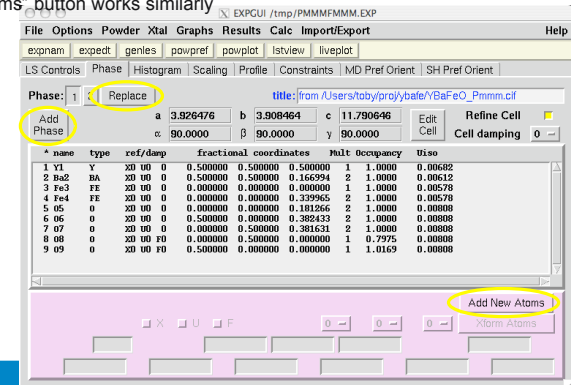


Problem 2: How do I get coordinates into GSAS without retyping them and other coordinate tricks

- EXPGUI makes importing coordinates easy
 - EXPGUI supports CIF (everything *should* write CIFs by now)
- EXPGUI can sort atoms in various ways
- EXPGUI can do Origin 1 to Origin 2 transforms
- Grouping atoms for easy access in GUI

2.0 EXPGUI makes importing coordinates easy

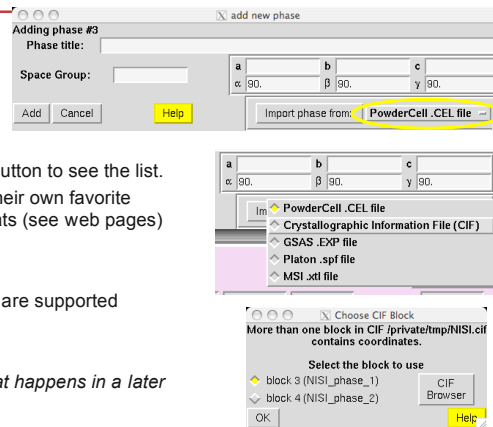
- “Replace Phase” or “Add Phase” button brings up add phase window
- “Add New Atoms” button works similarly



2.1 EXPGUI makes importing coordinates easy

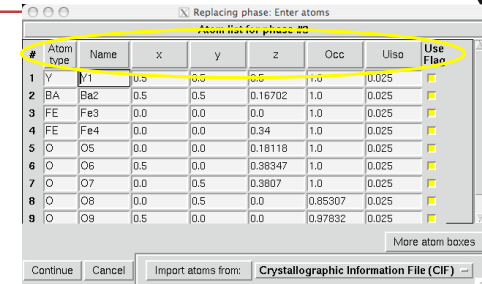
- Note that EXPGUI can read coordinates in several formats (including other GSAS .EXP files)
 - Click on the format button to see the list.
 - Users can add their own favorite coordinate formats (see web pages)
- FYI, multiblock CIFs are supported

We will see exactly what happens in a later part of the talk



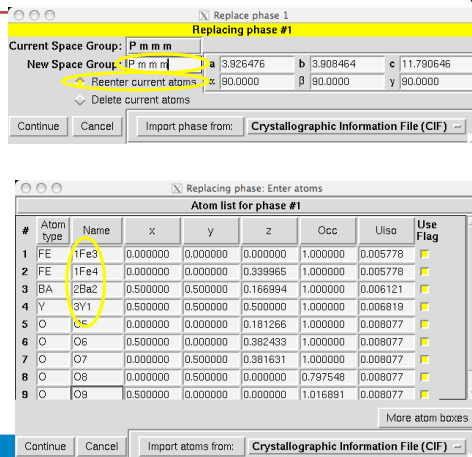
2.2 Sort atoms

- Sort buttons order atoms by type, label or by planes, etc.
- Remove unneeded atoms by unchecking the “use flag”



2.3 Replace phase can be used to reorder atoms

- Press "Replace" on Phase panel
- Reenter space group unchanged
- Select "Reenter current atoms" so that atoms already in phase show up in list
- Trick: add numbers in front of labels to force order.
 - Remove them before pressing continue.

