Loading a .txt or .cif crystal file

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- 3 kinds kinds of crystal files

1. jems .txt files (default). Many are found in folders jemsData/cubic, jemsData/hexagonal...

2. ICSD or AMS .cif files.

3. Selectable crystal structures.

1.1 Opening .txt crystal structure

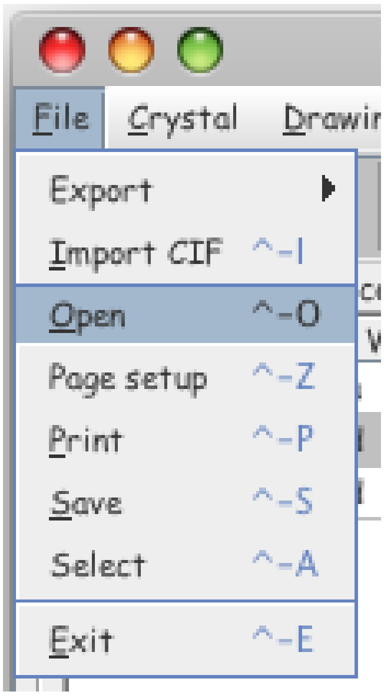

Figure 1: **File** → **Open**.

Naturally a particular crystal structure is usually not found in the jems set of crystal structures. You have to look for it either in the ICSD or AMS data bases or to define it using published data.

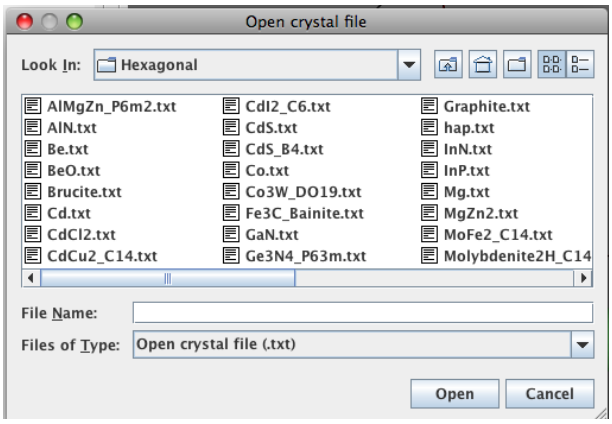

Figure 2: Selecting a crystal file.

1.2 Importing a .cif crystal structure

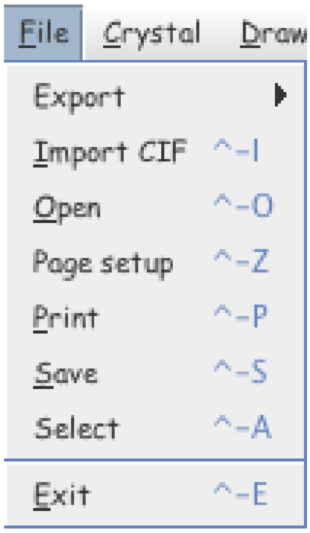

Figure 3: **File** → **Import**.

A **.cif** file can contains up to 100 different crystal structures. A particular one can be selected using the **CIF dataset selector dialogue**.

