736$, room-temperature data collection, final $R = 0{\cdot}062$ for 1930 reflections. The decalone skeleton adopts a chair–chair conformation which is essentially undistorted even in the presence of the 1,3-diaxial substituents. The mean torsion angle in ring *A*, the cyclohexanone ring, is 51·4°; the mean in ring *B* is 53·4°. The *N*-morpholinoethyl substituent is extended with an all-*trans* orientation of bonds C(9)—C(8), C(8)—C(17), C(17)—C(18), C(18)—N(19), N(19)—C(24). The mean distances in the morpholine ring are C—N 1·458, C—C 1·499, and C—O 1·410 Å.

Introduction. Reactions in which a proton alpha[‡] to a carbonyl group is abstracted by a general base are important in the function of many enzymes (Spencer, 1979; Westheimer, 1970; Wood, 1971). In our earlier research (Roberts, Ferran, Gula & Spencer, 1980; Hupe, Kendall & Spencer, 1973) we focused on elucidating why these biochemical alpha proton transfers so often occur *via* iminium ion formation, and concluded that this pathway has an inherent kinetic advantage, at physiological pH, of *ca* 10^5 compared with direct deprotonation of the carbonyl compound.



The current emphasis in our research concerns the geometry of alpha proton abstraction. Having the functional groups involved in a reaction localized in the correct positions, rather than free in solution, is generally considered to be an important component of enzymatic catalysis (Jencks, 1969). Accordingly, we have been trying to assess the further contribution to enzymatic rate acceleration of alpha proton transfer

---

[*] 4a-Methyl-8-[2′-(*N*-morpholino)ethyl]-2-oxo-*trans*-decahydro-8a-naphthyl acetate.

[†] To whom correspondence should be addressed.

[‡] The word 'alpha' is used to denote the position of carbons relative to the carbonyl group and the symbols α and β are used to denote substituents underneath and above, respectively, the plane of the decalin ring system.

0108-2701/86/121782-04$01.50

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *for the non-hydrogen atoms, with estimated standard deviations in parentheses, and equivalent isotropic temperature factors,* U_{eq}($\text{Å}^2 \times 10^4$)

$$U_{eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta).$$

	x	y	z	U_{eq}
C(1)	6024 (4)	−661 (3)	4097 (1)	448
C(2)	4776 (4)	306 (3)	4225 (2)	521
C(3)	5372 (5)	1631 (3)	4317 (2)	666
C(4)	6540 (4)	2024 (3)	3845 (2)	583
C(5)	8904 (4)	1486 (3)	3230 (2)	627
C(6)	10106 (5)	510 (4)	3054 (2)	754
C(7)	9277 (5)	−732 (4)	2882 (2)	700
C(8)	8269 (4)	−1246 (3)	3396 (1)	463
C(9)	7102 (3)	−235 (2)	3595 (1)	366
C(10)	7902 (4)	1061 (3)	3763 (1)	419
O(11)	3372 (3)	28 (3)	4289 (1)	746
O(12)	6031 (2)	104 (2)	3034 (1)	410
C(13)	4973 (4)	−706 (3)	2736 (2)	516
O(14)	4755 (3)	−1764 (2)	2888 (1)	772
C(15)	4129 (5)	−67 (4)	2185 (2)	710
C(16)	9007 (4)	1011 (3)	4369 (1)	515
C(17)	9362 (4)	−1859 (3)	3924 (1)	484
C(18)	9587 (4)	−3247 (3)	3785 (2)	540
N(19)	10868 (3)	−3857 (2)	4179 (1)	450
C(20)	12451 (4)	−3476 (3)	4001 (2)	621
C(21)	13767 (5)	−4155 (4)	4382 (2)	824
O(22)	13611 (3)	−5481 (2)	4321 (1)	742
C(23)	12090 (6)	−5859 (4)	4495 (2)	832
C(24)	10735 (4)	−5224 (3)	4118 (2)	669

which could result from such a correct juxtaposition of the proton and the general basic group that accepts it. Such assessments are made by comparing the rate of intramolecular reaction of a suitable model system with the rates of analogous intermolecular reactions. For use as our intramolecular reactant, we synthesized the title compound (I) (Jacobs, Nelson & Spencer, 1980), a compound in which the morpholino nitrogen can readily attain a position directly above the 1β alpha proton, as judged from molecular models. This geometric analysis, however, was based on the assumption that the cyclohexane ring of (I) exists in an undistorted chair conformation. The present study was undertaken to determine whether or not in fact the presence of the 8β and 10β 1,3-diaxial substituents results in significant distortion of this decalone system. The results of the kinetic study of the intramolecular alpha deprotonation of (I) and appropriate intermolecular analogs will be reported subsequently (Gula, Vitale & Spencer, to be published).

