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)		
$F\ d\ d\ 2$ (43)	C_2	$(0,0,z)$
$F\ d\ d\ d$ (70)	C_2	$(x,0,0)$
$F\ d\ d\ d$ (70)	D_2	$(0,0,0)$
$F\ d\ d\ d$ (70)	D_2	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$F\ d\ \bar{3}$ (203)	C_2	$(x,0,0)$
$F\ d\ \bar{3}$ (203)	T	$(0,0,0)$
$F\ d\ \bar{3}$ (203)	T	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$F\ 4_1\ 3\ 2$ (210)	C_2	$(x,0,0)$
$F\ 4_1\ 3\ 2$ (210)	T	$(0,0,0)$
$F\ 4_1\ 3\ 2$ (210)	T	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$F\ d\ \bar{3}\ m$ (227)	C_{2v}	$(x,0,0)$
$F\ d\ \bar{3}\ m$ (227)	T_d	$(0,0,0)$
$F\ d\ \bar{3}\ m$ (227)	T_d	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
A (Body-centered lattice)		
$I\ 4_1$ (80)	C_2	$(0,0,z)$
$I\ 4_1/a$ (88)	C_2	$(0,0,z)$
$I\ 4_1/a$ (88)	S_4	$(0,0,0)$
$I\ 4_1/a$ (88)	S_4	$(0,0,\frac{1}{2})$
$I\ 4_1\ 2\ 2$ (98)	C_2	$(0,0,z)$
$I\ 4_1\ 2\ 2$ (98)	D_2	$(0,0,0)$
$I\ 4_1\ 2\ 2$ (98)	D_2	$(0,0,\frac{1}{2})$
$I\ 4_1\ m\ d$ (109)	C_{2v}	$(0,0,z)$
$I\ \bar{4}\ 2\ d$ (122)	C_2	$(0,0,z)$
$I\ \bar{4}\ 2\ d$ (122)	S_4	$(0,0,0)$
$I\ \bar{4}\ 2\ d$ (122)	S_4	$(0,0,\frac{1}{2})$
$I\ 4_1/a\ m\ d$ (141)	C_2	$(x,x,0)$
$I\ 4_1/a\ m\ d$ (141)	C_{2v}	$(0,0,z)$
$I\ 4_1/a\ m\ d$ (141)	D_{2d}	$(0,0,0)$
$I\ 4_1/a\ m\ d$ (141)	D_{2d}	$(0,0,\frac{1}{2})$
$I\ 4_1/a\ c\ d$ (142)	C_2	$(x,x,\frac{1}{4})$
B (Face-centered lattice)		
$F\ d\ d\ d$ (70)	C_i	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ d\ d\ d$ (70)	C_i	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$F\ d\ \bar{3}$ (203)	C_{3i}	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ d\ \bar{3}$ (203)	C_{3i}	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$F\ 4_1\ 3\ 2$ (210)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ 4_1\ 3\ 2$ (210)	D_3	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$F\ d\ \bar{3}\ m$ (227)	D_{3d}	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ d\ \bar{3}\ m$ (227)	D_{3d}	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
B (Body-centered lattice)		
$I\ 4_1/a$ (88)	C_i	$(0,\frac{1}{4},\frac{1}{8})$
$I\ 4_1/a$ (88)	C_i	$(\frac{1}{4},0,\frac{3}{8})$
$I\ 4_1/a\ m\ d$ (141)	C_{2h}	$(0,\frac{1}{4},\frac{1}{8})$
$I\ 4_1/a\ m\ d$ (141)	C_{2h}	$(0,\frac{1}{4},\frac{5}{8})$
C		
$I\ 4_1/a\ m\ d$ (141)	C_2	$(x,\frac{1}{4},\frac{1}{8})$
$I\ 4_1/a\ c\ d$ (142)	C_2	$(\frac{1}{4},y,\frac{1}{8})$
D		
$P\ 3\ 1\ c$ (159)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{3}\ 1\ c$ (163)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{3}\ 1\ c$ (163)	D_3	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ \bar{3}\ 1\ c$ (163)	D_3	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3$ (173)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3/m$ (176)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3/m$ (176)	C_{3h}	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ 6_3/m$ (176)	C_{3h}	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3\ 2\ 2$ (182)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3\ 