

A The special settings considered in our space-group determination program

The space groups and the settings in each of A – O have the same set of systematic absences. (As a result of basis transformations, unit cells of different centering can have the same set, as in A , B and F .)

Table 1: List of the space groups and settings with specific sets of systematic absences

Space group (No. ^a)	H^b	coordinate						
A (Face-centered lattice)			B (Body-centered lattice)			$P \bar{4} 3 n$ (218)	C_2	$(x, 0, \frac{1}{2})$
$F d d d$ (43)	C_2	$(0, 0, z)$	$I 4_1/a$ (88)	C_i	$(0, \frac{1}{4}, \frac{1}{8})$	$P m \bar{3} n$ (223)	C_2	$(\frac{1}{4}, y, y + \frac{1}{2})$
$F d d d$ (70)	C_2	$(x, 0, 0)$	$I 4_1/a$ (88)	C_i	$(\frac{1}{4}, 0, \frac{1}{8})$	$P m \bar{3} n$ (223)	C_{2v}	$(x, \frac{1}{2}, 0)$
$F d d d$ (70)	D_2	$(0, 0, 0)$	$I 4_1/a m d$ (141)	C_{2h}	$(0, \frac{1}{4}, \frac{1}{8})$	$P m \bar{3} n$ (223)	C_{2v}	$(x, 0, \frac{1}{2})$
$F d d d$ (70)	D_2	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$I 4_1/a m d$ (141)	C_{2h}	$(0, \frac{1}{4}, \frac{1}{8})$	F (Body-centered)		
$F d \bar{3}$ (203)	C_2	$(x, 0, 0)$	C			$I \bar{4} 3 d$ (220)	C_3	(x, x, x)
$F d \bar{3}$ (203)	T	$(0, 0, 0)$	$I 4_1/a m d$ (141)	C_2	$(x, \frac{1}{4}, \frac{1}{8})$	$I a \bar{3} d$ (230)	C_3	(x, x, x)
$F d \bar{3}$ (203)	T	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$I 4_1/a c d$ (142)	C_2	$(\frac{1}{4}, y, \frac{1}{8})$	G		
$F 4_1 3 2$ (210)	C_2	$(x, 0, 0)$	D			$P 4_2 3 2$ (208)	D_2	$(\frac{1}{4}, 0, \frac{1}{2})$
$F 4_1 3 2$ (210)	T	$(0, 0, 0)$	$P 3 1 c$ (159)	C_3	$(\frac{1}{2}, \frac{1}{2}, z)$	$P 4_2 3 2$ (208)	D_2	$(\frac{1}{4}, \frac{1}{2}, 0)$
$F 4_1 3 2$ (210)	T	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P \bar{3} 1 c$ (163)	C_3	$(\frac{1}{2}, \frac{1}{2}, z)$	$P \bar{4} 3 n$ (218)	S_4	$(\frac{1}{4}, 0, \frac{1}{2})$
$F d \bar{3} m$ (227)	C_{2v}	$(x, 0, 0)$	$P \bar{3} 1 c$ (163)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$P \bar{4} 3 n$ (218)	S_4	$(\frac{1}{4}, \frac{1}{2}, 0)$
$F d \bar{3} m$ (227)	T_d	$(0, 0, 0)$	$P \bar{3} 1 c$ (163)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$P m \bar{3} n$ (223)	D_{2d}	$(\frac{1}{4}, 0, \frac{1}{2})$
$F d \bar{3} m$ (227)	T_d	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 6_3$ (173)	C_3	$(\frac{1}{2}, \frac{1}{2}, z)$	$P m \bar{3} n$ (223)	D_{2d}	$(\frac{1}{4}, \frac{1}{2}, 0)$
A (Body-centered lattice)			$P 6_3/m$ (176)	C_3	$(\frac{1}{2}, \frac{1}{2}, z)$	H		
$I 4_1$ (80)	C_2	$(0, 0, z)$	$P 6_3/m$ (176)	C_{3h}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$P 4_3 3 2$ (212)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$I 4_1/a$ (88)	C_2	$(0, 0, z)$	$P 6_3/m$ (176)	C_{3h}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$P 4_3 3 2$ (212)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$I 4_1/a$ (88)	S_4	$(0, 0, 0)$	$P 6_3 2 2$ (182)	C_3	$(\frac{1}{2}, \frac{1}{2}, z)$	$P 4_1 3 2$ (213)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$I 4_1/a$ (88)	S_4	$(0, 0, \frac{1}{2})$	$P 6_3 2 2$ (182)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$P 4_1 3 2$ (213)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$I 4_1 2 2$ (98)	C_2	$(0, 0, z)$	$P 6_3 2 2$ (182)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	I		
