

C R Y S C A L C user's guide

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C R Y S C A L C

(CRYSTALLOGRAPHIC CALCULATIONS)

*makes crystallographer life easier !*

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[with courtesy of JRC and JGP for CFML]

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## Introduction

**CRYSCALC** has been created to perform basic crystallographic calculations or get crystallographic informations. **CRYSCALC** has been written in Fortran 95, and uses the crystallographic calculations potential of the Crystallographic Fortran Modules Libraries written by J. Rodriguez-Carvajal (ILL-Grenoble, France) and J. Gonzalez (Univ. La Laguna, Spain).

Principal tools implemented in **CRYSCALC** :

- unit cell volume calculation
- space group informations: space group features, Wyckoff positions, symmetry operators, extinctions ...
- calculation of  $d_{hkl}$ ,  $Q_{hkl}$ ,  $2\theta_{hkl}$  (including with a propagation wave vector)
- hkl generation for a given space group (simulation of a Debye-Scherrer film with equal intensities Bragg peaks)
- structure factor calculation (Xrays, neutrons, electrons)
- simulation of powder diffraction pattern (X, neutrons)
- geometric calculations: interatomic distances, angles, connectivity, bond valence sums (BVS), centroid coordinates, angles between 2 vectors in direct and reciprocal space, ...
- atomic features: weight, density, electronic configuration, ionic and Shannon radii, neutron data, X-rays data ...
- molecular informations: molecular weight, density ...
- absorption coefficient calculation (X-rays, neutrons) and transmission calculation
- transformation of unit cell, atomic coordinates and hkl files
- statistics on hkl file and sort of hkl data
- search for systematic extinctions and space group
- ADP parameters conversion
- create HTML report from a CIF file
- . etc.

**CRYSCALC** can be run through an input file containing a list of keywords, defining the type of crystallographic calculations that will be performed, or in an interactive mode, by entering keywords at the **CRYSCALC** prompt.

Crystallographic features can be read from different types of input files :

- .CFL
- .INS/.RES file (SHELXL)
- .CIF file
- .PCR file (FullProf)

- .CEL file (PowderCELL)

Alternatively, particular jobs can be performed by **CRYSCALC** when special arguments are passed to **CRYSCALC** through the command line (see **CRYSCALC** command line arguments section).

Online help can be obtained by typing **MAN** or **HELP** at the "Enter input file" (menu option #2) or "Enter keyword:" (menu option #1) prompt:

```
d:\> cryscalc  
> Enter keyword : man
```

or launching **CRYSCALC** program with **MAN** or **HELP** as argument:

```
d:\> cryscalc man
```

Details on the meaning of keywords can be obtained by typing the corresponding keyword at the "Enter keyword : " prompt or launching **CRYSCALC** program with the corresponding keyword(s) as argument(s):

```
d:\> cryscalc MAN CELL
```

Recommendations:

To get all potential of **CRYSCALC**, it is recommended to define the **CRYSCALC** environment variable, that has to point to the folder where **CRYSCALC** has been installed (ex: d:\>progs). Furthermore, some special options of **CRYSCALC** can not be fully executed if **WinPLOT** has not been installed previously.

## List of **CRYSCALC** keywords

- ABSENT\_HKL
- ABSORPTION
- ACTA
- ANG
- APPLY\_OP
- ATOM
- ATOM\_LIST
- BARY
- BEAM
- BVPARAM
- CELL
- CELL\_ESD
- CHEM
- CIF\_EXTRACT
- CLONE
- CONN
- CONT
- CREATE\_ACE
- CREATE\_CEL
- CREATE\_CFL
- CREATE\_CIF
- CREATE\_FST
- CREATE\_FHZ
- CREATE\_HKF5
- CREATE\_INS
- CREATE\_PCR
- CREATE\_PDB
- CREATE\_REPORT
- CREATE\_SOLVE
- CREATE\_TIDY

- CREATE\_XYZ
- D\_HKL
- D\_HKL\_MAX
- D\_REC
- DATA\_ATOMIC
- DATA\_NEUTRONS
- DATA\_XRAYS
- DIAG\_MAT
- DIFF
- DIR\_ANG
- DIST
- DIST\_DHA
- DIST\_MULT
- DIST\_NEW
- DIST\_NEW\_COL
- DIST\_PLUS
- EDIT
- EQUIV\_ATOMS
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- EULER\_TO\_KAPPA
- EXIT
- FILE
- FIND\_HKL
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- FRIEDEL
- GEN\_HKL
- GET\_FORMAL\_CHARGES
- GET\_TRANS\_MAT
- HEADER
- HEX\_RHOMB
- HKL
- HKL\_DIFF

- HKL\_MULT
- HKL\_NEG
- HKL\_POS
- INSIDE
- KAPPA\_TO\_EULER
- LIST\_EXTI
- LIST\_HKL\_MAX
- LIST\_HKL\_FC\_MAX
- LIST\_KEYS
- LIST\_LAUE
- LIST\_MATR
- LIST\_MATR\_USER
- LIST\_SG
- MAG
- MAN
- MAN\_HTML
- MATMUL
- MATRIX
- MENDEL
- MERGE
- MONOCLINIC
- NEWS
- NIGGLI
- OBV\_REV
- PAUSE
- PERMUT
- PLANE
- Q\_HKL
- QVEC
- READ\_ACE
- READ\_CEL
- READ\_CIF

- READ\_EXP
- READ\_FACES
- READ\_FCF
- READ\_HKLF5
- READ\_INS
- READ\_LST
- READ\_NREPORT
- READ\_P4P
- READ\_PCR
- READ\_PDB
- READ\_SEQ
- READ\_SFRM
- READ\_SPF
- READ\_TIDY\_OUT
- READ\_XYZ
- REC\_ANG
- REDUCE\_CELL
- RESET
- RINT
- RHOMB\_HEX
- SAVE\_SETTINGS
- SEARCH\_EXTI
- SEARCH\_MONO
- SEARCH\_P3P6
- SEARCH\_SPGR
- SEARCH\_SYMM
- SEARCH\_TETRA
- SET
- SETTING
- SFAC
- SF\_HKL
- SG

- SG\_ALL
- SG\_EXTI
- SG\_INFO
- SG\_SUB
- SHANNON
- SHELL
- SHIFT\_2TH
- SIZE
- SORT
- STAR\_K
- STL
- SUPERCELL
- SYMM
- SYST
- THERM
- THERM\_SHELX
- THETA
- TITL
- TOLMAN\_ANGLE
- TRANSLATION
- TRANSMISSION
- TRICLINIC
- TWIN\_HEX
- TWIN\_PSEUDO\_HEX
- TWO\_THETA
- UB\_MATRIX
- UNIT
- UPDATE
- USER\_MAT
- WATER\_H
- WAVE
- WEB

- WRITE\_ADP
- WRITE\_BEAM
- WRITE\_CELL
- WRITE\_CHEM
- WRITE\_DEVICE
- WRITE\_QVEC
- WRITE\_REF
- WRITE\_SG
- WRITE\_SUPERCELL
- WRITE\_SYM\_OP
- WRITE\_WAVE
- WRITE\_ZUNIT
- X\_WAVE
- ZUNIT

## Details of **CRYSCALC** keywords

### • **ABSENT\_HKL**

. type: OUTPUT keyword  
. meaning: search for observed reflections (with  $F2 > 0$ .) that should be absent for a given space group  
. optional arguments: . arg = "ALL": all the violations reflections are output  
. arg = "OUT": requested reflections are output on the screen  
. arg = "WRITE": requested reflections are output in a HKL file  
. arg = real\_value (n\_sig): only reflections with  $I/\text{sig} > n\_sig$  are output  
. mandatory keyword: FILE, SPGR  
. identical keywords: ABSENT\_HKL, HKL\_ABSENT

[top of CRYSCALC keywords list]

### • **ABSORPTION**

. type: CALCULATION keyword  
. arguments: no argument  
. meaning: absorption coefficient calculation  
. mandatory keywords: CELL, WAVE, CONT / CHEM  
. identical keywords: ABSORPTION, ABSORPTION\_CALC, CALC\_ABSORPTION, MU, CALC\_MU, MU\_CALC

[top of CRYSCALC keywords list]

### • **ACTA**

. type: OUTPUT keyword  
. arguments: no argument  
. meaning: create CRYSCALC.CIF file containing calculation results in a CIF format  
. identical keywords: ACTA

[top of CRYSCALC keywords list]

### • **ANG**

. type: CALCULATION keyword  
. arguments: 3 characters strings  
. meaning: calculation of the angle defined by three atoms

```

labelled by the atom labels (cf ATOM keyword)
. example:      ANG C8 C10 C9
or
. arguments:    4 characters strings
. meaning:      calculation of the angle defined by the segments
                  constituted by atoms couples labelled as S_1, S_2
                  and S_3, S_4 respectively (cf ATOM keyword)
. remark:       atom label can refer to equivalent position through
                  a particular symmetry operator (cf SYMM keyword).
                  This is specified by adding "$n" to the
                  atomic label, with n referring to the number of
                  symmetry operator in the list.
. example:      ANG 01 C8 C9 C10_$1
. identical keywords:  ANG, ANGLE

```

[top of CRYSCALC keywords list]

- **APPLY\_OP**

```

. type:          OUTPUT keyword
. arguments :    no argument
. outputs:       apply the symmetry operators on the atomic
                  positions
. mandatory keyword: SYMM, ATOM
. identical keywords: APPLY_OP, APPLY_SYMMETRY_OPERATOR,
                  APPLY_SYM_OP, APPLY_SYMM_OP, APPLY_SYMOP

```

[top of CRYSCALC keywords list]

- **ATOM**

```

. type:          INPUT keyword
. arguments:     2 characters strings and 5 reals
. meaning:       . string #1: atomic label
                  . string #2: atom type (can contain oxidation state)
                  . x,y,z atomic reduced coordinates
                  . Biso, site occupancy (%)
. remarks:       . if Biso is missing: Biso = 0.0
                  . if Occ(%) is missing: Occ(%) = 1.0 (site is fully occupied)
. example:       ATOM 01  O  0.04356 0.03008 0.39001 0.35 1.
                  ATOM C8  C  0.02071 -0.12436 0.36957 0.30 1.
                  ATOM C9  C -0.27497 -0.07538 0.27585 0.30 1.
                  ATOM C10 C -0.16896 -0.18823 0.36382 0.32 1.
                  ATOM Si1 Si+4 0.53245 0.53245 0.5
                  ATOM 01  O-2 0.58566 0.85594 0.61727
. identical keywords: ATOM, ATM

```

[top of CRYSCALC keywords list]

- **ATOM\_LIST**

type: OUTPUT keyword  
 optional argument: "CART", "IN\_A", "NO\_H"  
 meaning: list the atoms (type, labels, coordinates, ...)  
   . if "CART" is present, cartesian atomic coordinates will be output. Derivative CART arguments are CART\_A (a//x) and CART\_C (x//c).  
   . if "IN\_A" is present, atomic coordinates are listed in A.  
   . if "NO\_H" is present, only non-hydrogen atoms are listed.  
   . if "ONLY\_X" is present, only X species atoms are listed.  
 optional keyword: SPGR  
 identical keywords: ATOM\_LIST, ATOM\_LST, LIST\_ATOM\_LIST, LIST\_ATOMS, LST\_ATOMS, WRITE\_ATOMS, WRITE\_ATMS

[top of CRYSCALC keywords list]

- **BARY**

. type: CALCULATION keyword  
 . arguments: n characters strings  
   or "ALL"  
 . optional argument: "No\_H"  
 . meaning: calculation of the coordinates of the centroid of the n atoms known by the atom label (cf ATOM keyword)  
   if arg<sub>2</sub> = ">", all atoms of same species from first and third arguments will be considered in the calculation. Note that this notation is not allowed with labels containing a letter after the number (ex: C10A).  
   if arg="ALL" : all input atoms are considered  
   if arg="no\_H": Hydrogen atoms are excluded  
 . examples: BARY C31 C32 C33 C34 C35  
   BARY C31 > C35  
   BARY C31 > C34 C35  
   BARY ALL  
 . identical keywords: BARY, CENTROID

[top of CRYSCALC keywords list]

- **BEAM**

. type: INPUT keyword  
 . arguments: characters string  
 . optional arguments: real value, following "WL=" for wavelength in Å or "E=" for energy (in KeV for X-rays and electrons or in meV for neutrons)  
 . optional arguments: real value (wavelength in Å or energy)  
 . meaning: type of the incident beam:

```

- BEAM NEUT for neutrons
- BEAM ELECTRONS for electrons
- X_Ag for X Rays (Silver K_alpha)
- X_Mo for X Rays (Molybdenum K_alpha)
- X_Cu for X Rays (Copper K_alpha)
- X_Ni for X Rays (Nickel K_alpha)
- X_Co for X Rays (Cobalt K_alpha)
- X_Fe for X Rays (Iron K_alpha)
- X_Cr for X Rays (Chromium K_alpha)

. examples:      BEAM X_Mo
                  BEAM X WL=1.5
                  BEAM X E=8.26
                  BEAM NEUT WL=1.2
                  BEAM NEUT E=56.8

. identical keyword: BEAM, JOBTYP, JPBTYP

```

[top of CRYSCALC keywords list]

#### • BVPARM

```

. type:          INPUT keyword
. arguments:     characters string
. meaning:       bond-valence parameters given by the user,
                  provided to the BVS calculation routine (see CONN keyword).
                  The order of BV parameters are as follows: cation anion d0 B0
. example:       BVPARM W+6 S-2 2.309 0.370
. identical keyword: BVPARM, BVPAR, BVPARAM

```

[top of CRYSCALC keywords list]

#### • CELL

```

. type:          INPUT keyword
. arguments:     6 reals or 1 characters string
. meaning:       - reals: unit cell parameters in A (a, b, c) and
                  angles in deg. (alfa, beta, gamma)
                  - characters string: file name containing unit cell
                  parameters.
                  Following files can be read:
                    . CIF file
                    . INS/RES file for SHELXL
                    . PCR file for FullProf
                    . P4P file created by SAINT
                    . M50 file created by JANA
                    . X file created by DENZO
                    . RMAT file created by DIRAX
                    . SUM file created by CRYVALIS
                    . SCA file created by SCALEPACK
                    . _CN file created by CELL_NOW

```

```

        . _Ls file created by SAINT
. output:    unit cell volume calculation
              direct and reciprocal unit cell parameters
. example:   CELL 7.6520 7.8450 11.0760 90. 90. 90.
              CELL import.CIF
              CELL my_saint_data.P4P
              CELL my_jana_data.m50
. identical keywords  CELL, CELL_PARAMETERS, READ_CELL

```

[top of CRYSCALC keywords list]

### • CELL\_ESD

```

. type:      INPUT keyword
. arguments: 6 reals max.
. meaning:   ESD for unit cell parameters in A (a, b, c) and
              angle in deg. (alfa, beta, gamma)
              . if only 1 real is input, metric is supposed to be cubic
              . if only 2 reals are input, metric is supposed to be tetragonal
              . if only 3 reals are input, metric is supposed to be
                orthorhombic
. output:    calculation of ESD for unit cell volume
. example:   CELL_ESD 0.0011 0.0013 0.0037 0.004 0.004 0.003
. identical keywords  CELL_ESD, ESD_CELL, CELLSD

```

[top of CRYSCALC keywords list]

### • CHEM

```

. type:      INPUT keyword
. arguments: n "El_i_n_i" characters strings (without blank
              character between label and number)
. optional argument: Friedif
. meaning:   Molecular chemical formula: El_i is the chemical
              symbol of the species i and n_i is the corresponding
              number of atoms in the formula unit.
              IF FRIEDIF optional argument is given, a Friedif value
              calculation is done, according to the spreadsheet
              by Flack and Shmueli (Acta Cryst. A 2007, 63, 257-265)
. output:    molecular weight, total number of electrons,
              atomic and weight percentage
. mandatory keyword: ZUNIT
. example:   CHEM C4 O6 H9 N1
. identical keywords: CHEM, CHEM_FORM, CHEMICAL_FORMULA

```

[top of CRYSCALC keywords list]

- **CIF\_EXTRACT**

```

. type:                OUTPUT keyword
. arguments:          DIST A B
                     ANG  A B C
                     TORS  A B C D
                     ACQ
                     ADP
                     ATOMS
                     CELL
                     CHEM
                     CRYSTAL
                     DATARED
                     SG
. meaning:            Extract interatomic distances, angles and torsion
                     angles from a CIF file
                     If arg=ACQ:      extract data collection features from a CIF file
                     If arg=ADP:      extract Atomic Displacement Parameters from a CIF
                     If arg=ATOMS:    extract atoms and corresponding coordinates from
                     If arg=CELL:     extract cell parameters from a CIF file
                     If arg=CHEM:    extract chemical formule from a CIF file
                     If arg=CRYSTAL:  extract crystal features from a CIF file
                     If arg=DATARED:  extract data reduction features from a CIF file
                     If arg=SG:       extract space group from a CIF file
. output:            If arg=DIST, ANG, TORS : ouput min and max values of requested pa
                     and calculation of the mean value.
. mandatory keyword: READ_CIF
. examples:          CIF_EXTRACT DIST Pd Br
                     CIF_EXTRACT DIST C1 C2
                     CIF_EXTRACT ANG  Br Pd Br
. identical keywords: CIF_EXTRACT, EXTRACT_CIF, EXTRACT_FROM_CIF

```

[top of CRYSCALC keywords list]

- **CLONE**

```

. type:                INPUT keyword
. arguments:          n character strings referring to n-1 atomic labels
                     describing a fragment. The last string argument
                     corresponds to the first atom of the cloned fragment.
. meaning:            calculation of atomic coordinates of a cloned fragment
. example:          CLONE C1 C2 C3 C4 C5 C6 C11
>> input fragment is defined by 6 atoms from C1 to C6 and
cloned fragment is calculated starting from C11 atom and
is generated with the following condistions:
vect(C11-C12) = vect(C1-C2)
vect(C12-C13) = vect(C2-C3)
vect(C13-C14) = vect(C3-C4)
...
. remark:            max number of atoms to define the fragment has been limited to 10

```

. identical keywords: CLONE, CREATE\_CLONE, CLONE\_FRAGMENT

[top of CRYSCALC keywords list]

- **CONN**

. type: INPUT keyword

. argument: atom\_label + dist\_max

. optional arguments: ALL, ALL\_X, NO\_X, ONLY\_X, ONLY\_Xn, LIGAND=, ANG, BVS, VOL, SHAPE, SELF, MIN=, MAX=, CONDENSED, No\_BD

. meaning:

- . Determine the connectivity around the atom "atom\_label" with interatomic distances calculated between MIN and MAX values.
- . Calculate the polyedron distortion as:  

$$\text{distortion} = \text{SUM}((\text{dist}-\text{dist\_av})/\text{dist\_av})^2) / n$$
 with n: number of ligands  
 dist\_av: average distance
- . Default values for MIN and MAX = 0.4 and 3.0 A.
- . if "ALL" is present, the program will calculate connectivity around all atoms.
- . if "ALL\_X" is present, the program will calculate connectivity around all atoms of the species X.
- . if "ONLY\_X" is present, the program will calculate connectivity between all atoms of the species X.
- . if "ONLY\_Xn" is present, the program will calculate connectivity around Xn atom.
- . if "LIGAND=L" (or LIGAND\_L, or L=L or, L\_L) is present, the program will output connectivity with ligand L.
- . if "NO\_X" is present, the program will exclude connectivity with all atoms of the species X.
- . if "ANG" is present, interatomic angles will also be calculated. If tetrahedral environment is found around a metal atom, tau4 index is calculated, following the formula introduced by L. Yang (Dalton Trans, 2007, 955-964):  

$$\text{tau4} = (360 - (\text{alfa}+\text{beta}))/141$$
 where alfa and beta are two largest angles at the four-coordinated metal atom.  
 In the case of five-coordinate system, tau5 trigonality index is calculated, following the formula  $\text{tau4} = (\text{alfa}-\text{beta})/60$ . where alfa and beta are two largest angles at the five-coordinate metal atom (Dalton Trans, 2007, 955-964)
- . if "BVS" is present, bond valence sums calculations are performed. Tolerance factor can be specified through the BVS\_xx keyword. Note that tolerance is defined in the same way than in FullProf, i. two atoms are considered as bonded if their distance is less than the sum of their respective ionic radii augmented by the value of TOLERANCE. The explicit expression is  $\text{dist}(A1,A2) < (r_{A1}+r_{A2})*(1+0.01*\text{TOL})$
- . if "BVS\_SUMM" is present, a summary is provided after BVS calculation.

- . if "VOL" is present, polyedron volume is calculated (ref. : VOLCAL program of L. W. FINGER included in CFML).
- . if "SHAPE" is present, an input file for SHAPE program (<http://www.ee.uib.es/>) is created.  
derivative SHAPE arguments : SHAPE\_A (a//x), SHAPE\_C (x//c)
- . if "SELF/AUTO" is present, output distances between atoms from the same label
- . if "CONDENSED" is present, short output is created
- . if "BD" is present, bonds distribution is ouput.  
ex: CONN Yb1 SELF MAX=10.  
ex: CONN Si1 MIN=1.5 MAX=2.7  
ex: CONN Nd1 VOL SHAPE No\_H  
ex: CONN Re1 L=Br1  
ex: CONN ONLY\_C ! output C-C distances  
ex: CONN ALL\_C L\_C ! output C-C distances  
ex: CONN ALL\_C L\_S ! output C-S distances  
ex: CONN ALL\_Nd  
ex: CONN ALL ANG CONDENSED  
ex: CONN Cu1 no\_H  
ex: CONN Cu1 MAX=3.1 BVS\_30
- . output: interatomic distances, bond distribution and optional BVS calculations.  
Effective distance is calculated as follows:  
 $r_{\text{eff}} = [N / \sum(r^{-3})]^{1/3}$   
If CIF/ACTA keyword is input, the created CIF file will contains all the calculated distances in CIF format.
- . mandatory keywords: SPGR, ATOM, CELL
- . identical keywords: CONN, CONNECT, CONNECTIVITY

[top of CRYSCALC keywords list]

#### • CONT

- . type: INPUT keyword
- . arguments: n "El\_i n\_i"(characters string, real) couples
- . meaning: unit cell contents: El\_i is the chemical symbol of the species i and n\_i is the corresponding number of atoms in the unit cell
- . optional keyword: ZUNIT
- . example: CONT C 16. 0 24. H 36. N 4.

[top of CRYSCALC keywords list]

#### • CREATE\_ACE

- . type: OUTPUT keyword
- . optional argument: OUT
- . meaning: create .ACE file for CaRIne from a CIF file

if "OUT" argument is given, CaRIne lines are written on screen  
if "FILE=xxx" argument is given, xxx is the name of  
the CaRIne output file

. mandatory keyword: READ\_CIF file.cif

[top of CRYSCALC keywords list]

#### • CREATE\_CEL

. type: OUTPUT keyword  
. optional argument: OUT  
. meaning: create .CEL file for PowderCELL from a CIF file  
if "OUT" argument is given, PowderCELL lines are written  
on screen.  
if "FILE=xxx" argument is given, xxx is the name of  
the PowderCELL output file.

. mandatory keyword: READ\_CIF file.cif, READ\_INS file.ins

[top of CRYSCALC keywords list]

#### • CREATE\_CFL

. type: OUTPUT keyword  
. optional argument: OUT, No\_H  
. meaning: create .CFL file for CRYSCALC from a CIF file  
if "OUT" argument is given, CFL lines are written on screen.  
if "FILE=xxx" argument is given, xxx is the name of  
the CFL output file.  
. if "no\_H" is present, Hydrogen atoms are excluded.

. mandatory keyword: READ\_CIF file.cif  
. dependent parameter: CREATE\_CFL parameter value in the CRYSCALC.INI  
setting file. If equal to 1, a .CFL file will be  
automatically created if a .CIF file is given as  
argument when CRYSCALC is launching from a command line:  
d:\> cryscalc file.cif

[top of CRYSCALC keywords list]

#### • CREATE\_CIF

. type: OUTPUT keyword  
. optional argument: output CIF file name  
if "FILE=xxx" argument is given, xxx is the name of  
the CIF output file.  
if "VIEW/RUN" argument is given, the CIF file is opened  
automatically by the associated CIF viewer (defined in  
[EXTERNAL APPLICATIONS] section in the cryscalc.ini file

through the "CIFVIEWER" item.

. meaning: create .CIF file from a .PCR, .INS/.RES or .CEL file.  
or structural data input from keywords.

. mandatory keyword: READ\_pcr file.pcr  
READ\_ins file.ins  
READ\_CEL file.cel

[top of CRYSCALC keywords list]

#### • CREATE\_FST

. type: OUTPUT keyword

. argument: POLY, RUN/VIEW, MOLE, No\_H, OUT, FILE=xxx

. meaning: create .FST file for FP Studio  
if argument="POLY" : include polyedra if  
connectivity calculation have been performed  
if argument="RUN/VIEW" : launch FP\_studio software  
if argument="MOLE": only atoms of the asymmetric  
unit cell are drawn.  
if argument="No\_H": H atoms and related bonds  
are excluded. This option is valid only if  
MOLE is specified.  
if argument="OUT": output FP\_Studio lines on screen.  
if "FILE=xxx" argument is given, xxx is the name of  
the FPStudio output file.

. mandatory keyword: READ\_CIF file.cif or READ\_INS file.ins

. dependent parameter: CREATE\_fst parameter value in the CRYSCALC.INI  
setting file. If equal to 1, a .fst file will be  
automatically created if a .CIF file is given as  
argument when CRYSCALC is launching from command line:  
d:\> cryscal file.cif

[top of CRYSCALC keywords list]

#### • CREATE\_FHZ

. type: OUTPUT keyword

. meaning: calculation of internal coordinates of a molecule  
from fractionnal coordinates:  
. cartesian coordinates  
. spherical coordinates  
. Z-matrix coordinates

This routine has been extracted from mol\_tpcr program  
of the FullProf Suite. Obviously, all the input atoms  
are considered to belong to a single molecule.

. optional argument: PCR/FP: PCR input files are created for Simulated Annealing  
FullProf.

[top of CRYSCALC keywords list]

- **CREATE\_HKF5**

. type: input keyword  
 . arguments: 9 integers or reals values  
 . meaning: transformation (3,3) matrix components  
 . optional keywords: MULT=xx: intensities and sigma are multiplied by xx factor.  
 . output: apply the transformation matrix on hkl file  
 and create hklf5 format data file.  
 Overlapping reflections criteria can be defined  
 in the setting file with "ref\_overlap\_criteria="  
 keyword in the [OPTIONS] section. Default value is 0.15  
 and allowed maximum value is 0.25.  
 . mandatory keyword: FILE  
 . identical keywords: HKLF5, CREATE\_HKLF5, WRITE\_HKLF5

[top of CRYSCALC keywords list]

- **CREATE\_INS**

. type: OUTPUT keyword  
 . optional argument: no\_H, PURGE/CLEAN, ISO, ANIS/ANISO, OUT, FILE=xxx, P1  
 . meaning: create .INS file for SHELXL  
 . if "no\_H" is present, the .INS file will not contain  
 Hydrogen atoms.  
 . if "PURGE/CLEAN" is present, the .INS file will exclude  
 spurious atoms with  $U_{eq} < 0.$  or  $U_{eq} > U_{threshold}$   
 (defined in setting file in the [CREATE\_INS] section).  
 . if "ISO" is present,  $U_{eq}$  are written in the atoms list,  
 even if anisotropic ADP have been input.  
 . if "ANIS/ANISO" is present, ANIS keyword is added  
 in the .INS created file.  
 . if "SIMU" is present, EADP keywords will be replaced by  
 "SIMU 0.003" keyword in the .INS created file.  
 . if "OUT" is present, INS lines are written on screen.  
 . if "FILE=xxx" argument is given, xxx corresponds to the name  
 of the INS output file.  
 . if "FLACK" argument is given, "TWIN" and "BASF 0.02" keywords  
 are inserted of the INS output file.  
 . if "VIEW/RUN" argument is given, the INS file is opened  
 automatically by the associated INS viewer (defined in  
 [EXTERNAL APPLICATIONS] section in the cryscalcalc.ini file  
 through the "INSVIEWER" item.  
 . if "P1" optional argument is specified, crystal structure is  
 described in P1 space group, with all atoms present in the  
 unit cell. If necessary, a translation is applied to atomic  
 coordinates to locate each molecule centroid inside the unit ce  
 . mandatory keyword: READ\_CIF file.cif  
 . example: CREATE\_INS PURGE no\_H

- . dependent parameter: CREATE\_INS parameter value in the CRYSCALC.INI setting file. If equal to 1, a .INS file will be automatically created if a .CIF file is given as argument when CRYSCALC is launching from command line:  
d:\> cryscal file.cif

[top of CRYSCALC keywords list]

- CREATE\_PCR

- . type: OUTPUT keyword
- . optional argument: ISO/FORCE\_ISO, MP, OUT, FILE=
- . meaning: create .PCR file for FullProf (pattern simulation)
  - . if "ISO" or "FORCE\_ISO" is present, the isotropic Uiso parameters will be written in the .PCR file, even if ADP parameters have been input as anisotropic values.
  - . if "MP" is present, multi-pattern format is used when PCR file is created.
  - . if "REF" is present, the create PCR file is for a diffraction pattern refinement.
  - . if "MP\_REF/REF\_MP" is present, the create PCR file is for a diffraction pattern refinement (multi-pattern format).
  - . if "No\_H" is present, only non Hydrogen atoms are written in the .PCR file.
  - . if "OUT" is present, PCR lines are written on screen.
  - if "FILE=xxx" argument is given, xxx is the name of the FullProf output file.
- . mandatory keyword: READ\_CIF file.cif, READ\_INS file.ins
- . example: CREATE\_PCR ISO
- . dependent parameter: CREATE\_PCR parameter value in the CRYSCALC.INI setting file. If equal to 1, a .PCR file will be automatically created if a .CIF or .INS file is given as argument when CRYSCALC is launching from command line:  
d:\> cryscal file.cif

[top of CRYSCALC keywords list]

- CREATE\_PDB

- . type: OUTPUT keyword
- . optional argument: OUT, FILE=xxx
- . meaning: create .PDB file containing atoms list with cartesian coordinates in PDB format, following documentation from <http://www.wwpdb.org/documentation/file-format-content/format33>  
The following Cartesian frame is used:  
x // a; z is in the ac-plane; y is  $x \wedge z = b^*$   
if "OUT" argument is given, PDB lines are written on screen.  
if "FILE=xxx" argument is given, xxx is the name of the PDB output file.

