

CANTFOUR
CANTERBURY FOURIER

CANTFOUR was written by R. J. Dellaca and W. T. Robinson of the University of Canterbury, New Zealand, and further modified by D. J. Hodgson at UMC. The basic logic is based on A. Zalkin's program FORDAP. CANTFOUR accepts observed and calculated structure factor amplitudes (ANVLSFOUR.DAT) and performs Fourier syntheses; output includes files containing Fourier peaks and the sectioned Fourier map for further use.

The program in its present form was modified by F. Rotella for the IPNS VAX where it is called TOFOUR. The format of the peak file was changed on the CHM VAX for compatibility with the program DIST.

COMMAND FILE (Name: CANTFOUR.COM)

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$ RENAME [directory]CANTFOUR.LOG [directory.subdirectory]CANTFOUR.LOG
$ SET DEF [directory.subdirectory]
$ ASSIGN POSITION.DAT FOR002
$ ASSIGN CANTFOUR.INP FOR005
$ ASSIGN ANVLSFOUR.DAT FOR012
$ ASSIGN CANTFOUR.FMP FOR013
$ RUN [NEUTRON.ANVLS]CANTFOUR
```

NOTES

- (1) POSITION.DAT is an output file containing Fourier peaks; it can be used with the program DIST to calculate distances between peaks or between atoms and peaks (see last page of this manual). If creation of this file is not desired (see LINE 2 below), omit this ASSIGN statement.
- (2) CANTFOUR.INP is an input file of operating parameters for use in CANTFOUR, created by the user and currently in the user's directory. For an explanation of the contents of CANTFOUR.INP, see INPUT DATA below.
- (3) ANVLSFOUR.DAT is the input file (FOURIER FILE) of observed and calculated F's created by ANVLS and currently in the user's

directory.

- (4) CANTFOUR.FMP is the output file containing the sectioned Fourier map suitable for use in contour plotting; it is written into the user's directory. If creation of CANTFOUR.FMP is not desired (see LINE 2 of input), omit this ASSIGN statement.

EXECUTION COMMAND

SUBMIT/NOPRINT/NOTIFY CANTFOUR

INPUT DATA

LINE 1 TITLE - Format(20A4)

A title of up to 80 Hollerith characters which will appear as a heading for the printed output.

LINE 2 PROGRAM CONTROL - Format(8I1,I2,F5.0,E15.6)

col. 1 ICALC: =0, no Fourier summation to be carried out, i.e., program will function on a map calculated previously and found on FOR013.
=1, new Fourier map to be calculated.

col. 2 ITRANS: =0, normal option; sections of the map will be calculated (or were calculated) along an axis parallel to one of the unit cell axes.
=1, sections will be calculated (or were calculated) parallel to a general plane and the U-matrix is supplied (see OPTIONAL LINE 5 below).
=2, sections will be calculated (or were calculated) parallel to a general plane and the equation of the plane is supplied (see OPTIONAL LINES 6 and 7 below).

col. 3 IPRINT: =0, no numeric printout of the Fourier map.
=1, numeric printout with single-spaced lines.
=2, numeric printout with double-spaced lines.
=3, numeric printout with triple-spaced lines.

col. 4 IPLOT: =0, no alphameric plot of the Fourier map.
=1, alphameric plot is desired (see

OPTIONAL LINE 12 below).
=2, contoured map is desired (see
CONTOURING PROGRAM information -
DOCUMENTATION NOT CURRENTLY (10/83)
AVAILABLE).

col. 5 ISEARCH: =0, no peak search to be carried out.
=1, search Fourier map for peaks (see
OPTIONAL LINE 11 below).

col. 6 ITFLS: =0, take no action.
=1, input on FOR012 was created previously
by TOFLS.

col. 9-10 NEQUIV: leave 0 or blank if ITFLS = 1.
The number of symmetry transformations to
be input (see OPTIONAL LINES 4 below).

col. 11-15 SCALE: usually 1.0.
