The program `BondStr` (or `Bond_Str`) and its GUI `GBond_Str`

Version March 2018, J. Rodríguez-Carvajal - ILL

The program BondStr calculates distances, angles and polyhedra volume and distortions pair distributions of bonds (PDB), Bond-Valence Sums (BVS), Bond-Valence Energy Landscapes (BVEL) for any kind of crystal structure. The program is fully based in CrysFML (Crystallographic Fortran 95 Modules Library).

The program needs an input file that can be either a standard CIF file or a CFL file containing just the necessary structural information and the ionic species. A CFL file is a file with a format that is recognized by all programs based in CrysFML. They have the extension `*.cfl` and contains keywords and numerical values that are in free format. A CFL file can be generated from a CIF file just running BondStr (or using other programs like `Formal_Charges`, see below). Example of CFL files are given below.

The main program BondStr call the following procedures of CrysFML depending on the input parameters in the CFL file:

```
Readn_set_Xtal_Structure      <- Set up of the crystal structure reading a
                                 CIF or CFL file
Write_Crystal_Cell
Write_SpaceGroup              <- Write crystal structure parameters read by
Write_Atom_List                  Readn_set_Xtal_Structure


Write_CFL                     <- Called when the input file is a CIF file
Write_Cif_Template            <- Called when the input file is a CFL file
                                 and BVEL is asked

Calc_Dist_Angle_Sigma         <- Calculates distances and angles

Calc_Distortion_IVTON         <- Calculates polyhedra volume and distortions
Calc_PDB                      <- Calculation of pair distributions of bonds
Calc_BVS                      <- Calculation of BVS for each site

Calc_Map_BVS                  <- Calculation of BVS mismatch map

Calc_Map_BVEL                 <- Calculation of BVEL map
Percolation_Calc              <- Calculates percolation (migration) energies
```

The most reliable bond-valence parameters (based in the file bvparm.cif from I.D. Brown) are stored in CFML_BVpar.f90, but, alternatively, SoftBVS parameters can be calculated or user-given bond-valence parameters can be read form the input file instead of using the internal (or calculated) parameters.

The program can be invoked from the command line together with the name of the file or the code (name without extension) of a CIF or CFL file. The program looks first for the existence of a CFL file with the given code, if there is no CFL file it looks for a CIF file.

Alternatively the program can be invoked with the name of a buffer file in which there is a list of CIF or CFL file. Depending on additional arguments the program perform different calculations.

Alternatively, the GUI GBond_Str program can be used directly to convert CIF files to CFL files. Remember that information about the chemical species (ionic oxidation states) is not always included in CIF files, so the user has to include it in the appropriate place in the atom string (see below) if he (she) wants to make bond-valence calculations (alternatively the user can run the program `Formal_Charges` for getting a proper CFL file).

All it is needed to know about the input files and running the program is explained in the following examples.

Example 1:

A CIF file, called `99677.cif`, exists in the current directory (and there is no file called `99677.cfl`); the program can be invoked as follows:

`Current_directory> Bond_Str 99677  <cr>`

`<cr>` corresponds to carriage return (ENTER key)

The screen output is the following:

```
               ==============================
               ====== PROGRAM BOND_STR ======
               ==============================
    **********************************************************************
    * Distances, angles and Bond-Valence Sums from  *.cfl or *.cif files  *
    *     Calculation of BVS and Bond-Valence Energy Landscape maps       *
    **********************************************************************
                    (JRC - ILL, version: March 2018)

 => Treating file #:    1  -> 99677.cif
 => A CFL-file has been generated from CIF -> CFL_file.cfl
    This file may be used to add instructions for BOND_STR

 => Normal End of: PROGRAM BOND_STR
 => Global results in File: 99677.bvs
 => CPU-time:   0 minutes  0.0156 seconds
 => TOTAL CPU-time:   0 minutes  0.0156 seconds
```

In the input CIF file there is no information to calculate the oxidation state of the different ions, so bond-valence calculations are not performed. Only distances up to 3.2 angstroms are calculated for the current structure. A file called `CFL_file.cfl` has also been generated and the user can include the necessary information to perform the complete calculations in

further runs (using the CFL file instead of the CIF file). This can be done more easily using the GUI GBond_Str and importing a CIF file that is automatically transformed into a CFL file.