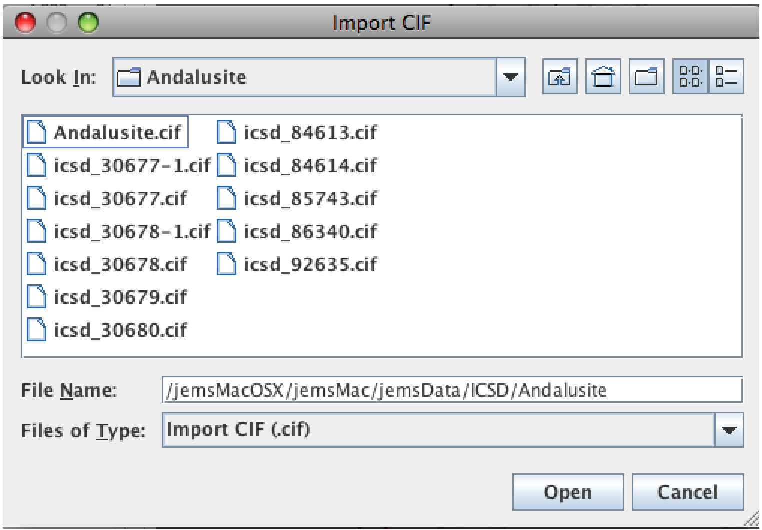

Figure 4: Selecting a **.cif** file.

1.3 CIF dataset selector dialogue

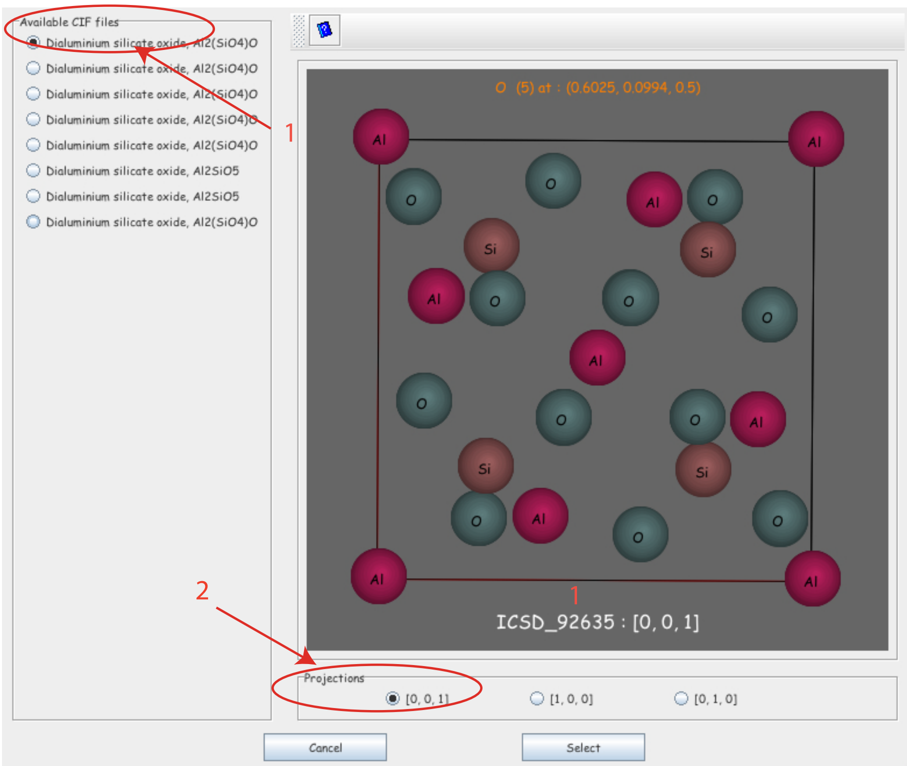

Figure 5: Selecting a **.cif** crystal structure, (1) crystal selection & (2) projected structure.

1.4 Checking the .cif structure

It is necessary to check the .cif structure since it may happen that its space-group description is non-standard. By default the .cif structure can't be saved (Fig. 6). The jems console (Fig. 7) displays some of the properties of the .cif file. Locate the space-group description and verify that it is recognized by jems.

Figure 6: The space-group must be confirmed before saving the crystal structure as a **.txt** jems cystal structure. The **File**→**Save** or **Save icon** (1) are unavailable.

