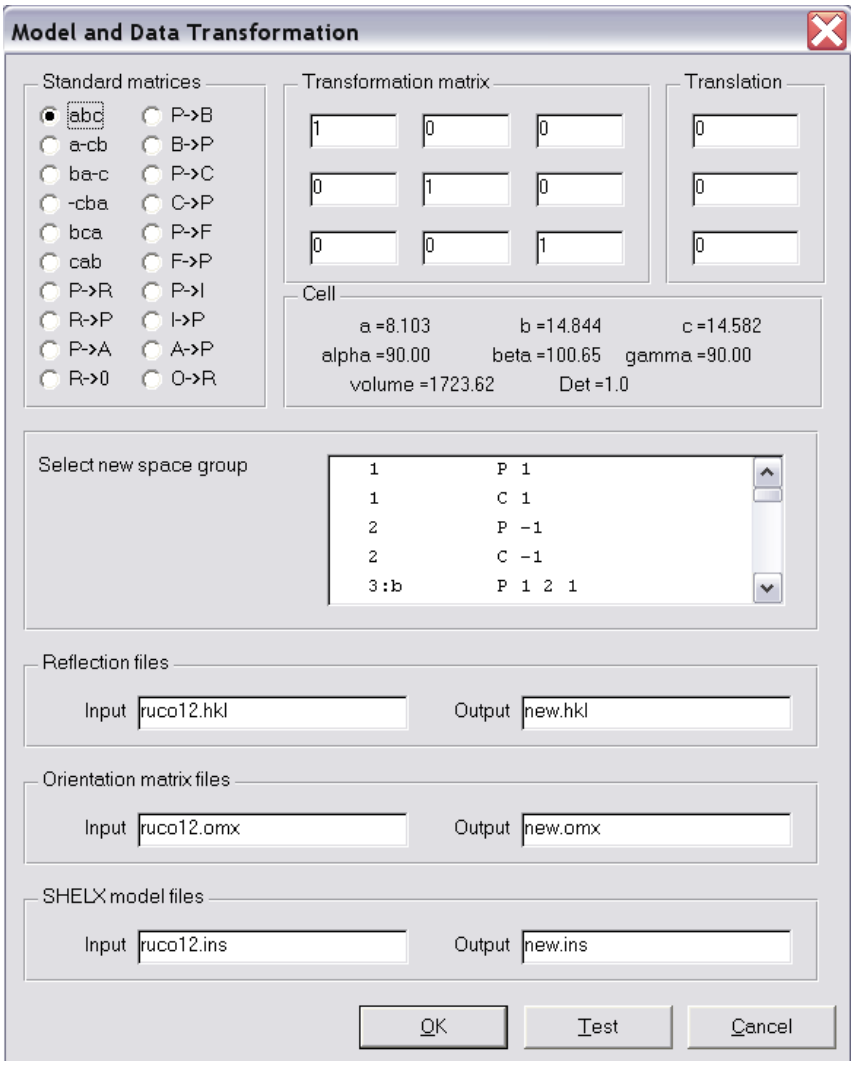
# Chapter 2.3

# TRANSFORM

## Transformation of current model

Louis J. Farrugia
Dept. of Chemistry
University of Glasgow
G4 9DS, Scotland, U.K.
email: louis@chem.gla.ac.uk

This program allows the user to transform the unit cell (with errors), the reflection indices (and if present the direction cosines), the atomic coordinates and the anisotropic thermal parameters according to a chosen transformation matrix R. A new model file NEW.INS and reflection file NEW.HKL are written. A number of standard transformation matrices are available, but the user can type in any matrix of choice. If the determinant of R is negative, the cell volume is reported as negative, indicating that the resultant cell is not right-handed. A new space group may be chosen from the list of 530 standard and non-standard settings. For an explanation of the various settings see below.




For instance, suppose a user has collected data and refined a structure in the non-standard orthorhombic space group *C*2cb, and wishes to transform the structure to the standard setting. Looking down the list of space groups in the TRANSFORM menu shows that *C*2cb is space group #41 with setting -cba. To perform the transformation, the user merely needs to select the -cba matrix button, and then

choose the standard setting for this spacegroup, which is *A*ba2. Clicking the OK button then gives transformed set (NEW.INS, NEW.HKL etc),which may be used for refinement without any further changes.
The TEST button allows the user to see the result of applying the matrix to the input cell.

## Conventions for space group settings in WinGX

| Monoclinic | unique axis b | | unique axis c | | unique axis a | |
|---|---|---|---|---|---|---|
| | abc | c-ba | abc | ba-c | abc | -acb |
| cell choice 1 | :b1 | :-b1 | :c1 | :-c1 | :a1 | :-a1 |
| 2 | :b2 | :-b2 | :c2 | :-c2 | :a2 | :-a2 |
| 3 | :b3 | :-b3 | :c3 | :-c3 | :a3 | :-a3 |

| | | |
|---|---|---|
| Orthorhombic | :ba-c | change of basis abc -> ba-c |
| | :1 | origin choice 1 |
| | :2ba-c | origin choice 2, change of basis abc -> ba-c |
| Tetragonal & Cubic | :1 | origin choice 1 |
| | :2 | origin choice 2 |
| Trigonal | :h | hexagonal axes |
| | :r | rhombohedral axes |