additional holes in the mask or, preferably, by rotating the mask in its own plane through 180° so that the zero-order hole is at the bottom right-hand corner of the mask. Values of cos $(hx+ky)$ for every atom can be obtained in this way and the values for similar atoms summed. For non-centrosymmetric projections the values of sin $(hx+ky)$ can be obtained in the same way, using the same masks and the same table, by setting the position of the masks from the values of x, marked along the edges of the table, corresponding to sin x.

The table can be prepared from the values of cos x given in *Internationale Tabellen* (1935). The masks can be made as required until a substantial number of the 500 necessary for a complete set has been acquired, and then the missing ones can be added. (100–200 masks may be required during the refinement of two zones of a structure of average complexity.) A master chart of the same dimensions as the mask, marked out in rectangles as in the table, in which are printed the values of x, is useful for making the masks. The corners of the rectangles corresponding to the values of ky for the required value of y can be pricked through to a blank mask placed below.

Geometrical structure factors for a centrosymmetric zone containing 10 similar atoms can be evaluated at the rate of 20–30 per hour.

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The crystallographic constants of acetoxy*nor*cafestenolide.

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The molecular structure of cafestol is unknown and has been the subject of several chemical investigations (Djerassi, Wilfred, Visco & Lemin, 1953; Haworth, Jubb & McKenna, 1954). Organic reactions indicate the presence of a furan ring attached to a six-membered ring and also a five-membered carbon ring with glycollic side chain. Combustion analyses suggest a formula $C_{20}H_{28}O_3$, which leads to possible structures involving five rings. The presence of two extra hydrogen atoms, which would admit a number of other structures involving fewer rings, cannot, however, be immediately dismissed. This work was undertaken to determine the exact number of hydrogen atoms per molecule, which must, in this compound, be even.

Crystals of the derivative acetoxy*nor*cafestenolide (Haworth, Jubb & McKenna, 1955), $C_{21}H_{28}O_4$, based upon the above formula for cafestol, proved to be easily obtainable as single crystals from ethereal solution. Furthermore, preliminary investigation showed them to be monoclinic with $\beta \fallingdotseq 92°$, so that the unit-cell volume is relatively insensitive to slight errors in β.

The primitive translations were obtained from single-crystal rotation photographs by the method suggested by Farquhar & Lipson (1946), the values being refined by least-squares extrapolation. Their arrangement of a van Arkel mounting was modified by the insertion of a shaped ebonite plug, drilled to take the collimator assembly, into the collimator opening of a Unicam 3 cm. camera to ensure that the film was wholly in contact with the camera. Normally, filtered Cu $K\alpha$ radiation was used, but where this did not result in spots at sufficiently high θ, as was the case for the b direction, filtered Ni $K\alpha$ radiation was found to be satisfactory. At least two determinations of each parameter involving different crystals were made; β was measured by the method of triangulation (Buerger, 1942), using a Weissenberg camera, as the method of angular lag becomes unreliable as β tends to 90°.

Results

Taking

Cu $K\alpha_1$ = 1·54051 Å, Ni $K\alpha_1$ = 1·65784 Å,
Cu $K\alpha_2$ = 1·54433 Å, Ni $K\alpha_2$ = 1·66169 Å,

we find

$$a \sin\beta = 8{\cdot}252 \pm 0{\cdot}002 \text{ Å},$$
$$b = 7{\cdot}683 \pm 0{\cdot}002 \text{ Å},$$
$$c \sin\beta = 14{\cdot}637 \pm 0{\cdot}002 \text{ Å},$$
$$\beta = 92° 36' \pm 30' \ (\sin\beta = 0{\cdot}9989 \pm 0{\cdot}0004).$$

The density is $1{\cdot}228_5$ g.cm.$^{-3}$ and hence the unit-cell volume is $929{\cdot}0 \pm 0{\cdot}5$ Å^3.

Systematic absences were $0k0$ when k is odd; the space group is therefore $P2_1$ or $P2_1/m$. Since there are only two molecules per unit cell and chemical evidence rejects the possibility of a molecular centre of symmetry, the space group is probably $P2_1$; and this is confirmed by the detection of a pyroelectric effect.

The molecular weight determined is then $343{\cdot}8 \pm 0{\cdot}5$ while that for $C_{21}H_{28}O_4$ is 344·4.

The density of the crystals was measured, after outgassing *in vacuo* for 12 hr., by the sink-or-float method, using variation of both the solution composition and the temperature.

The crystals were elongated along b. The refractive index parallel to b was considerably less than the indices perpendicular to b. These observations are consistent with a roughly planar molecular arrangement, the planes being stacked normal to the screw axis. These observations thus show that the structure of cafestol must contain five rings.

We wish to thank the B.S.A. Group Research Centre for the loan of a Weissenberg camera and are indebted to Mr H. S. Peiser for many facilities. The derivative was prepared by Mr A. H. Jubb.

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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).

Tables for Harmonic Synthesis

The authors of the above tables (see *Acta Cryst.* (1949), **2**, 194, and *Math. Tab. Wash.* (1949), **3**, 413) have drawn attention to the following errors:

$F = 69$. Read 470 instead of 370.
$F = 99$. Read 405–460 instead of 505–560.
$F = 16$. Read 350–380 instead of 550–580.
$F = 98$. Read 240 instead of 230.

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Two charts for setting the Buerger precession camera: correction

An error occurs in Fig. 1 of the above article by M. V. King (*Acta Cryst.* (1955), **8**, 53): the symbol $\bar{\gamma}$ (twice) should read $\bar{\nu}$.