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

****

C R Y S C A L C

(CRYSTALLOGRAPHIC CALCULATIONS)

makes crystallographer life easier !

Ver. 25.04

T. Roisnel

CDIFX/PRTS/ISCR

UMR6226 CNRS-Univ Rennes, France

[with courtesy of JRC and JGP for CFML]

contact : thierry.roisnel@univ-rennes.fr

web site : https://cdifx.univ-rennes1.fr/cryscalc

****

Tables of contents

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 Librairies 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, 2theta_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
- ...

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 WinPLOTR has not been installed previously.

List of **CRYSCALC** keywords

- ABSENT_HKL
- ABSORPTION
- ACTA
- ANG
- APPLY_OP
- ATOM
- ATOM_LIST
- BARY
- BEAM
- BVPARM
- CELL
- CELL_ESD
- CHEM
- CIF_EXTRACT
- CONN
- CONT
- CREATE_ACE
- CREATE_CEL
- CREATE_CFL
- CREATE_CIF
- CREATE_FST
- CREATE_FHZ
- CREATE_INS
- CREATE_PCR
- CREATE_PDB
- CREATE_REPORT
- CREATE_SOLVE
- CREATE_TIDY
- CREATE_XYZ
- D_HKL

- D_HKL_MAX
- D_REC
- DATA_ATOMIC_DENSITY
- DATA_ATOMIC_RADIUS
- DATA_ATOMIC_WEIGHT
- DATA_NEUTRONS
- DATA_XRAYS
- DIAG_MAT
- DIFF
- DIR_ANG
- DIST
- DIST_DHA
- DIST_MULT
- DIST_NEW
- DIST_PLUS
- EDIT
- EQUIV_HKL
- EULER_TO_KAPPA
- EXIT
- FCF_FILE
- FILE
- FIND_HKL
- FIND_HKL_LIST
- FRIEDEL
- GEN_HKL
- GET_TRANS_MAT
- HEADER
- HEX_RHOMB
- HKL
- HKL_DIFF
- HKL_MULT
- HKL_NEG

- HKL_POS
- HKLF5
- 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_EXP
- READ_CEL
- READ_CIF

- READ_FACES
- READ_HKLF5
- READ_INS
- READ_LST
- READ_NREPORT
- READ_P4P
- READ_PCR
- READ_PDB
- READ_P4P
- READ_SFRM
- READ_SPF
- READ_TIDY_OUT
- REC_ANG
- REDUCE_CELL
- REF_ABS_CRYSALIS
- REF_D8V_CU
- REF_D8V_MO
- REF_APEX
- REF_DENZO
- REF_EVAL
- REF_KCCD
- REF_SADABS
- REF_SHELX
- REF_SIR
- REF_SUPERFLIP
- REF_SUPERNOVA
- REF_X2S
- REF_XCALIBUR
- 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
- SITE_INFO
- SIZE
- SORT
- STAR_K
- STL
- SUPERCELL
- SYMM
- SYST
- THERM
- THERM_SHELX
- THETA
- TITL
- TOLMAN_ANGLE
- TRANSLATION

- TRANSMISSION
- TRICLINIC
- TWIN_HEXA
- TWIN_PSEUDO_HEXA
- 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_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/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 refering to the number of symmetry operator in the list.

. example: ANG O1 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 oxdation 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 O1   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 O1  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.
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_2 = ">", 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 numor (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 A
                       or "E= for energy (in KeV for X-rays and electrons or
                       in meV for neutrons)
. optional arguments:  real value (wavelength in A 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, JOBTYPE, 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 CRYSALIS
                         . 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]

- 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 distorsion as:
                          distorsion = SUM((dist-dist_av)/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 ouput 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):
                        tau4 = (360 - (alfa+beta)/141
                        where alfa and beta are two largest angles at the
                        four-coordinated metal atom.
                        In the case of five-ccordinate system, tau5 trigonality index
                        is calculated, following the formula tau4 = (alfa-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_TOL keyword.
                      . 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.ub.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
                       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_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.  O 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
. 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.
. 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 asymetric 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:\> cryscalc 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

