



InfoChems'

Structure Input and Search Documentation

Version 1.2

November 2005

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Please note:

This manual will be upgraded continuously. Please visit our homepage www.infochem.de to download the latest version of this manual.

Version 1.2, Summer 2005

- Description of InfoChems' Editor – implemented.

Autumn 2005

- Description of Use in ChemDraw
- Description of Use in Enso Applet

Winter 2005

- Search strategies

1. Query Features on a molecule

A query feature on a molecule is a definition or a restriction on an atom or a bond that specifies the retrieval of certain types of molecule records from a database.

1.1 Atom query features

* Allow or exclude specific atoms

ANY ATOM


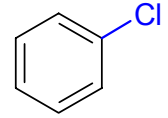
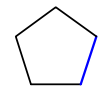
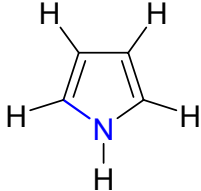
Format

A

Description

To allow any atom except hydrogen at a specific position, choose A as Atom Symbol.

Example

Query	Example of Molecules retrieved
/A	
	
	
	

Use in ISIS/Draw

1. Select an atom.
2. Double-click the selected atom.
3. Drop down the Atom Symbol box.
4. Select Atom Symbol "A"
5. Click ok.

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Open the P-Table
5. Select Atom Symbol "A"
6. Click ok.

Q-ATOM


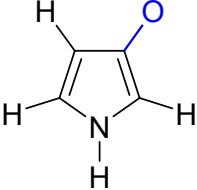
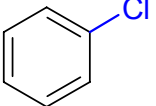
Format

Q

Description

To allow any atom *except hydrogen or carbon* at a specific position, choose Q as Atom Symbol.

Example

Query	Example of Molecules retrieved
Q	
	
	

Use in ISIS/Draw

1. Select an atom.
2. Double-click the selected atom.
3. Drop down the Atom Symbol box.
4. Select Atom Symbol "Q"
5. Click ok.

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Open the P-Table
5. Select Atom Symbol "Q"
6. Click ok.

LIST

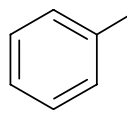
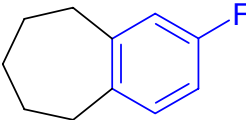
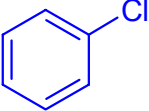
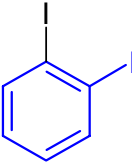
Format

[A,B,C]

Description

To allow one atom from a list of atoms of your choice at a specific position, choose List as Atom Symbol.

Example

Query	Example of Molecules retrieved
 [F,Cl,Br,I]	
	
	

Use in ISIS/Draw

1. Select an atom.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Drop down the Atom Symbol box.
5. Select "List..." to open the Periodic Table.
6. Click an atom symbol to add it to your list of allowed atoms. (Click an atom symbol a second time to remove it.)
7. Click OK.

Use in ChemDraw

Use in InfoChem's Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Select "List" to open the Periodic Table.
5. Click an atom symbol to add it to your list of allowed atoms. (Click an atom symbol a second time to remove it)
6. Click ok.

NOTLIST

Format

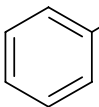
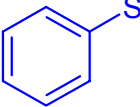
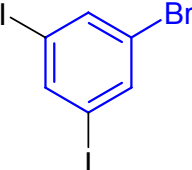
NOT[A,B,C]

Description

To exclude both hydrogens and any atom on your list at that position, choose Not List.

(This query feature also specifies no hydrogen atoms.)

Example

Query	Example of Molecules retrieved
 NOT [C,N,O]	
	

Use in ISIS/Draw

1. Select an atom.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Drop down the Atom Symbol box.
5. Select "Not List..." to open the Periodic Table.
6. Click an atom symbol to add it to your list of excluded atoms. (Click an atom symbol a second time to remove it.)
7. Click OK.

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Select "Not List" to open the Periodic Table.
5. Click an atom symbol to add it to your list of allowed atoms. (Click an atom symbol a second time to remove it.)
6. Click ok.

* Specify explicit hydrogen atoms

Use the following procedure to draw an explicit hydrogen on an existing atom.

Format

-H

Description

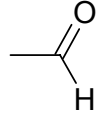
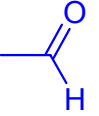
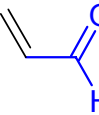
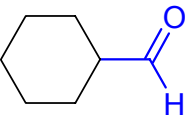
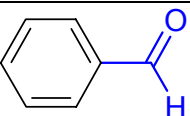
To allow solely hydrogen atoms at specified positions in the structures retrieved, you must draw explicit hydrogens in your search query. You can also draw explicit hydrogens to block substitutions at specific positions in the structures retrieved.

Note: implicit hydrogens are not recognized in a search query, even if you show them. If you want to create a search query that allows solely hydrogen atoms at specified positions in the structures retrieved, you must draw explicit hydrogens.

EXPLICIT HYDROGEN

An explicit hydrogen is a hydrogen that is attached to an atom by a visible bond.

Example

Query	Example of Molecules retrieved
	
	
	
	

Use in ISIS/Draw

1. Select the Drawing Tool "Single Bond"
2. Draw a single Bond from the atom, which you want to have a Hydrogen Atom attached.
3. Select the atom you want to be defined as the explicit hydrogen.
4. Choose Object > Edit Atom.
5. Drop down the Atom Symbol box.
6. Select Atom Symbol "H".
7. Click OK.

Use in InfoChems' Editor

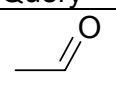
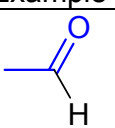
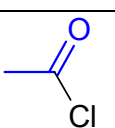
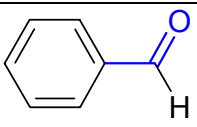
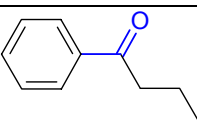
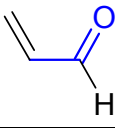
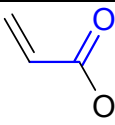
1. Select the Drawing Tool "Single Bond"
2. Draw a single Bond from the atom, which you want to have a Hydrogen Atom attached.
3. Select the atom you want to be defined as the explicit hydrogen.
7. Open the context menu "Edit Atom" to open the P-Table
4. Select Atom Symbol "H".
5. Click OK.

IMPLICIT HYDROGEN – no valid query feature!! -

An implicit hydrogen is a hydrogen that is either assumed to be present (invisible) or attached to an atom by an invisible bond.

Note: implicit hydrogens are not recognized in a search query, even if you show them. If you want to create a search query that allows solely hydrogen atoms at specified positions in the structures retrieved, you must draw explicit hydrogens.

Example

Query	Example of Molecules retrieved
 Hydrogen Display OFF	
$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$ Hydrogen Display ON	
	
	
	
	

* Prohibit hydrogens on an atom

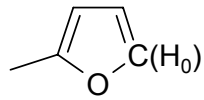
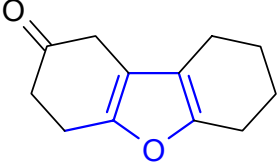
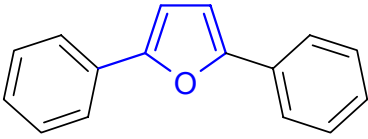
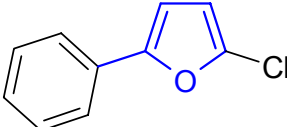
Format

(H₀)

Description

Use this procedure to mark atoms with (H₀) to prohibit any hydrogen attachments to the atom.

Example

Query	Example of Molecules retrieved
	
	
	

Use in ISIS/Draw

1. Select the atom on which to prohibit hydrogens.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the check box: No implicit hydrogens.
5. Click OK. The selected atom is marked with (H₀)

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom on which to prohibit hydrogens.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the check box: No implicit hydrogens.
5. Click OK. The selected atom is marked with (H₀).

* Specify an unsaturated atom

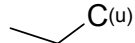

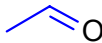
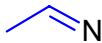
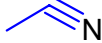
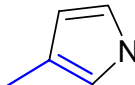
Format

(U)

Description

Use this procedure to mark an atom unsaturated (U) to specify that the atom must be attached to at least one multiple bond: double, triple, or aromatic.

Example

Query	Example of Molecules retrieved
 C(u)	
	
	
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as unsaturated.
2. Double-click the selected atom(s).
3. Click the Query Atom tab.
4. Click the check box: Unsaturated atoms.
5. Click OK. The selected atom is marked with (U).

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom that you want to specify as unsaturated.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the check box: Unsaturated atoms.
5. Click OK. The selected atom is marked with (U).

* **Specify the number of attachments (substituents)**

Use this procedure to specify the number of allowed non-hydrogen attachments (substituents) on an atom.

NO NON-HYDROGEN ATTACHMENTS

Format

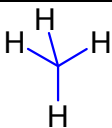
s0

Description

Use this procedure to specify the number of allowed non-hydrogen attachments (substituents) on an atom as 0.

The query atom feature s0 allows you to specify that the records retrieved must have NO non-hydrogen attachments at the specified position. All open valences at that position have solely implicit hydrogen atoms. This query feature implies the retrieval of a single atom with attached hydrogens (if any).

Example

Query	Example of Molecule retrieved
C(s0)	

Use in ISIS/Draw

1. Draw a single atom.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 0.
5. Click OK. The selected atom is marked with (s0).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 0.
5. Click OK. The selected atom is marked with (s0).

