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A Fully Automatic Program for Finding the Unit Cell from Powder Data

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A description is given of a fully automatic program, written in ALGOL 60, that finds the constants of the reciprocal lattice from powder data. The progress of the program is illustrated with the (nearly) complete computer output for one selected case. Planes through the origin of the reciprocal lattice (zones) are found first. After evaluating these, the program selects pairs of zones with a common row in order to find reciprocal lattices, which are then reduced in a simple way. Each solution is compared with the experimental data and a figure of merit is calculated. The program is most suited for compounds of orthorhombic or lower symmetry.

Introduction

The problem of finding the unit cell from powder diffraction data can be formulated with the help of the reciprocal lattice:

$$(2 \sin \theta/\lambda)^2 = 1/d^2 = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + kl \,.\, 2b^*c^* \cos \alpha^* + hl \,.\, 2a^*c^* \cos \beta + hk \,.\, 2a^*b^* \cos \gamma^* \,. \quad (1)$$

We define $Q = 10^4/d^2$ and write

$$Q(hkl) = h^2A + k^2B + l^2C + klD + hlE + hkF \,. \quad (2)$$

The task of finding, in the general case, the six constants $A \ldots F$ all at the same time is, at present, too big a problem; for lattices in which not more than two parameters have to be determined, there exist graphical methods (*e.g.* Hull–Davey charts), while for lattices with orthogonal zones the methods of Lipson (1949) and Hesse (1948) are suitable.

The systematic trial-and-error method of Werner (1964) is based on the use of a computer. It is generally applicable, but the computing time (even for present-day machines) becomes prohibitive for triclinic lattices (Taupin, 1968).

A perfectly general approach to the problem is the method given by Runge (1917), rediscovered by Ito (1949, 1950) and refined by de Wolff (1957). According to this approach we first try to find zones (net-planes in the reciprocal lattice containing the origin); any two true zones will have a line of intersection. If the angle between two such zones is found, we have determined a reciprocal lattice. Sometimes this lattice can be reduced, that is, described on symmetry axes in the reciprocal lattice. The main difference between the method described here and the one proposed by Ito is that Ito deliberately ignores the symmetry of the reciprocal lattice, whereas we try to establish the reduced lattice as soon as possible.

The reduction procedure used in this program was kept simple and therefore it does not handle lattices with more than twofold symmetry very well. One- and two-parameter problems can probably be solved more effectively by a systematic trial-and-error method (Werner, 1964; Jamard, Taupin & Guinier, 1966; Taupin, 1968).

The program

The program is based mainly on suggestions given by de Wolff (1958). It consists of the following steps:

(1) Find zones and reduce these.

(2) Test whether any or both of the base vectors should be halved. Refine the parameters with a least-squares (LS) method. Calculate the probability that the zone is found by pure chance (quality figure).

(3) Find pairs of zones with a common row and determine the angle between these zones.

(4) Reduce the lattices found and transform if necessary so that the lattice is described in a standard way.

(5) Try to index the first 20 lines of the pattern and repeat this after a LS-refinement of the parameters. Note the number of lines actually indexed and calculate the figure of merit.

These steps in the program will be considered in some detail in the following sections. They will be illustrated with the nearly complete computer output for a well known problem.

The example

The $\sin^2 \theta$ values of KNO_3, obtained by Hesse (1948) with Cr $K\alpha$ radiation, were used for the example. They are reproduced in Table 1. These data were also taken by Hesse (1948), Lipson (1949) and Ito (1950, page 205) to illustrate their methods.

As we usually have much smaller Q values to deal with (the first Q is often smaller than 100), the program is not really adapted to this kind of pattern, especially as the limit for the difference between two 'equal' values is too small for this case.