. mandatory keyword: READ\_CIF file.cif, READ\_INS file.ins  
 . dependent parameter: CREATE\_PDB parameter value in the CRYSCALC.INI setting file.  
 If equal to 1, a .PDB file will be automatically created if  
 a .CIF or .INS file is given as argument when CRYSCALC is  
 launching from command line :  
 > cryscalc file.cif  
 . identical keywords: CREATE\_PDB, WRITE\_PDB

[top of CRYSCALC keywords list]

### ● CREATE\_REPORT

. type: output keyword  
 . optional argument: .CIF file name  
 . meaning: create a STRUCTURAL\_REPORT.HTML file in HTML format  
 from the reading of the ARCHIVE.CIF file present in  
 the current folder, and launch the browser with this  
 HTML file. The .CIF file can be explicitly defined  
 with the argument.  
 If "LONG" or "TXT" is given as argument, a longer  
 report will be created, containing more informations,  
 included distances and angles.  
 . identical keywords: REPORT, CREATE\_REPORT  
 . examples: report  
 report long my\_struct.cif

[top of CRYSCALC keywords list]

### ● CREATE\_SOLVE

. type: output keyword  
 . meaning: if no argument is given, input files for SIR97, SHELXS/T  
 and SUPERFLIP/EDMA structure solving softwares are created.  
 . optional arguments: SIR, SXT, SPF to specify the files to be created.  
 SPF\_PROT: add protein options for Superflip  
 SPF\_JANA: add creation of JANA .m81 output file for Superflip.  
 . dependent parameter: CELL parameters, cell content, space group and  
 hkl file has to be provided  
 . examples: SOLVE SPF\_PROT JANA  
 . identical keywords: CREATE\_SOLVE, CREATE\_TO\_SOLVE, CREATE\_FILES\_TO\_SOLVE,  
 SOLVE

[top of CRYSCALC keywords list]

### ● CREATE\_TIDY

. type: OUTPUT keyword  
 . optional argument: OUT, FILE=xxx  
     if "OUT" argument is given, PDB lines are written on screen.  
     if "FILE=xxx" argument is given, xxx is the name of  
     the TIDY output file.  
 . meaning: create xx\_tidy.dat file for TIDY (standardisation  
     of inorganic crystal-structure data [Acta Cryst.  
     1984, A40, 169-183] from a .CIF or .INS file  
     if "OUT" argument is given, TIDY lines are written on screen  
 . mandatory keyword: READ\_CIF file.cif or READ\_INS file.ins  
 . identical keywords: CREATE\_TIDY, CREATE\_TIDY\_FILE, CREATE\_TIDY\_INPUT\_FILE

[top of CRYSCALC keywords list]

### • CREATE\_XYZ

. type: OUTPUT keyword  
 . optional argument: OUT, FILE=xxx  
 . meaning: create .XYZ file containing atoms list with cartesian  
     coordinates. The following Cartesian frame is used:  
     x // a; z is in the ac-plane; y is  $x \wedge z = b^*$   
     if "OUT" is given as argument, XYZ lines are written on screen.  
     if "FILE=xxx" argument is given, xxx is the name of the XYZ  
     output file.  
     if "VIEW/RUN" argument is given, the XYZ file is opened  
     automatically by the associated XYZ viewer (defined in  
     [EXTERNAL APPLICATIONS] section in the cryscalcalc.ini file  
     through the "XYZVIEWER" item.  
 . mandatory keyword: READ\_CIF file.cif, READ\_INS file.ins  
 . dependent parameter: CREATE\_XYZ parameter value in the CRYSCALC.INI setting file.  
     If equal to 1, a .XYZ file will be automatically created  
     if a .CIF or .INS file is given as argument when CRYSCALC is  
     launching from command line:  
     > cryscalcalc file.cif  
 . identical keywords: CREATE\_XYZ, WRITE\_XYZ

[top of CRYSCALC keywords list]

### • D\_HKL

. type: CALCULATION keyword  
 . argument: real values  
 . meaning: d\_hkl(A) values  
 . outputs: Q(A-1), SinTheta/lambda(A-1)  
     theta(deg) for known wavelength  
 . optional keyword: WAVE  
 . identical keywords: D\_HKL, DHKL  
 . example: DHKL 0.77

[top of CRYSCALC keywords list]

- **D\_HKL\_MAX**

```
. type:          CALCULATION keyword
. argument:     one optional integer value, corresponding
                to the number of listed reflexions
. meaning:     output the features for the highest values of d_hkl
                Cell parameters and space group has to be known
. outputs:     h,k,l, m, Q(A-1), SinTheta/lambda(A-1), d(A)
. optional keywords: CELL, SPACE_GROUP
. identical keywords: D_HKL_MAX, DMAX, DHKL_HIGH, DHIGH
. example:     DMAX 4
```

[top of CRYSCALC keywords list]

- **D\_REC**

```
. type:          CALCULATION keyword
. argument:     real values
. meaning:     1/d_hkl (A-1)
. outputs:     d(A)
                theta(deg)
. optional keyword: WAVE
. identical keywords: D_STAR, D_STAR_HKL, DSTAR, DSTARHKL, DSTAR_HKL,
                D_REC, D_REC_HKL, DREC, DRECHKL, DREC_HKL
. example:     D_STAR 0.5
```

[top of CRYSCALC keywords list]

- **DATA\_ATOMIC**

```
. type:          OUTPUT keyword
. optional arguments: . RADIUS
                    . COVALENT_RADIUS
                    . VDW_RADIUS
                    . VOLUME
                    . DENSITY
                    . WEIGHT
                    . EC (Electronic configuration)
                    . ALL
                    . PLOT
. meaning:     list atomic data for all atoms
                if arg=PLOT: create a PGF file and plot it with WinPLOTR
                if arg=ALL: all atomic features are listed
. identical keywords: DATA_ATOMIC, ATOMIC_DATA
```

[top of CRYSCALC keywords list]

- **DATA\_NEUTRONS**

. type: OUTPUT keyword

. optional argument: PLOT

. optional argument: Sm\_nat, Sm\_149, Eu\_nat, Eu\_151, Gd\_nat, Gd\_155, Gd\_157, Dy\_164, Er\_nat, Er\_167, Yb\_nat, Yb\_168, Yb\_174 and Lu\_176

. meaning: list neutrons data for all atoms (coherent scattering length, incoherent scattering cross-section, absorption cross-section)  
Neutron data are extracted from :  
V.F. Sears  
Neutron News, vol.3-3, 1992, 26-37  
excepted scattering lengths of particular rare earths given as argument:  
Atom. data and nuc. data tables 44, 191-207 (1990)  
J.E. Lynn and P.A. Seeger, L.A.N.L.  
if arg=PLOT: create a PGF file and plot it with WinPLOTR  
if arg=PLOT\_ALL: create a PGF file containing Re, Im, parts and modulus of scattering length (available only for input rare earth). PGF file is then plotted with WinPLOTR

. see: Xrays\_DATA

. example: DATA\_NEUTRONS Gd\_157 PLOT\_all

. identical keywords: DATA\_NEUTRONS, NEUTRONS\_DATA, DATA\_NEUTRON, NEUTRON\_DATA

[top of CRYSCALC keywords list]

- **DATA\_XRAYS**

. type: OUTPUT keyword

. optional argument: PLOT

. meaning: list X-ray data for all atoms (total interaction cross section for Ag, Mo, Cu, Co, Fe and Cr radiations)  
X-ray data are extracted from :  
Tables Internationales vol.C 1995, p.200-206,  
Tables Internationales vol.C 1995, p. 193-199  
if arg=PLOT: create a PGF file and plot it with WinPLOTR

. see: Xrays\_DATA

. identical keywords: DATA\_XRAYS, XRAYS\_DATA, DATA\_XRAY, XRAY\_DATA

[top of CRYSCALC keywords list]

- **DIAG\_MAT**

. type: INPUT keyword  
 . arguments: 9 reals  
 . meaning: transformation (3,3) matrix components  
 . examples: MATR 0 0 1 0 1 0 -1 0 -1  
 MATR 0.5 0.5 0 -0.5 0.5 0 0 0 1  
 MATR 1/2 1/2 0 -1/2 1/2 0 0 0 1  
 . output: Diagonalization of the 3\*3 matrix and output  
 the Eigen values and Eigen vectors  
 . identical keywords: DIAG, DIAG\_MAT, DIAG\_MATR, DIAG\_MATRIX

[top of CRYSCALC keywords list]

### • DIFF

. type: CALCULATION keyword  
 . arguments: 2 characters strings  
 . meaning: calculation of the components of the difference vector  
 between atoms labelled by their atom labels (cf ATOM keyword)  
 diff. vector = coordinates atom\_2 - coordinates atom\_1  
 . remark: atom label can refer to equivalent position through  
 a particular symmetry operator (cf SYMM keyword)  
 atomic label, with n referring to the number of  
 symmetry operator in the list.  
 If the symmetry operator is unknown, "\_" option allows  
 to generate all equivalent positions from the current  
 space group operators. Corresponding difference vectors  
 are output.  
 . example: DIFF C8 C10  
 DIFF C10 C9  
 DIFF C10 C9\_\$1  
 DIFF C10 C9\_\*  
 . identical keywords: DIFF, DIFFERENCE, DIFF\_CALC, DIFFERENCE\_CALCULATION

[top of CRYSCALC keywords list]

### • DIR\_ANG

. type: CALCULATION keyword  
 . arguments: 2\*3 reals  
 . meaning: calculation of the angle between 2 vectors in the  
 direct space. The 3 first real values are related  
 to the coordinates of the first vector and the 3  
 last real values to the coordinates of the second  
 vector  
 . mandatory keyword: CELL  
 . identical keywords: DIR\_ANG, DIRANG, DIRECT\_ANGLE  
 . example: DIR\_ANG 1. 0. 0. 0. 1. 0.

[top of CRYSCALC keywords list]

- **DIST**

. type: CALCULATION keyword  
 . arguments: 2 characters strings  
 . meaning: calculation of the interatomic distance between 2 atoms labelled by their atom labels (cf ATOM keyword)  
 . remark: atom label can refer to equivalent position through a particular symmetry operator (cf SYMM keyword) atomic label, with n referring to the number of symmetry operator in the list.  
 If the symmetry operator is unknown, "\_" option allows to generate all equivalent positions from the current space group operators and distances smaller than d\_max are output.  
 . example: DIST C8 C10  
 DIST C10 C9  
 DIST C10 C9\_\$1  
 DIST C10 C9\_\*  
 . identical keywords: DIST, DISTANCE, ATOMIC\_DISTANCE

[top of CRYSCALC keywords list]

- **DIST\_DHA**

. type: CALCULATION keyword  
 . arguments: 2 characters strings (D A)  
 . optional argument: 1 real d\_H (default value=0.9 Ang.)  
 . meaning: - calculation of the interatomic distance between donor (D) and acceptor atoms (A)  
 . - calculation of the coordinate of H atom  
 with :  $d_{DH} = d_{AD} - d_H$   
 . examples: DIST\_DHA N1 O2  
 DHA N1 O2 0.92  
 . identical keywords: DIST\_DHA, DHA, POS\_H, CALC\_POS\_H

[top of CRYSCALC keywords list]

- **DIST\_MULT**

. type: CALCULATION keyword  
 . arguments: 2 characters strings (A B) + 1 real (x)  
 . meaning: - calculation of the interatomic distance between 2 atoms labelled by their atom labels A and B  
 . - calculation of the coordinate of the point M  
 with :  $d_{AM} = d_{AB} * x$   
 . example: DIST\_X C8 C10 1.2  
 . identical keywords: DIST\_MULT, DIST\_X

[top of CRYSCALC keywords list]

- **DIST\_NEW**

. type: CALCULATION keyword  
. arguments: 2 characters strings (A B) + 1 real (x)  
. meaning: - calculation of the interatomic distance between 2 atoms labelled by their atom labels A and B  
. - calculation of the coordinate of the point M with :  $d_{AM} = x$   
. example: DIST\_NEW C8 O10 0.95

[top of CRYSCALC keywords list]

- **DIST\_NEW\_COL**

. type: CALCULATION keyword  
. arguments: 3 characters strings (referring to atoms A,B,C)  
. meaning: - calculation of atomic coordinates of D with  $\text{vect}(AB) = \text{vect}(CD)$   
. example: DIST\_NEW\_COL C1 C2 C11  
. identical keywords: DIST\_NEW\_COL, DIST\_COL

[top of CRYSCALC keywords list]

- **DIST\_PLUS**

. type: CALCULATION keyword  
. arguments: 2 characters strings (A B) + 1 real (x)  
. meaning: - calculation of the interatomic distance between 2 atoms labelled by their atom labels A and B  
. - calculation of the coordinate of the point M with :  $d_{AM} = d_{AB} + x$   
. example: DIST\_PLUS C8 C10 1.2  
. identical keywords: DIST\_PLUS, DIST\_+

[top of CRYSCALC keywords list]

- **EDIT**

. type: output keyword  
. argument: 1 characters string (filename)  
. meaning: open the file given as argument with the editor defined in the CRYSCALC.ini setting file  
. example: edit my\_cryscalcalc.cfl  
. related keywords: SET, SETTING

[top of CRYSCALC keywords list]

- **EQUIV\_ATOMS**

```
. type:                OUTPUT keyword
. optional arguments : list of atomic labels (characters strings)
. outputs:             give information on Wyckoff atomic positions and
                       apply the symmetry operators of the current space
                       group on the atomic positions
                       if no argument:      all atoms of the atoms list
                                               (cf ATOM keyword) are considered
                       if arg = "ALL":      all atoms of the atoms list
                                               (cf ATOM keyword) are considered
                       if arg = "PCR":      list of equivalent atoms is
                                               output in a FullProf format.
                       if arg = "PCR_MAG":  list of magnetic atoms is
                                               output in a FullProf format.

. mandatory keyword:  SPGR, ATOM
. example:            SITE_INFO 01 C8
. identical keywords: EQUIV_ATOMS, EQUIV_ATOM, SITE_INFO, INFO_SITE, ATOM_SITE, SITE_AT
                       LIST_SITE_INFO, GEN_EQUIV_ATOMS, WYCKOFF
```

[top of CRYSCALC keywords list]

- **EQUIV\_HKL**

```
. type:                OUTPUT keyword
. arguments:           3 integer values: h, k, l
. meaning:             search for equivalent reflections (Space group is
                       mandatory)
. output:              list of required hkl reflections
. mandatory keyword:  SPGR
. identical keywords: EQUIV, EQUIV_HKL, SEARCH_EQUIV, SEARCH_EQUIV_HKL,
                       FIND_EQUIV, FIND_EQUIV_HKL
. example:            EQUIV 1 1 0 FRIEDEL
```

[top of CRYSCALC keywords list]

- **EULER\_TO\_KAPPA**

```
. type:                calculation keyword
. argument:           3 real values, corresponding to phi, omega and chi
                       values (in degrees)
. meaning:            convert motors angles values of single crystal
                       diffractometer from Eulerien to Kappa
                       geometry, given Phi, Omega and Chi values.
. identical keywords: EULER, EULER_TO_KAPPA
```

[top of CRYSCALC keywords list]

- **EXIT**

```
. type:          OUTPUT keyword
. argument:      no
. meaning:       exit from the "enter keyword" procedure to come
                  back to the CRYSCALC main menu
. identical keywords: EXIT, X, QUIT, END, STOP
```

[top of CRYSCALC keywords list]

- **FILE**

```
. type:          INPUT keyword
. arguments:     1 characters string
. meaning:       read .HKL file name, containing a list of
                  h, k, l, F2, sig_F2
                  . available formats for HKL file:
                    . SHELX type: 3I4, 2F8.2
                    . CIF format
                    . RAW format (created by SAINT)
                    . MUL format (created by SAINT for twinned crystals)
                    . M91/M95 format (created by JANA)
                    . SCA format (created by SCALEPACK)
. output:        . analysis of the hkl reflections:
                  . number of hkl reflections
                  . d(A) and sinTheta/lambda collected ranges
                    (dependent keyword = CELL)
                  . Theta collected range (dependent keyword = CELL, WAVE)
                  . statistic on collected data
                  . if space group is known (see SPGR keyword), the
                    number of reflections in agreement is output
                  . if F2_max > 999999.99, all intensities are divided
                    by 10 until F2_max is lower than this upper value.
                    Sigmas are of course divided by the same coefficient
                    and a new *_sx.hk file is then created (Shelx format).
. optional arguments: NEG: negative reflections are treated as follows:
                    if (F2 < 0.0001) F2 = 0.0001
                    if (sig_F2_ < 0.00001) sig_F2_ = sqrt(abs(F2))
                    if (sig_F2_ < 0.00001) sig_F2_ = sqrt(abs(F2))
                    EXCLUDE_NEG: reject all negative intensity reflections
                    OUT_n : write every n reflections
                    MAX_n : list the n most intensive reflections
                    MAX_ALL: list all reflections in decreasing intensities order
                    STAT : statistics output on hkl reflections
                    NO_STAT: no statistics output on hkl reflections
                    FREE : free format for hkl data (only h,k,l,F2
                        and sig_F2 are read).
                    SEMIFREE : semifree format for hkl data : fixed 3I4 format
```

only h,k,l and free for F2 and sig\_F2  
 FMT= : format of the hkl file (default format  
 corresponds to the SHELX format (3I4, 2F8.2)  
 EXTRACT\_P4P/CREATE\_P4P : create a P4P file containing  
 cell parameters and esd's, orientation matrix, radiation  
 source, symmetry and Bravais lattice.  
 EXTRACT\_EDIT\_P4P/CREATE\_EDIT\_P4P/EXTRACT\_P4P\_EDIT/  
 CREATE\_P4P\_EDIT: create and edit a P4P file.  
 MULT=xx: intensities and sigma are multiplied by xx factor.  
 . action: plot the  $F_2=f(\sin\Theta/\lambda)$  curve with WinPLOTR  
 . examples: FILE my\_HKL\_FILE.HKL MAX\_10  
 FILE import.CIF plot  
 FILE file.HKL FMT=(3i4,2f15.2)  
 . identical keywords: FILE, READ\_HKL

[top of CRYSCALC keywords list]

#### • FIND\_HKL

. type: OUTPUT keyword  
 . arguments: 3 integer values: h, k, l  
 or  
 characters with one or two index characters being h,  
 k or l  
 . optional arguments: EQUIV, FRIEDEL (only for integer values of h, k and l  
 . meaning: search a particular hkl reflection in a  
 reflections list  
 . arg = EQUIV: search for equivalent reflections  
 (Space group is mandatory)  
 . arg = FRIEDEL: search for Friedel reflections  
 . output: list of required hkl reflections  
 . mandatory keyword: FILE  
 . identical keywords: FIND\_HKL, FINDHKL, SEARCH\_HKL  
 . examples: FIND\_HKL 1 1 0 FRIEDEL  
 FIND\_HKL h 0 0  
 FIND\_HKL 2 k 0  
 FIND\_HKL -1 k l

[top of CRYSCALC keywords list]

#### • FIND\_HKL\_LIST

type: OUTPUT keyword  
 mandatory argument: 1 integer value corresponding to the numor in the  
 following the extinction rules list:

1.	h00	h=2n+1	21	.	.
2.	0k0	k=2n+1	.	21	.
3.	00l	l=2n+1	.	.	21
4.	0kl	k=2n+1	b	.	.

```

5. Okl      l=2n+1  c  .  .
6. Okl      k+l=2n+1 n  .  .
7. h0l      h=2n+1  .  a  .
8. h0l      l=2n+1  .  c  .
9. h0l      h+l=2n+1 .  n  .
10. hk0     h=2n+1  .  .  a
11. hk0     k=2n+1  .  .  b
12. hk0     h+k=2n+1 .  .  n
13. hhl     h+l=2n+1 .  .
14. hkk     k+h=2n+1 .  .
15. hkh     h+k=2n+1 .  .
16. hkl     k+l=2n+1 (A)
17. hkl     h+l=2n+1 (B)
18. hkl     h+k=2n+1 (C)
19. hkl     not all odd/even (F)
20. hkl     h+k+l=2n+1 (I)
21. h00     h/=4n  41 .  .
22. Ok0     k/=4n  .  41 .
23. 00l     l/=4n  .  .  41
24. Okl     k+l/=4n d  .  .
25. h0l     h+l/=4n .  d  .
26. hk0     h+k/=4n .  .  d
27. h-hl, h0l, Okl  l=2n+1
28. hkl     h=2n+1
29. hkl     k=2n+1
30. hkl     l=2n+1
31. hkl     h=2n+1 and k=2n+1
32. hkl     h=2n+1 and l=2n+1
33. hkl     k=2n+1 and l=2n+1
34. hkl     -h+k+l=3n (Robv)
35. hkl     h-k+l=3n (Rrev)

```

or a characters string in the following list :  
A, B, C, I, F corresponding to the #13, #14, #15,  
#16 and #17 in the previous list.

meaning: If the integer value is negative, the opposite condition will be searched in the HKL file.

optional arguments: search, in a reflections list, those obeying to the selected extinction rule

- . arg = "OUT": the requested list will be output on the screen
- . arg = "ALL": no condition about F2 and F2/sig is required
- . arg = "WRITE": requested list is stored in a HKL file
- . arg = "SUPPRESS"/"REMOVE": requested list is removed from the initial file
- . arg = real value: F2/sig value

mandatory keyword: FILE

examples: FIND\_HKL\_LIST 5 OUT ALL  
FIND\_HKL\_LIST I WRITE SUPPRESS

identical keywords: FIND\_HKL\_LIST, FIND\_HKL\_LST, EXTRACT\_HKL\_LIST, EXTRACT\_HKL\_LST

[top of CRYSCALC keywords list]

- **FRIEDEL**

. type: CALCULATION keyword  
 . optional argument: symmetry (characters string): "TRIC", "MONO", "ORTHO", "TETRA", "TRIG", "HEXA", "CUB"  
 . meaning: calculate the number of Friedel pairs in a hkl file  
 . mandatory keyword: FILE, SPGR if no symmetry argument  
 . identical keywords: FRIEDEL, FRIEDEL\_PAIRS  
 . example: FRIEDEL mono

[top of CRYSCALC keywords list]

- **GEN\_HKL**

. type: calculation keyword  
 . arguments: characters strings  
 . meaning: generate a hkl reflections list in a particular scattering range:  
 . STL\_min=xx STL\_max=xx for SinTheta/lambda range, in A-1  
 . d\_min=xx d\_max=xx for d range, in A  
 . Q\_min=xx Q\_max=xx for  $Q=4\pi*\text{SinTheta}/\text{lambda}$  range, in A  
 . Theta\_min=xx Theta\_max=xx for Theta range, in deg.(dependent keyword = WAVE)  
 . 2Theta\_min=xx 2Theta\_max=xx for 2Theta range, in deg. (dependent keyword = WAVE)  
 If atoms are unknown, a simulation of a Debye Scherrer film, with equal intensities of Bragg peaks, is created. Format is .PGF type with "DATA: X COMM" and "data\_type=3" identifiers and can be plotted with the latest version of WinPLOTR software, downloaded from:  
<https://cdifx.univ-rennes.fr/progs/winplotr/winplotr.exe>  
 If this latest version of WinPLOTR has been installed, this Debye-Scherrer film (cryscalcalc\_DSf.pgf file) is automatically plotted.  
 If atoms are input, a structure factor calculation is done. In the case where scattering variable is 2theta, a list of I/Imax values is output.  
 . optional arguments . "OUT": a list of generated reflections will be output  
 . "OUT\_n": sort the reflections list by decreasing F2calc and output the n more intensive ones.  
 . "OUT\_ALL": sort the reflections list by decreasing F2calc and output all of them.  
 . "PM2K": hkl reflections list stored in the PM2K format

- . "PAT": In the case where scattering variable is 2theta, atoms are input and space group is known, a diffraction pattern is then created. Two different files are output :
  - cryscalcalc\_pat.xy (2 columns)
  - cryscalcalc\_pat.prf (FullProf format)
 If WinPLOTR is installed on the workstation, it is automatically launched with the PRF file.  
 If "PAT\_NOPLOT" is used instead of "PAT", WinPLOTR is not launched.  
 If "PAT\_PLOT" is used instead of "PAT", WinPLOTR will be launched, independently of the value of "plot\_PRF" value in the setting file.  
 If "PAT\_PLOT\_XY" is used instead of "PAT", WinPLOTR will be launched, independently of the value of "plot\_XY" value in the setting file.  
 If "PAT\_NORMA\_xxx", the simulated diffraction pattern is normalized to xxx value, i.e. maximum counting is set to xxx.  
 If "\_PDPF" string is added to "PAT" or "PAT\_PLOT", a Powder Diffraction Pattern File (.pdf) is created, containing hkl list, 2theta, d\_hkl values and relative intensities.
- . "SIZE=XXX" : specify particles size (XXX in A)
- . "SIZE\_Y=xxx" : specify particles size effects(xxx) (HL=size\_Y/cosTheta)
- . "STRAIN=XXX" : specify strains (1.E-06 - 0.02 range)
- . "STRAIN\_U=xxx": specify strains effects (HG\*\*2=strain\_U\*tanTheta)\*\*2
- . output:
  - calculation of interplanar distance d\_hkl, in A (dependent keyword = CELL)
  - calculation of Bragg angle 2theta\_hkl, in deg. (dependent keyword = CELL, WAVE)
  - structure factor calculation (dependent keywords = ATOM)
- . mandatory keywords: CELL, SPGR
- . examples
  - GEN\_HKL theta\_min=0. THETA\_max=25. OUT
  - GEN\_HKL d\_min=0.5. d\_max=5.
  - GEN\_HKL 2THETA\_min=0. 2THETA\_max=125. OUT PAT
  - GEN\_HKL 2THETA\_min=0. 2THETA\_max=125. OUT PAT SIZE=150
- . identical keywords: GEN\_HKL, GENERATE\_HKL, GENERATE\_HKL\_LIST

[top of CRYSCALC keywords list]

### ● GET\_FORMAL\_CHARGES

type: calculation keyword  
 argument: no  
 meaning: determination of the formal charges of atoms using bond-valence sums, in a crystal structure read from a .CIF, .INS, .PCR file.

