

are given at the points $u = n/120$, on the one side for $n = 0, 2, \dots, 30$, and on the other for $n = 1, 3, \dots, 29$. Now any strip, $A \cos 2\pi h_1 u$ for instance, can be looked upon as presenting the values of the function at the point $u_1 = h_1/120$, for the values of $h = n = 0, 2, \dots, 30$ and $h = n = 1, 3, \dots, 29$ respectively, (or at $u_1 = h_1/60$ for $h = 1, 2, \dots, 15$, on the even side of the strip). Consequently the value of the function

$$C(u, w) = \sum_h \sum_l D_{hl} \cos 2\pi hu \cdot \cos 2\pi lz = \sum_h B_h(w) \cos 2\pi hu,$$

at points (u_i, w_j) , at intervals of $1/60$, can be calculated in the following way. First one prepares, in the conventional way, the figure table $B_h(w) = \sum_l D_{hl} \cos 2\pi lw$, then, laying the strip $A = 10$ (or 100, according to the accuracy needed) and $h = 60u_i$ of the cos function under the line of figures corresponding to w_j on the $B_h(w)$ table, one multiplies the two lines of figures additively, as can be conveniently done with most business computing machines. When the figure field is desired at point intervals of $1/120$, a set of strips with $A = 10$ (or 100) and the values of the function for $n = 1, 2, \dots, 30$ all written on the same side, should be prepared. The sine term

$$S(u, w) = \sum_h \sum_l D_{hl} \sin 2\pi hu \cdot \sin 2\pi lw$$

can be calculated in exactly the same way, using the sin strips. To obtain the value of $D(u_i, w_j)$, the tables for the different terms, with the respective strips on them, are laid side by side and the additive multiplication is carried through the lines $w = w_j$, on the different tables. The results can be copied from the computing machine right to the figure map, this being also facilitated by the fact that the indices (i, j) on the tables and strips coincide with those of the points on the map.

This technique was applied, with considerable success, to the refinement of the atomic coordinates in the structure analysis of dianthrone (Harnik & Schmidt, 1954). It is fairly rapid and, as one gets accustomed, can be performed almost automatically. Compared to the conventional technique the time needed to perform a cycle of refinement is reduced by approximately 50%.

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The X-ray crystallography of 2,6-dimethyl- γ -pyrone. By GEORGE M. BROWN and HILLYER G. NORMENT, *Department of Chemistry, University of Maryland, College Park, Maryland, U.S.A.*

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The unusual chemical behavior of the γ -pyrones (reviewed by Fried, 1950) has prompted an investigation in this laboratory of the structure of 2,6-dimethyl- γ -pyrone by single-crystal X-ray methods. Rotation, Weissenberg, and precession photographs have been taken using $\text{Cu K}\alpha$ radiation. Analysis of the films yields the following data:

$$a = 7.672 \pm 0.007, \quad b = 7.212 \pm 0.007, \quad c = 13.92 \pm 0.01 \text{ \AA}, \\ \beta = 120^\circ 59' \pm 2';$$

axial ratios: 1.0638:1:1.9301; space group: $C_{2h}^5-P2_1/c$.

The transformation $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = -\mathbf{b}$, $\mathbf{c}' = -\mathbf{a} - \mathbf{c}$ gives a cell with axial ratios 1.0638:1:1.6563 and $\beta = 92^\circ 28'$ (space group $P2_1/n$), in fair agreement with the ratios 1.0599:1:1.6441 and angle $\beta = 92^\circ 30'$ determined goniometrically by Wyrouboff (1909) and recorded by Groth (1919).

The space group $P2_1/c$ is uniquely established by the extinction of reflections $0k0$ for odd values of k and of reflections $h0l$ for odd values of l . The absence of centrosymmetry in the molecules of 2,6-dimethyl- γ -pyrone requires that there be at least four molecules in the unit cell. The calculated density for four molecules is 1.249 g.cm.^{-3} ; the observed density by the flotation method is 1.254 g.cm.^{-3} .

The equi-inclination, multiple-film Weissenberg method has been used to collect intensity data. The crystal specimens used were approximately cylindrical, about 0.4 mm. in diameter, enclosed in thin-wall glass capillaries

to prevent evaporation. Of the 1450 reflections theoretically accessible, using $\text{Cu K}\alpha$ radiation, about 1200 have been recorded, and their intensities have been estimated visually. After correction for the Lorentz and polarization factors, the data have been put on an absolute basis by the Wilson (1942) method; and the B value of the temperature factor has been established as $4.15 \times 10^{-16} \text{ cm.}^2$. Preliminary calculations are in progress for application of the Hauptman-Karle (1953) method of solution.

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