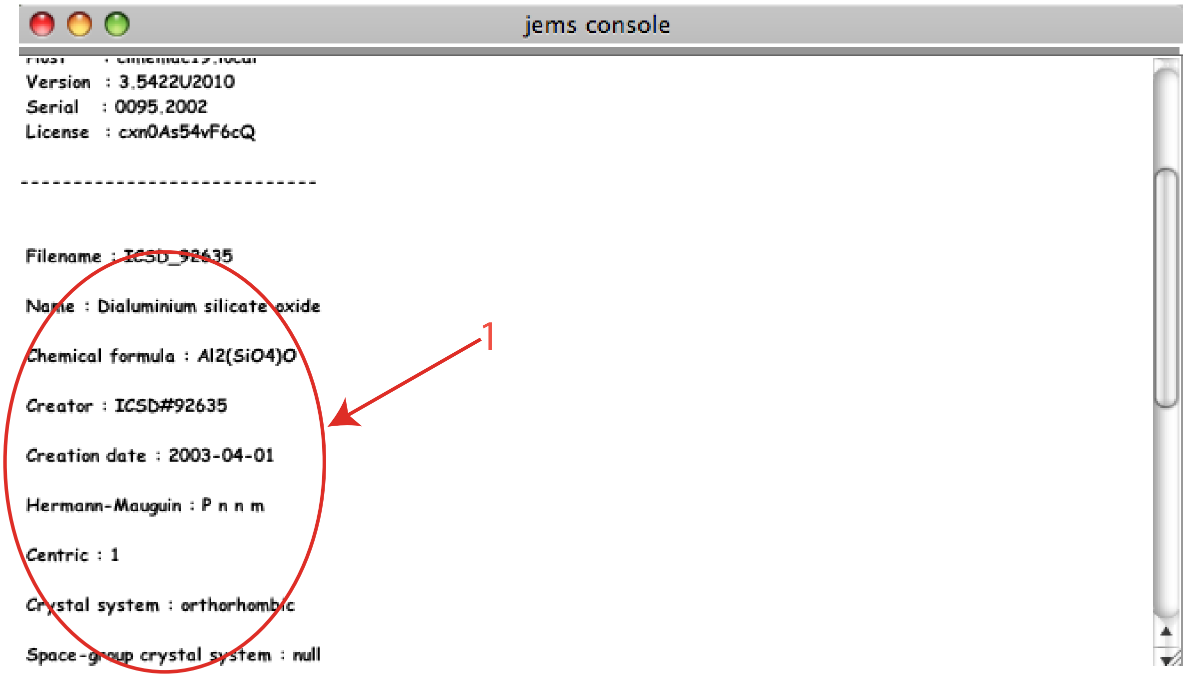

Figure 7: The jems console displays the crystal system and space-group read from the .cif structure.

1.5 Checking the space-group

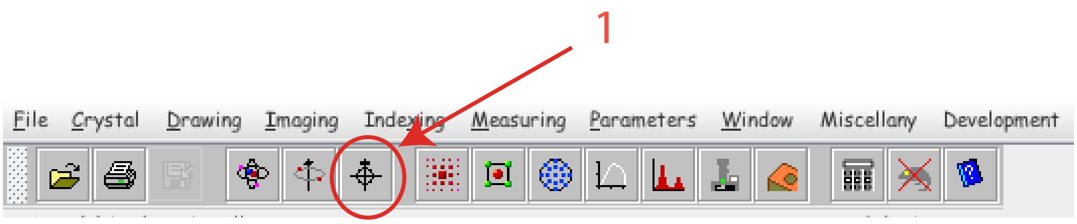

Figure 8: *Open the space-group dialogue using either **Crystal→System→Space-group** or the **Space-group icon** (1).*

