

we measure is the average over  $\beta$  of  $H$ , which brings the problem back to one of cylindrical symmetry:

$$\frac{H(\zeta, \xi)}{V} = \frac{1}{2\pi} \int_{\beta} \int_{\alpha} \int_z \int_x \phi(z, x, \alpha) \times \exp[2\pi i\{\zeta z + \xi x \cos(\alpha + \beta)\}] x dx dz d\alpha d\beta.$$

Expanding,

$$\exp\{2\pi i \xi x \cos(\alpha + \beta)\} = \sum_{-\infty}^{+\infty} i^l I_l(2\pi \xi x) \exp\{il(\alpha + \beta)\},$$

$$\text{and } \phi(z, x, \alpha) = \sum_{-\infty}^{+\infty} \phi_m(z, x) \exp(-im\alpha). \quad (5)$$

The integration over  $\alpha$  gives

$$\frac{H(\zeta, \xi)}{V} = \int_{\beta} \int_z \int_x \sum_{-\infty}^{+\infty} \phi_l(z, x) i^l I_l(2\pi \xi x) \times \exp(il_{\beta} + 2\pi i \zeta z) x dx dz d\beta.$$

Integrating over  $\beta$ , all terms of the sum over  $l$  give zero, with the exception of  $l=0$ :

$$\frac{H(\zeta, \xi)}{V} = 2\pi \int_z \int_x \phi_0(z, x) I_0(2\pi \xi x) \exp(2\pi i \zeta z) x dx dz,$$

where, from (5),

$$\phi_0(z, x) = \frac{1}{2\pi} \int_0^{2\pi} \phi(z, x, \alpha) d\alpha.$$

This leads us back to the case of the fibre diagram, equation (1b).

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## Short Communications

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Rapid publication will be easier if the contributions are without illustrations.*

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### A preliminary examination of the crystal structure of 2, 2'-bipyridyl and its relation to biphenyl.

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Crystals of 2,2'-bipyridyl suitable for a single-crystal study are difficult to obtain. The material usually crystallizes in very complex aggregates. Small but satisfactory prisms were prepared by Prof. Francis H. Case, Temple University, Philadelphia, Pennsylvania. The compound had been carefully purified (m.p. 69–70° C.).

Rotation and Weissenberg patterns were taken about the  $b$ - and  $c$ -axes. The unit cell has the dimensions  $a=5.51$  A.,  $b=6.24$  A.,  $c=13.68$  A.,  $\beta=120^\circ$ . When indexed, the following interferences were found:  $hkl$  in all orders,  $h0l$  when  $l=2n$ ,  $0k0$  when  $k=2n$ . These data are consistent with the choice of the space group  $P2_1/c-C_{2h}^5$ . The density of the crystals, determined by flotation in a solution of potassium iodide, was 1.26 g.cm.<sup>-3</sup> From this and the unit-cell dimensions we calculate that it contains 1.97 molecules. This indicates two molecules per unit cell and would require that these have a center of symmetry. This, taken with the observation (Feldman & Cagle, unpublished) that the ultra-violet spectrum of 2,2'-bipyridyl dissolved in a non-polar solvent is like that reported for biphenyl (O'Shaughnessy & Rodebush, 1940), indicates considerable resonance energy.

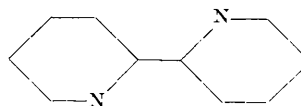
The entire problem of coplanarity of the benzene rings in biphenyl and its analogues, which are not substituted in the  $o,o'$ -positions, has attracted a great deal of interest. Pickett, Walter & France (1936), as well as O'Shaughnessy & Rodebush (1940) and Rodebush & Feldman

(1946), have suggested, based on ultra-violet absorption data, that the rings of such compounds tend toward coplanarity.

On the other hand, Karle & Brockway (1944) have put forth objections to the coplanar structure for biphenyl. It was found that electron diffraction data could be fitted as well by a non-coplanar molecule as by a coplanar one. In addition, it was observed that one might expect some interference between the hydrogen atoms in the  $o,o'$ -positions.