Example 2:

A CFL file, called mfepo5.cfl, exists in the current directory; the program is invoked as follows:

```
Current_directory> Bond_Str mfepo5  <cr>
....
```

The screen output is the following:

```
                    =============================
                    ====== PROGRAM BOND_STR ======
                    =============================
     **********************************************************************
     * Distances, angles and Bond-Valence Sums from  *.cfl or *.cif files  *
     *      Calculation of BVS and Bond-Valence Energy Landscape maps      *
     **********************************************************************
                       (JRC - ILL, version: March 2018)

 => Treating file #:    1  -> NiFePO5.cfl
  Subroutine Calc_BVS (JRC-LLB, version: March-2005)
  Title: Summary of Bond-Valence calculations for file: NiFePO5.cfl
   Atom      Coord  D_aver Sigm    Distort(x10-4)      Valence     BVSum(Sigma)
    Ni        6.00  2.0801(   6)          3.128        2.000       1.906(   3)
    Fe        6.00  2.0470(  21)         72.020        3.000       3.015(  20)
    P         4.00  1.5301(  20)          0.968        5.000       5.064(  28)
    O1        4.00  2.0251(  31)         15.651       -2.000       1.784(  19)
    O2        4.00  2.0538(  17)        231.642       -2.000       1.929(  18)
    O3        2.00  1.7029(  32)        132.641       -2.000       2.032(  21)
    O4        3.00  1.8603(   7)        156.069       -2.000       2.120(   5)

 => Old Global Instability Index (GII=SQRT{SUM{|BVS-abs(q)|^2}/Num_Atoms})=10.71/100
 => Normalized   GII(a)=SUM {|BVS-abs(q)|  *mult}        /N_Atoms_UCell =   9.15 /100
 => Normalized   GII(b)=SUM {|BVS-abs(q)|  *mult/abs(q)}/N_Atoms_UCell =   4.31 %
 => Normalized   GII(c)= SQRT{ SUM {|BVS-abs(q)|^2*mult}/N_Atoms_UCell}=  10.88/100

 => Normal End of: PROGRAM BOND_STR
 => Global results in File: NiFePO5.bvs
 => Summary of BVS in File: NiFePO5_sum.bvs
 => CPU-time:   0 minutes   0.0156 seconds
 => TOTAL CPU-time:   0 minutes   0.0156 seconds
```

The information given in the screen output corresponds to the content of the summary file mfepo5_sum.bvs. All details are in the output file mfepo5.bvs. A CIF file is generated from the CFL file (NiFePO5_gen.cif) containing the relevant structural information.

The content of the CFL corresponding to the above calculation is the following:

```
------------------- Start of the mfepo5.cfl file --------------------

Title   NiFePO5
!         a            b            c         alpha    beta    gamma
Cell   7.1882(2)   6.3924(2)   7.4847(3)   90.000  90.000  90.000
!       Space Group
Spgr  P n m a
!   label Spc       x            y            z           Biso      occ
Atom  Ni   NI2+  0.0000       0.0000       0.0000       0.74      0.5
Atom  Fe   FE+3  0.1443(9)    0.2500       0.7074(2)    0.63      0.5
Atom  P    P5+   0.3718(9)    0.2500       0.1424(2)    0.79      0.5
Atom  O1   O2-   0.3988(9)    0.2500       0.64585(2)   0.71      0.5
Atom  O2   O-2   0.19415(4)   0.2500       0.0253(4)    0.70      0.5
Atom  O3   O-2   0.0437(2)    0.2500       0.4728(2)    0.83      0.5
Atom  O4   O-2   0.3678(2)    0.0566(1)    0.2633(2)    0.77      1.0


! Instructions for Bond_STR
DISTANCE        ! Calculation and output of distances and angles
!RESTRAINS      ! Uncomment for restraints file for FullProf
DMAX  3.4 2.7   ! Fixing maximum distances dmax_dis and dmax_angl
                ! For angle calculations dmax_angl /= 0 (defaults: 3.2 0.0)
------------------- End of the mfepo5.cfl file --------------------
```