2\ 2$ (182)	D_3	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ 6_3\ 2\ 2$ (182)	D_3	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3\ m\ c$ (186)	C_{3v}	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{6}\ 2\ c$ (190)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{6}\ 2\ c$ (190)	C_{3h}	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ \bar{6}\ 2\ c$ (190)	C_{3h}	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3/m\ m\ c$ (194)	C_{3v}	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3/m\ m\ c$ (194)	D_{3h}	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ 6_3/m\ m\ c$ (194)	D_{3h}	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
E		
$P\ 6_2$ (171)	C_2	$(\frac{1}{3},\frac{1}{3},z)$
$P\ 6_4$ (172)	C_2	$(\frac{1}{3},\frac{1}{3},z)$
$P\ 6_2\ 2\ 2$ (180)	C_2	$(\frac{1}{2},0,z)$
$P\ 6_2\ 2\ 2$ (180)	D_2	$(\frac{1}{2},0,0)$
$P\ 6_2\ 2\ 2$ (180)	D_2	$(\frac{1}{2},0,\frac{1}{2})$
$P\ 6_4\ 2\ 2$ (181)	C_2	$(\frac{1}{2},0,z)$
$P\ 6_4\ 2\ 2$ (181)	D_2	$(\frac{1}{2},0,0)$
$P\ 6_4\ 2\ 2$ (181)	D_2	$(\frac{1}{2},0,\frac{1}{2})$
F (Primitive)		
$P\ 4_2\ 3\ 2$ (208)	C_2	$(x,\frac{1}{2},0)$
$P\ 4_2\ 3\ 2$ (208)	C_2	$(x,0,\frac{1}{2})$
$P\ \bar{4}\ 3\ n$ (218)	C_2	$(x,\frac{1}{2},0)$
$P\ \bar{4}\ 3\ n$ (218)	C_2	$(x,0,\frac{1}{2})$
$P\ m\ \bar{3}\ n$ (223)	C_2	$(\frac{1}{4},y,y+\frac{1}{2})$
$P\ m\ \bar{3}\ n$ (223)	C_{2v}	$(x,\frac{1}{2},0)$
$P\ m\ \bar{3}\ n$ (223)	C_{2v}	$(x,0,\frac{1}{2})$
F (Body-centered)		
$I\ \bar{4}\ 3\ d$ (220)	C_3	(x,x,x)
$I\ a\ \bar{3}\ d$ (230)	C_3	(x,x,x)
G		
$P\ 4_2\ 3\ 2$ (208)	D_2	$(\frac{1}{4},0,\frac{1}{2})$
$P\ 4_2\ 3\ 2$ (208)	D_2	$(\frac{1}{4},\frac{1}{2},0)$
$P\ \bar{4}\ 3\ n$ (218)	S_4	$(\frac{1}{4},0,\frac{1}{2})$
$P\ \bar{4}\ 3\ n$ (218)	S_4	$(\frac{1}{4},\frac{1}{2},0)$
$P\ m\ \bar{3}\ n$ (223)	D_{2d}	$(\frac{1}{4},0,\frac{1}{2})$
$P\ m\ \bar{3}\ n$ (223)	D_{2d}	$(\frac{1}{4},\frac{1}{2},0)$
H		
$P\ 4_3\ 3\ 2$ (212)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$P\ 4_3\ 3\ 2$ (212)	D_3	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$P\ 4_1\ 3\ 2$ (213)	D_3	$(\frac{3}{8},\frac{3}{8},\frac{3}{8})$
$P\ 4_1\ 3\ 2$ (213)	D_3	$(\frac{7}{8},\frac{7}{8},\frac{7}{8})$
I		
$I\ 4_1\ 3\ 2$ (214)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$I\ 4_1\ 3\ 2$ (214)	D_3	$(\frac{7}{8},\frac{7}{8},\frac{7}{8})$
J		
$I\ 4_1\ 3\ 2$ (214)	D_2	$(\frac{1}{8},0,\frac{1}{4})$
$I\ 4_1\ 3\ 2$ (214)	D_2	$(\frac{5}{8},0,\frac{1}{4})$
K		
$I\ \bar{4}\ 3\ d$ (220)	S_4	$(\frac{7}{8},0,\frac{1}{4})$
$I\ \bar{4}\ 3\ d$ (220)	S_4	$(\frac{3}{8},0,\frac{1}{4})$
L		
$I\ 4_1\ 3\ 2$ (214)	C_2	$(x,0,\frac{1}{4})$
$I\ \bar{4}\ 3\ d$ (220)	C_2	$(x,0,\frac{1}{4})$
$I\ a\ \bar{3}\ d$ (230)	C_2	$(\frac{1}{8},y,-y+\frac{1}{4})$
M		
$I\ a\ \bar{3}\ d$ (230)	C_2	$(x,0,\frac{1}{4})$
N		
$I\ a\ \bar{3}\ d$ (230)	D_2	$(\frac{1}{8},0,\frac{1}{4})$
$I\ a\ \bar{3}\ d$ (230)	S_4	$(\frac{3}{8},0,\frac{1}{4})$
O		
$I\ a\ \bar{3}\ d$ (230)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$