[top of CRYSCALC keywords list]

- CREATE_INS

```
. type:                 OUTPUT keyword
. optional argument:    no_H, PURGE/CLEAN, ISO, ANIS/ANISO, OUT, FILE=xxx
. 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 Ueq < 0. or Ueq > U_threshold
                          (defined in setting file in the [CREATE_INS] section).
                        . if "ISO" is present, Ueq 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 "VIEW/RUN" argument is given, the INS file is opened
                          automatically by the associated INS viewer (defined in
                          [EXTERNAL APPLICATIONS] section in the cryscalc.ini file
                          through the "INSVIEWER" item.
. 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:\> cryscalc 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:\> cryscalc 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 ^ 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
```

[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 explicitely 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 ^ 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 cryscalc.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:
> cryscalc file.cif

[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_DENSITY

. type: OUTPUT keyword
. optional argument: PLOT
. meaning: list atomic density data for all atoms
if arg=PLOT: create a PGF file and plot it with WinPLOTR
. identical keywords: DATA_DENSITY, DENSITY_DATA, DATA_ATOMIC_DENSITY, ATOMIC_DENSITY

[top of CRYSCALC keywords list]

- DATA_ATOMIC_RADIUS

. type: OUTPUT keyword
. optional argument: PLOT
. meaning: list atomic radius data for all atoms
if arg=PLOT: create a PGF file and plot it with WinPLOTR
. identical keywords: DATA_RADIUS, RADIUS_DATA, DATA_ATOMIC_RADIUS, ATOMIC_RADIUS

[top of CRYSCALC keywords list]

- DATA_ATOMIC_WEIGHT

. type: OUTPUT keyword
. optional argument: PLOT
. meaning: list atomic weight data for all atoms
if arg=PLOT: create a PGF file and plot it with WinPLOTR
. identical keywords: DATA_WEIGHT, WEIGHT_DATA, DATA_ATOMIC_WEIGHT, ATOMIC_WEIGHT

[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
```

[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 refering 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 refering 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_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_cryscalc.cfl
  . related keywords: SET, SETTING

[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]

- FCF_FILE

```
. type:                 INPUT keyword
. argument :            1 characters string
. meaning:              read .FCF file name, created by SHELXL and containing
                        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
. 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]

- 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 coeffficient
```

```
                          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 ouput 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 multipled by xx factor.
. action:                plot the F2=f(sinTheta/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. 0kl     l=2n+1  c  .  .
                           6. 0kl   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. 0k0     k/=4n  .  41 .
                          23. 00l     l/=4n  .  . 41
                          24. 0kl   k+l/=4n  d  .  .
                          25. h0l   h+l/=4n  .  d  .
                          26. hk0   h+k/=4n  .  .  d
                          27. h-hl, h0l, 0kl    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.

                       If the integer value is negative, the opposite
                       condition will be searched in the HKL file.
meaning:               search, in a reflections list, those obeying
                       to the selected extinction rule
optional arguments:    . 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=4pi*SinTheta/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-rennes1.fr/progs/winplotr/winplotr.exe
                          If this latest version of WinPLOTR has been installed,
                          this Debye-Scherrer film (cryscalc_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 ouput
                        . "OUT_n": sort the reflections list by decreasing F2calc
                                   and ouput the n more intensive ones.
                        . "OUT_ALL": sort the reflections list by decreasing F2calc
                                   and ouput 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 ouput :
                            - cryscalc_pat.xy (2 columns)
                            - cryscalc_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 (.pdpf) 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_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:
                       tol = ABS(p1_t1 - p1_2) + ABS(p2_t1 - p2_2) +
                             ABS(p3_t1 - p3_2) + ABS(p4_t1 - p4_2) +
                             ABS(p5_t1 - p5_2) + 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 A
                        (dependent keyword = CELL)
                        calculation of Bragg angle 2theta_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
. relared keyword: HKL_NEG

[top of CRYSCALC keywords list]

