

Beilstein
Commander TM
Getting Started

Distributed by

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Manual Version 5.0, July 2000, for Beilstein Commander Version 2000 and CrossFire Server Version 2000.

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6.2 THE F

Introduction

1

1 Introduction

1.1 General

The Beilstein Commander provides the user interface suite for Beilstein's products. The current version supports access to the CrossFire system as well as to AutoNom.



CrossFire:

CrossFire is a client-server based database system, which lets you search and display information in a way which is most applicable to you; the artificially created barriers of information about Substances (molecules and properties), Reactions and Citations have been broken.



Autonom:

AutoNom (Automatic Nomenclature) is a fully automatic and practical computerized system for the generation of IUPAC systematic nomenclature directly from the structure diagrams of organic compounds.

Since the different products have different interface requirements, the Commander configures itself accordingly.

When using CrossFire, the Commander is configured with a Structure and Reaction editor, a Fact editor and the Display Hits module. These are all linked together through the Commander to give one coherent interface unit.

The Commander provides the means to access the CrossFire server, Beilstein and Gmelin databases and your own customer databases; allowing searches to be carried out, results displayed and the database to be browsed - thus giving you the ability to navigate through the world of chemistry.


1.2 Manuals

The manuals of the CrossFire package are delivered as a hard copy and as the original Microsoft Word for Windows files. You will find the files on CD-ROM.

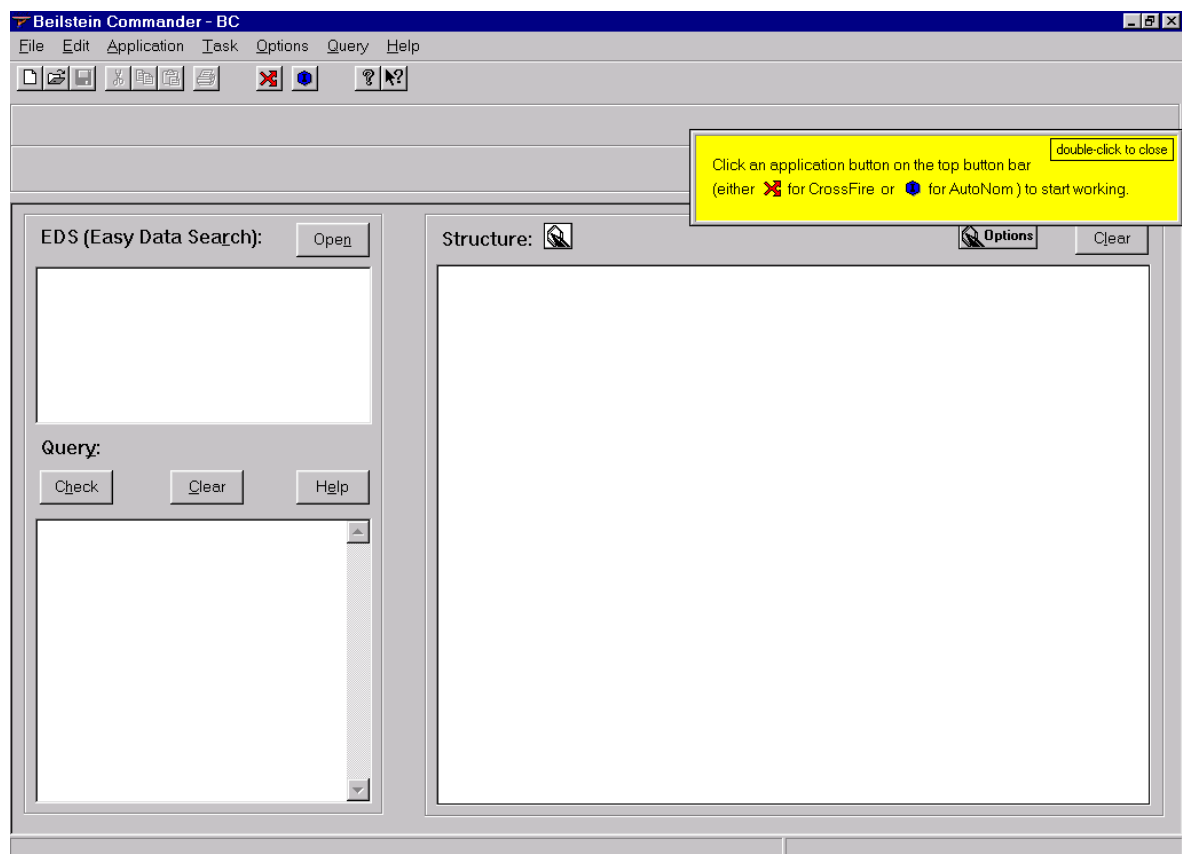
Starting the Beilstein Commander

2

2 Starting the Beilstein Commander

After a successful installation, you can start the Commander by double-clicking the  icon in the Program Manger.


