Table 2. *Anisotropic temperature factors* ($\times 10^4$)

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1) DR	217	46	177	62	−67	21
SM	206	44	151	59	−47	16
σSM	6	1	6	4	10	4
O(2) DR	233	52	118	44	25	−10
SM	227	53	91	46	18	−10
σSM	7	1	5	4	10	3
C(1) DR	169	27	142	6	−59	12
SM	149	25	119	−6	−18	−8
σSM	6	1	7	4	10	4
N DR	176	41	99	14	−13	−3
SM	150	36	88	5	12	2
σSM	6	1	6	4	8	4
C(2) DR	163	36	121	42	−8	−1
SM	138	28	98	15	5	−4
σSM	6	1	7	4	10	4
C(3) DR	195	62	163	−26	−35	−2
SM	177	58	153	−38	−61	−15
σSM	8	2	9	5	12	5

The goodness of fit for both sets of data to their corresponding models is about the same; for our data $R=0{\cdot}061$, $R''=0{\cdot}049$, for the SM data $R=0{\cdot}049$, $R''=0{\cdot}070$, with R'' based on the 489 reflexions common to both data sets ($R=\Sigma_i |F_o-F_c|/\Sigma_i |F_o|$). We conclude that the small differences between our model and that of SM arise mainly from systematic errors in the data.

In carrying out the Hamilton tests, weights for the SM data were estimated from SM's expression for $\sigma(F_o^2)$ using $\sigma(F_o)\sim\sigma(F_o^2)/2F_o$. For our data, and also in the latter stages of our refinement, we employed a weighting system $w_i=64/F_o^2, F_o\geq 8$; $w_i=F_o^2/64, F_o\leq 8$, which was found empirically to give a reasonably constant value of $\Sigma_i w_i(F_o-F_c)^2/n$ in different ranges of F_o. Some earlier calculations were carried out with weights based on the estimated intensity errors arising solely from statistical counting fluctuations. Since the diffractometer operates on a fixed-time counting mode, weak reflexions are here assigned in general low weights, while strong reflexions are assigned a high and more or less constant weight. The unsuitability of this weighting scheme soon became apparent from the $\Sigma_i w_i(F_o-F_c)^2/n$ test, but it is interesting that it led to large errors not only in the thermal parameters but also in the positions of the atoms. The change in the position of C(3) amounted to 0·035 Å, about ten times the estimated standard deviation, with a concomitant change in the C(2)–C(3) bond length from 1·525 Å (SM) to 1·553 Å!! This impresses the importance to be attached to a suitable weighting system for least-squares refinement.

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A program to contour Fourier maps by use of an incremental CRT display.

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A method of automatically contouring Fourier syntheses by use of the on-line incremental CRT display type 340 has been developed as one of a series of programs written for the University of Western Australia's PDP 6 computer. The display unit operates on a network of 1024×1024 points which occupy a screen area of $10''\times 10''$. The two principal modes of operation are (i) *the point mode* where the coordinates of an individual point are stored in a 36-bit word and (ii) *the vector mode* where the components of a vector are stored in an 18-bit half-word. The vector mode can also be used to increment the display coordinates without intensifying the screen. The time required to display a point is 30 μ sec, while a vector is drawn at a speed corresponding to 1·5 μ sec per point.

A method of plotting syntheses on a point by point principle has been developed for an *X–Y* plotter by Cherin, Madigan & Martin (1965). It would be possible to apply this technique directly to the CRT display. However, the figures given above show that the display is much more efficient with regard to both speed and storage required when used in the vector mode. The present method was therefore developed so as to utilize this feature as much as possible.

The details of the calculation are best understood by reference to Fig. 1. This represents a grid unit *ABCD* with electron density values of 30, 20, 60 and 10 at the corners. It is assumed that contours are required at 25 and 50 with the first level broken. A linear interpolation is performed along *AB* to obtain the coordinates of the point *P* where the electron density has the value 25. Points *Q*, *R* and *S* are similarly located. To resolve the ambiguity as to whether the contours at $\varrho=25$ are along *PS* and *RQ* or *RS* and *PQ*, the function $|\varrho_A+\varrho_C-25|-|\varrho_B+\varrho_D-25|$ is examined. In this example the function is positive, so the contours are taken to be *RS* and *PQ*. Vectors are then set up as follows.

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Firstly, an unintensified vector AP is drawn to increment the display coordinates to the point P. An intensified vector is then drawn in the direction PQ, but only up to the point Q' (where $PQ' = \frac{1}{2} PQ$) to give the appearance of a broken vector. An unintensified vector $Q'R$ increments the coordinates to R and the broken vector RS' is displayed. The interpolation is then repeated to obtain the coordinates of the points T and U which correspond to $\varrho = 50$, the unintensified vector $S'T$ is drawn and this is followed by the intensified vector TU. Finally, as all the contours have now been set up for this grid square, an unintensified vector UD is drawn to initialize the coordinates for the next grid unit. The calculation is repeated for all grid units in the section until all the contours are drawn. Vectors are then set up to enclose the section and the title and section number are displayed with the use of a character mode which is also a feature of the display unit.

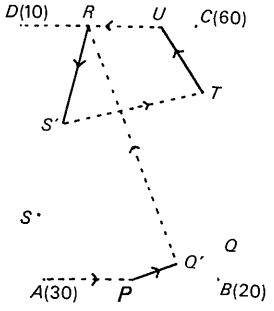

Fig. 1. An example of the method used to draw the contours. Continuous lines represent intensified, and broken lines unintensified, vectors. The parallelogram $ABCD$ represents one grid unit. PQ' and RS' are the broken contours at $\varrho = 25$. TU is the continuous contour at $\varrho = 50$.

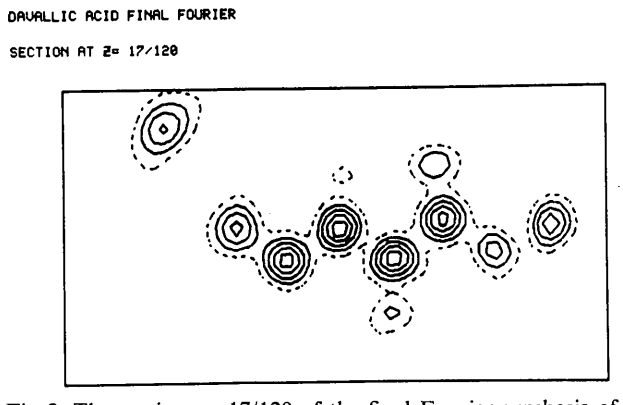

Fig. 2. The section $z = 17/120$ of the final Fourier synthesis of davallic acid. The broken contour is at 1·0 e.Å^{-3} and the contour interval is 1·0 e.Å^{-3}. The limits of the section are $x = 0$ to a (vertical) and $y = 16/60$ to $76/60$ (horizontal).

Although the words 'draw' and 'display' are used above, no data are actually transferred to the display unit during the calculation. Rather, the information is stored sequentially in the computer's core storage and only when all the data for a section have been set up are they displayed as a block. This output is repeated continuously until interrupted by use of a light pen, after which the next section is processed.

Fig. 2 shows the results of contouring the section $z = 17/120$ of the final Fourier synthesis evaluated on the plant product davallic acid. The grid consists of 30 intervals, each of 13 display points along the vertical axis (x) and 60 intervals each of 14 points along the y (horizontal) axis. The time required to set up a section was about 15 sec and the map was displayed once every 0·1 sec. The linear interpolation and straight line approximations have led to some jaggedness in the contours, but all the principal features of the map are retained and it is considered that the method produces results which are sufficiently accurate for most purposes.

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