Resultats

L'approximation obtenue par cette méthode se révêle excellente à l'usage pour un intervalle (0; 0,7). Si l'on agrandit l'intervalle en faisant toujours passer la courbe par cinq points (polynôme $P(x)$ du quatrième degré), la précision diminue mais reste assez longtemps acceptable.

Par exemple, dans le cas du tungstène, une approximation des valeurs de Eichhorn (1958) dans l'intervalle (0; 1,8), en faisant passer la courbe par les points 0,1 — 0,3 — 0,6 — 1,2 — 1,8 entraîne une erreur $\Delta f/f$ qui n'excède jamais 1,8%.

L'intervalle utile dans les calculs courants étant (0; 0,7) les résultats sont évidemment bien meilleurs (cf. Tableaux 1 et 2).

On trouvera une comparaison entre les méthodes de Vand, Eiland & Pepinsky (1951), de Freeman & Smith (1958) et la méthode proposée dans le Tableau 3.

Sur la machine Gamma E. T. Bull dont nous disposons, le calcul de f est à peu près deux fois plus rapide que celui de l'approximation en double exponentielle.

L'auteur remercie pour ses conseils, M. E. F. Bertaut, conseiller scientifique du Laboratoire de Diffraction Neutronique au Centre d'Etudes Nucléaires de Grenoble.

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Unit cell and space group of alpha- and beta-parachloral.

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(*Received* 26 *October* 1961 *and in revised form* 10 *February* 1962)

The following first results on the crystallography of α and β parachloral have been obtained on material furnished by Dr Máximo Barón, of Atanor's (S.A.M.) Scientific Department, who prepared the compounds in connection with his studies on cyclic polymers of aldehydes. Both α and β parachloral have formula $(CCl_3CHO)_3$. Their molecular structure was studied by Novak & Whalley (1958).

α-Parachloral crystallizes from ethanol as transparent prismatic crystals with two different habits: (1) elongated parallel to b axis; (2) elongated parallel to [101].

From rotating crystal and Weissenberg photographs, taken with Co $K\alpha$ radiation, the following results were obtained:

System: Orthorhombic

$$a_0 = 10{\cdot}55,\ b_0 = 15{\cdot}40,\ c_0 = 9{\cdot}34\ \text{Å}\ .$$

The morphology, studied on several stereograms, showed the point group to be *mmm*.

The conditions for the presence of reflections are:

hkl	no conditions
h0l	no conditions
*hk*0	$h = 2n$
0*kl*	$k + l = 2n$

which leads to space group *Pnma*.

The observed density, obtained by the flotation method in aqueous solutions of potassium iodomercurate, is $1{\cdot}89 \pm 0{\cdot}01$ g.cm.$^{-3}$. There are four molecules in the unit cell. The calculated density is 1·93 g.cm.$^{-3}$.

β-Parachloral crystallizes from ethanol as six or eight-sided acicular crystals, elongated parallel to b axis. Most stereograms show a binary symmetry axis. The predominant forms are {100}, {101}, {001}, {10$\bar{1}$}.

Strange extinctions obtained from a Weissenberg photograph were accounted for assuming a twinning on [100]. On several stereograms twinning on [101] was observed.

From rotating crystal and Weissenberg photographs, taken with Co $K\alpha$ radiation, the following results were obtained:

System: Monoclinic

$$a_0 = 20{\cdot}20,\ b_0 = 5{\cdot}91,\ c_0 = 13{\cdot}04\ \text{Å},\ \beta = 100°.$$

The conditions for the presence of reflections are:

hkl	no conditions
*h*0*l*	$h = 2n$
0*k*0	$k = 2n$

which leads to space group $P2_1/a$.

The observed density, obtained by the flotation method in aqueous solutions of potassium iodomercurate is $1{\cdot}92 \pm 0{\cdot}02$ g.cm.$^{-3}$. There are four molecules in the unit cell. The calculated density is 1·92 g.cm.$^{-3}$.

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