ONE NON-HYDROGEN ATTACHMENTS

Format

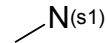
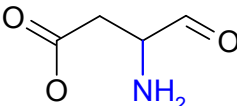
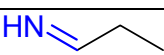
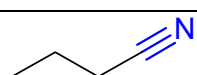
s1

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as ONE.

The query atom feature s1 allows you to specify that the records retrieved must have exactly ONE non-hydrogen attachment of any bond type at the specified position.

Example

Query	Example of Molecules retrieved
	
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 1.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s1).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 1.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s1).

TWO NON-HYDROGEN ATTACHMENTS

Format

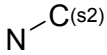
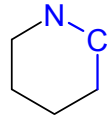
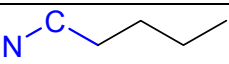
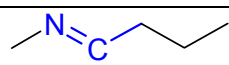
s2

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as TWO.

The query atom feature s2 allows you to specify that the records retrieved must have exactly TWO non-hydrogen attachments of any bond type at the specified position.

Example

Query	Example of Molecules retrieved
	
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 2.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s2).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 2.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s2).

THREE NON-HYDROGEN ATTACHMENTS

Format

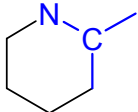
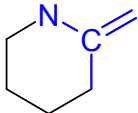
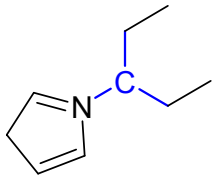
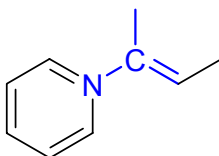
s3

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as THREE.

The query atom feature s3 allows you to specify that the records retrieved must have exactly THREE non-hydrogen attachments of any bond type at the specified position.

Example

Query	Example of Molecules retrieved
$\text{N}-\text{C}(\text{s}3)$	
	
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 3.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s3).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 3.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s3).

FOUR NON-HYDROGEN ATTACHMENTS

Format

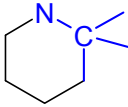
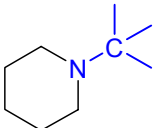
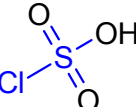
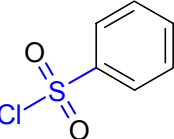
s4

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as four.

The query atom feature s4 allows you to specify that the records retrieved must have exactly FOUR non-hydrogen attachments of any bond type at the specified position.

Example

Query	Example of Molecules retrieved
$\text{N}-\text{C}(\text{s4})$	
	
$\text{Cl}-\text{S}(\text{s4})$	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 4.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s4).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 4.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s4).

FIVE NON-HYDROGEN ATTACHMENTS

Format

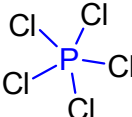
s5

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as five.

The query atom feature s5 allows you to specify that the records retrieved must have exactly FIVE non-hydrogen attachments of any bond type at the specified position.

Example

Query	Example of Molecules retrieved
P(s5)	

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 5.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s5).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 5.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s5).

SIX NON-HYDROGEN ATTACHMENTS

Format

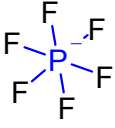
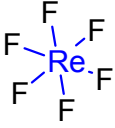
s6

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as six.

The query atom feature s6 allows you to specify that the records retrieved must have exactly SIX non-hydrogen attachments of any bond type at the specified position.

Example

Query	Example of Molecules retrieved
Q(s6) (Q represents any atom except carbon or hydrogen)	 

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose 6.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s6).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Substitution count box and choose 6.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (s6).

NON-HYDROGEN ATTACHMENTS “AS DRAWN”

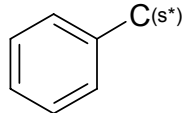
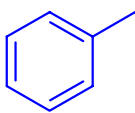
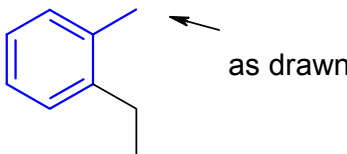
Format

s*

Description

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as exactly those non-hydrogen attachments that you have drawn at the specified position in your query.

Example

Query	Example of Molecules retrieved
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Substitution count box and choose * (asterisk).
5. Click OK. The selected atom is marked with (s*).

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu “Edit QueryFeature”
4. Click the spin buttons of the Substitution count box and choose * (asterisk).
5. Click OK. The selected atom is marked with (s*).

* Specify the number of ring bond attachments

A Ring Bond is a bond that is part of a ring structure.

Use this procedure to specify the number of allowed ring bonds on an atom.

NO RING BOND ATTACHMENTS

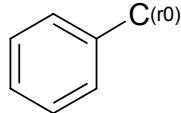
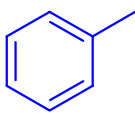
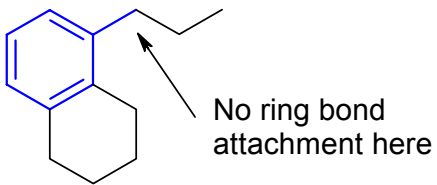
Format

r0

Description

The query atom feature r0 allows you to specify that the records retrieved must have NO ring bond attachment at the specified position. All atoms with this mark must not be part of a ring.

Example

Query	Example of Molecules retrieved
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having ring bond attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Ring bond count box and choose 0.
Note: Count double or triple bonds as one attachment.
6. Click OK. The selected atom is marked with (r0).

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom that you want to specify as having ring bond attachments.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Ring Bond count box and choose 0.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r0).

TWO RING BOND ATTACHMENTS

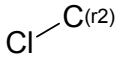

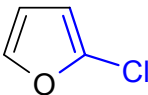
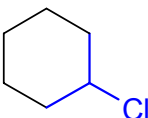
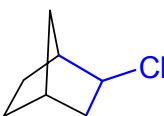
Format

r2

Description

The query atom feature r2 allows you to specify that the records retrieved must have exactly TWO ring bond attachments at the specified position.

Example

Query	Example of Molecules retrieved
	
	
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having ring bond attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Ring bond count box and choose 2.
Note: Count double or triple bonds as one attachment.
6. Click OK. The selected atom is marked with (r2).

Use in ChemDraw

Use in InfoChem's Editor

1. Select the atom that you want to specify as having ring bond attachments.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Ring Bond count box and choose 2.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r2).

THREE RING BOND ATTACHMENTS


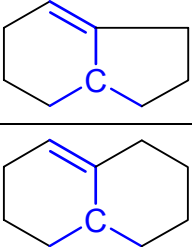
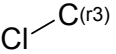
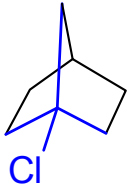
Format

r3

Description

The query atom feature r3 allows you to specify that the records retrieved must have exactly THREE ring bond attachments at the specified position.

Example

Query	Example of Molecules retrieved
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having ring bond attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Ring bond count box and choose 3.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r2).

Use in ChemDraw

Use in InfoChem's' Editor

1. Select the atom that you want to specify as having ring bond attachments.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Ring Bond count box and choose 3.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r3).

FOUR RING BOND ATTACHMENTS

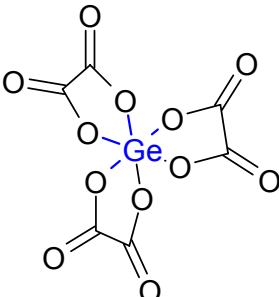
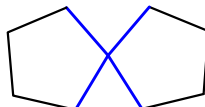
Format

r4

Description

The query atom feature r4 allows you to specify that the records retrieved must have AT LEAST FOUR ring bond attachments at the specified position.

Example

Query	Example of Molecules retrieved
Ge(r4)	
C(r4)	

Use in ISIS/Draw

1. Select the atom that you want to specify as having ring bond attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Ring bond count box and choose 4.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r4).

Use in ChemDraw

Use in InfoChem's Editor

1. Select the atom that you want to specify as having ring bond attachments.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Ring Bond count box and choose 4.
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r4).

RING BOND ATTACHMENTS “AS DRAWN”

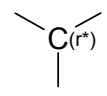
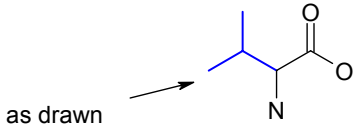
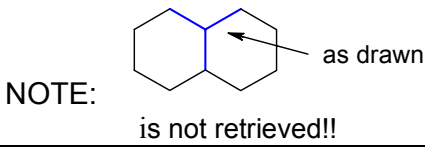
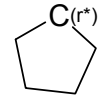
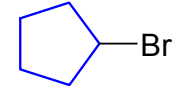
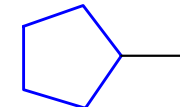
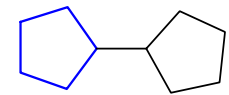
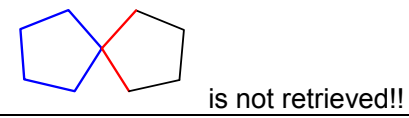
Format

r^*

Description

The query atom feature r^* allows you to specify that the records retrieved must have exactly THOSE ring bond attachments that you have drawn at the specified position in your query.

Example

Query	Example of Molecules retrieved
	
	<p>NOTE:</p> 
	
	
	
	

Use in ISIS/Draw

1. Select the atom that you want to specify as having ring bond attachments.
2. Double-click the selected atom.
3. Click the Query Atom tab.
4. Click the Ring bond count box and choose * (asterisk).
Note: Count double or triple bonds as one attachment.
6. Click OK. The selected atom is marked with (r^*).

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom that you want to specify as having ring bond attachments.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Ring Bond count box and choose * (asterisk)..
Note: Count double or triple bonds as one attachment.
5. Click OK. The selected atom is marked with (r*).