After the Beilstein Commander has been started it will present to you a screen with buttons and windows:

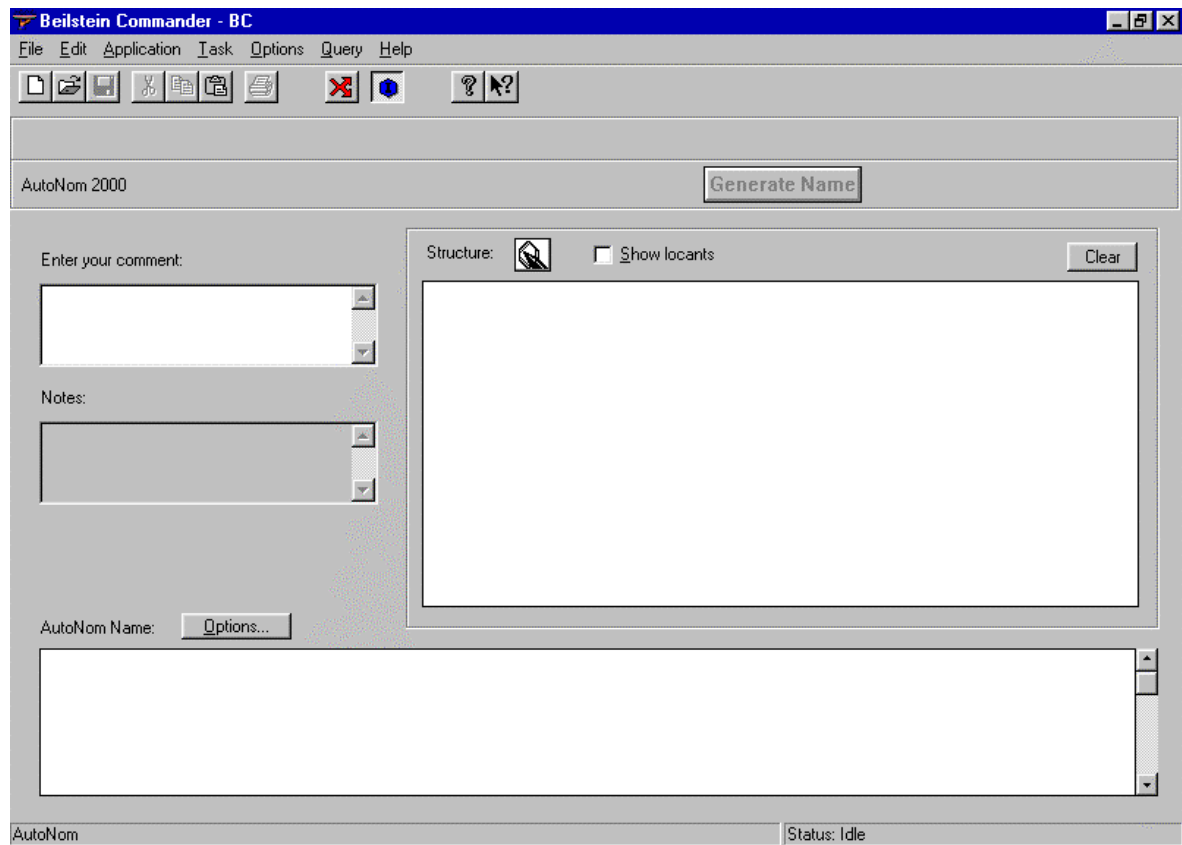


2.1.1 Starting CrossFire

Select from the menu **Application: CrossFire** or click the  - button. Please follow the instructions in section 2.2.1

2.1.2 Starting Autonom

Select from the menu **Application: AutoNom** or click the -button. The Commander configures itself in the following way:

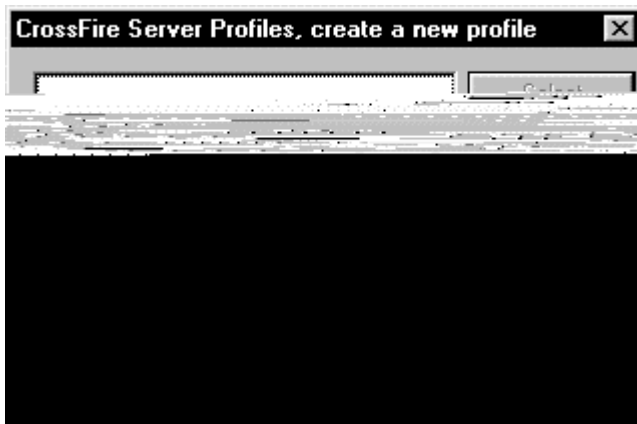


Please see further description in section 7.

2.2 Starting CrossFire

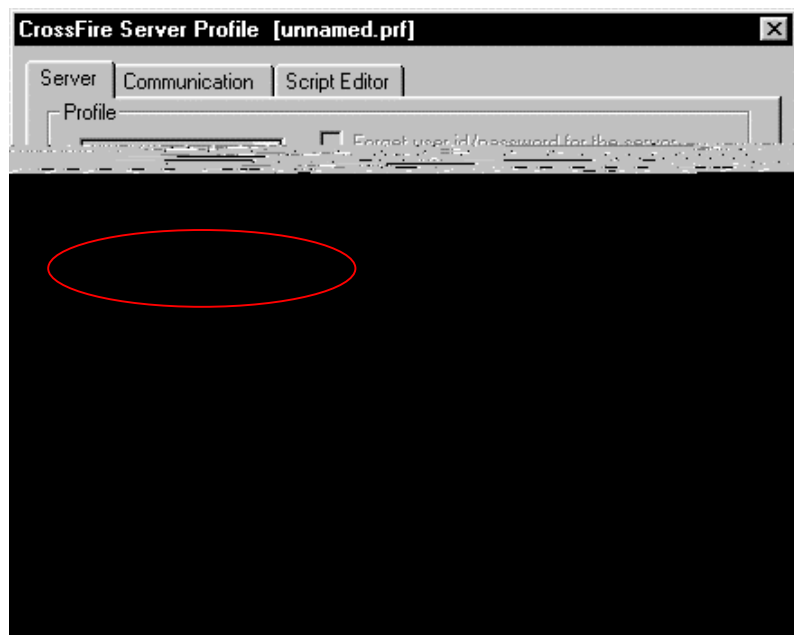
2.2.1 Connections Settings

If no communication profile has been created yet (e.g. by your system administrator), you will get the following dialog box:



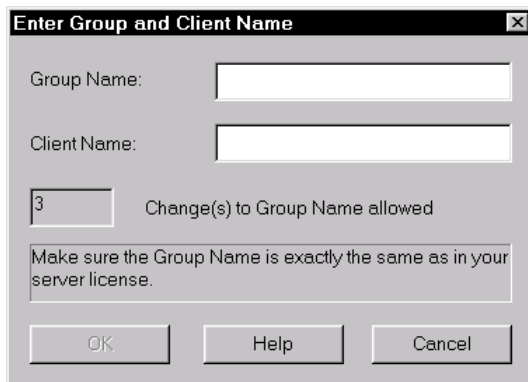
Click the 'New'-button and you will get the following dialog box:

- Enter the host name (name or IP address) of your CrossFire server.
- Enter the operating system (OS)
- Click 'OK'



- You are requested to enter a file name, in order to save the settings.
- Select the profile name *.prf.


After the first start of CrossFire you have to enter your Group Name and a Client Name.



The dialog box titled "Enter Group and Client Name" contains the following elements:

- Group Name: [Text input field]
- Client Name: [Text input field]
- 3 [Text input field] Change(s) to Group Name allowed
- Make sure the Group Name is exactly the same as in your server license.
- Buttons: OK, Help, Cancel

If you do not know your Group Name, please ask your system administrator. The Client Name should be a unique name for your PC.