It may be otherwise used to scale the
height of peak in the map if the input
data are not on an absolute scale (e.g.,
C-centered cell, SCALE = 2.0) or if the
input data is doubled (e.g., a data set
containing Friedel pairs, SCALE = 0.5).

col. 16-30 RMAX: usually 0.0E0 or blank.
If ICALC = 0 and printing or plotting is
being carried out, entry here of the
maximum value in the map will save a
search throughout the data set on FOR013;
alternatively, entry of a different value
here will change the normalized scale so
that the maximum value will no longer be
999.
NOTE THE E-format!

OPTIONAL LINE 3 REAL UNIT CELL CONSTANTS - Format(6F10.6)

Omit if ITFLS = 1 (see LINE 2 above).

col. 1-10 A: a-axis length in Angstroms.

col. 11-20 B: b-axis length in Angstroms.

col. 21-30 C: c-axis length in Angstroms.

col. 31-40 ALPHA: interaxial angle alpha in degrees,
or COSA: cosine of interaxial angle alpha.

col. 41-50 BETA: interaxial angle beta in degrees,
or COSB: cosine of interaxial angle beta.

col. 51-60 GAMMA: interaxial angle gamma in degrees,
or COSG: cosine of interaxial angle gamma.

OPTIONAL LINE 4 SYMMETRY TRANSFORMATIONS - Format(3(F15.10,3I3))

Omit is ITFLS = 1 (see LINE 2 above).

Include one line for each of the NEQUIV positions (see LINE 2 above). These should include all of the equivalent positions in the space group excluding those related by a center of symmetry at the origin or by a unit cell centering condition. Transformed coordinates (x',y',z') may be obtained from input coordinates (x,y,z) through the following parametric equations:

$$\begin{aligned}x' &= T1 + S11*x + S12*y + S13*z \\y' &= T2 + S21*x + S22*y + S23*z \\z' &= T3 + S31*x + S32*y + S33*z\end{aligned}$$

col. 1-15 T1

col. 16-18 S11

col. 19-21 S12

col. 22-24 S13

col. 25-39 T2

col. 40-42 S21

col. 43-45 S22

col. 46-48	S23
col. 49-63	T3
col. 64-66	S31
col. 67-69	S32
col. 70-72	S33

OPTIONAL LINE 5 U-MATRIX ELEMENTS - Format(F8.4)

Present only if ITRANS = 1 (see LINE 2 above).

The elements of the U-matrix (see NOTES ON GENERAL PLANES below):

col. 1- 8	U11
col. 9-16	U12
col. 17-24	U13
col. 25-32	U21
col. 33-40	U22
col. 41-48	U23
col. 49-56	U31
col. 57-64	U32
col. 65-72	U33

OPTIONAL LINE 6 GENERAL PLANE EQUATION - Format(7F10.5)

Present only if ITRANS = 2 (see LINE 2 above).

General plane equation and orthogonalized unit cell constants
(see NOTES ON GENERAL PLANES below):

col. 1-10	P1
col. 11-20	P2
col. 21-30	P3
col. 31-40	D
col. 41-50	CELL(1)
col. 51-60	CELL(2)
col. 61-70	CELL(3)

OPTIONAL LINE 7 TRANSFORMED MAP LIMITS AND RESOLUTION -
Format(9F8.5)

Present only if ITRANS = 2 (see LINE 2 above).

Limits over which the calculation is to be performed for the
transformed map and the resolution along each of the output axes
(in Angstroms) (see NOTES ON GENERAL PLANES below):

col. 1- 8	XMIN: limits along
col. 9-16	XMAX: x-axis in Angstroms.
col. 17-24	YMIN: limits along
col. 25-32	YMAX: y-axis in Angstroms.
col. 33-40	ZMIN: limits along
col. 41-48	ZMAX: z-axis in Angstroms.
col. 49-56	DX: intervals between sampling points
col. 57-64	DY: parallel to the x-, y- and
col. 65-72	DZ: z-axes, respectively, in Angstroms.