The Set\_Formal\_Charges CFML routine written by Nebil Ayape Katcho is used  
 identical keywords: GET\_FORMAL\_CHARGES, FORMAL\_CHARGES, GET\_FORMAL\_CHARGE, FORMAL\_CHA

[top of CRYSCALC keywords list]

- **GET\_TRANS\_MAT**

type: calculation keyword  
 argument: no  
 meaning: determination of the transformation matrix between two primitive unit cells (matrix determinant is equal to 1). if CELL keyword has been previously input, the input parameters are corresponding to cell #1, and only cell #2 parameters will be asked to input. If no transformation matrix is founded, the user is invited to enter its own tolerance value (default value = 0.3). This tolerance factor is defined as follows:  

$$\text{tol} = \text{ABS}(p1\_t1 - p1\_2) + \text{ABS}(p2\_t1 - p2\_2) + \text{ABS}(p3\_t1 - p3\_2) + \text{ABS}(p4\_t1 - p4\_2) + \text{ABS}(p5\_t1 - p5\_2) + \text{ABS}(p6\_t1 - p6\_2)$$
 where p1 ... p6 are parameters of transformed cell #1 and parameters for input cell #2.  
 Remark: range of indices for transformation matrix has been fixed to -2 to 2 (step=1, i.e. only integer matrix elements are allowed)  
 identical keywords: GET\_TRANS\_MAT, GET\_TRANSF\_MAT, GTM, GET\_MAT, SEARCH\_MAT, SEARCH\_TRANSF\_MAT

[top of CRYSCALC keywords list]

- **HEADER**

type: OUTPUT keyword  
 argument: no  
 meaning: write header text of CRYSCALC  
 identical keywords: HEADER, HEAD

[top of CRYSCALC keywords list]

- **HEX\_RHOMB**

. type: OUTPUT keyword  
 . arguments : no argument  
 . outputs: give transformation matrix from hexagonal to rhomboedral setting  
 . mandatory keyword: no  
 . identical keywords: HEX\_RHOMB, HEXA\_RHOMB, HEX\_TO\_RHOMB, HEXA\_TO\_RHOMB

[top of CRYSCALC keywords list]

- **HKL**

. type: INPUT keyword  
. arguments: 3 reals  
. meaning: h,k,l, Miller indices  
. output: calculation of interplanar distance  $d_{hkl}$ , in Å  
(dependent keyword = CELL)  
calculation of Bragg angle  $2\theta_{hkl}$ , in deg.  
(dependent keyword = CELL, WAVE)  
. identical keywords: HKL, HKL\_CALC, CALC\_HKL  
. example: HKL 1. 0. 1.  
. mandatory keyword: CELL

[top of CRYSCALC keywords list]

- **HKL\_DIFF**

. type: INPUT keyword  
. arguments: 2 characters strings  
. meaning: hkl\_1 and hkl\_2 files:  
.HKL (SHELX format)  
.INT (for FullProf; format is specified in the second line)  
. output: calculation of difference F2 for common hkl reflections  
create HKL\_diff.hkl output file (SHELX format) containing  
h k l F2 and sig, with:  
 $F2 = F2_1 - F2_2$   
 $sig = \sqrt{sig_1^2 + sig_2^2}$   
. remark: This can be usefull to extract magnetic contribution from data  
collections in the magnetic and paramagnetic temperature  
ranges.  
. identical keywords: HKL\_DIFF, DIFF\_HKL  
. example: HKL\_diff 2K.int 10K.int

[top of CRYSCALC keywords list]

- **HKL\_MULT**

. type: output keyword  
. arguments: no  
. meaning: provides multiplicity of input HKL reflexion  
. mandatory keyword: SPGR  
. identical keywords: MULT\_HKL, MULT, HKL\_MULT, MUL\_HKL, MUL, HKL\_MUL

[top of CRYSCALC keywords list]

- **HKL\_NEG**

```
. type:                output keyword
. arguments:           no
. meaning:             search for negative intensity reflections in a HKL
                      file
. optional keywords:  . arg = "OUT": requested reflections are output on the
                      screen
                      . arg = "WRITE": requested reflections are output in a
                      HKL file
. mandatory keyword:  FILE
. identical keywords: HKL_NEG, HKL_NEGATIVE, NEG_HKL, NEGATIVE_HKL
. related keyword:    HKL_POS
```

[top of CRYSCALC keywords list]

- **HKL\_POS**

```
. type:                output keyword
. arguments:           no
. meaning:             search for positive intensity reflections in a HKL
                      file
. optional keywords:  . arg = "OUT": requested reflections are output on the
                      screen
                      . arg = "WRITE": requested reflections are output in a
                      HKL file
                      . arg = real_value (n_sig): only positive reflections
                      with  $I > n\_sig * sig(F2)$  are output
. mandatory keyword:  FILE
. identical keywords: HKL_POS, HKL_POSITIVE, POS_HKL, POSITIVE_HKL
. related keyword:    HKL_NEG
```

[top of CRYSCALC keywords list]

- **INSIDE**

```
. type:                output keyword
. arguments:           no
. meaning:             put the atoms of the atom list inside the unit cell
. output:             list of atoms with atomic coordinates in the 0.0 - 1.0 range
. mandatory keyword:  ATOM or atom list in a .INS/.RES file
```

[top of CRYSCALC keywords list]

- **KAPPA\_TO\_EULER**

. type: calculation keyword  
 . argument: 3 real values, corresponding to phi, omega and kappa values (in degrees)  
 . meaning: convert motors angles values of single crystal diffractometer from Kappa to Eulerien geometry, given Phi, Omega and Kappa values.  
 . identical keywords: KAPPA, KAPPA\_TO\_EULER

[top of CRYSCALC keywords list]

- LIST\_EXTI

type: OUTPUT keyword  
 argument: no  
 meaning: list the extinction rules implemented in CRYSCALC  
 identical keywords: LIST\_EXTI, LIST\_EXTI\_RULE, LST\_EXTI, LST\_EXTI\_RULE

[top of CRYSCALC keywords list]

- LIST\_HKL\_MAX

. type: OUTPUT keyword  
 . argument: 1 integer, corresponding to the number n of reflections to list. HKL file has to be read first.  
 . meaning: output the n most intensive observed reflections  
 . identical keywords: LIST\_HKL\_MAX, HKL\_MAX, MAX, LIST\_F2\_MAX, F2\_MAX  
 . example: HKL\_MAX 25

[top of CRYSCALC keywords list]

- LIST\_HKL\_FC\_MAX

. type: OUTPUT keyword  
 . optional argument: 1 integer, corresponding to the number n of reflections to output. A crystal structure has to be input first through READ\_INS/READ\_CIF/READ\_PCR keywords. Default value for n = 10.  
 . meaning: output the n most intensive calculated reflections  
 . identical keywords: LIST\_HKL\_FC\_MAX, HKL\_FC\_MAX, FC\_MAX, FC\_MAX, MAX\_FC, MAX\_FC  
 . example: FC\_MAX 10

[top of CRYSCALC keywords list]

- LIST\_KEYS

```
. type:                OUTPUT keyword
. optional argument:   characters string containing "*" character
. meaning:            list of keywords:
                    . if no argument: all the keywords are listed
                    . if "*" character is present in the character
                      string: all the keywords containing the
                      the characters string before or after the "*"
                      will be listed
. identical keywords: KEY, KEYS, LST_KEYS, LIST_KEYS, LST_KEYWORDS,
                    LIST_KEYWORDS
. examples:          . KEYS
                    . KEYS HKL*
```

[top of CRYSCALC keywords list]

- **LIST\_LAUE**

```
. type:                OUTPUT keyword
. argument:           no
. meaning:            list of Laue classes
. identical keywords: "LST_LAUE", "LIST_LAUE", "LST_LAUE_CLASS",
                    "LIST_LAUE_CLASS"
. examples:          . LIST_LAUE
```

[top of CRYSCALC keywords list]

- **LIST\_MATR**

```
. type:                OUPUT keyword
. arguments:          no
. meaning:            list of transformation matrices implemented in CRYSCALC
                    (direct and inverse matrices) and defined by the user
                    in the CRYSCALC.INI setting file.
. identical keywords: LST_MAT, LST_MATR, LST_MATRIX, LIST_MAT, LIST_MATR,
                    MAT_LST, MAT_LIST, MATR_LST, MATR_LIST, LIST_MATRIX,
                    LIST_TRANSFORMATION_MATRIX
```

[top of CRYSCALC keywords list]

- **LIST\_MATR\_USER**

```
. type:                OUPUT keyword
. arguments:          no
. meaning:            list of transformation matrices defined by the user
                    in the CRYSCALC.INI setting file.
. identical keywords: LST_MAT_USER, LST_MATR_USER, LST_MATRIX_USER, LIST_MAT_USER,
                    LIST_MATR_USER, MAT_LST_USER, MAT_LIST_USER, MATR_LST_USER,
```

MATR\_LIST\_USER, LIST\_MATRIX\_USER,  
LIST\_TRANSFORMATION\_MATRIX\_USER

[top of CRYSCALC keywords list]

- LIST\_SG

```
. type:          OUPUT keyword
. arguments:     characters strings
                  available arguments (order is not important):
. symmetry arguments: "all", "centric", "acentric",
                    "triclinic", "monoclinic", "orthorhombic",
                    "tetragonal", "trigonal", "hexagonal", "cubic"
. "chiral", "enantio", "polar"
. Bravais arguments: "P", "A", "B", "C", "I",
                    "F", "R"
. Laue class arguments: "laue_n", with n relative
  to the numor of Laue class of the space group:
    n=1: -1                n=8: -3m (rhomb. axes)
    n=2: 2/m              n=9: -31m (hex. axes)
    n=3: mmm              n=10: -3m1 (hex. axes)
    n=4: 4/m              n=11: 6/m
    n=5: 4/mmm           n=12: 6/mmm
    n=6: -3 (rhomb. axes) n=13: m-3
    n=7: -3 (hex. axes)  n=14: m-3m
. "mult/multi/multiplicity": output the general multicplicity
  of the space group
. meaning:       list space groups with corresponding IT number, Laue group and
                  point group.
                  if POLAR is given as argument: list only the non-centrosymmetric
                  space groups containing mirror planes.
                  if CHIRAL is given as argument: list only the 65 chiral
                  space groups (Sohncke groups), i.e. containing only rotation
                  or screw axes (no inversion center, no mirror plane, no glide
                  plane)
                  if ENANTIO is given as argument: list only the 11 pairs of
                  enantiomorphic space groups (screw axes of opposite handedness)
. examples:     LST_SG tetragonal centric: list tetragonal and centric
                  space groups
                  LST_SG acentric monoclinic C: list monoclinic,
                  acentric and C centred space groups
                  LST_SG laue_4: list tetragonal space groups with 4/m
                  Laue class
                  LST_SG trigonal enantio
                  LST_SG cubic chiral
                  LST_SG chiral
. identical keywords: LIST_SG, LST_SG, LIST_SPACE_GROUPS
```

[top of CRYSCALC keywords list]

- **MAG**

```
. type:                OUTPUT keyword
. arguments :          characters string (atom or ion label)
. outputs:             list magnetic features of the current ion or atom:
                      electronic configuration, level, magnetic moment ...
                      for 3d and 4f elements
. identical keywords: MAG, MAGNETIC
. examples:           mag Mn3+
.                   mag TB
```

[top of CRYSCALC keywords list]

- **MAN**

```
. type:                OUTPUT keyword
. optional arguments: characters strings
. meaning:             get the CRYSCALC manual
. output:             list the meaning and use of CRYSCALC keywords
                      . if no arguments: all the keywords are listed
                      . optional arguments are keywords name
                      . if "*" character in the characters string: all the
                        keywords containing the characters string before
                        or after the "*" will be listed
. examples:           MAN wave cell
                      MAN ANG*
. identical keywords: MAN, HELP
```

[top of CRYSCALC keywords list]

- **MAN\_HTML**

```
. type:                OUTPUT keyword
. optional argument:   'browse'
. meaning:             get the CRYSCALC manual in HTML format
                      open the HTML file with the current browser
. output:             list the meaning and use of CRYSCALC keywords
. examples:           MAN_HTML
. identical keywords: MAN_HTML, HTML_MAN, HTML
```

[top of CRYSCALC keywords list]

- **MATMUL**

```
. type:                calculation keyword
. arguments:          no
. meaning:           input of components of 3*3 matrices as follows:
```

. ouput: M11, M12, M13, M21, M22, M23, M31, M32, M33  
 calculation of the MixM2 matrix

[top of CRYSCALC keywords list]

- **MATRIX**

. type: INPUT keyword  
 . arguments: 9 reals (+ 3 optional reals)  
 . meaning: transformation (3,3) matrix components  
 if 3 optional extra reals are input, they are  
 considered as origin shift to apply to new  
 coordinates  
 . examples: MATR 0 0 1 0 1 0 -1 0 -1  
 MATR 0.5 0.5 0 -0.5 0.5 0 0 0 1  
 MATR 1/2 1/2 0 -1/2 1/2 0 0 0 1

or

. arguments: "#" 1 integer  
 . meaning: number of matrix in the matrices list implemented in  
 CRYSCALC (see LIST\_MATR keyword)  
 . example: MATR #3  
 . special arguments : "I" : identity matrix  
 "-I" : inverse matrix

or

. arguments: 3 characters strings among a, -a, b, -b, c, -c and  
 combinations.  
 . meaning: setting of the unit cell  
 . examples: MATR -c b a  
 MATR -a-c -b c

or

. arguments: 2 characters strings: P, A, B, C, I, F, R\_rev, R\_obv  
 Following transformations are allowed:  
 MAT P R (MAT #9, for rhomboedral to hexagonal  
 transformation)  
 MAT R P (MAT #10, for hexagonal to rhomboedral  
 transformation)  
 MAT R\_rev R\_obv (MAT #11, for observe/reverse  
 transformation in hexagonal type R setting)  
 MAT R\_obv R\_rev (MAT #12, for reverse/observe  
 transformation in hexagonal type R setting)  
 MAT P A (MAT #13)  
 MAT A P (MAT #14)  
 MAT P B (MAT #15)  
 MAT B P (MAT #16)  
 MAT P C (MAT #17)  
 MAT C P (MAT #19)  
 MAT P F (MAT #19, for rhomboedral to cubic F transformation)  
 MAT F P (MAT #20, for cubic F to rhomboedral transformation)  
 MAT P I (MAT #21, for rhomboedral to cubic I transformation)  
 MAT I P (MAT #22, for cubic I to rhomboedral transformation)

MAT F R (MAT #36, for cubic F to hexagonal R transformation)  
 MAT R F (MAT #37, for hexagonal R to cubic F transformation)  
 MAT C I (MAT #38, for mono/ortho C to mono/ortho I transformation)  
 MAT I C (MAT #39, for mono/ortho I to mono/ortho C transformation)

. meaning: Bravais lattices of the original and final cells.  
 The transformation matrices are related to matrices  
 from #9 to #22 and #36 and #37 in the matrix list

. example: MATR C P  
 MATR R\_obv R\_rev

. optional argument: UPDATE/NO\_UPDATE: update or not cell parameters and atomic  
 coordinates after transformation (independently of the  
 "update\_parameters" value in the setting file)

. output: . calculation of new cell parameters (dependent keyword = CELL),  
 new atomic coordinates (dependent keyword = ATOM) if matrix  
 determinant is equal to 1., and new hkl Miller indices  
 (dependent keyword = HKL)  
 . create a new file containing the new hkl indices (dependent  
 keyword = FILE)

. identical keywords: MAT, MATR, MATRIX, TRANS, TRANSF

[top of CRYSCALC keywords list]

#### • MENDEL

. type: OUTPUT keyword

. arguments: characters strings

. meaning: atom type or atomic number

. output: get atomic features: atomic number, weight,  
 density, electronic configuration, oxydation  
 states, ionic radius, ...  
 get neutron data: scattering length, scattering  
 and absorption cross sections  
 get Xrays data: mass attenuation coefficient,  
 total interaction cross sections, coefficient)  
 for scattering factor calculation =f(stl),  
 values of D\_fp and D\_fpp anomalous dispersion  
 coefficient (for Cr, Fe, Cu, Mo and Ag radiations)

. optional arguments: - PLOT: create a .PGF file containing the scattering factor  
 values versus SinTheta/lambda and plot it with WinPLOTR  
 - EXTRACT\_WGT : output only atomic weight  
 - EXTRACT\_CR : output only covalent radius  
 - EXTRACT\_IR : output only ionic radius  
 - EXTRACT\_VDWR: output only Van der Waals radius  
 - EXTRACT\_VOL : output only atomic volume  
 - EXTRACT\_X : output only Xrays data  
 - EXTRACT\_N : output only neutrons data  
 - EXTRACT\_EC : output only electronic configuration

. examples: MENDEL TI C  
 MENDEL Cu+2 PLOT  
 MENDEL 59

[top of CRYSCALC keywords list]

- **MERGE**

. type: CALCULATION keyword  
. optional argument: symmetry (characters string): "TRIC", "MONO", "ORTHO",  
"TETRA", "TRIG", "HEXA", "CUB"  
. meaning: merge the data in the current symmetry and create  
a xxx\_merge.HKL file  
. mandatory keyword: FILE, SPGR if no symmetry argument  
. example: merge monoclinic

[top of CRYSCALC keywords list]

- **MONOCLINIC**

. type: OUTPUT keyword  
. outputs: . list the transformation matrices for equivalent  
monoclinic settings  
. if CELL exists: apply the transformation matrices  
to give new monoclinic cell parameters  
. mandatory keyword: NO\_OUT  
. optional keyword: CELL  
. identical keywords: MONOCLINIC, MONOC, MONOCL

[top of CRYSCALC keywords list]

- **NEWS**

. type: OUTPUT keyword  
. outputs: list the last new possibilities implemented in CRYSCALC  
. optional argument: specified year or LAST to get CRYSCALC news from a specific  
year of the latest month.  
. example: NEWS 2010  
. identical keywords: NEWS

[top of CRYSCALC keywords list]

- **NIGGLI**

. type: OUTPUT keyword  
. arguments : no argument  
. output: transform the current triclinic cell to the Niggli  
cell.  
. related keyword: CELL  
. identical keywords: NIGGLI, NIGGLI\_CELL

[top of CRYSCALC keywords list]

- **OBV\_REV**

. type: OUTPUT keyword  
. arguments : 1 integer  
. meaning: twin matrix number:  
. 1: matrix law = (-1 0 0 0 -1 0 0 0 1): twofold  
axis parallel to threefold  
. 2: matrix law = ( 0 -1 0 -1 0 0 0 0 -1): twofold  
axis parallel to (a-b)  
. outputs: analysis of the reflections versus the parity  
. remark: if no argument is given, first matrix law is taken  
. mandatory keyword: FILE  
. identical keywords: OBV\_REV, OBVERSE\_REVERSE, TWIN\_OBVERSE\_REVERSE  
TWIN\_OBV\_REV, TWINNING\_OBVERSE\_REVERSE  
TWINNING\_OBV\_REV

[top of CRYSCALC keywords list]

- **PAUSE**

PAUSE:

. type:  
. arguments : no  
. meaning: create a break in the execution of the requested  
commands. This keyword can be useful when commands  
are executed through a .CFL command file

[top of CRYSCALC keywords list]

- **PERMUT**

. type: OUTPUT keyword  
. arguments : no  
. meaning: apply matrix #3, #4, #5, #6 and #7 (see LIST\_MATR  
keyword) to the initial cell parameters, independently  
to the update\_parameters value in the setting file. This  
corresponds to axes permutation.  
. outputs: new cell parameters and new volume, obtained after  
applying matrix #n  
if cell parameters are unknown: list the  
transformation matrix

[top of CRYSCALC keywords list]

- **PLANE**

. type: OUTPUT keyword  
 . arguments : 3 atom labels minimum (max.=20)  
 . meaning: calculate the equation of the mean plane ( $Ax+By+Cz+D=0$ )  
 containing input atoms.  
 . outputs: output the four components A, B, C and D of the plane  
 equation.  
 . identical keywords: PLANE, PLAN

[top of CRYSCALC keywords list]

- **Q\_HKL**

. type: CALCULATION keyword  
 . argument: real values  
 . meaning:  $Q=4\pi \cdot \sin\theta / \lambda$  values  
 . outputs: d\_hkl(A),  $\sin\theta / \lambda(A-1)$   
 theta(deg) for known wavelength  
 . optional keyword: WAVE  
 . identical keywords: QHKL, Q\_HKL  
 . example: QHKL 10.

[top of CRYSCALC keywords list]

- **QVEC**

. type: input keyword  
 . arguments : 3 reals  
 . meaning: components of the propagation vector  
 . outputs: apply the propagation vector on the hkl list and  
 calculate the corresponding d value  
 . mandatory keyword: HKL  
 . identical keywords: QVEC, Q\_VEC, Q\_VECTOR, KVEC, K\_VEC, K\_VECTOR,  
 MOD\_VEC, MODULATION\_VECTOR  
 . example: QVEC 0.5 0.5 0.

[top of CRYSCALC keywords list]

- **READ\_ACE**

. type: input keyword  
 . argument: 1 characters string corresponding to a ACE file name  
 . meaning: read a ACE format file (CarINE format) to extract  
 structural features as: space group, cell parameters  
 and atomic positions.  
 . identical keywords: READ\_ACE, READ\_ACE\_FILE, READ\_CARINE, FILE\_ACE, OPEN\_ACE, ACE  
 . example: READ\_ACE my\_file.ace

[top of CRYSCALC keywords list]

- **READ\_CEL**

. type: input keyword  
. argument: 1 characters string corresponding to a CEL file name  
. meaning: read a CEL format file (PowderCELL format) to extract structural features as: space group, cell parameters and atomic positions.  
. identical keywords: READ\_CEL, READ\_CEL\_FILE, READ\_POWDERCELL, FILE\_CEL, OPEN\_CEL, CEL  
. example: READ\_CEL my\_file.cel

[top of CRYSCALC keywords list]

- **READ\_CIF**

. type: input keyword  
. argument: 1 characters string corresponding to a CIF file name  
If not extension is given, .cif is assumed.  
. meaning: read a CIF format file to extract structural features:  
as: space group and/or symmetry operators, cell parameters, atomic positions, wavelength ...  
if "VOIDS" optional argument is specified: calculation of porosity through Monte-Carlo method  
. identical keywords: READ\_CIF, READ\_CIF\_FILE, CIF\_FILE, FILE\_CIF, OPEN\_CIF, CIF  
. examples: READ\_CIF my\_file.cif  
READ\_CIF my\_cif\_file

[top of CRYSCALC keywords list]

- **READ\_EXP**

. type: input keyword  
. argument: 1 characters string corresponding to a .EXP file name,  
created by APEX3/APEX4 software and containing data collection strategy.  
. meaning: read a EXT format file to extract experimental scans features.  
. example : READ\_EXP my\_Mo\_EXP.EXP  
. identical keywords: READ\_EXP, FILE\_EXP, OPEN\_EXP

[top of CRYSCALC keywords list]

- **READ\_FACES**

. type: input keyword  
. optional argument: 1 characters string corresponding file name

containing crystal shape habitus :  
 - absorb.ins file created by Collect software (Nonius).  
 - faces.def file created by WinGX.  
 if absent, shape file = absorb.ins  
 . meaning: read a file containaing crystal shape as  
 (h,k,l,dim) list.  
 . identical keywords: READ\_FACES, FACES  
 . examples: READ\_FACES my\_absorb.ins  
 READ\_FACES faces.def

[top of CRYSCALC keywords list]

### • READ\_FCF

. type: INPUT keyword  
 . argument : 1 characters string  
 . meaning: read .FCF file name, created by SHELXL with (LIST 4, LIST 6  
 or LIST 8 instruction) a list of h, k, l, F2\_calc, F2\_obs, sig\_F2  
 . outputs: . calculation of R1 and wR2 agreement factors  
 . list of strange reflections with  $(F2o - F2c)/sig < -100$ .  
 . list of strange reflections with  $(F2o - F2c)/sig < -10$   
 and  $theta < 3$ .  
 . list of strange reflections with  $ABS(F2o - F2c)/sigW > 10$ .  
 . list of strange reflections with  $F2o < -2sigW$   
 . optional arguments:  
 PLOT : create a \*\_FCF.PGF file for WinPLOTR  
 (F2c = f(F2o) curve)  
 PLOT\_STL : create a \*\_FCF\_stl.PGF file for WinPLOTR  
 (F2c - F2o = f(FSinTheta/lambda) curve)  
 OUT\_n : output every n reflections  
 HKL/CREATE\_HKL : creation of .hkl file (free format)  
 OMIT : list outliers reflections preceded by OMIT instruction  
 for SHELXL refinement program  
 OMIT\_UPDATE: update .INS file with OMIT keywords for outliers  
 reflections.  
 . examples: FCF\_FILE my\_FCF\_FILE.FCF  
 FCF\_FILE FCF.fcf out\_n plot  
 . identical keywords: FCF\_FILE, FILE\_FCF, READ\_FCF

[top of CRYSCALC keywords list]

### • READ\_HKLF5

. type: input keyword  
 . argument: 1 characters string corresponding to a HKLF5 file  
 name  
 . optional argument: "OUT", "ANA", "NOR", "ONLY\_1"  
 . meaning: read a HKLF5 format data file containing structure factors  
 of a twinned crystal.

Output statistics for all reflections as well as overlapping and non-overlapping reflections for each twin component.

If "OUT" is given as argument, the list of clusters of reflections (> 2 components) will be output.

If "ANA" is given as argument, an analysis of redundant reflections is performed.

If "NOR" is given as argument, a file containing only non-overlapping reflections is created.

If "ONLY\_1" is given as argument, a file containing only reflections of domain #1 (non-overlapping and overlapping reflections) is created.

. identical keywords: READ\_HKLF5, FILE\_HKLF5, OPEN\_HKLF5  
 . example: READ\_HKLF5 twin5.hkl

[top of CRYSCALC keywords list]

- **READ\_INS**

. type: input keyword  
 . argument: 1 character string corresponding to a INS/RES file name (SHELX)  
 If any extension is given, ".ins" will be assumed.  
 . optional arguments: WGHT, HFIX, No\_H  
 . meaning: read a .INS/.RES SHELX format file to extract structural features as: space group and/or symmetry operators, cell parameters, atomic positions, ...  
 If input file is a .RES file and second argument is WGHT the refined weighting scheme is updated in the corresponding .INS file.  
 If optional argument "HFIX" is specified, HFIX instructions are listed after the "PLAN" line. This can be useful after automatic introduction of Hydrogene atoms with the following PLATON command: platon -f job.ins  
 "No\_H/remove\_H" argument for READ\_INS keyword: remove Hydrogen atoms from the .INS file  
 if "VOIDS" optional argument is specified: calculation of porosity through Monte-Carlo method  
 . identical keywords: READ\_INS, READ\_INS\_FILE, INS\_FILE, FILE\_INS, OPEN\_INS, INS\_READ\_RES, READ\_RES\_FILE, RES\_FILE, FILE\_RES, OPEN\_RES, RES  
 . examples: READ\_INS my\_file.ins  
 READ\_INS my\_ins\_file

[top of CRYSCALC keywords list]

- **READ\_LST**

. type: input keyword  
 . argument: 1 characters string corresponding to a LST file name  
 If no extension is given, .lst is assumed.

```

. optional arguments: . ADP:   extract principal mean square atomic displacements U
.                   . AFIX:   extract default effective X-H distances
.                   . ATOMS:  extract final atomic coordinates and ADP's
.                   . CONN:   extract connectivity table
.                   . DIST/BONDS: extract interatomic distances and angles
.                   . FLACK:  extract Flack parameter (if calculated)
.                   . H:      extract Idealized hydrogen atom generation
.                   . HKL/DATARED: extract rejected reflections, number of total
                                reflections, Rint ...
.                   . HKL_STAT: extract reflection statistics
.                   . HTAB:   extract Hydrogen bonds (if exist) and extract from
                                .RES file instructions for potential hydrogen bonds
.                   . LS:     extract least-squares features
.                   . MDR:    extract Most Disagreeable Reflections with
                                Error/esd > 5.0
.                   . MDR_OMIT: extract Most Disagreeable Reflections with
                                Error/esd > 5.0 and output hkl list,
                                preceded by OMIT keyword (format compatible with
                                .INS/.RES SHELXL input file)
.                   . MDR_crit/MDR_OMIT_crit: extract Most Disagreeable Reflections
                                with Error/esd > MDR_crit
                                Note that default criteria value for MDR keyword is equal to 5.
                                but can be specified through the MDR_crit/MDR_OMIT_crit options
.                   . MPLA:   extract least-squares planes
.                   . RHO:    extract difference Fourier peaks
.                   . SPLIT:  extract atoms to split and create part of .INS SHELXL
                                input file containing coordinates splitted atoms and
                                corresponding EADP constraints.
.                   . SPLIT_EDIT: same behavior as SPLIT option but edit the .INS
                                created file if an editor has been specified in
                                the cryscalcalc.ini setting file
.                   . TORSION: extract torsion angles
.                   . UNIT:   extract unit-cell contents from UNIT instruction and
                                atom list and write SFAC/UNIT lines to include in
                                .INS SHELXL input file.
.                   . VAR:    extract analyse of variance for reflections used
                                in refinement

. meaning:          read a LST output file from SHELX to extract hkl,
                    structural and refinement features

. identical keywords: READ_LST, READ_LST_FILE, LST_FILE, FILE_LST, OPEN_LST, LST
. examples:         READ_LST my_file.lst
                    READ_LST my_lst_file MDR_8
                    READ_LST my_lst_file MDR_OMIT_10

```

[top of CRYSCALC keywords list]

- **READ\_NREPORT**

READ\_NREPORT:

. type: input keyword  
. optional argument: browse  
. meaning: read nreport.html file created by the Nonius software suite for KCCD diffractometer.  
If 'browse' is given as argument, launch the browser defined in the 'crystalcalc.ini' setting file.  
If not, outputs the HTML file on screen (without tags).  
. identical keywords: READ\_NREPORT, READ\_report%HTML, READ\_NREPORT\_HTML

[top of CRYSCALC keywords list]

• **READ\_P4P**

READ\_P4P:

. type: OUTPUT keyword  
. optional arguments : P4P file name  
. meaning: read the .P4P file (created by SAINT) present in the current folder (if more than one .P4P file is present, select a P4P file in a .P4P file list) and create a P4P.cif file containing cell parameters (and esd's), wavelength, number of reflections used to refine the cell parameters and related theta\_min and theta\_max.  
. identical keywords: READ\_P4P, READ\_P4P\_FILE, P4P\_FILE, FILE\_P4P, OPEN\_P4P, P4P

[top of CRYSCALC keywords list]

• **READ\_PCR**

. type: input keyword  
. argument: 1 characters string corresponding to a PCR file name  
If not extension is given, .pcr is assumed.  
. meaning: read a PCR FullProf format file to extract structural features as: space group and/or symmetry operators, cell parameters, atomic positions, wavelength ...  
. identical keywords: READ\_PCR, READ\_PCR\_FILE, PCR\_FILE, FILE\_PCR, OPEN\_PCR, PCR  
. examples: READ\_PCR my\_file.pcr  
READ\_PCR my\_pcr\_file

[top of CRYSCALC keywords list]

• **READ\_PDB**

. type: input keyword  
. argument: 1 characters string corresponding to a PDB file name

from the Protein Data Bank.  
 If not extension is given, .pdb is assumed.

. meaning: read a PDB format file to extract structural features as: space group, cell parameters, atomic positions

. identical keywords: READ\_PDB, READ\_PDB\_FILE, PDB\_FILE, FILE\_PDB, OPEN\_PDB, PDB

. examples: READ\_PDB my\_file.pdb  
 READ\_PDB my\_pdb\_file

[top of CRYSCALC keywords list]

- **READ\_SEQ**

. type: OUTPUT keyword

. optional arguments : SEQ file name

. meaning: read the .SEQ file (created by FULLPROF in sequentail mode) create a xx\_tables.seq file in a multicolumns format. Default separator is the "TAB" character but it can be specified in the[OPTIONS] section of the CRYSCAL.ini setting file through "separator=" keyword : separator can be "tab", "space" or "comma"

. identical keywords: READ\_SEQ, SEQ, READ\_SEQ\_FILE, FILE\_SEA, OPEN\_SEQ, SEQ

[top of CRYSCALC keywords list]

- **READ\_SFRM**

. type: input keyword

. argument: 1 characters string corresponding to SUPERFLIP/EDMA input file name.

. meaning: read SUPERFLIP/EDMA input file to extract cell parameters, wavelength, symmetry operators list, centering vectors and deduce space group.

. identical keywords: READ\_SPF, READ\_SUPERFLIP, READ\_EDMA, FILE\_EDMA

. example: READ\_SPF my\_file\_SPF.in

[top of CRYSCALC keywords list]

- **READ\_SPF**

. type: input keyword

. argument: 1 characters string corresponding to the .SFRM file name (diffraction frame from BAXS diffractometers) to be read.

. optional argument: "SHORT" : condensed output from header

. meaning: read the header of a SFRM diffraction frame to extract experiment features (sample temperature, detector temperature, wavelength, target voltage and intensity, motors positions, rotation axis, ...)

. identical keywords: READ\_SFRM, READ\_SFRM\_HEADER, SFRM, OPEN\_SFRM

. example: READ\_SFRM mo\_test\_01\_0001.sfrm

[top of CRYSCALC keywords list]

- **READ\_TIDY\_OUT**

. type: input keyword  
. optional argument: 1 characters string corresponding to the TIDY output file to be read. Default name=stidy.out  
. meaning: read a output file created by TIDY and extract all structural features as: space group, cell parameters, atomic positions.  
. example: READ\_TIDY\_OUT  
. identical keywords: READ\_TIDY\_OUT, READ\_TIDY, OPEN\_TIDY\_OUT, OPEN\_TIDY

[top of CRYSCALC keywords list]

- **READ\_XYZ**

. type: input keyword  
. argument: 1 characters string corresponding to .XYZ input file name  
. optional arguments: H/H\_included, NO\_SORT  
. meaning: read .XYZ file (atom list in cartesian coordinates) and output interatomic distance towards the first atom in the list. By default, Hydrogen atoms are excluded from the list and distances are sorted by increasing values.  
. identical keywords: READ\_XYZ, READ\_CART\_XYZ  
. example: READ\_XYZ my\_file.XYZ H

[top of CRYSCALC keywords list]

- **REC\_ANG**

. type: CALCULATION keyword  
. arguments: 2\*3 reals  
. meaning: calculation of the angle between 2 vectors in the reciprocal space. The 3 first real values are related to the coordinates of the first vector and the 3 last real values to the coordinates of the second vector  
. mandatory keyword: CELL  
. identical keywords: REC\_ANG, RECANG, RECIPROCAL\_ANGLE  
. example: REC\_ANG 1. 0. 0. 0. 1. 0.