* **Allow additional atoms and/or bonds in a chain or a ring**

Use a link node to specify the addition of variable numbers of identical repeating units to a ring or chain.

Not yet implemented

* Specify a mass (isotope) on an atom

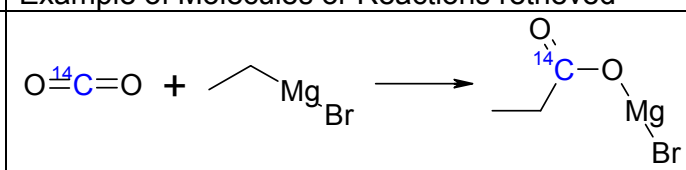
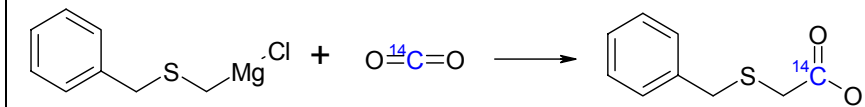
Format



Description

This atom feature allows you to specify that the records retrieved must have the isotopes that you have drawn at the specified position in your query.

Example (Database COFGT)

Query	Example of Molecules or Reactions retrieved
${}^{14}\text{C}$	 $\text{O}=\text{}^{14}\text{C}=\text{O} + \text{CH}_3\text{CH}_2\text{MgBr} \longrightarrow \text{CH}_3\text{CH}_2\text{O}(\text{}^{14}\text{C})\text{O}(\text{Mg})\text{Br}$
	 $\text{C}_6\text{H}_5\text{CH}_2\text{S}(\text{Mg})\text{CH}_2\text{Cl} + \text{O}=\text{}^{14}\text{C}=\text{O} \longrightarrow \text{C}_6\text{H}_5\text{CH}_2\text{S}(\text{Mg})\text{CH}_2\text{C}(\text{}^{14}\text{C})\text{O}$

Use in ISIS/Draw

1. Select the atom where you want to place the isotope.
2. Double-click the selected atom.
3. Click the Atom tab.
4. Increase or reduce the mass in the Isotope box by clicking on the arrow.
5. Click OK. The isotope is displayed as superscript on the selected atom.

Use this procedure to enter isotopes and their atom symbols using the keyboard.

1. Select the atom where you want to place the isotope.
2. Enter the isotope number, followed by the atom symbol. For example, to label an atom ${}^{14}\text{C}$, enter 14C.
3. Press the Return key. The isotope is displayed as superscript on the selected atom.

Note: If an atom you typed is not recognized as a legal atom type, it is added as an atom alias, not as isotope. An alias is not a legal atom type.

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom where you want to place the isotope.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit Atom"
4. Increase or reduce the mass by clicking on the spin buttons of the Isotope box
5. Click OK. The isotope is displayed as superscript on the selected atom.

* **Specify an explicit valence on an atom**

Format
 $X^{(I,II,III,...)}$

Description

This atom feature allows you to specify that the records retrieved must have exactly the valence that you have specified at the selected position in your query.

Each atom type has assigned one or more legal standard valence states, e.g. C: 4, N: 3, P: 3,5, S: 2,4,6.

When connecting bonds to an atom, always implicit H-atoms will be added to the atom, until the next legal valence state is reached.

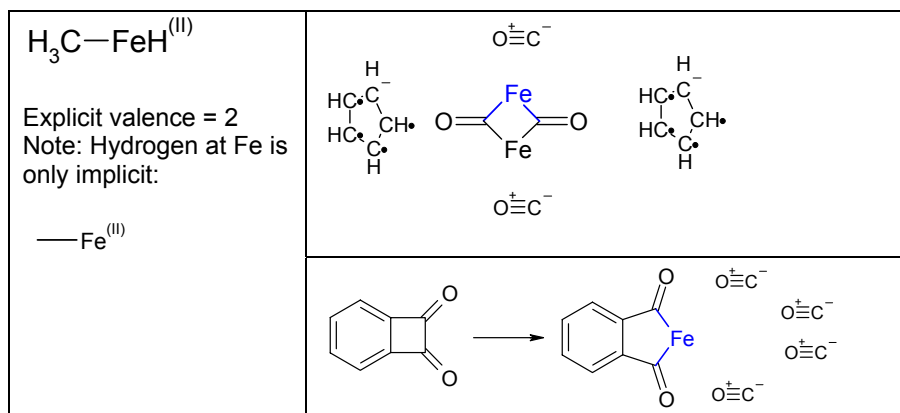
Transition metal atoms have no standard valence assigned, therefore no implicit hydrogens will be added.

To override the standard valence you may specify an explicit valence to an atom. Only explicit valency settings will be used for retrieving database records with identical valency settings.

Please also refer to chapter "allow a specific number of attachments" and use this procedure to specify the number of allowed non-hydrogen attachments (substituents) on an atom.

Examples (Database EROS Build 4, 2004)

Query	Example of Molecules or Reactions retrieved
<p>H_3C-Fe</p> <p>Unspecified Valence: implicit valence = 1 \Rightarrow Valence in query is set to 1: $-Fe^{(I)}$</p>	



Use in ISIS/Draw

1. Select the atom where you want to place the valence.
2. Double-click the selected atom.
3. Click the Atom tab.
4. Click the Valence count box and enter a valence from 0 to 14 or increase or reduce the value by clicking on an arrow.
5. Click OK.

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom where you want to place the valence.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit Atom"
4. Increase or reduce the valence by clicking on the spin buttons of the Valence box
5. Click OK.

* Specify a charge on an atom

For Salts: please see also chapters
4.1 Standardization of Functional Groups
4.2 Salts, Complexes and Organometallics

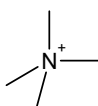

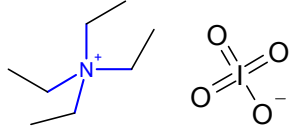
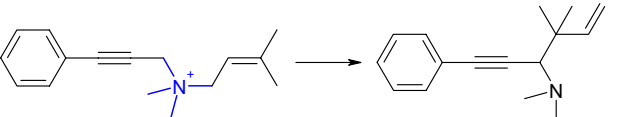
Format

X^+ , X^{2+} , X^- , X^{3-}

Description

This atom feature allows you to specify that the records retrieved must have exactly the charge that you have specified at the selected position in your query.

Examples (Database eEROS, Build 4, 2003)

Query	Example of Molecules or Reactions retrieved
	
	
	

Use in ISIS/Draw

1. Select the atom where you want to place the charge.
2. Double-click the selected atom.
3. Click the Atom tab.
4. Click the Charge count box and enter a charge from -15 to +15 or increase or reduce the value by clicking on an arrow.
5. Click OK.

Use this procedure to enter atoms and their charges using the keyboard.

1. Select the atom where you want to place the atom charge.
2. Enter the atom symbol, followed by the number of charges, followed by + for a positive charge or - for a negative charge. For example, to label an atom Ca^{2+} , enter Ca2+.

Note: You do not need to enter 1 to specify one charge.

3. Press the Return key. The atom charge is displayed as superscript on the selected atom.

Note: If an atom you typed is not recognized as a legal atom type, it is added as an atom alias, not as isotope. An alias is not a legal atom type.

Use in ChemDraw

Use in InfoChems' Editor

1. Select the atom where you want to place the charge.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit Atom"
4. Increase or reduce the charge by clicking on the spin buttons of the Charge box
5. Click OK.

1.2 Bond query features

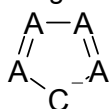
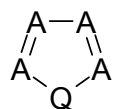
* Specific bond type

You can retrieve molecules that allow variations in bond type at specified positions.

Definition of Aromaticity

The following ring systems are aromatic:

- * Five-membered rings such as the structures shown below:

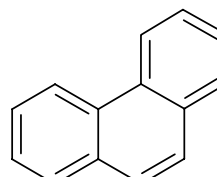
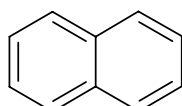
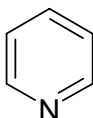
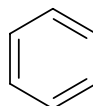


where
A = any atom except H
Q = any atom except C or H

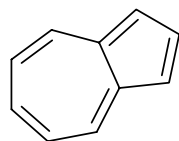
For example:



- * Six-membered rings that can be drawn with alternating double and single bonds:



- * Perimeter bonds in azulenes:



Note: The bonds of six-membered aromatic ring systems and the perimeter bonds of azulenes are stored as aromatic bonds in the database. The bonds of five-membered aromatic rings, however, are stored as single and double bonds and interpreted as aromatic during a search. The differences between five-membered rings and other types of aromatic rings can cause different search results for five- and six-membered rings/azulenes when you use the following bonds in queries: Single, Double, and Single/Double query bonds.

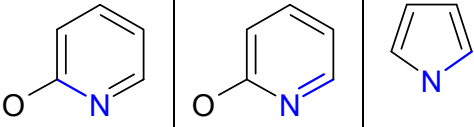



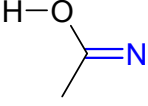

ANY BOND

Format

Description

To allow any bond type at the specified positions in your query, choose Any.

Example

Query	Example of Molecules retrieved
-----N	
	
	
	
	
	

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Bond Type box and select "Any" from the drop down list.
5. Click OK.

Use in ChemDraw

Use in InfoChem's Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Click the Bond Type box and select "Any" from the scroll list.
5. Click OK.

