

Acta Cryst. (1984). C40, 1957–1960

Structures of Three Photodimers of 5-Fluoro-1,3-dimethyluracil: (I) an *anti* Cyclobutene Dimer, $C_{12}H_{13}FN_4O_4$;^{*} (II) the *trans-anti* Cyclobutane Dimer, $C_{12}H_{14}F_2N_4O_4$; and (III) the *cis-syn* Cyclobutane Dimer, $C_{12}H_{14}F_2N_4O_4$

BY JUDITH L. FLIPPEN-ANDERSON AND RICHARD GILARDI

Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC 20375, USA

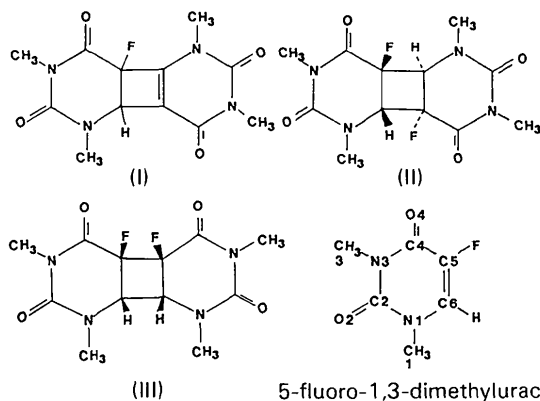
(Received 19 March 1984; accepted 18 June 1984)

Abstract. (I): $M_r = 296.3$, monoclinic, Pc , $a = 8.456$ (8), $b = 11.229$ (12), $c = 7.386$ (8) Å, $\beta = 112.55$ (8)°, $V = 647.7$ Å³, $Z = 2$, $D_x = 1.52$ g cm⁻³, Cu $K\alpha$, $\lambda = 1.54178$ Å, $\mu = 11$ cm⁻¹, $F(000) = 308$, $T = 295$ K, $R = 7.4\%$ for 675 reflections, $S = 1.2$. (II): $M_r = 316.3$, orthorhombic, $P2_12_12_1$, $a = 12.259$ (12), $b = 12.842$ (12), $c = 8.576$ (8) Å, $V = 1350.1$ Å³, $Z = 4$, $D_x = 1.56$ g cm⁻³, Cu $K\alpha$, $\lambda = 1.54178$ Å, $\mu = 12$ cm⁻¹, $F(000) = 656$, $T = 295$ K, $R = 5.3\%$ for 1254 reflections, $S = 2.5$. (III): $M_r = 316.3$, orthorhombic, $Pbca$, $a = 13.962$ (12), $b = 25.418$ (15), $c = 7.815$ (2) Å, $V = 2773.4$ Å³, $Z = 8$, $D_x = 1.51$ g cm⁻³, Cu $K\alpha$, $\lambda = 1.54178$ Å, $\mu = 17$ cm⁻¹, $F(000) = 1312$, $T = 295$ K, $R = 6.1\%$ for 1379 reflections, $S = 1.6$. (I), (II) and (III) are dimers formed by photoirradiation of the antineoplastic drug 5-fluoro-1,3-dimethyluracil. (II) and (III) are normal cyclobutane dimers similar to several previously reported photoproducts of nucleic acid bases. (I) is a strained cyclobutene dimer formed from an intermediate cyclobutane dimer by loss of HF. The structure of (I) was solved by Patterson-search techniques followed by tangent-formula expansion.

Introduction. Photodimers of nucleic acid bases and their derivatives which are formed by UV irradiation of frozen aqueous solutions have been extensively studied (Wang, 1976) since these compounds have been linked to the photobiological effects caused by UV irradiation of DNA. This paper reports on the structures of three materials derived from the irradiation of the antineoplastic drug 5-fluoro-1,3-dimethyluracil. Compound (I) is formed by heating the *cis-anti* dimer with the resultant loss of HF. Molecules (II) and (III) are simple *trans-anti* and *cis-syn* homodimers of the parent monomer.

Experimental. All crystals provided by Dr S. Y. Wang of Johns Hopkins University. Crystal sizes 0.1 × 0.2 × 0.35 mm for (I), 0.4 × 0.45 × 0.7 mm for (II),

^{*} (I) is 4a-fluoro-4a,8b-dihydro-1,3,5,7-tetramethylcyclobuta-[1,2-*d*:3,4-*d'*]dipyrimidine-2,4,6,8(1*H*,3*H*,5*H*,7*H*)-tetrone and names for (II) and (III) may be similarly derived. Note that this numbering differs from that used throughout the text.