Notice the way of giving the oxidation state of the ions: the name of the element followed by +/-n or n+/- being "n" the assumed valence. Notice also that the standard deviations can be given in parenthesis (as usual) but immediately following the last number. No space is permitted between the value and its standard deviation. The minimal set of keywords in a CFL file for being used as input of the program Bond_Str are: cell, spgr and atom. They are case insensitive.

The symbol "!" is used as a comment. The items following an atom keyword are: Label of the atom, element or species, fractional coordinates x, y, z, isotropic displacement parameter (Biso) and occupation factor (proportional to the multiplicity of the site, e.g. occ=m/M).

Two more items can be given: magnetic moment value and ionic charge as real values. If instead of the ionic species only the element symbol is provided the two additional items are needed: even if the magnetic moment is not used it should be given. An alternative atom-line corresponding to the first line in the above example can be written as follows:

```
!     Label Element    x       y       z       Biso   occ   MagM  Charge
Atom   ni      ni    0.0000  0.0000  0.0000  0.74   0.5   1.80  2.00
```

The keywords DISTANCE and RESTRAINS in the above examples do not need numerical values. They just instruct the program to change the output with respect to the default values.

The keyword DMAX is for limiting distance and angle calculations and it is followed by two real values (dmax_dis and dmax_angl).
Be careful not giving a high number for dmax_angle because the number of possible angles between three atoms that are at or below a distance dmax_angl increases strongly with dmax_angl.

If user-given bond-valence parameters are to be provided, the instruction in the CFL file is as follows (for instance in the case of La^{3+}-O^{2-} and Mn^{3+}-O^{2-}):
```
BVPARM LA+3 O-2  2.172   0.370
```

```
BVPARM MN+3 O-2  1.760   0.370
```

