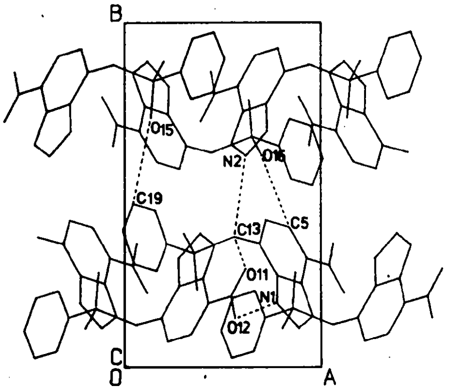

Fig. 3. Projection of the crystal structure along the *c* axis.

The phenyl ring of the $C_6H_5SO_2CH_2$— substituent is inclined to the indazole system at 13·4 (1)°. Its interatomic distances are in the range 1·368 (4)–1·386 (4) Å, with a mean value of 1·380 (4) Å, which is somewhat shorter than the ordinary aromatic bond length. The C(17)—S(14) bond distance of 1·764 (3) Å is comparable to the C(sp^2)—S single bond, *e.g.* 1·766 (2) Å (Sim, 1987), while that of S(14)—C(13), 1·783 (3) Å, is slightly shorter than the C(sp^3)—S (1·81 Å) single bond (*International Tables for X-ray Crystallography*, 1974). The bond distances S(14)—O(15) [1·437 (2) Å] and S(14)—O(16) [1·436 (2) Å] of the —SO_2— group are near to the expected value of 1·432 (3) Å for an S—O double bond (*International Tables for X-ray Crystallography*, 1974). A projection of the crystal structure is shown in Fig. 3. A hydrogen bond exists between the nitrogen and oxygen atoms with the following geometry: N(1)---O(12^i) 3·006 (3), H(11)---O(12^i) 2·18 (3) Å, N(1)—H(11)---O(12^i) 172 (2)°, (i) $-0·5 + x, 0·5-y, 0·5 + z$. Moreover, weak intermolecular C—H---O and C—H---N hydrogen bonds were observed (Fig. 3).

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References

DUDZINSKA-USAREWICZ, J., WRZECIONO, U., FRANKIEWICZ, A., LINKOWSKA, E., KOHLER, T. & NUHN, P. (1987). *Pharmazie*. In the press.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

JASKÓLSKI, M. (1982). *Fourth Symp. Org. Cryst. Chem.*, Poznań, September 1982, *Coll. Abstr.*, edited by Z. KAŁUSKI, pp. 70–71.

LEBAN, I., STANOVNIK, B. & TIŠLER, M. (1978). *Acta Cryst.* B**34**, 293–295.

LEHMANN, M. S. & LARSEN, F. K. (1974). *Acta Cryst.* A**30**, 580–584.

MAKOSZA, M., KINOWSKI, A., DANIKIEWICZ, W. & MUDRYK, B. (1986). *Annalen*, pp. 69, and references therein.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

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

SIM, G. A. (1987). *Acta Cryst.* C**43**, 778–780.

SUTTON, L. E. (1958). *Tables of Interatomic Distances and Configuration in Molecules and Ions*. London: The Chemical Society.

Acta Cryst. (1989). C**45**, 644–647

Azoles. 20.* Structure of a 2/1 Molecular Complex of 3,5-Dinitroindazole with Morpholine

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Abstract. $C_{18}H_{17}N_9O_9$, $M_r = 503·19$, monoclinic, $P2_1/n$, $a = 8·753$ (1), $b = 21·723$ (2), $c = 11·888$ (1) Å, $\beta = 99·39$ (1)°, $V = 2230·2$ (3) Å^3, $D_m = 1·50$ (1), $D_x = 1·50$ Mg m^{-3}, $Z = 4$, λ(Cu $K\alpha$) = 1·54178 Å, μ(Cu $K\alpha$) = 0·954 mm^{-1}, $F(000) = 1040$, room temperature, final $R = 0·051$ for 2508 observed reflections. The asymmetric unit contains a molecular complex consisting of one morpholine and two 3,5-

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* Part 19: Gzella, Wrzeciono, Dudzińska-Usarewicz & Borowiak (1989).

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dinitroindazole molecules. The first forms the ammonium cation as a result of the incorporation of one proton from the pyrrole nitrogen atom of one of the two indazole moieties. Both indazole systems are approximately planar and lie in the same plane. The morpholine cation has a chair conformation, the least-squares plane through this cation is inclined to the indazole moieties at approximately 87°. The molecules in the complex are hydrogen bonded.