Finding zones

Any two points in the reciprocal lattice, together with the origin, define a plane in the reciprocal lattice, cor-

responding to a crystallographic zone. Let the values of Q (the square of the distance from the origin to the point) be Q' and Q''. We can find other points in this zone by calculating

$$Q_{m,n}=m^2Q'+n^2Q''+mnR\,, \qquad (3)$$

where $R=2\sqrt{Q'Q''}\cos\varphi$, φ being the angle between the directions from the origin to the points whose Q values are Q' and Q''. Reversing equation (3) we might be able to find the value of R belonging to the Q' and Q'' of a set of Q values:

$$R=(Q_{m,n}-m^2Q'-n^2Q'')/mn\,. \qquad (4)$$

For Q' and Q'' we try combinations of the first three with the first six lines of the Q list (Table 2), unless specific combinations are given in the input.

By inserting for $Q_{m,n}$ all observed Q values up to a reasonable limit and for m and n a few positive integer values, and by storing the absolute value of R, we get a great number of $|R|$ values, some of which are equal within the limits of error. We found empirically that there is not much to be gained by extending the index field beyond $n,m=2$.* In this case we can expect at most 8 equal values of R when $R\neq 0$ and 4 equal values when $R=0$.

In the program we multiply R by a constant factor, round off to the nearest integer value and add one to the memory space corresponding to that number. When finished, we go through the memory in small overlapping steps, summing the contents of 6 successive memory spaces. If the sum exceeds a preset number (*e.g.* 4 if $Q'\neq Q''$) then a weighted mean is calculated and stored. The tolerance in R has thus a fixed absolute value, determined by the constant by which R was multiplied. This is the first tolerance given in Table 1.

The first five columns of Table 2 give the output of the zone-finding procedure. NR means only a serial number; NUMBER (4th column) is the number of times that the value of R was found.

When the multiplicity-factor of a powder diffraction line is greater than two, its Q value represents more than one (significant) point in the reciprocal lattice. Therefore it is useful to try combinations of Q values of the type $Q'=Q''$ (Table 2). In an orthorhombic lattice, for example, each $Q(h,k,l)$ with $h,k,l\neq 0$ represents 8 points in the reciprocal lattice. These points define three different zones. In the program, we accept for the same pair, Q', Q'', up to four significant values of R (which is the maximum one can expect from the combination of two general orthorhombic reflexions).

A transformation of the zone axes is carried out if $R>Q'$ and if there are equalities between Q', Q'' and R. The new values of Q', Q'' and R are in the last three columns of Table 2.

In the first case ($R>Q'$) there is at least one reciprocal lattice point, *i.e.* $(1,\bar{1})$, whose Q value $(Q'+Q''-R)$ is less than that of one or both of the axes on which the lattice was described. In this case a transformation is carried out to describe the zone on shorter axes (zones 8 and 9, Table 2). This process is repeated if necessary.

In the second case (equalities between Q', Q'' and R) there are pairs of Q's which are systematically equal.

* This was suspected and subsequently proved empirically by ir. F. Kuypers of our laboratory (internal report).

Table 1. *sin² θ values of* KNO_3^*

The first part of the output reproduces the tolerances and the Q values of the input.