[a] Number assigned to every space group in the international tables vol. A.
[b] Site 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.

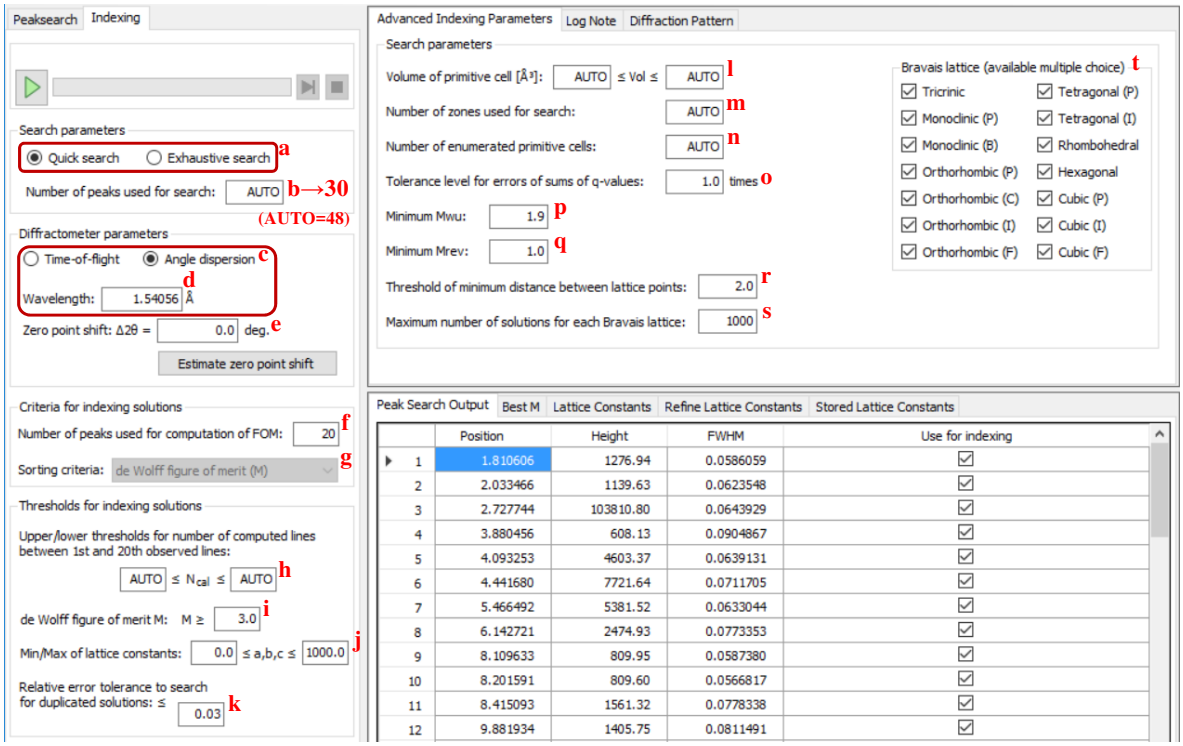

Figure 1: Default parameters (1/2) used in *CONOGRAPH*; For the software comparison, the parameter b was changed to 30.

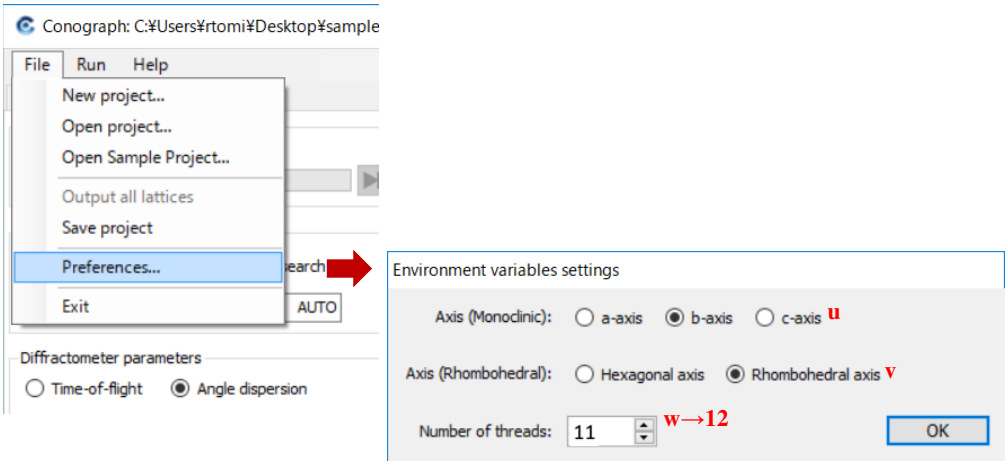

Figure 2: Default parameters (2/2) used in *CONOGRAPH*; the default value of w is the number of threads of the computer minus one. For the software comparison, w was set to the number of all the threads.