0.05 × 0.1 × 0.9 mm for (III). Picker FACS-I diffractometer, $\theta/2\theta$ data collection, scan width 2°, scan rate 2° min⁻¹, 10 s background count; $(\sin\theta/\lambda)_{\max}$ 0.500 Å⁻¹ for (I) and (III), 0.562 Å⁻¹ for (II); range of hkl : $\pm hkl$ for (I), hkl for (II) and (III). For (I), 857 unique reflections with 625 having $|F_o| > 3\sigma(F_o)$; for (II), 1277 unique reflections with 1254 having $|F_o| > 3\sigma(F_o)$; for (III), 1379 unique reflections all considered observed. Standard reflections 300, 040, 102 for (I), 10,0,0, 080, 004 for (II), 502, 0,10,1, 220 for (III) monitored every 100 measurements; intensity variations 3.27% (I), 3.5% (II) and 2.5% (III). Lattice parameters from 10 reflections out to $2\theta_{\max} = 76.5^\circ$ (I), 12 reflections out to $2\theta_{\max} = 90^\circ$ (II) and 12 reflections out to $2\theta_{\max} = 67^\circ$ (III). Corrections for Lorentz and polarization but not for absorption.

Structures of (II) and (III) were solved by routine application of the symbolic addition procedure (Karle & Karle, 1966). Structure of (I) was solved by combination of Patterson-search techniques and the tangent formula. Space group Pc was chosen over $P2/c$ since with $Z = 2$ the latter space group would have required a full molecule disorder across a twofold axis or a center of symmetry. The orientation for the twelve-atom planar segment of (I) was obtained from analysis of the Patterson map. Since in space group Pc the location of the molecule in the xz plane is arbitrary it was only necessary to calculate a one-dimensional translation function along y to position the fragment

properly with respect to a cell origin. The remaining atoms appeared after one iteration through the tangent-formula recycling procedure (Karle, 1968). (I) and (III) were refined by restrained least-squares methods using program *RESLSQ* (Flippin-Anderson, Gilardi & Konnert, 1983). Molecule (I) was not explicitly restrained to fix the xz location of the Pc cell origin, since we have found empirically that the sparse-matrix refinement program *RESLSQ* does not shift the origin in such cases. (This may be due to the neglect of most atom-atom correlation terms; the only off-diagonal elements of the refinement matrix kept by *RESLSQ* are those relating bonded and next-nearest neighbors.) (II) was refined by full-matrix least squares using program *ORFLS* (Busing, Martin, Levy, Ellison, Hamilton, Ibers, Johnson & Thiessen, 1975). In all cases the function minimized was $\sum w(|F_o| - |F_c|)^2$ where the weights w are calculated based on counting statistics with a term included for random error (0.02 in this work) (Gilardi, 1973). Parameters refined: atomic coordinates and anisotropic thermal parameters for all nonhydrogen atoms. All H atoms initially put in at calculated positions. For (I) H positions refined, thermal parameters fixed equal to those of covalently bonded atoms, for (II) H atoms held constant, for (III) H coordinates refined, thermal parameters constant. Scattering factors from *International Tables for X-ray Crystallography* (1962). (I) $R = 7.4\%$, $R_w = 6.5\%$ for 675 reflections, (II) $R = 5.3\%$, $R_w = 6.90\%$ for 1254 reflections, (III) $R = 6.1\%$, $R_w = 4.0\%$ for 1379 reflections. Ratio of maximum least-squares shift to error, exclusive of H atoms, 1:3 for (I), 1:2 for (II) and (III); final difference Fourier $\Delta\rho$ excursions 0.33 and $-0.36 \text{ e } \text{\AA}^{-3}$ for (I), 0.25 and $-0.22 \text{ e } \text{\AA}^{-3}$ for (II), 0.22 and $-0.23 \text{ e } \text{\AA}^{-3}$ for (III). No corrections for secondary extinction.

