BondStr

Welcome

Bond_Str

A program for calculating distances and angles in crystal structures.

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Introduction

The program ***Bond_Str*** calculates distances and angles in crystal structures. It is based in old Fortran 77 versions but is has been completely re-written and it is now based in ***CrysFML*** (Crystallographic Fortran 95 Modules Library).

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

Running the program

You can run ***Bond_Str*** program from:

- Console
- by clicking on the  icon on the Toolbar of FullProf Suite (***GBond_Str*** program)

Console version

You can run ***Bond_Str*** from a console as follows:

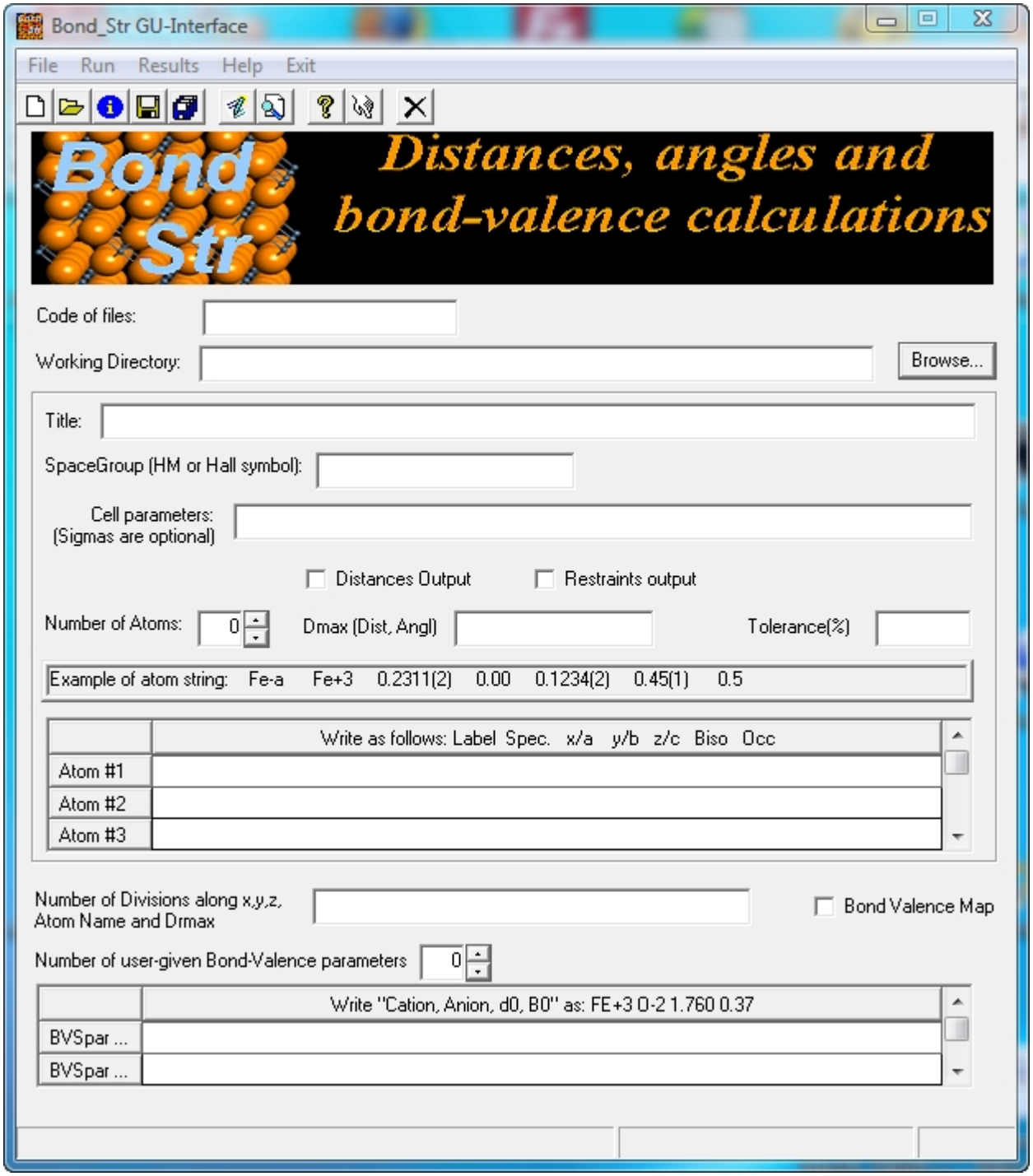
Local_Prompt> *bond_str My_file <cr>*

My_file is the code of the input file that can be either a standard **CIF** file or a **CFL** file containing just the necessary structural information and the ionic species.

GBond_Str

Gbond_Str program is a simple GUI for ***Bond_Str*** program.

The main windows is similar to the next figure.