- HKLF5

. type: input keyword
. arguments: 9 integers or reals values
. meaning: transformation (3,3) matrix components
. optional keywords: MULT=xx: intensities and sigma are multipled 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

[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, FCMAX, MAX_FC, MAXFC
. 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 multiciplicity
                          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:
                        M11, M12, M13, M21, M22, M23, M31, M32, M33
. ouput:                calculation of the M1xM2 matrix
```

[top of CRYSCALC keywords list]

- MATRIX

```
. 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
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 transformatio
                         MAT I C (MAT #39, for mono/ortho I to mono/ortho C transformatio
. 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 keyword:    PLOT: create a .PGF file containing the scattering
                           factor values versus SinTheta/lambda and plot it
                           with WinPLOTR
  . 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

  . 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 mininum (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

  . argument: real values
  . meaning: Q=4pi*sinTheta/lambda values
  . outputs: d_hkl(A), SinTheta/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_EXP

. 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_CEL

. 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 ...
. 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_CIF

  . 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_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.
  Ouput 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 redondant 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 at from the .INS file
. 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 paramter (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 containning 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 cryscalc.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

```
  . 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 'cryscalc.ini' setting file.
                          If not, ouputs the HTML file on screen (without tags).
  . identical keywords:   READ_NREPORT, READ_report%HTML, READ_NREPORT_HTML
```

[top of CRYSCALC keywords list]

- 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, wave ...
  . 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_P4P

  . 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 vetors 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
. optional argument: 1 characters string corresponding to the .SFRM file name (diffraction frame from BAXS diffractometers) to be read.
. 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.
. identical keywords: READ_TIDY_OUT, READ_TIDY_OUTPUT, READ_TIDY_OUTPUT_FILE
. example: READ_TIDY_OUT

[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]

- REF_ABS_CRYSALIS

. type: OUTPUT keyword
. argument: no
. meaning: write in CIF format absorption correction procedure implemented in CRYSALIS software (Agilent Technologies)
. optional argument: CIF/ACTA
. identical keywords: REF_ABS_CRYSALIS

[top of CRYSCALC keywords list]

- REF_D8V_CU

. type: OUTPUT keyword
. argument: no
. meaning: write APEXII diffractometer programs and device references
. optional argument: CIF/ACTA
. identical keywords: REF_APEX, REF_APEXII, WRITE_APEX, WRITE_APEXII, APEX, APEXII

[top of CRYSCALC keywords list]

- REF_D8V_MO

. type: OUTPUT keyword
. argument: no
. meaning: write D8 Venture diffractometer programs and device references
. optional argument: CIF/ACTA
. identical keywords: REF_D8V_Cu, REF_D8_VENTURE_CU

[top of CRYSCALC keywords list]

- REF_APEX

. type: OUTPUT keyword
. argument: no
. meaning: write D8 Venture diffractometer programs and device references
. optional argument: CIF/ACTA
. identical keywords: REF_D8V_Mo, REF_D8_VENTURE_Mo

[top of CRYSCALC keywords list]

- REF_DENZO

  . type: OUTPUT keyword
  . argument: no
  . meaning: write EVALCCD references
  . optional argument: CIF/ACTA
  . identical keywords: REF_EVAL, REF_EVALCCD, WRITE_EVAL, WRITE_EVALCCD, EVAL, EVALCCD

[top of CRYSCALC keywords list]

- REF_EVAL

  . type: OUTPUT keyword
  . argument: no
  . meaning: write DENZO/SCALEPACK references
  . optional argument: CIF/ACTA
  . identical keywords: REF_DENZO, WRITE_DENZO, DENZO

[top of CRYSCALC keywords list]

- REF_KCCD

  . type: OUTPUT keyword
  . argument: no
  . meaning: write KCCD diffractometer software and device references
  . optional argument: CIF/ACTA
  . identical keywords: REF_KCCD, KCCD

[top of CRYSCALC keywords list]

- REF_SADABS

  . type: OUTPUT keyword
  . argument: no
  . meaning: write SADABS references
  . optional argument: CIF/ACTA
  . identical keywords: REF_SAD, SADABS

[top of CRYSCALC keywords list]