Introduction. The reaction of 2,5-dinitroindazole with morpholine yields 3-morpholine-5-nitroindazole and a second product consisting of two molecules of 3,5-dinitroindazole and one molecule of morpholine (Wrzeciono & Linkowska, 1980). The present work has been undertaken to elucidate the structure of the latter compound.

Experimental. The title compound, m.p. 491–492 K, was prepared by the method described by Wrzeciono & Linkowska (1980); yellow prismatic crystals recrystallized from methanol, D_m by flotation, crystal dimensions 0·5 x 0·2 x 0·2 mm, Syntex $P2_1$ diffractometer, graphite-monochromated Cu $K\alpha$ radiation, accurate cell parameters refined from setting angles of 15 reflections with $11° \leq 2\theta \leq 32°$, θ–2θ scan technique, two standard reflections monitored every 100 reflections, no significant intensity variation, profiles measured for 3453 reflections with $2\theta \leq 115°$, 3036 unique reflections, $R_{\rm int} = 0{\cdot}033$, range of *hkl*: h −9→9, k 0→23, l 0→12, profile analysis according to Lehmann & Larsen (1974), no absorption correction, 2508 reflections with $I \geq 1{\cdot}96\sigma(I)$ considered observed and used in the refinement, structure solved by direct methods using *SHELX76* (Sheldrick, 1976), refinement on F by full-matrix least-squares method, anisotropic non-H atoms, H atoms generated from ΔF map and refined with isotropic temperature parameters, $w^{-1} = \sigma^2(F)$, empirical isotropic extinction parameter x used to correct F_c according to $F_c' = F_c\ (1-xF/\sin\theta)$, x converged to 0·023 (1), final $R = 0{\cdot}051$ and $wR = 0{\cdot}055$, $S = 5{\cdot}474$, $(\Delta/\sigma)_{\rm max} = 0{\cdot}03$, max. and min. peak heights in the final ΔF map 0·19 and −0·21 e Å^{-3}; computer programs: *SHELX76* (Sheldrick, 1976) and local programs (Jaskólski, 1982), molecular illustrations drawn using *PLUTO* (Motherwell & Clegg, 1978). Atomic scattering factors from Sheldrick's programs.

Discussion. The labeling scheme of the title compound is given in Fig. 1. A stereoview of the molecular structure is shown in Fig. 2. Atomic coordinates are given in Table 1.* The bond distances and angles with their standard deviations are given in Table 2.

The asymmetric unit consists of the 2:1 molecular complex of 3,5-dinitroindazole with morpholine. On incorporation of one proton from the N(1*A*) atom the morpholine molecule forms an ammonium cation. Both indazole systems *A* and *B* are nearly planar within 0·010 (3) and 0·015 (3) Å, respectively. Moreover, they are almost parallel and lie in the same plane. The morpholine cation is inclined at approximately 87° to this plane. The molecules forming the complex are connected by three hydrogen bonds with the following geometry: N(1*A*)---H(11*B*) 1·68 (4), N(1*A*)···N(1*B*) 2·727 (4) Å, N(1*A*)---H(11*B*)—N(1*B*) 174 (3)°; N(2*A*)---H(161) 1·90 (4), N(2*A*)···N(16) 2·839 (4) Å, N(2*A*)---H(161)—N(16) 164 (3)°; N(2*B*)---H(162) 2·14 (4), N(2*B*)···N(16) 2·976 (4) Å, N(2*B*)---H(162)—N(16) 149 (3)°. The hydrogen-bonded N(1*A*), N(2*A*), N(1*B*), N(2*B*) and N(16) atoms form a ring planar within 0·008 (3) Å.

The geometry of the six-membered ring of both indazole molecules is deformed owing to the influence of a pyrazole ring fused to it along the C(8)—C(9) bond and to the presence of a strongly electronegative nitro

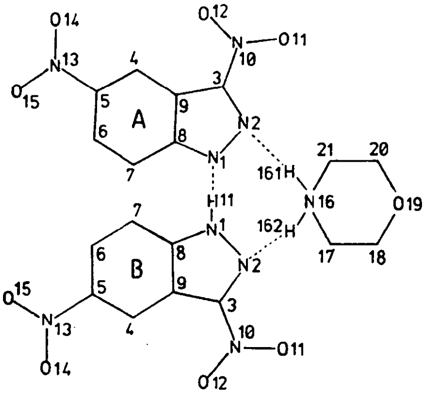

Fig. 1. Labeling scheme.