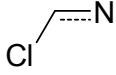
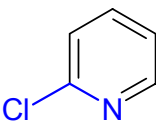
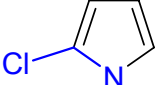
AROMATIC BOND

Format

Description

To allow solely aromatic bonds at the specified positions of your query, choose Aromatic.

Example

Query	Example of Molecules retrieved
	
	

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Bond Type box and select "Aromatic" from the drop down list.
5. Click OK.

Use in ChemDraw

Use in InfoChems' Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Click the Bond Type box and select "Aromatic" from the scroll list.
5. Click OK.

SINGLE/DOUBLE

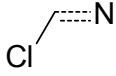
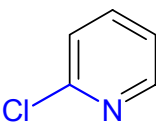
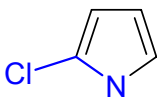
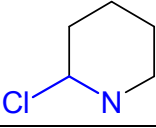
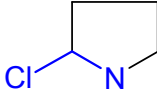
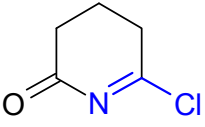
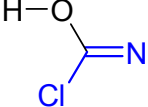
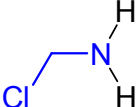
Format

.....

Description

To allow either single or double bonds at the specified positions of your query, choose Single/Double.

Example

Query	Example of Molecules retrieved	
		
		
		
		
		

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Bond Type box and select "Single/Double" from the drop down list.
5. Click OK.

Use in ChemDraw

Use in InfoChem's Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Click the Bond Type box and select "Single/Double" from the scroll list.
5. Click OK.

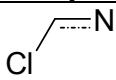
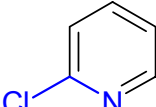
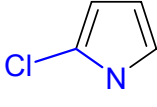

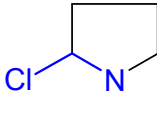
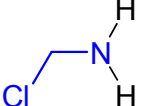
SINGLE/AROMATIC

Format

Description

To allow either single or aromatic bonds at the specified positions of your query, choose Single/Aromatic.

Example

Query	Example of Molecules retrieved	
		
		
		

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Bond Type box and select "Single/Aromatic" from the drop down list.
5. Click OK.

Use in ChemDraw

Use in InfoChems' Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Click the Bond Type box and select "Single/Aromatic" from the scroll list.
5. Click OK.

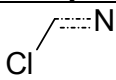
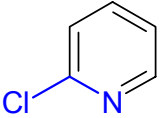
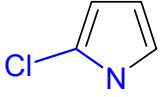
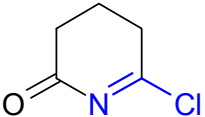
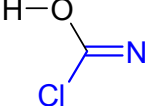
DOUBLE/AROMATIC

Format

Description

To allow either double or aromatic bonds at the specified positions of your query, choose Double/Aromatic.

Example

Query	Example of Molecules retrieved	
		
		
		

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Bond Type box and select "Double/Aromatic" from the drop down list.
5. Click OK.

Use in ChemDraw

Use in InfoChems' Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Click the Bond Type box and select "Double/Aromatic" from the scroll list.
5. Click OK.

* Topology (chain or ring bond)

CHAIN BOND

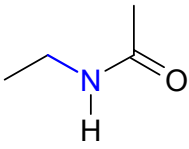
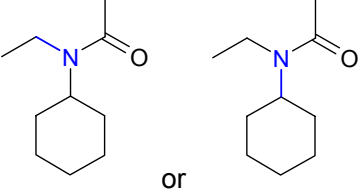
Format

—Ch—

Description

Use this procedure to mark a bond Ch to specify that the bond must be part of a chain, not part of a ring. The chain may be of any size:

Example

Query	Example of Molecules retrieved
—Ch—N	
	

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Topology box and choose “Chain” from the drop down list..
5. Click OK. The selected bond is marked with Ch.

Use in ChemDraw

Use in InfoChems' Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu “Edit Bond”
4. Click the spin buttons in the Topology box and select “Chain”.
5. Click OK. The selected bond is marked with Ch.

RING BOND

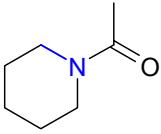
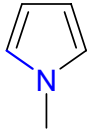
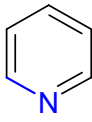
Format



Description

Use this procedure to mark a bond Rn to specify that the bond must be part of a ring, not part of a chain. The ring may be of any size:

Example

Query	Example of Molecules retrieved
—Rn—N	
	
	

Use in ISIS/Draw

1. Select a bond.
2. Double-click the selected bond.
3. Click the Bond tab.
4. Click the Topology box and choose “Ring” from the drop down list.
5. Click OK. The selected bond is marked with Rn.

Use in ChemDraw

Use in InfoChem's Editor

1. Select a bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu “Edit Bond”
4. Click the spin buttons in the Topology box and select “Ring”.
5. Click OK. The selected bond is marked with Rn.

* **Allow additional atoms and/or bonds in a chain or a ring**

Use a link node to specify the addition of variable numbers of identical repeating units to a ring or chain.

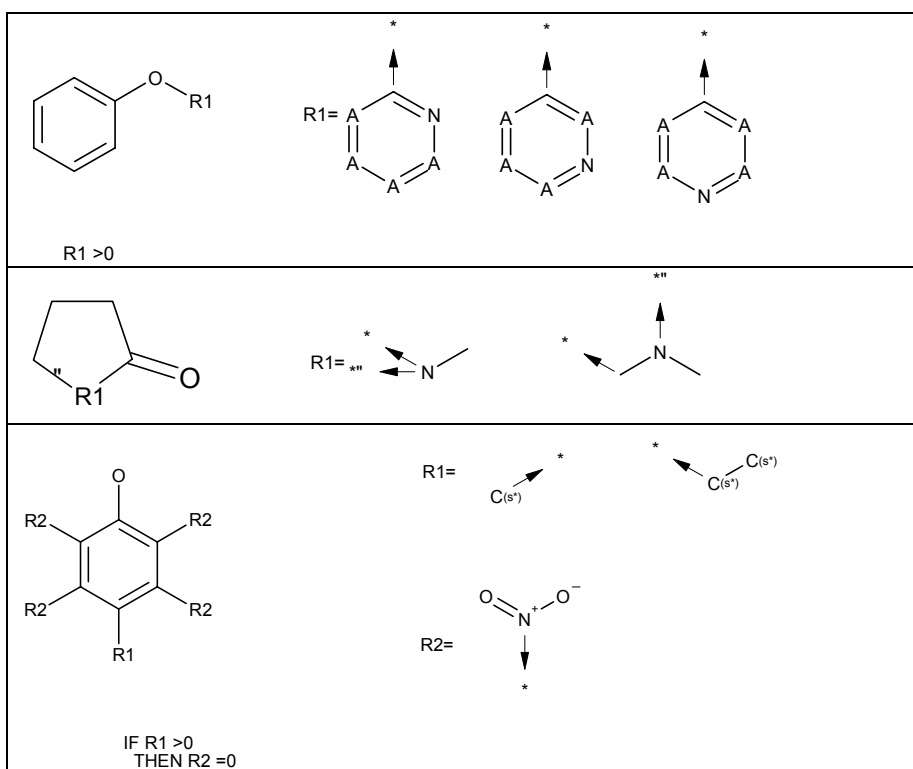
Not yet implemented.

1.3 Rgroup query features

An Rgroup (RGROUP) search finds molecule records that contain your query as a substructure wholly within a larger structure with additional restrictions. For example, you can:

- Specify the structural fragments (such as functional groups or atoms) of your choice at specific sites within a molecule.
- Exclude structural fragments of your choice at specific sites within a molecule.
- Specify that the presence of one structural fragment requires the presence of another (Rgroup conditions).

Examples for Rgroup queries:



1.4. Specifying attached data

- * For an exact search in a molecule database
- * For a substructure search in a molecule database

Not yet implemented

1.5. Stereochemistry

Please also refer to chapter 5. Advanced Stereochemistry

* UP and DOWN BOND

Format




Description

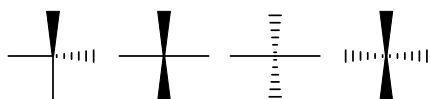
You can create a query with an UP bond or a DOWN bond on the asymmetric center of atoms C, N, O, P, S or Si.

An Up bond or a Down bond on the asymmetric tetrahedral center of atoms C, N, O, P, S, or Si allows you to retrieve molecules with matching stereochemistry. Without creating a chiral flag for the query, stereochemistry will be treated as relative, i.e. searching the query structure or its mirror image will result in identical hitsets.

NOTE:

Atom-centered stereo chemistry is defined by up and/or down bonds: . However, draw only one bond with stereo information (up or down). If stereochemistry is not absolutely clear, add hydrogens to stereocenters.

The following combinations of up and down bonds are correct:

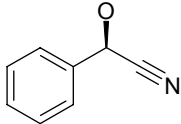
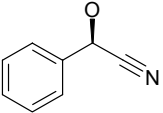
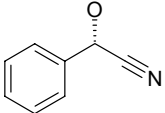
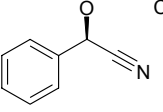
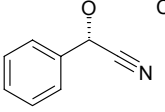
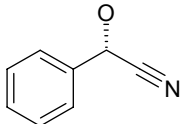
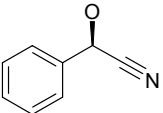
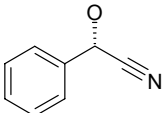
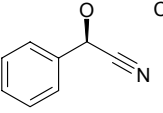
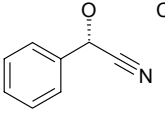


The following combinations of up and down bonds are INCORRECT:



The direction of the stereo bonds is essential to specify the stereochemical center (the narrow end of the bond specifies the stereo chemical center, the flat end specifies the substituent for this stereochemical center).