NOTES ON GENERAL PLANES

Use of this option is normally very time consuming and is not recommended; the program uses a brute force method of calculating the transformed Fourier map.

(a) ITRANS = 1.

The transformation matrix (U) is supplied, where:

$$\begin{array}{rcccl} & \text{(New cell)} & = & U & \text{(Old cell)} \\ \text{i.e.,} & \text{(a')} & & \text{(U11 U12 U13)} & \text{(a)} \\ & \text{(b')} & = & \text{(U21 U22 U23)} & \text{(b)} \\ & \text{(c')} & & \text{(U31 U32 U33)} & \text{(c)} \end{array}$$

(b) ITRANS = 2.

The equation of the general plane is supplied as:

$$P1*X + P2*Y + P3*Z = D$$

where D is the distance in Angstroms of the plane from the origin of the unit cell. P1, P2, P3 and D can be obtained via the FORTRAN program PLANE, available in the crystallographic program library of the Chemistry Division at ANL, or a similar routine to calculate least-squares planes through arbitrary points in a crystallographic unit cell. If the equation is printed by PLANE as:

$$R*X + S*Y + T*Z = D$$

then:

$$\begin{array}{l} P1 = R \\ P2 = R*\text{COS}(\text{gamma}) + S*\text{SIN}(\text{gamma}) \\ P3 = R*\text{COS}(\text{beta}) - S*\text{COS}(\text{alpha})*\text{SIN}(\text{beta}) + \\ \quad T*\text{SIN}(\text{alpha})*\text{SIN}(\text{beta}) \end{array}$$

where alpha, beta and gamma are the interaxial angles within the unit cell. For this option, the new x-axis is set normal to the plane, the new y-axis is set parallel to the plane and to the projection of the original unit cell vector which has the largest component on this plane (i.e., the unit cell axis having a minimum P-value), and the new z-axis completes the orthogonal right-handed system. Thus, NORIEN (see LINE 9 below) is set to 100 by the program. The length of each new axis is set to the maximum of four quantities:

$$\text{ABS}(2.0*X\text{MAX}(I)), \text{ABS}(2.0*X\text{MIN}(I)), 10.0, \text{CELL}(I)$$

in Angstroms. The longer the axis, the greater the accuracy (i.e., unless the elements of the U-matrix are integers, errors will be introduced when the indices are transformed by it). For a section through the plane, set:

$$XMIN = XMAX = ABS(D)$$

The U-matrix is printed out as:

$$NEWA1 = U11*A1 + U12*A2 + U13*A3 + \dots$$

The determinant of the U-matrix is equal to the ratio of the volumes of the transformed and untransformed unit cells.

OPTIONAL LINE 8 FOURIER CONTROL - Format(4I5,F5.2)

Omit if ICALC = 0 (see LINE 2 above).

col. 1- 5	NREF:	usually 10 or 20 is normal. The number of input reflections for which equivalent forms and Fourier coefficients are to be listed; this is useful primarily as a check on the calculation.
col. 6-10	NCODE:	code number to indicate the source of the reflection data and the type of calculation required. =0, input reflection data from OPTIONAL LINES 10, compute a Patterson function. =1, input reflection data based on F's from FOR012, compute a difference Fourier excluding "unobserved" data (Fobs < 0.0). =2, input reflection data based on F's from FOR012, compute a difference Fourier with no rejection based on the value of Fobs. =3, input reflection data based on F's from FOR012, compute a Fourier based on Fobs with phases from Fcalc. =4, input reflection data based on F's

from FOR012, compute a Fourier based on Fcalc.

=5, input reflection data based on F's from FOR012, compute a Patterson based on (Fobs)**2.

=6, input reflection data based on F's from FOR012, compute a Patterson based on (Fcalc)**2.

=7, input reflection data based on F's from FOR012, compute an alpha synthesis, where:

$$A = Fobs * Fcalc * \cos(\alpha)$$

$$B = Fobs * Fcalc * \sin(\alpha)$$

alpha is the phase angle for a reflection.