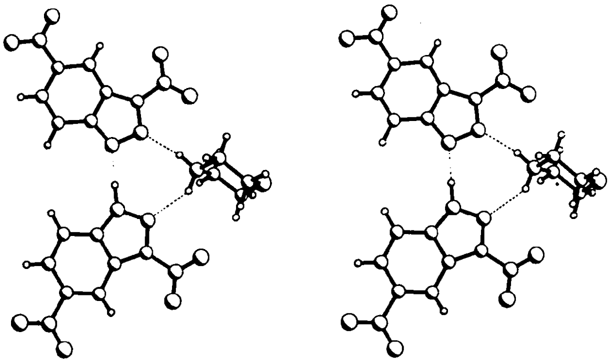

Fig. 2. Computer drawing of the molecular complex.

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* Lists of structure factors, anisotropic thermal parameters, hydrogen-atom coordinates, torsion angles and weak hydrogen bonds have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51450 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters* (Å^2)

$$U_{eq} = \tfrac{1}{3}\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j.$$

	x	y	z	U_{eq}
N(1*A*)	0·6111 (3)	0·2151 (1)	0·3156 (2)	0·0550 (9)
N(2*A*)	0·5544 (3)	0·1594 (1)	0·3352 (2)	0·055 (1)
C(3*A*)	0·4236 (3)	0·1677 (1)	0·3775 (2)	0·046 (1)
C(4*A*)	0·2756 (4)	0·2655 (1)	0·4279 (2)	0·046 (1)
C(5*A*)	0·2937 (3)	0·3281 (1)	0·4226 (2)	0·050 (1)
C(6*A*)	0·4166 (4)	0·3573 (2)	0·3813 (3)	0·056 (1)
C(7*A*)	0·5289 (4)	0·3231 (1)	0·3442 (3)	0·055 (1)
C(8*A*)	0·5144 (3)	0·2586 (1)	0·3477 (2)	0·045 (1)
C(9*A*)	0·3897 (3)	0·2303 (1)	0·3887 (2)	0·041 (1)
N(10*A*)	0·3418 (4)	0·1152 (1)	0·4070 (2)	0·063 (1)
O(11*A*)	0·3978 (3)	0·0637 (1)	0·4011 (2)	0·086 (1)
O(12*A*)	0·2153 (3)	0·1244 (1)	0·4367 (2)	0·084 (1)
N(13*A*)	0·1770 (4)	0·3672 (1)	0·4624 (3)	0·071 (1)
O(14*A*)	0·0709 (3)	0·3438 (1)	0·4996 (3)	0·110 (1)
O(15*A*)	0·1909 (3)	0·4231 (1)	0·4561 (3)	0·104 (1)
N(1*B*)	0·8762 (3)	0·2009 (1)	0·2256 (2)	0·053 (1)
N(2*B*)	0·9152 (3)	0·1417 (1)	0·2122 (2)	0·054 (1)
C(3*B*)	1·0459 (3)	0·1438 (1)	0·1704 (2)	0·048 (1)
C(4*B*)	1·2194 (4)	0·2327 (2)	0·1125 (3)	0·050 (1)
C(5*B*)	1·2171 (4)	0·2951 (2)	0·1099 (3)	0·055 (1)
C(6*B*)	1·1029 (4)	0·3314 (2)	0·1469 (3)	0·060 (1)
C(7*B*)	0·9821 (4)	0·3046 (1)	0·1886 (3)	0·055 (1)
C(8*B*)	0·9809 (3)	0·2401 (1)	0·1915 (2)	0·046 (1)
C(9*B*)	1·0962 (3)	0·2043 (1)	0·1543 (2)	0·044 (1)
N(10*B*)	1·1173 (3)	0·0866 (1)	0·1458 (2)	0·065 (1)
O(11*B*)	1·0513 (3)	0·0386 (1)	0·1596 (3)	0·095 (1)
O(12*B*)	1·2422 (3)	0·0906 (1)	0·1130 (2)	0·091 (1)
N(13*B*)	1·3436 (4)	0·3269 (2)	0·0647 (3)	0·075 (1)
O(14*B*)	1·4481 (4)	0·2962 (2)	0·0400 (3)	0·128 (2)
O(15*B*)	1·3364 (3)	0·3825 (1)	0·0557 (3)	0·109 (1)
N(16)	0·6998 (4)	0·0486 (1)	0·2826 (3)	0·064 (1)
C(17)	0·5948 (5)	0·0159 (2)	0·1914 (4)	0·073 (2)
C(18)	0·6795 (5)	−0·0375 (2)	0·1525 (4)	0·074 (2)
O(19)	0·7298 (3)	−0·0778 (1)	0·2450 (2)	0·070 (1)
C(20)	0·8372 (5)	−0·0476 (2)	0·3290 (4)	0·074 (2)
C(21)	0·7645 (6)	0·0062 (2)	0·3764 (4)	0·079 (2)