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H11834D/1-3-68/VISSER/AUTOMATIC INDEXING
PERMITTED RANGE IN R (MAAS) IS+,500000000000E+ 1
PERMITTED RANGE IN D IS+,500000000000E+ 1
   923.0     943.0    1271.0    1392.0    1427.0    1720.0    1789.0    1853.0    1877.0    1898.0
  2264.0    2339.0    2411.0    2496.0    2678.0    2731.0    2818.0    3060.0    3122.0    3263.0
  3462.0    3481.0    3513.0    3689.0    3766.0    4177.0    4223.0    4287.0    4500.0    4600.0
  4663.0    4963.0    5239.0    5427.0    5551.0    5624.0    5693.0    5748.0    6151.0    6699.0
```

* Hesse, 1948.

Table 2. *Results of the zone-finding procedure*

NR is a serial number, MAAS stands for R, NUMBER is the number of times a value of R(MAAS) was found. The next three columns contain the reduced values of Q', Q'' and R respectively.

NR	Q1	Q2	MAAS	NUMBER	REDUCED		
1.0	923.0	923.0	566.5	5.0	319.9	603.1	0.0
2.0	923.0	923.0	1414.8	4.0	107.8	815.2	0.0
3.0	923.0	943.0	15.2	4.0	923.0	943.0	15.2
4.0	923.0	1271.0	1270.8	4.0	317.8	605.3	0.0
5.0	923.0	1392.0	1372.9	4.0	923.0	942.1	473.1
6.0	943.0	943.0	515.0	4.0	342.8	600.3	0.0
7.0	943.0	943.0	991.7	4.0	223.6	719.4	0.0
8.0	943.0	1271.0	1272.5	4.0	941.5	943.0	613.5
9.0	943.0	1392.0	1411.9	4.0	923.1	943.0	474.1
10.0	1271.0	1271.0	1617.6	4.0	231.0	1040.0	0.0
11.0	1271.0	1271.0	1419.4	3.0	280.6	990.4	0.0
12.0	1271.0	1271.0	1638.1	3.0	176.0	1095.0	0.0

This means that there is a mirror-line in the zone and the zone is redefined on orthogonal axes. In Table 2 the zones 1 and 2 illustrate the reduction when $Q'=Q''$; zone 4 illustrates the case for $R=Q''$.

Improvement and evaluation of zones

The zones found are recalculated up to $0{\cdot}8\times Q_{max}$, with $Q'/4$, $Q''/4$ and $R/4$ as parameters. If, for example, the number of observed Q values which match calculated Q values with odd h (and even k) is sufficient, then we assume that $Q'/4$ is the correct parameter. The same sort of test is carried out for Q'' (condition: odd k, even h) and for centring of the old zone (condition: $h=2n$, $k=2n$, $h+k=4n$) and the new zone ($h+k=2n$). With the parameters thus obtained a round of least-squares is carried out. At the same time the zones can be printed (Table 3). The bottom line of this Table contains the refined parameters and the quality figure (next paragraph).

At the same time we calculate the probability that this zone has been found by pure chance. Both the parameters of the zones and the observed Q values will contain deviations from the ideal value. When the difference between a Q_{calc} and a Q_{obs} is less than 0·3% (with a minimum of 3·0 in $Q=10^4/d^2$) we regard this near coincidence as support for the zone. Associated with each Q_{obs} in the list there is thus a certain range, ΔQ, (0·3% on both sides) of significant Q values; any Q_{calc} falling within this range will be considered 'fitting'. If Q_{max} is the highest observed Q value in the zone, then the probability, p, that an arbitrary Q value fits, is obviously the sum of the ranges associated with all observed Q values up to Q_{max}, divided by the value of Q_{max}: $p=(\Sigma\,\Delta Q)/Q_{max}$. If there are N_c calculated Q values in the zone, N_0 of which give a fit, then the probability that this should occur by pure chance is

$$C=\frac{N_c!}{N_0!(N_c-N_0)!}\cdot p^{N_0}(1-p)^{N_c-N_0}\,.$$

Table 3. *Zones*

Only the first of all the printed zones is shown. The top line gives the original parameters, the bottom line contains the refined parameters followed by the probability that this zone was found by chance. The reciprocal of this figure is found under QUALITY in Table 4 (new number 6).

In the zone the calculated Q's that match an observed Q are marked with an ×.

