
NBS TECHNICAL NOTE 1141

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

# NBS*AIDS80: A FORTRAN Program for Crystallographic Data Evaluation

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# NBS*AIDS80:
## A FORTRAN Program for Crystallographic Data Evaluation

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# NBS*AIDS80: A FORTRAN PROGRAM FOR CRYSTALLOGRAPHIC DATA EVALUATION†

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Techniques for the computer-assisted evaluation of crystallographic data have been developed to improve the data compilations of the NBS Crystal Data Center and the JCPDS--International Centre for Diffraction Data. The resulting computer program, NBS*AIDS80, can be used for the analysis of unit-cell and powder diffraction data by the general scientific community as well. Research and analysis components include calculation of standard cells and space groups, determination of metric symmetry, checking the data for consistency, generation of d-spacings and indices, and analysis of powder patterns with calculation of figures of merit. Detailed input and output specifications are given.

Key Words: Computer evaluation; crystallographic data analysis; JCPDS--International Centre for Diffraction Data; metric symmetry; NBS Crystal Data Center; powder diffraction; unit cell.

## 1.0 Introduction

The computer program NBS*AIDS80 is derived from several years of experience at the National Bureau of Standards in the computer-assisted evaluation of crystallographic data. The program or its precursor has been used routinely by the NBS Crystal Data Center for the analysis of crystallographic data in the preparation of Crystal Data Determinative Tables,[1] and it has recently been expanded in collaboration with the JCPDS--International Centre for Diffraction Data for analysis of powder data for the Powder Diffraction File.[2] The combined evaluation of single-crystal and powder data in a common format enhances the quality of the data in both data compilations.

NBS*AIDS80 was originally intended for use by the data base builders in the evaluation of literature data and the creation of master data files. With such files, research studies can be carried out, indexes can be generated, and publications can be prepared. In addition, the files can be searched in an on-line or batch mode. However, it has become apparent that the data evaluation routines in NBS*AIDS80 are of value as a research and analysis tool for the general scientific community as well. In our evaluation of thousands of entries for the Crystal

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[1] Raised figures indicate literature references on page 24.

Data and Powder Diffraction Files, we have noted an unexpectedly large number of errors in the published crystallographic data, especially with respect to symmetry determination, unit cell transformation, density calculation, and the indexing of powder data. It is our hope that by using NBS*AIDS80 research scientists and journal editors will find and correct such errors prior to publication, and that additional analysis routines will be suggested for incorporation into the program.

## 2.0 Research and Analysis Applications

NBS*AIDS80 may be used as a research aid in conjunction with routine diffractometry for materials identification and characterization, in addition to the areas mentioned above. For example, in the determination of a crystal structure the program can be used once unit-cell dimensions have been determined to establish the probable symmetry of the lattice, the transformation matrix to the standard setting of the cell and space group, the calculated density for a check on unit cell contents, and the determinative ratios needed to find out if the same or a similar compound previously has been solved. The program should be used again at the end of the structure determination to give final values for publication. NBS*AIDS80 is also valuable in powder diffraction analyses. The program can generate d-spacings for any symmetry and input cell, and input powder data can be indexed based on a known unit cell. Once the pattern has been indexed, the program compares the observed and calculated d-spacings, flags systematic absences if present, and calculates the figures of merit F(N) and M(20). In addition, a table of powder data for publication can be prepared. The research and analysis applications of NBS*AIDS80 are summarized in the following sections.

### 2.1 Cell and Space Group Transformations

In order to compare unit-cell and space-group data from separate experimental determinations, it is essential that all data be reported in a standard orientation. NBS*AIDS80 transforms the input cell and space group to the Crystal Data setting, and the space-group number is assigned. The Crystal Data cell provides a standard setting for the publication and comparison of unit-cell parameters, and the determinative ratios can be used for direct entry into Crystal Data Determinative Tables for identification of unknowns and location of isostructural materials.

Errors are commonly made in the transformation of unit-cell axes and space groups, especially when unusual centerings are encountered. For example, SbSn and NiO crystallize in a rhombohedrally-distorted sodium chloride structure. These cells are frequently reported using F-centered rhombohedral axes; the corresponding hexagonal axes are calculated ignoring the face-centering, leading to incorrect axes and erroneous indexing of powder data. A more common use of NBS*AIDS80 would be the calculation of hexagonal unit-cell axes from primitive rhombohedral cell parameters.

Perhaps more importantly, it is essential that a given lattice be characterized by the same cell before comparisons are made. De Camp[3] has given an excellent example involving a lattice that has two different unit cells which appear to be based on the same three lattice translations. Crystals from two samples of condelphine hydroiodide gave apparently the same triclinic unit-cell dimensions when the cells were reduced using two separate reduction algorithms, with only the angle gamma differing significantly (Figure 1). The other differences were assumed to arise from experimental errors. The two cells are shown to define the same lattice when they are transformed using the NBS*AIDS80 algorithm.

| | Cell 1 | Cell 2 | Cell 1' |
|---|---|---|---|
| a | 9.34Å | 9.32Å | 9.34Å |
| b | 17.39 | 17.45 | 17.39 |
| c | 9.10 | 9.09 | 9.10 |
| α | 94.85° | 94.84 | 94.85° |
| β | 119.15 | 118.83 | 119.15 |
| γ | 88.57 | 86.50 | 86.71 |

Figure 1. Unit cell dimensions for condelphine hydroiodide. Cell 1 is transformed to cell 1' by the matrix $(\bar{1}01,010,001)$.

## 2.2 Determination of Metric Symmetry

The reduced cell[4] and the reduced form number are calculated by NBS*AIDS80 to give the metric symmetry of the lattice.[5] The metric symmetry is the highest symmetry possible for the lattice based solely on geometric considerations. A systematic analysis of the Crystal Data File has shown that the metric symmetry is almost always the same as the true symmetry of the lattice.[6] The metric symmetry is determined from the Niggli reduced cell by the values of the following vector products[5] known as the reduced form:

$$\begin{pmatrix} \underset{\sim}{a}\cdot\underset{\sim}{a} & \underset{\sim}{b}\cdot\underset{\sim}{b} & \underset{\sim}{c}\cdot\underset{\sim}{c} \\ \underset{\sim}{b}\cdot\underset{\sim}{c} & \underset{\sim}{a}\cdot\underset{\sim}{c} & \underset{\sim}{a}\cdot\underset{\sim}{b} \end{pmatrix}$$

The reduced form can thus be used to indicate the probable symmetry of the lattice. If the reduced form indicates the possibility of higher symmetry than the input lattice, the program will print the cell with the highest possible lattice symmetry. It is well known that cell reduction provides a practical way to prove that a lattice must be triclinic, as the crystal symmetry can never be higher than the symmetry indicated by the reduced form. The use of the reduced form to indicate probable lattice symmetry is particularly important in light of the current trend towards determining the unit cell of a compound solely from diffractometer data. An example of the use of this procedure is given in Figure 2.

| | Initial Cell | Reduced Cell | Metric Cell |
|---|---|---|---|
| a | 8.095Å | 8.096Å | 11.698Å |
| b | 8.096 | 8.095 | 25.990 |
| c | 30.62 | 25.990 | 11.194 |
| α | 88.67° | 90.00° | 90.00 |
| β | 58.08 | 90.00 | 90.01 |
| γ | 87.48 | 92.52 | 90.00 |

Reduced Form

$$\begin{pmatrix} 65.5 & 65.5 & 675.5 \\ 0.0 & 0.0 & -2.9 \end{pmatrix} = \begin{pmatrix} a\cdot a & a\cdot a & c\cdot c \\ 0 & 0 & -|a\cdot b| \end{pmatrix}$$

Figure 2. Determination of the metric cell for an unknown antimony tartrate. The metric cell was found by the program to be orthorhombic B-centered, reduced form number 13.

| | Cell 1 | Cell 2 | Cell 3 | Common Cell |
|---|---|---|---|---|
| a | 9.407Å | 9.407Å | 9.416Å | 9.407Å |
| b | 13.773 | 13.800 | 13.768 | 9.407 |
| c | 12.829 | 12.801 | 12.822 | 9.416 |
| α | 90.06° | 90.05° | 90.00° | 94.06° |
| β | 96.15 | 95.99 | 96.14 | 94.30 |
| γ | 89.84 | 90.01 | 89.84 | 94.07 |

Figure 3. Alternate A-centered cells for chabazite, all leading to a common cell.

It should be emphasized that the reduced form as given by NBS*AIDS80 must be carefully analyzed in order to determine the true metric symmetry, as the assignment of symmetry is often dependent on the assessment of experimental errors. A new routine for symmetry determination is being developed and will be added to the program. This routine will give all possible symmetries and pseudosymmetries. In addition, we plan to add evaluation routines to handle specialized reduced forms that can result from, for example, the mis-indexing of a powder pattern, the determination of the subcell of a lattice, or twinning.

One example of metric pseudosymmetry involves the mineral chabazite, $Ca_2Al_4Si_8O_{24}\cdot 12H_2O$. Chabazite has been reported as having rhombohedral, monoclinic, or triclinic symmetry. Although the metric symmetry is nearly rhombohedral, analysis in our laboratory reveals the symmetry to be monoclinic or lower. Figure 3 gives three similar but distinct A-centered cells that can be related to a common pseudo-rhombohedral cell.[7]

Much of the effort involved in the solution of crystal structures can be avoided if the metric symmetry is determined prior to data collection. In a systematic analysis of organic compounds, we noted a number of cases in which rhombohedral symmetry was incorrectly reported as monoclinic or even triclinic symmetry. While the molecular geometries determined were correct, many more structural parameters than necessary were determined and refined leading to a lower overall accuracy of the structure parameters. Figure 4 gives one such example.

| | Input Cell | Rhombohedral Cell (Hexagonal Axes) | Reduced Cell |
|---|---|---|---|
| a | 19.900Å | 11.489Å | 11.489Å |
| b | 11.489 | | 11.489 |
| c | 21.258 | 60.590 | 21.258 |
| α | | | 74.32° |
| β | 108.18° | | 74.32 |
| γ | | | 60.00 |

Reduced Form

$$\begin{pmatrix} 132.0 & 132.0 & 451.9 \\ 66.0 & 66.0 & 66.0 \end{pmatrix} = \begin{pmatrix} a\cdot a & a\cdot a & c\cdot c \\ \frac{a\cdot a}{2} & \frac{a\cdot a}{2} & \frac{a\cdot a}{2} \end{pmatrix}$$

Figure 4. Example of a rhombohedral cell reported as a C-centered monoclinic cell. The reduced form (number 9) is clearly rhombohedral.

## 2.3 Identification of Unknowns

The standard Crystal Data cell and determinative ratios calculated by NBS*AIDS80 can be used for the identification of unknown compounds. For example, the unknown antimony tartrate mentioned above (see Figure 2) was identified using Volume 3 of Crystal Data Determinative Tables. The B-centered orthorhombic cell (a = 11.694(5), b = 25.961(9), c = 11.192(5), a/b = 0.4504, c/b = 0.4311) was readily identified as potassium antimony tartrate trihydrate using the portion of the Tables given in Figure 5.

| | a/b | c/b | a | b | c | Formula |
|---|---|---|---|---|---|---|
| | 0.4502 | 0.3664 | 8.76 | 19.43 | 7.13 | $C_{15}H_{10}Cl_2$ |
| | 0.4506 | 0.3361 | 9.251 | 20.53 | 6.901 | $C_{15}H_{23}Br$ |
| → | 0.4510 | 0.4316 | 11.696 | 25.932 | 11.192 | $K_2Sb_2C_8H_4O_{12}\cdot 3H_2O$ |
| | 0.4511 | 0.4473 | 8.746 | 19.388 | 8.672 | $CaC_6H_{12}O_6\cdot 3H_2O$ |

Figure 5. Identification of an unknown antimony tartrate using Crystal Data Determinative Tables.

Even though the compound is supposedly known, it is always advisable to obtain the standard cell and check for identification prior to data collection. The crystal used for data collection frequently does not correspond to the analysis of the bulk material. For example, data on orthorhombic sulfur has mistakenly been collected many times.

An alternative identification scheme will soon be available using the reduced cells of all materials given in Crystal Data. This Identification File currently exists at NBS, and it will soon be available as part of the NIH-EPA Chemical Information System (CIS).[8] It will also be issued in a printed format, in which the reduced cell as given by NBS*AIDS80 can be used for identification.

## 2.4 Checking the Data for Consistency

The program performs a check of the consistency of the unit cell, Z, and formula through a density calculation. The molecular weight is computed based on the input formula, and the cell volume is calculated. Although these computations may seem trivial, our recent experience as editors reveals that the density calculation is incorrectly reported in 15% of the cases. The examples given in Figure 6 are taken from reports of quantitative structure determinations, so there should be no questions about the unit cell contents. The discrepancies often arise owing to calculation of the density using preliminary cell dimensions or unit cell contents. Other sources of error include incorrect computation of molecular weight, cell volume, and Z or an approximate (or missing) value for Avogadro's number.

| Formula | Measured Density | Calculated Density | NBS*AIDS80 Density |
|---|---|---|---|
| $Cd_2P_2O_7$ | 4.90 | 5.04 | 4.886 |
| $Ba_3P_2$ | 4.1 | 4.52 | 3.371 |
| $GeLi_2Zn$ | 4.035 | 4.15 | 4.353 |
| $Mn_3(PO_4)_2$ | 4.1 | 3.92 | 3.798 |

Figure 6. Comparison of measured and calculated densities reported in the literature with densities calculated by NBS*AIDS80.