NOTE

For example, NCODE = 5 indicates a Patterson map with data on FOR012;

NCODE = 1 indicates a difference Fourier map;

NCODE = 3 indicates an observed Fourier map.

Add 100 to NCODE if input is F**2.

col. 11-15 NONTAP: =0, use all input data in the Fourier summation.
 =N, use only the first N reflections in the summation.

col. 16-20 NREC: =0, normal; program provides 1000 data storage blocks for the map.
 =M, the number of data storage blocks required, where:

$$M = (\text{no. of lines}) * (\text{no. of sections}) + 2$$
 (see OPTIONAL LINE 9 below).

col. 21-25 SNLMAX: =0.0, use all input data in the Fourier summation.
 =S, value of $[1/(2*D)]$, where D is the d-spacing of the reflection (see Equation (8) in INTRODUCTION above), above which reflections will be rejected from the summation.

OPTIONAL LINE 9 FOURIER LIMITS AND RESOLUTION - Format(9F5.5,I5)

Omit if ICALC = 0 or if ITRANS = 2 (see LINE 2 above).

col. 1- 5	XMIN:	limits along x-axis
col. 6-10	XMAX:	in fractional coordinates.
col. 11-15	YMIN:	limits along y-axis
col. 16-20	YMAX:	in fractional coordinates.
col. 21-25	ZMIN:	limits along z-axis
col. 26-30	ZMAX:	in fractional coordinates.
col. 31-35	DX:	interval between sampling points
col. 36-40	DY:	parallel to the x-, y- and z-axis,
col. 41-45	DZ:	respectively, in Angstroms.
col. 46-50	NORIEN:	=100, compute sections along x-axis, with z-axis along top of page and y-axis down page. = 10, compute sections along y-axis, with x-axis along top of page and z-axis down page. = 1, compute sections along z-axis, with y-axis along top of page and x-axis down page.

NOTES

- (1) The maximum number of grid points printed across a page of output is 28, and with single-spacing (IPRINT = 1; see LINE 2 above) it is possible to fit 52 grid points down the page. The number of grid points to be considered along the x-axis is calculated by:

$$NGP = [(XMAX - XMIN)*A]/DX$$

where A is the axial length along x in Angstroms; analogous calculations may be carried out for the y- and z-axes.

- (2) The program adjusts the intervals DX, DY and DZ so that there is an integral number of grid points along each axis by using the expression:

$$DX = [(XMAX - XMIN)]/AINT[\{(XMAX - XMIN)*A\}/DX] + 0.5]$$

where A is the length of the x-axis in Angstroms; analogous adjustments are performed on DY and DZ. If a particular number of grid points is required, enter an exact increment for DX, DY and DZ.

- (3) Values for (XMAX - XMIN), etc., greater than 1.0 are not allowed.
- (4) In general, calculation time for a given problem will be minimized when there are a maximum number of sampling points per line and a minimum number of sections (e.g., pages of printed output). Thus, some thought should be given to the selection of limits, since for most space groups there are various ways in which the asymmetric unit can be chosen. By choosing the appropriate orientation, it is always possible to minimize calculation time.
- (5) If the peak interpolation routine (see OPTIONAL LINE 11 below) is to interpolate the position and intensity of peaks on the borders of the map correctly, an exact asymmetric unit must be chosen.

OPTIONAL LINES 10 REFLECTION DATA - Format (3I5,5X,2F10.2)

Present only if NCODE = 0 (see LINE 8 above).

One line for each reflection to be input.

col. 1- 5	J: Miller indices
col. 6-10	K: of the reflection
col. 11-20	L: (h,k,l)
col. 21-30	A: Fourier coefficients for
col. 31-40	B: the reflection (h,k,l)

Terminate LINES 10 with a line with J greater than or equal to 99.

OPTIONAL LINE 11 PEAK SEARCH CONTROL - Format(6I5,F5.0)

Omit if ISEARCH = 0 (see LINE 2 above).

