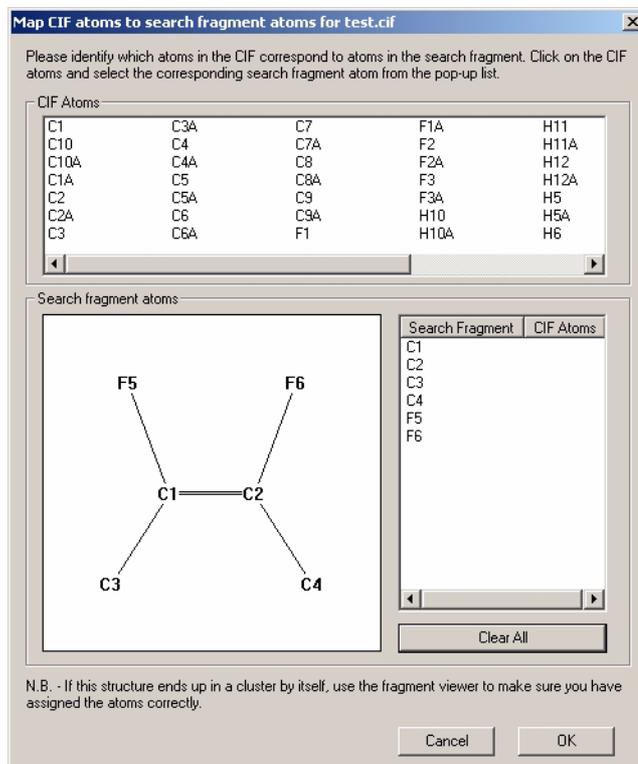


Including your own CIFs

Input:

In *dSNAP* it is possible to include new structures that are not yet present in the database and to compare these against related structures returned from a CSD search. To do this click the *Select CIFs to include in calculation* checkbox at the bottom of the input window. Once all other details have been provided as normal, clicking *OK* will open a new input window that asks for the location of the CIFs to be included. Multiple CIFs can be selected at the same time, but these must all be in the same folder so they can be selected simultaneously. Clicking *OK* opens a new window:



As the included CIF is separate from the returned database entries, *dSNAP* has no information on how to compare them properly. The user must provide information on which atoms in the CIF correspond to atoms of the search fragment.

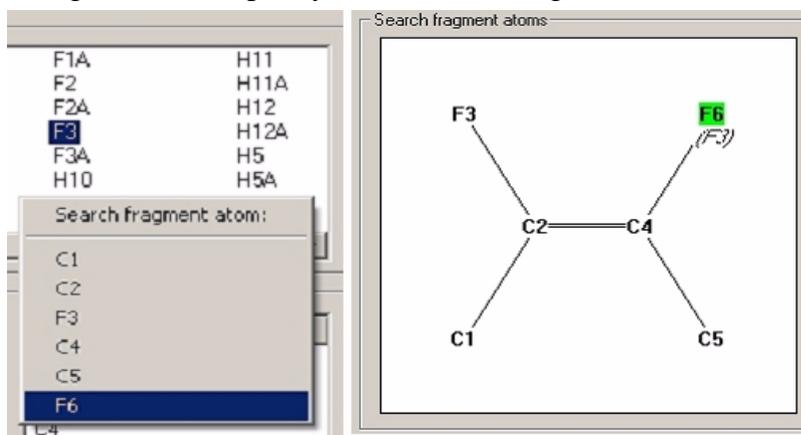
To do this there are three sections in the window. The first section, *CIF atoms*, gives a list of **all** the atoms in the CIF. Only some of these will be relevant to *dSNAP*. Below that there is *Search Fragment atoms* section which displays the original fragment as a 2D diagram. Finally there is a section where all the search fragment atoms are listed in a table, with a column for all of the corresponding CIF atoms.

Nomenclature:

It is important to note that assignment of search fragment atoms must be done by viewing the CIF structure in a viewing program like *Mercury* to establish which CIF-labelled atoms are part of the fragment.

Assignment:

Once the user has determined which CIF atoms are part of the fragment this information must be provided to *dSNAP*. For example if CIF atom F3 corresponded to search fragment atom F6, then this information would be specified by clicking on the atom F3 in the *CIF atoms* section of the window. This tells *dSNAP* that F3 is part of the fragment. Once this is done a pull down menu appears asking where in the fragment this atom belongs by asking the user to specify which search fragment atom F3 corresponds to:



Selecting F6 from this menu tells *dSNAP* that CIF atom F3 corresponds to search fragment atom F6. With this done the other two sections change. The assigned atom (F6) now has the corresponding atom (F3) written in italics below. The corresponding atom also appears listed on the table. The process must then be repeated for every search fragment atom on the diagram until the whole fragment is assigned. If multiple CIFs have been included then each CIF has to be assigned in turn. It is possible to import more than one fragment from a CIF.

Results display:

Once analysis is complete the included fragment can be easily identified in the results display as it is labelled with a + followed by the name of the parent CIF.



If the included fragment is assigned in a cluster of its own and is not similar to any of the other clusters then this may suggest that a mistake has been made in the assignment. If the included fragment does not look sensible in the 3D fragment viewer then this is another sign that the assignment may be wrong. A more detailed description including your own CIFs is given in the program manual.