Table 2. *Bond distances* (Å) *and angles* (°) *and their standard deviations*

N(1*A*)—N(2*A*)	1·342 (3)	C(3*B*)—N(10*B*)	1·441 (4)
N(1*A*)—C(8*A*)	1·364 (3)	C(4*B*)—C(5*B*)	1·358 (4)
N(2*A*)—C(3*A*)	1·335 (4)	C(4*B*)—C(9*B*)	1·401 (4)
C(3*A*)—C(9*A*)	1·404 (4)	C(5*B*)—C(6*B*)	1·399 (5)
C(3*A*)—N(10*A*)	1·420 (4)	C(5*B*)—N(13*B*)	1·478 (4)
C(4*A*)—C(5*A*)	1·371 (4)	C(6*B*)—C(7*B*)	1·369 (5)
C(4*A*)—C(9*A*)	1·397 (4)	C(7*B*)—C(8*B*)	1·401 (4)
C(5*A*)—C(6*A*)	1·404 (4)	C(8*B*)—C(9*B*)	1·402 (4)
C(5*A*)—N(13*A*)	1·466 (4)	N(10*B*)—O(11*B*)	1·216 (3)
C(6*A*)—C(7*A*)	1·362 (5)	N(10*B*)—O(12*B*)	1·222 (3)
C(7*A*)—C(8*A*)	1·407 (4)	N(13*B*)—O(14*B*)	1·207 (4)
C(8*A*)—C(9*A*)	1·407 (4)	N(13*B*)—O(15*B*)	1·214 (4)
N(10*A*)—O(11*A*)	1·228 (3)	N(16)—C(17)	1·484 (5)
N(10*A*)—O(12*A*)	1·232 (3)	N(16)—C(21)	1·485 (5)
N(13*A*)—O(14*A*)	1·204 (4)	C(17)—C(18)	1·491 (5)
N(13*A*)—O(15*A*)	1·223 (3)	C(18)—O(19)	1·419 (4)
N(1*B*)—N(2*B*)	1·345 (3)	O(19)—C(20)	1·416 (5)
N(1*B*)—C(8*B*)	1·362 (4)	C(20)—C(21)	1·485 (5)
N(2*B*)—C(3*B*)	1·321 (4)		
C(3*B*)—C(9*B*)	1·409 (4)		

N(2*A*)—N(1*A*)—C(8*A*)	108·2 (2)	N(2*B*)—C(3*B*)—N(10*B*)	118·5 (3)
N(1*A*)—N(2*A*)—C(3*A*)	108·0 (2)	C(9*B*)—C(3*B*)—N(10*B*)	128·3 (3)
N(2*A*)—C(3*A*)—C(9*A*)	111·9 (3)	C(5*B*)—C(4*B*)—C(9*B*)	116·0 (3)
N(2*A*)—C(3*A*)—N(10*A*)	118·9 (3)	C(4*B*)—C(5*B*)—C(6*B*)	124·3 (3)
C(9*A*)—C(3*A*)—N(10*A*)	129·2 (3)	C(4*B*)—C(5*B*)—N(13*B*)	117·8 (3)
C(5*A*)—C(4*A*)—C(9*A*)	115·7 (3)	C(6*B*)—C(5*B*)—N(13*B*)	117·9 (3)
C(4*A*)—C(5*A*)—C(6*A*)	124·4 (3)	C(5*B*)—C(6*B*)—C(7*B*)	120·6 (3)
C(4*A*)—C(5*A*)—N(13*A*)	118·0 (3)	C(6*B*)—C(7*B*)—C(8*B*)	116·3 (3)
C(6*A*)—C(5*A*)—N(13*A*)	117·7 (3)	N(1*B*)—C(8*B*)—C(9*B*)	107·5 (3)
C(5*A*)—C(6*A*)—C(7*A*)	120·1 (3)	C(7*B*)—C(8*B*)—C(9*B*)	122·6 (3)
C(6*A*)—C(7*A*)—C(8*A*)	117·4 (3)	C(3*B*)—C(9*B*)—C(8*B*)	102·5 (2)
N(1*A*)—C(8*A*)—C(9*A*)	110·3 (2)	C(4*B*)—C(9*B*)—C(8*B*)	120·2 (3)
C(7*A*)—C(8*A*)—C(9*A*)	121·6 (3)	O(11*B*)—N(10*B*)—O(12*B*)	124·9 (3)
C(3*A*)—C(9*A*)—C(8*A*)	101·7 (2)	O(14*B*)—N(13*B*)—O(15*B*)	124·1 (4)
C(4*A*)—C(9*A*)—C(8*A*)	120·9 (3)	C(17)—N(16)—C(21)	111·5 (3)
O(11*A*)—N(10*A*)—O(12*A*)	123·3 (3)	N(16)—C(17)—C(18)	108·6 (3)
O(14*A*)—N(13*A*)—O(15*A*)	122·1 (3)	C(17)—C(18)—O(19)	110·3 (3)
N(2*B*)—N(1*B*)—C(8*B*)	111·5 (2)	C(18)—O(19)—C(20)	110·3 (3)
N(1*B*)—N(2*B*)—C(3*B*)	105·3 (2)	O(19)—C(20)—C(21)	110·9 (4)
N(2*B*)—C(3*B*)—C(9*B*)	113·1 (3)	N(16)—C(21)—C(20)	109·7 (3)