$I 4_1 2 2$ (98)	D_2	$(0, 0, 0)$	$P 6_3 m c$ (186)	C_{3v}	$(\frac{1}{2}, \frac{1}{2}, z)$	$I 4_1 3 2$ (214)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$I 4_1 2 2$ (98)	D_2	$(0, 0, \frac{1}{2})$	$P \bar{6} 2 c$ (190)	C_3	$(\frac{1}{2}, \frac{1}{2}, z)$	$I 4_1 3 2$ (214)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$I 4_1 m d$ (109)	C_{2v}	$(0, 0, z)$	$P \bar{6} 2 c$ (190)	C_{3h}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	J		
$I \bar{4} 2 d$ (122)	C_2	$(0, 0, z)$	$P \bar{6} 2 c$ (190)	C_{3h}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$I 4_1 3 2$ (214)	D_2	$(\frac{1}{2}, 0, \frac{1}{4})$
$I \bar{4} 2 d$ (122)	S_4	$(0, 0, 0)$	$P 6_3/m m c$ (194)	C_{3v}	$(\frac{1}{2}, \frac{1}{2}, z)$	$I 4_1 3 2$ (214)	D_2	$(\frac{1}{2}, 0, \frac{1}{4})$
$I \bar{4} 2 d$ (122)	S_4	$(0, 0, \frac{1}{2})$	$P 6_3/m m c$ (194)	D_{3h}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	K		
$I 4_1/a m d$ (141)	C_2	$(x, x, 0)$	$P 6_3/m m c$ (194)	D_{3h}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{4})$	$I \bar{4} 3 d$ (220)	S_4	$(\frac{7}{8}, 0, \frac{1}{4})$
$I 4_1/a m d$ (141)	C_{2v}	$(0, 0, z)$	E			$I \bar{4} 3 d$ (220)	S_4	$(\frac{7}{8}, 0, \frac{1}{4})$
$I 4_1/a m d$ (141)	D_{2d}	$(0, 0, 0)$	$P 6_2$ (171)	C_2	$(\frac{1}{2}, \frac{1}{2}, z)$	L		
$I 4_1/a m d$ (141)	D_{2d}	$(0, 0, \frac{1}{2})$	$P 6_4$ (172)	C_2	$(\frac{1}{2}, \frac{1}{2}, z)$	$I 4_1 3 2$ (214)	C_2	$(x, 0, \frac{1}{4})$
$I 4_1/a c d$ (142)	C_2	$(x, x, \frac{1}{4})$	$P 6_2 2 2$ (180)	C_2	$(\frac{1}{2}, 0, z)$	$I \bar{4} 3 d$ (220)	C_2	$(x, 0, \frac{1}{4})$
B (Face-centered lattice)			$P 6_2 2 2$ (180)	D_2	$(\frac{1}{2}, 0, 0)$	$I a \bar{3} d$ (230)	C_2	$(\frac{1}{8}, y, -y + \frac{1}{4})$
$F d d d$ (70)	C_i	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 6_2 2 2$ (180)	D_2	$(\frac{1}{2}, 0, \frac{1}{2})$	M		
$F d d d$ (70)	C_i	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 6_4 2 2$ (181)	C_2	$(\frac{1}{2}, 0, z)$	$I a \bar{3} d$ (230)	C_2	$(x, 0, \frac{1}{4})$
$F d \bar{3}$ (203)	C_{3i}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 6_4 2 2$ (181)	D_2	$(\frac{1}{2}, 0, 0)$	N		
$F d \bar{3}$ (203)	C_{3i}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 6_4 2 2$ (181)	D_2	$(\frac{1}{2}, 0, \frac{1}{2})$	$I a \bar{3} d$ (230)	D_2	$(\frac{1}{8}, 0, \frac{1}{4})$
$F 4_1 3 2$ (210)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	F (Primitive)			$I a \bar{3} d$ (230)	S_4	$(\frac{1}{8}, 0, \frac{1}{4})$
$F 4_1 3 2$ (210)	D_3	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 4_2 3 2$ (208)	C_2	$(x, \frac{1}{2}, 0)$	O		
$F d \bar{3} m$ (227)	D_{3d}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P 4_2 3 2$ (208)	C_2	$(x, 0, \frac{1}{2})$	$I a \bar{3} d$ (230)	D_3	$(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$
$F d \bar{3} m$ (227)	D_{3d}	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$P \bar{4} 3 n$ (218)	C_2	$(x, \frac{1}{2}, 0)$			

^aNumber assigned to every space group in the international tables vol. A.