Example

Query	Example of Molecules retrieved	
		
	 Chiral	 Chiral
		
	 Chiral	 Chiral

Use in ISIS/Draw



1. Do one of the following:



To sprout an Up bond from an atom, click



To sprout a Down bond from an atom, click







2. Click the atom of your choice, from which the up or down bond shall be drawn.
3. You may change the direction of the stereo bond by clicking on the existing stereo bond with the buttons  or .

Note: please don't use  for up bonds and  for down bonds.

Use in ChemDraw

Use in InfoChems' Editor

1. To sprout an Up bond from an atom, click 
To sprout a Down bond from an atom, click 
2. Click the atom of your choice, from which the up or down bond shall be drawn.
3. You may change the direction of the stereo bond by clicking on the existing stereo bond with the buttons  or .

* Stereochemistry at double bonds

Not yet supported. E / Z (Cis / trans) configurations drawn in the query will be ignored during searches.

* Chiral flag

Format

Chiral

Description

You can create a query with a CHIRAL FLAG on a molecule with at least one asymmetric center or on a molecule that is asymmetric to retrieve solely the absolute stereo configuration but not relative stereo configurations.

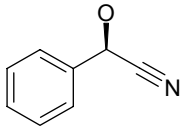
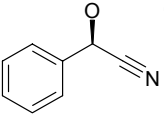
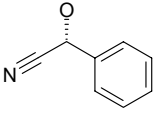
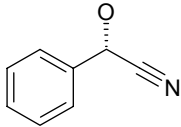
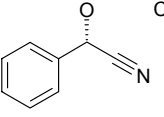
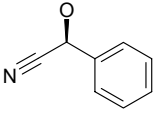
When you create a query without a chiral flag on a molecule that contains at least one asymmetric center or on a molecule that is asymmetric, you retrieve all the relative stereoconfigurations.

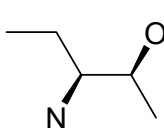
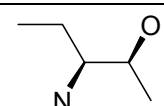
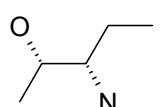
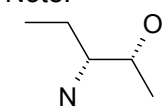
The chiral flag eliminates the relative stereoconfigurations.

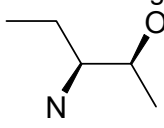
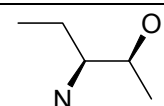
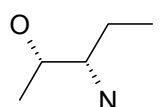
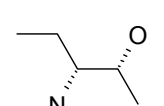
You can use queries with:

Geometric stereochemistry for the following atoms that are separated by a double bond: C, O, S (sulfoxide), Si, and trivalent N and P. (Ignored by the InfoChem/ICFSE. You always retrieve both the cis and trans configuration.)
Tetrahedral stereochemistry for the following atoms: C, N, O, S (sulfate and sulfoxide), P, Si, and pentavalent N and P (3 or 4 attachments with 1 double bond).

Example

Query	Example of Molecules retrieved	
1 stereo center:  Chiral	 Chiral	 Chiral
 Chiral	 Chiral	 Chiral

2 stereo centers: WITH Chiral flag Chiral 	 Chiral
	 Chiral
	Note:  Chiral will NOT be retrieved

2 stereo centers: NO Chiral flag 	 Chiral
	 Chiral
	 Chiral will be retrieved

Use in ISIS/Draw

1. Select the structure that you want to label as chiral.
2. Choose Chemistry > Create Chiral Flag. You see the word "Chiral" at the right of the structure. With the Select tool you may change the position of the CHIRAL flag within the molecule, what affects only the display, but not the chemical information.

Use in ChemDraw

Use in InfoChems' Editor

2. Query Features on a Reaction

2.1 Specific Query Features on a Reaction

A query feature on a reaction is a restriction on the reacting centers or on the spatial arrangement of stereo bonds or on atoms that specifies the retrieval of certain types of reaction records from the database.

* **Reacting center query features**

A Reacting Center is a bond that changes in the reactant and in the product. Markings on the bonds of reactants and products specify exactly which bonds change (or do NOT change).

If you don't mark Reaction Centers, only the "pure" structures (reactant and product) of your query will be searched as substructures in the reaction database, not considering the chemistry of the reaction.

On the other hand, specifying Reaction Centers in your query is a method to cut down a large hitlist of "pure substructure hits" to a shorter list of chemically corresponding hits.

NOT CENTER

Format




Description

The marked bond must not change.

Example (Database eEROS, Release 5)

Query	Examples of Reactions retrieved

Use in ISIS/Draw

1. Click  ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.
2. Click the bond on which to mark a reacting center. Each time you click the bond, you see a different reacting center mark. Keep clicking the bond until you see the desired reacting center mark:
X: The bond must not change

Alternative method:

1. Double Click on the bond you want to specify as reacting bond.
2. Click the Bond Tab
3. Select "Not Center" from the Reacting center drop down list.
4. Click ok. The selected bond is marked with "x".

Use in ChemDraw

Use in InfoChems' Editor

1. Select the bond you want to specify as reacting bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Select "Not Center" by clicking the spin buttons of the Reacting center box.
5. Click ok. The selected bond is marked with "x".

CENTER

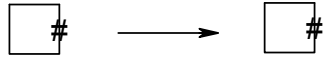
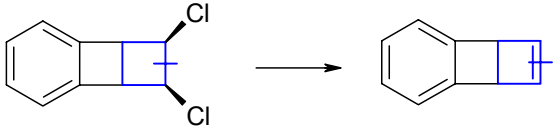
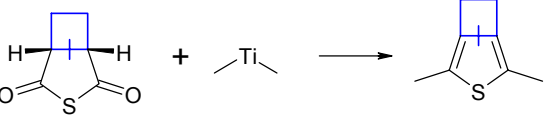
Format

—#—


Description

The marked bond changes unspecifically (may be formed or broken).

Example (Database eEROS Release 5 and SOS Release November 2003)

Query	Example of Reactions retrieved
	
	 <p>Bond gets aromatic</p>

Use in ISIS/Draw

1. Click . ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.
2. Click the bond on which to mark a reacting center. Each time you click the bond, you see a different reacting center mark. Keep clicking the bond until you see the desired reacting center mark:
#: The bond changes unspecifically (may be formed or broken).

Alternative method:

5. Double Click on the bond you want to specify as reacting bond.
6. Click the Bond Tab
7. Select "Center" from the Reacting center drop down list.
8. Click ok. The selected bond is marked with "#".

Use in ChemDraw

Use in InfoChems' Editor

1. Select the bond you want to specify as reacting bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Select "Center" by clicking the spin buttons of the Reacting center box.
5. Click ok. The selected bond is marked with "#".

CHANGE

Format




Description

The marked bond changes its bond type

Example (Database SOS, Release November 2003)

Query	Example of Reactions retrieved

Use in ISIS/Draw

1. Click 
ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.
2. Click the bond on which to mark a reacting center. Each time you click the bond, you see a different reacting center mark. Keep clicking the bond until you see the desired reacting center mark:
|: The bond changes its bond type

Alternative method:

1. Double Click on the bond you want to specify as reacting bond.
2. Click the Bond Tab
3. Select "Change" from the Reacting center drop down list.
4. Click ok. The selected bond is marked with "|"

Use in ChemDraw

Use in InfoChem's Editor

1. Select the bond you want to specify as reacting bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Select "Change" by clicking the spin buttons of the Reacting center box.
5. Click ok. The selected bond is marked with "|".

MAKE/BREAK

Format




Description

The marked bond is either formed or broken.

Example (Databases eEROS Release 5, and COFGT)

Query	Example of Reactions retrieved

Use in ISIS/Draw

1. Click 
ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.
2. Click the bond on which to mark a reacting center. Each time you click the bond, you see a different reacting center mark. Keep clicking the bond until you see the desired reacting center mark:
||: The bond is either formed (product) or broken (reactant).

Alternative method:

1. Double Click on the bond you want to specify as reacting bond.
2. Click the Bond Tab.
3. Select "Make/Break" from the Reacting center drop down list.
4. Click ok. The selected bond is marked with "||"

Use in ChemDraw

Use in InfoChems' Editor

1. Select the bond you want to specify as reacting bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Select "Make/Break" by clicking the spin buttons of the Reacting center box.
5. Click ok. The selected bond is marked with "||".

MAKE/CHANGE

Format



Description


The marked bond is either formed or broken and changes its bond type.

NOT supported by InfoChem Search Engine.

Example

Query	Example of Reactions retrieved
	0 Hits NOT supported by InfoChem Search Engine

Use in ISIS/Draw

1. Click 
ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.
2. Click the bond on which to mark a reacting center. Each time you click the bond, you see a different reacting center mark. Keep clicking the bond until you see the desired reacting center mark:
|||: The bond s either formed or broken and changes its bond type

Alternative method:

1. Double Click on the bond you want to specify as reacting bond.
2. Click the Bond Tab
3. Select "Make/Change" from the Reacting center drop down list.
4. Click ok. The selected bond is marked with "|||"

Use in ChemDraw

Use in InfoChems' Editor

1. Select the bond you want to specify as reacting bond.
2. Click the selected bond with the right mouse button.
3. Open the context menu "Edit Bond"
4. Select "Make/Change" by clicking the spin buttons of the Reacting center box.
5. Click ok. The selected bond is marked with "|||".