[top of CRYSCALC keywords list]

- **REDUCE\_CELL**

. type: CALCULATION keyword  
. argument: 1 character string, corresponding to the Bravais lattice:

P, A, B, C, I, R, F (default = P)

. meaning: calculation of conventional unit cell parameters and transformation matrix between input cell and conventional cell(s). The routine is based on Get\_conventional\_Unit\_Cells program written by JRC using procedures implemented in CRYSFML.

. mandatory keyword: CELL

. identical keywords: REDUCE, REDUCE\_CELL, REDUCED, REDUCED\_CELL

. example: REDUCE F

[top of CRYSCALC keywords list]

#### ● RESET

. type: input keyword

. argument: no

. meaning: initialization of all input parameters and arrays

. identical keywords: RESET, RAZ, INIT, INITIALIZATION

[top of CRYSCALC keywords list]

#### ● RINT

. type: CALCULATION keyword

. optional arguments: symmetry (characters string): "TRIC", "MONO", "ORTHO", "TETRA", "TRIG", "HEXA", "CUB", "SHELL"

. meaning: calculate the internal Rint value  
calculate the completeness of the data collection  
if SHELL argument is present: calculate Rint and completeness in different resolution shells. This option is equivalent to "Rint\_shell = ns" in th cryscal.ini setting file.  
rem : ns\_max = 10

. mandatory keyword: FILE, SPGR if no symmetry argument

. identical keywords: RINT, R\_INT

. example: RINT mono

[top of CRYSCALC keywords list]

#### ● RHOMB\_HEX

. type: OUTPUT keyword

. arguments : no argument

. outputs: give transformation matrix from rhomboedral to hexagonal setting

. mandatory keyword: no

. identical keywords: RHOMB\_HEX, RHOMB\_HEXA, RHOMB\_TO\_HEX, RHOMB\_TO\_HEXA

[top of CRYSCALC keywords list]

- **SAVE\_SETTINGS**

. type: OUTPUT keyword  
. arguments : no argument  
. outputs: create a cryscalcalc.ini setting file in the current folder  
. identical keywords: SAVE\_SETTINGS, SAVE\_SETTING

[top of CRYSCALC keywords list]

- **SEARCH\_EXTI**

. type: OUTPUT keyword  
. arguments: 1 optional characters string or 2 optional real arguments:  
n\_sig, ratio\_criteria  
. meaning: analyse hkl reflections list and search systematic  
extinctions  
if arg="ALL" : all reflections are considered. In the  
other case,  
    . n\_sig: only reflections with  $I/\text{sig} > n\_sig$  will  
    be analysed  
    . ratio\_criteria:  
    if  $\langle F2\_odd \rangle / \langle F2\_even \rangle < \text{ratio\_criteria}$ , the current  
    reflection type is considered as extinction rule.  
. mandatory keyword: FILE  
. identical keywords: SEARCH\_EXTI, FIND\_EXTI  
. example: SEARCH\_EXTI 2 0.02  
. example: SEARCH\_EXTI ALL

[top of CRYSCALC keywords list]

- **SEARCH\_MONO**

. type: OUTPUT keyword  
. optional argument: criterias for searching monoclinic angle  
. meaning: determine monoclinic angle from hkl data integrated  
in a pseudo-orthorhombic unit cell by calculating  
internal R values for "P 2 1 1", "P 1 2 1" and  
"P 1 1 2" space groups (case of primitive Bravais lattice).  
For C centered Bravais orthorhombic lattices, "C 2 1 1" and  
"C 1 2 1" the following space groups are tested.  
Criterias correspond to the max. shift of the angles  
respect to 90. and minimum value of Rint respect to the  
other Rint values respectively.  
Default values of these criteria are 2.5 and 0.2 respectively.  
Criteria\_1: if more than one angle shift towards 90. deg. is  
greater than this criteria value, monoclinic angle search



space groups are listed.

If "ACENTRIC/ONLY\_ACENTRIC" argument is present, only acentric space groups are listed.

In the monoclinic case, if "OMA/ONLY" is given as argument, only space groups with monoclinic angle compatible with unit cell parameters will be output. For example, if beta is the monoclinic angle, only "L 1 x 1" space groups will be considered. Monoclinic angle in unit cell parameters has to be far from 90. of "search\_mono\_criteria" value (default value=2.5, defined in the setting file ([OPTIONS] section) This OMA/ONLY option can also be defined through "search\_SG\_only\_mono" field in the setting file ([OPTIONS] section)

```
. mandatory keyword: FILE
. examples: SEARCH_GROUP 3 0.05
SEARCH_GROUP mono
SEARCH_GROUP centered
. identical keywords: SEARCH_SPGR, SEARCH_SPACE_GROUP, SEARCH_GROUP, SEARCH_SG
CHECK_SPGR, CHECK_SPACE_GROUP, CHECK_GROUP, CHECKGROUP
```

[top of CRYSCALC keywords list]

#### • SEARCH\_SYMM

```
. type: OUTPUT keyword
. optional argument: 1 criteria for searching symmetry
. meaning: calculation of internal R values for different symmetries
and Laue groups and deduction of the most probable one.
Criteria corresponds to the ratio minimum value of Rint with
respect to Rint values calculated in different Laue groups.
Default value is 0.5.
If criteria > 1. : criteria = criteria / 100.
If crystal system is known and corresponds to tetragonal, trigonal
hexagonal or cubic system, this crystal system is taken into account
and calculation for all Laue group is not realized.
If "ALL/FORCE_ALL" argument is present, calculation for all
Laue groups are performed.
If "T/TRICLINIC/FORCE_T/FORCE_TRICLINIC" argument is present,
Rint for P -1 triclinic space group is also performed.
. mandatory keyword: FILE
. identical keywords: SEARCH_SYMM, SEARCH_LAUE
```

[top of CRYSCALC keywords list]

#### • SEARCH\_TETRA

```
. type: OUTPUT keyword
. optional argument: 3 criterias for searching tetragonal axis
. meaning: determine tetragonal axis from hkl data integrated
```

in a pseudo-cubic unit cell by calculating internal R values in abc, cab and bca settings. Criterias correspond to the max. shift for cell parameters respect to mean cell parameter values and max. shift for the angles respect to 90. respectively and minimum value of Rint respect to the other Rint values. Default values for these criteria are: 0.5, 2.5 and 0.2. Criteria\_1: if more than one cell parameter towards the mean cell parameter value greater than this criteria value, tetragonal axis search will be stopped. Criteria\_2: if more than one angle shift towards 90. deg. is greater than this criteria value, tetragonal axis search will be stopped. Criteria\_3: Rint for the right tetragonal axis has to be lower than criteria\_2\*Rint for the others.

```
. example:          SEARCH_TETRA 0.7 3. 0.25
. mandatory keyword: FILE
. identical keywords: SEARCH_TETRA, SEARCH_TETRAGONAL, SEARCH_TETRA_AXIS, SEARCH_TETRAGONAL_AXIS
.                  GET_TETRA, GET_TETRAGONAL, GET_TETRA_AXIS, GET_TETRAGONAL_AXIS
```

[top of CRYSCALC keywords list]

- SET

```
. type:             INPUT keyword
. arguments:        2 string arguments
. meaning:          definition of external applications:
.                  . if arg(1) = "EDITOR": arg(2) is the browser application
.                  . if arg(1) = "BROWSER": arg(2) is the editor application
. example:          set browser "C:\Program Files\Mozilla Firefox\firefox.exe"
```

[top of CRYSCALC keywords list]

- SETTING

```
. type:             OUTPUT keyword
. arguments:        no
. meaning:          output the different parameters defined in the CRYSCALC.INI
.                  setting file
. identical keywords: SETTING, SETTINGS, SETUP
```

[top of CRYSCALC keywords list]

- SFAC

```
. type:             INPUT keyword
. arguments:        n characters strings
```

```

. meaning.: list of chemical elements in the molecule
. output:  - atomic density calculation, in at/cm3
            (dependent keyword = CELL)
            - absorption coefficient calculation
            (dependent keywords = CELL, BEAM)
            - determination of the molecular formula
            (dependent keywords = Z)
            - calculation of the molecular weight
            (dependent keywords = Z)
            - calculation of the atomic and weight
              percentage (dependent keywords = Z)
            - determination of the density
            (dependent keywords = CELL, Z)

. mandatory keyword: UNIT
. example: SFAC C O H N

```

[top of CRYSCALC keywords list]

- **SF\_HKL**

```

. type: INPUT keyword
. arguments: 3 reals
. optional argument: FRIEDEL, SCAT
. meaning: h,k,l, Miller indices
. output: calculation of crystallographic structure
            factor for the hkl reflection
            (dependent keyword = CELL, WAVE, SPGR, ATOM)
            if "FRIEDEL" is specified, a crystal structure factor
            calculation is also performed for -H reflection
            if "SCAT" is specified, atomic scattering factor coefficients
            are output

. example: HKL 1 0 1 FRIEDEL SCAT
. mandatory keyword: CELL, WAVE, SPGR, ATOM
. related keyword : BEAM
. identical keywords: SF_HKL, SFAC_HKL

```

[top of CRYSCALC keywords list]

- **SG**

```

. type: INPUT keyword
. arguments : characters string
. meaning: space group (Hall Mauguin symbol, number in IT)
. outputs: . general informations on the input space group
            . if HKL file has been previously read (see FILE
              keyword), the number of reflections in agreement
              with the space group is output

. see: SG_INFO, SG_EXTI, LST_SYM_OP, SITE_INFO
. example: SPGR P 21 21 21

```

. identical keywords: SPGR, SG, SPACE\_GROUP

[top of CRYSCALC keywords list]

- **SG\_ALL**

. type: OUTPUT keyword  
. arguments : no argument  
. outputs: get informations on the current space group: symmetry operators (complete and reduced set), Wyckoff positions, extinction rules ...  
. mandatory keyword: SPGR  
. identical keywords: SG\_ALL, SP\_ALL

[top of CRYSCALC keywords list]

- **SG\_EXTI**

. type: OUTPUT keyword  
. arguments : no argument  
. outputs: list extinctions rules for the current space group.  
. mandatory keyword: SPGR  
. identical keywords: SP\_EXTI, SP\_EXTI, SG\_EXTINCTIONS, SPACE\_GROUP\_EXTI, SPACE\_GROUP\_EXTINCTIONS

[top of CRYSCALC keywords list]

- **SG\_INFO**

. type: OUTPUT keyword  
. outputs: informations on the space group: list the reduced set of symmetry operators and symmetry symbols.  
. mandatory keyword: SPGR  
. optional argument: ALL: list all symmetry operators (including inversion and lattice centring translations), Wyckoff positions and extinctions rules for current space group.  
. identical keywords: SG\_INFO, SP\_INFO, SPACE\_GROUP\_INFO, LIST\_SPACE\_GROUP\_INFO

[top of CRYSCALC keywords list]

- **SG\_SUB**

```
. type:          OUTPUT keyword
. outputs:      informations on the space group: list the
                Translationengleische Subgroups for the current
                space group.
. mandatory keyword: SPGR
. identical keywords: SG_SUB, SG_SUBGROUP
```

[top of CRYSCALC keywords list]

- SHANNON

```
. type:          OUTPUT keyword
. argument:      characters string
. outputs:      get effective ionic radii from the Shannon table
                (Acta Cryst 1976, A32, 751)
                . ec: electronic configuration
                . CN: coordinence
                . SP: configuration de spin
                . CR: crystal radius
                . IR: effective radius
. identical keywords: SHAN, SHANNON
. examples:     SHANNON Pb
                SHANNON CU+2
```

[top of CRYSCALC keywords list]

- SHELL

```
. type:          CALCULATION keyword
. arguments:     2 characters strings (one mandatory argument) + 2 reals
. meaning:      arg_1 = d:    keeps reflections in the d_min and
                        d_max range
                        created hkl file: HKL_shell_d.hkl
                        dependent keyword: CELL
                arg_1 = stl:  keeps reflections in the stl_min and
                        stl_max range
                        created hkl file: HKL_shell_stl.hkl
                        dependent keyword: CELL
                arg_1 = theta: keeps reflections in the theta_min and
                        theta_max range
                        created hkl file: HKL_shell_theta.hkl
                        dependent keyword: CELL, WAVE
                arg_1 = int:  keeps reflections in the int_min and
                        int_max range
                        created hkl file: HKL_shell_i.hkl
                arg_1 = isig: keeps reflections in the i/sig_min and
                        i/sig_max range
                        created hkl file: HKL_shell_isig.hkl
                arg_2 = plot: create a .PGF file from the created
```

```

                                HKL file and plot it with WinPLOTR
                                (excepted for arg_1=int and
                                arg_1 = isig)
                                real_1:      X_min value
                                real_2:      X_max value
. mandatory keyword:  FILE
. optional argument:  arg_2 = plot
. examples:          SHELL d plot
                   SHELL theta

```

[top of CRYSCALC keywords list]

- **SHIFT\_2TH**

```

. type:                INPUT keyword
. arguments :          3 reals
. meaning:             diffractometer 2theta shift: constant, cos dependent
                       and sin dependent values
. outputs:            apply the diffractometer 2theta shift to the
                       calculated 2theta value:
                       2theta = 2theta_calc + shift_2theta
. mandatory keyword:   HKL, GEN_HKL, GEN_SAT
. identical keywords:  SHIFT_2TH, SHIFT_2THETA, 2TH_SHIFT, 2THETA_SHIFT

```

[top of CRYSCALC keywords list]

- **SIZE**

```

. type:                INPUT keyword
. arguments:           3 reals
. meaning:             crystal dimensions in mm
. output:             crystal volume calculation
                       calculation of the radius of a sphere with identical
                       volume
. example:            SIZE 0.11 0.13 0.122
. identical keywords:  SIZE, CRYSTAL_SIZE

```

[top of CRYSCALC keywords list]

- **SORT**

```

. type:                CALCULATION keyword
. arguments:           2 characters strings
. meaning:            arg_1 = d:      sort HKL file in increasing d_hkl
                       (dependent keyword: CELL)
                       created hkl file: HKL_sort_d.hkl
                       arg_1 = stl:   sort HKL file in increasing

```

```

sinTheta/lambda
(dependent keyword: CELL)
created hkl file: HKL_sort_stl.hkl
arg_1 = theta: sort HKL file in increasing Theta
(dependent keyword: CELL, WAVE)
created hkl file: HKL_sort_theta.hkl
.
arg_1 = int: sort HKL file in decreasing F2
created hkl file: HKL_sort_i.hkl
.
arg_1 = isig: sort HKL file in decreasing F2/sigma
created hkl file: HKL__sort_isig.hkl
.
arg_2 = plot: create a .PGF file from the created
HKL file and plot it with WinPLOTR
(excepted for arg_1=int and
arg_1 = isig)
arg_2 = out_n: list the n first sorted reflections
. mandatory keyword: FILE
. optional argument: arg_2 = plot
. examples: SORT d plot
SORT stl
SORT theta OUT_10

```

[top of CRYSCALC keywords list]

- **STAR\_K**

```

. type: CALCULATION keyword
. argument: no
. meaning: apply rotational parts of symmetry operators
. of the current space group on propagation wave components
. to determine the star of k.
. outputs: list of k vectors and arms of the k star
. mandatory keywords: SPGR, QVEC

```

[top of CRYSCALC keywords list]

- **STL**

```

. type: CALCULATION keyword
. argument: real values
. meaning: sinTheta / lambda values
. outputs: d_hkl(A), Q(A-1)
theta(deg) for known wavelength
. optional keyword: WAVE
. identical keywords: STL, STL_HKL, SINTHETA/WAVE, SINTHETA/LAMBDA
. example: STL 0.70

```

[top of CRYSCALC keywords list]

- **SUPERCELL**

```
. type:                input keyword
. arguments :          3 reals + 1 optional characters string
. meaning:             components of a superstructure cell
. outputs:            if atoms are input, atomic coordinates in the
                    superstructure cell are calculated.
. mandatory keyword:  CELL
. identical keywords: SUPERCELL
. optional arguments: "pcr": output list of atomic coordinates in a .PCR
                    FullProf format.
                    "ins": output list of atomic coordinates in a .INS
                    SHELXL format.
. example:            SUPERCELL 2 2 2 pcr
```

[top of CRYSCALC keywords list]

- **SYMM**

```
. type:                INPUT keyword
. arguments :          12 reals
. meaning:             symmetry operator in numeric form:
                    S11 S12 S13  T1  S21 S22 S23 T2  S31 S32 S33 T3
                    Sij: components of the rotational part of the
                        symmetry operator
                    Ti:  components of the translationnal part of
                        the symmetry operator
. example:            SYMM  1  0  0  0.5  0 -1  0  0.5  0  0 -1  0.
or
. arguments :          string
. meaning:             symmetry operator in alphanumeric form
. example:            SYMM  x+1/2, -y+1/2, -z
. outputs:            apply the current symmetry operator to atomic
                    coordinates (dependent keyword = ATOM)
. optional keyword:   APPLY_OP, SYM_OP
. identical keywords: SYMM, SYM, SYMM_OP, SYM_OP, SYMMETRY_OPERATOR
```

[top of CRYSCALC keywords list]

- **SYST**

```
. type:                EXTERNAL keyword
. arguments:           1 characters string
. meaning:             launch an external command or program
. example:            SYST dir *.CFL / P
. identical keywords: SYST, CMD, COMMAND, DOS, DOS_COMMAND
```

[top of CRYSCALC keywords list]

- **THERM**

```
. type: INPUT/OUTPUT keyword
. arguments: 1 characters string + reals
. meaning: conversion of atomic displacement parameters:
. available arguments:
- "Uiso", "U_iso": conversion from Uiso to Biso
- "Biso", "B_iso": conversion from Biso to Uiso
- "U_ij", "Uij" : conversion from U_ij to B_ij and
beta_ij
- "U_ij", "Uij" : conversion from U_ij to B_ij and
beta_ij
- "beta_ij", "betaij", "beta"": conversion from
beta_ij to B_ij and U_ij
. reals values correspond to isotropic thermal
parameters values (Biso or Uiso) or anisotropic
thermal parameters (Uij, Bij, Beta) in the following
order: 11, 22, 33, 12, 13, 23
. examples: THERM Biso 0.52 0.76 0.35
THERM B_ij 0.01 0.01 0.01 0.0 0.0 0.0
. mandatory keyword CELL for anisotropic thermal parameters conversion
. identical keywords: THERM, THERMAL, ADP
```

[top of CRYSCALC keywords list]

- **THERM\_SHELX**

```
. type: INPUT/OUTPUT keyword
. arguments: 1 characters string + reals
. meaning: conversion of atomic displacement parameters:
. available arguments:
- "Uiso", "U_iso": conversion from Uiso to Biso
- "Biso", "B_iso": conversion from Biso to Uiso
- "U_ij", "Uij" : conversion from U_ij to B_ij and
beta_ij
- "U_ij", "Uij" : conversion from U_ij to B_ij and
beta_ij
- "beta_ij", "betaij", "beta"": conversion from beta_ij
to B_ij and U_ij
. reals values correspond to isotropic thermal
parameters values (Biso or Uiso) or anisotropic
thermal parameters (Uij, Bij, Beta) in the following
order: 11, 22, 33, 23, 13, 12 (as in SHELXL program)
. examples: THERM Biso 0.52 0.76 0.35
THERM B_ij 0.01 0.01 0.01 0.0 0.0 0.0
. mandatory keyword CELL for anisotropic thermal parameters conversion
. identical keywords: THERM_SHELX, THERMAL_SHELX, ADP_SHELX
```

[top of CRYSCALC keywords list]

- **THETA**

```
. type:          CALCULATION keyword
. argument:     real values
. meaning:      Theta (deg) values
. outputs:      d_hkl(A), Q(A-1), SinTheta/lambda
. mandatory keyword: WAVE
. identical keywords: THETA, THETA_HKL
. example:      THETA 27.5
```

[top of CRYSCALC keywords list]

- **TITL**

```
. type:          INPUT keyword
. arguments:     characters strings
. meaning:      title of the job
. example:      Ammonium bitartrate
. identical keywords: TITL, TITLE
```

[top of CRYSCALC keywords list]

- **TOLMAN\_ANGLE**

```
. type:          INPUT keyword
. arguments:     5 characters strings, corresponding to metal, centered atom
                  and 3 ligand atoms respectively
. optional arguments: 3 optional arguments can be input to specify the van der
                  Waals radii that will be used in the calculation. If not
                  defined, default values are extracted from CRYSFML library,
                  excepted for Hydrogen (r=1.2 A).
. meaning:      calculation of the Tolman cone angle, as defined
                  in "Transition Met. Chem. 20, 533 (1995)
. example:      TOLMAN_ANGLE S1 P1 H1a HC2a H3a
                  TOLMAN_ANGLE S1 P1 H1a HC2a H3a 1.25 1.25 1.25
. identical keywords: TOLMAN_CONE_ANGLE, TOLMAN_CONE
                  TOLMAN_ANGLE, CONE_ANGLE, CONE, TOLMAN
```

[top of CRYSCALC keywords list]

- **TRANSLATION**

```
. type:          INPUT keyword
. arguments :    translation components (3 reals) + 1 sign (optional)
```

. outputs: apply the translation on atomic coordinates  
 if sign is input, new atomic coordinates become :  
 $t(1) + x.sign, t(2) + y.sign, t(3) + z.sign$   
 as in SHELXL with the MOVE keyword  
 if sign > 0 : sign = 1  
 if sign < 0 : sign = -1

. mandatory keyword: ATOM

. examples: TRANSLATION 0.5 0.5 0.5  
 MOVE 1. 1. 1.5 -1.

. identical keywords: TRANSLATION, TRANSLATE, MOVE, SHIFT

[top of CRYSCALC keywords list]

### ● TRANSMISSION

. type: INPUT/OUTPUT keyword

. arguments : list of distances (in mm)

. outputs: calculation of transmission coefficient for  
 different distances values given as arguments

. mandatory keyword: CELL, UNIT, SFAC

[top of CRYSCALC keywords list]

### ● TRICLINIC

. type: OUTPUT keyword

. arguments : no argument

. outputs: . list the transformation matrices for equivalent  
 triclinic unit cells  
 . if CELL exists: apply the transformation matrices  
 to give new triclinic cell parameters

. mandatory keyword: no

. optional keyword: CELL

. identical keywords: TRICLINIC, TRICL

[top of CRYSCALC keywords list]

### ● TWIN\_HEXA

. type: OUTPUT keyword

. arguments : no argument

. outputs: . list the transformation matrices for hexagonal setting  
 . if CELL exists: apply the transformation matrices  
 to give new cell parameters

. mandatory keyword: no

. optional keyword: CELL

. identical keywords: HEXA\_TWIN, HEXA\_TWINNING, HEXAGONAL\_TWIN, HEXAGONAL\_TWINNING  
 TWIN\_HEXA, TWIN\_HEXAGONAL, TWINNING\_HEXA, TWINNING\_HEXAGONAL

[top of CRYSCALC keywords list]

- **TWIN\_PSEUDO\_HEX**

. type: OUTPUT keyword  
. arguments : no argument  
. outputs: . list the transformation matrices for pseudo-hexagonal setting in a monoclinic unit cell  
. if CELL exists: apply the transformation matrices to give new cell parameters  
. mandatory keyword: no  
. optional keyword: CELL  
. identical keywords: TWIN\_PSEUDO\_HEX

[top of CRYSCALC keywords list]

- **TWO\_THETA**

. type: CALCULATION keyword  
. argument: real values  
. meaning: 2Theta (deg) values  
. outputs: d\_hkl(A), Q(A-1), SinTheta/lambda  
. mandatory keyword: WAVE  
. identical keywords: TWO\_THETA, 2THETA, 2THETA\_HKL, TWO\_THETA\_HKL  
. example: TWO\_THETA 50.

[top of CRYSCALC keywords list]

- **UB\_MATRIX**

. arguments: 9 reals or 1 character string  
. meaning: UB matrix components in the following order:  
11 21 31 12 22 32 13 23 33  
If a tenth argument is input and corresponds to "111213212223313233" or "P4P" or "ORT", the UB components are read in the following order: 11 12 13 21 22 23 31 32 33  
If only 1 argument, it has to correspond to a CIF file name: UB matrix is then extracted from it.  
. output: cell parameters deduced from the UB matrix  
. identical keywords: UB\_MAT, UB\_MATRIX

[top of CRYSCALC keywords list]

- **UNIT**

```

. type:                INPUT keyword
. arguments:           n characters strings
. meaning:             list of chemical elements in the molecule
. output:              - atomic density calculation, in at/cm3
                       (dependent keyword = CELL)
                       - absorption coefficient calculation
                       (dependent keywords = CELL, BEAM)
                       - determination of the molecular formula
                       (dependent keywords = Z)
                       - calculation of the molecular weight
                       (dependent keywords = Z)
                       - calculation of the atomic and weight
                         percentage (dependent keywords = Z)
                       - determination of the density
                       (dependent keywords = CELL, Z)

. mandatory keyword:  SFAC
. example:            UNIT 16. 24. 36. 4.

```

[top of CRYSCALC keywords list]

#### • UPDATE

```

. optional arguments: BETA/TMP/TEMP/ZIP
. meaning:            download latest version of CRYSCALC
                       from the CRYSCALC web site:
                       https://cdifx.univ-rennes.fr/progs/cryscalcc/cryscalcc.exe
                       If TMP is given as argument, a temporary uncompactd version
                       of CRYSCALC will be downloaded from:
                       https://cdifx.univ-rennes.fr/progs/cryscalcc/temp/cryscalcc.exe
                       If BETA is given as argument, a beta uncompactd version
                       of CRYSCALC will be downloaded from:
                       https://cdifx.univ-rennes.fr/progs/cryscalcc/beta/cryscalcc.exe
                       If ZIP is given as argument, a zipped file containing
                       cryscalcc.exe will be downloaded from:
                       https://cdifx.univ-rennes.fr/progs/cryscalcc/cryscalcc.zip
. remark:            browser has to be defined in the setting file
                       [EXTERNAL APPLICATIONS] section.
. examples:          UPDATE
. examples:          UPDATE ZIP
. identical keywords: UPDATE, DOWNLOAD

```

[top of CRYSCALC keywords list]

#### • USER\_MAT

```

. arguments:         "#" + 1 integer
. meaning:           number of user matrix in the matrices list defined by
                       the user in the cryscalcc.ini setting file
. example:           USER_MAT #3

```

or

```
. arguments:      "$" characters string
. meaning:       this characters string has to be one of the comment text
                 accompagnying the matrix defined by the user in the
                 cryscalc.ini setting file

. example:      MATR $2a
. output:       calculation of new cell parameters (dependent keyword = CELL)
                 calculation of new atomic coordinates (dependent keyword = ATOM)
                 calculation of new hkl Miller indices (dependent keyword = HKL)
                 create a new file containing the new hkl indices
                 (dependent keyword = FILE)

. identical keywords: USER_MAT, USER_MATR, USER_MATRIX, MAT_USER, MAT_USER,
                     MATRIX_USER
```

[top of CRYSCALC keywords list]

- **WATER\_H**

```
. type:          INPUT keyword
. optional argument: EDIT
. meaning:       . read "hatoms.out" output file from CALC-OH (M. Nardelli,
                 J. Appl. Cryst. 1999, 32, 563-571) and create "hatoms_out.INS"
                 file in SHELXL format with:
                 - coordinates of Hydrogen atoms with AFIX constraints
                 - distances constraints between atoms of the water molecules
                 . if EDIT is given as optional argument, hatoms_out.INS is
                 automatically edited with the editor specified in the
                 cryscalc.ini setting file.

. identical keywords: WATER, WATER_H
```

[top of CRYSCALC keywords list]

- **WAVE**

```
. type:          INPUT keyword
. arguments:     1 real or 1 characters string
. meaning:       . real value: wavelength value in A
                 . characters string:
                 - "X_Ag" or "XAG": wavelength = 0.556363 A
                 - "X_Mo" or "XMO": wavelength = 0.71073 A
                 - "X_Cu" or "XCU": wavelength = 1.5406 A
                 - "X_Ni" or "XNI": wavelength = 1.65794 A
                 - "X_Co" or "XCO": wavelength = 1.78892 A
                 - "X_Fe" or "XFE": wavelength = 1.93597 A
                 - "X_Cr" or "XCR": wavelength = 2.28962 A

. examples:     WAVE 0.71073
                 WAVE XMO

. identical keywords: WAVE, WAVELENGTH, WL, LAMBDA
```

[top of CRYSCALC keywords list]

- **WEB**

. type: OUTPUT keyword  
. argument: web site name or address  
. meaning: web site name can be one of the following: CDIFX, CRYSCALC  
or site name defined in the cryscalcalc.ini setting file  
in the [WEB] section  
. identical keywords: WEB, INTERNET

[top of CRYSCALC keywords list]

- **WRITE\_ADP**

. type: OUTPUT keyword  
. optional argument: DETAILS, NO\_H  
. meaning: write anisotropic displacements parameters for all atoms  
if DETAILS is given as argument, output details on ADP  
if NO\_H is present, only non-hydrogen atoms are listed.  
. mandatory action : ADP have to be read previously in a .INS or .CIF file  
. identical keywords: WRITE\_ADP, WRITE\_UIJ

[top of CRYSCALC keywords list]

- **WRITE\_BEAM**

. type: OUTPUT keyword  
. argument: no  
. meaning: write incident beam type  
. mandatory keyword : WAVE  
. identical keywords: WRITE\_BEAM, WRITE\_INCIDENT\_BEAM, OUTPUT\_BEAM  
OUTPUT\_INCIDENT\_BEAM

[top of CRYSCALC keywords list]

- **WRITE\_CELL**

. type: OUTPUT keyword  
. optional argument: CART\_A/CART\_C  
. meaning: write cell parameters (direct and reciprocal space) and metric  
tensors and Busing-Levy B-matrix if required  
if arg="CART\_A", Cartesian frame is follows:  
x // a; z is in the ac-plane; y is  $x \wedge z = b*$   
if arg="CART\_C", Cartesian frame is follows:  
z // c; y is in the bc-plane; x is  $y \wedge z = a*$   
. mandatory keyword : CELL or FILE .CIF or READ\_CIF or READ\_INS or READ\_PCR  
. identical keywords: WRITE\_CELL, OUTPUT\_CELL

