because different sets of incident and absorption edge wavelengths have been used. The differences amount to no more than some tenths of an electron except for wavelengths close to an absorption edge; these values are particularly uncertain and have been marked with an asterisk.

The dispersion corrections calculated in this paper are not regarded as being necessarily superior to those of Cromer (1965).

The variation of the absorption coefficient follows closely a  $\lambda^p$  relation, where  $\lambda$  is the wavelength. The exponents pdepend on the electron shell and on the atomic number involved. They have been chosen according to the examples given by Parratt & Hempstead.

Neither damping effects nor variation with diffraction angle were taken into account in evaluating  $\Delta f'$ .

It is quite difficult to evaluate the total error in the final values of  $\Delta f'$ ; they are given to one decimal place, but this should not be taken as an indication of their accuracy.

The present table is intended as an aid in the use of the two-wavelength method for solving centrosymmetric crystal structures. The use of this method requires a suitable selection of two wavelengths  $\lambda_1$  and  $\lambda_2$  so that, for the anomalous scatterers in the structure, the difference  $\Delta f'(\lambda_1) - \Delta f'(\lambda_2)$  is as great as possible. For a given element, the maximum difference ranges between 20% or more to about 6.5% of the atomic number. Only the elements in the range Z = 38

to Z=48 have a difference less than 10% for the wavelengths included in the present table. If necessary longer wavelengths can be used to remove this limitation.

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## References

CATICHA-ELLIS, S. (1962). Acta Cryst. 15, 863.

CAUCHOIS, Y. & HULUBEI, H. (1947). Longueurs d'Onde des Émissions X et des Discontinuités d'Absorption X. Paris: Hermann et Cie.

COOPER, M. J. (1963). Acta Cryst. 16, 1067.

CROMER, D. T. (1965). Acta Cryst. 18, 17.

- DAUBEN, C. H. & TEMPLETON, D. H. (1955). Acta Cryst. 8, 841.
- PARRATT, L. G. & HEMPSTEAD, C. F. (1954). *Phys. Rev.* 94, 1593.
- TEMPLETON, D. H. (1962). International Tables for X-Ray Crystallography, Vol. III. Birmingham: Kynoch Press.

Acta Cryst. (1966). 20, 930

Crystal data (I) for some cholestane derivatives. By BARBARA HANER and DORITA A. NORTON, Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York, U.S.A.

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The lattice constants of seven cholestane derivatives given in Table 1 have been determined by procedures described in earlier papers (Haner & Norton, 1964; Ohrt, Haner & Norton, 1964). No further work is anticipated on these compounds at the present time.

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## References

HANER, B. & NORTON, D. A. (1964). Acta Cryst. 17, 1610.

OHRT, J. M., HANER, B. & NORTON, D. A. (1964). Acta Cryst. 17, 1611.

		•	•				
	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Formula	$C_{27}H_{48}$	$C_{27}H_{48}O \cdot 2H_2O$	$C_{27}H_{46}O$	$C_{27}H_{44}O$	$C_{27}H_{44}O$	$C_{27}H_{46}O_2$	$C_{27}H_{44}O_2$ . H <sub>2</sub> O
Mol. wt.	372.65	424.68	386.64	384.62	384.62	402.64	418.64
$D_m$ (g.cm <sup>-3</sup> )	1.010	0.957	1.025	1.077	1.080	0.996	1.022
$D_x$ (g.cm <sup>-3</sup> )	1.024	0.959	1.035	1.080	1.069	1.070	1.023
Space group	$P2_1$	$P_1$	$P2_1$	$P2_1$	$P2_{1}2_{1}2_{1}$	$P_1$	P21
Z	4	4	12	2	4	2	4
a (Å)*	19.509	11.235	34.120	14.625	11.236	10.716	23.245
b (Å)*	11.093	23.941	19.967	7.851	19.137	19.963	12.284
c (Å)*	11.479	11.118	11.036	10.672	11.110	6.138	9.663
α (°)	<u> </u>	103-48	_	—		90.94	
β (°)	103.40	89.82	98.33	105.13		107.33	100.02
γ (°)		96.22				94·22	_
Volume (Å <sup>3</sup> )	2417	2941	7439	1183	2389	1250	2717
Solvent	Ethanol	Toluene	Methanol–	Ethanol	Methanol–	Unknown	Ethanol-
•			acetone		acetone		acetone
(1) $5\alpha$ -Cholestane				(5) 5-Cholesten-3-one			
	(2) $5\alpha$ -Cholestan-3 $\beta$ -ol . 2H <sub>2</sub> O (3) $5\alpha$ -Cholestan-3-one			(6) $5\alpha$ -Cholestan-3 $\beta$ -ol-6-one (7) 5-Cholesten-3 $\beta$ -ol-7-one . H <sub>2</sub> O			
	(4) 4	-Cholesten-3-one			-	-	

## Table 1. Crystal data for some cholestane deriwatives

\* Estimated standard deviation 0.04 %.