Discussion. Tables 1–3 list final refined coordinates and B_{eq} values for the non-hydrogen atoms in molecules (I)–(III).*

Bond lengths and angles for all three molecules are listed in Tables 4 and 5 and the conformations of the molecules are illustrated in Figs. 1–3. Overall, the distances and angles for (II) and (III) agree well with values found for other cyclobutyl photodimers. The bonds connecting the two six-membered rings appear to be affected by the location of substituent moieties. In the uracil-uracil dimer, with no substituents, the bonds are equal. In the 6-methyluracil dimer and in the methylene-bridged thymine-thymine dimer the bond with the methyls attached is significantly longer than

* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39598 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates and B_{eq} values for molecule (I)*

Standard deviations, given in parentheses, are based solely on least-squares results. The B_{eq} values are calculated according to the equation: $B_{eq} = \frac{1}{3} \sum_i \sum_j \beta_{ij} a_i \cdot a_j$, where the β_{ij} values are the final refined anisotropic thermal parameters.

	x	y	z	$B_{eq}(\text{\AA}^2)$
N(1)	0.1558 (13)	0.0878 (10)	0.3701 (19)	3.9 (7)
C(1)	-0.0205 (16)	0.0621 (14)	0.3619 (27)	4.3 (9)
C(2)	0.2474 (15)	-0.0053 (16)	0.3540 (24)	3.9 (8)
O(2)	0.2042 (12)	-0.1083 (8)	0.3499 (18)	5.2 (6)
N(3)	0.4156 (13)	0.0193 (10)	0.3530 (17)	2.7 (6)
C(3)	0.5190 (20)	-0.0835 (14)	0.3497 (26)	4.4 (8)
C(4)	0.4881 (17)	0.1322 (14)	0.3693 (23)	3.5 (8)
O(4)	0.6299 (10)	0.1463 (10)	0.3725 (18)	4.8 (6)
C(5)	0.3805 (18)	0.2350 (12)	0.3672 (25)	4.1 (8)
F	0.4698 (10)	0.3117 (7)	0.5168 (15)	5.3 (5)
C(6)	0.1903 (17)	0.2107 (13)	0.3557 (24)	3.7 (8)
N(1')	0.3280 (12)	0.3566 (9)	-0.0382 (16)	2.9 (6)
C(1')	0.5103 (17)	0.3916 (14)	0.0686 (28)	4.9 (9)
C(2')	0.1898 (19)	0.3879 (12)	-0.1491 (27)	4.6 (8)
O(2')	0.2239 (13)	0.4378 (8)	-0.2689 (17)	5.0 (6)
N(3')	0.0329 (13)	0.3574 (10)	-0.1441 (20)	3.2 (6)
C(3')	-0.1167 (21)	0.3970 (16)	-0.3357 (26)	6.4 (11)
C(4')	-0.0263 (18)	0.2992 (13)	-0.0194 (24)	4.0 (8)
O(4')	-0.1651 (11)	0.2749 (10)	-0.0335 (18)	5.6 (6)
C(5')	0.1343 (16)	0.2712 (12)	0.1641 (21)	2.6 (7)
C(6')	0.2873 (16)	0.3056 (14)	0.1693 (23)	3.6 (8)

Table 2. *Fractional coordinates and B_{eq} values for molecule (II)*

Standard deviations, given in parentheses, are based solely on least-squares results. The B_{eq} values are calculated according to the equation: $B_{eq} = \frac{1}{3} \sum_i \sum_j \beta_{ij} a_i \cdot a_j$, where the β_{ij} values are the final refined anisotropic thermal parameters.