```
319.9    603.1      6.6

5118.5

2878.9    3482.6 X  5291.4

1279.5    1882.6 X  3692.6 X

 319.9     923.6 X  2732.4 X

           603.1    2412.5 X
319.6     602.7      6.6   .419E-  1
```

The numbers N_c and N_0 should refer to significant points only.

A line, together with its higher orders is, therefore, counted as one single observation, both for N_0 and N_c. Also, we deduct the number of parameters involved from the number of significant points to obtain N_0 and N_c.

For technical reasons we assign the reciprocal value, $1/C$, of the above probability as a quality figure, to the zone. The zones are sorted on this quality figure (Table 4); only the best six zones are used in the rest of the program.

The program accepts up to four different values of R for every Q'–Q'' combination. In this way it collects many false zones. The criterion described above has proved to be a very powerful tool in separating the true zones from the false ones.

Combinations of zones and determination of the angle between them

In order to find a lattice, all possible combinations (including the combinations of each zone with itself) of the six best zones (*cf.* preceding section) are tried. For every pair of zones we must first find the line of intersection, whence the angle between them can be determined.

The line of intersection of two zones is a row of common points; the Q value of the first point of this row must be a low Q value occuring in both zones. In order to find this point we compute the Q values of the four points nearest to the origin in each zone (Q', Q'', $Q'+Q''+R$, $Q'+Q''-R$) and compare these with the points of the other zone. If a common Q value is found the zones are redefined (if necessary) with the common value as one of the axes and the smallest remaining Q value as the other (Table 5). Provisionally labelling the parameters of the first zone, A, B and F and those of the second zone A, C and E, we can use equation (2) to determine the remaining parameter, D:

$$D=(Q-h^2A-k^2B-l^2C-hlE-hkF)/(kl)\,.$$

For Q we insert all observed Q values in the list, for h,k,l we take:

$$-2\leq h\leq +2;\ k=-2,-1,1,2;\ l=1,2\ (kl\neq 0!)\,.$$

The actual calculation is carried out in much the same way as the selection of values of R (see the section *Finding zones*). Apart from the most frequently occurring value of D, three other values are retained, but only if they are not much less frequent than the best values (Table 6). In the example shown, none of the combinations yields more than two values of D. The example also shows that it is indeed useful to combine zones with themselves.

Reduction of lattices

Some of the sets of constants $A\ldots F$ that we have found might be different descriptions of the same lat-

tice; other lattices could be described in a simpler way. Therefore the lattices are reduced and brought to a standard description.

The reduction of the lattices is carried out in two steps. In the first step we determine the shortest non-coplanar translations in the reciprocal lattice by calculating the Q values of half the number of reciprocal lattice points close to the origin (the inversion-equivalent points are left out), selecting the smallest Q values and storing their indices (h_n, k_n, l_n, $n=1,2,3$). The translations are coplanar if the determinant of the matrix $/h_1,k_1,l_1/h_2,k_2,l_2/h_3,k_3,l_3/$ equals zero. In this case we try the next smallest Q value as the third translation, *etc.* until a non-coplanar set is found. The second step in the reduction is a test for symmetry.

We need only test two kinds of symmetry relations:

(*a*) Two of the translational constants (A,B,C) are equal while the angle between their directions differs from 90°, *e.g.* $A=B$ and $F\neq 0$. In this case the reduced constants (primed) are: $A'=(A+B-F)/4$; $B'=(A+B+F)/4$; $C'=C$; $D'=(D-E)/2$; $E'=(D+E)/2$; $F'=0$. This case is illustrated by lattices numbered 6–10 in Tables 6 and 7.

(*b*) An angle-factor is equal to one of the translational constants which defines one limit of the angle, *e.g.* $F=A$ or $F=B$. If $F=A$ the reduced constants are: $A'=A/4$, $B'=B-A/4$, $C'=C$, $D'=D-E/2$, $E'=E/2$, $F'=0$. Lattice number 4 (Tables 6 and 7) illustrates this case.