Experimental. A 0·15 × 0·20 × 0·25 mm crystal of (I) was grown by slow evaporation of solution in ether. Data to 2θ of 130° on a Syntex $P2_1$ diffractometer, $\theta/2\theta$, variable-speed (2·0 to 29·0° min^{-1} in 2θ) scans. Cell constants by least squares of 15 reflections widely separated in reciprocal space with $58 \leq 2\theta \leq 66°$. 3131 independent observations, 18 reflections excluded owing to secondary extinction, 1930 of 3113 remaining had $I \geq 2\sigma(I)$ and were used in the structure solution and refinement. A check reflection, measured after every 99 reflections, showed no diminution in intensity.

Lorentz, polarization and empirical absorption corrections, the latter determined from a ψ scan, applied; scattering factors for C, N and O from Cromer & Waber (1965), for H from Stewart, Davidson & Simpson (1965); direct methods [*MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980)], full-matrix least-squares refinement minimizing $\sum w||F_o|-|F_c||^2$ with weights $w^{1/2} = 1$ for $|F_o| \leq 8{\cdot}0$ and $w^{1/2} = 8{\cdot}0/|F_o|$ for $|F_o| > 8{\cdot}0$ (program based on *FMLS* by P. K. Gantzel, R. A. Sparks and K. N. Trueblood, modified by A. T. McPhail); all H atoms located in a difference synthesis; anisotropic temperature factors for non-hydrogen atoms, isotropic factors for H atoms; convergence at $R = 0{\cdot}062$, $wR = 0{\cdot}070$, $S = 0{\cdot}721$, max. $(\Delta/\sigma) = 0{\cdot}171$ for the non-hydrogen atoms, max. $\Delta\rho$ peak 0·23 e Å^{-3}; *ORTEP* (Johnson, 1965) for molecular drawings.

Table 2. *Interatomic distances* (Å), *bond angles* (°) *and selected torsion angles* (°), *with estimated standard deviations in parentheses*

C(1)—C(2)	1·498 (5)	C(9)—O(12)	1·488 (3)
C(1)—C(9)	1·519 (4)	C(10)—C(16)	1·537 (4)
C(2)—C(3)	1·501 (5)	O(12)—C(13)	1·355 (4)
C(2)—O(11)	1·218 (4)	C(13)—O(14)	1·189 (4)
C(3)—C(4)	1·512 (5)	C(13)—C(15)	1·494 (5)
C(4)—C(10)	1·544 (4)	C(17)—C(18)	1·520 (4)
C(5)—C(6)	1·506 (6)	C(18)—N(19)	1·460 (4)
C(5)—C(10)	1·532 (5)	N(19)—C(20)	1·451 (4)
C(6)—C(7)	1·522 (6)	N(19)—C(24)	1·463 (4)
C(7)—C(8)	1·534 (5)	C(20)—C(21)	1·501 (6)
C(8)—C(9)	1·529 (4)	C(21)—O(22)	1·420 (5)
C(8)—C(17)	1·543 (4)	O(22)—C(23)	1·400 (5)
C(9)—C(10)	1·560 (4)	C(23)—C(24)	1·496 (6)
C(2)—C(1)—C(9)	112·2 (2)	C(4)—C(10)—C(9)	108·1 (2)
C(1)—C(2)—C(3)	116·3 (3)	C(4)—C(10)—C(16)	108·7 (2)
C(1)—C(2)—O(11)	122·2 (3)	C(5)—C(10)—C(9)	109·4 (2)
C(3)—C(2)—O(11)	121·4 (3)	C(5)—C(10)—C(16)	108·8 (3)
C(2)—C(3)—C(4)	113·1 (3)	C(9)—C(10)—C(16)	112·5 (2)
C(3)—C(4)—C(10)	113·8 (3)	C(9)—O(12)—C(13)	123·8 (2)
C(6)—C(5)—C(10)	113·0 (3)	O(12)—C(13)—O(14)	125·2 (3)
C(5)—C(6)—C(7)	111·3 (3)	O(12)—C(13)—C(15)	109·5 (3)
C(6)—C(7)—C(8)	113·2 (3)	O(14)—C(13)—C(15)	125·2 (3)
C(7)—C(8)—C(9)	109·9 (3)	C(8)—C(17)—C(18)	109·8 (2)
C(7)—C(8)—C(17)	111·0 (3)	C(17)—C(18)—N(19)	114·4 (3)
C(9)—C(8)—C(17)	116·1 (2)	C(18)—N(19)—C(20)	110·8 (3)
C(1)—C(9)—C(8)	114·0 (2)	C(18)—N(19)—C(24)	110·1 (3)
C(1)—C(9)—C(10)	111·2 (2)	C(20)—N(19)—C(24)	108·5 (2)
C(1)—C(9)—O(12)	107·5 (2)	N(19)—C(20)—C(21)	110·8 (3)
C(8)—C(9)—C(10)	114·8 (2)	C(20)—C(21)—O(22)	111·7 (3)
C(8)—C(9)—O(12)	107·2 (2)	C(21)—O(22)—C(23)	109·7 (3)
C(10)—C(9)—O(12)	101·1 (2)	O(22)—C(23)—C(24)	112·3 (3)
C(4)—C(10)—C(5)	109·4 (2)	N(19)—C(24)—C(23)	110·6 (3)
Ring *A*			
C(9)—C(1)—C(2)—C(3)	−47·8 (3)	C(3)—C(4)—C(10)—C(9)	55·2 (3)
C(1)—C(2)—C(3)—C(4)	44·0 (3)	C(4)—C(10)—C(9)—C(1)	−58·1 (3)
C(2)—C(3)—C(4)—C(10)	−48·3 (3)	C(10)—C(9)—C(1)—C(2)	54·9 (3)
Ring *B*			
C(10)—C(5)—C(6)—C(7)	56·3 (3)	C(7)—C(8)—C(9)—C(10)	−51·1 (3)
C(5)—C(6)—C(7)—C(8)	−55·5 (3)	C(8)—C(9)—C(10)—C(5)	51·7 (3)
C(6)—C(7)—C(8)—C(9)	52·2 (3)	C(9)—C(10)—C(5)—C(6)	−53·4 (3)
Ring *C*			
C(24)—N(19)—C(20)—C(21)	−56·0 (3)	C(21)—O(22)—C(23)—C(24)	57·6 (4)
N(19)—C(20)—C(21)—O(22)	57·8 (3)	O(22)—C(23)—C(24)—N(19)	−58·0 (3)
C(20)—C(21)—O(22)—C(23)	−57·2 (3)	C(23)—C(24)—N(19)—C(20)	55·8 (3)