	x	y	z	$B_{eq}(\text{\AA}^2)$
N(1)	0.2724 (3)	0.2313 (4)	0.9677 (5)	3.6 (4)
C(1)	0.2546 (6)	0.2458 (6)	1.1342 (7)	6.2 (7)
C(2)	0.1878 (4)	0.2471 (4)	0.8700 (6)	3.7 (4)
O(2)	0.0998 (3)	0.2798 (4)	0.9142 (6)	5.9 (5)
N(3)	0.2056 (4)	0.2290 (3)	0.7091 (5)	3.6 (4)
C(3)	0.1145 (5)	0.2547 (6)	0.6041 (8)	6.6 (7)
C(4)	0.3041 (5)	0.2076 (4)	0.6411 (5)	3.6 (4)
O(4)	0.3210 (4)	0.2145 (3)	0.5043 (4)	5.8 (6)
C(5)	0.3902 (4)	0.1683 (3)	0.7480 (5)	2.9 (3)
F(5)	0.4893 (2)	0.2072 (2)	0.7044 (3)	4.5 (4)
C(6)	0.3698 (4)	0.1783 (4)	0.9245 (5)	2.8 (3)
N(1')	0.4874 (3)	-0.0071 (3)	0.7243 (4)	3.3 (4)
C(1')	0.5051 (5)	-0.0265 (5)	0.5549 (6)	5.1 (4)
C(2')	0.5690 (4)	-0.0287 (4)	0.8257 (6)	3.6 (3)
O(2')	0.6560 (3)	-0.0631 (4)	0.7847 (5)	5.5 (4)
N(3')	0.5483 (4)	-0.0120 (3)	0.9827 (5)	3.9 (4)
C(3')	0.6387 (6)	-0.0342 (6)	1.0907 (9)	7.6 (7)
C(4')	0.4505 (5)	0.0131 (4)	1.0471 (6)	4.0 (4)
O(4')	0.4304 (4)	0.0072 (4)	1.1872 (5)	7.1 (7)
C(5')	0.3676 (4)	0.0558 (4)	0.9366 (5)	2.9 (3)
F(5')	0.2659 (2)	0.0192 (2)	0.9756 (4)	4.8 (4)
C(6')	0.3900 (4)	0.0458 (4)	0.7649 (5)	2.9 (3)

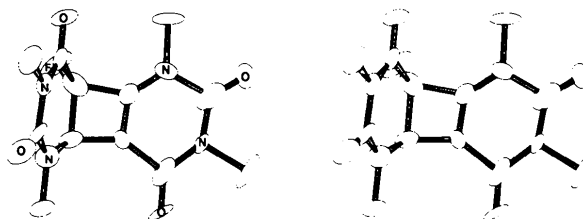


Fig. 1. *ORTEP* drawing (Johnson, 1965) of the cyclobutene dimer (I) (one arbitrarily selected antipode).

Table 3. Fractional coordinates and B_{eq} values for molecule (III)

Standard deviations, given in parentheses, are based solely on least-squares results. The B_{eq} values are calculated according to the equation: $B_{eq} = \frac{1}{3} \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$, where the β_{ij} values are the final refined anisotropic thermal parameters.

	x	y	z	$B_{eq}(\text{\AA}^2)$
N(1)	0.3688 (1)	0.3409 (1)	0.2826 (3)	3.9 (4)
C(1)	0.3580 (3)	0.3532 (1)	0.0990 (4)	6.4 (7)
C(2)	0.2879 (2)	0.3302 (1)	0.3682 (4)	4.1 (5)
O(2)	0.2088 (3)	0.3356 (1)	0.3069 (3)	6.2 (5)
N(3)	0.2960 (1)	0.3109 (1)	0.5375 (3)	3.9 (4)
C(3)	0.2053 (2)	0.2988 (1)	0.6280 (5)	6.5 (8)
C(4)	0.3797 (2)	0.3002 (1)	0.6184 (4)	3.7 (5)
O(4)	0.3830 (1)	0.2770 (1)	0.7550 (3)	5.3 (4)
C(5)	0.4675 (2)	0.3204 (1)	0.5329 (4)	3.5 (5)
F(5)	0.5434 (1)	0.2881 (1)	0.5731 (2)	5.1 (3)
C(6)	0.4649 (2)	0.3310 (1)	0.3422 (4)	3.7 (5)
N(1')	0.5050 (1)	0.4305 (1)	0.2913 (3)	4.0 (4)
C(1')	0.5528 (2)	0.4419 (1)	0.1279 (5)	6.0 (6)
C(2')	0.4299 (2)	0.4608 (1)	0.3379 (4)	4.4 (5)
O(2')	0.4024 (1)	0.4975 (1)	0.2510 (3)	6.3 (4)
N(3')	0.3855 (1)	0.4500 (1)	0.4956 (3)	3.7 (4)
C(3')	0.3020 (2)	0.4826 (1)	0.5385 (5)	5.8 (7)
C(4')	0.4168 (2)	0.4144 (1)	0.6143 (4)	4.0 (5)
O(4')	0.3801 (1)	0.4110 (1)	0.7532 (3)	6.2 (4)
C(5')	0.4981 (2)	0.3789 (1)	0.5623 (4)	3.9 (5)
F(5')	0.5696 (1)	0.3851 (1)	0.6805 (2)	5.7 (3)
C(6')	0.5265 (2)	0.3821 (1)	0.3775 (4)	3.8 (5)

