

MKS 04-0002

Editing Molecular Structure

ρ	ΔH_v	T_c	ΔG
η_l	D_{ab}	γ_{12}	Tf_{cc}
δ_h	P_{vp}	σ	C_p
T_b	λ_v	S_f	P_c

Molecular Knowledge Systems

info@molecularknowledge.com

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Helpful Prerequisites

Recommended Courses

The following courses can be found on [MKS's Training Webpage](#):

- 04-0001: Basic and common operations

Additional Resources

1. Estimating the Properties of Chemicals ([video](#))
2. Estimating the Properties of Mixtures ([video](#))

Topics Presented

Editing Molecular Structure

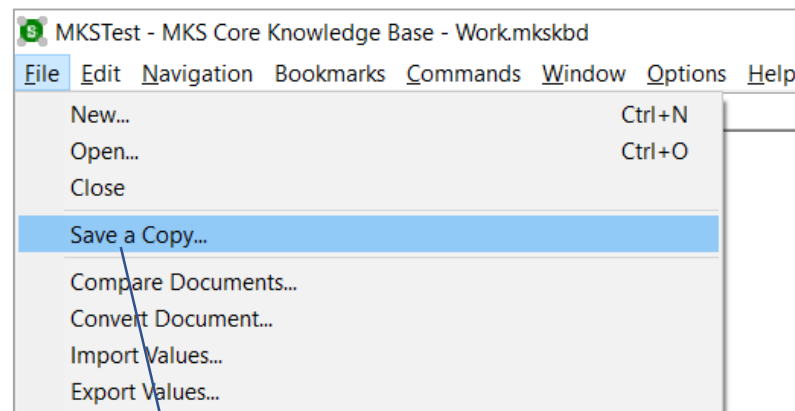
The molecular structure of chemicals and groups is essential for estimating physical properties and designing chemical products. Cranium and Synapse provide molecular structure editors that enable quick and easy entry.

- Molecular Structures
- Editing Atoms and Bonds
- Standard Structures
- Importing Structures
- Groups and Free Atoms
- Non-subtractable Atoms
- Utilizing Groups

Create a Working Copy

The actions taught in this course will permanently change the contents of the database file being used. It is highly recommended that a 'working copy' of a knowledge base be used.

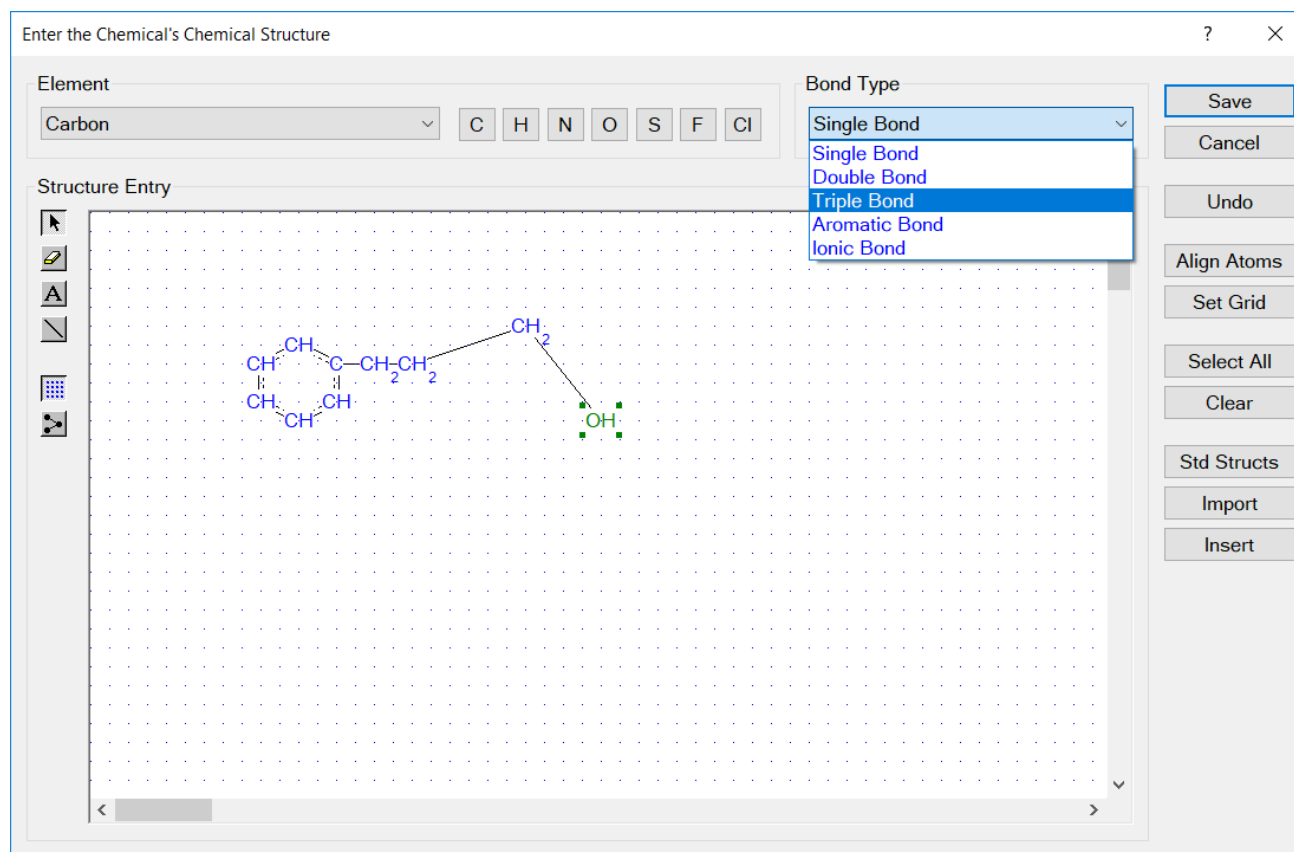
To create a working copy, open a knowledge base and then select the Save a Copy command from the File menu. Enter a name for the working copy. Open and use the working copy once the copy operation is complete.