- REF_SHELX

  . type: OUTPUT keyword
  . argument: no
  . meaning: write SHELXS/T and SHELXL references
  . optional argument: CIF/ACTA
  . identical keywords: REF_SHELX

[top of CRYSCALC keywords list]

- REF_SIR

  . type: OUTPUT keyword
  . argument: no
  . meaning: write SIR team programs references
  . optional argument: no
  . identical keywords: REF_SIR

[top of CRYSCALC keywords list]

- REF_SUPERFLIP

  . type: OUTPUT keyword
  . argument: no
  . meaning: write SUPERFLIP program reference
  . optional argument: no
  . identical keywords: REF_SPF, REF_SUPERFLIP

[top of CRYSCALC keywords list]

- REF_SUPERNOVA

  . type: OUTPUT keyword
  . argument: no
  . meaning: write SUPERNOVA diffractometer programs and device references
  . optional argument: CIF/ACTA
  . identical keywords: REF_SUPERNOVA

[top of CRYSCALC keywords list]

- REF_X2S

  . type: OUTPUT keyword
  . argument: no
  . meaning: write SMART X2S diffractometer programs and device references
  . optional argument: CIF/ACTA
  . identical keywords: REF_X2S, REF_SMART_X2S

[top of CRYSCALC keywords list]

- REF_XCALIBUR

  . type: OUTPUT keyword
  . argument: no
  . meaning: write XCALIBUR diffractometer sotware and device references
  . optional argument: CIF/ACTA
  . identical keywords: REF_SUPERNOVA

[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 argument: symmetry (characters string): "TRIC", "MONO", "ORTHO", "TETRA", "TRIG", "HEXA", "CUB"
  . meaning: calculate the internal Rint value
  calculate the completeness of the data collection
  . 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 cryscalc.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/sig > n_sig will
                            be analysed
                          . ratio_criteria:
                             if <F2_odd>/<F2_even> < 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
                        will be stopped.
                        Criteria_2: Rint for the right monoclinic angle has to be
                        lower than criteria_2*Rint for the others.
. mandatory keyword:    FILE
. identical keywords:   SEARCH_MONO, SEARCH_MONOCLINIC, SEARCH_MONO_ANGLE, SEARCH_MONOCLI
                        GET_MONO, GET_MONOCLINIC, GET_MONO_ANGLE, GET_MONOCLINIC_ANGLE
                        , SEARCH_MONO_AXIS, SEARCH_MONOCLINIC, AXIS, GET_MONO_AXIS, GET_M
```

[top of CRYSCALC keywords list]

- SEARCH_P3P6

```
. type:                 OUTPUT keyword
. optional argument:    criteria for searching symmetry
. meaning:              calculation of internal R values for different trigonal and
                         hexagonal Laue groups and ouput the most probable ones.
```

Criteria corresponds to the ratio minimum value of Rint with respect to Rint values calculated in different Laue groups. Default value is 0.2.

. mandatory keyword: FILE
. identical keywords: SEARCH_P3P6, P3P6

[top of CRYSCALC keywords list]

- SEARCH_SPGR

. type: calculation keyword
. optional arguments: 2 real : n_sig and threshold
1 characters string, defining the crystal system: M/mono, O/ortho, T/tetra, R/trig, H/hexa, C/cub, GET, ALL, P, CENTERED/NOT_P, OMA/ONLY, CENTRIC, ACENTRIC
. meaning: search in a hkl file systematic extinctions and propose space groups in agreement with observed extinctions.
. n_sig: only reflections with I/sig > n_sig are considered. Default value is n_sig=3.
. a threshold is also applied: only the reflections with F2 > threshold * max(F2) are considered. Default value is threshold=0.03
If P is input as argument, only primitive space groups will be output.
If ALL is given as argument, all space groups (centered and primitive) will be output.
If CENTERED/NOT_P is given as argument, only non primitive (centered) space groups will be output.
If GET is input as argument, the most probable space group will be considered.
If "CENTRIC/ONLY_CENTRIC" argument is present, only centric 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 ouput. 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, trigona
                        hexagonal or cubic system, this crystal systel is taken into acco
                        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_TETRAG
.                       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, COEF
. 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 aalso performed for -H reflection
                          if "SCAT" is specified, atomic scattering factor corefficients
                          are output
  . example:              HKL 1 0 1
  . 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 reducet 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]

- SITE_INFO