Table 4. Comparison of bond lengths (Å)

	Molecule (I)	Molecule (II)	Molecule (III)
N(1)—C(1)	1.498	1.457	1.476
N(1)—C(2)	1.332	1.349	1.340
N(1)—C(6)	1.422	1.423	1.443
C(2)—O(2)	1.211	1.218	1.212
C(2)—N(3)	1.454	1.417	1.416
N(3)—C(3)	1.453	1.472	1.482
N(3)—C(4)	1.393	1.369	1.356
C(4)—O(4)	1.203	1.194	1.220
C(4)—C(5)	1.466	1.486	1.488
C(5)—C(6)	1.603	1.540	1.515
N(1')—C(1')	1.523	1.490	1.470
N(1')—C(2')	1.473	1.354	1.352
N(1')—C(6')	1.279	1.418	1.433
C(2')—O(2')	1.172	1.206	1.214
C(2')—N(3')	1.385	1.387	1.407
N(3')—C(3')	1.562	1.472	1.469
N(3')—C(4')	1.374	1.359	1.368
C(4')—O(4')	1.168	1.228	1.203
C(4')—C(5')	1.543	1.494	1.505
C(5')—C(6')	1.337	1.503	1.500
C(5)—C(6')	1.585	1.580	
C(5)—C(5')			1.565
C(6)—C(5')	1.475	1.574	
C(6)—C(6')			1.582
C(5)—F(5)	1.375	1.366	1.377
C(5')—F(5')		1.374	1.369
Avg. s.d.	0.020	0.006	0.004

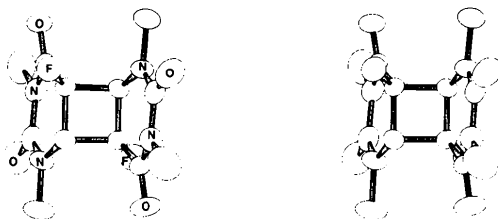


Fig. 2. ORTEP drawing of the *trans-anti* dimer (II).

the unsubstituted one (Karle, 1976). With F as the substituent the opposite effect seems to be present, the C(5)—C(5') bond in (III) is 0.017 (7) Å shorter than the unsubstituted C(6)—C(6') bond. The F...F distance is 2.629 (7) Å. In (II), which has the F atoms bonded at opposite corners of the four-membered ring, the two

Table 5. Comparison of bond angles (°)

	Molecule (I)	Molecule (II)	Molecule (III)
C(1)—N(1)—C(2)	116.6	118.3	116.2
C(1)—N(1)—C(6)	114.4	116.2	116.5
C(2)—N(1)—C(6)	127.7	123.7	126.0
N(1)—C(2)—N(3)	117.1	117.5	118.0
N(1)—C(2)—O(2)	124.9	122.7	123.3
N(3)—C(2)—O(2)	117.9	119.7	118.7
C(2)—N(3)—C(4)	124.8	125.7	125.0
C(2)—N(3)—C(3)	116.5	116.2	116.7
C(3)—N(3)—C(4)	118.6	117.0	118.1
N(3)—C(4)—C(5)	117.8	115.5	115.5
N(3)—C(4)—O(4)	121.5	123.8	122.5
C(5)—C(4)—O(4)	120.5	120.5	121.9
C(4)—C(5)—C(6)	118.1	117.6	118.9
C(4)—C(5)—C(6')	119.4	113.2	
C(4)—C(5)—C(5')			119.1
C(4)—C(5)—F(5)	109.8	109.6	109.0
C(6)—C(5)—F(5)	112.7	112.6	110.4
C(6)—C(5)—C(6')	84.3	89.6	
C(6)—C(5)—C(5')			89.0
F(5)—C(5)—C(6')	110.8	112.9	
F(5)—C(5)—C(5')			108.8
N(1)—C(6)—C(5)	113.1	115.6	111.7
N(1)—C(6)—C(6')			114.8
N(1)—C(6)—C(5')	121.4	116.5	
C(5)—C(6)—C(6')			87.8
C(5)—C(6)—C(5')	85.4	89.1	
C(1')—N(1')—C(2')	118.1	119.0	118.2
C(1')—N(1')—C(6')	123.6	116.2	118.9
C(2')—N(1')—C(6')	118.2	124.3	121.7
N(1')—C(2')—N(3')	109.7	117.2	117.7
N(1')—C(2')—O(2')	119.2	122.7	122.2
N(3')—C(2')—O(2')	130.9	120.1	120.1
C(2')—N(3')—C(4')	137.7	126.4	125.7
C(2')—N(3')—C(3')	110.9	116.3	116.0
C(3')—N(3')—C(4')	111.4	117.0	118.1
N(3')—C(4')—C(5')	104.9	115.4	117.0
N(3')—C(4')—O(4')	131.7	124.0	121.5
C(5')—C(4')—O(4')	123.3	120.5	121.5
C(4')—C(5')—C(6')	119.1	111.9	115.3
C(4')—C(5')—C(6)	141.9	113.3	
C(4')—C(5')—C(5)			113.8
C(4')—C(5')—F(5')		109.7	107.4
C(6')—C(5')—F(5')		112.0	116.8
C(6')—C(5')—C(6)	98.9	91.1	
C(6')—C(5')—C(5)			88.9
F(5')—C(5')—C(6)		111.9	
F(5')—C(5')—C(5)			114.0
N(1')—C(6')—C(5')	130.2	115.8	116.3
N(1')—C(6')—C(6)			120.6
N(1')—C(6')—C(5)	137.7	117.0	
C(5')—C(6')—C(6)			88.9
C(5')—C(6')—C(5)	90.9	90.3	
Avg. s.d.	1.3	0.4	0.3

