Lattice Matching

A method is proposed for aligning unit cells for a group of crystals so that they all appear as nearly similar as possible to a selected cell. Related unit cells with varying cell parameters or indexed with different lattice centering can be accommodated. (Andrews&Bernstin, 2021, submitted to J. Appl. Cryst.)

Input unit cells have various forms that they can enter in: Input is case insensitive.

Type of cell input	Label	Example
unit cell parameters	Any of P,A,B,C,I,F,R,H	P 10 10 10 66 66 66
S^6	S or S6	S 0 0 0 -100 -100 -100
G^6	G or G6 or V	G 100 100 200 0 0 0
D^7	D7	
C^3	C3	C3 followed by the real parts, then imaginary
Random	random	random

For R and H: If R is input and the angles are all equal, it is assumed that the input is a primitive rhombohedral cell; if the angles are 90, 90, 120, then it is assumed that the input is a triply-primitive rhombohedral cell. If the input is H, it is assumed to be a primitive cell, rhombohedral if the angles are equal, and hexagonal if the angles are 90, 90, 120. The choice and use of R or H in the literature is quite inconsistent (including in the Protein Data Bank).

INPUT UNIT CELL DATA

The forms of input data are in the table above. They can be used mix-and-match. Invalid cells (including misspelling of the type) will be rejected with a console message. Data following the numeric specification is ignored.

BUILDING AND RUNNING LatticeMatching

The zip file contains the source code, this file, and the project files for Visual Studio 2019. No other files are needed for the source.

To build in Linux, gcc version 9.3.0 has been used. From the folder, the following command suffices to build:
g++ *.cpp -o lm
to create the executable file “lm”.

Visual Studio 2019 can be used to build also. The .sln file and project files are included with the source. VS 2022 (initial Preview) also compiled the source correctly.

The input is described above, and examples are given below.

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EXAMPLE OF INPUT

The first input cell will be used as the reference to be matched as well as possible. The following cells will have a large number of alternate presentations searched to find the best match to the reference. These input cells are selected from a small region of the Protein Databank.
1DPY R 57.98 57.98 57.98 92.02 92.02 92.02 To be used as the reference cell
1FE5 R 57.98 57.98 57.98 92.02 92.02 92.02
1G0Z H 80.36 80.36 99.44 90 90 120
1G2X C 80.95 80.57 57.1 90 90.35 90
1U4J H 80.36 80.36 99.44 90 90 120
2OSN R 57.1 57.1 57.1 89.75 89.75 89.75

INPUT

R 57.98 57.98 57.98 92.02 92.02 92.02 To be used as the reference cell
R 57.98 57.98 57.98 92.02 92.02 92.02
H 80.36 80.36 99.44 90 90 120
C 80.95 80.57 57.1 90 90.35 90
H 80.36 80.36 99.44 90 90 120
R 57.1 57.1 57.1 89.75 89.75 89.75
end

OUTPUT:

R 57.98 57.98 57.98 92.02 92.02 92.02
R 57.98 57.98 57.98 92.02 92.02 92.02
R 57.02 57.02 57.02 90.39 90.39 89.61
R 57.10 57.11 57.11 90.27 90.25 89.75
R 57.02 57.02 57.02 90.39 90.39 89.61
R 57.10 57.10 57.10 90.25 90.25 89.75