Notes about the GUI `GBond_Str`

The program `GBond_Str` is a GUI for running `Bond_Str` without direct editing the input file. The interface has only a single window, except when the internal editor is invoked to
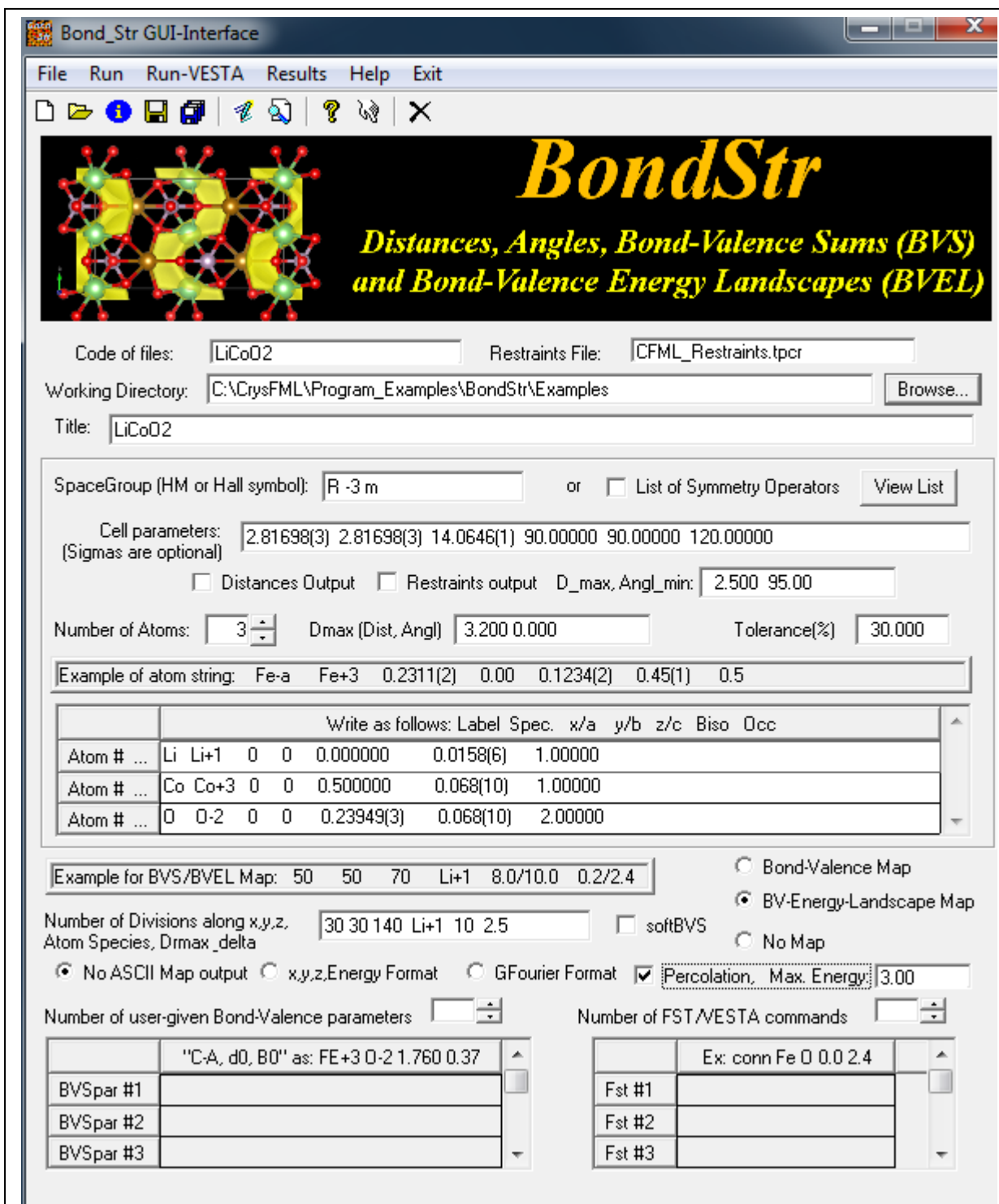

Figure 1: Screen shot of the GUI for `Bond_Str` after importing a CFL file. Notice that the calculation that will be performed correspond to a Bond-Valence Energy Landscape map followed by the estimation of the percolation energy.

visualise the results.

The aspect of the interface after importing a CFL file is shown in Figure 1.

The content of the CFL file is:

```
Title LiCoO2
!   Unit cell parameters:  a, b, c, Alpha, Beta, Gamma
Cell  2.81698(3)  2.81698(3)  14.0646(1)  90.00000  90.00000  120.00000
!      Space Group
Spgr  R -3 m
!  Atom-strings in the order: Label, Species, x, y, z, Biso, Occ [,2*Spin, charge]
Atom Li   Li1+   0   0    0.000000     0.0158(6)     1.00000
Atom Co   Co+3   0   0    0.500000     0.068(10)     1.00000
Atom O    O-2    0   0    0.23949(3)   0.068(10)     2.00000
!   Bond_STR instructions
!   Nx, Ny, Nz, Species, Dmax, Delta(eV): Values within Emin+delta are counted for
!   fractional volume estimation
BVEL 30 30 140  Li1+  10  2.5
PERCOLATION   3.00
```

This interface to `BondStr` may be used to transform CIF files to CFL files with just a click as shown in Figure 2. In fact the previous CFL file has been converted from a CIF file. If the CIF files does not contain information about charges, the user may change that in the interface by completing the appropriate atom strings using a simple editor or by hand in `GBond_Str`.