## 2.5 Powder Pattern Analysis

The program can be used to generate 2θ and d-spacings based on input-cell and space-group information for any crystal system. This feature was derived from the program "Lattice Parameter Least Squares Refinement"[9] with minor modifications. If reflection data are input (2θ, d, sinθ/λ, or Q) without hkℓ's assigned to any or all of the reflections, NBS*AIDS80 will assign the indices of the nearest reflection provided that $|\Delta(2\theta)| < 0.5°$. A small segment of the computer printout from the hkℓ/d-generation and indexing segment is shown in Figure 7. The "C" following each observed d-spacing (D OBS) indicates that the computer code has assigned the indices. If proper hkℓ's were given as input this column would be blank. However, if a given hkℓ is

not allowed in the input space group the column would contain an "N". Unindexable lines are marked with a "U". The maximum 2θ value for hkℓ/d-generation is an input parameter or, if left blank, determined by the range of input lines. The extinction conditions are generated automatically from the aspect symbol, space group symbol, or cell centering symbol. They may optionally be entered as input data as well.

Following the hkℓ, d and 2θ table, a pattern summary is printed as shown in Figure 8. Included are the number of lines possible out to 2θ max, the number of lines resolvable based on an estimated resolution factor, and the number of lines observed. This summary expresses the coverage of the experimental measurements. Next is a tabulation of the number of lines input, number indexed and number remaining unindexed. For the indexed lines the average and maximum magnitude of $\Delta(2\theta)$ are given. An average $|\Delta(2\theta)|$ of $<0.02°$ should be expected for high quality data. Data of this quality, or better, have been reported for nearly two decades primarily due to the use of internal 2θ standards. Another assessment of the fit between the observed and calculated 2θ's is the number of lines with $|\Delta(2\theta)|$ greater than some arbitrary limit. The JCPDS--International Centre for Diffraction Data currently uses a limit of 0.05° for "★" quality patterns and a limit of 0.20° for "I" quality patterns. (However, for a PDF card to be assigned either of these quality marks, chemical and intensity data criteria must also be satisfied.)

Two other assessments of the fit of the input cell and observed pattern are calculated by the program. M(20) is an indication of the correctness of the unit cell. According to de Wolff[10] a value of M(20) >10 coupled with two or fewer unindexed lines indicates that the cell is substantially correct. A value of M(20) <5 and/or several unindexed lines strongly suggests that the cell is not appropriate. The Smith-Snyder figure of merit F(N)[11] assesses the overall fit of the experimental data and cell as well as the coverage or completeness of the observations. For every one of the 105 patterns reported in Monograph 25, Section 16 and Section 17,[12] M(20) exceeded 15 and F(30) exceeded 13. However, in evaluating data in the literature, we often find indexed lines with $|\Delta(2\theta)|$ >0.5°, and patterns with M(20) <5 and F(30) <5. Often the reasons for the low quality of fit cannot be explained. However sometimes large discrepancies are typographical in origin. NBS*AIDS80 has a d/I/hkℓ/2θ table generation subroutine to help eliminate these errors (Figure 9). The subroutine determines the appropriate number of significant digits for each d-value based on the average magnitude of error in 2θ for the entire pattern. This keeps the round-off errors due to formatting of d-values less than the average magnitude of the error in 2θ.

```
**MESSAGE**POWDER PATTERN GENERATION/ANALYSIS FOR SYSTEM TET

       2-THETA(MAX) = 100.23            D(MIN) = 1.003868

       2 CONDITIONS FOR NON-EXTINCTION CALLED FOR
              CLASS CONDITION(S)
              HKL   H+K+L = 2N
              HHL   2H+L  = 4N
```

| | | | | AUTHORS | PROGRAM | OBS | CALC | DIFF |
|---|---|---|---|---|---|---|---|---|
| N | D CALC | D OBS | INT | H K L | H K L | 2-THETA | 2-THETA | 2-THETA |
| 1 | 5.4508 | | | | 1 0 1 | | 16.248 | |
| ** | 5.4508 | 5.4502C | 80 | 1 0 1 | | 16.250 | 16.248 | -.002 |
| 2 | 3.8489 | | | | 2 0 0 | | 23.090 | |
| ** | 3.8489 | 3.8472C | 65 | 2 0 0 | | 23.100 | 23.090 | -.010 |
| 3 | 3.1485 | | | | 1 1 2 | | 28.323 | |
| 4 | 3.1441 | | | | 2 1 1 | | 28.364 | |
| ** | 3.1441 | 3.1434C | 100 | 2 1 1 | | 28.370 | 28.364 | -.006 |
| 5 | 2.7254 | | | | 2 0 2 | | 32.836 | |
| ** | 2.7254 | 2.7250C | 15 | 2 0 2 | | 32.840 | 32.836 | -.004 |
| 6 | 2.7216 | | | | 2 2 0 | | 32.883 | |
| ** | 2.7216 | 2.7194C | 20 | 2 2 0 | | 32.910 | 32.883 | -.027 |

Figure 7. A segment of the hkℓ/d-generation output of NBS*AIDS80 for $NH_4H_2AsO_4$.

```
     REFLECTION SUMMARY FOR ENTIRE PATTERN:
     ESTIMATED RESOLUTION = .075 DEG. 2-THETA

          THEORETICAL LINES TOTAL = 75
          THEORETICAL RESOLVABLE  = 47
          UNIQUE OBSERVED LINES   = 39

          TOTAL LINES INPUT = 39
          NUMBER INDEXED    = 39
          NUMBER UNINDEXED  =  0

************FOR INDEXED LINES************

          AVERAGE 2-THETA DIFFERENCE = .012
          MAXIMUM 2-THETA DIFFERENCE = .030
          # WITH DIFF>0.05 (STAR LIMIT) = 0
          # WITH DIFF>0.20 (I LIMIT)    = 0
          M(20) = 59.49 (DLIMIT = 1.3589, # POSSIBLE = 33)
          F(30) = 47.69 (DELTA 2 THETA = .0123, # POSSIBLE = 51)
```

Figure 8. Pattern summary for $NH_4H_2AsO_4$.

| | | | | | |
|---|---|---|---|---|---|
| 5.450 | 80 | 1 | 0 | 1 | 16.25 |
| 3.847 | 65 | 2 | 0 | 0 | 23.10 |
| 3.143 | 100 | 2 | 1 | 1 | 28.37 |
| 2.725 | 15 | 2 | 0 | 2 | 32.84 |
| 2.719 | 20 | 2 | 2 | 0 | 32.91 |
| 2.438 | 4 | 1 | 0 | 3 | 36.83 |
| 2.433 | 4 | 3 | 1 | 0 | 36.92 |
| 2.058 | 45 | 3 | 2 | 1 | 43.96 |
| 1.9291 | 1 | 0 | 0 | 4 | 47.07 |
| 1.9241 | 3 | 4 | 0 | 0 | 47.20 |
| 1.8166 | 9 | 3 | 0 | 3 | 50.18 |

Figure 9: d/I/hkℓ/2θ Table Generation for $NH_4H_2AsO_4$.

## 3.0 Input Information

Any number of cells or powder patterns may be processed in a given run. The input consists of a single CONTROL CARD followed by one or more sets of DATA CARDS. All data sets in a given run will be processed as a homogeneous group as indicated by the control card. A typical input deck thus consists of one control card followed by data set 1, data set 2, etc. Examples of input decks and output listings are given in Appendix C.

The following card types may be input for each data set:

| | |
|---|---|
| CARD 1 | Cell parameters and crystal system (always required) |
| CARD 2 | Cell parameter standard deviations (optional) |
| CARD 3 | Space group, Z, Dm, Dx (required) |
| CARD 6 | Compound name (optional) |
| CARD 7 | Chemical formula (optional) |
| CARD 8 | Empirical formula (optional, but necessary for full analysis) |
| CARD B | Comments (optional) |
| CARD F | Pattern information (1) (required if powder data is input) |
| CARD G | Pattern information (2) (optional if powder data is input) |
| CARD H | Extinction conditions (optional) |
| CARD I | Powder pattern (required for powder data input) |
| CARD K | Entry termination (always required) |

Each set of data cards must begin with CARD 1 and must end with CARD K. In addition, CARD F and CARD I are required for powder data analysis. The card types are indicated in column 80 and each data set must have the cards ordered in the above sequence. The following table gives the card types required for typical analyses:

| Program analysis functions | Cards required |
|---|---|
| Cell analysis (reduced cell, Crystal Data cell, and metric symmetry determination) | 1, 3, K |
| Cell analysis, density, molecular weight | 1, 3, 7 or 8, K |
| Cell analysis, powder pattern analysis | 1, 3, F, I, K |
| Cell analysis, density, molecular weight, powder pattern analysis | 1, 3, 7 or 8, F, I, K |
| Generation of d-spacings, cell analysis | 1, 3, F, K |

CONTROL CARD (processing codes)

| Column | Format | Item |
|---|---|---|
| 5 | I1 | IJØB - type of run<br>0 = data analysis (cell or cell and powder pattern)<br>2 = d-spacing generation (no input powder data) |
| 35 | I1 | MØN25 - key for printing table of powder data in the format of NBS Monograph 25<br>0 = no output<br>1 = print |
| 46-50 | I5 | ITHMX - 2θ limit for d-spacing generation (if IJØB = 2) given as an integer, right justified |
| 55 | I1 | ICØL - print control<br>Blank = 120 columns or greater<br>1 = 80 column printing |

CARD 1 CELL PARAMETERS

| Column | Format | Item |
|---|---|---|
| 1-9 | F9.5 | a (original data) in Å |
| 10-18 | F9.5 | b |
| 19-27 | F9.5 | c |
| 28-35 | F8.3 | α (original data) in degrees |
| 36-43 | F8.3 | β |
| 44-51 | F8.3 | γ |
| 73-78 | 6A1 | Reference code, alphanumeric (ID for data set) |
| 79 | A1 | Crystal system code<br>A = anorthic (triclinic)<br>M = monoclinic<br>Ø = orthorhombic<br>T = tetragonal<br>H = hexagonal<br>R = rhombohedral (H or R axes)<br>C = cubic |
| 80 | A1 | 1 (card type 1) |

Note: Important: To prevent program malfunction, enter only those cell parameters required to define the cell:

| | |
|---|---|
| anorthic (triclinic) | a, b, c, α, β, γ |
| monoclinic (a-unique) | a, b, c, α |
| monoclinic (b-unique) | a, b, c, β |
| monoclinic (c-unique) | a, b, c, γ |
| orthorhombic | a, b, c |
| tetragonal | a, c |
| hexagonal | a, c |
| rhombohedral (H axes) | a, c |
| rhombohedral (R axes) | a, α |
| cubic | a |

For the rhombohedral crystal system, it is necessary to use the crystal system code "R" (even when the input cell is based on hexagonal axes) in order to obtain the correct reduced cell and metric symmetry analysis.

CARD 2 CELL PARAMETER STANDARD DEVIATIONS (optional)

| Column | Format | Item |
|---|---|---|
| 1-9 | F9.5 | $\sigma(a)$ |
| 10-18 | F9.5 | $\sigma(b)$ |
| 19-27 | F9.5 | $\sigma(c)$ |
| 28-35 | F8.3 | $\sigma(\alpha)$ |
| 36-43 | F8.3 | $\sigma(\beta)$ |
| 44-51 | F8.3 | $\sigma(\gamma)$ |
| 80 | A1 | 2 (card type 2) |

CARD 3 SPACE GROUP, Z, DENSITY

| Column | Format | Item |
|---|---|---|
| 1-8 | 8A1 | Space group, aspect in Laue class, or cell centering (left justified) |
| 20-25 | F6.0 | Z (may be entered as an integer, right justified, or as a decimal number) |
| 30-35 | F6.3 | Dm (measured density) |
| 38-43 | F6.3 | Dx (calculated density) |
| 80 | A1 | 3 (card type 3) |

Note: Enter the space group or aspect, left justified. The symbols may be in upper and lower case, or all upper case.

$P2_1/c \rightarrow$ P21/C (or P21/c) $R\bar{3}m \rightarrow$ R-3M (or R-3m)

$P4_32_12 \rightarrow$ P43212 I*/* → I*/*

If only the cell centering is known, enter the appropriate symbol (P, C, F, etc.) in column 1 under space group. If no centering is indicated, a primitive cell is assumed. The following symbols may be input:

| | |
|---|---|
| anorthic (triclinic) | P, A, B, C, F, I |
| monoclinic | P, A, B, C, F, I |
| orthorhombic | P, A, B, C, F, I |
| tetragonal | P, C, F, I |
| hexagonal | P |
| rhombohedral (H axes) | R |
| rhombohedral (R axes) | R, F, I |
| cubic | P, F, I |

CARD 6 COMPOUND NAME (optional)

| Column | Format | Item |
|---|---|---|
| 1-67 | 67A1 | Compound name (left justified) |
| 80 | A1 | 6 (card type 6) |

CARD 7 CHEMICAL FORMULA (optional)

| Column | Format | Item |
|---|---|---|
| 1-67 | 67A1 | Chemical formula (left justified) |
| 80 | A1 | 7 (card type 7) |

Note: If the chemical formula is input using the conventions specified below, the program will calculate the empirical formula and Card 8 is not required. The formula must be consistent with Z.

The formula is expressed as a sequence of discrete units. Each unit ends with a space. The following symbols are allowed:

1. Chemical element and number. Each element is followed by the number of atoms of that element; the element-number unit is terminated by a space. If the number of atoms of a given element is 1, then the 1 may be omitted. The element symbols may be in upper and lower case, or all upper case. Decimal multipliers are allowed.

   Ba Cℓ2 (or BA CL2)  Na2 S Ø4 (or NA2 S Ø4)

   BiO.5 CaO.5 Sr Ø3  (or BIO.5 CAO.5 SR Ø3)

2. Parentheses. A left parenthesis is always preceded and followed by a blank. A right parenthesis is always preceded by a blank and may be followed by a multiplier.