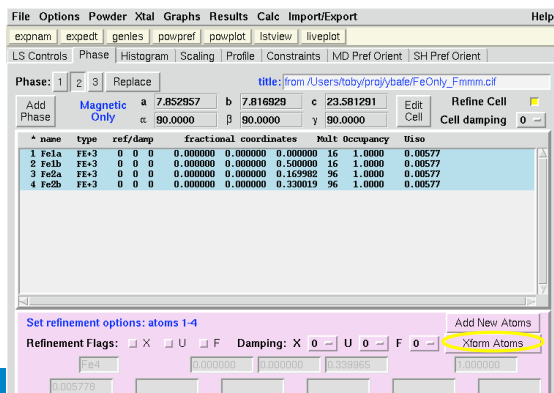


2.4A Transforming Origin 1 settings (Background)

- Have to pick an origin to define symmetry operations. For example:
 - (-x,-y,-z) is center of symmetry at origin
 - (-x,y,1/2+z) is a c-glide \perp a @ x=0
- Crystallographic convention: place origin @ highest symmetry location in unit cell
- Note: Computations are simplified when center of the symmetry is at the origin
- But, in 33 [centrosymmetric] space groups, a center of symmetry does not occur at the highest symmetry point in cell
- In these cases, the International Tables offer 2 choices:
 - Origin 1: origin @ highest symmetry point (not at center of symmetry)
 - Origin 2: center of symmetry at origin
- *Origin 2 is required for GSAS (and almost all crystallographic codes).*

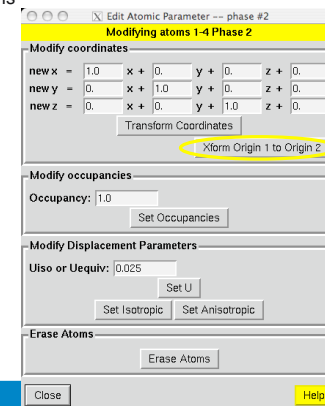
2.4B Transforming Origin 1 settings (How to)

- Select atoms to be transformed (usually all)
 - Shortcut: right mouse selects all atoms
- Press "Xform Atoms"



2.4C Transforming Origin 1 settings (How to)

- Select atoms to be transformed (usually all)
 - Shortcut: right mouse selects all atoms
- Press "Xform Atoms"
- If space group is one of 33 that has both origin 1 & origin 2 settings the "Xform Origin..." button will be active (standard axes only).
- Press the button and the selected atoms will be translated to shift the origin
 - *(in version 1.78 of EXPGUI or later, atom multiplicities are then updated)*



2.5 Atoms can be viewed sorted in different orders

- Use Options/Sort atoms by
- or click on atoms header to sort
 - Sort order is shown by * in header

File Options Powder Xtal Graphs Results Calc Import/Export

expnam | expedt | genies | powpref | powplot | lstview | liveplot

LS Controls | Phase | Histogram | Scaling | Profile | Constraints | MD Pref Orient | SH Pref Orient

Phase: 1 2 Replace title: from /Users/abey/proj/ybafey/BaFeO_Pmnm.cif

Add Phase a 3.926476 b 3.908464 c 11.790647 Edit Refine Cell
 c 90.0000 β 90.0000 γ 90.0000 Cell Cell damping 0

name	type	ref/damp	fractional coordinates (x*)			alt	occupancy	diso
3 Fe3	FE	2X 00 0	0.000000	0.000000	0.000000	*	1.0000	0.00576
8 O8	O	2X 00 F0	0.000000	0.500000	0.000000		1	0.7975
9 O9	O	2X 00 F0	0.500000	0.000000	0.000000		1	1.0163
2 Ba2	BA	2X 00 0	0.500000	0.500000	0.166993		2	1.0000
5 O5	O	2X 00 0	0.000000	0.000000	0.101527		2	1.0000
4 Fe4	FE	2X 00 0	0.000000	0.000000	0.339965		2	1.0000
7 O7	O	2X 00 0	0.000000	0.500000	0.381632		2	1.0000
6 O6	O	2X 00 0	0.500000	0.000000	0.382413		2	1.0000
1 Y1	Y	2X 00 0	0.500000	0.500000	0.500000		1	1.0000

Add New Atoms 40