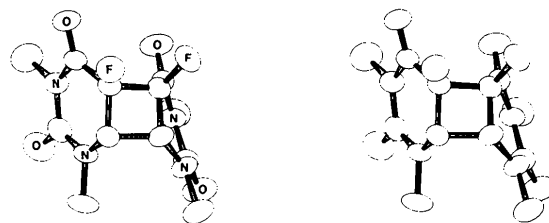


Fig. 3. ORTEP drawing of the *cis-syn* dimer (III) (one arbitrarily selected antipode).

bonds are equivalent. Table 6 lists pertinent torsion angles for the three molecules. The cyclobutyl ring in (II) is planar. The six-membered rings (including substituents) are essentially planar (to within 0.25 Å) and parallel to one another. There is an approximate (non-crystallographic) center of symmetry at the middle of the cyclobutyl ring. In (III) the four-membered ring is twisted and the six-membered rings also show significant deviation from planarity. The *cis-syn* dimers are not as stable as the *trans-anti* dimers and evidence has been found for monomerization of these dimers under prolonged exposure to X-rays during data collection (Karle, 1976). Some deterioration of (III) was noted during data collection; however, no evidence of a coexisting monomer was found. The crystal of (I) used in this study was a very weak scatterer and refinement of the resultant data set gave fairly high e.s.d.'s (on the order of 0.02 Å for bonds and 1.3° for angles). However, the X-ray results do indicate that the molecule is under considerable strain. The double bond formed by the loss of HF across the C(6')-C(5') bond is delocalized over the C(6)-C(5')-C(6')-N(1') system. The strain on the four-membered ring is clearly evidenced by the long C(5)-C(6) bond [1.60 Å as opposed to 1.54 and 1.52 Å in (II) and (III)], the small internal angles at C(5) and C(6) [84.3 and 85.4° compared to 89.6 and 89.1° for (II) and 89.0 and 87.8° for (III)] and the large external angles at the non-fluorinated corners. The N(1)-C(6)-C(5') angle is 121.4°, C(6)-C(5')-C(4') is 141.9° and C(5)-C(6')-N(1') is 137.7°; values for these angles in (II) are 116.5, 113.3 and 117.0°, for equivalent angles in (III) the values are 114.8, 120.6 and 113.8°. All N atoms are methylated, precluding the formation of hydrogen bonds. In molecule (I), however, there are some short intermolecular C...O approaches [C(6')...O(2') at 2.99 Å, C(6')...O(2) at 3.12 Å, C(2')...O(2') at 3.14 Å and C(1)...O(4) at 3.13 Å]. In (II) and (III) the closest intermolecular approaches are van der Waals separations.