Notice that the user can provide bond-valence parameters by filling the appropriate box that is activated as soon as one increases the number of user-given bond-valence parameter that is initially put to zero.
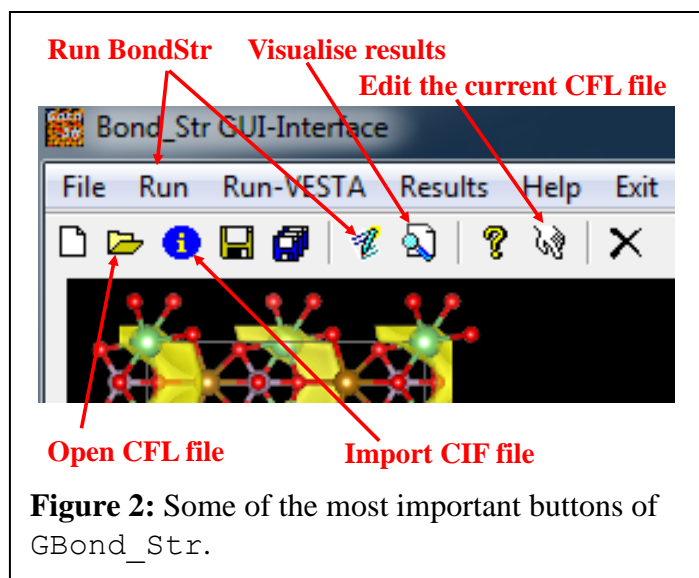

Figure 2: Some of the most important buttons of `GBond_Str`.

The program `GBond_Str` is just a tool for manipulating CIF and CFL files. There is no calculation inside `GBond_Str`. When the user clicks on the run button (or select Run in the menu) the program saves the current CFL file and invokes `Bond_Str` with the code of the current file as argument. The normal output of `Bond_Str` is directed to the screen in a terminal console. As soon as `Bond_Str` finish the calculations `GBond_Str` takes the control and edit the output file from `Bond_Str`.

The program `GBond_Str` can be used to create the appropriate keywords for output of distance and angles, restraint files and the conditions for generating it. The keywords recognized by `Bond_Str` are TITLE, DISTAN, FST_CMD, BVPAR, DMAX, RESTDA, RESTR_FILE, SOFTBVS, TOL, RESTR, BVELPAR, PERCOLATION, MAP, BVEL, and VDIST.

The major part of these keywords (and the corresponding values) can be generated by `GBond_Str`, by clicking or checking the appropriate check boxes or radio buttons (the meaning of the keywords can be deduced from the text written in the GUI). However, VDIST can presently only be introduced in the CFL by hand, is VDIST is present the calculation of

pair distributions of bond distances and volumes of polyhedra are calculated and output in the general output file of extension `*.bvs`.