1.6 Space-group dialogue

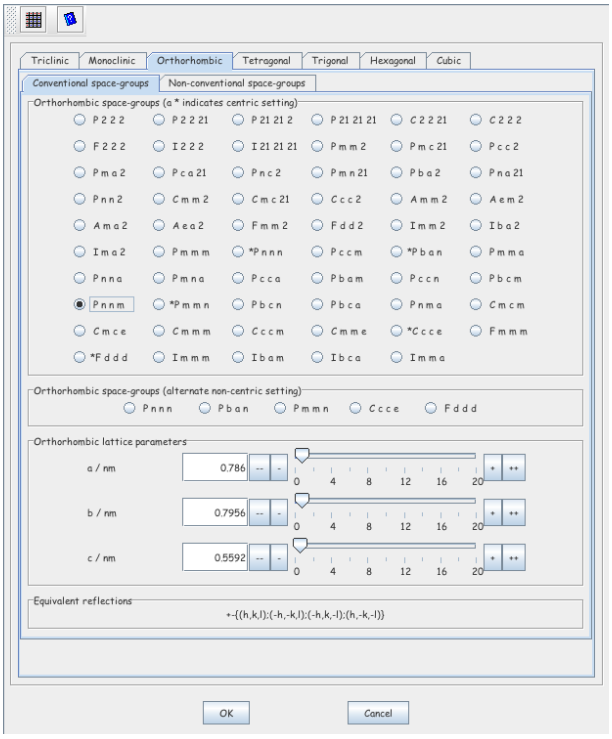

Figure 9: *Select the proper crystal system and the space-group (even when it is already selected). This will make the* ***File→Save*** *or* ***Save icon*** *(1) available to save the* ***.cif*** *structure as a* ***.txt*** *one.*