[top of CRYSCALC keywords list]

- **WRITE\_CHEM**

. type: OUTPUT keyword  
. argument: no  
. meaning: write molecular features (formula, weight )  
. mandatory keywords: CHEM, CONT/ZUNIT, SFAC/UNIT/ZUNIT  
. identical keywords: WRITE\_CHEM, WRITE\_CHEMICAL\_FORMULA,  
. OUTPUT\_CHEM

[top of CRYSCALC keywords list]

- **WRITE\_DEVICE**

. type: OUTPUT keyword  
. argument: no  
. meaning: write device features defined in the cryscalcalc.ini setting file  
. identical keywords: WRITE\_DEVICE, OUTPUT\_DEVICE, DEVICE, WRITE\_DIFFRACTO,  
OUTPUT\_DIFFRACTO, DIFFRACTO, WRITE\_DIFFRACTOMETER,  
OUTPUT\_DIFFRACTOMETER, DIFFRACTOMETER

[top of CRYSCALC keywords list]

- **WRITE\_QVEC**

. type: OUTPUT keyword  
. argument: no  
. meaning: write modulation wave vector components  
. mandatory keyword : QVEC  
. identical keywords: WRITE\_QVEC, OUTPUT\_QVEC

[top of CRYSCALC keywords list]

- **WRITE\_REF**

. type: OUTPUT keyword  
. arguments: APEX, CRYCALIS, D8V, DENZO, EVAL, KCCD, SADABS, SIR, SHELX,  
SUPERFLIP, SUPERNOVA, X2S, XCALIBUR, FULLPROF, WINPLOTR  
PLATON, SQUEEZE  
. meaning: output reference of the given argument  
. optional argument: CIF/ACTA  
. identical keywords: WRITE\_REF, WRITE\_REFERENCE, REF, REFERENCE

[top of CRYSCALC keywords list]

- **WRITE\_SG**

```
. type:                OUTPUT keyword
. argument:            no
. meaning:             write space group features
. mandatory keyword : SPGR
. identical keywords: WRITE_SG, WRITE_SPGR, WRITE_SPACE_GROUP
```

[top of CRYSCALC keywords list]

- **WRITE\_SUPERCELL**

```
. type:                OUTPUT keyword
. argument:            no
. meaning:             write superstructure cell
. mandatory keyword : CELL, SUPERCELL
. identical keywords: WRITE_SUPERCELL, OUTPUT_SUPERCELL
```

[top of CRYSCALC keywords list]

- **WRITE\_SYM\_OP**

```
. type:                OUTPUT keyword
. optional arguments : SHELX, SHELX:A, ONE_LINE, CONDENSED
. outputs:             list of symmetry operators (SYMM keyword, followed by
                      rotational and translational parts, in alphanumeric form)
                      if argument="SHELX": output reduced set of symmetry
                      operators for the given space group in a SHELX format
                      (NLAT, SYMM)
                      if argument="SHELX:1": output all symmetry operators
                      of the current space group in a SHELX format
                      if argument="SPF" or "SUPERFLIP": output symmetry operators
                      for the given space group in a SUPERFLIP format (x y z)
                      if argument="SPF_X" or "SUPERFLIP_X": output symmetry
                      operators for the given space group in a SUPERFLIP format
                      (x1 x2 x3).
                      if argument="ONE_LINE": all the symmetry operators are merged
                      in a single line, separated by ";" character, for
                      Symmetry Calculator [Cryscalc] distributed within the FullProf
                      Suite.)
                      if argument="CONDENSED": symmetry operators are output
                      in a condensed way.
. mandatory keyword:  SPGR or SYMM
. identical keywords: WRITE_SYM_OP, WRITE_SYMM_OP, WRITE_SYMP, WRITE_SYMM,
                      WRITE_SYMMETRY_OPERATORS, WRITE_SYMOP, WRITE_OP
                      LIST_SYM_OP, LIST_SYMM_OP, LST_SYM_OP, LST_SYMM_OP, LIST_OP
```

[top of CRYSCALC keywords list]

- **WRITE\_WAVE**

. type: OUTPUT keyword  
. argument: no  
. meaning: write current wavelength features  
. mandatory keyword : WAVE  
. identical keywords: WRITE\_WAVE, OUTPUT\_WAVE

[top of CRYSCALC keywords list]

- **WRITE\_ZUNIT**

. type: OUTPUT keyword  
. argument: no  
. meaning: write Z unit (number of molecular unit)  
. mandatory keyword : ZUNIT  
. identical keywords: WRITE\_ZUNIT, WRITE\_Z

[top of CRYSCALC keywords list]

- **X\_WAVE**

. type: output keyword  
. optional argument: target nature (Ag, Mo, Cu, Ni, Co, Fe, Cr)  
. meaning: if no optional argument, output Ka1 and Ka2 wavelength value (in Å) for main radiations: Ag, Mo, Cu, Ni, Co, Fe and Cr  
. identical keywords: XRAYS\_WAVELENGTH, X\_WAVE

[top of CRYSCALC keywords list]

- **ZUNIT**

. type: INPUT keyword  
. arguments: 1 real  
. meaning: number of formula units  
. example: 4  
. identical keywords: ZUNIT, Z, Z\_UNIT

[top of CRYSCALC keywords list]

## List of **CRYSCALC** command line arguments

- **MAN**

Create 'cryscalc.txt' file user's guide (text format).  
Same behavior can be obtained with the following arguments:  
MAN, /MAN, -MAN, --MAN, /M, -M, HELP, /HELP, -HELP, --HELP, /H , -H, /?  
ex : > cryscalc man  
      > cryscalc /?

- **HTML**

Create 'cryscalc.html' file user's guide (HTML format).  
ex : > cryscalc HTML

- **HTML\_BROWSE**

Create 'cryscalc.html' file user's guide (HTML format) and launch the browser previously defined in the 'cryscalc.ini' setting file'  
ex : > cryscalc HTML\_BROWSE

- **KEY/KEYS**

Create 'cryscalc\_keys.txt' file containing the keywords list  
ex : > cryscalc KEYS

- **P4P**

. List the .P4P files in the current folder.  
. Select a .P4P file  
. Search for the corresponding .HKL file and output SADABS file to create an 'import.cif' file.  
ex : > cryscalc P4P

- **filename.P4P**

Search for the corresponding .HKL file and output SADABS file to create an 'import.cif' file.  
ex : > cryscalc mycrystal.P4P  
.P4P, .HKL and . ABS files can be specified in the command line  
ex : > cryscalc P4P=mycrystal.P4P HKL=mycrystal.HKL ABS=mycrystal.ABS  
RAW file can be specified to create the 'import.cif' file.  
ex : > cryscalc mycrystal.P4P RAW=mycrystal.RAW

- **filename.RAW**

Read the filename.RAW file (created by SAINT) and create a HKL file with the SHELX format (3I4,2F8.2).  
ex : > cryscalc mycryscalc.RAW

- **REPORT\_REPORT\_LONG**

Create a HTML report from 'archive.cif' file or from the .CIF file give as a second argument.

```
ex : > cryscalc report
ex : > cryscalc report my_archive.cif
```

- **REPORT\_TXT**

Create a .TXT report from 'archive.cif' file or from the .CIF file give as a second argument.

```
ex : > cryscalc report_txt
ex : > cryscalc report_txt my_archive.cif
```

- **ARCHIVE.CIF**

. Read 'archive.cif' CIF file  
. Complete this 'archive.cif' with additionnal CIF fields related to absorption correction, squeeze procedure, hydrogen treatment, diffractometer features, structure solution program ...  
A new 'crystalcalc\_archive.cif' file is then created.  
Remark : diffractometer and structure solution program can be defined in the 'crystalcalc.ini' setting file in the [DEVICE] and [PROGRAMS] parts respectively.

- **CREATE\_ARCHIVE**

. create global 'crystalcalc\_archive.cif' CIF file from CIF files given as arguments, first argument being related to structural parameters file created by the refinement program.  
Example : CRYSCALC ambi struct

- **CIFDEP**

Combined with 'ARCHIVE.CIF' argument, this optional argument completes the 'crystalcalc\_archive.cif' file with CIF fields related to the author of the deposition (name, address), extracted from the 'crystalcalc.ini' setting file ([AUTHOR/USER] part)

- **EXTRACT**

Combined with 'ARCHIVE.CIF' argument, this optional argument extracts .res and .hkl files embedded in the archive.cif file

- **EXTRACT\_CIF**

Combined with a multiple global CIF file given as argument, this option allows to extract individual CIF files.

- **ADD\_HKL**

Combined with 'ARCHIVE.CIF' and 'job.cif' arguments, this optional argument adds hkl data into archive\_hkl.cif file. Syntax is as follows:  
d:\cifs>CRYSCALC ADD\_HKL archive.cif job.cif  
where archive.cif is a final archive CIF file and job.cif the CIF file created by SHELXL and containing hkl data, starting with \_shelx\_hkl\_file item and finishing with \_shelx\_hkl\_checksum item.

- **CREATE\_GLOBAL\_CIF**

Global CIF file containing several structures can be created through CREATE\_GLOBAL\_CIF command line argument. The list of CIF structures files is specified in a buffer file. The name of this buffer file can be given through a second argument in the command line. If not, default buffer file is called 'CIF\_files.buf'.

A list of authors to be included can be specified in a special file named 'authors\_list.txt'. The syntax is as follows :

```
[AUTHOR]
  Name, first_name
  address
  address2 (optional)
```

Note that :

- . input items can contain characters with accents
- . address has to be input in a single line. On the other hand, a second line will be interpreted as a second address. Carriage return can be applied using '\\\'' character.

Example:

```
[AUTHOR]
ROISNEL, Thierry
```

```
Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR6226 \\\ F-35
```

- **CREATE\_CIF\_BUFFER**

Create CIF buffer file containing the list of CIF structures files to be used with the help of CREATE\_GLOBAL\_CIF argument. The name of this buffer file can be given through a second argument in the command line. If not, default buffer file is called 'CIF\_files.buf'.

- **SOLVE\_TO\_INS\_CREATE\_INS**

- . read STRUCT.CIF file and get cell parameters with esd's
- . read import.RES created by SIRxx or SHELXS/T
- . create job.INS file for SHELXL with correct esd's and different useful SHELXL keywords (ACTA, BOND\$H ...)

- **DEBUG**

Combined with all previous arguments, this optional argument will create a 'cryscalc\_debug.txt' file containing informations about the values of some variables during the CRYSCALC run. This argument can be useful to detect the origin of the bug in a CRYSCALC crash.

- **NO\_OUT**

Combined with all previous arguments, this optional argument avoids to write CRYSCALC results lines in the screen and in the 'cryscalc.log' file.

## What's new in CRYSCALC?

CRYSCALC version: 26.06

Main new features implemented in CRYSCALC:  
(for more details, see the CRYSCALC manual)

### June 2026

# "plot\_PRF" item in the setting file can have a negative value to prevent output text on the screen.

### May 2026

# Pattern simulation: CTML and Rpolar values can now be input in the setting file through X\_pattern\_CTHM and X\_pattern\_Rpolar items.  
# new VOIDS argument for READ\_INS and READ\_CIF keyword: calculation of porosity (voids) through Monte-Carlo method

### April 2026

# FLACK argument for CREATE\_INS keyword has been added, in order to insert "TWIN/BASF lines" in the created INS file.  
# If CREATE\_INS/CREATE\_PCR keywords are input after SUPERCELL keyword, "P 1" space group is considered. If you want to obtain the full list of atomic positions in the supercell, use previously EQUIV\_ATOMS keyword to generate all atoms in the primary cell.  
# DATA\_DENSITY, DATA\_WEIGHT and DATA\_RADIUS keywords has been replaced by a single DATA\_ATOMIC keyword and DENSITY/WEIGHT/RADIUS/COVALENT\_RADIUS/VDW\_RADIUS/VOLUME/EC argument.  
# Simulation of powder diffraction pattern: scale factor can be adjusted automatically to provide countings in the range  $10^{*3}$  -  $10^{*4}$  above the background. This option can be specified through the auto\_scaling option in the [PATTERN SIMULATION] section of the setting file  
# New GET\_FORMAL\_CHARGES keyword allows to determine formal charge of atoms in a crystal structure read from a .CIF, .INS or .PCR file  
The Set\_Formal\_Charges CFML routine written by Nebil Ayape Katcho (ILL) is used.

### March 2026

# BVS calculation:  
. new BVS\_SUMM optional argument for CONN keyword will provided a summary of BVS calculation.  
# New keyword :  
- DIST\_COL/DIST\_NEW\_COL : calculation of atomic coordinates of a fourth atom A4 given 3 atoms and with A1A2 = A3A4.

```
ex: DIST_COL C4 C5 C11
    >> calculation of the atomic coordinates of C12 with
        vect(C11-C12) = vect(C4-C5).
- CLONE/CREATE_CLONE : calculation of atomic coordinates of a fragment defined
  by n-1 input atoms. Starting atom of the cloned fragment is the input atom n.
ex: CLONE C1 C2 C3 C4 C5 C6 C11
    >> input fragment is defined with C1 to C6 atoms and the cloned one is calculated
        starting from C11 atom. Cloned fragment is generated with the following
        conditions :
        vect(C11-C12) = vect(C1-C2)
        vect(C12-C13) = vect(C2-C3)
        vect(C13-C14) = vect(C3-C4)
        vect(C14-C15) = vect(C4-C5)
        ...
Rem: max number of atoms in the fragment has been limited to 10
```

### February 2026

```
# If "Rint_shell = ns" is present in the [OPTIONS] part of the setting
file, Rint calculation is performed in ns different Theta shells.
```

### January 2026

```
# Refinement of twinning crystals:
- in case of refinement towards a HKLF4 dataset created by TWINABS,
  the archive.cif contains h, k, l limits and the value of Rint.
- structural reports contains some sentences about the treatment of
  twinning in the final refinement.
```

### October 2025

```
# New "P1" option for "CREATE_INS": create .INS file in P1 space group,
  containing all atoms present in the unit cell. Note that input atoms
  are supposed to belong to a single molecule entity. After applying
  symmetry operators of the current space group, all the equivalent molecules
  are considered as residus in a SHELXL sense and then conserve the labelling.
  If necessary, a translation is applied to atomic coordinates to
  locate each molecule centroid inside the unit cell.
# New "WRITE_REF" keyword: replaces all the existing REF_XXX keywords.
# New "READ_XYZ" keyword: read xyz file (list of atoms in cartesian coordinates)
  and outputs interatomic distances.
# New "SHORT" optional argument for "READ_SFRM" keyword:
  outputs only main scan features.
```

### September 2025

```
# New ONLY_X optional argument for WRITE_ATOMS keyword :
  outputs only X species atoms.
# New SO_XXX keyword : allows to decode a character string as
  n_klm, composed as follows: n refers to the symmetry operation
  that is applied to atomic coordinates and k,l and m refer to
  the translations to apply to atomic coordinates.
```

## July 2025

```
# Import.cif file can be created starting from .P4P, .HKL and .CIF
files created by CRYNALIS software on Rigaku diffractometer.
This operation can be run if this kind of diffractometer is specified
in the [DEVICE] section of the setting file through following line:
diffractometer = XtaLAB Synergy, Dualflex, Eiger 1M
Diffractometer features are :
CIF_parameter_DEVICE_SYNERGY%diffrn_measurement_device_type      = "XtaLAB Synergy, Dual
CIF_parameter_DEVICE_SYNERGY%diffrn_measurement_method          = "omega scans"
CIF_parameter_DEVICE_SYNERGY%diffrn_detector                    = "Hybrid Pixel Array D
CIF_parameter_DEVICE_SYNERGY%diffrn_radiation_wavelength        = "0.71073"
CIF_parameter_DEVICE_SYNERGY%diffrn_radiation_monochromator     = "mirror"
CIF_parameter_DEVICE_SYNERGY%diffrn_radiation_probe            = "x-ray"
CIF_parameter_DEVICE_SYNERGY%diffrn_radiation_source            = "micro-focus sealed X
CIF_parameter_DEVICE_SYNERGY%diffracto_radiation_wavelength     = "0.71073"
CIF_parameter_DEVICE_SYNERGY%diffracto_radiation_monochromator  = "mirror"
CIF_parameter_DEVICE_SYNERGY%diffracto_radiation_probe         = "x-ray"
CIF_parameter_DEVICE_SYNERGY%diffracto_radiation_source        = "micro-focus sealed X
CIF_parameter_DEVICE_SYNERGY%diffracto_temperature             = "?"
CIF_parameter_DEVICE_SYNERGY%diffrn_source                     = "?"
CIF_parameter_DEVICE_SYNERGY%diffrn_detector_area_resol_mean   = "13.3333"
CIF_parameter_DEVICE_SYNERGY%diffrn_source_target              = "?"
CIF_parameter_DEVICE_SYNERGY%diffrn_source_current             = "1"
CIF_parameter_DEVICE_SYNERGY%diffrn_source_voltage             = "50"
CIF_parameter_DEVICE_SYNERGY%diffrn_source_power               = "?"
```

## June 2025

```
# RHOMB_HEX and HEX_RHOMB keywords allows to switch cell parameters, hkl file,
atomic coordinates ... from one to other setting

# RHOMB_HEX and HEX_RHOMB keywords hkl file created by FullProf can now been read.
Format is as follows:
. n lines : 3I4,I6,2F15.3, 2F13.5 (h,k,l, m, F2,sig, Theta, Q)
```

## May 2025

```
# New OMIT_update optional argument for READ_FCF keyword: list outliers reflections
and update .INS file with OMIT instruction.
```

## April 2025

```
# Minor changes in the structure factor calculation routine :
for expert use, calculation is performed using three different
routine of CRYSFML : Structure_Factors, Calc_StrFactor and
Calc_hkl_StrFactor
```

## February 2025

```
# New HKL_mult keyword: provides multiplicity of a given hkl reflexion
# Routine to find equivalent reflections has been modified:
  "Friedel" argument is now useless.
# Creation of archive.cif file: chemical formula is now in agreement
  with new CHECKCIF requirement:
  example : C9 H11 N1 O1 is replaced by C9 H11 N O
# Creation of archive.cif file: in the case of absolute structure
  determination, the "_chemical_absolute_configuration" CIF field
  is now fullfilled automatically :
. "ad"                if Flack parameter is < 0.2 and esd < 0.1
. "rm/ad/rmad/syn/unk/" if Flack parameter is < 0.2 and esd > 0.1
. "unk"              if Flack parameter is > 0.2
```

### January 2025

```
# New "CREATE_FHZ" keyword allows to calculate internal coordinates
  of a molecule given fractional coordinates :
. cartesian coordinates
. spherical coordinates
. Z-matrix coordinates
This routine has been extracted from mol_tpcr program of the FullProf Suite.
Obviously, all the input atoms are considered to belong to a single molecule.
PCR input files can be created for FullProf (simulated annealing).
```

### December 2024

```
# In the case of Rint calculation Rint > Bad_Rint_Criteria, Rint calculations
  are also performed considering new point groups:
. "-3" instead of "-3m"
. "m-3" instead of "m-3m"
. "-31m" instead of "-3m1"
. "-3m1" instead of "-31m"
. "4/m" instead of "4/mmm"
. "6/m" instead of "6/mmm"
# hkl file statistics now included Rmerge, Rmes and Rpim in different d_hkl
  ranges.
```

### November 2024

```
# "Read_Shx_Atom" routine in CRYSFML has been adapted to
  read .INS/.RES files coming from PLATON and OLEX2.
# New argument for WRITE_SYM_OP keyword : SHELX:1 allows to
  output ALL the symmetry operators in SHELX format and considering a
  acentric lattice. This can be useful to describe a structure in a
  setting where the origin is not at the inversion center.
# "Read_Shx_Atom" routine in CRYSFML has been adapted to
  read .INS/.RES files coming from Olex2.
```

### October 2024

- # CELL keyword : input \_CN file created by CELL\_NOW software and \_LS file created by SAINT software can now be read (only cell parameters are extracted).
- # Creation of import.cif file: in the case of twinned data, the twin law is now extracted from \*\_Om.\_ls created after integration with SAINT, taking into account the presence of two domains.

### September 2024

- # Search\_group routine will output only space groups with point group in agreement with point group present in the import.cif input file.

### July 2024

- # Highest resolution value is now output in the import.CIF created by CRYSCALC.
- # Wavelength used for powder diffraction pattern simulation can now be specified through "X\_pattern\_wave=" and "N\_pattern\_wave=" keywords in the CRYSCALC.ini setting file.

### April 2024

- # "DIST\_new A1 A2 x" keyword routine to calculate the position of a new atom at the distance x from the A1 atom in the A1-A2 direction was wrong. This has been fixed.
- # New "No\_H/REMOVE\_H" argument for READ\_INS keyword: remove Hydrogen atoms from the .INS file
- # New "HFIX" argument for READ\_INS keyword:  
HFIX instructions are listed after the "PLAN" line. This can be useful after automatic introduction of Hydrogen atoms with the following PLATON command:  
platon -f job.ins
- # Creation of structural report: when Hydrogen atoms are not in calculated positions, the sentence concerning the treatment of Hydrogen atoms is created consequently.
- # Creation of archive.cif file: in the case of Hydrogen bonds list, the D-H...A angle value is rounded if no standard deviation is given. This has been implemented to avoid a G-type alert in the CHECKCIF procedure.
- # New Hbond\_limit keyword in the [ARCHIVE\_AND\_REPORT] section of the cryscalcalc.ini setting file: Definition of a limit in Å, beyond which the Hbond distance is excluded from the archive.CIF file.

### March 2024

- # New "DIST\_new A1 A2 x" keyword allows to calculate atomic coordinates of a new M atom with at a distance  $d_{(A1-M)} = x$ , in the A1-A2 direction.
- # In the case of Rint calculation for centric space groups, listing of missing reflections can be output if "Rint\_missing\_reflections = 1" is specified in the [OPTIONS] section of the cryscalcalc.ini setting file.

### February 2024

```
# Simulation of powder diffraction pattern: by default, background is described
  by a constant value but also by a polynomial function (max. 8 deg.). Coefficient
  of the polynom can be specified in the setting file in the [PATTERN SIMULATION].
  section.
  ex:X_pattern_background      = 31.5  4.80  30.52 -200.18  212.64
# New READ_PDB keyword allows to read .PDB file from Protein Data Bank.
# When creating import.cif file, Friedif value is output, considering
  wavelength and chemical formula present in .P4P file.
# Routine to read chemical formula from .P4P file
  has been modified to be more robust and avoid crashes. As examples :
"C1_H2_O3_N4_Ni5_Au6_S7"  will be interpreted as "C1 H1 O1 N1 Ni1 Au1 S1"
"C_H_O_N_Ni_Au_S"        will be interpreted as "C1 H1 O1 N1 Ni1 Au1 S1"
"C1H2O3N4Ni5Au6S7"      will be interpreted as "C1 H2 O3 N4 Ni5 Au6 S17"
"C H O N Ni Au S"        will be interpreted as "C1 H1 O1 N1 Ni1 Au1 S1"
"CHONNiAuS"              will be interpreted as "C1 H1 O1 N1 Ni1 Au1 S1"
```

### January 2024

```
# Creation of import.cif file: format of writing intensities and sigmas has been changed,
  to be compatible with input .hkl file.
# "CREATE_CFL_file=2" in the [OPTIONS] section of the setting file will
  create CRYSCALC.CFL in append mode.
# Some _CDFIX_ items are included in the import.CIF file created by CRYSCALC.
# Structural report creation: FRAME and CRYSTAL PICTURE .PNG / .JPG files
  to be included in the report can be specified in the command line
  through FRAME= and PICTURE= keywords respectively.
  Example : CRYSCALC create_report FRAME=job_FRAME.PNG PICTURE=cristal.PNG
```

### December 2023

```
# Structural report creation: ORTEP file to be included in the report can be
  specified in the command line through ORTEP= keyword.
  Example : CRYSCALC create_report ORTEP=molecule.PNG
# Routine to read chemical formula from .P4P file
  has been modified to be more robust and avoid crashes. As examples :
"CHON"      will be interpreted as "C1 H1 O1 N1"
"C H O N"   will be interpreted as "C1 H1 O1 N1"
"C1H2O3N"   will be interpreted as "C1 H2 O3 N1"
"C_H_O_N"   will be interpreted as "C1 H1 O1 N1"
# Completeness calculation was wrong for non-standard space groups settings.
  This has been corrected.
# When creating archive.cif file with squeezed data, "[+ solvent]" string is added
  in the "_chemical_formula_moiety" line.
```

### October 2023

```
# CREATE_FST keyword: COLOR argument is now added in the ATOM list
# Correction of a output error in the TRANSF keyword routine. This bug
  was present since the version of July 2023
```

### September 2023

```
# If "checkCIF_PLATON page 2.htm" (created by online CHECKCIF procedure)
is present in the current folder, a "condensed CHECKCIF" is included in
the structural report, containing numbers of A-type, B-type, C-type
and G-type alerts.
# New arguments for EXTRACT_CIF/CIF_EXTRACT/EXTRACT_FROM_CIF keyword:
. arg=ACQ extracts data collection features from a CIF file, ie CIF comments
  lines from "DATA COLLECTION" section present in the header of
  import.CIF file created by CRYSCALC.
. arg=ADP extracts Atomic Displacement Parameters from a CIF file
. arg=ATOMS extracts atoms list from a CIF file
. arg=DATARED extracts data reduction features from a CIF file, ie CIF comments
  lines from "DATA REDUCTION" section present in the header of import.CIF file
  created by CRYSCALC.
. arg=CELL extracts cell parameters features from a CIF file, ie CIF comments
  lines from "SPACE GROUP AND UNIT CELL INFORMATION" section present in the
  header of import.CIF file created by CRYSCALC.
. arg=CHEM extracts chemical formula from a CIF file
. arg=CRYSTAL extracts crystal features from a CIF file, ie CIF comments
  lines from "CRYSTAL INFORMATION" section present in the header of
  import.CIF file created by CRYSCALC.
. arg=DEVICE extracts diffractometer features from a CIF file
. arg=SID extracts sample identifiers
. arg=SG  extracts space group
# F000 calculation is now also performed for neutrons radiation
# New READ_EXP keyword: extract data collection features (number of scans,
  motor positions, type of scan, exposition time ...
```

### July 2023

```
# New report_txt_table_X argument, allowing to create tables
from CIF file. X value corresponds to the numor of table
in the general TXT report.
example: CRYSCALC report_txt_table_2 archive.cif will create
         a archive_structural_report.txt file containing
         table of crystal data and structural refinement features.
# Two new transformations matrices has been implemented in the
CRYSCALC matrices list:
. Mat #38: 0 0 -1  0 1 0  1 0 1, corresponding to C to I transformation.
. Mat #39: 1 0  1  0 1 0 -1 0 0, corresponding to I to C transformation.
# P4P files created are now compatible with APEX4
# CHEM keyword is now providing Friedif parameter value, if FRIEDIF
argument is given. Friedif parameter value is calculated according to the
spreadsheet by Flack and Shmueli (Acta Cryst. A 2007, 63, 257-265)
# Creation of archive.CIF file:
If "INCLUDE_VRF = Y" item is specified in the cryscalcalc.ini setting file
([ARCHIVE_AND_REPORT] section), VRF syntax is included in the
REFINEMENT INFORMATION section of the archive.cif file.
```

### June 2023

```
# New routine to calculate atomic coordinates in a supercell.
```

### April 2023

# Creation of import.cif file : Correction of a bug when reading CELL\_now output file with different domains and selected cell from the possible cells list different than first one.

### Feb. 2023

# New "CREATE\_REPORT\_SUMM" item in the [option] section of the setting file allows to create a summary of structural\_report files from the command line after reading a .CIF file.

Example:

```
d:\progs> cryscalcc xxx.CIF
```

This summary file can also be created by specifying REPORT\_SUMM as argument in a command line.

Example:

```
d:\progs> cryscalcc report_SUMM
```

If "checkCIF\_PLATON page 2.htm" (created by online CHECKCIF procedure) is present in the current folder, the numbers of A-type, B-type, C-type and G-type alerts are included in the summary file.

### Dec. 2022

# FILE keyword : input SCA file created by DENZO/SCALEPACK software can now be read (cell parameters and integrated intensities are extracted)

# CELL keyword : input SCA file created by DENZO/SCALEPACK software can now be read (only cell parameters are extracted).

### Nov. 2022

# Compilation of CRYSCALC with the latest version of CRYSMFL, allowing to deal with trigonal space groups in rhomboedral cell specified by :R at the end of the space group symbol (ex: SPGR R -3 c:R)

# CREATE\_INS SXT : when creating .INS input file for SHELXT, the Laue group specified in the import.cif file is taken into account.

### Oct. 2022

# "CREATE\_SOLVE SXT" keyword : the temperature written in the import.ins file is now extracted from the import.cif file, independently of the "temperature" value in the [CREATE\_INS] section in the setting file.

# New SEQ=SEQ\_file command line argument where SEQ\_file is a .SEQ file coming from FullProf sequential refinement : a xxx\_tabl.seq file in columns format is then created. Default columns separator is tabulation, but can also be defined through "separator=tab/space.comma" item in the [OPTIONS] section of the setting file.