In view of these facts, one is led to conclude that in solutions of compounds of this type, there is a definite tendency toward coplanarity. In the crystalline state this tendency results in coplanar molecules. It is significant to observe that there have been three published determinations of the space group of biphenyl (Clark & Pickett, 1931; Dhar, 1932; Hengstenberg & Mark, 1929). All of these agree that it is  $P2_1/c-C_{2h}^5$  with two molecules per unit cell, and any error seems most unlikely.

In the case of 2,2'-bipyridyl, one concludes that the molecule exists in the crystal with the rings coplanar and with the nitrogen atoms *trans* to the bond joining the rings:



It is perhaps worthy of note that in this configuration the 3,3'-hydrogen atoms would not interfere, whereas should the *cis*-configuration (without a center of symmetry) have been chosen this would not be the case.

A study of the molecular configuration is now under way. It can be stated that the planes whose interferences are strong and which seem well fitted by the trial structure under consideration are of high index.

The writer wishes to thank Profs. G. L. Clark, of the University of Illinois, and J. Turkevich, of Princeton University, for the use of their laboratories. In addition, he wishes to thank Mr J. S. Fritz, of the University of Illinois, who kindly prepared a Debye-Scherrer pattern of high resolution by means of which final values of the unit-cell parameters were obtained.

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**Note sur la cristallographie de la cantharidine, C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>.** Par J. GARRIDO. *Instituto Nacional de Física y Química, Serrano 119, Madrid, Espagne*

(Reçu le 18 mai 1948)

La cantharidine, C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>, cristallise dans le système orthorhombique; les cristaux employés dans cette étude ont été obtenus par évaporation lente d'une solution de cantharidine 'Kalbaum' dans de l'acetone.

Les formes observées sont, par ordre d'importance: (100), (010), (011), (210). Les angles mesurés au goniomètre conduisent à la relation des axes:

$$a : b : c = 0,88_3 : 1 : 0,53_9$$

d'accord avec les valeurs données par Negri (1889). Le faciès des cristaux étudiés est représenté sur Fig. 1.

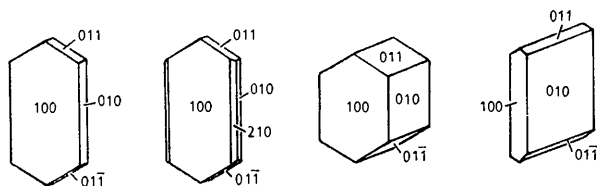


Fig. 1. Le faciès des cristaux de la cantharidine.

J'ai obtenu un certain nombre de diagrammes de Laue, tournants, et de Weissenberg (spectres: *hk0*, *hk1* et *h0l*). Les dimensions de la maille sont:

$$a_0 = 11,05 \text{ \AA}, \quad b_0 = 12,54 \text{ \AA}, \quad c_0 = 6,74 \text{ \AA}.$$

- ### References
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Une détermination de la densité m'a donné la valeur: 1,41 g.cm.<sup>-3</sup> Le nombre de molécules par maille est de 4 (densité calculée: 1,38 g.cm.<sup>-3</sup>). Les extinctions observées sur les diagrammes sont les suivantes:

- hk0*—quand *h* est impair;
- 0kl*—quand *k* + *l* est impair;
- h0l*—pas d'extinctions.

Ceci donne comme groupe probable le  $D_{2h}^{18}$ -*Pnma*.

La structure de la molécule de la cantharidine a été établie par Gadamer (1904), Diels & Alder (1929), et récemment par Woodward & Lotfield (1944). Ces auteurs admettent une formule avec un plan de symétrie. Les conditions de multiplicité du groupe *Pnma* et la présence de 4 molécules par maille confirment l'existence du plan de symétrie des molécules et exigent que celles-ci soient placées dans le cristal de façon à ce que leur plan de symétrie coïncide avec le plan *m* d'orientation (010).

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## Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).*

### International Union of Crystallography

The adhesion of Great Britain has already been announced in this column (*Acta Cryst.* (1948) **1**, 45). Further formal notification of adhesion has now been given as follows:

On 7 April 1948 by the United States of America through the National Research Council.

On 28 April 1948 by Canada through the National Research Council.

On 31 May 1948 by Norway through the Norwegian Academy of Science.