Discussion. Final atomic parameters for the non-hydrogen atoms are listed in Table 1; Table 2 contains bond lengths, bond angles and selected torsion angles.* Fig. 1 shows the molecular conformation and numbering scheme for (I).

The decalone system adopts a relatively undistorted chair–chair conformation. The mean torsion angle in ring *A* is 51·4°, identical to that in (II), a molecule like (I) but lacking the axial 8β substituent (Onan, Mayer & Spencer, 1984). This value is, however, smaller than that for unsubstituted cyclohexanone (54·2°) (Bucourt, 1974) or for the crowded cyclohexanone ring in 9-carbomethoxy-4,6,6-trimethyl-*trans*-decal-3-one† (54·7°) (Huber & Gabe, 1974).

Even though (I) possesses 1,3-diaxial substituents in ring *B* the mean torsion angle in this ring is 53·4°; that in (II) is 54·0°. While these means are very similar, the conformations of the rings differ. In (II), ring *B* is most flattened at the C(6) end (torsion angles *ca* 52°). This is caused by α-side interactions between O(12) and the axial hydrogens on C(5) and C(7) [O···$H(5)_{ax}$ 2·49, O···$H(7)_{ax}$ 2·68 Å] which result in a relatively large $H(5)_{ax}$···$H(7)_{ax}$ separation, 2·81 Å. In (I) these α-side interactions [O···$H(5)_{ax}$ 2·49, O···$H(7)_{ax}$ 2·62, $H(5)_{ax}$···$H(7)_{ax}$ 2·60 Å] are opposed by β-side interactions involving larger species, the C(10) methyl and the C(8) methylene. In (I) C(16)···C(17) is 3·22 Å while in (II) C(16)···$H(8)_{ax}$ is only 2·69 Å. The C···C transannular separation in (I) is similar to those in (III) (3·22, 3·22 Å) and (IV) (3·24, 3·04 Å) (Bernardinelli & Giersch, 1985). This C···C interaction results in a flattening at C(9) (torsion angles *ca* 51°) and a puckering at C(6) (torsion angles *ca* 56°) in (I).

