have an edge of about 3·8 Å. The number of lines actually observed up to $\sin\theta = 0{\cdot}8$ was roughly five times the number a 4 Å cubic cell could have produced in this interval. At higher values of $\sin\theta$ the lines were too diffuse to measure or even count.

The following observations were sufficient to select a unit cell. The 'cubic 200' reflection was split into two lines with the one of smaller Bragg angle more intense than the other; this was accounted for by assuming the a and c axes about equal and the b axis somewhat shorter. The 'cubic 110' reflection appeared split into four lines consisting of one line and a close doublet on opposite sides of a very strong line; these were accounted for by also taking β different from 90°. Weak lines corresponding to spacings greater than 4 Å were present; these were accounted for by doubling the cell edges. The resulting cell had the following dimensions:

$$a \fallingdotseq c = 7{\cdot}61\pm0{\cdot}01,\quad b = 7{\cdot}54\pm0{\cdot}01\ \text{Å};\quad \beta = 92^\circ\ 56'\pm6'.$$

All but two very weak lines were indexable with this cell. Indices were assigned on the basis of Bragg-angle agreement with no consideration as to the possible space group. Except for 504 and 070, however, all the indices are consistent with $P2_1/n$. Both of these exceptions are ambiguous, and, in view of the discussion by Vousden (1951), should be considered less probable than their listed alternates (Table 1).

If a is not exactly equal to c (they are not likely to differ by more than 0·015 Å however), the crystals are probably monoclinic. If a is exactly equal to c, choosing the diagonals of the a–c face as new a and c axes results in a cell which is orthogonal, B centered, and has cell edges of 10·49, 7·54 and 11·04 Å. This cell would imply that the crystals are orthorhombic. The orthorhombic a and c axes could be halved if the monoclinic cell were end centered, but the 332 and $\bar{5}24$ or 504 reflections, both very weak, prevent this possibility.

Another possibility is that the cell is similar to that of $NaNbO_3$ (Vousden, 1951). In this case we would expect the dimensions of the orthorhombic cell to be 5·24, 15·08 and 5·52 Å. If one takes into account the ambiguities in some of the indexing, no reflections prevent this possibility. In fact, this cell could also account for the two previously non-indexed reflections. A decision as to which unit cell is correct, as well as any detailed evaluation of the structure, will probably have to await the growing of satisfactory single crystals.

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A rapid numerical method of calculating structure factors.

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Simple, rapid methods of calculating structure factors usually depend on the use of some geometrical, mechanical or electrical analogue. The methods of Vand (1948), Llewellyn (1951), Phillips (1952), Stanley (1952) and Grenville-Wells (1954) all suffer from some disadvantages such as limited accuracy, the necessity of preparing preliminary tables of $(hx+ky)$, or the inconvenience of the presentation of the result as the length of a line or the deflection of a galvanometer. Numerical methods for calculating the product $\frac{\cos}{\sin}(hx)\frac{\cos}{\sin}(ky)$ are convenient only when a single product is required. The method here described is more accurate than most analogue devices and is numerical.

The basis of the method is a single table of values of $\cos x$ at intervals of 0·001 in x, arranged in a rectangular array so that successive rows overlap. In the present table each value of $\cos x$ is contained in a rectangle 1·0 cm. × 0·5 cm. and the values of x in successive rows run thus:

$$0{\cdot}000\text{–}0{\cdot}040,\ 0{\cdot}020\text{–}0{\cdot}060,\ 0{\cdot}040\text{–}0{\cdot}080,\ \ldots,\ 0{\cdot}980\text{–}0{\cdot}020,$$
$$0{\cdot}000\text{–}0{\cdot}040,\ 0{\cdot}020\text{–}0{\cdot}060,\ \ldots,\ 0{\cdot}980\text{–}0{\cdot}020\,.$$

Positive and negative values of $\cos x$ are distinguished by the use of different coloured inks and the values of x for both $\sin x$ and $\cos x$ are marked along the edges of the table. This type of arrangement of four complete cycles is necessary in order that the masks, described below, can be moved over the table and the correct relationship between the positions of the values of $\cos x$ preserved. The particular arrangement is flexible and the present table, which can be mounted on a board 18 in. × 20 in., has been designed for convenient desk use.

Masks are prepared, which cover the area of one cycle of the table, from which are cut rectangular holes 1·0 cm. × 0·5 cm. at positions corresponding to ky. One mask is required for each value of y punched with holes corresponding to successive orders of k up to, say, 20, and the holes are marked with the values of k. On the scale proposed the masks are approximately quarto size.

To use the method a table of values of hx is prepared for each atom and the appropriate mask for the y value of the first atom is selected. The mask is placed with the zero-order hole at 000 in the table. The values of $\cos ky$ appear in the holes marked k from 0 to 20. These values are conveniently noted on a recording adding machine. The mask is then moved until the zero-order hole is at x in the table when all the values of $\cos(x+ky)$ appear in the holes marked k and are similarly recorded. This procedure is repeated with the zero-order hole at $2x$, $3x$, etc. until all the values of $\cos(hx+ky)$ have been recorded. Negative values of k can be obtained by punching

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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 $\beta \fallingdotseq 92^\circ$, 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

$$\mathrm{Cu}\,K\alpha_1 = 1\cdot54051\ \text{Å}, \qquad \mathrm{Ni}\,K\alpha_1 = 1\cdot65784\ \text{Å}\,,$$
$$\mathrm{Cu}\,K\alpha_2 = 1\cdot54433\ \text{Å}, \qquad \mathrm{Ni}\,K\alpha_2 = 1\cdot66169\ \text{Å}\,,$$

we find

$$\begin{aligned} a\sin\beta &= 8\cdot252\pm0\cdot002\ \text{Å}\,, \\ b &= 7\cdot683\pm0\cdot002\ \text{Å}\,, \\ c\sin\beta &= 14\cdot637\pm0\cdot002\ \text{Å}\,, \\ \beta &= 92^\circ\ 36'\pm30'\ (\sin\beta = 0\cdot9989\pm0\cdot0004)\,. \end{aligned}$$

The density is $1\cdot228_5$ g.cm.$^{-3}$ and hence the unit-cell volume is $929\cdot0\pm0\cdot5$ 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 $343\cdot8\pm0\cdot5$ 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.