The use of `Bond_Str` to treat many files in one single run

The program `Bond_Str` can be used from a terminal to perform more complex data treatment. One can prepare a buffer file containing CIF or CFL files. The most interesting use of `Bond_Str` is when we have available a buffer file containing CFL files with oxidation states included in the structural information. This buffer file can be prepared using the program `Formal_Charges`. How to prepare this kind of file is described in the short manual of the program `Formal_Charges`. The program `Bond_Str` can be invoked in the command line giving the name of the buffer file as the first argument as:

```
C:\Database\CIFs>Bond_Str cfl_buffer.buf

                    ==============================
                    ====== PROGRAM BOND_STR ======
                    ==============================
      **********************************************************************
      * Distances, angles and Bond-Valence Sums from  *.cfl or *.cif files  *
      *     Calculation of BVS and Bond-Valence Energy Landscape maps       *
      **********************************************************************
                    (JRC - ILL, version: March 2018)

=> Treating file #:    1  -> 10069_gen_fch.cfl

 => Calculation of Bond-Valence Energy Landscape Map (it can take few minutes) ....
 => Volume  fraction for ion mobility in the unit cell:     12.41 %
 => Minimum Energy (in eV):   -4.7915

 => Computing a first rough estimation of percolation energies (it can take several
minutes) ....
    a-axis
      Searching percolation between  2.00 and  2.51 eV
      Searching percolation between  2.00 and  2.11 eV
        Percolation energy above Emin:   2.03 eV,   Isosurface for VESTA:  -2.76 eV

    b-axis
      Searching percolation between  1.00 and  1.51 eV
      Searching percolation between  1.30 and  1.41 eV
        Percolation energy above Emin:   1.35 eV,   Isosurface for VESTA:  -3.44 eV

    c-axis
      Searching percolation between  3.00 and  3.51 eV
      Searching percolation between  3.20 and  3.31 eV
        Percolation energy above Emin:   3.22 eV,   Isosurface for VESTA:  -1.57 eV

 => Normal End of: PROGRAM BOND_STR
 => Global results in File: 10069_gen_fch.bvs
 => Bond Valence Energy Landscape in File: 10069_gen_fch_bvel.map
 => VESTA File: 10069_gen_fch_str.vesta
 => CPU-time:   0 minutes 59.7640 seconds


                    ==============================
                    ====== PROGRAM BOND_STR ======
                    ==============================
      ****************************************************************
```

```
    * Distances, angles and Bond-Valence Sums from  *.cfl or *.cif files  *
    *     Calculation of BVS and Bond-Valence Energy Landscape maps       *
    **********************************************************************
                      (JRC - ILL, version: March 2018)


 => Treating file #:    2  -> 10645_gen_fch.cfl

 => Calculation of Bond-Valence Energy Landscape Map (it can take few minutes) ....
 => Volume  fraction for ion mobility in the unit cell:     10.49 %
 => Minimum Energy (in eV):   -0.3524

 => Computing a first rough estimation of percolation energies (it can take several
minutes) ....

 => Normal End of: PROGRAM BOND_STR
 => Global results in File: 10645_gen_fch.bvs
 => Bond Valence Energy Landscape in File: 10645_gen_fch_bvel.map
 => VESTA File: 10645_gen_fch_str.vesta
 => CPU-time:   0 minutes  4.1028 seconds
. . . . . . . . . . . . . . .
```

A part from the normal files generated by Bond_Str a global file called in this case `cfl_buffer_glb.res` containing a summary of the results. A rough output of this file in the screen can be obtained as:

```
C:\Database\CIFs>more cfl_buffer_glb.res
 GLOBAL RESULTS OF THE BVEL ANALYSIS OF BUFFER FILE: cfl_buffer.buf
   1 10069_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):   46.327    Fraction(%):
12.414     Emin:   -4.792    Emig(a):    2.030    Emig(b):    1.350    Emig(c):    3.220
Energy(percol,a,b,c):  -2.762  -3.442  -1.572
   2 10645_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    7.446    Fraction(%):
10.493     Emin:   -0.352    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   3 10669_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    8.123    Fraction(%):
11.316     Emin:   -0.379    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   4 10670_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    8.321    Fraction(%):
11.575     Emin:   -0.387    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   5 10671_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    3.986    Fraction(%):
11.150     Emin:   -0.404    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   6 10693_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):   23.465    Fraction(%):
8.408     Emin:   -3.828    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   7 11282_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    8.817    Fraction(%):
11.575     Emin:    0.276    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   8 11283_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    8.798    Fraction(%):
11.575     Emin:    0.288    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
   9 11284_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    8.674    Fraction(%):
11.575     Emin:    0.233    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
  10 11285_gen_fch.cfl           LI+1 delta(eV):    3.000   Vol(A^3):    8.682    Fraction(%):
11.619     Emin:    0.214    Emig(a):    0.000    Emig(b):    0.000    Emig(c):    0.000
Energy(percol,a,b,c):   0.000   0.000   0.000
```

One can edit this file in order to see more clearly the content of the information that is included in a line per treated file. For each line there is the number in the sequence of the treated file, the name of the file, the mobile chemical species, the parameter delta in electron volts, the available volume for migration, the fraction of the total volume, the minimum energy, the migration (activation) energies (along *a*, *b*, and *c*) and the percolation energies (along *a*, *b*, and *c*).