Save a copy of a knowledge base to be used for practice and experimentation.

Molecular Structure

Molecular structures are represented as simple atom-bond connectivity graphs. Editing a structure typically involves placing atoms on the editing pane and then connecting them with bonds.

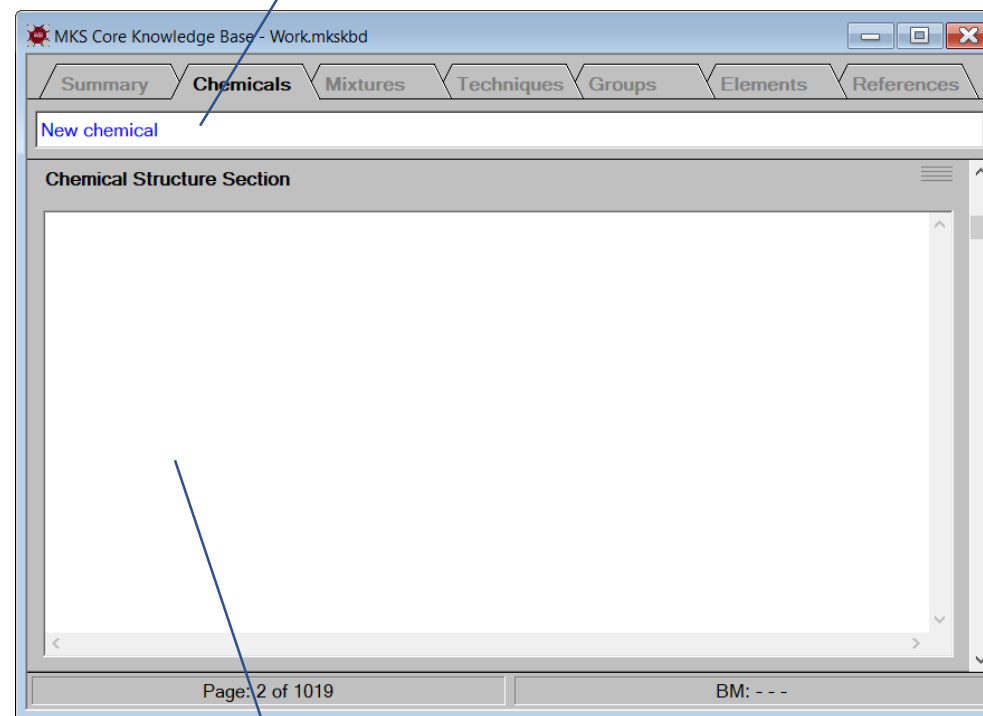


Editing Atoms and Bonds

Exercise – In a working copy of a knowledge base:

1. Add a new chemical (use the Add New Page command or the “+” toolbar button)
2. Assign a name to the chemical
3. Scroll to the Chemical Structure section
4. Click the left mouse button on the field’s large edit control

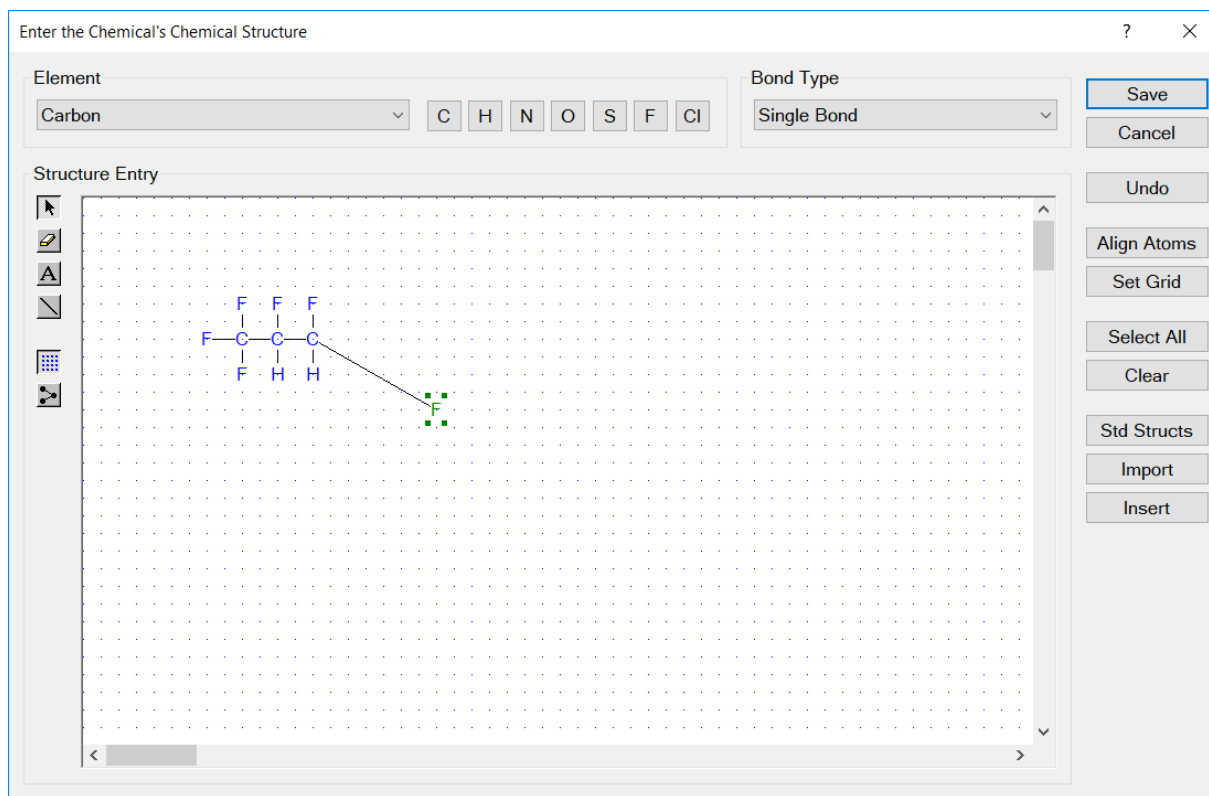
Click the left mouse button on the identifier field and enter a name for the new chemical



Molecular structure field

Editing Atoms and Bonds

Exercise – Click the left mouse button in the molecular structure field. The application will activate the chemical structure editor dialog.