```
  . 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 O1 C8
  . identical keywords: SITE_INFO, INFO_SITE, ATOM_SITE, SITE_ATOM, LIST_SITE_INFO,
                        GEN_EQUIV_ATOMS, WYCKOFF
```

[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

[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_HEXA

. 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_HEXA

[top of CRYSCALC keywords list]

- TWO_THETA

. 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

```
. meaning:              download lastest version of CRYSCALC
                        from the CRYSCALC web site:
                        https://cdifx.univ-rennes1.fr/progs/cryscalc/cryscalc.exe
                        If TMP is given as argument, a temporary uncompacted version
                        of CRYSCALC will be downloaded from:
                         https://cdifx.univ-rennes1.fr/progs/cryscalc/temp/cryscalc.exe
                        If BETA is given as argument, a beta uncompacted version
                        of CRYSCALC will be downloaded from:
                         https://cdifx.univ-rennes1.fr/progs/cryscalc/beta/cryscalc.exe
                        If ZIP is given as argument, a zipped file containing
                        cryscalc.exe will be downloaded from:
```

https://cdifx.univ-rennes1.fr/progs/cryscalc/cryscalc.zip
. remark: browser has to be defined in the setting file [EXTERNAL APPLICATIONS] section.
. examples: UPDATE
. examples: UPDATE ZIP

[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 cryscalc.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 cryscalc.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
                        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 ^ z = b*
if arg="CART_C", Cartesian frame is follows:
z // c; y is in the bc-plane; x is y ^ 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 cryscalc.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_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 rotationaland 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 ina 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 [Cryscal] distributed within the FullProf Suite.)
  if argument="CONDENSED": symmetry operators are ouput 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, LIST_SYM_OP, LIST_SYMM_OP, LST_SYM_OP, LST_SYMM_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 A) 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 bevahior 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 'cryscalc_archive.cif' file is then created.
Remark : diffractometer and structure solution program can be defined
         in the 'cryscalc.ini' setting file in the [DEVICE] and [PROGRAMS]
         parts respectively.
```

- CREATE_ARCHIVE

```
. create global 'cryscalc_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 'cryscalc_archive.cif' file with CIF fields related
to the author of the deposition (name, address), extracted from
the 'cryscalc.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: 25.04

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

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 perfomed 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 discribe 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 *_0m._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 if now output in the import.CIF created by CRYSCALC.
Wavelength used for powder diffraction pattern simulation cen 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 "AFIX" argument for READ_INS keyword:
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

```
# 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 bons list, the D-H...A angle
  value is rounded if no standart 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 cryscalc.ini
  setting file: Definition of a limit in A, beyond wich 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 cryscalc.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 ouput, 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 intensites 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"
# Completness 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 cryscalc.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> cryscalc xxx.CIF
This summary file can also be created by specifying REPORT_SUMM
as argument in a command line.
Example:
d:\progs> cryscalc 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 tetraedral 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 tetraedral atom site has to be performed.

July 2022

# Images file to be included in the structural reports cab be specified by user by edditing "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 < -2sigW