Code files
Common code of files for the run

Working directory
Complete path name of the working directory. This may be selected using the Browse button.

Title
A character string used as a title for the run

SpaceGroup
A character string with the Hermann-Mauguin or Hall symbol for the space group information

Cell parameters
Cell parameters with the sigmas are optional. In the last case the sigma is written between parenthesis.

Distance Output

Selecting this option active the calculation of distance and angles

Restraints Output
Selecting this option a restraint file is created for ***FullProf*** Program

Number of Atoms
Number to atoms to introduce in the program

Dmax (Dist, Ang)
Introduce two values indicating the distance maximum and angle to do the geometric calculations

Tolerance (%)
Set a particular tolerance for geometric calculations

Atoms information
Introduce the atom information according to keyword ATOM

BVS Information
If a BVS map is desidered then the user need activate it in the checkbox Bond Valence Map and introduce the grid points for the map. Also the label of the atom point and the maximum distance to cut neighbors contributions.

Also the user can modify the d0 and B0 parameters or introduce them if they aren't defined into the program.

Input File

The input file for ***Bond_Str*** program can be a **CFL** or **CIF** file. **CFL** file is a format that is recognized by all programs based in ***CrysFML***. They have the extension *.cfl and are in free format. The different items are recognized thanks to keywords. A CFL file can be generated from a CIF file just running ***Bond_Str***.

Alternatively, the GUI for ***Bond_Str*** program (***GBond_Str***) 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.

CFL Format

This is an example of input file as CFL format

```
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)
```

Giving the oxidation state of the ions
Name of the element followed by +/-n or n+/- being "n" the assumed valence.

Giving the standard deviations
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.

Comments
The symbol "!" is used as a comment.

Keywords

The values associated with for keywords are the following:

- ATOM
- BVPARM

ATOM

The items following an atom keyword are:

- Label of the atom
- Element or species
- Fractional coordinates `x`, `y`, `z`
- Isotropic displacement parameter (`Biso`)
- Occupation factor (proportional to the multiplicity of the site, e.g. `occ=m/M`).

Two more items can be given:

- Magnetic moment value
- Ionic charge

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.

Example:

```
!    Label  Element     x       y        z     Biso   Occ   MagM  Charge
Atom   Ni1    Ni     0.0000  0.0000   0.0000   0.74   0.5   1.80   2.00
```

BVPARM

If user wants give bond-valence parameters.

Example:

```
BVPARM LA+3 O-2  2.172   0.370
BVPARM MN+3 O-2  1.760   0.370
```

CELL

Cell parameters. Optionally standard deviation can be use.

Example:

```
!   Unit cell parameters:  a, b, c, Alpha, Beta, Gamma
Cell  5.518761   5.518761   7.810852  90.000000  90.000000  90.000000
```

DISTANCE

Active the calculation and output of distance and angles

Example:

```
! Activating Distance calculations
Distance
```

DMAX

This keyword is for limiting the distance and angle calculations. The sentence to use is:

DMAX *dmax_dis dmax_angle*

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_dis* increases strongly with *dmax_angle*.

Example:

```
! Bond_STR instructions
DMAX  3.900 2.500
```

MAP

Active the BVS Maps procedure. The setence is

MAP *nx ny nz AtomName Dmax*

where

NX NY NZ	Grid points for BVS map
AtomName	Is the representative point on the Map. It could be an atom from structure. In this case, the atom was not included in the BVS calculations
Dmax	is the maximum distance to search BVS contributions

Example:

```
!   Bond Valence Map Calculations
Map  32  32  64  Ca1  4.0
```

RESTRAINTS

Active the restraints file for ***Bond_STR*** program

Example:

```
! Bond_STR Instructions
Restrains
```

SPGR

A string containing the Hermann-Mauguin or Hall symbol of the space group.

Example:

```
! Space Group
Spgr  P n m a
```

TITL

String to give a Title

Example:

```
! Title of Job
Title Geometric Calculations on BaTiO3
```

TOL

Tolerance parameter for geometric calculations

Example:

```
! Tolerance parameter
Tol   20.0
```

VDIST

Active the procedure to calculates distortion parameter for a coordination polyhedra. The procedure was described by Balic Zunic & Vickovic in *J. Appl. Cryst*. (1996), **29**, 305-306.

Example:

```
!Bond_STR instructions
VDISTOR
```

Output File

All details are written in the output file. In general called *codefile.bvs*

Bibliography

Recommended references:

- Altermatt, D. & Brown, I.D., *Acta Cryst*. (1985). **B41**, 244-247
- Brown, I. D.; The Chemical Bond in Inorganic Chemistry - The Bond Valence Model. IUCr monographs on Crystallography 12, Oxford University Press, (2002).
- www.ccp14.ac.uk/ccp/web-mirrors/i_d_brown