

Acta Cryst. (1961). **14**, 1208

Parametres cristallins de quelques naphtoquinones 1-4. Par J. GAULTIER, *Laboratoire de Minéralogie et de Rayons X. Faculté des Sciences de Bordeaux, France*

(Reçu le 21 avril 1961)

Naphtoquinone 1-4

La Naphtoquinone 1-4 cristallise dans le système monoclinique sous forme de prismes jaunes allongés suivant la direction [100]. Les paramètres de maille ont été déterminés à partir des clichés de De Jong et de Bragg:

$$a = 8,27 \pm 0,02, \quad b = 7,86 \pm 0,03, \quad c = 12,03 \pm 0,03 \text{ \AA}; \\ \beta = 80^\circ \pm 30'.$$

Densité calculée: 1,37 g.cm.⁻³.
Nombre de molécules par maille: 4.
Groupe spatial: $P2_1/c$.

Bromo 2-naphtoquinone 1-4

La bromo 2-Naphtoquinone 1-4 cristallise dans le système monoclinique sous forme de plaquettes jaunes allongées suivant la direction [010].

Les paramètres de maille sont les suivants:

$$a = 13,88 \pm 0,03, \quad b = 3,98 \pm 0,02, \quad c = 15,74 \pm 0,03 \text{ \AA}; \\ \beta = 104^\circ \pm 1'.$$

Densité calculée: 1,87 g.cm.⁻³.
Nombre de molécules par maille: 4.
Groupe spatial: $P2_1/c$.

Chloro 2-naphtoquinone 1-4

Ce composé donne difficilement des cristaux propres à l'examen aux rayons X; il se présente sous forme de plaquettes brunâtres allongées suivant la direction [010]. Paramètres de la maille orthorhombique:

$$a = 23,84 \pm 0,04, \quad b = 3,88 \pm 0,02, \quad c = 9,12 \pm 0,02 \text{ \AA}.$$

Densité calculée: 1,52 g.cm.⁻³.
Nombre de molécules par maille: 4.
Groupe spatial: $P2_12_12_1$, ou $P2_122_1$.

Acta Cryst. (1961). **14**, 1208

A correction to photometrically measured intensities to allow for α_1, α_2 splitting. By A. I. M. RAE, *Department of Physics* and W. W. BARKER, *Department of Chemistry, University of Western Australia, Nedlands, Western Australia*

(Received 24 January 1961 and in revised form 16 May 1961)

When a set of X-ray intensities is measured using a non-integrating camera, the shape of the spots is observed to vary over the film. Four factors may be involved: irregular crystal shape, disorder in the crystal, imperfectly focused X-rays, and increasing separation of the α_1, α_2 doublets. If a micro-photometer is used to measure the intensities, allowance must be made for this change of shape by integrating the area under the photometer trace of each reflection. Brentano (1945) and Buerger (1960) suggest dividing each peak into a number of narrow strips, but these methods are tedious because a large number of measurements are required for each reflection, and are inaccurate when the breadth of the peaks is small. The authors' experience of a number of compounds shows that, in this latter case, the shape of a resolved peak is very frequently triangular to a close approximation. In this paper, it is assumed that a resolved reflection can be represented by a triangle and that doublet separation is the only factor contributing to the variations in line width. The individual α_1 and α_2 traces of a reflection will then be triangles of equal base and the base size will be constant for all reflections. A correction function $C(\theta)$ is derived by which the maximum height of the trace obtained from a reflection of Bragg angle θ should be multiplied to give a measure proportional to the intensity of the reflection.

There are three cases to be considered:

(1) at fairly low Bragg angle where the α_1, α_2 doublets are unresolved;

(2) where resolution occurs but is not complete;

(3) where the doublets are completely resolved.

Case 1

Fig. 1(a) shows the result of combining two triangular peaks of equal base and of heights in the ratio of 1.82:1 (corresponding to the ratio of the peak intensities of $\text{Cu } K\alpha_1$ and $K\alpha_2$ radiations respectively) whose centres are separated by a distance $\Delta < b$ where b is half the base of either triangle and Δ is the angular separation of the α_1 and α_2 peaks. It is seen that the position of maximum occurs at the point P . The maximum height H is given by

$$H = h_1 + h_2 - h_2\Delta/b, \quad (1)$$

where h_1 and h_2 are the heights of the α_1 and α_2 peaks respectively. Now the total area of both triangles is given by

$$A = b(h_1 + h_2). \quad (2)$$

Thus combining (1) and (2), with $r = h_1/h_2$,

$$A = bH \{1 + 1/[(1+r)b/\Delta - 1]\}. \quad (3)$$

Now, from the Bragg equation, $\lambda = 2d \sin \theta$,

$$\Delta = (2\Delta\lambda/\lambda) \tan \theta, \text{ for } \Delta \text{ small}, \quad (4)$$

$\Delta\lambda$ = difference in wavelength between α_1 and α_2 radiations.

The factor 2 appears because the angular movement