Molecular Structure Editor Dialog

Atom selection controls

Bond selection control

Tools palette

Editor pane

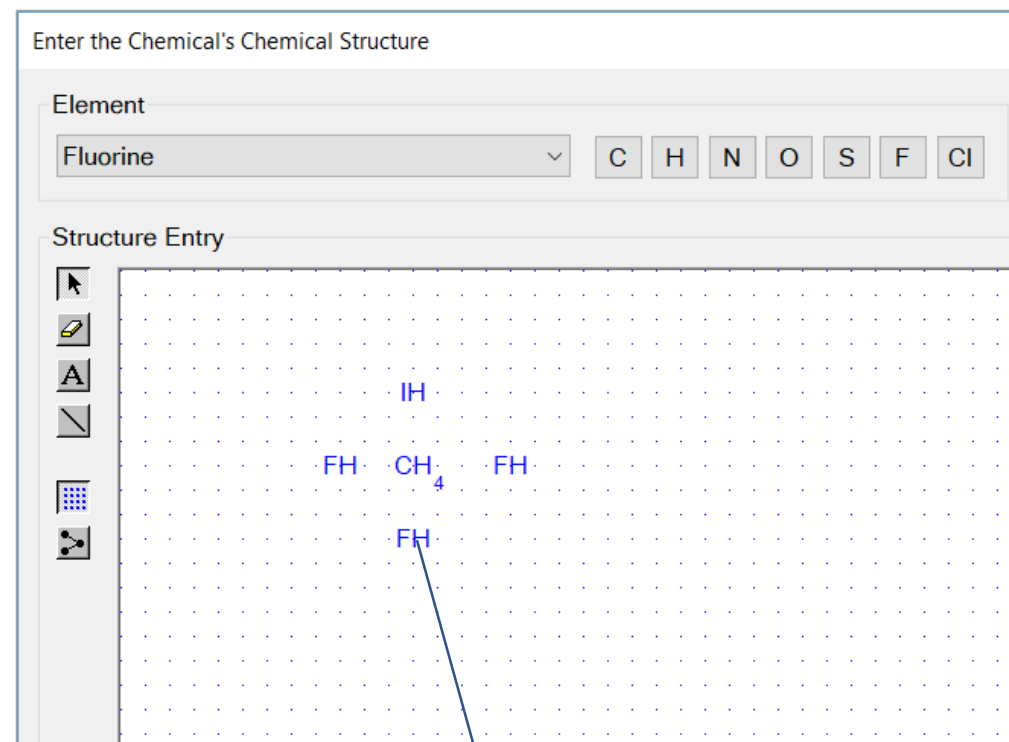
Command buttons

The image shows a software dialog titled "Enter the Chemical's Chemical Structure". At the top, there are two dropdown menus: "Element" (set to "Carbon") and "Bond Type" (set to "Single Bond"). Below these are buttons for elements: C, H, N, O, S, F, and Cl. The main area is a "Structure Entry" grid with a chemical structure of 1,1,1-trifluoroethane (F₃CH-CH₃) drawn on it. A new fluorine atom is being added to the right of the structure. On the left is a "Tools palette" with icons for selection, deletion, and drawing. On the right is a vertical stack of "Command buttons": Save, Cancel, Undo, Align Atoms, Set Grid, Select All, Clear, Std Structs, Import, and Insert.

Editing Atoms and Bonds

Exercise – Enter the structure for trifluoroiodomethane:

1. Press the Atom tool button
2. Select Carbon from Elements menu
3. Click the left mouse button in the editor pane
4. Repeat this process adding one iodine atom and three fluorine atoms
5. Use the eraser tool to remove any unwanted atoms

