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

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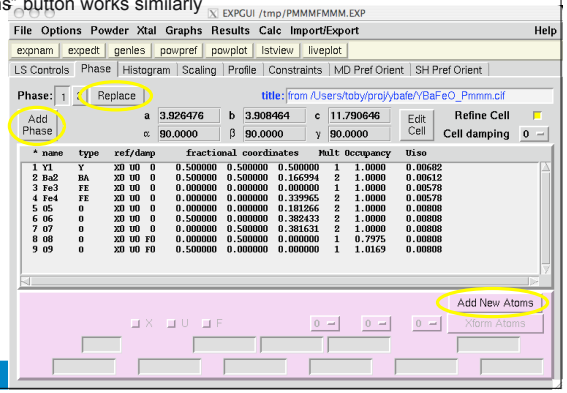
2.0 EXPGUI makes importing coordinates easy

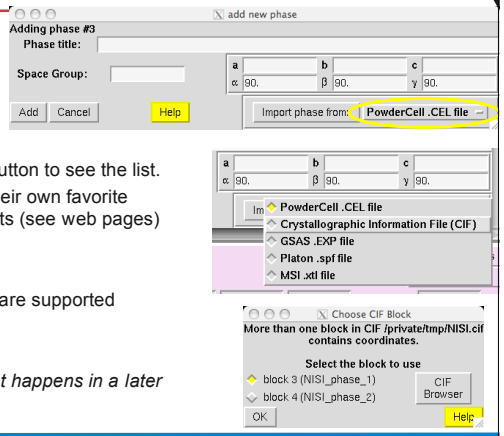
- "Replace Phase" or "Add Phase" button brings up add phase window
- "Add New Atoms" button works similarly



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



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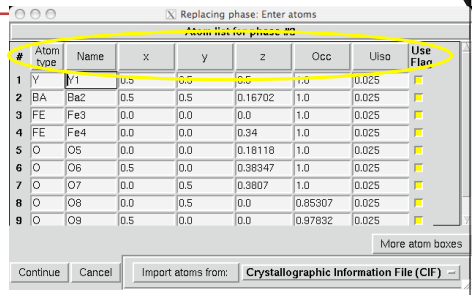
2.2 Sort atoms

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



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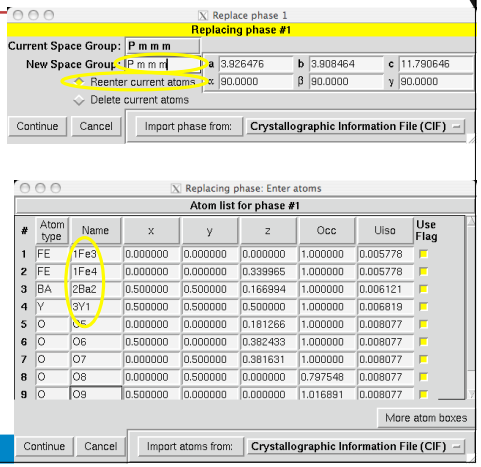
2.3 Replace phase can be used to reorder atoms

- 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.

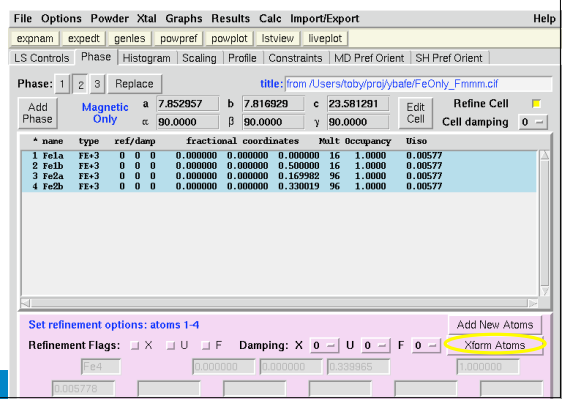


2.4A Transforming Origin 1 settings (Background)

- 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 ⊥ *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).*

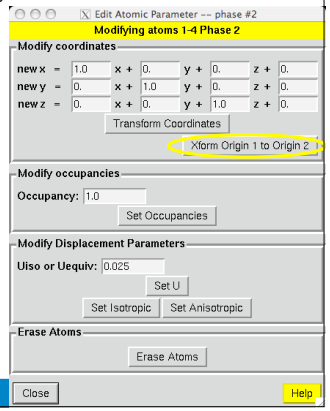
2.4B Transforming Origin 1 settings (How to)

- 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