7·428 (2), $b = 9·108$ (5), $c = 11·550$ (3) Å, $\beta = 96·71$ (3)°, $V = 776$ Å^3, $Z = 4$; $R_F = 0·026$ for 782 Cu $K\alpha$ data]. Both groups worked with needle-shaped crystals of form (II) prepared from crystallization in aqueous methanol.

References

ABDEL KADER, M. M., ABDEL HAY, A., KAMEL, G., TALAAT, M. & FAYEK, K. I. (1970). *Acta Biol. Med. Ger.* **24**, 1–11.

CLASTRE, J. (1964). *C. R. Acad. Sci.* **259**, 3267–3269.

FISCHER, M. S., TEMPLETON, D. H. & ZALKIN, A. (1970). *Acta Cryst.* **B26**, 1392–1397.

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 55, 99, 149. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

SHELDRICK, G. M. (1982). *Computational Crystallography*, edited by D. SAYRE, pp. 506–514. Oxford Univ. Press.

SHELDRICK, G. M. (1985). *Crystallographic Computing* 3, edited by G. M. SHELDRICK, C. KRÜGER & R. GODDARD, pp. 175–189. Oxford Univ. Press.

VOGT, H. (1966). *Arch. Gefluegelkd.* **30**, 283–298.

Acta Cryst. (1990). C**46**, 719–720

Structure of (2*R*,3*R*)-3-Acetoxy-5,7-dihydroxy-6-methylflavanone

BY M. C. CHENG, Y. S. CHENG, C. F. CHANG AND YU WANG*

Department of Chemistry, National Taiwan University, Taipei, Taiwan

(*Received* 5 *April* 1989; *accepted* 17 *May* 1989)

Abstract. $C_{18}H_{16}O_6$, $M_r = 328·32$, monoclinic, $I2$, $a = 14·488$ (5), $b = 8·034$ (1), $c = 14·341$ (5) Å, $\beta = 110·76$ (3)°, $V = 1561$ (2) Å^3, $Z = 4$, $D_x = 1·40$, $D_m = 1·39$ g cm^{-3}, $\mu = 1·0$ cm^{-1}, $F(000) = 680$, $T = 298$ K, λ(Mo $K\alpha$) = 0·71069 Å, final $R = 0·050$ for 1827 reflections. The structure of a new flavanone (extracted from the heartwood of *Pinus morrisonicola*) was characterized by X-ray diffraction. All single- and double-bond characters are as expected for a flavanone structure. The saturated heterocyclic ring in the molecule is not planar. The acetoxy and phenyl groups make a torsion angle of 53·0°.

Experimental. Crystal (Fang, Chang & Cheng, 1987) 0·2 × 0·3 × 0·4 mm, CAD-4 diffractometer. Unit cell: 25 reflections, 2θ range 19·58 to 23·56°. D_m by flotation (*n*-hexane/CCl_4). $2\theta_{max} = 60°$. Ranges of h, k, l: −20 to 20, 0 to 11, 0 to 20, respectively. 2θ scan range $(1·4 + 0·7\tan\theta)°$. Three standard reflections monitored every hour: variation < 2%. 2449 unique reflections, 1827 observed with $I > 1·5\sigma(I)$. $R(F) = 0·050$, $wR(F) = 0·037$, $S = 3·8$. Weighting scheme from counting statistics. Structure solved by direct method using the *MULTAN* program. H atoms calculated according to the ideal geometry. Only one of the methyl H atoms and the hydroxyl H atoms are found in a difference Fourier map after isotropic refinement. $(\Delta/\sigma)_{max} = 0·01$. Peak in final map < ±0·18 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Computing programs: *NRCC SDP VAX* Package (Gabe, 1985), *MULTAN* and *ORTEP* from Enraf–Nonius (1979) *Structure Determination Package*. Atomic parameters are given in Table 1,† bond distances and angles in Table 2. A drawing of the molecule is shown in Fig. 1.

† Lists of anisotropic temperature factors of the non-hydrogen atoms, positional and isotropic thermal parameters of the H atoms and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51919 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic parameters and* B_{eq} *values*

E.s.d.'s refer to the last digit printed.