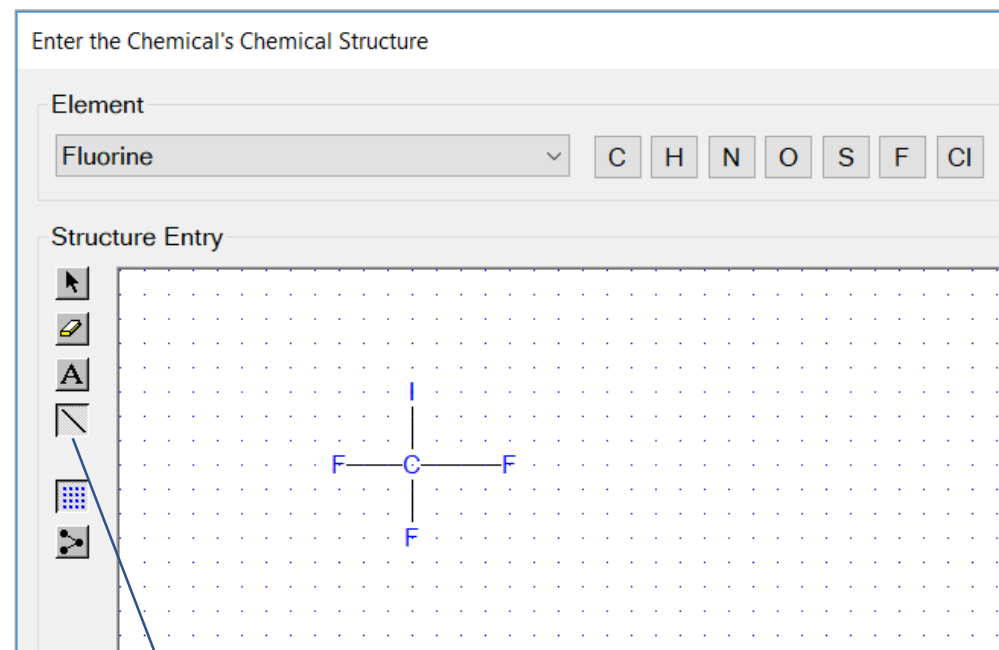


Atoms added to editor pane
(hydrogen automatically added)

Editing Atoms and Bonds

Exercise – Enter the structure for trifluoroiodomethane:

1. Press the Bond tool button
2. Click the left mouse button on the Carbon atom and then on the iodine atom
3. Repeat the process for each of the fluorine atoms
4. All atom should now be bonded
5. Use the eraser tool to remove any unwanted bonds



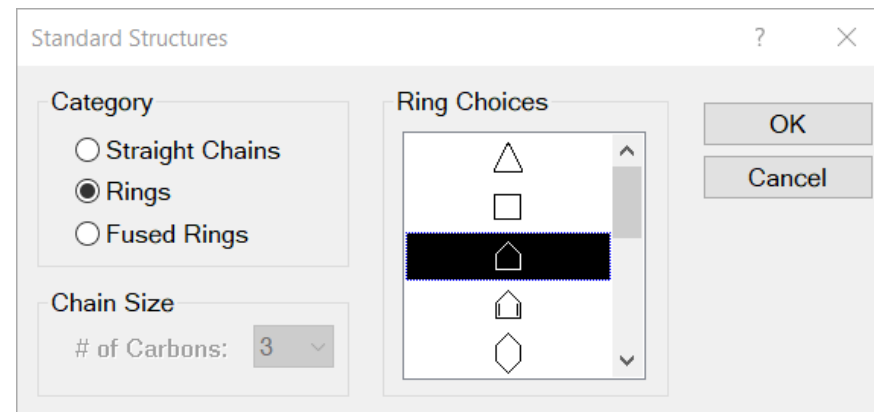
Use the bond tool to connect all atoms.
(The current Bond Type is used to create bonds.)

Standard Structures

The structure editor contains a selection of standard structures that can be used as a starting point for new structures.

Exercise – Enter the structure for tetrahydrofuran:

1. Press the Std Structs button on the structure editor dialog
2. Select the Rings category
3. Select the cyclopentane ring
4. Press the OK button



Standard Structures

Exercise – Enter the structure for tetrahydrofuran:

1. Press the selection tool button
2. Double-click the left mouse button on one of the carbon atoms in the cyclopentane ring
3. Select Oxygen from the activated Atoms dialog
4. Press the OK button

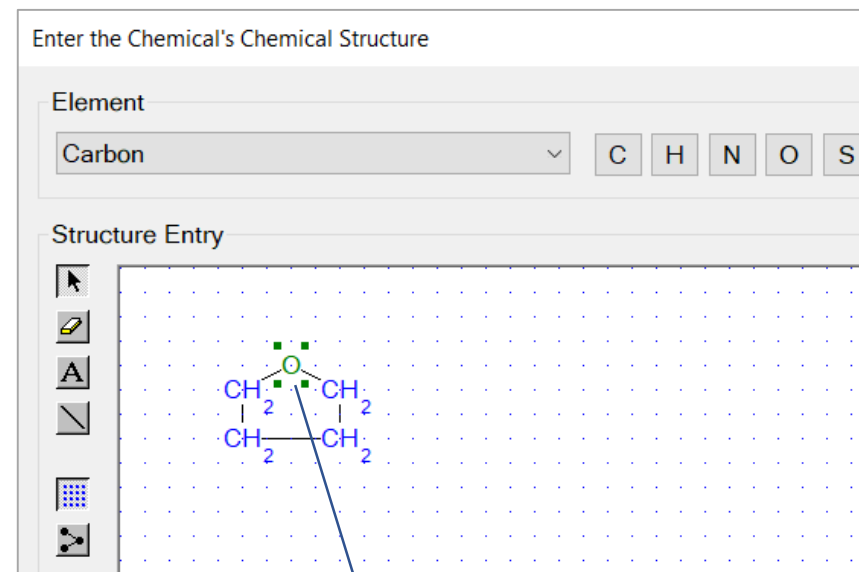
The screenshot shows a software window titled "Enter the Chemical's Chemical Structure". At the top, there is an "Element" dropdown menu set to "Carbon" and a row of buttons for "C", "H", "N", "O", "S", "F", and "Cl". To the right, a "Bond Type" dropdown is set to "Single Bond". Below this is the "Structure Entry" area, which contains a grid of dots and a partially drawn cyclopentane ring with five carbon atoms labeled "CH₂". A dialog box titled "Edit Atom Attributes (Modified)" is open over the structure. It has an "Element" dropdown menu currently showing "Oxygen", a "Subtractable" dropdown menu set to "Yes", and "OK" and "Cancel" buttons. A blue arrow points from the text below to the "Oxygen" dropdown menu.