### Sept. 2022

```
# CONN keyword: in the case of five-coordinate system,
tau5 trigonality index is calculated, following the formula introduced
by L. Yang (Dalton Trans, 2007, 955-964):
tau5 = (alfa-beta)/60
Angles calculation for five-coordinate atom has to be performed.
# CONN keyword: in the case of tetrahedral metal environment,
tau4 index is calculated, following the formula introduced
by L. Yang (Dalton Trans, 2007, 955-964):
tau4 = (360 - (alfa+beta))/141
Angles calculation for tetrahedral atom site has to be performed.
```

### July 2022

```
# Images file to be included in the structural reports cab be specified
by user by edditng "report.img" file in the current folder. The format
of "report.img" file is as follows:
  CRYSTAL=my_job.png
  FRAME=my_job_sfrm.png
  STRUCTURE=my_job_ORTEP.png
# New PLOT_XY/PLOT_PRF options in the [PATTERN SIMULATION] section
of the cryscalc.ini file allows to plot (or not) PRF file (FullProf format)
or XY (2 columns) simulated diffraction pattern.
```

### March 2022

```
# READ_FCF keyword output outliers reflections with  $F2o < -2\sigma$ 
```

### January 2022

```
# New "ONLY_1" argument for READ_HKLF5 keyword: allows to create
a file containing only reflections of the domain #1 (single and
common reflections)
# New EXTRACT_CIF/CIF_EXTRACT/EXTRACT_FROM_CIF keyword: extracts
geometrical features (distances, angles and torsion angles) from
a CIF file and outputs min., max, and mean values for requested
parameters. Arguments are as follows:
. DIST A B
. ANG A B C
. TORS A B C D
```

### November 2021

```
# Some changes in the import.CIF creation routine has been performed
to fit measurements with PHOTONIII BAXS detector.
```

### October 2021

```
# New OMIT optional argument for READ_FCF keyword: list outliers reflections
preceded by OMIT keyword for SHELXL refinement program.
# New way to launch browser with a local file (add "file:///folder_name/" before
```

HTML file name)  
# EXTRACT from CIF: .fcf files are extracted if included in the CIF file.  
# Shelxl weighting scheme is now included in structural reports.  
# READ\_FCF xxx.fcf keyword outputs list of outliers reflections with  
ABS( $F_o^2 - F_c^2$ )/sig\_WI > 10.  
where sig\_WI = 1./sqrt(wI) and wI calculated from weighting scheme  
used by SHELXL :  
 $w_I = 1 / [\text{sig}(F_o^2) + (aP)^2 + bP]$  where  $P = (F_o^2 + 2F_c^2) / 3$   
a and b values are extracted from xxx.INS file.

### September 2021

# Creation of archive.CIF file:  
INCLUDE\_FCF\_file keyword can be specified in the [ARCHIVE\_AND\_REPORT] section  
of the setting file to embed .FCF file in the final archive.CIF file.

### July 2021

# Creation of import.CIF file:  
Twinning details extracted from CELL\_NOW output file are now included  
in the header of the import.CIF file. Integration with several domains  
followed by TWINABS data reduction has to be realized previously.

### June 2021

# New "D<sub>MAX</sub>/D<sub>HKL\_MAX</sub>/DHKL\_HIGH/DHIGH" keyword: output the highest  
d<sub>hkl</sub> values  
# Cell parameters and space group has to be input previously.  
New "beam\_stop\_limit" item can be defined in the [DEVICE] section  
of the setting file : its correspond to the theta value below which  
reflexions are hidden behind the beam stop. Default value is 2.0 deg.  
# Routine for creation of archive.cif with formatted output lines  
(CIF\_format80=1 in the [ARCHIVE\_AND\_REPORT] section of the setting file)  
has been optimized for .CIF files created by old versions of SHELXL  
(previous 2014)

### May 2021

# Creation of archive.cif file  
Instrument type in the header is recovered from import.cif and not yet  
from the setting file. Then, it avoids to adapt the instrument item  
in the setting file to the current experiment.  
# Creation of crystal reports (HTML and LATEX):  
references are now linkable with DOI URL addresses previously  
specified in the setting file ([PROGRAMS] section)

### April 2021

# Creation of import.CIF file:  
. Initial and refined XYZ boxes are output for all scans of the data  
collection from the xxx.\_ls files created by SAINT.  
. Rint are output for all scans (extracted from .ABS file)

### March 2021

- # New optimized routine for creation of archive.cif with formatted output lines (CIF\_format80=1 in the [ARCHIVE\_AND\_REPORT] section of the setting file), in order to minimize the number of lines exceeding 80 characters. A warning is now output in such a case.
- # New optional arguments for READ\_LST keyword: AFIX, ATOMS, FLACK, HTAB, MPLA

### February 2021

- # Max. atoms value has been extended from 1200 to 2000.
- # New "WATER" keyword: read atoms.out output file from CALC-OH (M. Nardelli, J. Appl. Cryst. 1999, 32, 563-571) and create:
  - coordinates of Hydrogen atoms with AFIX constraints
  - distances constraints between atoms of the water moleculesIf EDIT is given as optional argument, hatoms\_out.INS is automatically edited with the editor specified in the cryscalc.ini setting file.
- # New "READ\_LST" keyword: read .LST SHELXL output file and extract extract hkl, structural and refinement features.
  - To extract particular items, following optional arguments are allowed: ADP, CONN, DIST, HKL, HKL\_STAT, LS, MDR/MDR\_OMIT/MDR\_crit/MDR\_OMIT\_crit, RHO, SPLIT/SPLIT\_EDIT, TORSION, UNIT, VAR.
  - Note that default criteria value for MDR keyword is equal to 3., leading to output only most disagreeable reflections with Error/Esd > 3.0
  - This criteria value can be specified through the MDR\_crit.
  - Example: READ\_lst job.lst MDR\_8
  - If MDR\_OMIT is used, the hkl indices of most disagreeable reflexions are output, preceded by OMIT keyword (format compatible with .INS/.RES input SHELXL file).
- # New "BD" argument for CONN keyword: include bonds distribution in the output. This new argument replaces the previous "no\_BD" one. By default, bond distribution is not yet output. To activate it, please use this new "BD" argument.
- # New "VIEW/RUN" argument for CREATE\_CIF keyword: view the created CIF in the CIF viewer. Note that CIF viewer can be specified in the [EXTERNAL APPLICATIONS] section of the cryscalc.ini setting file through the CIFviewer item.
- # New "VIEW/RUN" argument for CREATE\_INS keyword: view the created INS in the INS viewer. Note that INS viewer can be specified in the [EXTERNAL APPLICATIONS] section of the cryscalc.ini setting file through the INSviewer item.
- # New "VIEW/RUN" argument for CREATE\_XYZ keyword: view the created XYZ in the XYZ viewer. Note that XYZ viewer can be specified in the [EXTERNAL APPLICATIONS] section of the cryscalc.ini setting file through the XYZviewer item.
- # New "No\_H" argument for CREATE\_PCR keyword: if used, only non Hydrogen atoms are output in the PCR file.
- # New READ\_SFRM/READ\_SFRM\_HEADER keyword:
  - Read header of .sfrm file (diffraction frame from Bruker AXS diffractometers) and output experimental features (date of experiment,

temperature, wavelength, target voltage and intensity, rotation axis, positions of motors ...)

### December 2020

# Tolerance factor value (TOL) for BVS calculation can be specified using the BVS\_TOL argument of CONN keyword.  
Ex: CONN cu1 MAX=3.1 BVS\_30

### November 2020

# Tolerance has been extended from 20 to 30% for the BVS calculation.  
# Some minor changes have been made in the CONNECTIVITY routine in order to provide a standard deviation value for calculated mean distance if atomic positions esd's are known.  
# CRYSCALC has been recompiled with the last CRYSFML library:  
Symmetry card for Ibam space group is now correctly interpreted.

### September 2020

# New "Rint\_centric" item in the [OPTION] section of the setting file: allows to calculate Rint and completeness for centric space group in the case of acentric detected space group. This calculation is performed only if CRYSCALC is launched with a .CFL or .OOL command file as argument.  
# "CIF lines can contain "#" character after the value of the CIF field  
# Matrices for HEX\_RHOMB and RHOMB\_HEX keywords and some matrices used in the MAT B1 B2 keywords (with B1 B2 initial and final Bravais lattices respectively) were wrong in the last versions of CRYSCALC. This has been corrected. Thanks to V. Demande (ISCR) to have reported these bugs.  
# New WGHT argument for READ\_INS keyword:  
If .RES file is input as first argument, the weighting scheme is updated in the corresponding .INS file.

### July 2020

# Correction of a bug when reading .RAW / .MUL files (created by SAINT) containing high countings.

### June 2020

# Creation of archive CIF file for powders:  
. JANA.CIF files can be read.  
. In case of FP CIF files containing several phases, only first phase structural CIF items are considered.  
# New option of CREATE\_INS keyword: SIMU will replace EADP keyword by "SIMU 0.003" keyword in the .INS file.

- # The value of `_exptl_absorpt_correction_T_max` CIF field was wrong in the final archive.CIF in the previous versions of CRYSCALC since April 2020. It has been corrected.
- # "Get\_champ\_value" routine is replaced by "Get\_champ\_value\_new" routine (more general) to extract CIF values from a CIF file for string values. "Get\_champ\_value" routine is still used for get real values.

#### June 2020

- # The value of `_exptl_absorpt_correction_T_max` CIF field was wrong in the final archive.CIF in the previous versions of CRYSCALC since April 2020. It has been corrected.

#### May 2020

- # New "CIF\_powder" item in the [ARCHIVE AND REPORT] section of the setting file: allows to create a CIF file for a powder structure refinement with FullProf: different CIF files can be specified in the command line after "CREATE\_ARCHIVE" argument and instrumental features can be stored in a particular file.
- Example:
- ```
CRYSCALC CREATE_ARCHIVE job.cif job_dis.cif job_prof.cif device.cif
```

#### April 2020

- # GEN\_HKL keyword routine : if "OUT" is given as argument to output the hkl generation list, a Debye Scherrer film simulation is then created : format is .PGF type format for the latest version of WinPLOTR software, downloaded from:  
<https://cdifx.univ-rennes.fr/progs/winplotr/winplotr.exe>
- # New "CREATE\_REPORT\_TXT", "CREATE\_REPORT\_LATEX" and "CREATE\_REPORT\_HTML" items in the [option] section of the setting file: allows to create structural\_report files from the command line after reading a .CIF file, in .TXT, LATEX and .HTML format respectively. Default values for CREATE\_REPORT\_TXT, CREATE\_REPORT\_LATEX and CREATE\_REPORT\_HTML are equal to 0.
- Example:
- ```
d:\progs> cryscalc xxx.CIF
```
- These possibilities are equivalent to the previous (still existing) commands:
- ```
d:\progs> cryscalc report_TXT xxx.CIF
d:\progs> cryscalc report_LATEX xxx.CIF
d:\progs> cryscalc report_HTML xxx.CIF
```
- # CRYSCALC web site has been moved from  
"http://www.cdifx.univ-rennes.fr/CRYSCALC" to  
"https://cdifx.univ-rennes.fr/CRYSCALC"
- # New "MPO" optional argument for CREATE\_PCR keyword: create .PCR file for FullProf for a pattern refinement with multi preferential orientation (NORI=2)
- # New "PRF\_header" item in the [PATTERN SIMULATION] section of the setting

file: allows to include (or not) a header containing diffraction pattern features and structural informations in PRF files created by the diffraction pattern simulation routine (same header than .XY file).  
This kind of PRF file with a header can be read by the latest version of WinPLOTR and "PRF\_header=Y" in the [OPTIONS] section of the WinPLOTR.ini setting file.

### March 2020

```
# EXTRACT from CIF: if only 1 structure is extracted from a CIF file
the xxx.res/hkl(/fab) files are copied as job.ins/hkl or sqz.ins/hkl/fab
files for further refinement with SHELXL. This facility is only available
for "CDIFX" user (ROISNEL, CORDIER, DORCET) in expert mode.
# New "CREATE_LOG_file=0/1" item in [option] section of the CRYSCALC.ini
setting file allows to create (or not) CRYSCALC.log and CRYCALC_cmd.log
output files. Default value is 1.
# New "CREATE_CFL_file=0/1" item in [option] section of the CRYSCALC.ini
setting file allows to create (or not) a CRYSCALC.CFL containing
input CRYSCALC instructions. Default value is 1.
# New REPORT type structure in CRYSCALC module.
# New report_CCDC and report_ACQ items in the [ARCHIVE_AND_REPORT] section
of the cryscalc.ini setting file: include CCDC and report_ACQ section
in the structural report. These new options are only for ROISNEL user.
# Correction of bug in the creation of import.cif file:
"_computing_data_collection" field is now correct.
# New "PAT_NORM_xxx" optional argument for "GEN_HKL" keyword:
diffraction pattern will be normalized to provide maximum
counting equal to xxx.
Example:
  GEN_HKL 2THETA_MIN=10 2THETA_MAX=120 PAT_NORMA_500
This normalization can also be specified through the "pdp_norma = xxx" line
in the [PATTERN SIMULATION] section of the CRYSCALC.INI setting file.
This feature will be used for pattern simulation from command line.
Example:
  d:\progs> cryscalc CRYSCALC.CIF PAT
Furthermore, normalization procedure can be specified in command line
through the "PAT_NORMA" argument, independently of the presence of
the "pdp_norma = xxx" line in the setting file.
Note that the following arguments are available:
  PAT_NORMA, PAT_NORMA_X, PAT_X_NORMA, PAT_NORMA_N, PAT_N_NORMA
Example:
  d:\progs> cryscalc CRYSCALC.CIF PAT_NORM
If pdp_norma = xxx is not specified in the setting file, normalization
value xxx is fixed to the default value xxx=1000.
# Changes in the "generate_HKL" routine : reflections multiplicity
has been multiplied by 2. for acentric space groups if no structure
factor calculation is performed (zero input atoms)
# Changes in the "search_equiv_hkl" routine : Friedel argument is not
yet activated.
```

### February 2020

```
# New "NORM_xxx" optional argument for "GEN_HKL" keyword and pattern
simulation: diffraction pattern is normalized to provide maximum
intensity at xxx counts.
# Final archive.cif and structural reports are suitable for H free compounds.
# Changes in the volume_calculation routine: all the CELL features
are now provided by create_CELL_object routine, including
the set_Crystal_Cell CFML routine.
# New "create_P4P"/"extract_P4P" second argument for CELL keyword when
first argument is a .CIF or .INS file.
Example : CELL import.cif create_P4P
Creation of a P4P file containing cell parameters and orientation matrix
# Distances calculations in the CONN routine outputs standard deviations
if they are provided through reading a CIF file for example.
```

### January 2020

```
# "ref" argument for CREATE_PCR keyword allows to create .PCR file for
FullProf for a pattern refinement: in such a cas, JobTyp will be equal to 0
for X-ray data refinement and 1 for neutrons data. Number of refinement
cycles (NCY) is put to 10. This can also be specified in the setting file
through create_pcr=-1 in the [COMMAND LINE ARGUMENTS] section.
# "ref_mp/mp_ref" argument for CREATE_PCR keyword allows to create .PCR file
for FullProf for a refinement and in a multipattern format.
This can also be specified in the setting file through create_pcr=-2
in the [COMMAND LINE ARGUMENTS] section.
```

### December 2019

```
# New "report_diffraction_frame", "report_crystal_picture" and
"report_structure_ortep" items have been added in the [ARCHIVE_AND_REPORT]
part of the setting file: these items allow to include (or not) diffraction
frame file, crystal picture and structural ORTEP drawing in the HTML/LATEX
report respectively.
```

### November 2019

```
# GET_TRANSF_MAT keyword:
. tolerance value can now be input by user if no transformation matrix
is founded with default value (0.3).
. Cell paramters can be input with esd values.
# "CART_A" and "CART_C" arguments of "WRITE_CELL" keyword are now
in agreement with new definitions in CRYSFML, ie:
CART_A: x // a; z is in the ac-plane; y is  $x \wedge z = b*$ 
CART_C: z // c; y is in the bc-plane; x is  $y \wedge z = a*$ 
```

### October 2019

```
# New "READ_ACE" keyword allows to read structural informations
from a .ACE file (CaRIne).
# New "holder" item in the [DEVICE] section of the setting file:
combined with report_details=1, it will specify the sample
```

holder type (ex: cryoloop, fiber glass) mounted on the diffractometer for the single crystal experiment.

- # New "report\_details" item has been added in the [ARCHIVE\_AND\_REPORT] part of the setting file : whole sentences and some cosmetics as crystal description are now added in HTML and LATEX structural reports.
- # Creation of crystal report: due to the extension of the dimension of an internal array, the list of "Symmetry transformations used to generate equivalent atoms" was not correct in previous versions of CRYSCALC. This has been corrected.
- # PCR files containing single crystal structural data are now read correctly.
- # PAT/PAT\_X/PAT\_N arguments can be used in command line after reading CIF, CEL, CFL, INS and PCR files given as argument, independantly of the value of "create\_PAT\_PRF" item in the "[COMMAND LINE ARGUMENTS]" of the setting file.

Examples:

```
d:\progs> cryscalc CRYSCALC.CIF PAT
d:\progs> cryscalc CRYSCALC.CFL PAT
```

In such a case, a powder pattern calculation is performed, using structural parameters from the input file and profile parameters defined in the CRYSCALC.INI setting file.

- # "READ\_CIF" and "READ\_INS" routines: min and max Ueq values for Carbon species are now output, as well as the Ueq\_max/Ueq\_min ratio value.

### September 2019

- # "CREATE\_CIF" routine is now available even if structural data are input by user and not read in a file (.PCR/.INS/.CEL) Ouput CIF file name can be specified as argument of "CREATE\_CIF" keyword.
- # Change in the SEARCH\_SYMM/SEARCH\_LAUE keyword routine: to increase the speed of Rint calculation, crystal system is now taken into account if known. To force the calculation for all Laue group, "ALL/FORCE\_ALL" argument can be used. To force the calculation for triclinic symmetry, "T/TRICLINIC/FORCE\_T/FORCE\_TRICLINIC" argument can be used.
- # New "NOR" optional argument for READ\_HKLF5 keyword: create HKLF5 file containing only non-overlapping reflections and HKL files for each twin component.
- # New "create\_ool" item has been added in the [OPTION] part of the setting file: create a cryscalc.OOL file, containing a list of CRYSCALC instructions, separated by ";" character (same content as .CFL file but on one line). Note that the contain on this line starts and ends with "\" character.

Example : \ MENDEL Ni ; MENDEL MN ; \

This .OOL file can then be a command line argument when CRYSCALC is launched from a command line :

```
d:\progs> cryscalc cryscalc.ool
```

Note that this facility is reserved for expert users.

- # New "OUT" optional argument for CREATE\_ACE, CREATE\_CEL, CREATE\_CFL,

CREATE\_INS, CREATE\_PCR, CREATE\_PDB, CREATE\_TIDY and CREATE\_XYZ keywords:  
output lines on screen for the created file.

### July 2019

- # New HKL/CREATE\_HKL argument for READ\_FCF keyword: creation of an .hkl file (SHELX format). To get the hkl file in a free format, \_FREE has to be added to the argument.  
Examples:  
    READ\_FCF job.fcf HKL  
    READ\_FCF job.fcf HKL\_FREE
- # New EXTRACT\_OLEX command line argument: extract .res file and hkl data from the hkl loop in an archive .CIF file. Syntax is as follows:  
    d:\cifs>CRYSCALC EXTRACT\_OLEX archive.cif

### June 2019

- # Orientation matrix (UB matrix) is now included in the final archive.CIF file
- # New CREATE\_CIF keyword is now running after reading a .CEL file coming from PowderCELL.
- # New "How to convert .PCR or .INS/.RES file to a CIF file?" tutorial
- # CRYSCALC user's guide can be created from command line and one of the following argument : /?, HELP, /HELP, -HELP, --HELP, /H, -H, MAN, /MAN, -MAN, --MAN, /M, -M
- # New "computing\_molecular\_graphics" and "computing\_publication\_material" items can be defined in the [PROGRAMS] section of the setting file.
- # New "atom\_adp\_type=0/1" option in the CRYSCALC.ini setting file: allows to define ADP type in CFL files:  
    0: B\_iso  
    1: U\_iso
- # When reading .PCR or .INS/.RES file from command line, a CIF file can be automatically created if "create\_cif=1" is specified in the [COMMAND LINE ARGUMENTS] section of the setting.file.
- # New CREATE\_CIF keyword allows to create a CIF file after reading structural features from a .PCR or .INS/.RES file.
- # CRYSCALC instructions can now be specified as command line arguments. In that case, first and last characters of the command line has to be ";" (or "\"), and ";" is used as keywords separators. (Thanks to C. Prestipino [ISCR] for the suggestion).  
Examples :  
    d:\>crystalcalc ; SG P 21/c ;  
    d:\>crystalcalc \ read\_pcr job.pcr ; create\_ins ; \  
Note that the total length of the command line must not exceed 1024.

### May 2019

- # "mp" argument for CREATE\_PCR keyword allows to create .PCR file for FullProf in multi-patterns format. This can also be specified in the setting file through create\_pcr=2 in the [COMMAND LINE ARGUMENTS] section.  
Note that FullProf has been modified to perform powder pattern simulation (JTyp=2 or Jtyp=3) from multipattern PCR file (FullProf needed a data file

previously). This corrected version will be available in near future.  
in the ILL FullProf web site:

<https://www.ill.eu/sites/fullprof/php/downloads.html>

#### April 2019

- # New "CSD\_affiliation" and "CSD\_country" items have been added in the [USER] part of the setting file : these fields are used to fill the header of archive.cif file ; they are useful for a CIF file deposition at CCDC or FIZ Karlsruhe.
- # New "WL=" and "E=" optional arguments for BEAM keyword, allowing to enter wavelength (in A) or beam energy values (in KeV for X-rays and electrons or in meV for neutrons).
- # New CREATE\_PDB keyword allows to create .PDB file containing atoms list with Cartesian coordinates in PDB format. This .PDB can be visualized for example with Pymol. Documentation on PDB format has been used from:  
<http://www.wwpdb.org/documentation/file-format-content/format33>  
In addition, "create\_PDB" field can be input in the "[COMMAND LINE ARGUMENTS]" part in the cryscalc.ini setting file.

#### March 2019

- # References in HTML and LATEX structural reports are now written following the edition typography (Thanks to B. Boitrel [ISCR] for the suggestion) :
  - . journal name in italic mode
  - . year in bold mode
  - . volume number in italic mode.
- # New EXTRACT\_CIF command line argument: extract .cif files embedded in multiple global archive .CIF file. Syntax is as follows:  
d:\cifs>CRYSCALC EXTRACT\_CIF multiple\_archive.cif
- # New MAX\_FC keyword : output the most intensive calculated reflections  
Crystal structure has to be read first with READ\_INS/READ\_CIF/READ\_PCR keywords.  
Example :  
READ\_CIF my\_structure.CIF  
MAX\_FC 15
- # Optional ISO argument for WRITE\_ADP keyword will output only atoms with isotropic ADP.

#### February 2019

- # Reports creation is embedding sample\_ID\_sfrm.png file if present in the current folder
- # Create import.cif file routine : if the ID\_01\_0001.sfrm does not exist, the routine is now looking for the first present frame of each scan to extract scan features.
- # Correction of a bug in the WRITE\_ADP keyword routine (rms values were wrong when calculated from U\_ij values extracted from .INS file.
- # New ADD\_HKL command line argument allows to embed hkl data into an archive\_hkl.cif file. Syntax is as follows:

```
d:\cifs>CRYSCALC ADD_HKL archive.cif job.cif
where archive.cif is a final archive CIF file and job.cif
the CIF file created by SHELXL and containing hkl data,
starting with _shelx_hkl_file item and finishing with
_shelx_hkl_checksum item.
```

# When creating a global CIF file for multiple structures deposition, the list of authors to be included can be specified in a special file named "authors\_list.txt". The syntax is as follows :

```
[AUTHOR]
```

```
Name, first_name
address
address2 (optional)
address3 (optional)
```

Note that :

- . input items can contain characters with accents
- . address has to be input in a single line. On the other hand, a second line will be interpreted as a second address. Carriage return can be applied using "\\\" separator character.

Example:

```
[AUTHOR]
ROISNEL, Thierry
Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes)
- UMR 6226 \\ F-35000 Rennes, France
```

### January 2019

- # Optional ISO/FORCE\_ISO argument for CREATE\_PCR keyword will force ADP parameters to be written as isotropic values, even if anisotropic ADP parameters values have been input.
- # Option 10 in the main menu provides the capability to get some examples of .cfl input files for CRYSCALC.
- # CRYSCALC solve\_to\_ins: protection to avoid problems in case of wrong SFAC/UNIT format in SHELXL file if more than 999 atoms of one atomic species.

### November 2018

- # New option for LIST\_HKL\_MAX keyword: followed by an integer (n), corresponding to the number n of the most intensive reflections to be output.
- # New optional argument for FILE/READ\_HKL keyword:  
MAX\_n : list the n most intensive reflections  
MAX\_ALL : list all reflections in decreasing intensity order.
- # New optional argument for GEN\_HKL keyword:  
OUT\_n : sort reflections list by decreasing F2calc and list the n most intensive ones.  
OUT\_ALL : sort reflections list by decreasing F2calc and list all of them.
- # Bad Rint criteria can be defined in OPTIONS section of the setting file through the bad\_rint\_criteria string (default value is 25.)
- # New argument for UPDATE keyword : if ZIP is given as argument, a zipped file containing cryscalc.exe will be downloaded from:

<https://cdifx.univ.rennes.fr/progs/cryscalcalc/cryscalcalc.zip>

### September 2018

- # Automatic installation of CRYSCALC can now be performed using the new CRYSCALC\_setup.exe program developed with Inno Setup (<http://www.jrsoftware.org/isinfo.php>). CRYSCALC\_setup.exe can be download from : [https://cdifx.univ-rennes.fr/progs/cryscalcalc/cryscalcalc\\_setup.exe](https://cdifx.univ-rennes.fr/progs/cryscalcalc/cryscalcalc_setup.exe)
- # Cryscalcalc tutorials (.pdf) are also available henceforth from the CRYSCALC main menu.
- # Simulation of powder diffraction pattern: random noise is now added to the Y\_obs values, using same random generator as in FullProf.

### July 2018

- # Some CRYSCALC tutorials has been written and are available from the HTML user's guide:
  - . How to install?
  - . How to get help?
  - . How to start?
  - . How to create import.cif file on a Bruker diffractometer?
  - . How to convert CIF/INS files?
  - . How to calculate a powder diffraction pattern from a CIF/INS file?
  - . How to create a final CIF archive?
  - . How to extract .res and .hkl from a cif file?
  - . How to create an experiment report and tables from a CIF file?
  - . How to create a global CIF archive from several CIF files?
- # New feature for UB\_MAT keyword: if only one argument is input, it has to correspond to a CIF file name and UB matrix will be extracted from "\_diffrn\_orient\_matrix\_UB\_xx" lines.
- # New "create\_PAT\_PDPF=0/1" option in [COMMAND LINE COMMANDS] section of the setting file allows to create a Powder Diffraction Pattern File (.pdpf) containing hkl list, 2theta, d\_hkl values and relative intensities when a simulation of powder diffraction pattern is performed through the command line.  
Example : `cryscalcalc 100604.cif PAT`  
This kind of pdpf file can also be created in CRYSCALC with GEN\_HKL keyword and PAT\_PDPF argument (see user's guide.

### June 2018

- # New SEARCH\_SYMM keyword : calculation of internal R values for different Laue group and deduction of the most probable one.

### May 2018

- # New "SIZE\_Y=" and "STRAIN\_U=" arguments can be used with "GEN\_HKL" keyword, combined with "PAT" argument, to generate broadened profiles due to size or strains effects respectively. In that case, diffraction peaks are broadened with the following expressions:

```

HL_broad = size_Y/cos(theta)
HG_broad = U.tan(theta)
Final diffraction profiles are calculated as follows:
HG**2 = HG_inst**2 + HG_broad**2
HL     = HL_inst     + HL_broad

```

Note that HG\_inst and HL\_inst, corresponding to the gaussian and lorentzian parts of the Voigt function used to describe the instrumental resolution function, are defined in the setting file ([PATTERN SIMULATION] section). They can be directly profile\_TCH\_\*\* values for TCH Voigt profile function or internally calculated from the profile parameters if pseudo-Voigt profile function is chosen.

# Thompson-Cox-Hastings Voigt profile function can be used for powder diffraction patterns simulation, using the "profile\_function = TCH" line in the [PATTERN SIMULATION] section of the setting file. Gaussian and lorentzian parts of TCH function are defined as follows:

```

HG**2 = U.tan(theta)**2 + V.tan(theta) + W
HL     = X.tan(theta)     + Y/cos(theta) + Z

```

Default values for U, V, W, X, Y, Z TCH parameters are internally defined but can also be defined by the user in setting file through :

```

X_profile_TCH_U      = 0.0046
X_profile_TCH_V      = 0.0375
X_profile_TCH_W      = 0.0027
X_profile_TCH_X      = 0.
X_profile_TCH_Y      = 0.014
X_profile_TCH_Z      = 0.

```

Similar parameters can also be defined for a neutron diffraction pattern simulation using "N\_profile\_TCH\_\*" instead of "X\_profile\_TCH\_\*" lines

# Powder diffraction patterns can be simulated taking into account presence of strains in the sample. Strains are specified through the "strain=" argument of the GEN\_HKL keyword.

Remark: only gaussian part of the Voigt profile function is affected by strains in the sample

Strains can also be defined in the setting file ([PATTERN SIMULATION] section), through the "strain =" instruction. Profile broadening effects will be applied for strains values in the 1.E-06 - 0.02 range.

# Pattern simulation with particles size effects: a small error has been corrected in the Thomson-Cox-Hastings formula. Simulated patterns are now in perfect agreement with size values provided by a profile refinement (ex: FullProf).

### April 2018

```

# New "atom_occ_type=0/1" option in the CRYSCALC.ini setting file:
allow to define occupation type :
0: occupation type = % of site occupancy (default value)
1: occupation type = K * m/M * % of site occupancy
    m: site multiplicity
    M: space group multiplicity
    K: proportionnal value

```

# New BVPARM keyword allows the user to input d0 and B0 parameters for Bond Valence Sum calculations (see CONN keyword). The order of BV parameters are as follows: cation anion d0 B0

Example: BVPARM W+6 S-2 2.309 0.370

### March 2018

- # New CREATE\_XYZ keyword allows to create .XYZ file containing atoms list with Cartesian coordinates. This .XYZ can be loaded for example with Mercury.
- # SEARCH\_P3P6 routine has been changed: Rint values are now calculated for different trigonal and hexagonal laue groups.
- # New "ANA/ANA\_OUT" arguments for READ\_HKLF5 keyword: search for redondant reflections.
- # GEN\_HKL keyword: if "PAT" argument is changed to "PAT\_NOPLOT", PRF file will not be plotted by winPLOTR.

