Acta Cryst. (1963). **16**, 707

Crystal data (I) for pregnanediol and some of its isomers.*

By BARBARA HANER and DORITA A. NORTON, *Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York, U.S.A.*

(*Received* 31 *December* 1962)

Pregnanediol (5β-pregnan-3α,20α-diol), the C_{21} steroid most abundantly present in pregnancy urine, is a recognized metabolite of progesterone. Smaller quantities of two isomers of pregnanediol are also present in pregnancy urine as progesterone metabolites. These are 5α-pregnan-3α,20α-diol and 5α-pregnan-3β,20α-diol (Fieser and Fieser, 1959).

Crystal data for pregnanediol and some of its isomers (including one of those present in human pregnancy urine) have been obtained (Table 1). The X-ray measurements were made with a goniostat on a General Electric XRD-5 X-ray diffraction unit; using Cu $K\alpha$ radiation.

Before measurements were made, the identities of the crystals were checked by determination of their melting points, which were found to be within known melting point ranges. Results before and after crystallization compared favorably, and showed little change due to the crystallization process. In general, the melting points of the recrystallized samples were from 0·5° to 1·0° higher.

Space groups were determined by systematic absences, the centrosymmetric space groups having been automatically ruled out by virtue of the optical activity of pregnanediol and its isomers. Flotation density measurements were made, and the number of molecules per unit cell calculated.

Reference

FIESER, L. F.& FIESER, M. (1959). *Steroids*, pp. 569, 570. New York: Reinhold.

* This investigation was supported in part by PHS grant CY-6183 from the National Cancer Institute, Public Health Service.

Table 1. *Crystal data for pregnanediol* ($C_{21}H_{36}O_2$, $MW = 320{\cdot}50$) and its isomers

1. 5β-Pregnan-3α,20α-diol (pregnanediol). 2. 5β-Pregnan-3α,20β-diol. 3. 5β-Pregnan-3β,20β-diol. 4. 5α-Pregnan-3β,20α-diol. 5. 5α-Pregnan-3β,20β-diol

	1.		2.		3.		4.		5.	
(g.cm^{-3}, meas.)	1·147		1·067		1·087		1·137		1·061	
(g.cm^{-3}, calc.)	1·139		1·078		1·097		1·150		1·077	
Z	4		8		8		2		4	
Space group	$P2_12_12_1$		$P2_12_12_1$		$P2_12_12_1$		P_1		C_2	
a (Å)	10·225	±0·009	14·430	±0·008	14·164	±0·004	9·576	*	25·539	±0·008
b (Å)	24·582		23·032		20·831		12·595		6·376	
c (Å)	7·438		11·887		13·145		8·339		12·136	
α	—		—		—		104·12°		—	
β	—		—		—		92·02°		91·39°	
γ	—		—		—		106·58°		—	
V (Å^3)	1869·55		3950·67		3878·44		925·58		1975·60	
Solvent	Ethanol		Methanol		Acetone		Ethanol		Chloroform	

* No correction factor.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reitdiepskade 4, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

Pittsburgh Diffraction Conference

The twenty-first annual Pittsburgh Diffraction Conference will be held November 6, 7, 8, 1963 at Mellon Institute, Pittsburgh, Pennsylvania. Sessions will be devoted to instrumentation and techniques, structures, metals and alloys, defect lattices and/or radiation damage, with special sessions on transmission microscopy, electron-probe microanalysis, lattice dynamics and/or neutron diffraction. Professor Caroline MacGillavry of the University of Amsterdam will be the guest speaker for the Thursday evening meeting. A placement service will be available. Further information can be obtained from W. M. Biagas, Crucible Steel Company, P. O. Box 7257, Pittsburgh 13, Pennsylvania, U.S.A.