* Stereo bond query features

Inversion and retention Marks specify how the stereochemistry of an asymmetric center in a reactant or product changes/ does NOT change in a reaction.

.ret. specifies that the asymmetric center RETAINS its stereo chemical configuration during the reaction.

.inv. specifies that the asymmetric center INVERTS its stereo chemical configuration during the reaction.

INVERSION

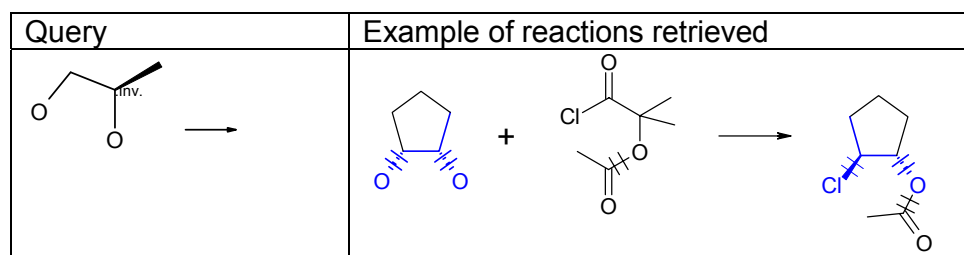
Format

.inv.

Description

.inv. specifies that the asymmetric center INVERTS its stereo chemical configuration during the reaction.

Example (Database eEROS, Release 5)



Use in ISIS/Draw

1. Select an atom.
2. Choose Object > Edit Atom or double click the atom.
3. Click the Query Atom tab.
4. Select "Inversion" from the Reaction Stereo drop down list.
5. Click OK. The selected atom is marked with .inv.

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Reaction Stereo box and choose "Inversion".
5. Click OK. The selected atom is marked with .inv.

RETENTION

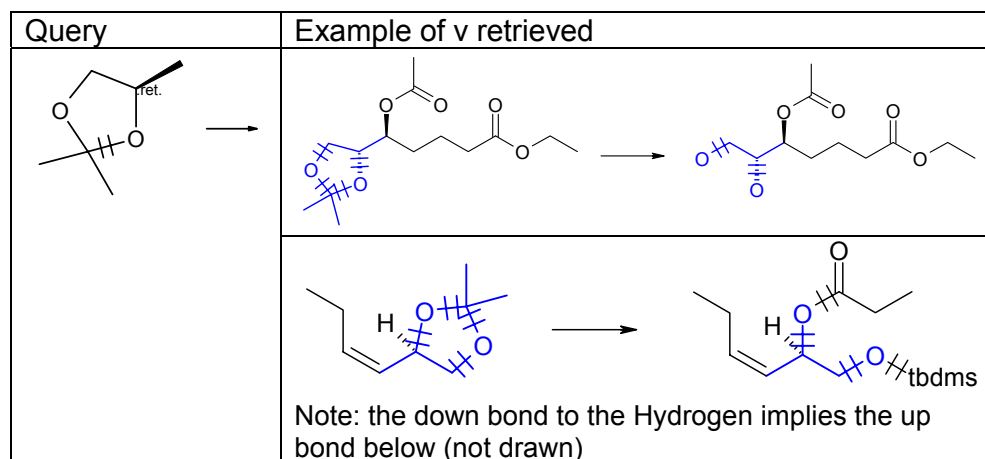
Format

.ret.

Description

.ret. specifies that the asymmetric center **RETAINS** its stereo chemical configuration during the reaction.

Example (Database eEROS, Release 5)



Use in ISIS/Draw

1. Select an atom.
2. Choose Object > Edit Atom or double click the atom.
3. Click the Query Atom tab.
4. Select "Retention" from the Reaction Stereo drop down list.
5. Click OK. The selected atom(s) are marked with ret.

Use in ChemDraw

Use in InfoChems' Editor

1. Select an atom.
2. Click the selected atom with the right mouse button.
3. Open the context menu "Edit QueryFeature"
4. Click the spin buttons of the Reaction Stereo box and choose "Retention".
5. Click OK. The selected atom is marked with .ret.

2.2 Atom-Atom Map on a Reaction

An atom-atom map on the reaction components in a query specifies exactly which atoms in the reactants correspond to the atoms in the products. You can specify the atoms that must (or must not) change in the transformations that you retrieve.

An atom-atom map eliminates additional, unwanted results.

You can atom-atom map AUTOMATICALLY or MANUALLY. If you map manually, you choose your own correspondence between the atoms in the reactants and in the products.

* Automapping a Reaction Query

Format

Description

Use this procedure to map all atoms in a reaction automatically. (Automatic atom-atom mapping is called automapping.)


To simplify the input of a RSS query using the InfoChem/Cartridge, your query will be mapped and assigned reaction centers automatically with the automap feature during transfer from ISIS/Draw to the Cartridge – **if desired**. This feature is currently only available if you use ISIS/Draw as input editor and the InfoChem map addin for ISIS/Draw has been installed.



Example (Database eEROS, Release 5)

Query	Example of reactions retrieved
<p>Automapping:</p>	
<p>Automapping:</p>	

Use in ISIS/Draw

1. Click on the InfoChems' Icon . You see the atom-atom maps and reacting centers in the reaction.
2. Visually inspect the atom-atom maps and reacting centers to be certain that the reactants and products are mapped correctly.
Note: If the automatic atom-atom map is incorrect, remove the atom-atom maps and centers and then manually atom-atom map the query.

Use in ChemDraw

Use in InfoChems' Editor

* Mapping a Reaction Query manually

Format

none

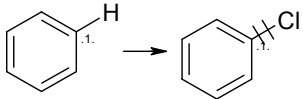
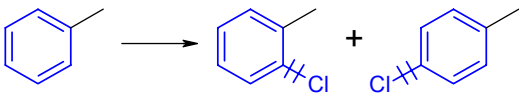
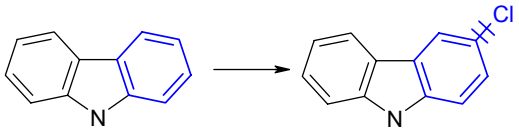
Description

If you map manually, you choose your own correspondence between the atoms in the reactants and in the products.

Use the following guidelines to help you to atom-atom map your query correctly:


- Always atom-atom map a query that contains an entire reaction (at least a portion of a reactant and at least a portion of a product). Do not attempt to atom-atom map a query that contains solely a reaction component and a reaction arrow.
- Only map those specific atoms that you see in both the reactants and the products.

Example

Query	Example of reactions retrieved
	
	

Use in ISIS/Draw



Use this procedure to manually map a pair of atoms in ISIS/Draw.

1. Click .
ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.
2. Click an atom in a reactant, and then click the corresponding atom in the product. The atom numbers (in the form .1.) display next to the atoms.
3. (Optional) To map a one-to-many relationship, first click an atom that is marked with an existing atom map. Then, click the corresponding atom.

Note: You cannot map a many-to-many relationship.

Use in ChemDraw

Use in InfoChems' Editor

1. Click 
2. Click an atom in a reactant, and then click the corresponding atom in the product. The atom numbers (in the form .1.) display next to the atoms.
3. (Optional) To map a one-to-many relationship, first click an atom that is marked with an existing atom map. Then, click the corresponding atom.
Note: You cannot map a many-to-many relationship.
4. To delete single mappings use 

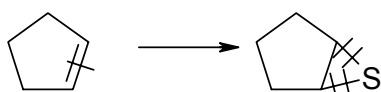
Atom-Atom-Mapping Guidelines

Use the following guidelines to help you to atom-atom map your query correctly:

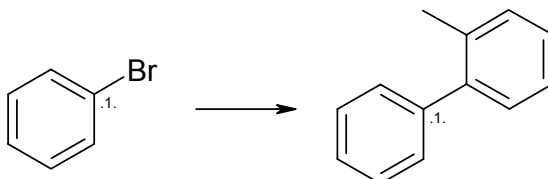
- Always atom-atom map a query that contains an entire reaction (at least a reactant and a product).
Do not attempt to atom-atom map a query that contains solely a reaction component and a reaction arrow.

Note: We strongly recommend that you draw solely the reacting fragments (and use query features where relevant) rather than draw each reactant and product in detail.

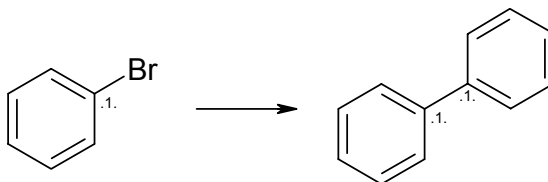
- Only map those specific atoms that you see in both the reactants and the products. For example, do not map the sulfur atom that you see only in the product:



- Map them manually:
 1. Select a reactant atom and a product atom that you want to specify as Atom 1 and map them manually.



2. Select the same atom in the reactant and another atom in the product that you want to specify as Atom 1 (a multiple mapping of Atom 1) and map them manually. For example:



- Always atom-atom map a reaction query at last, after you added all other structures, stereochemistry, and/or query features to your query.

3. Search Types - Basics

3.1 SSS (Substructure Search)

A Molecule **S**ubstructure **S**earch (SSS) finds molecule records in your database that contain your query as a substructure wholly within a larger structure. Your substructure query is a two-dimensional representation of a portion of a molecule (a 2D substructure).

You can also increase the power of an SSS search by the addition of specific restrictions (called query features) on atoms and/or bonds. There are a number of query features available for use.