### February 2018

- # CREATE\_CIF\_BUFFER command line argument: create a buffer file containing the list of CIF files present in the current folder. The name of this buffer file can be given through a second argument in the command line. If not, default buffer file is named "CIF\_files.buf".
- # New LIGAND= argument for CONN keyword will output only connectivity with a particular atom.  
ex: CONN RE1 LIGAND=Br1

### January 2018

- # Global CIF file containing several structures can be created through CREATE\_GLOBAL\_CIF command line argument. The list of CIF structures files is specified in a buffer file. The name of this buffer file can be given through a second argument in the command line. If not, default buffer file is called "CIF\_files.buf".
- # CONN keyword provided connectivity list with the whole symmetry operators used to generate the ligands (combination of "(tx,ty,tz)" and "Sym. Op."
- # New "No\_BD" argument for CONN keyword: exclude bonds distribution in the output
- # Maximum number of reflections in a HKL file has been extended to 1500000.

### December 2017

- # New SEARCH\_P3P6 keyword : calculate internal R values for P 3 and P 6 space group and deduce if symmetry is rather trigonal or hexagonal.
- # Minor changes in .HTML/.PDF reports

### November 2017

- # New "MAX\_geom" keyword in the [ARCHIVE\_AND\_REPORT] section of the setting file:  
allows to define the max. number of molecular geometry features (distances, angles, torsion angles and htab values) in a .CIF file. Max. and default values are 2000.
- # New "READ\_SPF" keyword: read SUPERFLIP/EDMA input files to extract cell parameters, wavelength, symmetry operators, centering vectors

and deduce current space group.

- # New "ANIS/ANISO" argument for CREATE\_INS keyword will add ANIS keyword in the .INS created file.
- # New optional arguments (SIR, SXT and SPF) for "SOLVE" instruction will specify the files to be created, for SIR, SHELXS/T and SUPERFLIP/EDMA respectively. In the case of SUPERFLIP/EDMA, the previous `cryscalc_superflip.in` and `cryscalc_edma.in` input files are now replaced by a single file called `xxx_SPF.in`, where `xxx` is the sample ID if exists or "cryscalc".
- # New argument for "FILE import.cif" instruction; "CREATE\_P4P" allows to create a .P4P file.
- # EXTRACT\_RES\_HKL keyword (Y/N) in the [COMMAND LINE ARGUMENTS] section of the setting file allows to extract .RES and .HKL file from archive.CIF file.
- # Some minor changes has been made in SUPERFLIP input file created by CRYSCALC:
  - . "derivesymmetry yes" is replaced by "derivesymmetry use"
  - . "symmetry ... endsymmetry" contains all symmetry operators of a primitive lattice
  - . "centers ... endcenters" card provides all centering vectors.
- # New "SPF\_X/SUPERFLIP\_X" argument for WRITE\_SYM\_OP keyword: ouput symmetry operators card in a x1 x2 x3 format, whereas SPF/SUPERFLIP keyword provides symmetry operators in x y z format.
- # Create\_archive routine is now adapted to extract Hydrogen bonds from CIF files created by the old and new version of SHELXL and the optionnal presence of "\_geom\_hbond\_publ\_flag" string.

#### October 2017

- # Routine to include .res/.hkl/.fab files into the final archive.cif file has been modified (new routine : `Include_file_into_CIF`).
- # New "SPF/SUPERFLIP" argument for WRITE\_SYM\_OP keyword
- # New "ISO" argument for CREATE\_INS keyword will force to ouput Ueq values in the atoms list, even if anisotropic ADP's are input.
- # CREATE\_INS keyword keeps the isotropic/anisotropic character of ADP's.

#### September 2017

- # New "PURGE" argument for CREATE\_INS keyword will exclude spurious atoms with  $U_{eq} < 0.$  or  $U_{eq} > U_{threshold}$ .  
`U_threshold` value can be defined in the [CREATE INS] section of the setting file through `U_threshold` keyword.
- # SOLVE keyword generates an input file (called `cryscal_EDMA.in`) for EDMA EDMA software.
- # New matrices implemented in the list of matrices, corresponding to the faces centered cubic unit cell to hexagonal R-centered unit cell transformations. These matrices correspond to #35 and #36 in the list of matrices.
- # Number of user matrices has been extended to 6.
- # Cosmetic changes in the PGF file created by the `READ_FCF` keyword.
- # New procedure to create final archive.cif file:
  - . extract all structural and refinement parameters from `xx.cif`
  - . extract all crystal and diffractometer features from `import.cif`

# Create\_archive routine is now adapted to extract Hydrogen bonds from CIF file created by the new version of SHELXL (july 2017) and the presence of "\_geom\_hbond\_publ\_flag" string.

#### July 2017

# Number of scans is now dimensionned dynamically. Default value is 50 but can be defined by user in the setting file through the "nb\_scans" keyword in the [ARRAYS DIMENSIONS] section.  
# When creating import.CIF from .P4P and .HKL files, experiment temperature is now extracted for each scan from first .sfrm image.  
# SEARCH\_MONO keyword is now operating for C-centered Bravais lattices.

#### June 2017

# No\_H argument for WRITE\_ADP and WRITE\_ATOMS keywords will output only non-hydrogen atoms.  
# Change in the READ\_CIF\_atom routine of CFML to read correctly anisotropic ADP in CIF files.  
# Cosmetic features for LATEX experimental report can be specified in the [ARCHIVE\_AND\_REPORT] section of the setting file, ie :  
latex\_cmb = 0 ! use Computer Modern Bright font in LaTeX report  
latex\_sans\_serif = 1 ! use Sans Serif font in LaTeX report  
latex\_title\_back\_color = #e3e6f7 ! Main title background color in LaTeX report  
latex\_title\_text\_color = #580a0a ! Main title text color in LaTeX report  
latex\_title\_border\_color = #000000 ! Main title border color in LaTeX report  
latex\_title1\_back\_color = #fafafa ! Title background color in LaTeX report  
latex\_title1\_text\_color = #580a0a ! Title background text in LaTeX report  
latex\_title1\_border\_color = #fafafa ! Title background text in LaTeX report  
latex\_title1\_text\_center = 1 ! Title text centering (0/1)  
# CELL keyword : crystal system is now deduced from cell parameters input by hand.  
# Maximum number of reflections in a HKL file has been extended to 750000.  
# Reorganization of several routines: CRYSCALC\_main.F90 and interactive.F90 global routines and particular cryscalclf95/fort routines for specific Fortran features (Command line, compiler type, PAUSE function).

#### May 2017

# Extraction of scan features in the creation of import.CIF files is now correct for diffraction experiments with more than 9 scans.

#### April 2017

# CELL keyword allows to extract cell parameters from a .PCR FullProf file  
ex: CELL 10K.pcr

#### March 2017

# Particles size (in A) for a diffraction pattern simulation can be defined in the setting file ([PATTERN SIMULATION] section), through the "particles\_size = " instruction. If the value of particles size is lower than 9999., profile broadening effects will be applied.

# CELL keyword : Bravais lattice and crystal system are extracted when reading a .P4P, .INS and .CIF file.

# SEARCH\_GROUP routine has been corrected for centered space group: by default, only space groups with Bravais lattice in agreement with the unit cell Bravais lattice are output.

# Maximum number of atoms has been extended to 1200 when reading a .INS/.CIF file.

# Compilation of CRYSCALC with latest version of CRYSFML (feb. 2017): standard deviations of atomic coordinates are taken into account in the calculation of plane equation (case of more than 3 input points).

### January 2017

# NEWS keyword can contain "EXPERT\_ONLY" as argument to output CRYSCALC news available only in expert mode.

# "EULER\_TO\_KAPPA" routine has been corrected for Chi values larger than 180 : Chi is then transformed to 360. - Chi).

# ABIN keyword allows to read and modify a .INS file by adding the ABIN SHELXL instruction (not included if .INS written by SXGRAPH interface of WinGX).

# The CRYSCALC routine associated to STAR\_K keyword has been changed to the "K\_Star" routine of CFML.  
The previous routine can still be output using the TR argument for STAR\_K (available only in expert mode)

# PLANE keyword accept more than 3 atoms for the calculation of a mean plane equation.

# Compilation of CRYSCALC with latest version of CRYSFML (December 2016)

# New CELL\_ESD keyword: input of esd's for cell parameters and calculation of corresponding unit cell volume ESD.

# New GET\_TRANSF\_MAT keyword provides the transformation matrix between two primitive unit cells (determinant of the matrix is equal to 1).

# New REDUCE keyword provides conventional unit cell parameters and transformation matrix between input cell and conventional cell(s). The routine is based on Get\_conventional\_Unit\_Cells program written by JRC using procedures implemented in CRYSFML.

### December 2016

# New WRITE\_BONDS, WRITE\_ANGLES, WRITE\_TORSION\_ANGLES, WRITE\_HTAB keywords are available after a READ\_CIF instruction.  
[only in EXPERT mode]

# When creating import.CIF from .P4P and .HKL files, scans features (type of scan, DX, exposition time, starting angles for theta, omega phi and chi motors) are extracted from .sfrm images.

### November2016

```
# "WRITE_ATOMS cart" keyword leads to the creation of a cryscalc.xyz file
for PyMOL (http://www.pymol.org/).
# NO_DETAILS keyword will lead to a very short and restricted output.
[only in EXPERT mode]
# TOLMAN keyword: van der Waals radius for ligands can be given as
arguments. If not specified, default values are coming from
CRYSFML library, excepted for H atoms (r=1.2A).
ex: TOLMAN C01 P1 H1A H11A H21A 1.22 1.22 1.22
# When creating import.CIF from .P4P and .HKL files, crystal to detector
distance is now extracted from .sfrm files for every scan of the data
collection.
# New "NO_H" argument for CREATE_INS keyword will exclude
hydrogen atoms from the created .INS file.
# New "NO_details" argument can be applied to most of the keywords,
excepted WRITE* keyword. This action will lead to a very short
and restricted output.
# New REM keyword: non interpreted command. Can be useful
to skip a command in a CFL input file. This keyword can
be replaced by "!" or "#" character.
```

### October 2016

```
# New READ_HKLF5 keyword: read HKLF5 format data file containing
structure factors of a twin crystal.
# New REF_SHELX keyword: output references for SHELXL and SHELXT
software.
# If a .png/.jpg file corresponding to the crystal picture is present
in the current folder (named as sample_ID.png/.jpg), it will be
embedded in the final structural report.
# New TOLMAN_ANGLE keyword: calculation of the Tolman cone angle
as defined from crystallographic data and Van der Waals radii in
"Transition Met. Chem. 20, 533 (1995)". The TOLMAN_ANGLE keyword
has to be followed by the labelling of the 5 atoms defining the cone,
corresponding to metal, centered atom and 3 ligand atoms respectively
```

### September 2016

```
# Cosmetic changes in the .HTML/.TXT/.PDF structural reports
# Redundancy is now calculated and output during Rint calculation.
# New "KAPPA_TO_EULER" AND "EULER_TO_KAPPA" keywords allow to convert
motors angles values of single crystal diffractometer from Kappa to
Eulerian geometry (and opposite)
```

### July 2016

```
# .FAB file created by SHELXL201x is now embedded in the
cryscalc_archive_hkl.cif file in the case of SQUEEZE
procedure has been used.
# Mean value of atomic volume for non H hydrogen atoms is now output after
molecular density calculation for compounds containing H atoms.
```

### June 202016

```
# New HKLF5 keyword: 9 arguments are necessary to input the 3*3
transformation matrix components. Combined with FILE keyword,
a hklf5 format data file is then created. Overlapping reflections
criteria can be defined in the cryscalc.ini setting file through
"ref_overlap_criteria=" keyword in the [OPTIONS] section. Defaut
value is 0.15 and max. value has been fixed to 0.25
# Corrections of minor bugs, specially when .CFL input file is read from
option #2 in the main menu.
# New EXTRACT command line argument: extract .res and .hkl files
embedded in an archive .CIF file. Syntax is as follows:
  d:\cifs>CRYSCALC EXTRACT archive.cif
# New features for SUPERCELL instruction:
  . cell parameters are updated
  . if space group of initial cell is know, space group is
    updated to P 1.
# STAR_K keyword: the arms of the K star are now correct
for primitive and centered space groups.
# New "CONDENSED" argument for WRITE_SYM_OP keyword:
output symmetry operators list in a condensed way.
```

### May 2016

```
# New ONLY_X argument for CONN keyword : output connectivity
between atoms of the same X species.
# CONN keyword: MIN and MAX arguments are now taken into
account correctly.
# Correction of bug in the "STAR_K" keyword routine :
The arms of the K star are now ouput for primitive
space groups (not yet ouput for others).
# new SAVE_SETTINGS keyword will save cryscalc.ini setting file
in the current folder. This can be useful if no setting file
is present in the CRYSCALC folder.
# WRITE_CELL keyword: standart deviations of cell parameters
and volume are ouput if they are known.
```

### April 2016

```
# Results of Rint calculation was bugged for successive
calculation without using RESET keyword. This is corrected.
# New FCF_FILE keyword: read .fcf file create by SHELX
IF "PLOT" is given as argument, a *_FCF.PGF file for WinPLOTR
is created (Fc2=f(Fo2) curve)
IF "PLOT_STL" is given as argument, a *_FCF_stl.PGF file
is created (Fc2 - Fo2 = f(sinThetal/lambda) curve).
If WinPLOTR is already installed, .PGF file is automatically
displayed.
```

### March 2016

# New features in the header of the import.cif file created from .P4P, .HKL and .ABS files coming from single crystal data reduction in APEX2 and APEX3 (Bruker AXS software).  
# MONOCLINIC keyword : condensed output if "no\_out" is given as argument.

### February 2016

# New DIFF keyword : calculation of the components of the difference atomic coordinates vector between 2 input atoms  
# New PLANE keyword : calculation of the 4 components of the plane equation  $Ax+By+Cz+D=0$ , given three atoms coordinates.  
# New SEARCH\_TETRA keyword : determine tetragonal axis from hkl data integrated in a pseudo-cubic unit cell by calculating successively internal R values for the most probable space group of following different setting: abc, cab, bca

### January 2016

# New UPDATE/NO\_UPDATE arguments for MAT keyword  
# New SUPERCELL input keyword: calculation of atomic coordinates in a superstructure cell.  
# \_shelx\_res\_checksum and \_shelx\_hkl\_checksum items are included in the archive.cif file for compatibility with PLATON Checkcif and cif files created by SHELXL-2014.

### December 2015

# Minor correction in the header of import.cif created from .P4P and .HKL files

### November 2015

# DIST keyword : "\_" option after second label allows to calculate interatomic distance between first input atome and the closest equivalent second atom (space group has of course to be known).  
example : DIST Mo1 Mo2\_\*

### October 2015

# HKL\_diff keyword : calculation of F2 difference for common reflections of 2 hkl files.  
# UPDATE keyword : download the lastest version of CRYSCALC from the web site (<https://cdifx.univ.rennes.fr/progs/cryscal/cryscal.exe>)  
Remark: Browser has to defined in the setting file.  
# Minor cosmetic changes in import.cif

### September 2015

```
# Polar character of space group has been corrected : point group
has to be one of the following :
1, 2, 3, 4, 6, mm2, m2m, 2mm, 3m, 3m1, 31m, 4mm, 6mm
# "include_experimenter" field can be input in the cryscalcalc.ini setting file :
experimenter features, coming from [AUTHOR] section, are then included
in the archive_cryscalcalc.cif file.
# import.cif file created from .P4P and .HKL files contains the number of scans
of the data collection and related features (exposition time, frames width,
number of frames)
# NIGGLI output: Niggli matrix is now output
```

### July 2015

```
# THERM output: some calculation outputs were wrong in the case of
"matrix U non-positive definite".
```

### June 2015

```
# SEARCH_EXTI keyword can have a string optional argument : if "ALL"
is given as argument, all reflections are considered, without applying
any criteria.
# A small bug has been corrected in the SEARCH_GROUP routine. It appeared
only when searching from only centered space groups and the symmetry
was unknown in the import.cif input file.
# Two logos for the structural_report.pdf can be specified in the
[OPTIONS] section of the setting file. These .jpg files will be used
included in the structural report (Latex and pdf formats). They
have first to be present in the \img folder of the CRYSCALC directory.
ex:
report_logo_1 = CDIFX_logo.jpg
report_logo_2 = ISCR_logo.jpg
```

### May 2015

```
# new SEARCH_MONO keyword : determine monoclinic angle
from hkl data integrated with a pseudo-orthorhombic
unit cell by calculating successively internal R values
for "P 2 1 1", "P 1 2 1" and "P 1 1 2" space groups.
# CONN output: polyedron distorsion is calculated as:
distorsion = SUM((dist-dist_av)/dist_av)**2) / n
with n: number of ligands
dist_av: average distance
# Minor changes for D8 Venture data file
```

### April 2015

```
# New DETAILS argument for WRITE_ADP keyword
```

### March 2015

```
# New CREATE_PCR keyword : create .PCR input file for FullProf
(pattern simulation). Structural data have to be previously input
through for example READ_CIF or READ_INS keywords. in such a case,
profile features can be specified in the setting file
([PATTERN SIMULATION (Pseudo-Voigt profile)] section).
# "create_pcr=1" can be spectified in the [COMMAND LINE ARGUMENTS]
section of the setting file to create automatic PCR file
from command line run of CRYSCALC
```

### February 2015

```
# New arguments for SEARCH_GROUP keyword :
. P : provide only primitive space groups
. ALL: provide primitive and centered space groups
. CENTERED/NOT_P: provide only centered space groups
# CIF files created by SHELXL2014 are correctly read (changes in
in CRYSFML to read new CIF strings as :
. _space_group_name_H-M_alt
. _space_group_symop_operation_xyz
. _space_group_crystal_system
# Parameters for D8 Venture diffractometer (Bruker AXS) has been included and
can be accessed from setting file in [DEVICE] section through :
"diffractometer = D8_VENTURE_Cu" or "diffractometer = D8V_Cu"
"diffractometer = D8_VENTURE_Mo" or "diffractometer = D8V_Mo"
for Cu and Mo radiations respectively.
# Flack parameter is now provided in HTML and TXT reports.
```

### December 2014

```
# Archive.cif command line argument can be followed by "NO_HKL",
allowing to exclude HKL file in final archive, independently
of the contain of cryscalcalc.ini setting file.
```

### November 2014

```
# New argument for DATA_neutrons keyword, allowing to provide
to the user neutron scattering length versus energy for
some rare earths and isotopes. The following arguments can be
input: Sm_nat, SM_149, Eu_nat, Eu_151, Gd_nat, Gd_155, Gd_157,
Dy_164, Er_nat, Er_167, Yb_nat, Yb_168, Yb_174 and Lu_176.
Thanks to Pierric Lemoine (ISCR) for taping neutron scattering
lengths from the following reference :
Atomic data and nuclear data tables 44, 191-207 (1990)
J.E. Lynn and P.A. Seeger, L.A.N.L.
# New PAT command line argument after .CIF or .INS file
allows to calculate a diffraction pattern from features given by
PDP_BEAM/PDP_WAVE keywords and details in the [PATTERN SIMULATION]
section of the setting file.
Example: cryscalcalc job.cif PAT
```

### October 2014

```

# New [USER SHORTCUTS] section of the cryscalc.ini, defining
some keywords shortcuts (max. = 10). The shortcut and its
details (CRYSCALC keyword) has to be separated by "=" character.
Example: RJC = READ_CIF job.cif
# New parameters in [PATTERN SIMULATION] section of the cryscalc.ini
setting file. These parameters are used for simulation
of powder diffraction file from command line and .CIF/.INS
file (create_PAT_PRF=1)
  pdp_beam   = N      ! N for neutrons / X for X-rays
  pdp_wave   = 1.22 ! wavelength used for diffraction pattern
                    simulation
If not specified, simulation pattern is calculated for
X-rays and Copper K_alpha1 radiation (1.5406 A)
# New command line argument:
CREATE_ARCHIVE argument, followed by the name of CIF files
(without extension), allows to create a whole archive.cif file.
First cif file corresponds to the main CIF file created by
refinement software and next ones to supplementary cif files
to complete the archive.
ex : d:\> CRYSCALC  CREATE_ARCHIVE my_job.cif import.cif
      . my_job.cif : main .CIF file, used to extract structural
                    parameters
      . import.cif : secondary .CIF file, containing experimental
                    parameters (crystal and experimental features, ...)

```

### September 2014

```

# new CREATE_SOLVE keyword:
. create input files for structure solving software as SIR97,
  SHELXS/T and SUPERFLIP.
# bugs corrections:
. site multiplicity calculation
. CRYSCALC reports (html, txt, latex): adp are in A^2
  and not in A^2x10^3 !
# Some statistics on F2_mean, sig_mean ... have been added in the
  output of the FILE keyword.

```

### July 2014

```

# "include_HKL_file" field can be input in the cryscalc.ini setting file to
embed the contain of hkl SHEXL file in the archive_cryscalc.cif file.
The SHELXL hkl file name corresponds to the last project ID in WinGX.
# TO AVOID CONFUSION, CRYSCAL PROGRAM HAS BEEN RENAMED AS
CRYSCALC. FEATURES OF THE SOFTWARE HAVE TO BE CHANGED
CONSEQUENTLY :
. environnement variable : CRYSCALC
. setting file : CRYSCALC.ini
. css files : CRYSCALC.css and CRYSCAL_report.css
CRYSCALC will be included in the distribution of the FullProf Suite
in a near future.

```

### June 2014

```
# New argument for CONN keyword:
  . NO_xx : exclude xx atoms type from listing
  ex ! CONN Cu1 NO_H
# "create_PAT_PRF" field has been added in the "[COMMAND LINE ARGUMENTS]"
part in the setting file (crystalcalc.ini) : X-ray diffraction pattern
is then created (PRF file FullProf format) after reading a CIF file.
By default, details (structural informations, hkl list ...) are not listed on
screen but can be output by replacing "create_PAT_PRF" by create_PAT_PRF_out.
```

### May 2014

```
# Corrections of bugs caused by the new CRYSFML library
specially in bond distribution routine
# New arguments for CONN keyword:
  . ANG : interatomic angle calculation
  . CONDENSED : short output
```

### March 2014

```
# ALL_X argument for CONN keyword:
output atomic connectivity for all atoms
of the X species.
ex: CONN ALL_Cu
# in_A argument for WRITE_ATOMS keyword:
Atomic coordinates are listed in A
# VOL argument for CONN keyword:
polyhedron volume calculation, based on VOLCAL program
of L. W. FINGER, included in CFML
```

### February 2014

```
# BARY keyword:
Centroid calculation can be applied with only 2 input atoms
# Bug has been corrected in the HTML report combined with
SQUEEZE option.
```

### November 2013

```
# STAR_K keyword:
Apply rotational parts of the symmetry operators of a given
space group on the components of a propagation wave vector.
```

### October 2013

```
# CONN keyword:
  . new argument for GEN_HKL keyword : PM2K
  PM2K_hkl.inp is created : its contains hkl reflections list
  to be copied in the input file for PM2K program (M. Leoni).
  . new MIN= and MAX= arguments (default values are defined
```

in cryscalc.ini setting file ([PARAMETERS] section)  
. calculation of effective interatomic distances

### September 2013

# new SELF argument for CONN keyword: output interatomic distance only between atoms with same labels.  
This can be useful for M-M distances in a organometallic complex.  
# New READ\_FACES keyword : read crystal habitus .  
ex. : READ\_FACES absorb.ins  
ex. : READ\_FACES faces.Def

### July 2013

# New DHA keyword : calculation of H position given donor and acceptor atoms.  
# Change in MENDEL argument that can be atomic number.:  
ex: MENDEL 59

### May 2013

# READ\_INS keyword: by default, Q peaks are not read.  
Q\_PEAKE argument has to be specified for not skipping Q peaks

### April 2013

# new arguments for CREATE\_FST keyword:  
MOLE : space group line is commented to draw only atoms of the asymmetric unit cell  
No\_H : Hydrogen atoms and related bonds are excluded from the drawing (lines are commented).  
No\_H argument is valid only with MOLE argument  
POLY : includes polyhedra drawing in Fp\_Studio if connectivity calculations have been performed  
RUN : launch FP\_Studio  
# argument "CART" after the "WRITE\_ATOMS" keyword outputs the cartesian coordinates of the atoms. Cartesian frame type can be specified by "CART\_A" (x//a) and "CART\_C" (x//c).  
# argument "SHAPE" after the "CONN" keyword creates an input for SHAPE program (<http://www.ee.ub.es/>)  
derivative SHAPE arguments : SHAPE\_A (a//x), SHAPE\_C (x//c)  
# Cartesian frame type (A: x//a or C: x//c) can be specified in the setting file, through the "cartesian\_frame\_type" keyword in the [OPTIONS] section. Default value for the cartesian frame is A (x//a)  
# argument "CART" after the "WRITE\_CELL" keyword outputs the cartesian frame, metric tensors and Busing-Levy B-matrix. Cartesian frame type can be specified by "CART\_A" (x//a) and "CART\_C" (x//c).  
argument.  
# DEBUG, DEBUG\_2 and DEBUG\_3 keywords : access to debug modes and create cryscalc\_debug.txt file. In level\_2 debug mode, this file contains the name of main called routines. In level\_3 mode, this file

contains more explanations.  
[only in EXPERT mode]

### March 2013

# New keywords related to TIDY software (standardisation of inorganic crystal-structure data (Acta Cryst. 1984, A40, 169-183):  
- CREATE\_TIDY : create input file for TIDY from a .CIF or .INS file  
- READ\_TIDY\_out : read output file from TIDY (default name = stidy.out)

### February 2013

# CONN keyword can have BVS argument for Bond Valence Sum Calculation. Oxidation state of the input atoms have to be provided through the ATOM keyword.  
ex: ATOM Fe1 Fe+3 0.11 0.22 0.33 0.4 1.  
example of CFL file :  
https://cdifx.univ-rennes.fr/progs/cryscalcalc/cryscalcalc\_y2o3\_bvs.cfl  
# Final.y file (coming from EVALCCD) are not read anymore, since they don't contain structure factors.  
# Connectivity calculation outputs symmetry operators used to generate atoms around a particular one. CFML has been modified to output this list.  
# Profile (U, V, W, eta0, eta1) and pattern (step, constant background, scale factor) parameters can be specified in the [PATTERN SIMULATION] section of the cryscalcalc.ini setting file, for X-ray and neutron pattern calculation.

### January 2013

# When creating archive\_cryscal.cif file, CRYSCALC is looking for output files creating by different versions of SQUEEZE procedure in PLATON, as platon.sqf or platon\_sqr.sqf (PLATON jan. 2013)  
# New argument for GEN\_HKL for powder diffraction pattern calculation : particle size (in A) can be specified through the "SIZE=" keyword. If not, particle size is considered as infinite and no line broadening is calculated.  
Example : GEN\_HKL 2theta\_min=20 2theta\_max=120 PAT SIZE=250  
Example of CFL file :  
https://cdifx.univ-rennes.fr/progs/cryscalcalc/cryscalcalc\_si\_x\_100.cfl  
# Import.cif file can be created from .P4P file and .RAW file (output of SAINT program). This has to be specified in the command line through the "RAW=" keyword.  
Example:  
d:\data\CRYSCALC file\_0m.P4P RAW=file\_0m.RAW  
# New "DIST\_X" and "DIST\_PLUS" keywords allow to calculate the coordinates of a particular point aligned with with the input atoms

### December

# New "FRIEDEL" keyword allows to get number pairs of Friedel in hkl file

### November 2012

```
# Particular format for .hkl file (h,k,l F2, sig) can be specified
  in the setting file in the [OPTIONS] section through the
  hkl_format keyword.
  example hkl_format = 3i4,2F15.2
  If not specified, default format is : 3I4,2F8.2 (SHELX format)
# new argument for WRITE_SYMM keyword : if argument="SHELX"
  the list of symmetry operators is output in a SHELX format
# news arguments for SITE_INFO keyword :
  . if argument="PCR", the list of symmetry equivalent atoms
    is output in a FullProf format (.PCR)
  . if argument="PCR_MAG", the list of magnetic atoms
    is output in a FullProf format (.PCR)
```

### October 2012

```
# "CIF file for Pymol can be created by putting "PYMOL" as
  argument of "READ_CIF", "READ_INS" and "READ_CEL"
  keywords (example: FILE file.cif pymol) or in the command line
  with a cif.file (example: d:\crystalcalc file.cif pymol
  "create_CIF_PYMOL" keyword (value = 0/1) can also be specified
  in the crystalcalc.ini setting file : file_pml.cif file is then
  automatically created after reading a CIF file.
# "Skip_start_menu" keyword (value = 0/1) can be input in the crystalcalc.ini
  setting file to skip the starting main menu of CRYSCALC.
# HTML structural report: torsion angles values greater
  than CIF_torsion_limit are excluded. Default value
  for CIF_torsion_limit is 170.0 but can be defined in the
  crystalcalc.ini setting file in the [OPTIONS] section
# Special format can be specified with the FILE keyword
  when reading .hkl file, with the FMT argument.
  Example : FILE filename.hkl fmt=3I4,2F15.2
```

### September 2012

```
# new argument for BARY keyword
# "HKL_statistics" keyword (value = 0/1) can be input in the crystalcalc.ini
  setting file to output or not statistics on hkl reflections.
# Export mode can be specified in the setting file through the expert_mode
  string in the setting file. If active, this mode allows to enter new
  specific keywords. This mode can also be activated through the
  "EXPERT_MODE" keyword and put OFF with "USER_mode" keyword.
Examples:
  FIC   : "FILE import.cif"
  ST25  : "SHELL THETA 2.5 25"
MAN_EXPERT keyword has been added to output the list of instructions in
  this expert mode.
The list of expert mode keywords can be output through the "MAN_EXPERT"
  keyword if this kind of mode is activated.
[only in EXPERT mode]
```

## July 2012

```
# FILE keyword: .COL file created by COLL5 (ILL / format =4)
    can be read
# FILE keyword: .INT file created by DATARED can be read
# CELL keyword: .RED file for DATARED can be read
# REPORT_LATEX argument can be specified when launching CRYSCALC
  for the command line. In such a case:
  . structural_report.ltx file is created, in a LATEX format
  . pdflatex is launched to create a .pdf file.
  If a .GIF file is present in the current folder for crystal
  structure visualization, it is first converted in .png file
  to be included in the final pdf document.
[only in EXPERT mode]
# New OUT_n argument for FILE keyword, allowing to output every
n reflection features (index, h,k,l,F2,sig)
```

## June 2012

```
# SHIFT_2TH keyword can now be followed by three values,
  corresponding to a constant, cos and sin dependent shifts
  respectively.
# css files for structural HTML report and user's guide
  are now available in the CRYSCALC folder (repertory that
  contains the cryscal.ini setting file. If present, these
  css files, called cryscal_report.css and cryscal.css
  for report and user's guide respectively, can be edited
  and modified by the user. These css files contains
  styles that are used in the HTML documents.
```

## April 12

```
# MOVE/TRANSLATE keyword accepts 4 arguments, as the MOVE
  instruction on SHELXL. Optional 4th argument corresponds to
  the sign to multiply atomic coordinates. New atomic
  are then : sign*x + t_x, sign*y + t_z, sign*z + t_z
  If input 3 arguments are given, they correspond to the
  t_x, t_y and t_z translation and the 4th argument is
  taken equal to +1.
```

## March 12

```
# GET argument can be input with SEARCH_GROUP keyword:
  the most probable space group is then considered
# Cell parameters are deduced from UB matrix when P4P file or
  import.cif file contain this information. Use WRITE_CELL
  keyword to output these cell parameters.
```

## January 12

```
# CRYSCALC has been compiled with the new CRYSFML library
# MOVE instruction for SHELXL (output of SG_INFO for acentric
  space group) is now correct for non conventional settings
```

#### December 2011

```
# Some minor changes have been performed in the code to be compiled
  with Intel Fortran Compiler
# HKL arrays are now dimensionned dynamically. Default dimension is
  500000 but can be defined by user in the setting file though the
  "hkl_reflections" keyword in the [ARRAYS DIMENSIONS] section.
# "LOCK_wave_value" field can be input in the cryscalcalc.ini setting file to
  to define the lock the input wavelength to the value of the closer
  Xray target (Cu, Mo ...). if not present in the setting file, the default
  value for this field is 0.02.
Examples :
- input wavelength = 1.53 and LOCK_wave_value = 0.02 : wl = 1.5406
- input wavelength = 1.53 and LOCK_wave_value = 0.005 : wl = 1.53
```

#### November 2011

```
# Minor corrections in the HTML report in the "symmetry transformations
  used to generate equivalent atoms" parts (distances, angles, torsion
  angles and hydrogen bonds)
# LST_SG keyword :
- "chiral" and "polar" arguments can se specified to output
  chiral and polar space groups respectively
# SG_INFO keyword outputs the MOVE instruction for SHELXL
  in the case of acentric space groups.
# CRYSCALC has been compiled with last version of CFML (5.00)
  and changes in the space_group routine have been made to be
  to be in agreement with the CFML library.
```

#### October 2011

```
# LST_SG keyword :
- "enantio" argument can se specified to output
  enantiomorphic space goupes
- Point group is output
# MU keyword : explicit keyword to perform absorption coefficient
  calculation. Cell paramaters, wave and cell content has to be
  known. This keyword can be useful after reading of parameters
  from an external file as CIF or INS file.
ex : READ_CIF UA12.cif
      WAVE X_cu
      MU

# DIAG keyword : diagonalization of a 3*3 matrix and ouput Eigen values
  and Eigen vectors
# THERM_SHELX keyword : ADP parameters are input in the following
```

SHELX order, i.e. 11 22 33 23 13 12

### July 2011

# Up to 5 extra matrices can be provided by the user in the cryscalc.ini setting file in the [USER TRANSFORMATION MATRICES] section. These matrices are defined through the "MAT\_n" keyword followed by the 9 components of the matrix m11 m12 m13 m21 m22 m23 m31 m32 m33 . and a comment text.  
New "USER\_MAT" keyword has been added to select a particular matrix provided by the user in the cryscalc.ini setting file.  
The matrix to be selected can be input either by the numor preceded by the "# symbol, either the comment text preceded by the "\$" symbol  
Examples : USER\_MAT #1  
          USER\_MAT \$2a

# "include\_RES\_file" field can be input in the cryscalc.ini setting file to embed the contain of last .res SHELXL file in the archive\_cryscalc.cif file to avoid PLAT005\_ALERT\_5G alert in the CHECK CIF procedure. The SHELXL .res file name corresponds to the last project ID in WinGX.