   Aℓ2 ( S Ø4 )3  Co ( C Ø )6  ( N H4 )2 S Ø4

3. Brackets. These are treated the same as parentheses.

   Ni3 [ Co ( C N )6 ]2

   Mg3 [ B ( Ø H )4 ]2 F ( Ø H ) S Ø4

4. Exclamation point. This symbol is used to indicate a center dot. It may be followed by a multiplier.

   Rb2 Zn ( Be F4 )2 !6 H2 Ø

   2 ( N H4 )2 S Ø4 ! H2 Ø

   La P Ø4 !0.5 H2 Ø

CARD 8 EMPIRICAL FORMULA (optional; not needed if Card 7 is input)

| Column | Format | Item |
|---|---|---|
| 1-67 | 67A1 | Empirical formula (left justified) |
| 80 | A1 | 8 (card type 8) |

Note: The empirical formula must be consistent with Z.

Follow each element symbol with a multiplier, and separate each element-multiplier unit with a space. A multiplier of 1 may be omitted.

Ca3 H2 Mg Ø24 Si C22 H36 Cℓ

The element symbols may be in upper and lower case, or all upper case; the first element symbol must begin in column 1.

CARD B COMMENTS (optional)

| Column | Format | Item |
|---|---|---|
| 1-67 | 67A1 | Any alphanumeric comments |
| 80 | A1 | B (card type B) |

CARD F PATTERN INFORMATION (1) (required only if powder data input or if d-generation is requested)

| Column | Format | Item |
|---|---|---|
| 7-15 | F9.5 | Wavelength in Å (Blank = 1.5405) |
| 30 | A1 | Code for original data<br>Blank = no data to be read (calculate hkℓ's and d's)<br>1 = $\theta$<br>2 = $2\theta$<br>D = d-spacings<br>S = $\sin^2\theta$<br>Q = $(d^*)^2 = 1/d^2$ |
| 80 | A1 | F (card type F) |

CARD G PATTERN INFORMATION (2) (optional if powder data input)

| Column | Format | Item |
|---|---|---|
| 17-20 | F4.2 | 2θ tolerance used in marking poor fit between observed and calculated 2θ's (Blank = 0.05) |
| 22 | A1 | Rhombohedral → hexagonal transformation code for hkℓ's<br>Blank = normal (no transformation)<br>R = input hkℓ's, based on rhombohedral axes, are to be transformed to hkℓ's based on hexagonal axes |
| 80 | A1 | G (card type G) |

CARD H EXTINCTION CONDITIONS (optional if powder data input or generated)

| Column | Format | Item |
|---|---|---|
| 21-47 | 27I1 | Extinction codes (see note) |
| 80 | A1 | H (card type H) |

Note: Extinction conditions will automatically be read from the extinction file for all space group and aspect settings given in Appendix A. Conditions must be input on this card for unusual orientations (e.g., c-unique monoclinic) or if the extinction file is not assigned.

If rhombohedral hkℓ's are to be transformed to hexagonal hkℓ's (column 22 on Card G = "R"), always input the special conditions for the rhombohedral cell based on hexagonal axes. The general rhombohedral condition (-h+k+ℓ=3n) need not be input.

See International Tables for X-ray Crystallography,[5] Volume 1, for the necessary extinctions for each space group. For each extinction, enter the integer value for "B" from the following table in the appropriate column:

| Indices | Condition | Column | Indices | Condition | Column |
|---|---|---|---|---|---|
| hkℓ | h+k=Bn | 21 | h0ℓ | h=Bn | 34 |
| hkℓ | h+ℓ=Bn | 22 | h0ℓ | ℓ=Bn | 35 |
| hkℓ | k+ℓ=Bn | 23 | h0ℓ | h+ℓ=Bn | 36 |
| hkℓ | h+k=Bx, h+ℓ=By, k+ℓ=Bz | 24 | hk0 | h=Bn | 37 |
| | | | hk0 | k=Bn | 38 |
| hkℓ | h+k+ℓ=Bn | 25 | hk0 | h+k=Bn | 39 |
| hkℓ | -h+k+ℓ=Bn | 26 | hh0 | h=Bn | 40 |
| hhℓ | h=Bn | 27 | h00 | h=Bn | 41 |
| hhℓ | ℓ=Bn | 28 | 0k0 | k=Bn | 42 |
| hhℓ | h+ℓ=Bn | 29 | 00ℓ | ℓ=Bn | 43 |
| hhℓ | 2h+ℓ=Bn | 30 | hℓℓ | h=Bn | 44 |
| 0kℓ | k=Bn | 31 | hℓℓ | ℓ=Bn | 45 |
| 0kℓ | ℓ=Bn | 32 | hℓℓ | h+ℓ=Bn | 46 |
| 0kℓ | k+ℓ=Bn | 33 | hℓℓ | h+2ℓ=Bn | 47 |

CARD I POWDER PATTERN (required only if powder data input)

Note: The data can be entered with either one, two, or three lines per card, in increasing $2\theta$ (decreasing d). Up to 200 lines may be entered for a given powder pattern; repeat Card I as necessary.

| Column | Format | Item |
|---|---|---|
| 1-7 | F7.n | $\theta$, $2\theta$, d, $\sin^2\theta$, or Q for line 1 (Data must agree with the data type indicated in column 30 of Card F. Give as many significant figures as possible.) |
| 8-10 | I3 | Relative intensity (any scale) |
| 12-14 | I3 | h |
| 15-17 | I3 | k |
| 18-20 | I3 | $\ell$ |
| 24-30 | F7.n | $\theta$, $2\theta$, d, $\sin^2\theta$, or Q for line 2 |
| 31-33 | I3 | Relative intensity |
| 35-37 | I3 | h |
| 38-40 | I3 | k |
| 41-43 | I3 | $\ell$ |
| 47-53 | F7.n | $\theta$, $2\theta$, d, $\sin^2\theta$, or Q for line 3 |
| 54-56 | I3 | Relative intensity |
| 58-60 | I3 | h |
| 61-63 | I3 | k |
| 64-66 | I3 | $\ell$ |
| 80 | A1 | I (card type I) |

CARD K ENTRY TERMINATION

| Column | Format | Item |
|---|---|---|
| 80 | A1 | K (card type K) |

## 4.0 Output Information

### Part 1. Warning and Error Messages

A warning message (**WARNING**) is printed if unusual data are entered. A warning is also given if the observed and calculated densities do not agree, if input hkℓ indices are not consistent with space group extinctions, or if the figure of merit indicates that the cell used in indexing a powder pattern is suspect. If the analysis of the reduced form indicates that a higher metric symmetry exists than was input, a warning message is printed and the cell parameters for the higher-symmetry cell are given along with the matrix for transformation of the initial cell to the higher-symmetry cell.

An error message (**ERROR**) usually indicates that an illegal parameter has been input or that the program has failed at some point. The input cards should be checked for accuracy.

A message (**MESSAGE**) relays information only, and does not indicate a warning or an error.

### Part 2. Cell Analysis

The input data and derived parameters are printed as a series of card images, with the type of data output summarized. Some or all of the following card images may be output:

CELL Initial cell, as input.

ESDS Standard deviations in the initial cell, if input; average standard deviation in axial lengths in parts per $10^5$; and quality index code. An "E" following the average standard deviation indicates that the program has assumed a value of 5 in the least significant digits.

| Average standard deviation (parts per $10^5$) | QI code | |
|---|---|---|
| 0 - 1 | A | |
| 2 - 5 | A- | |
| 6 - 10 | B | |
| 11 - 50 | B- | (typical single-crystal diffractometer) |
| 51 - 100 | C | |
| 101 - 500 | C- | |
| 501 - 1000 | D | |
| 1001 - 5000 | D- | |
| 5001 - 9999 | F | |

SG-1 Space group as input; space group or aspect number (see Appendix A); Z, Dm, and Dx as input; initial cell volume.

SG-2 Space group for Crystal Data cell; space group number; Z for Crystal Data cell; Dx calculated by the program; molecular weight; volume of Crystal Data cell. If no Z is input, then a value of 1 is assumed in the calculation of Dx; Dx is then followed by a "G".

NAME Compound name as input.

CHEM Chemical formula as input.

EMPR Empirical formula as input or as calculated from the chemical formula.

COMM Comments as input.

MATX Transformation matrices:
Initial cell to reduced cell (T-2)
Determinant and initial cell to Crystal Data cell
Inverse of initial cell to Crystal Data cell, if not identity matrix.

C-IN Initial cell and cell volume, as interpreted by the program.

C-RD Reduced cell, reduced cell volume, and reduced form number (see Appendix B). An "X" following the reduced form number indicates that the metric symmetry exceeds the input crystal symmetry.

C-CD Crystal Data cell and determinative ratios. For the conventions used to define the Crystal Data cell see the Introduction to Volume 3 or 4 of Crystal Data Determinative Tables.[1] The first determinative ratio is $\underline{a}/\underline{b}$ for anorthic, monoclinic, and orthorhombic; $\underline{c}/\underline{a}$ for tetragonal, hexagonal, and rhombohedral (hexagonal axes); and $\underline{a}$ for cubic. The second determinative ratio is $\underline{c}/\underline{b}$ for anorthic, monoclinic, and orthorhombic.

E-CD Standard deviations of the Crystal Data cell parameters, if initial standard deviations were input.

DOTM Dot product matrix ($\underset{\sim}{a}\cdot\underset{\sim}{a}$, $\underset{\sim}{b}\cdot\underset{\sim}{b}$, $\underset{\sim}{c}\cdot\underset{\sim}{c}$, $\underset{\sim}{b}\cdot\underset{\sim}{c}$, $\underset{\sim}{a}\cdot\underset{\sim}{c}$, $\underset{\sim}{a}\cdot\underset{\sim}{b}$) of the reduced cell. The values given for the dot products should be compared with the data in Appendix B to determine metric symmetry.

PDF1 Pattern information (1) as input (card F).

PDF2 Pattern information (2) as input (card G).

EXTC Extinction conditions as input (card H).

HIST Date processed; number of warnings generated; number of errors generated; year-version of NBS*AIDS80.

Part 3. Powder Pattern Analysis

The data are sorted on increasing 2θ, and intensities are rescaled to I(max) = 100. Observed and calculated d-spacings, 2θ's and hkℓ's are given, as well as Δ(2θ) for indexed lines. Any line that is unindexed on input will be assigned the indices of the closest calculated line provided that the observed and calculated 2θ's agree within 0.5°. The following editorial marks may be assigned to a given line by the program:

C = hkℓ assigned by the program
U = unindexed
N = not permitted by the space group

The reflections exceeding the $|\Delta(2\theta)|$ tolerance are listed. A reflection summary is given for the entire pattern, including the following: the theoretical number of lines possible, the number of lines resolvable, the number of unique observed lines, the total number of lines input, and the number of lines indexed and unindexed. For the indexed lines, the average and maximum $|\Delta(2\theta)|$ are given, along with the number of lines exceeding the tolerance of the PDF "★" limit ($|\Delta(2\theta)| \leq 0.05°$) and "I" limit ($|\Delta(2\theta)| \leq 0.20°$).

The figures of merit M(N) and F(N) proposed by de Wolff[10] and by Smith and Snyder,[11] respectively, are calculated for indexed powder patterns. Unindexed lines are not included in the calculation of either figure of merit. M(N) is defined by the equation

$$M(N) = \frac{Q(N)}{2\langle|\Delta Q|\rangle N}$$

where N is 20 or the number of indexed lines input if less than 20, Q(N) is the Q-value ( = $1/d^2$ ) of the $N^{th}$ line, and $\langle|\Delta Q|\rangle$ is the average magnitude of the difference between Q(obs) and Q(calc). According to de Wolff, a value of M(20) > 10 will indicate the essential correctness of the indexing provided that there are not more than two unindexed lines with $2\theta < 2\theta(N)$. The Smith-Snyder figure of merit is defined by

$$F(N) = \frac{1}{\langle|\Delta 2\theta|\rangle} \quad \frac{N}{N(poss)}$$

where N is 30 or the number of indexed lines input if less than 30, and N(poss) is the number of theoretical lines possible (excluding space-group extinct lines) up to and including the $N^{th}$ observed and indexed line. Co-positional lines (e.g. cubic indices 221 and 300) are counted as one possible line. The recommended format for reporting this figure of merit is F(N) [ $\langle|\Delta 2\theta|\rangle$, N(poss) ]. The factor N/N(poss) is a

measure of the completeness of the measurements while $<|\Delta 2\theta|>$ indicates the consistency of the unit cell with the experimental $2\theta$ values. For both M(N) and F(N) the average error values are based on the assigned $hk\ell$'s. If a line is input with multiple indices, then all possible differences (obs - calc) for that line are used in calculating the average error value.

Part 4. Table of Powder Data for Publication

A table of d-spacings, intensities, $hk\ell$ indices, and $2\theta$'s is prepared if MØN25 = 1 on the control card. The number of significant figures given for the spacings is determined by the overall $|\Delta(2\theta)|$ for the pattern.

## 5.0 Program Details

Examples of input card decks and output listings for typical data analysis runs are given in Appendix C. NBS*AIDS80 is written in FORTRAN and is currently running on a UNIVAC 1100 series computer. As overlayed, it occupies about 21K words of memory and requires from one second for cell analysis to five seconds for cell and powder data analysis. To improve portability of the program, we have grouped all ENCODE and DECODE statements together in a single subroutine. Laboratories with compilers that do not handle ENCODE and DECODE statements may have to write assembly language subroutines. The program makes use of the full 128 character ASCII character set. However, input may be restricted to only upper case for formulas and space group symbols. The program will be provided free of charge provided that a new, unlabeled 9 track magnetic tape, certified to 1600 bpi, accompanies the request. The supplied tape will be written unblocked in ASCII at 1600 bpi.

