

Nomenclature in dSNAP

Fragment:

The term *fragment* refers to the part of the molecule matching the database search query. This is only the part of the molecule that was searched for, not the structure as a whole.

Hit/Structure:

The terms *structure* and *hit* refer to the entire molecule that was returned from the database. This includes the search fragment, but is not limited to it.

Consequences:

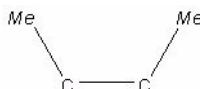
When faced with a structure that has matched the conditions of the database search, the *fragment* is only the section of the structure that matches the requirements specified in the search.

A single hit structure can therefore contain one or more fragments. When multiple fragments are observed for a hit, these fragments frequently lie in chemically distinct environments and thus may exhibit significantly different geometries. They are therefore treated independently.

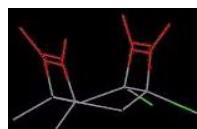
In such circumstances the software will suffix the individual refcode with an integer consistent with the order in which the fragment is output. This allows reference back to the correct fragment when studying the structures within the *ConQuest* search program.

Example:

A database search for the a carbon-carbon double bond with a methyl substituent on each carbon was performed.



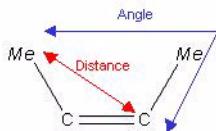
This is the search fragment. One of the hit structures returned by the search had the refcode HAFTEN. This hit has two instances of the fragment that was searched for, highlighted on the structure below in red.



Within dSNAP these will be labelled separately (in this case HAFTEN_01 and HAFTEN_02).

Variables:

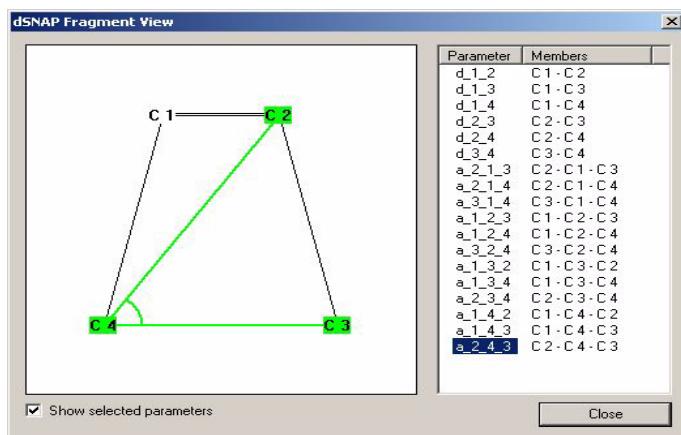
Variables are the geometric information defining the structure of the fragment being investigated. These include both angles between and distances between all atoms, not just the bonded distances and angles. Using the same search fragment as an example:



All interatomic distances and angles are considered. A single fragment will have many variables and the complete list of distances and angles completely defines a fragment.

Numbering scheme:

The variables are numbered in dSNAP according to the atoms that make up that variable. For example d_{1_4} represents the distance between atom 1 and 4 where $a_{2_4_3}$ is the angle between atoms 2, 4 and 3, with atom 4 at the vertex. The atoms are numbered according to the order in which they were drawn in the original database search.



To help in relating these names back to the actual variables they represent there is a 2D fragment viewer that can be accessed at any time from the results screen by using the F2 function key or selecting *Show Fragment Variables in 2D Viewer...* from the *Tools* menu. Clicking on any name on the list will highlight that variable on the 2D fragment diagram.