The third possible relation, *e.g.* $D=E$ only leads to a reduction if $A=B$, which is treated above, or if $F=2A$ or $F=2B$, which is impossible when the lattice has been defined by the shortest translations. By cyclic permutation of the constants they are all made to pass the few simple tests mentioned above. In this way all orthorhombic, and most of the monoclinic, lattices are recognized as such. Only one extra test is applied in order to pick out a few special cases of monoclinic centred lattices. Both symmetry-relations mentioned point to a probable centring of the lattice. This centring is, however, disregarded at this point of the program. The reduction of the lattice will establish the

Table 4. *Evaluated zones*

The evaluated zones are printed in descending order of the quality figure. The notation has been changed from Q', Q'', R to A, B, F respectively. The quality has been determined with the parameters before refinement [see nos. (NEW NR) 4 and 11].

EVALUATED ZONES

NEWNR	A	B	F	QUALITY	OLDNR
1	922.4	942.0	14.7	1448.9	3.0
2	317.5	624.1	0.0	1126.7	8.0
3	107.8	814.7	0.0	46.3	2.0
4	922.7	941.8	472.3	39.9	5.0
5	317.8	604.0	0.0	23.9	4.0
6	319.6	602.7	0.0	23.9	1.0
7	223.2	718.5	0.0	1.7	7.0
8	281.1	986.3	0.0	1.1	11.0
9	230.7	1043.2	0.0	1.1	10.0
10	176.1	1094.0	0.0	1.1	12.0
11	922.7	941.8	472.3	1.0	9.0
12	343.4	598.2	0.0	0.2	6.0

Table 5. *Combined zones*

The possible combinations of the six best (first) zones of Table 4 are given. The value of D is not zero but needs to be determined.

COMBINED ZONES

COMBINATION		A	B	C	D	E	F	NEW NR
1	1	922.4	942.0	942.0	0.0	14.7	14.7	11
1	2	941.8	922.4	317.5	0.0	635.0	14.7	12
1	3	922.4	942.0	107.8	0.0	215.6	14.7	13
1	4	922.5	942.0	941.8	0.0	472.3	14.7	14
1	5	922.1	942.0	317.8	0.0	635.5	14.7	15
1	6	922.4	942.0	319.6	0.0	639.2	14.7	16
2	2	317.5	624.1	624.1	0.0	0.0	0.0	22
2	4	941.7	317.5	922.7	0.0	472.3	635.0	24
2	5	317.6	624.1	604.0	0.0	0.0	0.0	25
3	3	107.8	814.7	814.7	0.0	0.0	0.0	33
3	4	922.6	107.8	941.8	0.0	472.3	215.6	34
3	5	922.1	107.8	317.8	0.0	635.5	215.6	35
3	6	922.4	107.8	319.6	0.0	639.2	215.6	36
4	4	922.7	941.8	941.8	0.0	472.3	472.3	44
4	5	922.2	941.8	317.8	0.0	635.5	472.3	45
4	6	922.5	941.8	319.6	0.0	639.2	472.3	46
5	5	317.8	604.0	604.0	0.0	0.0	0.0	55
5	6	922.6	317.8	319.6	0.0	639.2	635.5	56
6	6	319.6	602.7	602.7	0.0	0.0	0.0	66

crystal system, the Bravais-type follows from the final indexing as shown in the next section. The reduced lattices are shown in Table 7.

Final test on the lattices found

With the lattices found the program tries to index the first 20 lines of the diagram. At the same time a least-squares refinement of the parameters is carried out. By counting the number of reflexions that can be indexed on the basis of a centred lattice (*A*, *B*, *C*, *I* or *F*) the Bravais-type is established. This procedure is repeated once, after which the number of non-indexable lines is noted and a figure of merit (de Wolff, 1968) is calculated (Table 8). This figure of merit is in fact the ratio of the expected average discrepancy between the observed and calculated Q values for an arbitrary reciprocal lattice of the same size and the actual aver-

Table 6. *Possible lattices*

The values of *D* have been determined. The tolerance on *D* (compare Table 1) was a little underestimated, whence the 'double' values (*e.g.* combinations 121 and 122). The number of times a value of *D* has been found is mentioned under MULT.

POSSIBLE LATTICES

SERIAL	A	B	C	D	E	F	MULT	COMBNR
1	941,8	922,4	317,5	635,5	635,0	14,7	11,0	121,0
2	941,8	922,4	317,5	637,0	635,0	14,7	11,0	122,0
3	922,1	942,0	317,8	636,4	635,5	14,7	13,0	151,0
4	317,6	624,1	604,0	624,2	0,0	0,0	14,0	251,0
5	317,6	624,1	604,0	622,5	0,0	0,0	10,0	252,0
6	922,7	941,8	941,8	1640,8	472,3	472,3	12,0	441,0
7	317,8	604,0	604,0	582,2	0,0	0,0	13,0	551,0
8	317,6	604,0	604,0	580,6	0,0	0,0	9,0	552,0
9	319,6	602,7	602,7	581,9	0,0	0,0	11,0	661,0
10	319,6	602,7	602,7	583,0	0,0	0,0	11,0	662,0

Table 7. *The reduced lattices*