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## APPENDIX A

## SPACE GROUPS AND ASPECTS

The following tables give the space groups and diffraction aspects allowed by NBS*AIDS80 for the assignment of space group and aspect numbers and for the generation of systematic absences. Although any valid space group or diffraction aspect may be entered on Card 3, only those listed in these tables (in addition to cell centering symbols) will result in the automatic generation of systematic absences. For the monoclinic system the b-axis is assumed to be unique.

### Part I (Space Groups)

The space group numbers assigned by the program correspond to those given in the International Tables for X-ray Crystallography.[5] The assigned number is followed by an orientation code when more than one orientation is permitted for a given space group. In the monoclinic system these codes are A, B, or C, and in the orthorhombic system they are A, B, C, D, E, or F.

### Part II (Aspects)

The diffraction aspect, if known, should be entered on Card 3 when the space group is not uniquely defined. The diffraction aspects for each Laue class have been given by Donnay and Kennard[13] and are reprinted in Supplement II of the 3rd Edition of Crystal Data Determinative Tables,[1] Volumes 1 and 2. The four aspects that begin with the Laue group symmetry should be rewritten so that the lattice type appears first, followed by the Laue group:

| | |
|---|---|
| $\bar{1}$P* → P*,-1 | $\bar{3}$P* → P*,-3 |
| $\bar{3}$mP*c1 → P*c1,-3m | $\bar{3}$mP*1c → P*1c,-3m |

An aspect number assigned by the program is preceded by an asterisk(*), and this number corresponds to the number of the highest symmetry space group that is consistent with the diffraction aspect. The aspects for the enantiomorphic space groups (e.g. $P4_12_12$ and $P4_32_12$) are assigned the number corresponding to the lower-numbered space group of the pair. The orientation codes for the monoclinic and orthorhombic systems are the same as those assigned to the space groups.

PART I

SPACE GROUPS

## Anorthic (Triclinic) System

| Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|
| 1 | 2 | P1 |
| 2 | 2 | $P\bar{1}$ |

## Monoclinic System

| Space Group No. | Aspect No. | Space Group Symbols A* | B | C |
|---|---|---|---|---|
| 3 | 10 | P2 | | |
| 4 | 11 | $P2_1$ | | |
| 5 | 12 | C2 | A2 | I2 |
| 6 | 10 | Pm | | |
| 7 | 13 | Pc | Pa | Pn |
| 8 | 12 | Cm | Am | Im |
| 9 | 15 | Cc | Aa | Ia |
| 10 | 10 | P2/m | | |
| 11 | 11 | $P2_1/m$ | | |
| 12 | 12 | C2/m | A2/m | I2/m |
| 13 | 13 | P2/c | P2/a | P2/n |
| 14 | | $P2_1/c$ | $P2_1/a$ | $P2_1/n$ |
| 15 | 15 | C2/c | A2/a | I2/a |

*Orientation code

## Orthorhombic System

| Space Group No. | Aspect No. | Space Group Symbols A | B | C | D | E | F |
|---|---|---|---|---|---|---|---|
| 16 | 47 | P222 | | | | | |
| 17 | | $P222_1$ | $P2_122$ | $P22_12$ | | | |
| 18 | | $P2_12_12$ | $P22_12_1$ | $P2_122_1$ | | | |
| 19 | | $P2_12_12_1$ | | | | | |
| 20 | | $C222_1$ | $A2_122$ | $B22_12$ | | | |
| 21 | 65 | C222 | B222 | A222 | | | |
| 22 | 69 | F222 | | | | | |
| 23 | 71 | I222 | | | | | |
| 24 | 71 | $I2_12_12_1$ | | | | | |
| 25 | 47 | Pmm2 | Pm2m | P2mm | | | |
| 26 | 51 | $Pmc2_1$ | $P2_1ma$ | $P2_1am$ | $Pb2_1m$ | $Pcm2_1$ | $Pm2_1b$ |
| 27 | 49 | Pcc2 | Pb2b | P2aa | | | |
| 28 | 51 | Pma2 | P2cm | P2mb | Pbm2 | Pc2m | Pm2a |
| 29 | 57 | $Pca2_1$ | $P2_1ca$ | $Pb2_1a$ | $P2_1ab$ | $Pc2_1b$ | $Pbc2_1$ |
| 30 | 53 | Pnc2 | Pcn2 | Pn2b | Pb2n | P2na | P2an |
| 31 | 59 | $Pmn2_1$ | $Pnm2_1$ | $P2_1nm$ | $Pn2_1m$ | $Pm2_1n$ | $P2_1mn$ |
| 32 | 55 | Pba2 | P2cb | Pc2a | | | |
| 33 | 62 | $Pna2_1$ | $Pbn2_1$ | $P2_1cn$ | $P2_1nb$ | $Pn2_1a$ | $Pc2_1n$ |
| 34 | 58 | Pnn2 | Pn2n | P2nn | | | |
| 35 | 65 | Cmm2 | Bm2m | A2mm | | | |
| 36 | 63 | $Cmc2_1$ | $A2_1am$ | $A2_1ma$ | $Bm2_1b$ | $Bb2_1m$ | $Ccm2_1$ |
| 37 | 66 | Ccc2 | A2aa | Bb2b | | | |
| 38 | 65 | Amm2 | Am2m | B2mm | C2mm | Bmm2 | Cm2m |

## Orthorhombic System (cont.)

| Space Group No. | Aspect No. | Space Group Symbols A | B | C | D | E | F |
|---|---|---|---|---|---|---|---|
| 39 | 67 | Abm2 | Bma2 | C2ma | Ab2m | Cm2a | B2am |
| 40 | 63 | Ama2 | C2cm | Bbm2 | B2mb | Cc2m | Am2a |
| 41 | 64 | Aba2 | Ab2a | C2ca | B2ab | Cc2a | Bba2 |
| 42 | 69 | Fmm2 | Fm2m | F2mm | | | |
| 43 | | Fdd2 | Fd2d | F2dd | | | |
| 44 | 71 | Imm2 | Im2m | I2mm | | | |
| 45 | 72 | Iba2 | Ib2a | I2aa | | | |
| 46 | 74 | Ima2 | Im2a | Ibm2 | I2am | Ib2m | I2ma |
| 47 | 47 | Pmmm | | | | | |
| 48 | | Pnnn | | | | | |
| 49 | 49 | Pccm | Pmaa | Pbmb | | | |
| 50 | | Pban | Pncb | Pcna | | | |
| 51 | 51 | Pmma | Pmcm | Pcmm | Pmam | Pbmm | Pmmb |
| 52 | | Pnna | Pnnb | Pnan | Pncn | Pbnn | Pcnn |
| 53 | 53 | Pmna | Pncm | Pbmn | Pman | Pcnm | Pnmb |
| 54 | | Pcca | Pbaa | Pbcb | Pccb | Pbab | Pcaa |
| 55 | 55 | Pbam | Pcma | Pmcb | | | |
| 56 | | Pccn | Pbnb | Pnaa | | | |
| 57 | 57 | Pbcm | Pcmb | Pbma | Pcam | Pmab | Pmca |
| 58 | 58 | Pnnm | Pnmn | Pmnn | | | |
| 59 | 59 | Pmmn | Pnmm | Pmnm | | | |
| 60 | | Pbcn | Pnab | Pnca | Pbna | Pcan | Pcnb |
| 61 | | Pbca | Pcab | | | | |

## Orthorhombic System (cont.)

| Space Group No. | Aspect No. | Space Group Symbols | | | | | |
|---|---|---|---|---|---|---|---|
| | | A | B | C | D | E | F |
| 62 | 62 | Pnma | Pmnb | Pbnm | Pmcn | Pcmn | Pnam |
| 63 | 63 | Cmcm | Bbmm | Amam | Amma | Ccmm | Bmmb |
| 64 | 64 | Cmca | Abam | Ccma | Abma | Bmab | Bbam |
| 65 | 65 | Cmmm | Bmmm | Ammm | | | |
| 66 | 66 | Cccm | Amaa | Bbmb | | | |
| 67 | 67 | Cmma | Abmm | Bmam | | | |
| 68 | | Ccca | Bbab | Abaa | | | |
| 69 | 69 | Fmmm | | | | | |
| 70 | | Fddd | | | | | |
| 71 | 71 | Immm | | | | | |
| 72 | 72 | Ibam | Imaa | Ibma | | | |
| 73 | | Ibca | | | | | |
| 74 | 74 | Imma | Ibmm | Imam | | | |

## Tetragonal System

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 75 | 83 | P4 | 76 | 76 | $P4_1$ |
| 77 | 84 | $P4_2$ | 78 | 76 | $P4_3$ |
| 79 | 87 | I4 | 80 | | $I4_1$ |
| 81 | 83 | $P\bar{4}$ | 82 | 87 | $I\bar{4}$ |
| 83 | 83 | P4/m | 84 | 84 | $P4_2/m$ |
| 85 | | P4/n | 86 | | $P4_2/n$ |
| 87 | 87 | I4/m | 88 | | $I4_1/a$ |

## Tetragonal System (cont.)

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 89 | 123 | P422 | 90 | 113 | $P42_12$ |
| 91 | 91 | $P4_122$ | 92 | 92 | $P4_12_12$ |
| 93 | | $P4_222$ | 94 | | $P4_22_12$ |
| 95 | 91 | $P4_322$ | 96 | 92 | $P4_32_12$ |
| 97 | 139 | I422 | 98 | | $I4_122$ |
| 99 | 123 | P4mm | 100 | 127 | P4bm |
| 101 | 132 | $P4_2cm$ | 102 | 136 | $P4_2nm$ |
| 103 | 124 | P4cc | 104 | 128 | P4nc |
| 105 | 131 | $P4_2mc$ | 106 | 135 | $P4_2bc$ |
| 107 | 139 | I4mm | 108 | 140 | I4cm |
| 109 | 122 | $I4_1md$ | 110 | | $I4_1cd$ |
| 111 | 123 | $P\bar{4}2m$ | 112 | 131 | $P\bar{4}2c$ |
| 113 | 113 | $P\bar{4}2_1m$ | 114 | | $P\bar{4}2_1c$ |
| 115 | 123 | $P\bar{4}m2$ | 116 | 132 | $P\bar{4}c2$ |
| 117 | 127 | $P\bar{4}b2$ | 118 | 136 | $P\bar{4}n2$ |
| 119 | 139 | $I\bar{4}m2$ | 120 | 140 | $I\bar{4}c2$ |
| 121 | 139 | $I\bar{4}2m$ | 122 | 122 | $I\bar{4}2d$ |
| 123 | 123 | P4/mmm | 124 | 124 | P4/mcc |
| 125 | | P4/nbm | 126 | | P4/nnc |
| 127 | 127 | P4/mbm | 128 | 128 | P4/mnc |
| 129 | | P4/nmm | 130 | | P4/ncc |
| 131 | 131 | $P4_2/mmc$ | 132 | 132 | $P4_2/mcm$ |
| 133 | | $P4_2/nbc$ | 134 | | $P4_2/nnm$ |

## Tetragonal System (cont.)

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 135 | 135 | $P4_2/mbc$ | 136 | 136 | $P4_2/mnm$ |
| 137 | | $P4_2/nmc$ | 138 | | $P4_2/ncm$ |
| 139 | 139 | $I4/mmm$ | 140 | 140 | $I4/mcm$ |
| 141 | | $I4_1/amd$ | 142 | | $I4_1/acd$ |

## Hexagonal and Rhombohedral System

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 143 | 147 | P3 | 144 | 144 | $P3_1$ |
| 145 | 144 | $P3_2$ | 146 | 148 | R3 |
| 147 | 147 | $P\bar{3}$ | 148 | 148 | $R\bar{3}$ |
| 149 | 162 | P312 | 150 | 164 | P321 |
| 151 | 151 | $P3_112$ | 152 | 152 | $P3_121$ |
| 153 | 151 | $P3_212$ | 154 | 152 | $P3_221$ |
| 155 | 166 | R32 | 156 | 164 | P3m1 |
| 157 | 162 | P31m | 158 | 165 | P3c1 |
| 159 | 163 | P31c | 160 | 166 | R3m |
| 161 | 167 | R3c | 162 | 162 | $P\bar{3}1m$ |
| 163 | 163 | $P\bar{3}1c$ | 164 | 164 | $P\bar{3}m1$ |
| 165 | 165 | $P\bar{3}c1$ | 166 | 166 | $R\bar{3}m$ |
| 167 | 167 | $R\bar{3}c$ | 168 | 175 | P6 |
| 169 | 169 | $P6_1$ | 170 | 169 | $P6_5$ |
| 171 | 171 | $P6_2$ | 172 | 171 | $P6_4$ |

## Hexagonal and Rhombohedral System (cont.)

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 173 | 176 | $P6_3$ | 174 | 175 | $P\bar{6}$ |
| 175 | 175 | P6/m | 176 | 176 | $P6_3/m$ |
| 177 | 191 | P622 | 178 | 178 | $P6_122$ |
| 179 | 178 | $P6_522$ | 180 | 180 | $P6_222$ |
| 181 | 180 | $P6_422$ | 182 | | $P6_322$ |
| 183 | 191 | P6mm | 184 | 192 | P6cc |
| 185 | 193 | $P6_3cm$ | 186 | 194 | $P6_3mc$ |
| 187 | 191 | $P\bar{6}m2$ | 188 | 193 | $P\bar{6}c2$ |
| 189 | 191 | $P\bar{6}2m$ | 190 | 194 | $P\bar{6}2c$ |
| 191 | 191 | P6/mmm | 192 | 192 | P6/mcc |
| 193 | 193 | $P6_3/mcm$ | 194 | 194 | $P6_3/mmc$ |