Acta Cryst. (1984). **C40**, 1960-1963

6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-1(3H)-isobenzofuranone [(−)-α-Narcotine], C₂₂H₂₃NO₇, a Structural Analogue of GABA

BY D. S. MOSS AND F. E. WATSON

Department of Crystallography, Birkbeck College, University of London, Malet Street, London WC1E 7HX, England

(Received 14 March 1983; accepted 2 July 1984)

Abstract. $M_r = 413.43$, orthorhombic, $P2_12_12_1$, $a = 1.386 \text{ g cm}^{-3}$, Cu K α radiation, $\lambda = 1.5418 \text{ \AA}$, $\mu = 15.295 (9)$, $b = 32.593 (20)$, $c = 7.945 (5) \text{ \AA}$, $V = 9.99 \text{ cm}^{-1}$, $F(000) = 1744$, $T = 298 \text{ K}$, $R = 0.078$ for 3960.7 \AA^3 , $Z = 8$, $D_m(\text{floatation}) = 1.38$, $D_x = 4166$ reflections. Each of the two molecules in the

0108-2701/84/111960-04\$01.50

Table 6. Selected torsion angles (°)

	Molecule (I)	Molecule (II)	Molecule (III)
N(1)-C(2)-N(3)-C(4)	0.5	-7.5	-2.9
C(2)-N(3)-C(4)-C(5)	-6.5	20.1	12.5
N(3)-C(4)-C(5)-C(6)	2.4	-13.1	-23.6
C(4)-C(5)-C(6)-N(1)	6.6	-4.2	24.3
C(5)-C(6)-N(1)-C(2)	-14.1	18.1	-15.4
C(6)-N(1)-C(2)-N(3)	11.0	-13.3	4.8
N(1')-C(2')-N(3')-C(4')	-6.2	7.8	6.4
C(2')-N(3')-C(4')-C(5')	4.9	-18.7	-8.4
N(3')-C(4')-C(5')-C(6')	0.4	12.7	-7.8
C(4')-C(5')-C(6')-N(1')	-3.6	2.0	25.2
C(5')-C(6')-N(1')-C(2')	2.3	-14.1	-29.1
C(6')-N(1')-C(2')-N(3')	2.0	10.2	13.5
C(5)-C(6')-C(5')-C(6)	5.8	-1.2	
C(6')-C(5')-C(6)-C(5)	-5.8	1.2	
C(5')-C(6)-C(5)-C(6')	4.8	-1.1	
C(6)-C(5)-C(6')-C(5')	-5.3	1.2	
C(5)-C(5')-C(6')-C(6)			17.2
C(5')-C(6')-C(6)-C(5)			-17.8
C(6')-C(6)-C(5)-C(5')			17.0
C(6)-C(5)-C(5')-C(6')			-18.0
C(4)-C(5)-C(6')-N(1')	-53.4	121.7	
C(4')-C(5')-C(6)-N(1)	57.4	-119.4	
C(4)-C(5)-C(5')-C(4')			-23.6
N(1)-C(6)-C(6')-N(1)			-25.0
Avg. s.d.	1.6	0.5	0.5

References

- BUSING, W. R., MARTIN, K. O., LEVY, H. A., ELLISON, R. D., HAMILTON, W. C., IBERS, J. A., JOHNSON, C. K. & THIESSEN, W. E. (1975). *ORXFLS3*. Oak Ridge National Laboratory, Tennessee.
- FLIPPEN-ANDERSON, J. L., GILARDI, R. & KONNERT, J. (1983). NRL Memorandum Report No. 5042. Naval Research Laboratory, Washington, DC 20375, USA.
- GILARDI, R. D. (1973). *Acta Cryst.* **B29**, 2089-2095.
- International Tables for X-ray Crystallography* (1962). Vol. IV. Birmingham: Kynoch Press.
- JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.
- KARLE, I. L. (1976). In *Photochemistry and Photobiology of Nucleic Acids*, Vol. I, edited by S. Y. WANG. New York: Academic Press.
- KARLE, J. (1968). *Acta Cryst.* **B24**, 182-186.
- KARLE, J. & KARLE, I. L. (1966). *Acta Cryst.* **21**, 849-859.
- WANG, S. Y. (1976) Editor. *Photochemistry and Photobiology of Nucleic Acids*, Vol. I. New York: Academic Press.