Click on the -button and you will get a further dialog box :



The dialog box titled "Server User ID and Password" contains the following elements:

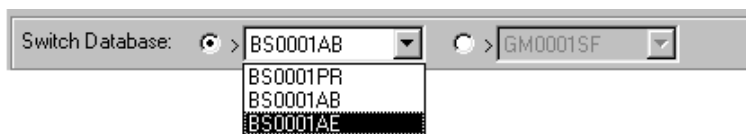
- Logon to CrossFire server [Text input field]
- Host 172.17.28.58
- User ID [Text input field]
- Password [Text input field]
- Change password... [Text input field]
- Save user id and password
- Buttons: OK, Cancel

Please enter your User ID and password. (If you do not know it, please ask your system administrator.)

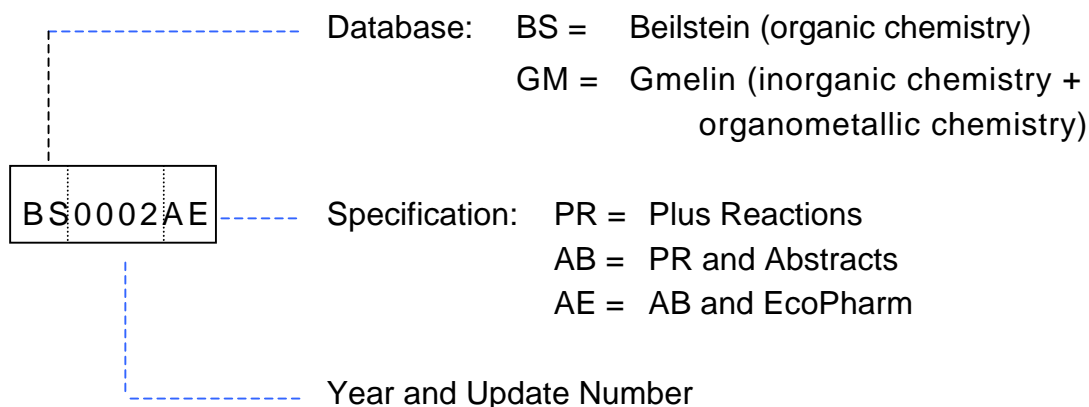
2.2.2 Select a Database

Database Selection Bar



After a connection to a CrossFire server has been established, the „Database Selection Bar “ will display the available databases:



The look of this bar depends on the licensed databases. Beilstein and Gmelin databases will be displayed in different list boxes. Every list box will display the different database versions. From within this listbox you can select a database. You can switch between Beilstein and Gmelin databases listbox on the spot.



2.2.3 Searching Procedure

- After drawing a query in the Structure Editor (chapter 3) and/ or entering a factual query in the EDS form (chapter 4) or Fact Editor (chapter 5), you are ready to perform a search in the specified database.
- Starting a search is **only** possible from the Commander !
- From Structure Editor or Display Hits, switch to the Commander using the -button or the 'F7'-key.
- To start a search within the Commander simply click the -button or use the 'F7'-key.


2.2.4 Opening the Structure Editor

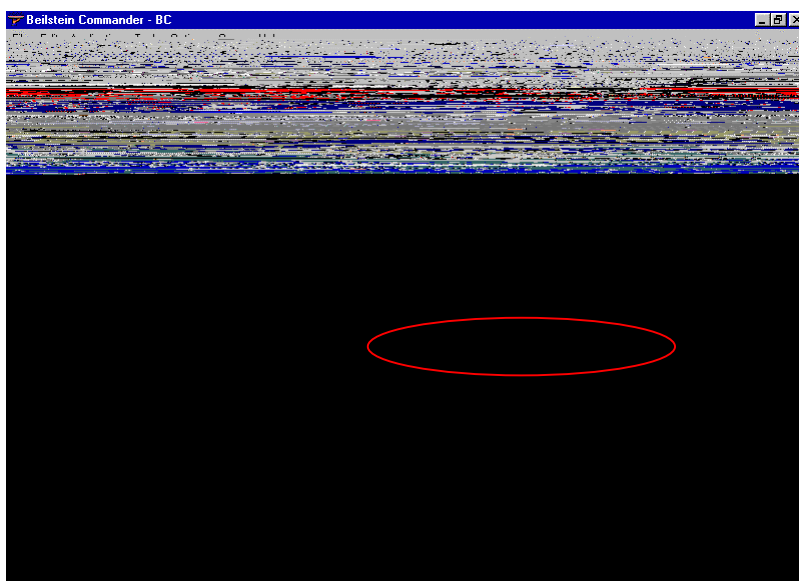
You may use either the Beilstein Structure editor or ISIS/Draw for drawing structures and reactions.