## Cubic System

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 195 | 200 | P23 | 196 | 202 | F23 |
| 197 | 204 | I23 | 198 | | $P2_13$ |
| 199 | 204 | $I2_13$ | 200 | 200 | Pm3 |
| 201 | | Pn3 | 202 | 202 | Fm3 |
| 203 | | Fd3 | 204 | 204 | Im3 |
| 205 | | Pa3 | 206 | | Ia3 |
| 207 | 221 | P432 | 208 | | $P4_232$ |
| 209 | 225 | F432 | 210 | | $F4_132$ |
| 211 | 229 | I432 | 212 | 212 | $P4_332$ |

## Cubic System (cont.)

| Space Group No. | Aspect No. | Space Group Symbols | Space Group No. | Aspect No. | Space Group Symbols |
|---|---|---|---|---|---|
| 213 | 212 | $P4_132$ | 214 | | $I4_132$ |
| 215 | 221 | $P\bar{4}3m$ | 216 | 225 | $F\bar{4}3m$ |
| 217 | 229 | $I\bar{4}3m$ | 218 | 223 | $P\bar{4}3n$ |
| 219 | 226 | $F\bar{4}3c$ | 220 | | $I\bar{4}3d$ |
| 221 | 221 | Pm3m | 222 | | Pn3n |
| 223 | 223 | Pm3n | 224 | | Pn3m |
| 225 | 225 | Fm3m | 226 | 226 | Fm3c |
| 227 | | Fd3m | 228 | | Fd3c |
| 229 | 229 | Im3m | 230 | | Ia3d |

# PART II

## ASPECTS

### Anorthic (Triclinic) System

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P*,$\bar{1}$ | 2 | P$\bar{1}$ (2), P1 (1) |

### Monoclinic System

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P*/* | 10 | P2/m (10), P2 (3), Pm (6) |
| $P2_1$/* | 11 | $P2_1$/m (11), $P2_1$ (4) |
| C*/* | 12A | C2/m (12A), C2 (5A), Cm (8A) |
| A*/* | 12B | A2/m (12B), A2 (5B), Am (8B) |
| I*/* | 12C | I2/m (12C), I2 (5C), Im (8C) |
| P*/c | 13A | P2/c (13A), Pc (7A) |
| P*/a | 13B | P2/a (13B), Pa (7B) |
| P*/n | 13C | P2/n (13C), Pn (7C) |
| C*/c | 15A | C2/c (15A), Cc (9A) |
| A*/a | 15B | A2/a (15B), Aa (9B) |
| I*/a | 15C | I2/a (15C), Ia (9C) |

### Orthorhombic System

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P*** | 47 | Pmmm (47), P222 (16), Pmm2 (25A), Pm2m (25B), P2mm (25C) |
| Pcc* | 49A | Pccm (49A), Pcc2 (27A) |
| P*aa | 49B | Pmaa (49B), P2aa (27C) |
| Pb*b | 49C | Pbmb (49C), Pb2b (27B) |
| P**a | 51A | Pmma (51A), $P2_1$ma (26B), Pm2a (28F) |
| P*c* | 51B | Pmcm (51B), Pmc$2_1$ (26A), P2cm (28B) |

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| Pc** | 51C | Pcmm (51C), $Pcm2_1$ (26E), Pc2m (28E) |
| P*a* | 51D | Pmam (51D), $P2_1am$ (26C), Pma2 (28A) |
| Pb** | 51E | Pbmm (51E), $Pb2_1m$ (26D), Pbm2 (28D) |
| P**b | 51F | Pmmb (51F), $Pm2_1b$ (26F), P2mb (28C) |
| P*na | 53A | Pmna (53A), P2na (30E) |
| Pnc* | 53B | Pncm (53B), Pnc2 (30A) |
| Pb*n | 53C | Pbmn (53C), Pb2n (30D) |
| P*an | 53D | Pman (53D), P2an (30F) |
| Pcn* | 53E | Pcnm (53E), Pcn2 (30B) |
| Pn*b | 53F | Pnmb (53F), Pn2b (30C) |
| Pba* | 55A | Pbam (55A), Pba2 (32A) |
| Pc*a | 55B | Pcma (55B), Pc2a (32C) |
| P*cb | 55C | Pmcb (55C), P2cb (32B) |
| Pbc* | 57A | Pbcm (57A), $Pbc2_1$ (29F) |
| Pc*b | 57B | Pcmb (57B), $Pc2_1b$ (29E) |
| Pb*a | 57C | Pbma (57C), $Pb2_1a$ (29C) |
| Pca* | 57D | Pcam (57D), $Pca2_1$ (29A) |
| P*ab | 57E | Pmab (57E), $P2_1ab$ (29D) |
| P*ca | 57F | Pmca (57F), $P2_1ca$ (29B) |
| Pnn* | 58A | Pnnm (58A), Pnn2 (34A) |
| Pn*n | 58B | Pnmn (58B), Pn2n (34B) |
| P*nn | 58C | Pmnn (58C), P2nn (34C) |
| P**n | 59A | Pmmn (59A), $Pm2_1n$ (31E), $P2_1mn$ (31F) |
| Pn** | 59B | Pnmm (59B), $Pnm2_1$ (31B), $Pn2_1m$ (31D) |

## Orthorhombic System (cont.)

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P*n* | 59C | Pmnm (59C), $Pmn2_1$ (31A), $P2_1nm$ (31C) |
| Pn*a | 62A | Pnma (62A), $Pn2_1a$ (33E) |
| P*nb | 62B | Pmnb (62B), $P2_1nb$ (33D) |
| Pbn* | 62C | Pbnm (62C), $Pbn2_1$ (33B) |
| P*cn | 62D | Pmcn (62D), $P2_1cn$ (33C) |
| Pc*n | 62E | Pcmn (62E), $Pc2_1n$ (33F) |
| Pna* | 62F | Pnam (62F), $Pna2_1$ (33A) |
| C*c* | 63A | Cmcm (63A), $Cmc2_1$ (36A), C2cm (40B) |
| Bb** | 63B | Bbmm (63B), $Bb2_1m$ (36E), Bbm2 (40C) |
| A*a* | 63C | Amam (63C), $A2_1am$ (36B), Ama2 (40A) |
| A**a | 63D | Amma (63D), $A2_1ma$ (36C), Am2a (40F) |
| Cc** | 63E | Ccmm (63E), $Ccm2_1$ (36F), Cc2m (40E) |
| B**b | 63F | Bmmb (63F), $Bm2_1b$ (36D), B2mb (40D) |
| C*ca | 64A | Cmca (64A), C2ca (41C) |
| Aba* | 64B | Abam (64B), Aba2 (41A) |
| Cc*a | 64C | Ccma (64C), Cc2a (41E) |
| Ab*a | 64D | Abma (64D), Ab2a (41B) |
| B*ab | 64E | Bmab (64E), B2ab (41D) |
| Bba* | 64F | Bbam (64F), Bba2 (41F) |
| C*** | 65A | Cmmm (65A), C222 (21A), Cmm2 (35A), C2mm (38D), Cm2m (38F) |
| B*** | 65B | Bmmm (65B), B222 (21B), Bm2m (35B), B2mm (38C), Bmm2 (38E) |
| A*** | 65C | Ammm (65C), A222 (21C), A2mm (35C), Amm2 (38A), Am2m (38B) |
| Ccc* | 66A | Cccm (66A), Ccc2 (37A) |
| A*aa | 66B | Amaa (66B), A2aa (37B) |

## Orthorhombic System (cont.)

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| Bb*b | 66C | Bbmb (66C), Bb2b (37C) |
| C**a | 67A | Cmma (67A), C2ma (39C), Cm2a (39E) |
| Ab** | 67B | Abmm (67B), Abm2 (39A), Ab2m (39D) |
| B*a* | 67C | Bmam (67C), Bma2 (39B), B2am (39F) |
| F*** | 69 | Fmmm (69), F222 (22), Fmm2 (42A), Fm2m (42B), F2mm (42C) |
| I*** | 71 | Immm (71), I222 (23), $I2_12_12_1$ (24), Imm2 (44A), Im2m (44B), I2mm (44C) |
| Iba* | 72A | Ibam (72A), Iba2 (45A) |
| I*aa | 72B | Imaa (72B), I2aa (45C) |
| Ib*a | 72C | Ibma (72C), Ib2a (45B) |
| I**a | 74A | Imma (74A), Im2a (46B), I2ma (46F) |
| Ib** | 74B | Ibmm (74B), Ibm2 (46C), Ib2m (46E) |
| I*a* | 74C | Imam (74C), Ima2 (46A), I2am (46D) |

## Tetragonal System

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| $P4_{1,3}$ | 76 | $P4_1$ (76), $P4_3$ (78) |
| P4/* | 83 | P4/m (83), P4 (75), $P\bar{4}$ (81) |
| $P4_2$/* | 84 | $P4_2$/m (84), $P4_2$ (77) |
| I4/* | 87 | I4/m (87), I4 (79), $I\bar{4}$ (82) |
| $P4_{1,3}22$ | 91 | $P4_122$ (91), $P4_322$ (95) |
| $P4_{1,3}2_12$ | 92 | $P4_12_12$ (92), $P4_32_12$ (96) |
| $P42_1$* | 113 | $P\bar{4}2_1m$ (113), $P42_12$ (90) |
| I4*d | 122 | $I\bar{4}2d$ (122), $I4_1md$ (109) |
| P4/*** | 123 | P4/mmm (123), P422 (89), P4mm (99), $P\bar{4}2m$ (111), $P\bar{4}m2$ (115) |

## Tetragonal System (cont.)

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P4/*cc | 124 | P4/mcc (124), P4cc (103) |
| P4/*b* | 127 | P4/mbm (127), P4bm (100), P$\bar{4}$b2 (117) |
| P4/*nc | 128 | P4/mnc (128), P4nc (104) |
| P4/**c | 131 | $P4_2$/mmc (131), $P4_2$mc (105), P$\bar{4}$2c (112) |
| P4/*c* | 132 | $P4_2$/mcm (132), $P4_2$cm (101), P$\bar{4}$c2 (116) |
| P4/*bc | 135 | $P4_2$/mbc (135), $P4_2$bc (106) |
| P4/*n* | 136 | $P4_2$/mnm (136), $P4_2$nm (102), P$\bar{4}$n2 (118) |
| I4/*** | 139 | I4/mmm (139), I422 (97), I4mm (107), I$\bar{4}$m2 (119), I$\bar{4}$2m (121) |
| I4/*c* | 140 | I4/mcm (140), I4cm (108), I$\bar{4}$c2 (120) |

## Hexagonal and Rhombohedral System

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| $P3_{1,2}$ | 144 | $P3_1$ (144), $P3_2$ (145) |
| P*,$\bar{3}$ | 147 | P$\bar{3}$ (147), P3 (143) |
| R* | 148 | R$\bar{3}$ (148), R3 (146) |
| $P3_{1,2}$12 | 151 | $P3_1$12 (151), $P3_2$12 (153) |
| $P3_{1,2}$21 | 152 | $P3_1$21 (152), $P3_2$21 (154) |
| P31* | 162 | P$\bar{3}$1m (162), P312 (149), P31m (157) |
| P*1c,$\bar{3}$m | 163 | P$\bar{3}$1c (163), P31c (159) |
| P3*1 | 164 | P$\bar{3}$m1 (164), P321 (150), P3m1 (156) |
| P*c1,$\bar{3}$m | 165 | P$\bar{3}$c1 (165), P3c1 (158) |
| R** | 166 | R$\bar{3}$m (166), R32 (155), R3m (160) |
| R*c | 167 | R$\bar{3}$c (167), R3c (161) |
| $P6_{1,5}$ | 169 | $P6_1$ (169), $P6_5$ (170) |
| $P6_{2,4}$ | 171 | $P6_2$ (171), $P6_4$ (172) |

Hexagonal and Rhombohedral System (cont.)

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P6/* | 175 | P6/m (175), P6 (168), $P\bar{6}$ (174) |
| $P6_3$/* | 176 | $P6_3$/m (176), $P6_3$ (173) |
| $P6_{1,5}22$ | 178 | $P6_122$ (178), $P6_522$ (179) |
| $P6_{2,4}22$ | 180 | $P6_222$ (180), $P6_422$ (181) |
| P6/*** | 191 | P6/mmm (191), P622 (177), P6mm (183), $P\bar{6}m2$ (187), $P\bar{6}2m$ (189) |
| P6/*cc | 192 | P6/mcc (192), P6cc (184) |
| P6/*c* | 193 | $P6_3$/mcm (193), $P6_3$cm (185), $P\bar{6}c2$ (188) |
| P6/**c | 194 | $P6_3$/mmc (194), $P6_3$mc (186), $P\bar{6}2c$ (190) |

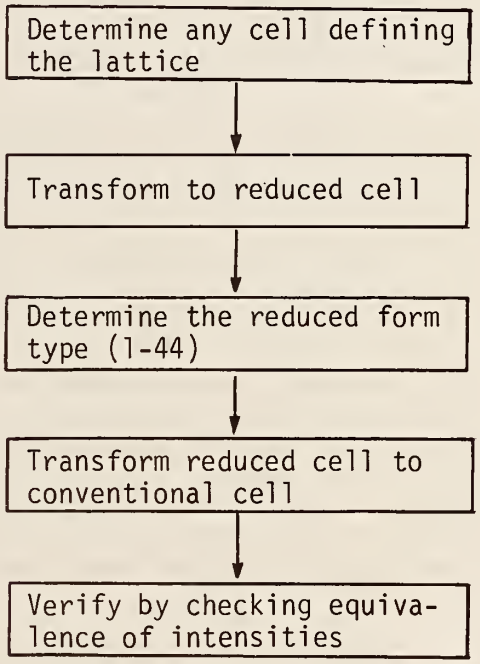
Cubic System

| Aspect | Number | Space Groups (Space Group Numbers) |
|---|---|---|
| P*3 | 200 | Pm3 (200), P23 (195) |
| F*3 | 202 | Fm3 (202), F23 (196) |
| I*3 | 204 | Im3 (204), I23 (197), $I2_13$ (199) |
| $P4_{1,3}32$ | 212 | $P4_332$ (212), $P4_132$ (213) |
| P*3* | 221 | Pm3m (221), P432 (207), $P\bar{4}3m$ (215) |
| P*3n | 223 | Pm3n (223), $P\bar{4}3n$ (218) |
| F*3* | 225 | Fm3m (225), F432 (209), $F\bar{4}3m$ (216) |
| F*3c | 226 | Fm3c (226), $F\bar{4}3c$ (219) |
| I*3* | 229 | Im3m (229), I432 (211), $I\bar{4}3m$ (217) |

## APPENDIX B

## LATTICE SYMMETRY DETERMINATION

There exists a close correlation between the metric symmetry (i.e. the symmetry determined from the cell parameters alone) and the crystal symmetry of the lattice. It has been shown that for 97 percent of the entries in the NBS Crystal Data File, the metric symmetry is the same as the crystal symmetry reported by the authors.[6] Thus it was concluded that more emphasis should be placed on cell determination and refinement algorithms used in routine diffractometry because of the basic importance of the metric lattice in crystallography. A convenient procedure to determine crystal symmetry is as follows:




The algorithm used by NBS*AIDS80 to calculate the reduced cell guarantees that both the main and special conditions for reduction are satisfied.[4] If only the main conditions for reduction are satisfied, one obtains a cell based on the shortest three non-coplanar translations. However, the special conditions must also be satisfied since in certain lattices two or more cells may be based on the shortest three translations.[4] In fact, Gruber[14] has shown that as many as five different cells of this type may exist in the same lattice. Thus the special conditions are necessary to define one and only one of these cells as the reduced cell. Table 1 gives the main and special conditions used by NBS*AIDS80 to determine the reduced cell.