All of them, except no. 6, basically represent the lattice of no. 4 (*e.g.* combination 122 in Tables 7, 8 and 10. A reduction of the refined values in Table 8 yields the same lattice as combination 251).
The coincidence of lattices 7 and 8, and of 9 and 10 is recognized; only one of each pair is retained.

LATTICES REDUCED

SERIAL	A	B	C	D	E	F	MULT	COMBNR
1	604,3	317,5	624,3	0,0	626,9	0,0	11,0	121,0
2	602,9	317,5	624,3	0,0	622,3	2,0	11,0	122,0
3	604,3	317,8	623,4	0,9	621,8	0,0	13,0	151,0
4	317,6	156,0	447,9	0,0	0,0	0,0	14,0	251,0
5	604,0	317,6	605,5	0,0	585,4	0,0	10,0	252,0
6	861,1	60,7	922,7	0,0	472,3	0,0	12,0	441,0
7	317,8	156,4	447,5	0,0	0,0	0,0	13,0	551,0
8	317,8	156,8	447,1	0,0	0,0	0,0	9,0	552,0
9	319,6	155,9	446,8	0,0	0,0	0,0	11,0	661,0
10	319,6	155,6	447,1	0,0	0,0	0,0	11,0	662,0

Table 8. *Lattices after indexing and LS refinement*

The column NUMBER gives the number of indexed lines among the first 20. The figure of merit is entered in the column QUALITY. In the column CENTER, 6 stands for a primitive lattice.
The refined parameters of the first two zones are equal, the number of indexed lines and the quality, however, are based on the parameters before refinement.

LATTICES AFTER INDEXING AND LS REFINEMENT

A	B	C	D	E	F	NUMBER	QUALITY	CENTER	COMBNR	BRAVAIS TYPE
317,9	156,1	447,1	0,0	0,0	0,0	20,0	28,2	6,0	251,0	P
317,9	156,1	447,1	0,0	0,0	0,0	17,0	17,7	6,0	552,0	P
318,2	156,1	447,1	0,0	0,0	0,0	17,0	16,1	6,0	661,0	P
624,1	318,0	603,0	0,4	623,6	0,0	13,0	18,7	6,0	122,0	P
603,3	318,1	603,4	0,0	581,9	0,0	12,0	26,2	6,0	252,0	P
603,3	318,0	624,3	0,6	623,5	0,0	12,0	15,2	6,0	151,0	P
603,3	318,2	624,5	0,0	624,4	0,0	11,0	22,3	6,0	121,0	P
880,4	60,6	923,9	0,0	472,0	0,0	10,0	24,8	6,0	441,0	P

age discrepancy. The four best lattices are printed layer by layer in the form of an array, in which the calculated Q values that match an observed value are marked with an X (Table 9). From this scheme any additional extinction is easily found by visual inspection. The final results for these four lattices are given in Table 10.

Experiences and results

This program has been in use, in various stages of development, since 1964. During that time quite a number of orthorhombic, monoclinic and triclinic compounds have been indexed correctly. None of these results have been published alone, they are incorporated in data sent by our laboratory to the Joint Committee on Powder Diffraction Standards for inclusion in the *X-ray Powder Data File* (ASTM-index). Some examples are given in Table 11.

The program proper is chiefly an administrative program; steps 2, 3, 4 and 5 of the section *The program* are separate procedures (subroutines). The computer used is a Telefunken TR4 computer (effective memory 20000 words of 52 (48) bits, cycle time 1 μ sec, addition 11 μ sec, multiplication 30 μ sec). The longest computing time on record up to now is 6 minutes; the usual time is less than 3 minutes.

The most frequent reason for failure in obtaining a correct reciprocal lattice is the inaccuracy of the input data. The errors in the diffraction angles should not exceed 0·03° (2θ). The first three lines especially should be as accurate as possible. Frequently it is possible to improve the Q values of the first lines with the aid of their higher orders. In one case a set of good diffractometer data failed to yield a good lattice. As a zero-error of the instrument was suspected we added 0·02° to all 2θ-values, whereupon the program found the correct lattice (confirmed later by single-crystal work).

The next most frequent reason for failure is the incompleteness of the input data. Systematic extinctions are sometimes a nuisance but they do not make indexing impossible. A multitude of non-systematic extinctions, however, can indeed make it impossible to find the correct solution, especially if many of the low-angle lines are missing.

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Table 9. *The four best lattices*

Only the first lattice is reproduced. It is printed in layers with ascending k. The space group could be *Pnam*. The number of non-systematic extinctions, however, does not make the n-glide plane very convincing.