3.2 RSS (Reaction Substructure Search)

A **R**eaction **S**ubstructure **S**earch (RSS) finds reaction records in your database that contain your query as a reaction substructure wholly within a larger reaction. Your reaction substructure query is a two-dimensional representation of a portion of a reaction (a 2D reaction substructure) with mapped atoms and your choice of restrictions on the reacting centers.

Your query can also contain restrictions (called query features) on the atoms, bonds and the reaction.

An atom-atom map on the reaction components in a query specifies exactly which atoms in the reactants correspond to the atoms in the products.

You can also add hydrogens with visible bonds (called explicit hydrogens) to your query to block substituents on specific atoms.

You can also search for an incomplete reaction, e.g. only the reactant or only the product is drawn, but always adding a reaction arrow left (for product search) or right to the molecule (for reactant search).

3.3 Role Search

The Role Search finds your query as a substructure (or as exact structure, if specified in your query) in a reaction, where the structure acts as reactant, catalyst, solvent or product according to the role you want to retrieve.

The following Role Searches are available:

Substructure as	reactant, catalyst, solvent or product
Exact structure as	reactant, catalyst, solvent or product

3.4 XSS (Exact Structure Search)

An **Exact Structure Search** (XSS) finds molecule records in your database that match your structure query exactly. For an exact match all stereo information (i.e. R/S) and all isotopic labels must match. Any stereo information of your query will be treated as absolute, even without setting the chiral flag for the query structure. Therefore only identical absolute stereochemistry will be retrieved. If you want to retrieve relative stereochemistry, you have to use the isomer exact structure search (IXSS, see below).

Please note, that currently geometrical stereo information (E/Z at double bonds) is ignored.

3.5 FlexXSS (Flexible Exact Structure Search)

A **Flexible Exact Structure Search** (FlexXSS) retrieves molecules from the database being

- stereo isomers
- isotopic isomers
- parent substructures and salts
- tautomers
- complexes

containing the structure(s) you specified in your query as component(s).

3.6 IXSS (Isomer Exact Structure Search)

An **Isomer Exact Structure Search** (IXSS) finds molecule records in your database that are geometric isomers, stereo isomers and isotopic isomers of your structure query.

3.7 PXSS (Parent Exact Structure Search)

A **Parent Exact Structure Search** (PXSS) search finds molecule records in your database where the main component of your query is the main component of the hit. With this search you will retrieve salts, complexes, identical or tautomeric structures.

This search type has additional functionality:

- Entering salt queries, consisting of more than one organic component, only the largest (main) organic component is used for parent searching.
- In addition to parents all other salt forms of the main organic component will be found.
- Non-salt organic queries are allowed as well. All salt forms of the organic component will be found (reverse parent search).
- Stereochemistry will be ignored during the search
- Isotopic labels will not be ignored.

3.8 TXSS (Tautomer Exact Structure Search)

A **Tautomer Exact Structure Search** (TXSS) finds all isomers, where hydrogens, radicals or metal atoms may be on variable positions, but where the σ -skeleton and the total number of hydrogen atoms must be identical after removing all bonds to metal atoms, all charges and all radical electrons.

Stereochemistry will be ignored during the search. Isotopic labels will not be ignored.

3.9 XSFS (exact sum formula search)

An **Exact Sum Formula Search** finds molecule records that contain the formula that you specify in your query.

Your formula query can be:

- * An exact formula and no other atoms, such as C₆H₆O
- * An exact formula containing ranges and no other atoms, such as C(1-6)H(0-99)N(0-5)

Your query can include ranges of atom counts but must include all standard atom symbols, including hydrogens. You can use a single space to separate atoms, but atom symbols must always begin with a capital letter. Multiple occurrences of atom counts will be accumulated.

For example:

To find phenol or isomers, enter: C₆H₆O or C₆H₅OH.

To find ethanol or isomers, enter: C₂H₆O or CH₃CH₂OH.

3.10 SFS (sum formula search)

A **Sum Formula Search** finds molecule records that contain the formula that you specify in your query as sub formula.

Your formula query can be:

- * A sub formula and any additional other atoms, such as C₁₇N₀O₃
- * A sub formula except specific atoms, such as C₅N₀, where N₀ represents zero nitrogens.
- * A sub formula containing ranges and any additional other atoms, such as C(1-6)N(0-5)

Your query can include a range of atom counts and typically excludes the hydrogens. You can use a single space to separate atoms, but atom symbols must always begin with a capital letter. Multiple occurrences of atom counts will be accumulated.

For example:

To find mono sodium salts, enter Na.

To find molecules that contain six carbons and any number of other atom types, enter: C6.

To find molecules that contain one to six carbon atoms, zero to five nitrogen atoms and any additional other atom types, enter: C(1-6)N(0-5).

3.11 XRS

A XRS search finds always the reaction records in the database that match your reaction query exactly. Any stereo information of your query will be treated as absolute, even without setting the chiral flag for the query structure.

3.12 XRSSUB

A XRSSUB search finds always the reaction records in the database that match your reaction query exactly. Additional reactants and products may be found in the reaction records from the database.

3.13 XRSRCT

A XRSRCT search finds always the reaction records in the database that match the reactant or reactants in your reaction query exactly. Additional reactants may be found in the reaction records from the database. The query input must not contain any products.

3.14 XRSPRD

A XRSPRD search finds always the reaction records in the database that match the product or products in your reaction query exactly. Additional products may be found in the reaction records from the database. The query input must not contain any reactants.

3.15 Examples for Search strategies

(coming soon)

4. Storing and Retrieving Structures in your Database

4.1 General rules for representing organic structures

Please see the following table to find out the normalized representation for your structure.

Scheme of general rules for bonding of atoms in organic structures in the database

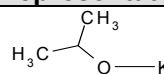
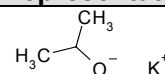
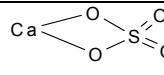
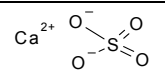

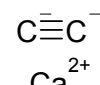
Halogens	Oxygen	Main group elements	Transition metals (and lanthanides, actinides)	Group IIa Alkali earth metals	Group Ia Alkali metals
Ionic	Ionic	Covalent	Covalent	Covalent	Covalent
Covalent	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	Covalent Exception: bonds between IIa and carbanions of alkenes or alkynes are ionic	Covalent	Covalent	Covalent
Covalent	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	No general rule defined	Covalent	Covalent	Covalent
Covalent	Covalent	Covalent	No general rule defined	Covalent Exception: bonds between IIa and carbanions of alkenes or alkynes are ionic	Covalent
Covalent	Covalent	Covalent	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	Covalent	Ionic
Covalent	Covalent	Covalent	Covalent	Covalent	Ionic

4.2 Standardization rules of functional groups

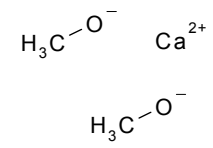
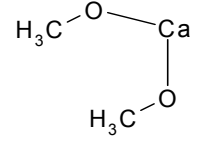
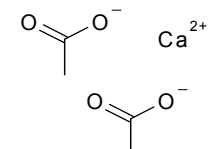
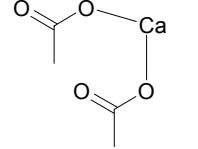
* Separation of covalent structures into ionic components

Automatically normalized structures are represented using standard MDL conventions. Therefore some covalent structures will be separated into ionic components according to the rules listed in 4.1.

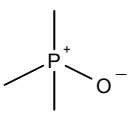
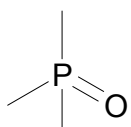
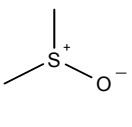
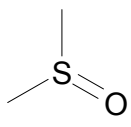
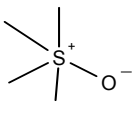
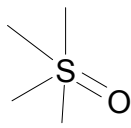
e.g.

Example	Original representation	Normalized representation
Alkali Alcoholates		
Complex ions and Q=Q-O ⁻ substructures		
Carbon to group IIa		

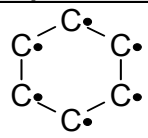
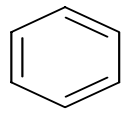
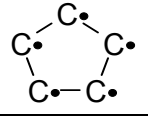
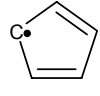
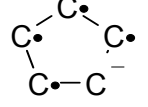
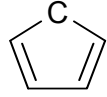
* Connecting ionic components

Example	Original representation	Normalized representation
		
		

* **Removing charge separations**

Example	Original representation	Normalized representation
4-bonded P-Atoms		
3-bonded S-Atoms		
5-bonded S-Atoms		

* **Radicals**

Example	Original representation	Normalized representation
		
		
		

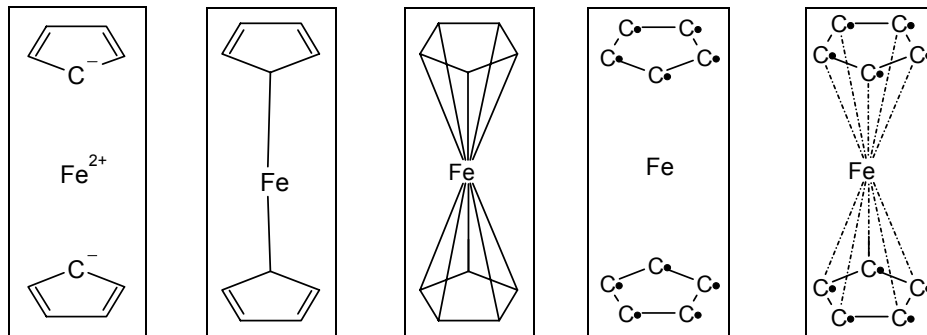
* **Normalisation of functional groups**

Additionally atoms in an unusual valence state or unusual representations of functional groups will be converted into a normalized representation.