Based on the reduced cell, NBS*AIDS80 calculates the vector products

defining the reduced form:

$$\begin{pmatrix} \underset{\sim}{a}\cdot\underset{\sim}{a} & \underset{\sim}{b}\cdot\underset{\sim}{b} & \underset{\sim}{c}\cdot\underset{\sim}{c} \\ \underset{\sim}{b}\cdot\underset{\sim}{c} & \underset{\sim}{a}\cdot\underset{\sim}{c} & \underset{\sim}{a}\cdot\underset{\sim}{b} \end{pmatrix}$$

From the reduced form, the reduced form type (1-44) is assigned. Table 2 gives the conditions for the 44 reduced forms, as well as the matrices relating each reduced form to a corresponding conventional cell of the Bravais lattice. This table[6] is derived from Table 5.1.3.1 of the International Tables for X-ray Crystallography,[5] including the published addenda and errata.[15,16] Thus to find the metric symmetry of an unknown, one can introduce any cell of the lattice on Card 1; if the cell is not primitive, the centering must be specified on Card 3. The program calculates the reduced cell, reduced form, and reduced form type. If the metric symmetry exceeds the input crystal symmetry, both the higher symmetry cell and the transformation matrix (input cell to Crystal Data conventional cell[1]) will be output. In practice we have found it convenient to determine a primitive triclinic cell on the diffractometer and use NBS*AIDS80 to suggest the lattice symmetry.

It is essential that the input cell be determined as accurately as possible. Usually the program will find the correct metric symmetry with the input of a refined cell determined from a diffractometer. However, caution should be used in the interpretation of metric symmetry. In its present form NBS*AIDS80 has the practical and theoretical limitation of determining only one metric cell when, in certain cases, more than one answer may be possible owing to experimental errors in the input cell. Thus the reduced cell and reduced form should be checked using Tables 1 and 2 to determine if an alternative symmetry might be considered. For example, the program may indicate a symmetry lower than the lattice symmetry because of inexact determination of cell angles; idealization of the experimental angles (e.g. 90°) may be necessary to obtain the correct analysis. Also, if the reduced form exhibits more specialization than is required to define the lattice type, it may signify that a subcell of the lattice has been input or that the material is twinned.

We have noted from our experience with obtaining cells from an automated diffractometer as well as from analysis of the data in the NBS Crystal Data File that the determination of a subcell of the lattice is a common source of error. A number of structure determinations have been carried out using only half of the available unique data; this error often results in apparent disorder in the refined structure. If it is suspected that a subcell of the lattice has been determined, one can obtain the cells of 2, 3, and 4 times the volume by applying the upper triangular $\underset{\sim}{Q}$ matrices given in Table 3 to any primitive cell of the lattice.[17] The seven cells of twice the original volume, thirteen cells of three times the volume, or 35 cells of four times the volume can be used to calculate the positions of the nodes in reciprocal space to be checked for diffraction intensity. Alternatively, one can apply the transpose of the inverse of the $\underset{\sim}{Q}$ matrices to the reciprocal cell to determine the nodes.

Table 1. Conditions for a Reduced Cell*

A. Positive reduced form, type I cell, all angles < 90°

Main conditions: $\underset{\sim}{a}\cdot\underset{\sim}{a} \leq \underset{\sim}{b}\cdot\underset{\sim}{b} \leq \underset{\sim}{c}\cdot\underset{\sim}{c}$ ; $\underset{\sim}{b}\cdot\underset{\sim}{c} \leq \frac{1}{2}\,\underset{\sim}{b}\cdot\underset{\sim}{b}$ ; $\underset{\sim}{a}\cdot\underset{\sim}{c} \leq \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$ ;

$\underset{\sim}{a}\cdot\underset{\sim}{b} \leq \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$

Special conditions:

(a) if $\underset{\sim}{a}\cdot\underset{\sim}{a} = \underset{\sim}{b}\cdot\underset{\sim}{b}$ then $\underset{\sim}{b}\cdot\underset{\sim}{c} \leq \underset{\sim}{a}\cdot\underset{\sim}{c}$

(b) if $\underset{\sim}{b}\cdot\underset{\sim}{b} = \underset{\sim}{c}\cdot\underset{\sim}{c}$ then $\underset{\sim}{a}\cdot\underset{\sim}{c} \leq \underset{\sim}{a}\cdot\underset{\sim}{b}$

(c) if $\underset{\sim}{b}\cdot\underset{\sim}{c} = \frac{1}{2}\,\underset{\sim}{b}\cdot\underset{\sim}{b}$ then $\underset{\sim}{a}\cdot\underset{\sim}{b} \leq 2\,\underset{\sim}{a}\cdot\underset{\sim}{c}$

(d) if $\underset{\sim}{a}\cdot\underset{\sim}{c} = \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$ then $\underset{\sim}{a}\cdot\underset{\sim}{b} \leq 2\,\underset{\sim}{b}\cdot\underset{\sim}{c}$

(e) if $\underset{\sim}{a}\cdot\underset{\sim}{b} = \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$ then $\underset{\sim}{a}\cdot\underset{\sim}{c} \leq 2\,\underset{\sim}{b}\cdot\underset{\sim}{c}$

B. Negative reduced form, type II cell, all angles ≥ 90°

Main conditions:

(a) $\underset{\sim}{a}\cdot\underset{\sim}{a} \leq \underset{\sim}{b}\cdot\underset{\sim}{b} \leq \underset{\sim}{c}\cdot\underset{\sim}{c}$ ; $|\underset{\sim}{b}\cdot\underset{\sim}{c}| \leq \frac{1}{2}\,\underset{\sim}{b}\cdot\underset{\sim}{b}$;

$|\underset{\sim}{a}\cdot\underset{\sim}{c}| \leq \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$ ; $|\underset{\sim}{a}\cdot\underset{\sim}{b}| \leq \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$

(b) $(|\underset{\sim}{b}\cdot\underset{\sim}{c}| + |\underset{\sim}{a}\cdot\underset{\sim}{c}| + |\underset{\sim}{a}\cdot\underset{\sim}{b}|) \leq \frac{1}{2}\,(\,\underset{\sim}{a}\cdot\underset{\sim}{a} + \underset{\sim}{b}\cdot\underset{\sim}{b}\,)$

Special conditions:

(a) if $\underset{\sim}{a}\cdot\underset{\sim}{a} = \underset{\sim}{b}\cdot\underset{\sim}{b}$ then $|\underset{\sim}{b}\cdot\underset{\sim}{c}| \leq |\underset{\sim}{a}\cdot\underset{\sim}{c}|$

(b) if $\underset{\sim}{b}\cdot\underset{\sim}{b} = \underset{\sim}{c}\cdot\underset{\sim}{c}$ then $|\underset{\sim}{a}\cdot\underset{\sim}{c}| \leq |\underset{\sim}{a}\cdot\underset{\sim}{b}|$

(c) if $|\underset{\sim}{b}\cdot\underset{\sim}{c}| = \frac{1}{2}\,\underset{\sim}{b}\cdot\underset{\sim}{b}$ then $\underset{\sim}{a}\cdot\underset{\sim}{b} = 0$

(d) if $|\underset{\sim}{a}\cdot\underset{\sim}{c}| = \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$ then $\underset{\sim}{a}\cdot\underset{\sim}{b} = 0$

(e) if $|\underset{\sim}{a}\cdot\underset{\sim}{b}| = \frac{1}{2}\,\underset{\sim}{a}\cdot\underset{\sim}{a}$ then $\underset{\sim}{a}\cdot\underset{\sim}{c} = 0$

(f) if $(|\underset{\sim}{b}\cdot\underset{\sim}{c}| + |\underset{\sim}{a}\cdot\underset{\sim}{c}| + |\underset{\sim}{a}\cdot\underset{\sim}{b}|) = \frac{1}{2}\,(\,\underset{\sim}{a}\cdot\underset{\sim}{a} + \underset{\sim}{b}\cdot\underset{\sim}{b}\,)$

then $\underset{\sim}{a}\cdot\underset{\sim}{a} \leq 2\,|\underset{\sim}{a}\cdot\underset{\sim}{c}| + |\underset{\sim}{a}\cdot\underset{\sim}{b}|$

---

*For further details see the discussion in Reference 5.

# Table 2. Metric Classification of Reduced Forms*

| Reduced Form No. | Reduced Form Matrix | | | | Reduced Form Type | Bravais Lattice | | Cell Transformation Reduced → Conventional |
|---|---|---|---|---|---|---|---|---|
| | First Row | Second Row | | | | | | |
| | $a\cdot a\ b\cdot b\ c\cdot c$ | $b\cdot c$ | $a\cdot c$ | $a\cdot b$ | | | | |
| a = b = c | | | | | | | | |
| 1 | $a\cdot a\ a\cdot a\ a\cdot a$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | + | Cubic | F | $1\bar{1}1/11\bar{1}/\bar{1}11$ |
| 2 | $a\cdot a\ a\cdot a\ a\cdot a$ | $b\cdot c$ | $b\cdot c$ | $b\cdot c$ | + | Rhombohedral | hR | $1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$ |
| 3 | $a\cdot a\ a\cdot a\ a\cdot a$ | 0 | 0 | 0 | - | Cubic | P | 100/010/001 |
| 4 | $a\cdot a\ a\cdot a\ a\cdot a$ | $-\lvert b\cdot c\rvert$ | $-\lvert b\cdot c\rvert$ | $-\lvert b\cdot c\rvert$ | - | Rhombohedral | hR | $1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$ |
| 5 | $a\cdot a\ a\cdot a\ a\cdot a$ | $-\frac{a\cdot a}{3}$ | $-\frac{a\cdot a}{3}$ | $-\frac{a\cdot a}{3}$ | - | Cubic | I | 101/110/011 |
| 6 | $a\cdot a\ a\cdot a\ a\cdot a$ | $\frac{-a\cdot a+\lvert a\cdot b\rvert}{2}$ | $\frac{-a\cdot a+\lvert a\cdot b\rvert}{2}$ | $-\lvert a\cdot b\rvert$ | - | Tetragonal | I | 011/101/110 |
| 7 | $a\cdot a\ a\cdot a\ a\cdot a$ | $-\lvert b\cdot c\rvert$ | $\frac{-a\cdot a+\lvert b\cdot c\rvert}{2}$ | $\frac{-a\cdot a+\lvert b\cdot c\rvert}{2}$ | - | Tetragonal | I | 101/110/011 |
| 8 | $a\cdot a\ a\cdot a\ a\cdot a$ | $-\lvert b\cdot c\rvert$ | $-\lvert a\cdot c\rvert$ | $-(\lvert a\cdot a\rvert-\lvert b\cdot c\rvert-\lvert a\cdot c\rvert)$ | - | Orthorhombic | I | $\bar{1}\bar{1}0/\bar{1}0\bar{1}/0\bar{1}\bar{1}$ |
| a = b | | | | | | | | |
| 9 | $a\cdot a\ a\cdot a\ c\cdot c$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | + | Rhombohedral | hR | $100/\bar{1}10/\bar{1}\bar{1}3$ |
| 10 | $a\cdot a\ a\cdot a\ c\cdot c$ | $b\cdot c$ | $b\cdot c$ | $a\cdot b$ | + | Monoclinic | C** | $110/1\bar{1}0/00\bar{1}$ |
| 11 | $a\cdot a\ a\cdot a\ c\cdot c$ | 0 | 0 | 0 | - | Tetragonal | P | 100/010/001 |
| 12 | $a\cdot a\ a\cdot a\ c\cdot c$ | 0 | 0 | $-\frac{a\cdot a}{2}$ | - | Hexagonal | P | 100/010/001 |
| 13 | $a\cdot a\ a\cdot a\ c\cdot c$ | 0 | 0 | $-\lvert a\cdot b\rvert$ | - | Orthorhombic | C | $110/\bar{1}10/001$ |
| 14 | $a\cdot a\ a\cdot a\ c\cdot c$ | $-\lvert b\cdot c\rvert$ | $-\lvert b\cdot c\rvert$ | $-\lvert a\cdot b\rvert$ | - | Monoclinic | C** | $110/\bar{1}10/001$ |
| 15 | $a\cdot a\ a\cdot a\ c\cdot c$ | $-\frac{a\cdot a}{2}$ | $-\frac{a\cdot a}{2}$ | 0 | - | Tetragonal | I | 100/010/112 |
| 16 | $a\cdot a\ a\cdot a\ c\cdot c$ | $-\lvert b\cdot c\rvert$ | $-\lvert b\cdot c\rvert$ | $-(a\cdot a-2\lvert b\cdot c\rvert)$ | - | Orthorhombic | F | $\bar{1}\bar{1}0/1\bar{1}0/112$ |
| 17 | $a\cdot a\ a\cdot a\ c\cdot c$ | $-\lvert b\cdot c\rvert$ | $-\lvert a\cdot c\rvert$ | $-(a\cdot a-\lvert b\cdot c\rvert-\lvert a\cdot c\rvert)$ | - | Monoclinic | I†† | $\bar{1}0\bar{1}/\bar{1}\bar{1}0/011$ |
| b = c | | | | | | | | |
| 18 | $a\cdot a\ b\cdot b\ b\cdot b$ | $\frac{a\cdot a}{4}$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | + | Tetragonal | I | $0\bar{1}1/1\bar{1}\bar{1}/100$ |
| 19 | $a\cdot a\ b\cdot b\ b\cdot b$ | $b\cdot c$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | + | Orthorhombic | I | $\bar{1}00/0\bar{1}1/\bar{1}11$ |
| 20 | $a\cdot a\ b\cdot b\ b\cdot b$ | $b\cdot c$ | $a\cdot c$ | $a\cdot c$ | + | Monoclinic | C† | $011/01\bar{1}/\bar{1}00$ |
| 21 | $a\cdot a\ b\cdot b\ b\cdot b$ | 0 | 0 | 0 | - | Tetragonal | P | 010/001/100 |
| 22 | $a\cdot a\ b\cdot b\ b\cdot b$ | $-\frac{b\cdot b}{2}$ | 0 | 0 | - | Hexagonal | P | 010/001/100 |
| 23 | $a\cdot a\ b\cdot b\ b\cdot b$ | $-\lvert b\cdot c\rvert$ | 0 | 0 | - | Orthorhombic | C | $011/0\bar{1}1/100$ |
| 24 | $a\cdot a\ b\cdot b\ b\cdot b$ | $-\frac{b\cdot b-\frac{a\cdot a}{3}}{2}$ | $-\frac{a\cdot a}{3}$ | $-\frac{a\cdot a}{3}$ | - | Rhombohedral | hR | $121/0\bar{1}1/100$ |
| 25 | $a\cdot a\ b\cdot b\ b\cdot b$ | $-\lvert b\cdot c\rvert$ | $-\lvert a\cdot c\rvert$ | $-\lvert a\cdot c\rvert$ | - | Monoclinic | C† | $011/0\bar{1}1/100$ |

