PROGRAM: Get_Conv_Cell

Author: J. Rodriguez-Carvajal (ILL)

Created: January 2008, Updated: March 2022

This program provides the conventional cell from the input of an arbitrary cell. The program needs as input the unit cell parameters and provides the conventional unit cell parameters and the transformation matrix between the input cell and the conventional cell(s). The program is similar to REDUC from Yvon Le Page but it has been developed from the scratch using new procedures that are in CrysFML. These procedures are based on well-known articles of the literature about reduced and conventional cells. In particular, the search of two-fold axes is based on the paper by Yvon Le Page in *J. Appl .Cryst.* **15**, 255 (1982) and the search of the Niggli cell is based on the algorithm developed by I. Krivy and B. Gruber, *Acta Cryst* **A32**, 297 (1976).

The source code of the program can be found in the CrysFML repository:
https://code.ill.fr/scientific-software/crysfml
within the program examples and metrics subdirectories:
https://code.ill.fr/scientific-software/crysfml/Program_Examples/Metrics.

The program runs in a console and does not need input files. The output appears on the screen, unless the user asks for an output file, and it is self-explanatory. An example of the use of the program is given below.

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    Program: Get_Conventional_Unit_Cells
 Author: J. Rodriguez-Carvajal, ILL(2008)
          Updated January 2011
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=> Output on the screen (<cr>) or in file (f) :
=> Enter the cell parameters: 5 5 5 60 60 60
=> Enter the centring type (P,A,B,C,I,R,F): P
=> Enter angular tolerance in degrees (<cr> = 3 deg.): 2
=> Enter distance tolerance in angstroms (<cr> = 0.2 A.): 0.15

            Input Cell (Aic):     5.0000    5.0000    5.0000   60.0000   60.0000   60.0000  Centring: P
  Primitive input Cell (Api):     5.0000    5.0000    5.0000   60.0000   60.0000   60.0000
           Niggli Cell  (AN):     5.0000    5.0000    5.0000   60.0000   60.0000   60.0000

            (Aic) formal column matrix containing the input cell vectors:
            (Api) formal column matrix containing the primitive cell vectors:
             (AN) formal column matrix containing the Niggli cell vectors:
            (Acc) formal column matrix containing the conventional cell vectors:

                          (Api) = M (Aic)                          (AN) = N (Api)
    TransF:        1.000000    0.000000    0.000000       -1.000000    0.000000    0.000000
    TransF:        0.000000    1.000000    0.000000       -1.000000    0.000000    1.000000
    TransF:        0.000000    0.000000    1.000000       -1.000000    1.000000    0.000000
=> Two-fold axes (indices in the Niggli cell)
=>       Direct       Reciprocal    Dot    Cross      Length
       0   1   0       1   2   1     2     0.000     5.00000
       1  -1   0       1  -1   0     2     0.000     5.00000
       0   1  -1       0   1  -1     2     0.000     5.00000
       0   0   1       1   1   2     2     0.000     5.00000
       1   0   0       2   1   1     2     0.000     5.00000
       1   0  -1       1   0  -1     2     0.000     5.00000
       1   1  -1       1   1   0     2     0.000     7.07107
       1  -1  -1       0   1   1     2     0.000     7.07107
       1  -1   1       1   0   1     2     0.000     7.07107

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=> The new Cell is Metrically Cubic, F-centred cell  and the transformation matrix from then Niggli cell is:
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                       /  1   1  -1 \
 (Acc) = Tr (AN);  Tr: |   1  -1  -1  |   Determinant:    4
                       \ -1   1  -1 /
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  Conventional Cell:    7.07107   7.07107   7.07107   90.000   90.000   90.000
                                 /   -1.000000   -1.000000    1.000000\
     Final Tranformation Matrix: |     1.000000   -1.000000   -1.000000 |       (Acc) = Ftr (Aic)
                                 \    1.000000   -1.000000    1.000000/

     Determinant:     4.000000

                                 /   -0.500000    0.000000    0.500000\
    Inverse Tranformation Matrix: |    -0.500000   -0.500000    0.000000 |       (Aic) = (Ftr)^(-1) (Acc)
                                 \    0.000000   -0.500000    0.500000/

 => There are   9 two-fold axes
 => Do you want to display the monoclinic cells? (<cr>=no): y
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 => MONOCLINIC CELLS: In this section each two-fold axis is considered as a unique b-axis of M-cells
    The metrics of the monoclinic cells may be of higher symmetry, e.g. beta=90.0
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The new Cell is Metrically Monoclinic, I-centred cell  and the transformation matrix from then Niggli cell is:
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                         / -1   0   1 \
  (Acc) = Tr (AN);  Tr: |   0   1   0  |   Determinant:    2
                         \ -1   1  -1 /

  Conventional Cell:    5.00000   5.00000   7.07107   90.000   90.000   90.000
                                 /    0.000000    1.000000    0.000000\
     Final Tranformation Matrix: |    -1.000000    0.000000    1.000000 |       (Acc) = Ftr (Aic)
                                 \    1.000000   -1.000000    1.000000/

     Determinant:     2.000000

                                 /    0.500000   -0.500000    0.500000\
    Inverse Tranformation Matrix: |     1.000000    0.000000    0.000000 |       (Aic) = (Ftr)^(-1) (Acc)
                                 \    0.500000    0.500000    0.500000/

  Equivalent C-centred Cell:    5.00000   5.00000   8.66025   90.000  125.264   90.000
                                 /    0.000000    1.000000    0.000000\
     Final Tranformation Matrix: |    -1.000000    0.000000    1.000000 |       (Acc) = Ftr (Aic)
                                 \    1.000000   -2.000000    1.000000/

     Determinant:     2.000000

                                 /    1.000000   -0.500000    0.500000\
    Inverse Tranformation Matrix: |     1.000000    0.000000    0.000000 |       (Aic) = (Ftr)^(-1) (Acc)
                                 \    1.000000    0.500000    0.500000/

 => Two-fold axis along monoclinic b-axis,  Angular Discrepancy (deg)    0.0000
 =>       Direct       Reciprocal    Dot    Cross      Length
        0   1   0       1   2   1     2     0.000     5.00000

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The new Cell is Metrically Monoclinic, I-centred cell  and the transformation matrix from then Niggli cell is:
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                         / -1   0   0 \
  (Acc) = Tr (AN);  Tr: |   0  -1   1  |   Determinant:    2
                         \ -1   1   1 /

  Conventional Cell:    5.00000   5.00000   7.07107   90.000   90.000   90.000
                                 /    1.000000    0.000000    0.000000\
     Final Tranformation Matrix: |     0.000000    1.000000   -1.000000 |       (Acc) = Ftr (Aic)
                                 \   -1.000000    1.000000    1.000000/

     Determinant:     2.000000

                                 /    1.000000    0.000000    0.000000\
    Inverse Tranformation Matrix: |     0.500000    0.500000    0.500000 |       (Aic) = (Ftr)^(-1) (Acc)
                                 \    0.500000   -0.500000    0.500000/

  Equivalent C-centred Cell:    5.00000   5.00000   8.66025   90.000  125.264   90.000
                                 /    1.000000    0.000000    0.000000\
     Final Tranformation Matrix: |     0.000000    1.000000   -1.000000 |       (Acc) = Ftr (Aic)
                                 \   -2.000000    1.000000    1.000000/

     Determinant:     2.000000

                                 /    1.000000    0.000000    0.000000\
    Inverse Tranformation Matrix: |     1.000000    0.500000    0.500000 |       (Aic) = (Ftr)^(-1) (Acc)
                                 \    1.000000   -0.500000    0.500000/
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