Functional group	Original representation	Normalized representation
5-bonded N-Atoms		
e.g. nitro group		
5-bonded N-Atoms		
5-bonded N-Atoms		
5-bonded N-Atoms		
enolate group		
thio-enolate group		
diazo group		
diazonium salt		
azide		
azide		
Carbon monoxide		

* **Special Molecules with alternative representations**

In the course of time several methods have been used to represent complexes and organometallics, e.g. ferrocene



4.3 GENERIC STRUCTURES

You can define the following generic structures

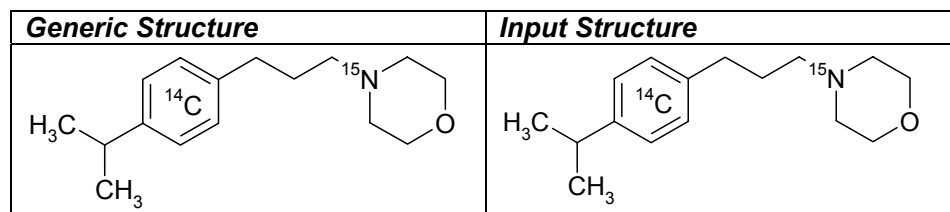
- * Isotopes at an unspecified position in rings
- * Substituents with unknown structure
- * Variable side chains
- * Substituents with unspecified position in rings and chains
- * Tautomers
- * Pseudotautomers

* Isotopes at unspecified positions in rings

Description

To define Isotopes at unspecified positions in a ring, draw a single atom and its corresponding mass WITHIN the ring. This mass will be assigned to all atoms of the same type in the smallest ring surrounding the isotope.

Example

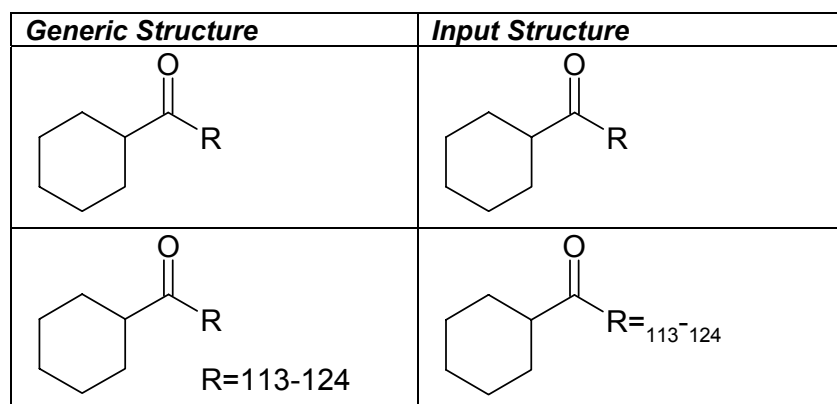


* Substituents with unknown structure

Description

To draw unspecified substituents, use the atom type R. You may assign a range for the mass (if known) by typing the range in the text field of the R atom.

Examples



* **Variable side chains**

Description

Resolve all brackets and additional explaining text to evaluate the longest chain possible. If this chain shall contain double bonds with unlocalized positions, assign the bond type “single/double” to all bonds of this chain.

Examples

Generic Structure	Input Structure
<p>$n = 10, 11, 12(60-70\%), 13$</p>	
<p>$n = 10, 11, 12(60-70\%), 13$</p>	

* **Substituents with unspecified position in rings and chains**

Description

To assign more than one possible position for one substituent, draw a bond from the substituent to each possible position and assign these bonds the bond type “Any”.

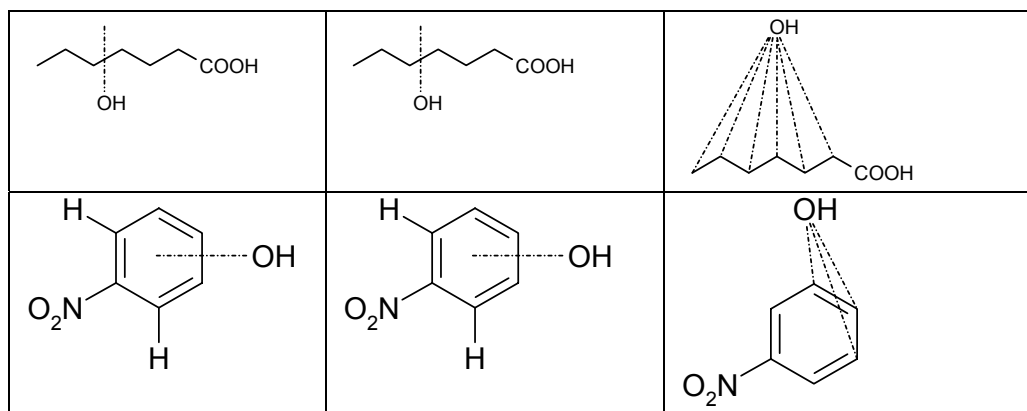
If the position of the substituent in a ring is not specified, draw a bond with bond type “Any” from the substituent to the middle of the ring.

If the position of the substituent in a chain is not specified, draw a bond with bond type “Any” from the substituent crossing the chain.

To exclude specific positions among several possible positions, block these positions by adding explicit Hydrogens.

Examples

Generic Structure	Input Structure	Database Representation*



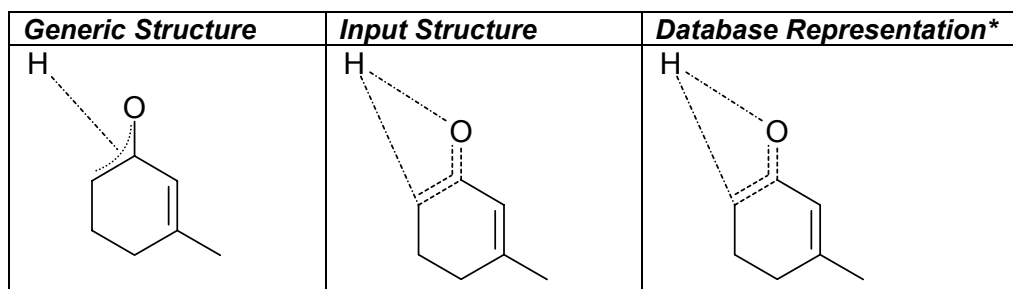
* The database representation will be generated automatically by the registration software.

* Tautomers

Description

To draw a mixture of tautomers, select the Hydrogen and draw it as substituent with unspecified position (Draw Any bonds from the Hydrogen to all possible positions). In addition assign the bond type “single/double” to all bonds of the σ -skeletal structure.

Example



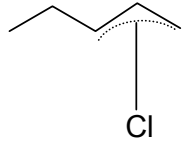
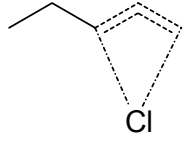
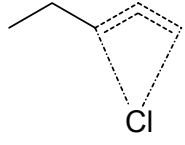
* The registration software will not modify the input structure.

* Pseudotautomers

Description

To draw a mixture of pseudotautomers, select the atom with variable position and draw it as substituent with unspecified position (Draw Any bonds from this atom to all possible positions). In addition assign the bond type “single/double” to all bonds of the σ -skeletal structure.

Example

Generic Structure	Input Structure	Database Representation*
		

* The input structure will not be modified by the registration software.

5. Advanced Stereochemistry

* Stereochemical centers

Description

Instead of using the chiral flag to specify absolute stereochemistry for a whole molecule, you may specify absolute and relative stereochemistry for single atoms in one molecule.

Select the stereochemical center and add an asterisk to the atom symbol to assign absolute stereochemistry.

Use this procedure for absolute stereochemistry only at the following atom types: C, N, Si, P, S, Ge, As, Sb, B, Sn.

Examples

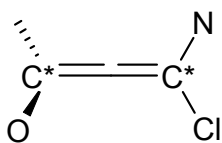
„C*“, „N*“, „N+*“

* Configuration at double bonds

Description

E or Z Configurations are assigned automatically to all double bonds (and higher homologues with odd numbered cumulated double bonds) following the CIP rules. Configurations at allenes are assigned by specifying up/down bond at one end of the double bonds. Use an asterisk in the atom label additionally to the atom symbol to specify absolute stereochemical configuration.

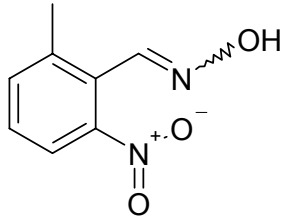
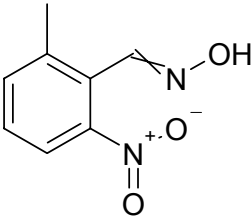
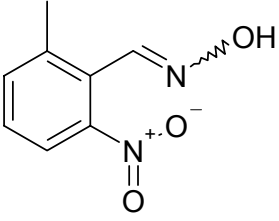
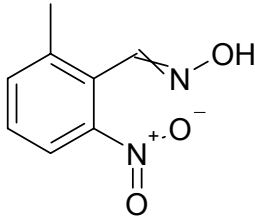
Please note that wedged bonds have to be drawn in pairs.



Allene with absolute stereochemistry

For unknown stereochemistry at double bonds, this bond has to be marked explicitly by assigning the bond type “double/either” or by drawing connecting a ligand with an “either” bond (wavy bond)

Example

Display Structure	Input Structure	Database Representation*
	 or 	

* The database representation will be generated automatically by the registration software.