```
    0,9     447,1    1788,6 X
  317,9     765,1    2106,5
 1271,5 X  1718,8 X  3060,2 X
 2861,2

  156,1     603,3    1944,7
  474,3     921,2 X  2262,6 X
 1427,7 X  1874,9 X  3216,3
 3017,3

  624,5    1071,6    2413,1 X
  942,4 X  1389,5 X  2731,0 X
 1896,1 X  2343,2 X

 1405,1    1852,2 X  3193,6
 1723,3 X  2170,1
 2676,7 X  3123,8 X

 2497,9 X  2945,0
 2815,8 X  3262,9 X
```

Table 10. *The end result*

The columns should have the same headings as Table 8. After the new round of parameter refinement the first three lattices have become equal. The figure of merit has improved considerably.
Reduction of the fourth lattice yields: 156·118, 318·061, 446·911, 0, 0, 0.

```
317,910   156,121   447,142   0,000     0,000     0,000   20,000   29,904   6,000   251,000   P
317,911   156,121   447,142   0,000     0,000     0,000   20,000   29,994   6,000   592,000   P
317,914   156,120   447,142   0,000     0,000     0,000   20,000   29,196   6,000   661,000   P
624,473   318,061   603,029   0,000   624,194     0,000   13,000   58,964   6,000   122,000   P
```

Table 11. *Examples of the use of the program*

		a/α	b/β	c/γ	M_{20}*	Space group	Confirmed
1	$Cd_4(OH)_6Br_2$[a]	7·513	10·031	6·856	29·5	*Pmnn?*†	—
		90	90	90			
2	$CuSeO_4.5H_2O$[b]	6·224	10·872	6·081	38	$P\bar{1}$	
		97·76	107·07	77·15			
3	UO_2WO_4[c]	13·60	5·489	7·22	33	$P2_1/a$	Single crystal
		90	104·49	90			
4	As_2O_5[d]	8·454	8·645	4·629	32	$P2_12_12_1$?	—
		90	90	90			
5	$H_5As_3O_{10}$[e]	5·717	7·258	4·667	45	$P\bar{1}$	Single crystal
		97·41	99·59	100·34			
6	$2H_3AsO_4.H_2O$[f]	8·229	13·244	7·651	15	$P2_1/a$	Single crystal
		90	111·18	90			
7	$Na_2Ca(CO_3)_2.5H_2O$[g]	11·579	7·776	11·207	35	$I2/a$	Single crystal
	Gaylussite	90	101·98	90		or Ia	

* The values of M_{20} (figure of merit) are by themselves a confirmation of the correct indexing (de Wolff, 1968).

† Space groups with a question mark are deduced from powder data. They denote the maximum of possible systematic extinctions compatible with the data, *e.g.* $P2_12_12_1$ for As_2O_5 excludes the presence of glide planes, but includes, for example, *Pmm*2 as the possible true space group.

[a] Sample obtained from Mme L. Walter-Lévy (Walter-Lévy & Groult, 1966).

[b] 2θ-values read by an inexperienced (new) assistant. Nevertheless the correct answer was found by computer. Isomorphous with $CuSO_4.5H_2O$ which gives an indirect conformation.

[c] Diffractometer data from a different laboratory. Example 2 of de Wolff (1968).

[d] The program gave a subcell (only 12 lines indexed, 'M_{20}'=64!). The first unindexed line, however, had an indexed second order, 102. Halving the appropriate axis gave the correct cell.

[e] Found independently of Worzala (1968).

[f] Found independently of Jost, Worzala & Thilo (1966).

[g] Mineral from Lake Tchaad, Central Africa. Determined independently of Monroe (1967). The program found the *I*-centred cell.

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