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(Fo^2 - Fc^2)/sig_WI > 10.
  where sig_WI = 1./sqrt(wI) and wI calculated from weighting scheme
  used by SHELXL :
  w_I=1/[sig(Fo^2)+(aP)^2+bP] where P=(Fo^2+2Fc^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 "DMAX/D_HKL_MAX/DHKL_HIGH/DHIGH" keyword: output the highest
  d_hkl 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 ouput 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 ouput 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 molecules
If 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 desagreable reflections with Eror/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 desagreable reflexions
  are ouput, 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 ouput in the PCR file.
# New READ_SFRM/READ_SFRM_HEADER kewyord:
  Read header of .sfrm file (diffraction frame from Bruber 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 of .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-rennes1.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-rennes1.fr/CRYSCALC" to
  "https://cdifx.univ-rennes1.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 lastest 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" filed 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 ^ z = b*
  CART_C: z // c; y is in the bc-plane; x is y ^ 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:\>cryscalc ; SG P 21/c ;
   d:\>cryscalc \ 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 perfom 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.
```

Febryary 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 ile 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 ouput.

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 trough 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.rennes1.fr/progs/cryscalc/cryscalc.zip

September 2018

Automatic installation of CRYSCALC can now been performed using the new CRYSCALC_setup.exe program developped with Inno Setup (http://www.jrsoftware.org/isinfo.php).
CRYSCALC_setup.exe can be download from :
https://cdifx.univ-rennes1.fr/progs/cryscalc/cryscalc_setup.exe

Cryscalc 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 : cryscalc 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 paramters if pseudo-Voigt profile
function is choosen.
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 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 profil 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 existsor "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 Ueq < 0. or Ueq > 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 cryscalc_lf95/ifort 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 lastest version of CRYSFML (feb. 2017):
  standart 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 lastest 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 EPERT 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, defaut values are coming from
  CRYSFML library, excepted for H atoms (r=1.2A).
  ex: TOLMAN CO1 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.rennes1.fr/progs/cryscalc/cryscalc.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 cryscalc.ini setting file :
  experimenter features, coming from [AUTHOR] section, are then included
  in the archive_cryscalc.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 ouput: Niggli matrix is now output
```

July 2015

```
# THERM ouput: 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 cryscalc.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: cryscalc 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 (cryscalc.ini) : X-ray diffraction pattern
  is then created (PRF file FullProf format) after reading a CIF file.
  By defauft, 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:
  polyedron 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_PEAKS 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 polyedra 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 programm (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 trough the
  ATOM keyword.
  ex: ATOM Fe1 Fe+3 0.11 0.22 0.33 0.4 1.
  example of CFL file :
    https:\\cdifx.univ-rennes1.fr\progs\cryscalc\cryscalc_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 cryscalc.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-rennes1.fr\progs\cryscalc\cryscalc_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:\cryscalc file.cif pymol
  "create_CIF_PYMOL" keyword (value = 0/1) can also be specified
  in the cryscalc.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 cryscalc.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
  cryscalc.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 cryscalc.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 crycsalc.ini setting file. If present, these
  css files, called cryscalc_report.css and cryscalc.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 cryscalc.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 goups
  - 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 UAl2.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-rennes1.fr/cryscalc)
# Some changes in output files :
   . cryscalc.log is renamed cryscalc_debug.txt
   . cryscalc.out is renamed cryscalc.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 (cryscalc.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_cryscalc.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 ouput 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 (cryscalc.ini)
  with the following fields :
   . create_CEL
   . create_INS
   . create_CFL
  Putting the corresponding values to 1 will create .CEL, .INS and .CFL
  respectively.
# cryscalc 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_HEXA keyword
# TWIN_HEXA keyword
# Bugs in the routine to create the archive_cryscalc.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 optained 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 cryscal_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 optained 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 CRYSCAL 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 defaut values about diffractometer, author, structure solution and refinement programs ... This setting file, called cryscalc.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-rennes1.fr/
cryscalc   = https://cdifx.univ-rennes1.fr/cryscalc
reciprocs  = https://cdifx.univ-rennes1.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             = htps://cdifx.univ-rennes1.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         ! Ouput 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_cryscalc.cif file
include_HKL_file          = 1        ! include .HKL file in the archive_cryscalc.cif file
include_experimenter      = 1        ! include experimenter name in the
                                     ! archive_cryscalc.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.
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
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
```

[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
RIJ                    = 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
SF2                    = SF_HKL  0 0 -2
```

List of **CRYSCALC** command line arguments

- 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
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

This user's guide has been created by **CRYSCALC** (25.04). Please report any bugs and problems to: thierry.roisnel@univ-rennes.fr.

Save trees and paper! Please do not print this document.