One way in which molecules can accommodate the strain of 1,3-diaxial substitution is to bend the substituents outwards, away from the ring. A measure of this is the angle between the ring-to-substituent bond and the plane containing the ring atom of attachment and its two flanking endocyclic atoms (V). A bridgehead methyl, therefore, will display two such angles. In (II) these angles are identical at 126·4°, a value only slightly larger than the 125·3° expected on the basis of ideal cyclohexane geometry (Johnson, Zito, Sarma & McKeever, 1978). In (I) these angles are 126·7 and 127·6°, with the latter involving ring *B*, the ring bearing two axial substituents. The C(8)–C(17) bond is bent outwards quite significantly, the angle being 134·1°. These values are similar to analogous angles in (III) and (IV). In both (III) and (IV) the C(10) methyl makes an angle of 126° from ring *A* and 130° from ring *B*. The methyl groups at C(4) and C(8) bend outwards 128 and 135° in (III) and 130 and 132° in (IV).

The small (3·2°) C(16)–C(10)···C(8)–C(17) virtual torsion angle in (I) shows that any distortion due to the 1,3-diaxial substitution is not alleviated by skeletal twisting of the molecule. This magnitude of twist corresponds to values of from 0·4 to 6·0° in (III) and (IV).

The 2′-(*N*-morpholino)ethyl substituent is extended and, in the solid state, points away from the decalone skeleton. The morpholine ring adopts the expected chair conformation and is linked equatorially. The distances in the morpholine are all unexceptional (means: C–N 1·458, C–C 1·499, C–O 1·410 Å) (*e.g.* Rømming, Nevstad & Songsted, 1982; Vilsmaier & Klein, 1982; Maia & Pérez, 1982).

The distances and angles throughout the molecule lie within normal ranges. The presence of the axial substituent at C(8) is reflected in a slightly lengthened C(9)–C(10) bond [1·560 (4) *vs* 1·546 Å in (II)], a diminished C(7)–C(8)–C(9) angle [109·9 (3) *vs* 111·6° in (II)] and an increased C(8)–C(9)–C(10) angle [114·8 (2) *vs* 111·7° in (II)].

The arrangement of molecules in the crystal as viewed in projection along the *b* axis is shown in Fig. 2. The smallest intermolecular separations [C(2)···C(2′)

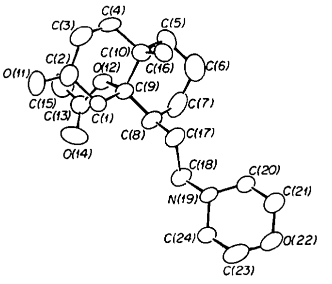


Fig. 1. View of the title compound with the atom-numbering scheme.

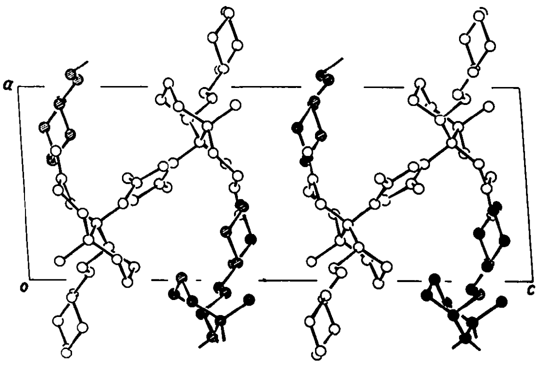


Fig. 2. Packing diagram for the title compound. Partial molecules are shaded for clarity.

---

* Lists of structure factors, anisotropic thermal parameters and hydrogen-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43184 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

† 1,7,7-Trimethyl-2-oxo-*trans*-decahydro-8a-naphthyl acetate.

3·39, C(2)···O(11′) 3·46 Å] occur between carbonyl units related by the crystallographic center of symmetry. All others conform to normal van der Waals contacts.

References

BERNARDINELLI, G. & GIERSCH, W. (1985). *Acta Cryst.* C**41**, 746–749.

BUCOURT, R. (1974). *Topics in Stereochemistry,* edited by E. L. ELIEL & N. L. ALLINGER, pp. 159–224. New York: John Wiley.

CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.

HUBER, C. S. & GABE, E. J. (1974). *Acta Cryst.* B**30**, 2519–2521.

HUPE, D. J., KENDALL, M. C. R. & SPENCER, T. A. (1973). *J. Am. Chem. Soc.* **95**, 2271–2278.

JACOBS, J. N., NELSON, J. A. & SPENCER, T. A. (1980). *J. Org. Chem.* **45**, 1645–1650.

JENCKS, W. P. (1969). *Catalysis in Chemistry and Enzymology,* ch. 1. New York: McGraw-Hill.

