the corrections for all the aberrations (see for example, Wilson, 1963) except for dispersion and the Lorentz-polarization factor.

Thus for the first iteration, we obtain the limits

$$\theta'_{01} = \sin^{-1}\left\{\frac{[\lambda_C + R(\lambda)/2]\sin\theta_{C0}}{\lambda_C}\right\} - \Delta_G$$

$$\theta'_{N1} = \sin^{-1}\left\{\frac{[\lambda_C - R(\lambda)/2]\sin\theta_{C0}}{\lambda_C}\right\} - \Delta_G\,. \qquad (6)$$

The angles θ'_{01}, θ'_{N1} are rounded to the nearest θ'_j values; because of this rounding an exact knowledge of the spectral distribution is not required and only an approximate value of λ_C need be used in equations (6). The accuracy of λ_C required for equations (6) depends of course both on the Bragg angle and on the magnitude of $\Delta\theta$; the weighted mean of the published peak values of α_1 and α_2 is sufficiently accurate for the back reflection region and the $\Delta\theta$ values given above.

3. The centroid θ'_{C1} of the distribution between the (rounded) limits θ'_{01} and θ'_{N1} is calculated from equation (2) (replacing the unprimed by the primed values) and an adjusted centroid θ_{C1} is found from

$$\theta_{C1} = \theta'_{C1} + \Delta_G\,. \qquad (7)$$

4. If $\theta_{C1} \neq \theta_{C0}$, then θ_{C1} replaces θ_{C0} in equations (6) to calculate new limits θ'_{02}, θ'_{N2}. A new centroid θ_{C2} is then calculated as in step 3.

5. The process is iterated i times until $\theta_{Ci} = \theta_{C(i-1)} = \theta_{Cn}$, at which point the limits are symmetric on a wavelength scale about the centroid. In practice, i is small — at most two or three iterations are required.

6. Finally, the corrected centroid $\theta_C(R)$ is found from

$$\theta_C(R) = \theta_{Cn} + \Delta_L \qquad (8)$$

where Δ_L is the correction of the centroid to account for the effects of dispersion and the Lorentz-polarization factor (Ladell, Mack, Parrish & Taylor, 1959).

The necessity of using an equivalent measure of line position for the powder diffraction line and the spectral line has been discussed by Ladell, Parrish & Taylor (1959) and Pike & Wilson (1959). Because of this requirement, the centroid λ_C of the incident spectral distribution for the same wavelength range as that used in determining $\theta_C(R)$ must be known accurately in order to solve the Bragg equation for d_{hkl}.

To determine λ_C for a selected wavelength range $R(\lambda)$, the procedure is as follows:

1. An approximate centroid λ_{C0} is chosen and the centroid λ_{C1} of the spectral distribution between the limits $\lambda_{01} = \lambda_{C0} + R(\lambda)/2$ and $\lambda_{N1} = \lambda_{C0} - R(\lambda)/2$ is calculated.

2. The difference $D_1 = \lambda_{C1} - \lambda_{C0}$ is used to determine new limits $\lambda_{02} = \lambda_{01} + D_1$ and $\lambda_{N2} = \lambda_{N1} + D_1$, and a new centroid λ_{C2} is calculated.

3. The process is iterated i times until $D_i = D_n = \lambda_{Cn} - \lambda_{C(n-1)} = 0$, at which point the centroid λ_{Cn} lies midway between the limits. Then $\lambda_{Cn} = \lambda_C$ is the spectral centroid for the range $R(\lambda)$.

It should be noted that experimental two-crystal spectrometer spectral distributions may require corrections for aberrations and that these corrections, if known, may be applied in a manner similar to that used for $\theta_C(R)$. Standard values of λ_C for a given radiation need be tabulated only once for a series of ranges for use in solving the Bragg equation. Results of the determination of λ_C for various ranges for Cu $K\alpha$ and Fe $K\alpha$ spectral distributions and the application of the above method to the determination of lattice parameters are being prepared for publication.

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Étude cristallographique préliminaire du perfluoxymolybdate monohydraté de potassium, $K_2MoO_3F_4,H_2O$.

