The program BondStr (or Bond_Str) and its GUI GBond_Str

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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 to be calculated

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 a simple bond-valence sum calculation (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
```

For calculating a bond valence energy landscape map, using softBVS parameters an average coordination must be given. For instance the line for Mn3+ should be written as:

```
BVPARM MN+3 O-2  1.760   0.370  6
```

In such a case the program calculates the Morse potential used in BVEL calculations from the BVS parameters provided in the BVPARM instruction. This is only true if the anions are in the internal list of chemical properties (ionic radius, electronegativity, etc.). Otherwise the user should provide the full list of parameters in the Morse potential using the instruction:

```
!     Cation  Anion  CN    R0   Cutoff    D0       Rmin        Alpha
BVELPAR MN+2  N-3     6    1.5    5     0.63394   1.81719     2.50000
```

For the meaning of the different parameters see the output file of BondStr for a case in which everything works with internal tables. The average coordination `CN` and the parameter `Cutoff` are not actually used for the calculations but should be provided for maintaining the format of the information provided in the output file.

In some cases the differences in the energies calculated by using softBVS parameters or using the most reliable internal tables (when the keyword SOFTBVS is not provided) may be important. The difference is less when one considers the activation energies, but it may attains values close to 1 eV.

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 visualise the results.

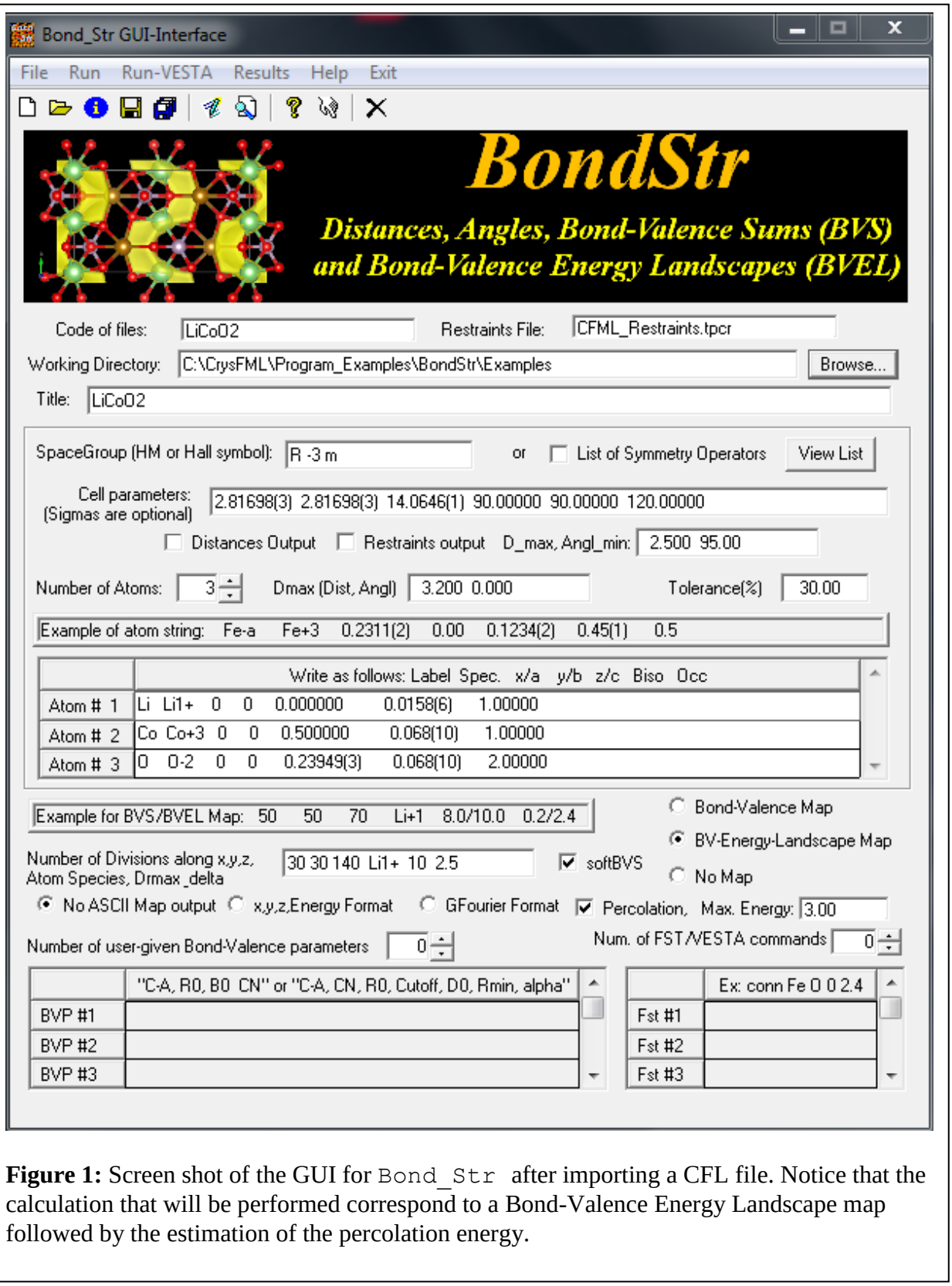

Figure 1: Screen shot of the GUI for `Bond_Str` after importing a CFL file. Notice that the calculation that will be performed correspond to a Bond-Valence Energy Landscape map followed by the estimation of the percolation energy.

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.

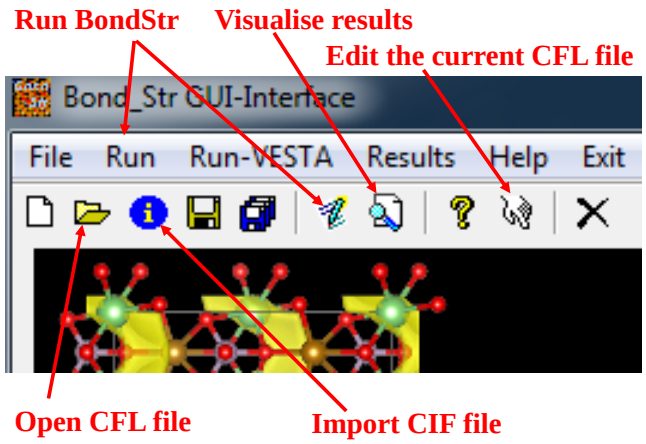

Figure 2: Some of the most important buttons of `GBond_Str`.

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`.

An example of the GUI content when the user provides directly the parameters defining the Morse potential for making a calculation of the BVEL map is given below in Fig. 3.

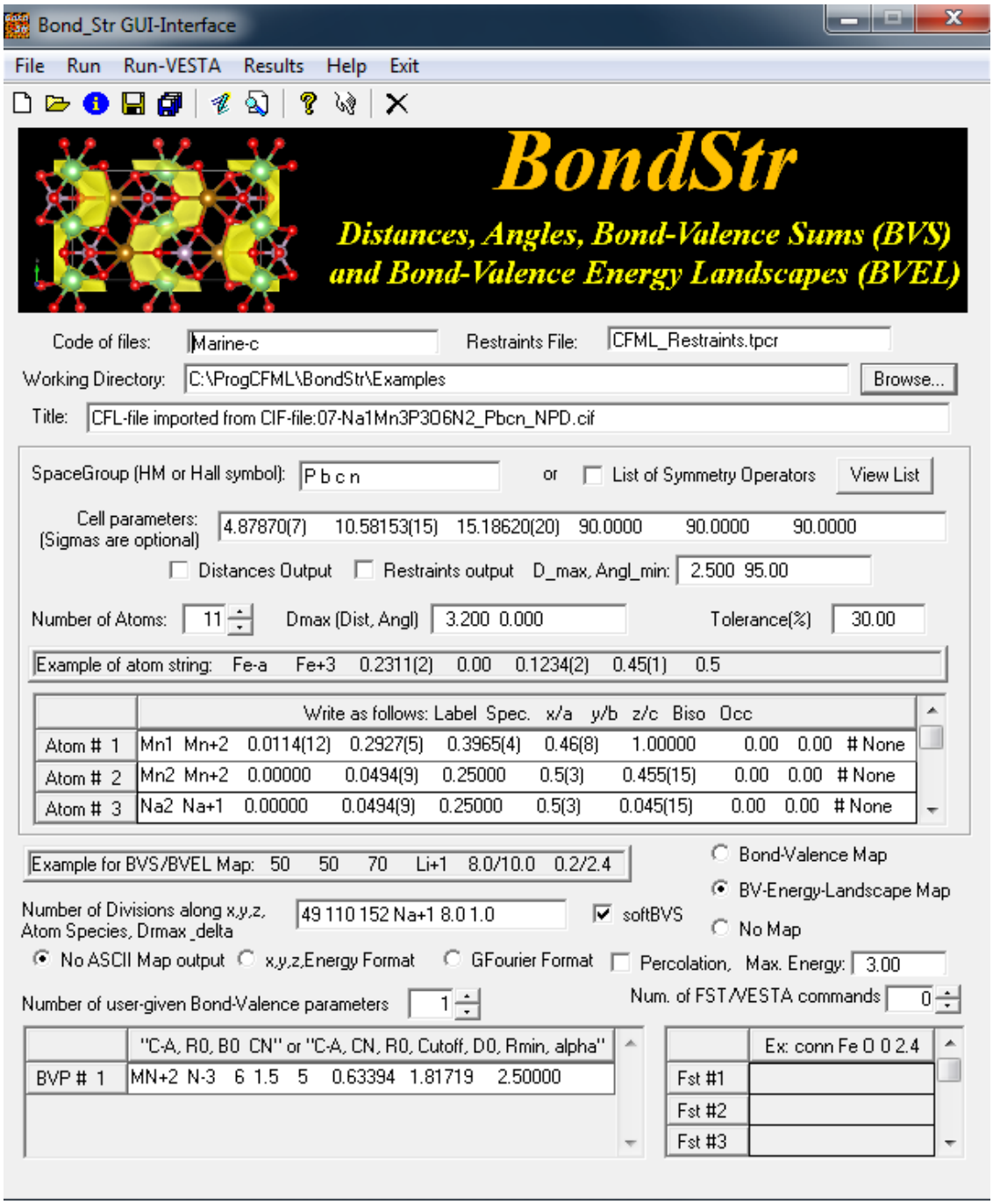

Figure 3: Artificial example in which the parameters of the Morse potential are provided by the user. When running the program, it generates a CFL file in which the instruction:

```
!      Cation  Anion  CN     R0    Cutoff     D0        Rmin        Alpha
BVELPAR MN+2   N-3      6    1.5     5      0.63394   1.81719     2.50000
```

In this case (for which the program will use softBVS parameters) the full set of parameters for the potential is not needed because the chemical properties of Mn^{2+} and N^{3-} are in the internal list of ions. It is only necessary to provide, the three parameters R0, B0 and CN in the BVP #1 box (e.g. `MN+2 N-3 1.849 0.37 6`), this generates the instruction:
`BVPARM MN+2 N-3 1.849 0.37 6,` in the CFL file.

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.