$B_{eq} = \frac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
O1	0·5622 (2)	0·68310	0·1532 (2)	4·6 (2)
C2	0·6382 (2)	0·6817 (6)	0·1178 (3)	3·7 (2)
C3	0·6592 (3)	0·5313 (6)	0·0843 (3)	3·9 (2)
C4	0·7368 (3)	0·5259 (6)	0·0500 (3)	3·8 (2)
C5	0·7966 (3)	0·6618 (6)	0·0502 (3)	3·9 (2)
C6	0·7718 (3)	0·8111 (6)	0·0829 (3)	4·2 (2)
C7	0·6905 (3)	0·8258 (6)	0·1155 (3)	3·6 (2)
C8	0·6584 (3)	0·9852 (6)	0·1389 (3)	3·9 (2)
C9	0·5616 (3)	0·9777 (6)	0·1550 (3)	4·0 (2)
C10	0·5598 (3)	0·8229 (6)	0·2151 (3)	3·9 (2)
C11	0·4720 (3)	0·8035 (6)	0·2456 (3)	4·0 (2)
C12	0·3784 (3)	0·8293 (7)	0·1813 (3)	6·4 (3)
C13	0·2993 (3)	0·8061 (10)	0·2103 (4)	8·1 (3)
C14	0·3120 (3)	0·7580 (9)	0·3038 (4)	7·6 (3)
C15	0·4049 (3)	0·7280 (9)	0·3693 (3)	8·3 (4)
C16	0·4861 (3)	0·7505 (7)	0·3419 (3)	6·0 (3)
O17	0·7601 (2)	0·3811 (4)	0·0152 (2)	4·7 (1)
C18	0·8825 (3)	0·6468 (6)	0·0153 (3)	5·4 (2)
O19	0·8242 (2)	0·9495 (5)	0·0792 (2)	5·8 (2)
O20	0·7028 (2)	1·1170 (5)	0·1417 (2)	5·2 (2)
O21	0·5474 (2)	1·1218 (5)	0·2066 (2)	4·7 (1)
C22	0·4695 (3)	1·2193 (6)	0·1588 (3)	4·3 (2)
O23	0·4173 (2)	1·1944 (5)	0·0749 (2)	6·0 (2)
C24	0·4587 (3)	1·3559 (6)	0·2231 (3)	5·7 (3)

* To whom all correspondence should be addressed.

0108-2701/90/040719-02$03.00

© 1990 International Union of Crystallography

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

O(1)—C(2)	1·366 (4)	C(8)—O(20)	1·232 (6)
O(1)—C(10)	1·439 (4)	C(9)—C(10)	1·518 (6)
C(2)—C(3)	1·374 (6)	C(9)—O(21)	1·427 (5)
C(2)—C(7)	1·391 (6)	C(10)—C(11)	1·494 (5)
C(3)—C(4)	1·379 (5)	C(11)—C(12)	1·359 (5)
C(4)—C(5)	1·393 (6)	C(11)—C(16)	1·389 (6)
C(4)—O(17)	1·354 (5)	C(12)—C(13)	1·363 (6)
C(5)—C(6)	1·381 (7)	C(13)—C(14)	1·344 (8)
C(5)—C(18)	1·502 (5)	C(14)—C(15)	1·363 (7)
C(6)—C(7)	1·418 (5)	C(15)—C(16)	1·378 (6)
C(6)—O(19)	1·358 (5)	O(21)—C(22)	1·344 (5)
C(7)—C(8)	1·442 (6)	C(22)—O(23)	1·189 (5)
C(8)—C(9)	1·502 (6)	C(22)—C(24)	1·477 (7)