^bSite symmetry

B Input parameters used for the software comparison

The input parameters used in the software comparison are presented.

B.1 Parameters for *ITO13*, *N-TREOR*, *DICVOL14*

For these programs, the uniquely fixed parameter sets were searched for by the authors to provide the best results. As far as we tested, the parameters concerning the searched range (c, d for *TREOR*, i–m for *DICVOL*) did not much change their computation times.

Table 2: Input parameters for *ITO13*

$9^a 0^b 0^c 9^d 1^e 1^f 1^g 1.54056^h 4.0^i$
0.000^j

a: option for the information printed out.

b: option for the information printed out.

c: option for reading intensities.

d: number of solutions printed out.

e: orthorhombic solutions are searched for.

f: monoclinic solutions are searched for.

g: triclinic solutions are searched for.

h: wavelength of *X*-rays.

i: at most 0.04° difference is allowed between computed and observed lines in 2θ .

j: this number is used as zero point-shift.

Table 3: Input parameters for *N-TREOR*

CHOICE=4 ^a ,
WAVE= 1.54056 ^b ,
VOL= 3500 ^c ,
CEM= 40 ^d ,

a: option for reading peak positions (= 3: input data are d-values, = 4: input data are d-values).

b: wavelength of *X*-rays.

c: upper threshold for unit-cell volumes.

d: upper threshold for unit-cell dimensions *a, b, c*.

Table 4: Input parameters for *DICVOL14*

30^a	3^b	1^c	1^d	1^e	1^f	1^g	1^h
40^i	40^j	40^k	0^l	3500^m	90^n	125^o	
1.54056^p	$0.^q$	$0.^r$	$0.^s$				
0.0^t	$3.^u$	0^v	0^w	1^x	1^y		

- a: number of lines used for peak indexing.
- b: option for reading peak positions (= 2: 2θ angle in degrees., = 3: d -Spacing in angstrom unit).
- c: cubic solutions are searched for.
- d: tetragonal solutions are searched for.
- e: hexagonal solutions are searched for.
- f: orthorhombic solutions are searched for.
- g: monoclinic solutions are searched for.
- h: triclinic solutions are searched for.
- i: upper threshold for unit-cell dimension a .
- j: upper threshold for unit-cell dimension b .
- k: upper threshold for unit-cell dimension c .
- l: lower threshold for unit-cell volume.
- m: upper threshold for unit-cell volume.
- n: lower threshold for β .
- o: upper threshold for β .
- p: wavelength of X -rays.
- q: if $q = 0$, nothing is assumed on molecular weight.
- r: if $r = 0$, nothing is assumed on measured density.
- s: if $s = 0$, nothing is assumed on measured density.
- t: if $t = 0.0$, at most 0.025° for triclinic system and 0.03° for the other systems are allowed between computed and observed lines in 2θ .
- u: minimum value of de Wolff figure of merit of accepted solutions.
- v: maximum number of accepted impurity lines.
- w: if $w = 1$, the zero-point shift is searched for before powder indexing.
- x: zero-point shift is refined by least squares.
- y: more exhaustive search is executed if $y = 1$.

B.2 Parameters for *CONOGRAPH*

On *CONOGRAPH*, although a lot of parameters are adjustable, the parameters to be changed are only a few: only those surrounded by dark red lines in Figure 1. What users have to do is to select **Exhaustive search** in a, and set information about the diffractometer in d. Although similarly good results may be obtained in shorter time by selecting **Quick search** or reducing the number of peaks in b, users do not need to do so, if they want to finish all in a single run of the software.

For comparison, the parameter b, w was changed as indicated in the figures.

The screenshot shows the 'Peaksearch' and 'Advanced Indexing Parameters' windows. The 'Search parameters' section includes:

- Volume of primitive cell [Å]: AUTO ≤ Vol ≤ AUTO (labeled **l**)
- Number of zones used for search: AUTO (labeled **m**)
- Number of enumerated primitive cells: AUTO (labeled **n**)
- Tolerance level for errors of sums of q-values: 1.0 times (labeled **o**)
- Minimum Mwu: 1.9 (labeled **p**)
- Minimum Mrev: 1.0 (labeled **q**)
- Threshold of minimum distance between lattice points: 2.0 (labeled **r**)
- Maximum number of solutions for each Bravais lattice: 1000 (labeled **s**)