1.7 Unconventional space groups: RPS code dialogue

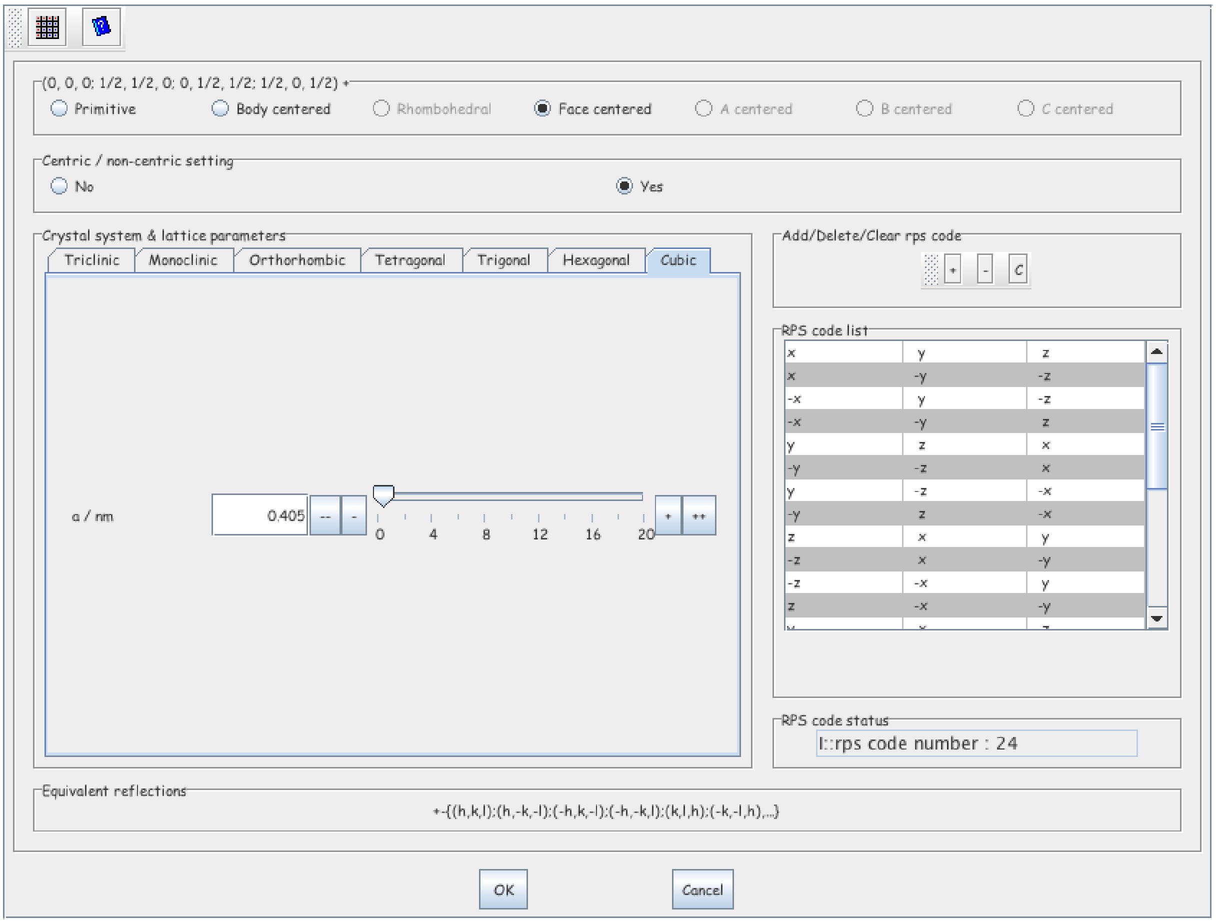

Figure 10: *For unconventional space-groups* use the *RPS code* dialogue to define the symmetry operations.

1.8 Selecting a crystal structure: File→Select

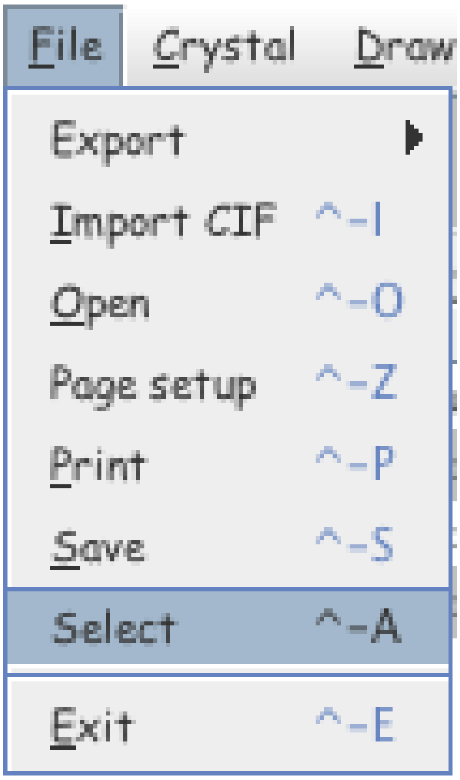

Figure 11: *Selecting a crystal structure among a set 42 predefined ones.*

1.9 Select crystal dialog

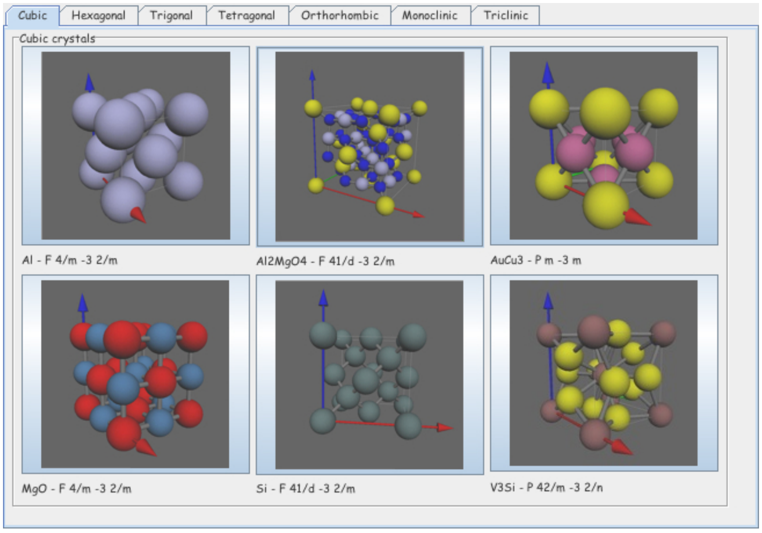

Figure 12: *The 42 defined crystals are grouped in 7 crystal systems.*