C(2)—O(1)—C(10)	115·7 (3)	C(9)—C(8)—O(20)	122·3 (4)
O(1)—C(2)—C(3)	116·4 (4)	C(8)—C(9)—C(10)	108·9 (3)
O(1)—C(2)—C(7)	121·3 (4)	C(8)—C(9)—O(21)	111·2 (3)
C(3)—C(2)—C(7)	122·3 (3)	C(10)—C(9)—O(21)	109·7 (3)
C(2)—C(3)—C(4)	117·5 (4)	O(1)—C(10)—C(9)	106·3 (3)
C(3)—C(4)—C(5)	124·1 (4)	O(1)—C(10)—C(11)	107·9 (3)
C(3)—C(4)—O(17)	120·0 (4)	C(9)—C(10)—C(11)	116·0 (3)
C(5)—C(4)—O(17)	116·0 (3)	C(10)—C(11)—C(12)	122·3 (4)
C(4)—C(5)—C(6)	116·4 (3)	C(10)—C(11)—C(16)	118·8 (3)
C(4)—C(5)—C(18)	121·7 (4)	C(12)—C(11)—C(16)	118·8 (4)
C(6)—C(5)—C(18)	122·0 (4)	C(11)—C(12)—C(13)	121·1 (4)
C(5)—C(6)—C(7)	122·1 (4)	C(12)—C(13)—C(14)	120·8 (4)
C(5)—C(6)—O(19)	118·8 (4)	C(13)—C(14)—C(15)	119·4 (4)
C(7)—C(6)—O(19)	119·1 (4)	C(14)—C(15)—C(16)	121·0 (4)
C(2)—C(7)—C(6)	117·5 (4)	C(11)—C(16)—C(15)	118·9 (4)
C(2)—C(7)—C(8)	120·7 (3)	C(9)—O(21)—C(22)	117·2 (3)
C(6)—C(7)—C(8)	121·6 (4)	O(21)—C(22)—O(23)	122·4 (4)
C(7)—C(8)—C(9)	113·3 (4)	O(21)—C(22)—C(24)	111·7 (3)
C(7)—C(8)—O(20)	124·3 (4)	O(23)—C(22)—C(24)	125·9 (4)

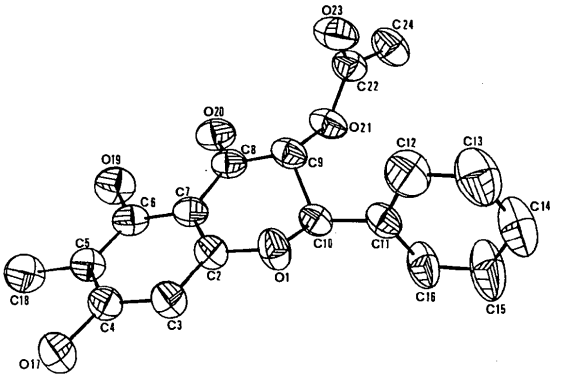

Fig. 1. *ORTEP* drawing of the title compound with 50% probability ellipsoids.

References

Enraf–Nonius (1979). *Structure Determination Package*. Enraf–Nonius, Delft, The Netherlands.

FANG, J. M., CHANG, C. F. & CHENG, Y. S. (1987). *Phytochemistry*, **26**, 2559–2561.

GABE, E. J. (1985). *Crystallographic Computing* III, edited by G. M. SHELDRICK, C. KRUGER & R. GODDARD, pp. 167–174. Oxford: Clarendon Press.

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

Acta Cryst. (1990). C**46**, 720–722

Structure of 6-Azabicyclo[3.2.0]heptan-7-one

BY GÜNTER RECK

Central Institute of Molecular Biology, Academy of Sciences of GDR, 1115 *Berlin-Buch, German Democratic Republic*

JIŘÍ JEČNÝ* AND KAREL HUML

Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, 162 06 *Praha* 6, *Czechoslovakia*

AND JINDŘICH SYMERSKÝ

Institute of Organic Chemistry and Biochemistry, Czechoslovak Academy of Sciences, 166 10 *Praha* 6, *Czechoslovakia*

(*Received* 16 *June* 1989; *accepted* 16 *October* 1989)

Abstract. C_6H_9NO, $M_r = 111{\cdot}15$, monoclinic, $P2_1/c$, $a = 10{\cdot}778$ (3), $b = 6{\cdot}147$ (2), $c = 9{\cdot}673$ (3) Å, $\beta = 109{\cdot}18$ (2)°, $V = 605{\cdot}3$ (8) Å^3, $Z = 4$, $D_x = 1{\cdot}22$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å (graphite monochromator), $\mu = 1{\cdot}02$ cm^{-1}, $F(000) = 240$, $T = 298$ K. Final $R = 0{\cdot}050$ for 785 observed reflections with $I > 2\sigma(I)$. The four-membered lactam ring is planar, and with the five-membered ring adopts a nearly ideal envelope conformation. The shared C—C bond is significantly longer than the other C—C bonds in the molecule. 2_1-related molecules are connected by N—H···O bridges forming chains in the [010] direction. The structure forms channels running along the [001] direction, which probably

* To whom correspondence should be addressed.

0108-2701/90/040720-03$03.00

© 1990 International Union of Crystallography