group. This deformation is observed in the C(4)—C(5) and C(6)—C(7) bonds and in the values of the internal angles C(5)—C(4)—C(9) and C(6)—C(7)—C(8) in both indazole molecules (Table 2). In both indazole systems the endocyclic angle at the *ipso* C(5) atom, α_{NO_2}, with mean value 124·4 (3)°, is about 2° wider than the value of 122·1 (1)° reported by Domenicano, Vaciago & Coulson (1975) for many nitrobenzene derivatives. The nitro group on C(5*A*) is practically coplanar with the indazole system *A*, while the same group attached to C(5*B*) is inclined at 5·3 (1)°, about the C(5*B*)—N(13*B*) bond, to the least-squares plane of indazole *B*. This twisting is probably caused by a weak hydrogen bond between O(15*B*) and C(21)(0·5 + x, 0·5 − y, −0·5 + z); the intermolecular contact O---H—C is 3·215 (5) Å.

No differences are noted in the distances for the N(1)—N(2) and N(1)—C(8) bonds in the pyrazole rings of both indazole systems, although some differences were expected because of the absence of a proton at atom N(1*A*). Only a difference in the valency angles is found for N(2*A*)—N(1*A*)—C(8*A*) and N(2*B*)—N(1*B*)—C(8*B*) (Table 2). Of particular interest are the exocyclic bonds C(3*A*)—N(10*A*) and C(3*B*)—N(10*B*) (Table 2), shortened with respect to the single C—N bond, 1·463 (2) Å, derived from many structural results on nitrobenzene derivatives (Domenicano, Vaciago & Coulson, 1975). This observation indicates some degree of resonance in the nitropyrazole part of both 3,5-dinitroindazole molecules. The difference in these interatomic distances indicates that the excess of the negative charge at the N(1*A*) atom raises the degree of resonance in the *A* molecule. The nitro groups attached to C(3*A*) and C(3*B*) are turned by 6·9 (1) and 4·7 (1)° out of the plane of the respective *A* and *B*

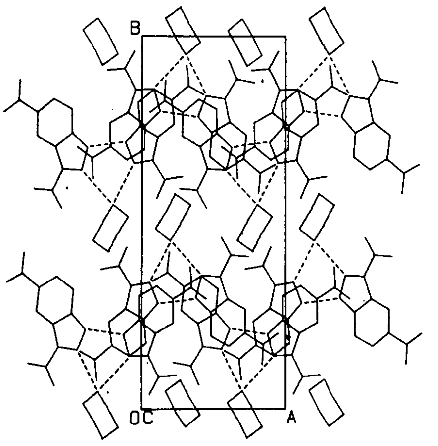

Fig. 3. Projection of the crystal structure along the *c* axis.