Select Oxygen as the replacement element

Standard Structures

The selected oxygen element replaces the carbon atom in the cyclopentane ring. The resulting molecular structure is not tetrahydrofuran.

Very often it is quicker to start with a standard structure and modify it then to build a structure atom by atom.



Oxygen has replaced Carbon

Importing Structures

A mol file is a standard file format for describing a chemical's molecular structure.

The Import button is used to import a mol file's structure into the edit pane.

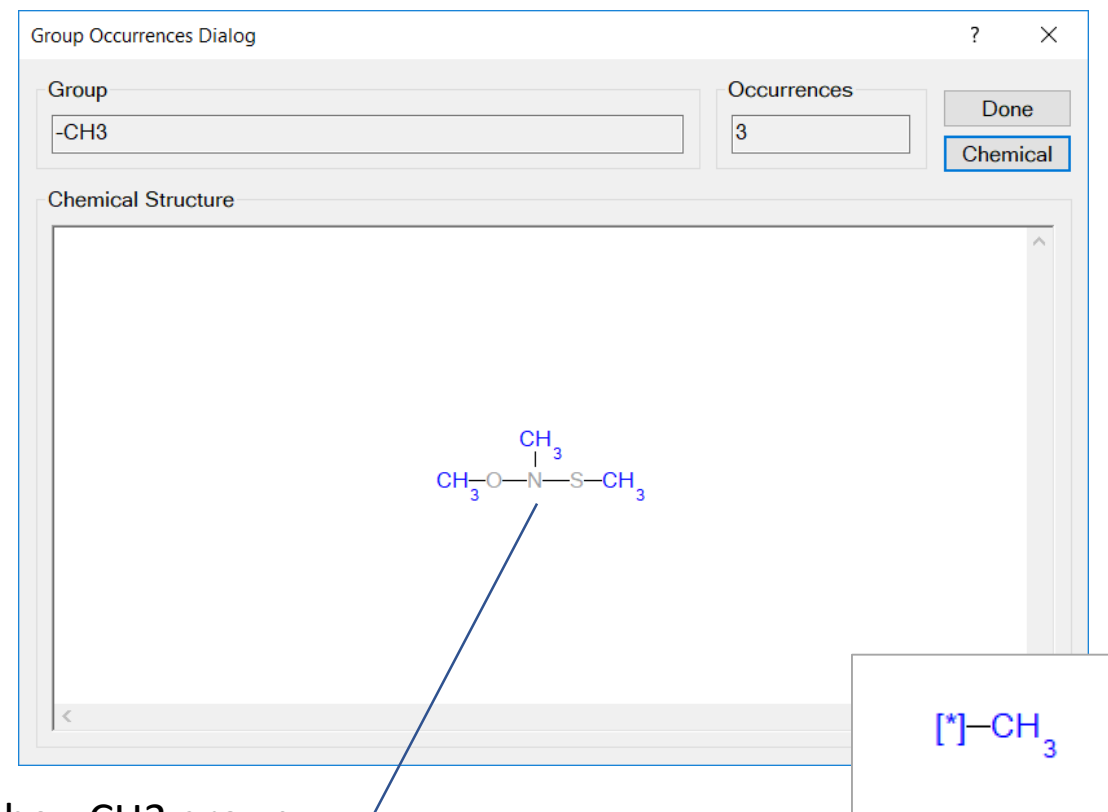
```
MKS      1204180118
Generated by Synapse:Version 2.3, Core 314
 5  5  0  0  0  0          999 v2000
 14.6000 -11.4000  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 14.6000 -14.8000  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 17.6000  -9.8000  0.0000 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 20.6000 -14.8000  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 20.6000 -11.4000  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 2  1  1  0  0  0
 1  3  1  0  0  0
 4  2  1  0  0  0
 3  5  1  0  0  0
 5  4  1  0  0  0
M  END
```