# After a matrix transformation of atomic coordinates, the list of atoms is updated with new coordinates.

# Search\_group procedure outputs only space groups those Bravais lattice corresponds to the Bravais lattice contained in the import.cif file

# Include "\_symmetry\_space\_group\_name\_H-M" string in the import.cif file created from .P4P and .HKL file

### June 2011

# CRYSCALC has been compiled with new version of CFML (5.00)

### May 11

# Bug has been corrected in the structure factor calculation routine  
# Total number of electrons is output after CHEM keyword.  
# The matrix used for the hexagonal to rhomboedral system was corrupted.

### April 2011

# Some changes in the routine to get new space group after matrix transformation  
# Some changes in the monoclinic transformation matrix list  
# A non systematic bug in the bonds distribution list (CONN keyword) has been corrected

### February 2011

# Stucture factors calculation can be performed for electrons diffraction (GEN\_HKL and SF\_HKL routines). This has to be specified by the BEAM keyword and "ELECTRONS" argument

```
# Some examples of CFL input files can be downloaded from the
CRYSCAL web site (https://cdifx.univ-rennes.fr/cryscal)
# Some changes in output files :
. cryscal.log is renamed cryscal_debug.txt
. cryscal.out is renamed cryscal.log
LOG argument has been replaced by DEBUG argument
# New PAT argument for GEN_HKL keyword allows to generate a
diffraction pattern. PRF file is automatically plotted
with the WinPLOTR program if installed.
# I/Imax is now calculated in the GEN_HKL routine when working
in the 2theta space and neutron or Cu_K_alpha1 X-ray radiation.
Intensity is calculated as follows:
      I=mult * Lp * F^2
where : mult is the multicicity of the reflection
      Lp the Lorentz-polarization factor, calculated by:
      Lp=(1-K+K*CTHM*cos2(2theta)/(2sin2(theta)cos(theta)
      CTHM=cos2(2theta_monok) [CTHM=0.79]
      K=0. for neutrons
      K=0.5 for unpolarized X-ray radiation
# Cosmetic changes in the Fortran codes to allow the compilation
with the free G95 Fortran compiler.
```

#### January 2011

```
# CREATE_FST keyword allows to create a .FST file for
FullProf Studio after reading a CIF file.
# "create_FST" field can be input in the "[COMMAND LINE ARGUMENTS]" part
in the setting file (cryscal.ini)
```

#### December 2010

```
# New extinction rules for FIND_HKL_LIST keyword:
. hhl with h+l=2n
. hkk with k+h=2n
. hkh with h+k=2n
# Cosmetic changes in archive_cryscal.cif file: in the case
of samples without H atoms, "_atom_sites_solution_hydrogens" and
"_refine_ls_hydrogen_treatment" cif field lines are removed
```

#### November 2010

```
# Connectivity calculations are followed by a bonds distribution list
# Transformation matrix components can be input as fractional values
Example : matrix 1/2 1/2 0. -1/2 1/2 0. 0. 0. 1
# Cosmetic changes in HTML structural report
```

#### October 2010

```
# A threshold value can be given as argument to the SEARCH_GROUP keyword
```

### September 2010

# FIND\_HKL\_list argument value can be negative and allows to search reflections with opposite rule than for positive value.  
# SIR\_TO\_INS command line argument has been replaced by SOLVE\_TO\_INS and allows now to create INS file for SHELXL from SHELXS output file as well as SIRxx output file.)  
# CREATE\_ACE keyword allows to create a .ACE file for CarIne after reading a CIF file.  
# "create\_CEL" field has been added in the "[COMMAND LINE ARGUMENTS]" part in the setting file (cryscalc.ini)  
# NIGGLI/NIGGLI\_CELL keyword has been added and allows to determine the Niggli cell from any triclinic cell  
# [CREATE INS] section has been added in the cryscalc.ini setting file to define temperature and thermal parameter threshold to skip atoms  
This avoids to enter these values related to the CREATE\_INS keyword

### June 2010

# Bugs in the FIND\_HKL\_LIST routine has been corrected

### April 2010

# Some items of the experimental part in the HTML structure report are now in italic in agreement with published articles.

### March 2010

# WRITE\_DEVICE keyword  
# WRITE\_HKL keyword has been replaced by FIND\_HKL\_LIST.  
The SUPPRESS/REMOVE argument for FIND\_HKL\_LIST keyword has been added, leading to the creation of a new file free of data obeying the current selection rule.  
# QVEC components can be input as fractionnal values.  
The following fractionnal absolute values are :  
1/2, 1/3, 2/3, 1/4, 3/4, 1/5, 2/5, 3/5, 4/5, 1/6, 5/6,  
1/7, 2/7, 3/7, 4/7, 5/7, 6/7, 1/8, 3/8, 5/8, 7/8,  
1/9, 2/9, 4/9, 5/9, 7/9 and 8/9  
# GEN\_HKL keyword leads to a structure factor calculation if atoms has been input.  
# SF\_HKL keyword leads to a structure factor calculation for a given hkl reflection  
# New WRITE\_BEAM and WRITE\_QVEC keywords

### February 2010

# CREATE\_CEL keyword allows to create a .CEL file for PowderCELL after reading a CIF file.  
# CREATE\_INS keyword allows to create a .INS file for SHELXL after reading a CIF file.  
# CREATE\_CFL keyword allows to create a .CFL file for CRYSCALC

after reading a CIF file.  
# New "[COMMAND LINE ARGUMENTS]" part in the setting file (cryscal.ini)  
with the following fields :  
  . create\_CEL  
  . create\_INS  
  . create\_CFL  
Putting the corresponding values to 1 will create .CEL, .INS and .CFL  
respectively.  
# cryscal file.p4p: if crystal faces are present in the .P4P file,  
  they are extracted and saved in the import.cif.

### January 2010

# Bug in \_trans.HKL file has been corrected.

### November 2009

# If a "platon\_ortep.gif" file is present in the current folder, it is  
automatically incorporated in the HTML report file  
# If final.y file contains QVEC field and related parameters,  
  a hklm file is created

### October 2009

# If a hkl file is input, the transformed hkl file is  
loaded automatically after MATRIX keyword  
# Shannon table value for magnesium is corrected (Mg+2)  
# Cosmetic changes in the HTML documents (report and user's guide) created  
  by CRYSCALC.  
# Space group number has been added in the HTML report  
# SHELX reference has been changed to :  
  G. M. Sheldrick, Acta Cryst A, 2008, A64, 112-122

### September 2009

# TWIN\_PSEUDO\_HEXAX keyword  
# TWIN\_HEXAX keyword  
# Bugs in the routine to create the archive\_cryscal.cif file has  
  been corrected, specially when the archive.cif file is created  
  from the "create CIF / ACTA-C" procedure in WinGX, where the  
  order of some CIF fields is changed.  
# CRYSCALC has been compiled with new version of CFML (4.00)  
# Bugs in the connectivity calculation routine has been corrected

### February 2009

# CHECK\_GROUP can now determine trigonal space group  
# SG\_ALL keyword output sub-groups of the current space group

### January 2009

# .RAW file can be given as argument in the command line  
i.e. d:\> CRYSCALC my\_file.RAW  
CRYSCALC is then reading my\_file.RAW and will create a  
my\_file\_RAW.HKL file in a SHELX format. This file also contains  
dir. cos. for further absorption correction.  
Same behavior can be obtained by associating a selected RAW file to  
CRYSCALC program in the Windows file folder

#### November 2008

# GEN\_HKL accepts now Q\_min and Q\_max arguments  
# SEARCH\_HKL arguments can be h, k or l letters.  
ex: SEARCH\_HKL h 0 0  
SEARCH\_HKL 1 k 0  
# SITE\_INFO keyword gets constraints on anisotropic ADP, using the  
routine implemented in FullProf  
# new available arguments for CRYSCALC in command line:  
- LOG : create a cryscalc.log file  
- NO\_OUT : no output information are written on screen

#### October 2008

# CRYSCALC archive.cif : for archive.cif files created with the new version of  
WinGX (sept. 2008), CRYSCALC is skipping the whole part of the cif file  
containing programs references, to created the cryscalc\_archive.cif file  
# new argument for CRYSCALC in command line : CRYSCALC CREATE\_INS/SIR\_TO\_INS  
Create job.ins file from :  
. output.RES file created by SIR programs  
. struct.cif file created by WinGX  
This job.ins can be directly used for structure refinement with  
SHELXL, and contains right cell parameters and esd's, Mo wavelength  
and useful instructions such as ACTA, BOND\$H, CONF, TEMP ...

#### September 2008

# CRYSCALC archive.cif : CRYSCALC is reading archive.cif and cryscalc.cif  
files and creating completed archive\_cryscalc.cif file  
# keyword PAUSE: pause in the execution of the requested commands  
This keyword can be useful when commands are executed from a CFL  
commands file

#### July 2008

# REPORT/REPORT\_long: CIF fields can be independly in lower and  
upper cases

#### April 2008

# CONN keyword: calculation of connectivity around a selected atom given as argument.

### September 2007

# SEARCH\_SPGR keyword: search for a space group, given a hkl list and a given crystal system (Thanks to JRC for the CHECK\_GROUP routine)

### July 2007

# MATMUL keyword for 3\*3 matrix multiplication  
# CIF file can be given as a second argument if "REPORT" or "REPORT\_long" is given at first. A CIF\_file\_structural\_report.HTML is then created  
ex: d:\cryscalc report\_long my\_CIF\_file.CIF  
# P4P file can be given as argument in the command line to run CRYSCALC, i.e. CRYSCALC my\_file.P4P.  
CRYSCALC is then reading my\_file.P4P and my\_file.HKL to create import.CIF file for WinGX  
Same behavior can be obtained by associating a selected P4P file to CRYSCALC program in the Windows file folder

### April 2007

# MERGE keyword: merge equivalent reflections of the current HKL file  
  
# REPORT keyword can be interpreted in command line:  
> cryscalc report  
CRYSCALC is looking in the current folder for the presence of a "archive.cif" file: "structural\_report.html" file is then created and contains text about the crystallographic study. The browser defined in the "cryscalc.ini" file is then launch

### March 2007

# .x file (created by DENZO) and .rmat file (created by DIRAX) can be passed as argument for CELL keyword

### February 2007

# RESET keyword for input parameters and arrays initialization

### January 07

# THERM keyword can performed conversion of anisotropic displacement parameters:  
new available arguments: U\_ij, B\_ij, Beta\_ij  
# DIR keyword has been added and corresponds to the DIR DOS command.  
Arguments may follow this keyword.  
# Wcryscalc for Windows has been created.

### November 2006

```
# X rays data for Ag, Fe and Cr have been tabulated
# Launch CRYSCALC with P4P argument in command line:
d:\> cryscalc P4P:
CRYSCALC is looking in the current folder, for a P4P file (created
by SAINT) and a HKL file (created by SADABS). Import.cif file is then
created and can be directly read by WinGX as a KappaCCD file
```

### October 2006

```
# MAG keyword:      output magnetic features for a 3d or 4f ion
# SHANNON keyword: get effective ionic radii from Shannon article
(Acta Cryst. 1976, A32, 751)
# P4P keyword:      read P4P file created by SAINT (Bruker-AXS)
```

### September 2006

```
# FILE keyword: .m91 and .m95 files created by JANA can be read
# CELL keyword: .m50 file can be read
```

## CRYSCALC.ini setting file

A setting file can be used by **CRYSCALC**, containing the definition of different parameters such as external applications that can be launched from **CRYSCALC** (browser, editor ...) or default values about diffractometer, author, structure solution and refinement programs ... This setting file, called `cryscal.ini` has to be located in the **CRYSCALC** folder defined through the **CRYSCALC** environment variable.

Example of setting file:

### [EXTERNAL APPLICATIONS]

```
browser = "C:\Program Files\Mozilla Firefox\firefox.exe"
editor  = "C:\Program Files\Keditw\KEDITW32.EXE"
```

### [WEB ADDRESS]

```
fps      = www.ill.fr/dif/Soft/fp/
cdifx    = https://cdifx.univ-rennes.fr/
cryscal  = https://cdifx.univ-rennes.fr/cryscal
reciprocs = https://cdifx.univ-rennes.fr/reciprocs
```

### [DEVICE]

```
diffractometer = APEXII AXS Bruker
laboratory     = CDIFX Rennes
radiation      = X_Mo
wave_A         = 0.71073
temperature_K  = 150(2)
beam_stop_limit = 3.0
holder         = cryoloop
fast_scan_included = 1
```

### [USER]

```
name          = ROISNEL
first_name    = Thierry
address       = Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes)
              UMR 6226
              F-35000 Rennes, France
email         = thierry.roisnel@univ-rennes.fr
CSD_affiliation = CDIFX ISCR CNRS Univ. Rennes
CSD_country   = France
web           = https://cdifx.univ-rennes.fr
team          = CDIFX/PRTS/ISCR
orcid         = 0000-0002-6088-4472
```

### [ARRAYS DIMENSIONS]

```
hkl_reflections = 200000 ! max. number of hkl reflections in a file
nb_scans        = 50     ! max. number scans in a single crystal diffraction experiment
```

### [CREATE INS]

```
get_sample_ID = 0          ! get sample ID (default=job)
temperature   = 100K       ! experimental temperature value
u_threshold   = 0.1        ! atoms with U_iso > U_threshold will be excluded
```

**[PARAMETERS]**

```

i_sig      = 3.          ! used in SEARCH_GROUP procedure
threshold  = 0.03       ! used in SEARCH_GROUP procedure
d_max_A    = 3.5        ! used with the CONN keyword (connectivity calculation)

```

**COMMAND LINE ARGUMENTS]**

```

create_ACE      = 1      ! .ACE file for Carine
create_CEL      = 1      ! .CEL file for PowderCELL
create_CFL      = 1      ! .CFL file for CRYSCALC
create_INS      = 1      ! .INS file for SHELXL
create_FHZ      = 1      ! .FHZ file (Z-matrix)
create_FST      = 1      ! .FST file for FP Studio
create_XYZ      = 0      ! .XYZ file (Cartesian coordinates)
create_CIF_pymol = 0      ! X_pml.CIF for PYMOL
create_PCR      = 0      ! .PCR file for FullProf
create_PAT_PRF  = 1      ! .PRF file for FullProf
create_PAT_PDPF = 0      ! .pdpf file

```

**[PROGRAMS]**

```

structure_solution_name      = SHELXT
structure_solution_reference  = G.M. Sheldrick, Acta Cryst. A71 (2015) 3-8
structure_solution_cif_ref    = SHELXT (G. Sheldrick, 2015)
structure_refinement_name     = SHELXL-2014
structure_refinement_reference = G.M. Sheldrick, Acta Cryst. C71 (2015), 3-8
structure_refinement_cif_ref  = SHELXL-2018/3 (G. Sheldrick, 2015)
absorption_correction_name    = SADABS
absorption_correction_reference = Sheldrick G.M. (2014), SADABS Bruker AXS Inc.,
                                Madison, Wisconsin, USA
absorption_correction_cif_ref = Sheldrick G.M. (2014), SADABS Bruker AXS Inc.,
                                Madison, Wisconsin, USA

```

**[OPTIONS]**

```

LOG_file      = 1          ! create CRYSCALC.log file
LOCK_wave_value = 0.02     ! lock current wavelength to anticathode value
update_parameters = 1      ! update parameters after transformation
                                ! (cell parameters, atomic coordinates)

skip_start_menu = 1        ! Skip start menu
hkl_statistics  = 1        ! Output statistics on hkl reflections
hkl_format      = 3I4,2F8.2 ! format for .hkl file (h,k,l,F2,sig)
cartesian_frame_type = A    ! A: x//a ; C: x //c
pdp_beam        = X        ! Beam for powder diffraction pattern calculation
                                ! (N for neutrons / X for X-rays)
pdp_wave        = 1.5406   ! Wavelength used for powder diffraction pattern
                                ! calculation
ref_overlap_criteria = 0.10 ! criteria on hkl index for overlapped reflections criteria
search_mono_criteria = 2.5  ! max. diff. between monoclinic angle and 90.
search_SG_only_mono = 1     ! output only monoclinic space groups compatible
                                ! with unit cell metrics
bad_rint_criteria = 25.     ! criteria to define bad value for Rint
atom_occ_type     = 0       ! 0: %occ ; 1: n_occ*%occ
atom_adp_type     = 1       ! 0: Biso ; 1: Uiso (only for CFL file)

```

**[ARCHIVE\_AND\_REPORT]**

```

CIF_powder           = 0           ! create archive.CIF file for single crystal data,
CIF_format80        = 0           ! formatted line, when creating a CIF file,
                        ! if more than 80 characters
CIF_torsion_limit    = 170.       ! exclude torsion angle if greater than this limit
CIF_author           = 0           ! include author name and address in CIF file
CIF_audit            = 0           ! include audit details in CIF file
include_RES_file     = 1           ! include .RES file in the archive_crystcalc.cif file
include_HKL_file     = 1           ! include .HKL file in the archive_crystcalc.cif file
include_experimenter = 1           ! include experimenter name in the
                        ! archive_crystcalc.cif file
report_header        = 1           ! Write header in structural report
latex_cmb            = 0           ! use Computer Modern Bright font in LaTeX report
latex_sans_serif     = 1           ! use Sans Serif font in LaTeX report
latex_title_back_color = #e3e6f7 ! Main title background color in LaTeX report
latex_title_text_color = #580a0a ! Main title text color in LaTeX report
latex_title_border_color = #000000 ! Main title border color in LaTeX report
latex_title1_back_color = #fafafa ! Title background color in LaTeX report
latex_title1_text_color = #580a0a ! Title background text in LaTeX report
latex_title1_border_color = #fafafa ! Title background text in LaTeX report
latex_title1_text_center = 0       ! Title text centering (0/1)

```

**[PATTERN SIMULATION (Pseudo-Voigt profile)]**

```

X_profile_U          = 0.0055     ! U value of the Cagliotti formula :
                        ! FWHM2 = U*TAN**2(theta) + V*TAN(theta) + W
X_profile_V          = -0.0015    ! V value
X_profile_W          = 0.0036     ! W value
X_profile_eta0       = 0.3         ! Lorentzian components : eta = eta0 + 2theta * eta1
X_profile_eta1       = 0.
X_profile_TCH_U      = 0.0046     ! Profile parameters for Voigt (TCH) function
X_profile_TCH_V      = 0.0375     ! HG**2 = U*TAN**2(theta) + V*TAN(theta) + W
X_profile_TCH_W      = 0.0027     ! HL      = X*TAN(Theta) + Y/cos(Theta) + Z
X_profile_TCH_X      = 0.
X_profile_TCH_Y      = 0.014
X_profile_TCH_Z      = 0.
X_pattern_step       = 0.01
X_pattern_xmin       = 0.
X_pattern_xmax       = 120.
X_pattern_wave       = 1.5406
X_pattern_scale      = 100.
X_pattern_background = 50.
S_profile_U          = 0.000271    ! U value of the Cagliotti formula : FWHM2 = U*TAN**2(theta)
S_profile_V          = 0.000022    ! V value
S_profile_W          = 0.0036     ! W value
S_profile_eta0       = 0.000055    ! Lorentzian components : eta = eta0 + 2theta * eta1
S_profile_eta1       = 0.
S_profile_TCH_U      = 0.000271    ! Profile parameters for Voigt (TCH) function
S_profile_TCH_V      = 0.000022    ! HG**2 = U*TAN**2(theta) + V*TAN(theta) + W
S_profile_TCH_W      = 0.000055    ! HL      = X*TAN(Theta) + Y/cos(Theta) + Z
S_profile_TCH_X      = 0.015206
S_profile_TCH_Y      = 0.005903

```

```

S_profile_TCH_Z      = 0.
S_pattern_step      = 0.01
S_pattern_xmin      = 0.
S_pattern_xmax      = 120.
S_pattern_wave      = 1.5406
S_pattern_scale     = 100.
S_pattern_background = 50.
S_pattern_shifts    = 0. 0 0
S_pattern_CTHM      = 0.
S_pattern_Rpolar    = 0.1
N_profile_U         = 0.0146
N_profile_V         = -0.0375
N_profile_W         = 0.0475
N_profile_eta0      = 0.01
N_profile_eta1      = 0.
N_profile_TCH_U     = 0.0097      ! Profile parameters for Voigt (TCH) function
N_profile_TCH_V     = -0.0356     ! HG**2 = U*TAN**2(theta) + V*TAN(theta) + W
N_profile_TCH_W     = 0.0493     ! HL   = X*TAN(Theta) + Y/cos(Theta) + Z
N_profile_TCH_X     = 0.
N_profile_TCH_Y     = 0.0089
N_profile_TCH_Z     = 0.
N_pattern_step      = 0.025
N_pattern_xmin      = 0.
N_pattern_xmax      = 120.
N_pattern_wave      = 1.23
N_pattern_scale     = 100.
N_pattern_background = 50.
particles_size      = 9999.
strains             = 0.
plot_DSF            = 1           ! plot Debye-Scherrer film
plot_PRF            = 1
plot_XY             = 0
auto_scaling        = 1
PRF_header          = 1
profile_function    = PV         ! PV / TCH
pdp_beam            = X         ! Beam for powder diffraction pattern calculation
                                ! (N for neutrons / X for X-rays)
pdp_wave            = 1.5406     ! Wavelength used for powder diffraction pattern
                                ! calculation
pdp_norma           = 0.         ! Normalization of powder diffraction pattern

```

[USER TRANSFORMATION MATRICES]

```

MAT_1      =    2.  0.  0.   0.  1.  0.   0.  0.  1.   ! 2abc
MAT_2      =    1.  0.  0.   0.  2.  0.   0.  0.  1.   ! a2bc
MAT_3      =    1.  0.  0.   0.  1.  0.   0.  0.  2.   ! ab2c
MAT_4      =    2.  0.  0.   0.  2.  0.   0.  0.  2.   ! 2a2b2c
MAT_5      =    0.  0.  1.   0.  1.  0.  -1.  0.  1.   ! C_to_I
MAT_6      =    1.  0. -1.   0.  1.  0.   1.  0.  0.   ! I_to_C

```

[USER SHORTCUTS] ! only in expert mode

```

RCJ          = READ_CIF job.cif

```

```
RJC          = READ_CIF job.cif
RIJ          = READ_INS job.ins no_out
RJI          = READ_INS job.ins no_out
CALC        = DOS calc
MAX_10       = GEN_HKL theta_min=0. theta_max=10 out_10
MAX_3        = GEN_HKL theta_min=0. theta_max=3 out
PAT_10_80    = GEN_HKL 2theta_min=10. 2theta_max=80
SF1          = SF_HKL 0 0 2
SF1          = SF_HKL 0 0 2
```

## Examples of .CFL input files

- Calculation of internal R factor from hkl data included in a import.cif file [.cfl]

```
FILE import.cif
SEARCH_GROUP get
RINT
```

- Pnma space group information [.cfl]

```
SG P n m a
SG_INFO
```

- Transformation from Pbnm to Pnma space group [.cfl]

```
CELL 5.5 5.7 7.7
SG P b n m
MAT b c a
```

- Simulation of a X-ray diffraction pattern for Si [.cfl]

```
CELL 5.43
SG F D -3 M
ATOM SI SI 1/8 1/8 1/8
WAVE 1.5406
GEN_HKL 2THETA_MIN=0. 2THETA_MAX=140. PAT
```

- Simulation of a X-ray diffraction pattern for Si (particles size=100A) [.cfl]

```
CELL 5.43
SG F D -3 M
ATOM SI SI 1/8 1/8 1/8
WAVE 1.5406
GEN_HKL 2THETA_MIN=0. 2THETA_MAX=140. PAT SIZE=100
```

- Simulation of a neutron diffraction pattern for Si [.cfl]

```
CELL 5.43
SG F D -3 M
ATOM SI SI 1/8 1/8 1/8
WAVE 1.59
BEAM NEUT
GEN_HKL 2THETA_MIN=0. 2THETA_MAX=140. PAT
```

- Simulation of a X-ray diffraction pattern in a supercell (quartz example) [.cfl]

```
TITL quartz
CELL 4.913 4.913 5.404 90.00 90.00 120.00
SG P 32 2 1
ATOM Si Si 0.47 0. 2/3
ATOM O O 0.4146 0.78543 0.0109
GEN_EQUIV_ATOMS
SUPERCELL 2 2 2
WAVE X_CU
GEN_HKL 2theta_min=0 2theta_max= 120 PAT
```

- Atom connectivity in  $Y_2O_3$  [.cfl]

```
CELL 10.601
SG I A -3
ATOM Y1 Y 1/4 1/4 1/4
ATOM Y2 Y 0.467 0. 1/4
ATOM O O 0.109 0.348 0.119
SITE_INFO
CONN Y1 3.
CONN Y2 3.
```

- Bond valence calculation in  $Y_2O_3$  [.cfl]

```
CELL 10.601
SG I A -3
ATOM Y1 Y+3 1/4 1/4 1/4
ATOM Y2 Y+3 0.467 0. 1/4
ATOM O O-2 0.109 0.348 0.119
SITE_INFO
CONN BVS
```

- X-ray absorption coefficient calculation (case of ammonium bitartrate) [.cfl]

```
TITLE Ammonium bitartrate C4H5O6, NH4
WAVE X_MO
CELL 7.641 7.767 11.033
ZUNIT 4
CHEM C4 H9 N1 O6
SIZE 0.1 0.2 0.3
MU
```

## How to's

- What is CRYSCALC?
- Install CRYSCALC?
- Get help in CRYSCALC?
- Start with CRYSCALC?
- Create import.cif file on a Bruker diffractometer?
- Convert CIF/INS files?
- Convert PCR or INS/RES to CIF format?
- Calculate of a powder diffraction pattern from a CIF/INS file?
- Create a final CIF archive?
- Extract .res and .hkl from a cif file?
- Create a experiment report and tables from a CIF file?
- Create a global CIF archive from several CIF files?

## CRYSCALC download and links

- Automatic install of **CRYSCALC** (for Windows)
- CRYSCALC.exe (for Windows 64 bits)
- CRYSCALC.exe (for Windows 32 bits)
- Example of CRYSCALC setting file
- Example of CSS file for HTML user's guide
- Example of CSS file for HTML structural report
- CRYSFML repository
- CrysFML: Crystallographic Fortran Modules Library, by J. Rodriguez-Carvajal and J. González-Platas

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This user's guide has been created by **CRYSCALC** (26.06). Please report any bugs and problems to: [thierry.roisnel@univ-rennes.fr](mailto:thierry.roisnel@univ-rennes.fr).

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