The 'Diffractometer parameters' section includes:

- Search parameters: **Quick search** (selected) and **Exhaustive search** (labeled **a**)
- Number of peaks used for search: AUTO (labeled **b**) with a note **b→30 (AUTO=48)**
- Wavelength: 1.54056 Å (labeled **d**)
- Zero point shift: Δ2θ = 0.0 deg. (labeled **e**)

The 'Criteria for indexing solutions' section includes:

- Number of peaks used for computation of FOM: 20 (labeled **f**)
- Sorting criteria: de Wolff figure of merit (M) (labeled **g**)
- Upper/lower thresholds for number of computed lines between 1st and 20th observed lines: AUTO ≤ N_{cal} ≤ AUTO (labeled **h**)
- de Wolff figure of merit M: M ≥ 3.0 (labeled **i**)
- Min/Max of lattice constants: 0.0 ≤ a,b,c ≤ 1000.0 (labeled **j**)
- Relative error tolerance to search for duplicated solutions: ≤ 0.03 (labeled **k**)

The 'Bravais lattice (available multiple choice)' section includes:

- Triclinic (checked)
- Monoclinic (P) (checked)
- Monoclinic (B) (checked)
- Orthorhombic (P) (checked)
- Orthorhombic (C) (checked)
- Orthorhombic (I) (checked)
- Orthorhombic (F) (checked)
- Tetragonal (P) (checked)
- Tetragonal (I) (checked)
- Rhombohedral (checked)
- Hexagonal (checked)
- Cubic (P) (checked)
- Cubic (I) (checked)
- Cubic (F) (checked)

The 'Peak Search Output' table is shown below:

	Position	Height	FWHM	Use for indexing
▶ 1	1.810606	1276.94	0.0586059	<input checked="" type="checkbox"/>
2	2.033466	1139.63	0.0623548	<input checked="" type="checkbox"/>
3	2.727744	103810.80	0.0643929	<input checked="" type="checkbox"/>
4	3.880456	608.13	0.0904867	<input checked="" type="checkbox"/>
5	4.093253	4603.37	0.0639131	<input checked="" type="checkbox"/>
6	4.441680	7721.64	0.0711705	<input checked="" type="checkbox"/>
7	5.466492	5381.52	0.0633044	<input checked="" type="checkbox"/>
8	6.142721	2474.93	0.0773353	<input checked="" type="checkbox"/>
9	8.109633	809.95	0.0587380	<input checked="" type="checkbox"/>
10	8.201591	809.60	0.0566817	<input checked="" type="checkbox"/>
11	8.415093	1561.32	0.0778338	<input checked="" type="checkbox"/>
12	9.881934	1405.75	0.0811491	<input checked="" type="checkbox"/>

Figure 1: Default parameters (1/2) used in *CONOGRAPH*; For the software comparison, the parameter b was changed to 30.

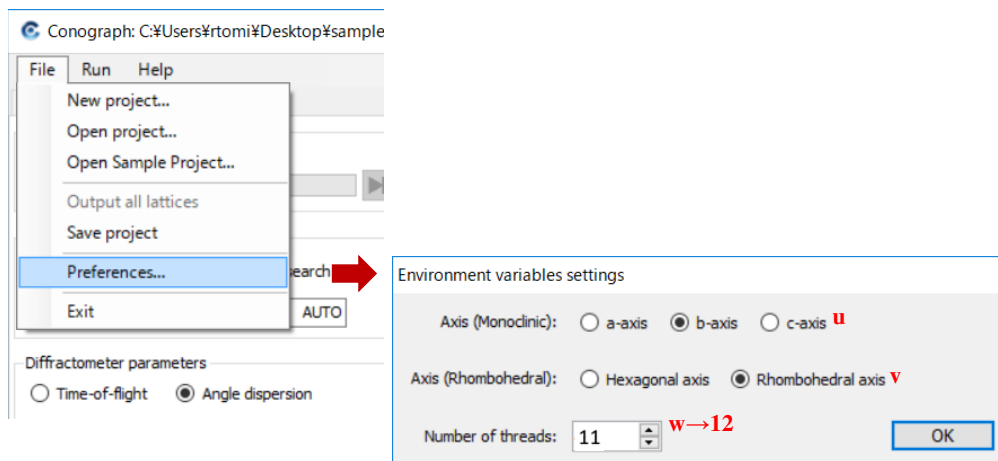


Figure 2: Default parameters (2/2) used in *CONOGRAPH*; the default value of w is the number of threads of the computer minus one. For the software comparison, w was set to the number of all the threads.