A mol file is a standard format for exchanging molecular structures

Groups and Free Atoms

Groups are molecular structures used for substructure search and physical property estimation. A group typically contains a special atom called a 'free atom'.

A free atom is denoted by the symbol '*'. When performing a structure match, a free atom can match any other atom.



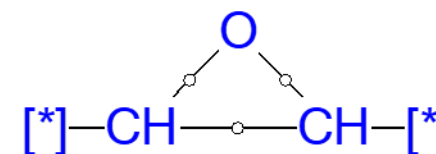
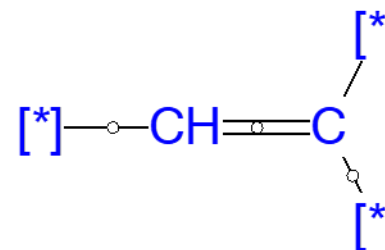
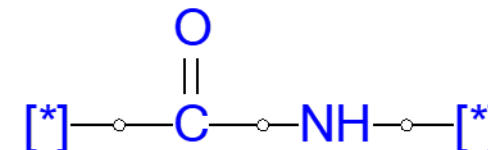
The free atom in the -CH3 group matches oxygen, nitrogen and sulfur

Groups and Free Atoms

When entering groups is also very important to specify “ring structure” by explicitly using ring bonds and aromatic bonds.

Ring bonds are denoted by small circles located in the center of the bond.

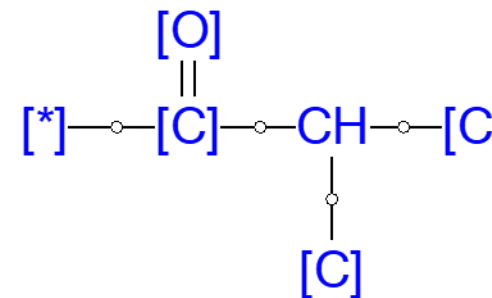
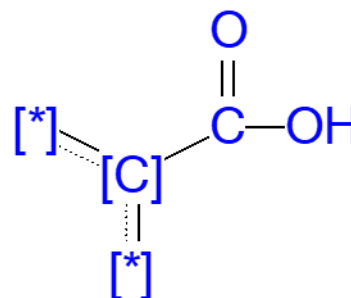
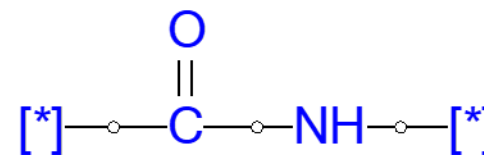
Groups must use explicit ring bonds for substructure matching



Non-subtractable Atoms

The brackets, i.e., “[” and “]” around the free atom’s symbol denotes that the atom is non-subtractable. When a substructure match is made, a groups subtractable atoms are removed for the next match. If an atom is non-subtractable, then it is not removed.

Other atoms, besides free atoms, can be marked as non-subtractable.



Utilizing Groups

The Groups chapter contains several commands that will search for a group in a technique, a specific chemical or in all the chemicals in the current knowledge base. This is a very useful tool for compiling chemicals having similar chemical classes.

Chemicals Containing this Group

Group
-I

10 Chemicals Found

- 1-Iodobutane
- 1-Iodoheptafluoropropane
- Candidate Chemical 001
- Diiodomethane
- Ethyl iodide
- Hydrogen iodide
- Iodine
- Iodobenzene
- Methyl iodide
- Trifluoroiodomethane

Chemical Structure

Chemical structure of Diiodomethane (I-CH₂-I) is displayed.

Buttons: Done, Go To, Bookmark, Detail

All chemicals containing a -I group were compiled.

Questions or Comments

info@molecularknowledge.com

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Thank You