One can use a buffer file without calculation of the percolation/migration energies. For instance, if we are only interested in the calculation of bond-valence sums (using the same buffer file) one can invoke the program as:

```
C:\Database\CIFs>Bond_Str cfl_buffer.buf GII_only

                     ==============================
                     ====== PROGRAM BOND_STR ======
                     ==============================
     ***********************************************************************
     * Distances, angles and Bond-Valence Sums from  *.cfl or *.cif files  *
     *     Calculation of BVS and Bond-Valence Energy Landscape maps        *
     ***********************************************************************
                      (JRC - ILL, version: March 2018 )

 => Treating file #:    1  -> 10069_gen_fch.cfl
  Subroutine Calc_BVS (JRC-LLB, version: March-2005)
  Title: Summary of Bond-Valence calculations for file: 10069_gen_fch.cfl
   Atom      Coord  D_aver Sigm   Distort(x10-4)    Valence     BVSum(Sigma)
    Li        6.00  2.1894(   0)      76.998         1.000       0.898(  0)
    O         4.00  2.0243(   0)      89.607        -2.000       2.112(  0)
    O         2.00  1.7408(   0)      26.375        -2.000       1.602(  0)
    O         3.00  1.9118(   0)      15.745        -2.000       2.411(  0)
    O         3.00  2.1353(   0)     300.440        -2.000       1.616(  0)
    O         4.00  2.0032(   0)       9.948        -2.000       2.300(  0)
    V         5.00  1.8177(   0)      55.709         4.500       4.951(  0)
    V         5.00  1.9016(   0)      43.497         4.500       4.192(  0)
 =>  Old Global Instability Index (  GII=SQRT{SUM{|BVS-abs(q)|^2}/Num_Atoms} ) =  33.28 /100
 =>  Normalized   GII(a)=      SUM {|BVS-abs(q)|  *mult}        /N_Atoms_UCell =  30.82 /100
 =>  Normalized   GII(b)=      SUM {|BVS-abs(q)|  *mult/abs(q)}/N_Atoms_UCell =  13.41 %
 =>  Normalized   GII(c)= SQRT{ SUM {|BVS-abs(q)|^2*mult}        /N_Atoms_UCell}=  33.28 /100

 => Normal End of: PROGRAM BOND_STR
 => Global results in File: 10069_gen_fch.bvs
 => Summary of BVS in File: 10069_gen_fch_sum.bvs
 => CPU-time:   0 minutes  0.0156 seconds


. . . . . . . . . . . .



                     ==============================
                     ====== PROGRAM BOND_STR ======
                     ==============================
     ***********************************************************************
     * Distances, angles and Bond-Valence Sums from  *.cfl or *.cif files  *
     *     Calculation of BVS and Bond-Valence Energy Landscape maps        *
     ***********************************************************************
                      (JRC - ILL, version: March 2018 )


 => Treating file #:   10  -> 11285_gen_fch.cfl
  Subroutine Calc_BVS (JRC-LLB, version: March-2005)
  Title: Summary of Bond-Valence calculations for file: 11285_gen_fch.cfl
   Atom      Coord  D_aver Sigm   Distort(x10-4)    Valence     BVSum(Sigma)
    O         6.00  2.1060(   0)       0.002        -2.000       1.824(  0)
    Li        6.00  2.1060(   0)       0.000         1.000       0.980(  0)
    Co        6.00  2.1060(   0)       0.000         2.140       1.944(  0)
 =>  Old Global Instability Index (  GII=SQRT{SUM{|BVS-abs(q)|^2}/Num_Atoms} ) =  15.26 /100
 =>  Normalized   GII(a)=      SUM {|BVS-abs(q)|  *mult}        /N_Atoms_UCell =  17.51 /100
 =>  Normalized   GII(b)=      SUM {|BVS-abs(q)|  *mult/abs(q)}/N_Atoms_UCell =   8.54 %
 =>  Normalized   GII(c)= SQRT{ SUM {|BVS-abs(q)|^2*mult}        /N_Atoms_UCell}=  17.99 /100

 => Normal End of: PROGRAM BOND_STR
 => Global results in File: 11285_gen_fch.bvs
 => Summary of BVS in File: 11285_gen_fch_sum.bvs
 => CPU-time:   0 minutes  0.0156 seconds
 => TOTAL CPU-time:   0 minutes  0.3120 seconds
```