Table 2. (continued)

| Reduced Form No. | Reduced Form Matrix | | | | Reduced Form Type | Bravais Lattice | | Cell Transformation Reduced → Conventional |
|---|---|---|---|---|---|---|---|---|
| | First Row††† | Second Row | | | | | | |
| | a·a b·b c·c | b·c | a·c | a·b | | | | |
| a≤b≤c 26 | a·a b·b c·c | $\frac{a\cdot a}{4}$ | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | + | Orthorhombic | F | 100/$\bar{1}$20/$\bar{1}$02 |
| 27 | a·a b·b c·c | b·c | $\frac{a\cdot a}{2}$ | $\frac{a\cdot a}{2}$ | + | Monoclinic | I*** | 0$\bar{1}$1/$\bar{1}$00/1$\bar{1}\bar{1}$ |
| 28 | a·a b·b c·c | $\frac{a\cdot b}{2}$ | $\frac{a\cdot a}{2}$ | a·b | + | Monoclinic | C | $\bar{1}$00/$\bar{1}$02/010 |
| 29 | a·a b·b c·c | $\frac{a\cdot c}{2}$ | a·c | $\frac{a\cdot a}{2}$ | + | Monoclinic | C | 100/1$\bar{2}$0/00$\bar{1}$ |
| 30 | a·a b·b c·c | $\frac{b\cdot b}{2}$ | $\frac{a\cdot b}{2}$ | a·b | + | Monoclinic | C | 010/01$\bar{2}$/$\bar{1}$00 |
| 31 | a·a b·b c·c | b·c | a·c | a·b | + | Triclinic | P | 100/010/001 |
| 32 | a·a b·b c·c | 0 | 0 | 0 | - | Orthorhombic | P | 100/010/001 |
| 33 | a·a b·b c·c | 0 | -\|a·c\| | 0 | - | Monoclinic | P | 100/010/001 |
| 34 | a·a b·b c·c | 0 | 0 | -\|a·b\| | - | Monoclinic | P | $\bar{1}$00/00$\bar{1}$/0$\bar{1}$0 |
| 35 | a·a b·b c·c | -\|b·c\| | 0 | 0 | - | Monoclinic | P | 0$\bar{1}$0/$\bar{1}$00/00$\bar{1}$ |
| 36 | a·a b·b c·c | 0 | $-\frac{a\cdot a}{2}$ | 0 | - | Orthorhombic | C | 100/$\bar{1}$0$\bar{2}$/010 |
| 37 | a·a b·b c·c | -\|b·c\| | $-\frac{a\cdot a}{2}$ | 0 | - | Monoclinic | C* | 102/100/010 |
| 38 | a·a b·b c·c | 0 | 0 | $-\frac{a\cdot a}{2}$ | - | Orthorhombic | C | $\bar{1}$00/120/00$\bar{1}$ |
| 39 | a·a b·b c·c | -\|b·c\| | 0 | $-\frac{a\cdot a}{2}$ | - | Monoclinic | C** | $\bar{1}\bar{2}$0/$\bar{1}$00/00$\bar{1}$ |
| 40 | a·a b·b c·c | $-\frac{b\cdot b}{2}$ | 0 | 0 | - | Orthorhombic | C | 0$\bar{1}$0/012/$\bar{1}$00 |
| 41 | a·a b·b c·c | $-\frac{b\cdot b}{2}$ | -\|a·c\| | 0 | - | Monoclinic | C† | 0$\bar{1}\bar{2}$/0$\bar{1}$0/$\bar{1}$00 |
| 42 | a·a b·b c·c | $-\frac{b\cdot b}{2}$ | $-\frac{a\cdot a}{2}$ | 0 | - | Orthorhombic | I | $\bar{1}$00/0$\bar{1}$0/112 |
| 43 | a·a b·b c·c | $-\frac{b\cdot b-\lvert a\cdot b\rvert}{2}$ | $-\frac{a\cdot a-\lvert a\cdot b\rvert}{2}$ | -\|a·b\| | - | Monoclinic | I | $\bar{1}$00/$\bar{1}\bar{1}\bar{2}$/0$\bar{1}$0 |
| 44 | a·a b·b c·c | -\|b·c\| | -\|a·c\| | -\|a·b\| | - | Triclinic | P | 100/010/001 |

† If $a\cdot a < 4|a\cdot c|$
* If $b\cdot b < 4|b\cdot c|$
** If $c\cdot c < 4|b\cdot c|$
} Premultiply Table Matrix by 00$\bar{1}$/010/101 (I centered)

†† If $3a\cdot a < c\cdot c + 2|a\cdot c|$
*** If $3b\cdot b < c\cdot c + 2|b\cdot c|$
} Premultiply Table Matrix by $\bar{1}$0$\bar{1}$/010/100 (C centered)

††† No required relationships between symmetrical scalars for reduced forms 26-44.

* Reprinted from Reference 6. Based on Table 5.1.3.1 prepared by A. Mighell, A. Santoro, and J. D. H. Donnay for the International Tables for X-ray Crystallography[5] and published revisions.[15,16]

Table 3. Unique $\underset{\sim}{Q}$ Matrices Generating Superlattices for $|\underset{\sim}{Q}| = 2, 3, 4$*

| $\lvert\underset{\sim}{Q}\rvert = 2$ | $\lvert\underset{\sim}{Q}\rvert = 4$ | $\lvert\underset{\sim}{Q}\rvert = 4$ |
|---|---|---|
| 100/010/002 | 100/010/004 | 111/020/002 |
| 100/011/002 | 100/011/004 | 111/021/002 |
| 101/010/002 | 100/012/004 | 100/040/001 |
| 101/011/002 | 100/013/004 | 110/040/001 |
| 100/020/001 | 101/010/004 | 120/040/001 |
| 110/020/001 | 101/011/004 | 130/040/001 |
| 200/010/001 | 101/012/004 | 200/010/002 |
| | 101/013/004 | 200/011/002 |
| $\lvert\underset{\sim}{Q}\rvert = 3$ | 102/010/004 | 201/010/002 |
| 100/010/003 | 102/011/004 | 201/011/002 |
| 100/011/003 | 102/012/004 | 200/020/001 |
| 100/012/003 | 102/013/004 | 210/020/001 |
| 101/010/003 | 103/010/004 | 400/010/001 |
| 101/011/003 | 103/011/004 | |
| 101/012/003 | 103/012/004 | |
| 102/010/003 | 103/013/004 | |
| 102/011/003 | 100/020/002 | |
| 102/012/003 | 100/021/002 | |
| 100/030/001 | 101/020/002 | |
| 110/030/001 | 101/021/002 | |
| 120/030/001 | 110/020/002 | |
| 300/010/001 | 110/021/002 | |

*For each value of $|\underset{\sim}{Q}|$ the matrices can be applied to any primitive cell of the original lattice, but they must be applied to the same cell.

## APPENDIX C

## EXAMPLES OF INPUT DECKS AND OUTPUT LISTINGS

### Example 1. Cell analysis for two data sets

**Input deck:**

```
1          0                                   0                          1
2       12.83      9.026    13.44               123.0                                TEST01M1
3         .02       .009      .05                  .5                                      2
4       CC                          4     1.46                                           3
5       Sodium carbonate decahydrate                                                     6
6       NA2 C 03 !10 H2 O                                                                7
7       Example of cell analysis and density calculation                                 8
8                                                                                        K
9       8.095     8.096     30.62     88.67    58.08    87.48                          TEST02A1
10      P                                                                                3
11      Example of symmetry determination                                                8
12                                                                                       K
```

**Output listing:**

```
                          ***  MONOCLINIC *****  TEST01 ***
     1     1     1     2     1     3     1     4     1     5     1     6     1     7
12.83      9.026    13.44               123.0                                        CELL
  .02       .009      .05                  .5                209  C-                 ESDS
Cc              9A          4      1.460                                1305.31      SG-1
Cc              9A          4                 1.456          286.14     1305.31      SG-2
Sodium carbonate decahydrate                                                         NAME
Na2 C 03 !10 H2 O                                                                    CHEM
C H20 Na2 C13                                                                        EMPR
Example of cell analysis and density calculation                                     COMM
T-2       .50    .50    .00 / -.50    .50    .00 /  .50   -.50  1.00               MATX
1.00:  1.00    .00    .00 /  .00 -1.00    .00 /-1.00    .00 -1.00                  MATX
INV     1.00    .00    .00 /  .00 -1.00    .00 /-1.00    .00 -1.00                  MATX
  12.830    9.026  13.440  90.00 123.00  90.00  1305.31                            C-IN
   7.843    7.843  12.175  98.77 105.91 109.75   652.65              17            C-RD
  12.830    9.026  12.546  90.00 116.05  90.00    1.4214  1.3900                   C-CD
    .020     .009    .104    .00    .35    .00                                     E-CD
  61.519   61.519 148.238 -14.562 -26.172 -20.785                                   DOTM
                         01/12/81   0   0 45 16/12/80                              HIST
```

```
                          ***   ANORTHIC  *****  TEST02 ***
**WARNING**AI,BI AND/OR CI > 30A
**WARNING**METRIC SYMMETRY EXCEEDS CRYSTAL SYMMETRY
     CRYSTAL DATA BRAVAIS LATTICE = AP  BRAVAIS LATTICE FROM REDUCED CELL=OB
     OB CELL PARAMETERS:  11.698  25.990  11.194   90.00   90.01   90.00
      MATRIX (INITIAL TO OB):,-1.0-1.0  .0/-2.0  .0 1.0/-1.0 1.0  .0
     1     1     1     2     1     3     1     4     1     5     1     6     1     7
8.095     8.096    30.62    88.67   58.08   87.48                                  CELL
                                                 95E C                           ESDS
P               0                                                1701.65          SG-1
P               0                                                1701.65          SG-2
Example of symmetry determination                                                COMM
T-2       .00  1.00    .00 /-1.00    .00    .00 /-2.00    .00  1.00               MATX
1.00: -1.00    .00    .00 /-2.00    .00  1.00 /  .00  1.00    .00                MATX
INV    -1.00    .00    .00 /  .00    .00  1.00 /-2.00  1.00    .00                MATX
   8.095    8.096  30.620  88.67  58.08  87.48  1701.65                           C-IN
   8.096    8.095  25.990  90.00  90.00  92.52  1701.65             13X           C-RD
   8.095   25.990   8.096  90.00  92.52  90.00     .3115   .3115                  C-CD
  65.545   65.529 675.473    .001   -.009  -2.982                                 DOTM
                         01/12/81   2   0 45 16/12/80                             HIST
```

## Example 2. Generation of d-spacings and hkl indices

### Input deck:

```
1          2                                   0              40     1
2       12.214                                                                TEST03C1
3       PA3                          4              1.670                             3
4       SODIUM ALUMINUM SULFATE HYDRATE (SODA ALUM)                            6
5       NA AL ( S O4 )2 t12 H2 O                                               7
6       Example of hkl/d-generation                                            8
7             1.540598                                                         F
8                                                                              K
```