JOHNSON, C. K. (1965). *ORTEP.* Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

JOHNSON, F., ZITO, S. W., SARMA, R. & MCKEEVER, B. M. (1978). *Tetrahedron Lett.* pp. 753–756.

MAIA, E. & PÉREZ, S. (1982). *Acta Cryst.* B**38**, 849–852.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P., WOOLFSON, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

ONAN, K. D., MAYER, B. J. & SPENCER, T. A. (1984). *Acta Cryst.* C**40**, 1044–1047.

ROBERTS, R. D., FERRAN, H. E. JR, GULA, M. J. & SPENCER, T. A. (1980). *J. Am. Chem. Soc.* **102**, 7054–7058.

RØMMING, C., NEVSTAD, G. O. & SONGSTED, J. (1982). *Acta Chem. Scand. Ser. A*, **36**, 399–405.

SPENCER, T. A. (1979). *Bioorganic Chemistry,* Vol. 1, edited by E. E. VAN TAMELEN, ch. 13. New York: Academic Press.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

VILSMAIER, E. & KLEIN, C. M. (1982). *Chem. Ber.* **115**, 1209–1223.

WESTHEIMER, F. H. (1970). *Search,* **1**, 34.

WOOD, W. A. (1971). *The Enzymes,* Vol. V, edited by P. D. BOYER, 3rd ed., p. 582. New York: Academic Press.

Acta Cryst. (1986). C**42**, 1785–1787

Structure of 3-Isopropyl-1*H*-2,1,3-benzothiadiazin-4(3*H*)-one 2,2-Dioxide (Bentazon)

BY LARRY E. MOSS, BARBARA A. KARCHER, JAMES W. RICHARDSON JR AND ROBERT A. JACOBSON*

Department of Chemistry, Iowa State University, Ames, Iowa 50011, *USA*

(*Received* 28 *February* 1986; *accepted* 25 *June* 1986)

Abstract. $C_{10}H_{12}N_2O_3S$, $M_r = 240.3$, monoclinic, space group $P2_1/c$, $a = 11.658$ (2), $b = 7.406$ (1), $c = 13.296$ (3) Å, $\beta = 110.55$ (2)°, $V = 1074.9$ (3) Å^3, $Z = 4$, $F(000) = 504$, $D_x = 1.48$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0.71007$ Å (graphite monochromator using Si standard), $\mu = 2.81$ cm^{-1} (no correction), $T = 173$ K, $R = 0.045$ for 1002 unique reflections with $|F_o| > 3\sigma(F)$. The nitrogen and carbon atoms in the heterocyclic ring are nearly coplanar with the aromatic carbon ring. However, the sulfur is displaced from this plane by 0·70 Å.

Introduction. Bentazon is one of many compounds known to have herbicidal activity. It is believed to inhibit CO_2 fixation and to inhibit the Hill reaction (photosynthetic electron transport) by binding within the chloroplast (Mine & Matsunaki, 1975). Precise structural information about herbicides can aid in drawing inferences concerning the binding sites in the chloroplast and the mechanism for inhibition of CO_2 fixation.

Experimental. Crystal (obtained from Environmental Protection Agency) 0·10 mm on a side, 2815 intensities measured (fixed width ω-scan, each background being measured for one-half of the total scan time), at ~ 173 K on a modified Nicolet four-circle diffractometer ($2\theta \leq 50°$, diffracted-beam monochromated Mo $K\alpha$ radiation); one standard reflection with no appreciable decay; no absorption correction; octants hkl and $\bar{h}\bar{k}l$, h −13→12, k −8→8, l 0→15; 1170 reflections with $F \gtrsim 3\sigma(F)$, averaging equivalent reflections gave 1002 unique reflections ($R_{\rm int} = 0.024$); cell constants refined from 2θ values of 16 reflections in range 22–37°; systematic absences $0k0$, $k = 2n + 1$ and $h0l$, $l = 2n + 1$.

Non-hydrogen-atom positions were identified using *MULTAN*76 (Main, Lessinger, Woolfson, Germain & Declercq, 1976). Hydrogen atoms located in electron difference synthesis (Powell & Jacobson, 1980) or calculated assuming C—H = 1·05 Å and H—C—H = 109·54°. Full-matrix refinement (Lapp & Jacobson, 1979) on $|F|$ to $R = 0.045$ and $wR = 0.045$, $w = 1/\sigma(F)^2$, non-hydrogens anisotropic; hydrogens isotropic; average $\Delta/\sigma = 0.12$; max. and min. heights in

---

* To whom correspondence should be addressed.

0108-2701/86/121785-03$01.50