Using the keyword `GII_only` in the command line invocation of the program the `cfl_buffer_glb.res` is simpler and contains only the value of the normalized `GII(c)` and the name of the corresponding CFL file. For instance in the present case we have:

```
C:\Database\CIFs>more cfl_buffer_glb.res

 GLOBAL RESULTS OF THE BVEL ANALYSIS OF BUFFER FILE: cfl_buffer.buf
    1 10069_gen_fch.cfl          Normalized   GII(c):    33.28
    2 10645_gen_fch.cfl          Normalized   GII(c):    19.33
    3 10669_gen_fch.cfl          Normalized   GII(c):    30.64
    4 10670_gen_fch.cfl          Normalized   GII(c):    31.03
    5 10671_gen_fch.cfl          Normalized   GII(c):    28.82
    6 10693_gen_fch.cfl          Normalized   GII(c):    61.54
    7 11282_gen_fch.cfl          Normalized   GII(c):    16.88
    8 11283_gen_fch.cfl          Normalized   GII(c):    16.96
    9 11284_gen_fch.cfl          Normalized   GII(c):    17.87
   10 11285_gen_fch.cfl          Normalized   GII(c):    17.99
```

If we are only interested in the calculation of BVEL without calculating the percolation energies one can invoke the program as:

```
C:\Database\CIFs>Bond_Str cfl_buffer.buf NPERCOLATION
```

The file `cfl_buffer_glb.res` is also simpler than in the general case, in our case it is as seen just below:

```
C:\Database\CIFs>more cfl_buffer_glb.res
 GLOBAL RESULTS OF THE BVEL ANALYSIS OF BUFFER FILE: cfl_buffer.buf
    1 10069_gen_fch.cfl LI+1 delta(eV): 3.000 Vol(A^3):46.327 Fraction(%): 12.414 Emin:    -
4.792
    2 10645_gen_fch.cfl LI+1 delta(eV): 3.000 Vol(A^3): 7.446 Fraction(%): 10.493 Emin:    -
0.352
    3 10669_gen_fch.cfl LI+1 delta(eV): 3.000 Vol(A^3): 8.123 Fraction(%): 11.316 Emin:    -
0.379
    4 10670_gen_fch.cfl LI+1 delta(eV): 3.000 Vol(A^3): 8.321 Fraction(%): 11.575 Emin:    -
0.387
    5 10671_gen_fch.cfl LI+1 delta(eV): 3.000 Vol(A^3): 3.986 Fraction(%): 11.150 Emin:    -
0.404
    6 10693_gen_fch.cfl LI+1 delta(eV): 3.000 Vol(A^3):23.465 Fraction(%):  8.408 Emin:    -
3.828
    7 11282_gen_fch.cfl  LI+1  delta(eV):  3.000  Vol(A^3):  8.817  Fraction(%):  11.575  Emin:
0.276
    8 11283_gen_fch.cfl  LI+1  delta(eV):  3.000  Vol(A^3):  8.798  Fraction(%):  11.575  Emin:
0.288
    9 11284_gen_fch.cfl  LI+1  delta(eV):  3.000  Vol(A^3):  8.674  Fraction(%):  11.575  Emin:
0.233
   10 11285_gen_fch.cfl  LI+1  delta(eV):  3.000  Vol(A^3):  8.682  Fraction(%):  11.619  Emin:
0.214
```

The information contained in the current document may be changed in forthcoming versions when more options will be available. More information about `Bond_Str` and its GUI can be obtained from the existing documentation in the FullProf Suite toolbar even if it is not currently updated.