Par DANIEL GRANDJEAN et RAYMOND WEISS, *Laboratoire de Chimie minérale structurale, Institut de Chimie, B.P. 296, Strasbourg (Bas-Rhin), France*

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Le perfluoxymolybdate monohydraté de potassium (Piccini, 1892) cristallise en lamelles monocliniques; les formes les plus courantes sont: {001}, {301}, {$\bar{3}$01}, {021}, {031}.

L'interprétation des diagrammes de cristal tournant et du diagramme de poudre de $K_2MoO_3F_4,H_2O$, conduit à une maille monoclinique de paramètres:

$$a = 6{,}31 \pm 0{,}015,\ b = 6{,}28 \pm 0{,}015,\ c = 18{,}15 \pm 0{,}015\ \text{Å};$$
$$\beta = 98^\circ\ 09' \pm 10'.$$
$$a:b:c = 1{,}0048:1:2{,}8901$$
$$\lambda\ \text{Cu}\ K\alpha = 1{,}5418\ \text{Å}.$$

Cette maille est reliée à celle trouvée par étude mor-

phologique par Piccini (1895; see also Groth), par un changement d'axes de matrice:

$$\begin{vmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

Les enregistrements des plans réciproques suivant les axes [100] et [010] ont été réalisés à l'aide d'un rétigraphe Rimsky-Nonius. Les extinctions systématiques relevées dans ces plans sont du type:

$$h0l \text{ avec } l = 2n+1 \text{ et } 0k0 \text{ avec } k = 2n+1$$

Ces extinctions systématiques sont caractéristiques du groupe de symétrie monoclinique $P2_1/c$.

Le nombre de groupements $K_2MoO_3F_4,H_2O$ par maille est de 4. (densité mesurée: 3,00 g.cm^{-3}, densité calculée: 2,96 g.cm^{-3}).

La détermination de la structure atomique est en voie d'achèvement.

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Crystal data (I) for some estrone-related compounds.*

By JEAN M. OHRT and DORITA A. NORTON, *Department of Biophysics, Roswell Park Memorial Institute, Buffalo, New York, U.S.A.*

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Estrone, $C_{18}H_{22}O_2$, the estrogenically active phenolic metabolite of estradiol, is used in the treatment of prostatic carcinoma and inoperable mammary carcinoma as well as for replacement therapy in estrogen deficiency. It is characterized by the presence of reactive groups at carbon atoms 3 and 17. Table 1 lists crystal data for a series of estrone derivatives with substituents in either or both of these positions.

Lattice constants were determined on a General Electric XRD-5 goniostat-equipped X-ray diffraction unit with Cu $K\alpha$ radiation. Space groups were established on the basis of systematic absences and optical activity. Flotation density measurements were used in calculating the number of molecules per unit cell. The measured and calculated densities agree within the experimental error (3·0%). Melting points, before and after crystallization, agreed with values recorded in the literature.

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Table 1. *Crystal data* (I) *for some estrone-related compounds*

1. 1,3,5(10)-Estratrien-3-ol-17-one 3-methyl ether
2. 1,3,5(10)-Estratrien-3-ol-17-one 3-acetate
3. 1,3,5(10)-Estratrien-3-ol-17-one 3-ethyl ether
4. 1,3,5(10),16-Estratetraen-3,17-diol diacetate
5. 1,3,5(10)-Estratrien-3-01-17-one 3-benzoate

	1	2	3	4	5
Formula	$C_{19}H_{24}O_2$	$C_{20}H_{24}O_3$	$C_{20}H_{26}O_2$	$C_{22}H_{26}O_4$	$C_{25}H_{26}O_3$
Mol.wt.	284·40	312·41	298·43	354·45	374·48
D_m (g.cm^{-3})	1·222	1·205	1·170	1·215	1·247
D_x (g.cm^{-3})	1·239	1·202	1·208	1·243	1·244
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_1$
Z (calc.)	4	4	4	4	2
a (Å)*	11·820	10·834	11·560	11·384	10·562
b (Å)*	18·449	14·838	19·504	21·902	10·146
c (Å)*	6·988	10·733	7·274	7·597	10·357
β (°)	—	—	—	—	115·78
V (Å^3)	1524	1725	1640	1894	999
Solvent	Acetone	Heptane	Acetone–methanol	95% Ethanol	Acetone

* ±0·005 Å