indazole systems. The first twisting is presumably due to a weak hydrogen bond between O(12A) and C(20)(1 − x, −y, 1 − z); the O---H—C distance is 3·343 (4) Å. The morpholine cation adopts a chair conformation. Bond lengths N(16)—C(17) and N(16)—C(21) (Table 2) due to the protonation of the nitrogen atom are slightly larger than the single N—C bond. Oxygen O(19) participates in the following hydrogen bonds: O(19)---H(71$A^{\rm i}$) 2·34 (3), O(19)···C(7$A^{\rm i}$) 3·310 (4) Å, O(19)---H(71$A^{\rm i}$)—C(7$A^{\rm i}$) 156 (2)°; O(19)---H(71$B^{\rm i}$) 2·38 (3), O(19)···C(7$B^{\rm i}$) 3·327 (4) Å, O(19)---H(71$B^{\rm i}$)—C(7$B^{\rm i}$) 157 (2)°; symmetry code (i) 1·5 − x, −0·5 + y, 0·5 − z.

Fig. 3 shows the molecular packing in the unit cell. In the crystal lattice the two independent molecules of 3,5-dinitroindazole are almost parallel and partly overlap. They form layers approximately perpendicular to z and about 3·3 Å distant. The molecules overlap in the following order: molecule A overlaps molecule B of a complex in the equivalent position −0·5 + x, 0·5 − y, 0·5 + z.

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References

Domenicano, A., Vaciago, A. & Coulson, C. A. (1975). *Acta Cryst.* B**31**, 221–234.

Gzella, A., Wrzeciono, U., Dudzińska-Usarewicz, J. & Borowiak, T. (1989). *Acta Cryst.* C**45**, 642–644.

Jaskólski, M. (1982). *Fourth Symp. Org. Cryst. Chem.*, Poznań, September 1982, *Coll. Abstr.*, edited by Z. Kałuski, pp. 70–71.

Lehmann, M. S. & Larsen, F. K. (1974). *Acta Cryst.* A**30**, 580–584.

Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

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

Wrzeciono, U. & Linkowska, E. (1980). *Pharmazie*, **35**(10), 593–595.

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Structure of 1-(2-Deoxy-β-D-ribofuranosyl)-5-[(1*S*)-2,2-dibromocyclopropyl]uracil

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Abstract. $C_{12}H_{14}Br_2N_2O_5$, $M_r = 426·07$, orthorhombic, $P2_12_12_1$, $a = 5·861$ (1), $b = 18·609$ (4), $c = 13·433$ (3) Å, $V = 1465·1$ (3) Å^3, $Z = 4$, $D_x = 1·931$ g cm^{-3}, λ(Cu $K\alpha_1$) = 1·5405 Å, $\mu = 73·1$ cm^{-1}, $F(000) = 840$, $T = 293$ K, $R = 0·037$, GOF = 2·6 for 2145 observed reflections. The absolute configuration about C(7) of the cyclopropane ring is *S*. The 5-substituted pyrimidine is *anti* with respect to the deoxyribose and the 2′-deoxyribose is in the 2′-*endo* pucker mode. The torsion angle about C(4′)—C(5′) is *gauche–gauche*.

Introduction. (*E*)-5-(2-Bromovinyl)-2′-deoxyuridine (BVDU) is a potent and selective antiviral agent against herpes simplex virus type 1 (HSV-1) and varicella-zoster virus (VZV) in cell culture, in animals and in the clinic (Jones, Sayers, Walker & De Clercq, 1988). Its activity is due to selective phosphorylation by HSV-1 encoded thymidine kinase and metabolic trapping within infected cells, but not in uninfected host cells (Cheng, Dutschman, Fox, Watanabe & Machida, 1981; De Clercq, Descamps, De Somer, Barr, Jones & Walker, 1979). Structure–activity correlations (Goodchild, Porter, Raper, Sim, Upton, Vitney & Wadsworth, 1983) for olefinic 5-substituted-2′-deoxyuridines indicate that optimum inhibition of HSV-1 occurs when the C(5) olefinic substituent is conjugated with the pyrimidine ring, is not longer than four carbon atoms in length, has *E* stereochemistry and includes a hydrophobic electronegative atom. Exploitation of differences between virus-specific enzymes and the corresponding host-cell enzymes provides a promising strategy in the design of more effective and less toxic antiherpes drugs. It was thus anticipated that 1-(2-deoxy-β-D-ribofuranosyl)uracil possessing a 5-(2,2-dibromocyclopropyl) substituent could act as a biological isostere of the 5-(2-bromovinyl) substituent present in BVDU. The hybridization of the cyclopropane ring results in a higher electron density along the C—C bonds, making them more like those of

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