col. 1- 5	NPOS:	maximum number of peaks in the map to be located and listed.
col. 6-10	NNEG:	maximum number of negative troughs in the map to be located and listed.
col. 11-15	NOINT:	maximum number of peaks and troughs in the map to be interpolated to a maximum of 250 (i.e., if non-zero, NOINT usually equals [NPOS + NNEG]); the program will always interpolate peaks first, then make up the difference in troughs.
col. 16-20	NPUNCH:	maximum number of peaks and troughs to be written to FOR002.
col. 21-25	NTRAN:	=0, Primitive or Rhombohedral unit cell. =1, A-centered unit cell. =2, B-centered unit cell. =3, C-centered unit cell. =4, I-centered unit cell. =5, F-centered unit cell.
col. 26-30	ICENT:	=1, centrosymmetric space group. =2, non-centrosymmetric space group.

NOTE

Patterson (Laue) groups are always centrosymmetric.

col. 31-35	RMIN:	=0, usually. If the peak search routine prints messages to the effect that the map contains too many "peaks", a positive value should be entered here; RMIN is the minimum value on the normalized scale for a point to be considered a peak.
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OPTIONAL LINE 12 ALPHAMERIC PLOTTING CONTROL - Format(7I5)

Present if IPLOT = 1 (see LINE 2 above).

Alphameric "plots" are actually output to the line printer; the term "plot" is used here to distinguish these maps from the normal printed output produced when IPRINT is non-zero (see LINE 2 above).

col. 1- 5	NHSP:	number of spaces between alphameric characters horizontally (minimum of 0, maximum of 3).
col. 6-10	NVSP:	=0, single-spaced lines of output. =1, double-spaced lines of output. =2, triple-spaced lines of output.
col. 11-15	NDISP:	=0, orthogonal grid is to be output. =N, each line is displaced N print positions left (N < 0) or right (N > 0) compared with the preceding line (e.g., NHSP = 2 and NVSP = 1 at 6 lines per inch carriage control, the angle between the two axes is approximately 120 degrees for NDISP = -2).
col. 16-20	RHOMIN:	summation answers between RHOMIN and RHOMAX (on the normalized scale) will be plotted as one of 40 alphameric characters; by judicious choice of these values, an appropriate scale can be obtained (e.g., to plot both positive and negative regions of the map, set RHOMAX = 1000 and RHOMIN = -1000; to plot positive regions only, set RHOMAX = 1000 and RHOMIN = 0).
col. 21-25	RHOMAX:	
col. 26-30	IPOS:	=0, summation answers which are greater than RHOMAX on the normalized scale will be plotted as blanks. =1, such grid points will be plotted as "+" characters.
col. 31-35	INEG:	=0, summation answers which are less than RHOMIN on the normalized scale will be

plotted as blanks.
=1, such grid points will be plotted as
"-" characters.

NOTE

As presently written, the plotting routine requires each line of the map to fit across one line printer page; if it will not do so, the input specifications must be changed. With a 132 print-position line printer, the maximum number of answers per line is:

116 for NHSP = 0
58 for NHSP = 1
38 for NHSP = 2
29 for NHSP = 3

A non-zero value for NDISP will further reduce these values.

NOTE ON SUBROUTINE REJECT

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SUBROUTINE REJECT  
COMMON /REJ/ AAA, BBB, COSAA, DEL, FCALC, FOBS, JJ, KK, LL, NREJ, SINAA
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This subroutine can be used to reject or modify reflection data.

The standard version of the program contains a routine in which NREJ equals zero, and all reflections are accepted; to reject a reflection include rejection criteria in the subroutine and for those reflections which are to be rejected under these criteria, set NREJ not equal to zero. JJ, KK and LL are the reflection indices, and AAA and BBB are the Fourier coefficients. For Fourier input from FOR002, COSAA, SINAA, FOBS, FCALC, and DEL are the cosine and sine of the phase angle, Fobs, Fcalc and (Fobs - Fcalc) for the reflection, respectively.