Calculs de distanes, angles et « bond valence » dans FullProf

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Les calculs de distances et angles interatomiques, ainsi que les calculs de «bond valence» [1] peuvent maintenant être exécuter par FullProf, sans utiliser de programme externe (BONDSTR par exemple). Ces calculs peuvent se faire à l'aide de la variable `JDIST`, en lui donnant la valeur 3 ou 4. Un fichier avec l'extension `.DIS` est alors généré pour chaque phase, contenant les résultats des calculs effectués.

Voici un exemple de fichier `.PCR` (cas d'une pérovskite de manganèse) permettant de faire ce genre de calculs ainsi que quelques explications (extraites du guide de l'utilisateur de FullProf `FullProf_manual.pdf`). Les paramètres importants dans le fichier `.PCR` sont en caractère gras et les caractères bleus sont relatifs aux calculs de Bond Valence.

```
LaMnO3
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ     Nvk   Npr More
  4   0   0  0.0 0.0 1.0  0   0   0   0   0    967.37   0 7 1
!
!Jvi Jdi Hel Sol Mom Ter Brind   RMua   RMub   RMuc     Jtyp
  0   3   0   0   0   0  1.0000  0.0000 0.0000 0.0000   1
!
! Max_dst(dist) (angles) Bond-Valence Calc.
  3.5000         0.0000   BVS
! N_cations N_anions Tolerance(%) / Name or cations/ and Anions
   2   1   0.00
LA+3 MN+3
O-2
!
P b n m <--Space group symbol
!Atom Typ X Y Z Biso Occ In Fin N_t Spc /Codes
La    LA    -0.00768     0.04908   0.25000   0.33853 0.50000  0  0  0  1
              111.00      121.00      0.00    181.00 0.00
Mn    MN     0.50000     0.00000   0.00000   0.20383 0.50000  0  0  0  2
               0.00        0.00      0.00    151.00 0.00
O1    O      0.07430     0.48732   0.25000   0.48818 0.50000  0  0  0  3
               91.00      101.00      0.00    141.00 0.00
O2    O      0.72563     0.30660   0.03843   0.42020 1.00000  0  0  0  3
               71.00       81.00     61.00    171.00 0.00
```

JDIST

- **=3** Distance and angle calculations will be performed for the current phase. Bond valence calculations may be also performed. The output is in the file CODFIL*n*.dis. An additional file helping to create strings for soft constraints is output. This file has a fixed name: "dconstr*n*.hlp"
- **=4** Only Bond Valence calculations are output to the file CODFIL*n*.dis for the current phase.

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[1] Se référer au document "ftp://129.20.75.88/pub/intranet/pdf/bond_valence_sum.pdf» pour quelques explications sur ce concept

LINE 20: DIS_MAX, ANG_MAX, BVS (2 Reals - Character) [FOR JDIST=3, 4]
Comment line: ! Max_dst(dist) (angles) Bond-Valence Calc

DIS_MAX
Maximum distance between atoms to output in file CODFIL*n*.dis.

ANG_MAX
Maximum distance between atoms to output angmes in file CODFIL*n*.dis. If ANG_MAX=0 no angle calculations are performed

BVS
If this character variable is equal to `BVS` then Bond Valence calculations are performed and the results output to file CODFIL*n*.dis. The line 21 is then read

LINE 21: N_CATIONS, N_ANIONS, TOLERANCE (2 Integers - 1 Real)
Comment line: ! N_cations N_anions Tolerance(%) / Name cations/ and Anions

N_CATIONS
Number of Cations

N_ANIONS
Number of Anions

TOLERANCE
Tolerance for the ionic radius in percentage. Two atoms are considered as bonded if their distance is less than the sum of their respective ionic radius augmented by the value of `TOLERANCE`. The explicit expression dor considering two atoms is:

$$Distance(Atom_1, Atom_2) = (R(Atom_1) + R(Atom_2)) \times (1+0.01 \times TOLERANCE)$$

If `TOLERANCE`=0 the program takes `TOLERANCE`=20

LINE 21-1: CATIONS (Character) (N_Cations)

CATIONS
Symbol of the cations in uppercase and putting the sign of the charge before the valence.
Example for three cations:
```
CU+2 Y+3 BA+2
```

The chemical species are numbered sequentially, so: CU^{2+} is the species number 1, Y^{3+} is the species number 2 and Ba^{2+} is the species number 3. This numbering is important to identify the chemical nature of the atoms in the asymmetric unit.

LINE 21-2: ANIONS (Character) (N_Anions)

ANIONS
Symbol of the anions in uppercase and putting the sign of the charge before the valence.
Example for two anions:
```
O-2 CL-1
```

O^{2-} is the species number 4 and Cl^{-1} is the species number 5.

`LINE 25-1`

N_Species
Number of the chemical species. Used for Bond Valence calculations, see LINE 21 for details