### Output listing:

```
                                ***     CUBIC     *****  TEST03 ***
     1     1     1     2     1     3     1     4     1     5     1     6     1     7
 12.214                                                                              CELL
                                                                  40E B-                ESDS
 Pa3          205           4                1.670                      1822.11       SG-1
 Pa3          205           4                1.671           458.27     1822.11       SG-2
 SODIUM ALUMINUM SULFATE HYDRATE (SODA ALUM)                                         NAME
 Na Al ( S O4 )2 t12 H2 O                                                            CHEM
 Al H24 Na O20 S2                                                                    EMPR
 Example of hkl/d-generation                                                         COMM
 T-2     1.00    .00    .00 /  .00   1.00    .00 /  .00    .00   1.00               MATX
 1.00:   1.00    .00    .00 /  .00   1.00    .00 /  .00    .00   1.00               MATX
   12.214  12.214  12.214  90.00  90.00  90.00  1822.11                             C-1N
   12.214  12.214  12.214  90.00  90.00  90.00  1822.11              3              C-RD
   12.214  12.214  12.214  90.00  90.00  90.00  12.2140                             C-CD
  149.182 149.182 149.182    .000    .000    .000                                   DOTM
       1.540598                                                                    PDF1
                          01/12/81  0  0 45 16/12/80                               H1ST

**MESSAGE**POWDER PATTERN GENERATION/ANALYSIS FOR SYSTEM CUB

          2-THETA(MAX)= 40.00     D(MIN)= 2.252212

           3 CONDITIONS FOR NON-EXTINCTION CALLED FOR
                     CLASS CONDITION(S)
                     CKL      K   =2N
                     HOL      L   =2N
                     HKO      H   =2N

                                  <AUTHORS>      <PROGRAM>       OBS      CALC     DIFF
  N    D CALC    D OBS    INT    H   K   L    H   K   L    2-THETA  2-THETA  2-THETA
  1    7.0518                                 1   1   1             12.542
  2    6.1070                                 0   2   0             14.492
  3    5.4623                                 2   1   0             16.214
  4    4.9863                                 1   2   1             17.773
  5    4.3183                                 2   2   0             20.551
  6    4.0713                                 2   2   1             21.812
  7    3.6827                                 1   3   1             24.147
  8    3.5259                                 2   2   2             25.238
  9    3.3876                                 2   3   0             26.287
 10    3.2643                                 2   3   1             27.298
 11    3.0535                                 0   4   0             29.223
 12    2.9623                                 2   3   2             30.144
 13    2.8789                                 1   4   1             31.039
 14    2.8021                                 3   3   1             31.912
 15    2.7311                                 2   4   0             32.764
 16    2.6653                                 2   4   1             33.597
 17    2.6040                                 3   3   2             34.412
 18    2.4932                                 2   4   2             35.994
 19    2.4428                                 4   3   0             36.762
 20    2.3954                                 3   4   1             37.517
 21    2.3506                                 1   5   1             38.259
 22    2.2681                                 2   5   0             39.708
```

## Example 3. Powder pattern analysis with calculation of figures of merit

### Input deck:

```
1          0                                        1                    1
2       8.8659              5.0433                                                TEST04H1
3        .0006               .0005                                                       2
4       P321                     3              2.729                                   3
5       Sodium Silicon Fluoride                                                         6
6       NA2 SI F6                                                                       7
7       Example of powder pattern analysis including calc of figures of merit          B
8            1.540598                    2                                          F
9       17.58   13   0  0  1   20.03  100   1  1  0   21.07   95   1  0  1   1      I
10      26.74   90   1  1  1   29.20   50   2  0  1   30.79    9   2  1  0   2      I
11      35.05    5   3  0  0   35.58    7   0  0  2   35.66   15   2  1  1   3      I
12      37.54    1   1  0  2   39.47   90   3  0  1   40.68    6   2  2  0   4      I
13      41.16    4   1  1  2   42.42    3   3  1  0   42.88    4   2  0  2   5      I
14      44.61    9   2  2  1   46.22    6   3  1  1   47.72   10   2  1  2   6      I
15      50.79   55   3  0  2   51.86    4   3  2  0   54.56    2   0  0  3   7      I
16      55.19   20   3  2  1   55.96    4   1  0  3   56.52    9   3  1  2   8      I
17      57.94   20   4  1  1   58.69    4   1  1  3   60.01    3   2  0  3   9      I
18      60.60    3   4  0  2   62.84   11   3  3  0   63.23    5   5  0  1  10      I
19      63.94    8   2  1  3   64.11    8   4  2  0   66.50    3   3  0  3  11      I
20      67.03    8   4  1  2   67.03    8   4  2  1                               I
21                                                                                  K
```

### Output listing:

```
                          ***  HEXAGONAL  *****  TEST04 ***
    1    1    1    2    1    3    1    4    1    5    1    6    1    7
 8.8659              5.0433                                                  CELL
  .0006               .0005                                        7  B       ESDS
 P321        150          3              2.729                          343.31  SG-1
 P321        150          3              2.729          188.06          343.31  SG-2
 Sodium Silicon Fluoride                                                     NAME
 Na2 Si F6                                                                   CHEM
 F6 Na2 Si                                                                   EMPR
 Example of powder pattern analysis including calc of figures of merit       COMM
 T-2      .00    .00   1.00 / 1.00    .00    .00 /  .00   1.00    .00        MATX
 1.00:  1.00    .00    .00 /  .00   1.00    .00 /  .00    .00   1.00        MATX
    8.866   8.866   5.043  90.00  90.00 120.00   343.31                      C-IN
    5.043   8.866   8.866 120.00  90.00  90.00   343.31            22        C-RD
    8.866   8.866   5.043  90.00  90.00 120.00    .5688                     C-CD
     .001    .001    .000    .00    .00    .00                               E-CD
  25.435  78.604  78.604 -39.302    .000    .000                             DGTM
       1.540598                2                                          PDF1
                          01/12/81  0  0 45 16/12/80                        HIST

**MESSAGE**POWDER PATTERN GENERATION/ANALYSIS FOR SYSTEM HEX

          2-THETA(MAX)= 68.03     D(MIN)= 1.376990

           0 CONDITIONS FOR NON-EXTINCTION CALLED FOR
                   CLASS CONDITION(S)

                                    <AUTHORS>     <PROGRAM>      OBS      CALC     DIFF
   N   D CALC   D OBS    INT      H   K   L     H   K   L   2-THETA   2-THETA  2-THETA
   1   7.6761                                   1   0   0              11.516
   2   5.0433                                   0   0   1              17.571
***    5.0433   5.0408   13       0   0   1                  17.580   17.571   -.009
   3   4.4329                                   1   1   0              20.014
***    4.4329   4.4294  100       1   1   0                  20.030   20.014   -.016
   4   4.2153                                   1   0   1              21.059
***    4.2153   4.2131   95       1   0   1                  21.070   21.059   -.011
   5   3.8390                                   2   0   0              23.150
   6   3.3296                                   1   1   1              26.753
***    3.3296   3.3312   90       1   1   1                  26.740   26.753    .013
   7   3.0547                                   2   0   1              29.212
***    3.0547   3.0559   50       2   0   1                  29.200   29.212    .012
   8   2.9020                                   2   1   0              30.785
***    2.9020   2.9016    9       2   1   0                  30.790   30.785   -.005
```

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 2.5594 | | | | | | 3 | 0 | 0 | | 35.032 | |
| *** | 2.5594 | 2.5581 | 5 | 3 | 0 | 0 | | | | 35.050 | 35.032 | -.018 |
| 10 | 2.5216 | | | | | | 0 | 0 | 2 | | 35.573 | |
| *** | 2.5216 | 2.5212 | 7 | 0 | 0 | 2 | | | | 35.580 | 35.573 | -.007 |
| 11 | 2.5153 | | | | | | 2 | 1 | 1 | | 35.666 | |
| *** | 2.5153 | 2.5157 | 15 | 2 | 1 | 1 | | | | 35.660 | 35.666 | .006 |
| 12 | 2.3958 | | | | | | 1 | 0 | 2 | | 37.511 | |
| *** | 2.3958 | 2.3939 | 1 | 1 | 0 | 2 | | | | 37.540 | 37.511 | -.029 |
| 13 | 2.2823 | | | | | | 3 | 0 | 1 | | 39.451 | |
| *** | 2.2823 | 2.2812 | 90 | 3 | 0 | 1 | | | | 39.470 | 39.451 | -.019 |
| 14 | 2.2165 | | | | | | 2 | 2 | 0 | | 40.673 | |
| *** | 2.2165 | 2.2161 | 6 | 2 | 2 | 0 | | | | 40.680 | 40.673 | -.007 |
| 15 | 2.1918 | | | | | | 1 | 1 | 2 | | 41.151 | |
| *** | 2.1918 | 2.1914 | 4 | 1 | 1 | 2 | | | | 41.160 | 41.151 | -.009 |
| . | | | | | | | | | | | | |
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| . | | | | | | | | | | | | |
| 32 | 1.5719 | | | | | | 1 | 1 | 3 | | 58.688 | |
| *** | 1.5719 | 1.5718 | 4 | 1 | 1 | 3 | | | | 58.690 | 58.688 | -.002 |
| 33 | 1.5399 | | | | | | 2 | 0 | 3 | | 60.029 | |
| *** | 1.5399 | 1.5404 | 3 | 2 | 0 | 3 | | | | 60.010 | 60.029 | .019 |
| 34 | 1.5356 | | | | | | 5 | 0 | 0 | | 60.215 | |
| 35 | 1.5274 | | | | | | 4 | 0 | 2 | | 60.574 | |
| *** | 1.5274 | 1.5268 | 3 | 4 | 0 | 2 | | | | 60.600 | 60.574 | -.026 |
| 36 | 1.4777 | | | | | | 3 | 3 | 0 | | 62.839 | |
| *** | 1.4777 | 1.4776 | 11 | 3 | 3 | 0 | | | | 62.840 | 62.839 | -.001 |
| 37 | 1.4690 | | | | | | 5 | 0 | 1 | | 63.250 | |
| *** | 1.4690 | 1.4695 | 5 | 5 | 0 | 1 | | | | 63.230 | 63.250 | .020 |
| 38 | 1.4547 | | | | | | 2 | 1 | 3 | | 63.949 | |
| *** | 1.4547 | 1.4548 | 8 | 2 | 1 | 3 | | | | 63.940 | 63.949 | .009 |
| 39 | 1.4510 | | | | | | 4 | 2 | 0 | | 64.128 | |
| *** | 1.4510 | 1.4514 | 8 | 4 | 2 | 0 | | | | 64.110 | 64.128 | .018 |
| 40 | 1.4440 | | | | | | 3 | 2 | 2 | | 64.475 | |
| 41 | 1.4180 | | | | | | 3 | 3 | 1 | | 65.806 | |
| 42 | 1.4051 | | | | | | 3 | 0 | 3 | | 66.490 | |
| *** | 1.4051 | 1.4049 | 3 | 3 | 0 | 3 | | | | 66.500 | 66.490 | -.010 |
| 43 | 1.3955 | | | | | | 4 | 1 | 2 | | 67.005 | |
| *** | 1.3955 | 1.3951 | 8 | 4 | 1 | 2 | | | | 67.030 | 67.005 | -.025 |
| *** | 1.3945 | 1.3951 | 8 | 4 | 2 | 1 | | | | 67.030 | 67.064 | .034 |
| 44 | 1.3945 | | | | | | 4 | 2 | 1 | | 67.064 | |
| 45 | 1.3790 | | | | | | 5 | 1 | 0 | | 67.916 | |

REFLECTION SUMMARY FOR ENTIRE PATTERN:
ESTIMATED RESOLUTION= .075 DEG. 2-THETA

THEORTICAL LINES TOTAL= 45
THEORETICAL RESOLVABLE= 42
UNIQUE OBSERVED LINES= 34

TOTAL LINES INPUT= 35
NUMBER INDEXED= 35
NUMBER UNINDEXED= 0

********FOR INDEXED LINES********

AVERAGE ABS(DEL 2-THETA)= .013
LARGEST 2-THETA DIFFERENCE= .034
# WITH DIFF>0.05 (STAR LIMIT)= 0
# WITH DIFF>0.20 (I LIMIT)= 0

AVERAGE 2-THETA DIFFERENCE= -.001
# WITH DIFF > +0.02(2-THETA)= 3
# WITH DIFF < -0.02(2-THETA)= 3

M(20) = 67.17 (DLIMIT = 1.7584, # POSSIBLE = 24)

F(30) = 70.27 (DELTA 2 THETA = .0115, # POSSIBLE = 37)

NBS-114A (REV. 2-8C)

| U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions) | 1. PUBLICATION OR REPORT NO. NBS Tech. Note 1141 | 2. Performing Organ. Report No. | 3. Publication Date April 1981 |
|---|---|---|---|

4. TITLE AND SUBTITLE

NBS*AIDS80: A FORTRAN Program for Crystallographic Data Evaluation

5. AUTHOR(S)

A.D. Mighell, C.R. Hubbard, and J.K. Stalick

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

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8. Type of Report & Period Covered

Final

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

Same as No. 6

10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

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Techniques for the computer-assisted evaluation of crystallographic data have been developed to improve the data compilations of the NBS Crystal Data Center and the JCPDS--International Centre for Diffraction Data. The resulting computer program, NBS*AIDS80, can be used for the analysis of unit-cell and powder diffraction data by the general scientific community as well. Research and analysis components include calculation of standard cells and space groups, determination of metric symmetry, checking the data for consistency, generation of d-spacings and indices, and analysis of powder patterns with calculation of figures of merit. Detailed input and output specifications are given.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

Computer evaluation; crystallographic data analysis; JCPDS--International Centre for Diffraction Data; metric symmetry; NBS Crystal Data Center; powder diffraction; unit cell.

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