Please use the menu item **Options: Structure Editors...** for selection.



For starting the structure editor:

- Choose from the menu 'Task: Structure Editor' or
- 'Double click' on the Structure Editor window or
- Click the button  (Structure Editor)



See further description of the Beilstein structure editor in chapter 3.

2.2.5 Opening an 'Easy Data Search' -Form

The following window makes a list of EDS forms available to you. In order to facilitate property searching some predefined EDS-forms are offered.

The availability of the EDS-forms depends on the kind of the available databases.



Select the desired EDS-form. Double click will open the form.
(See further description in chapter 4).

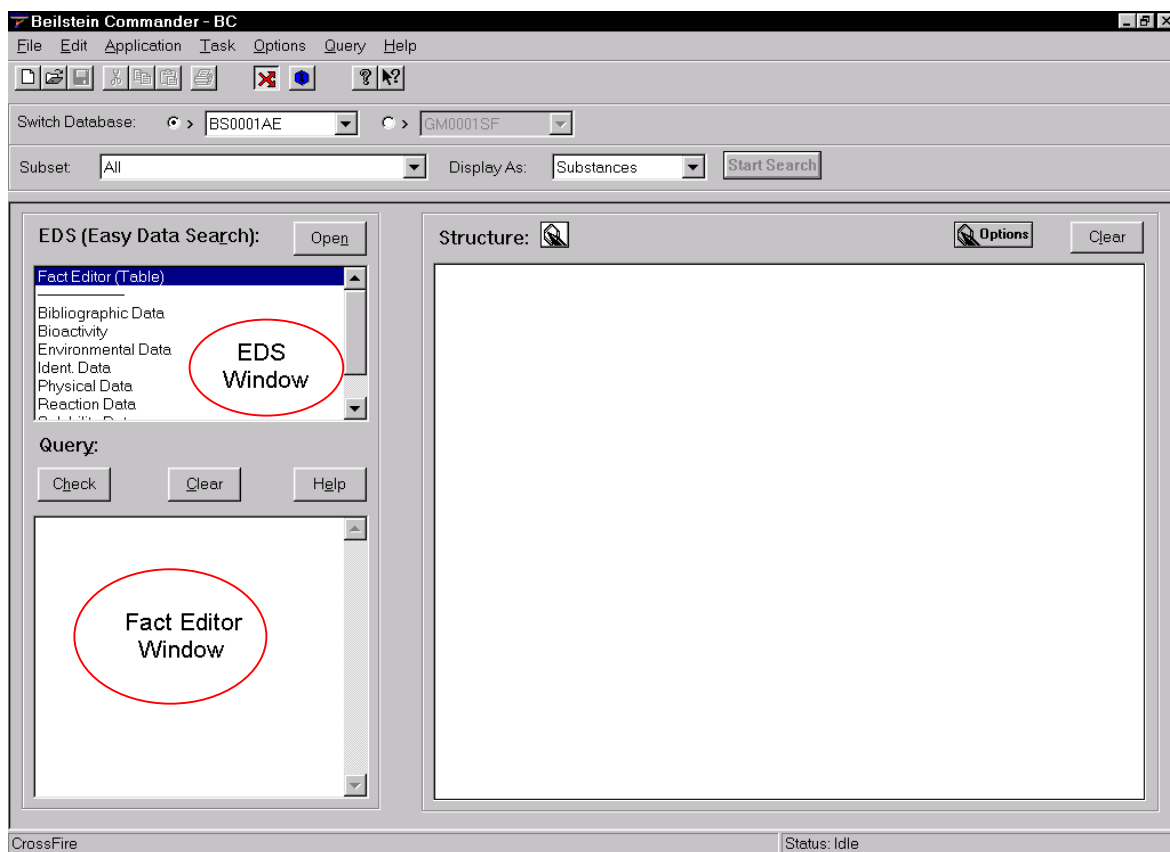
2.2.6 Opening the Fact Editor (Table)

The Tabular Form

The tabular form of the Fact Editor allows a guided and flexible, comfortable and quick input of all kind of factual queries.

Please select the top entry „Fact Editor (Table)“ in the EDS-window **first**.

- ‘Double click’ on the entry „Fact Editor (Table)“ in the EDS-window **or**
- Double click on the Fact Editor window **or**
- Choose from the menu **Task: Fact Editor or EDS Form** (same as ‘F8’-key)

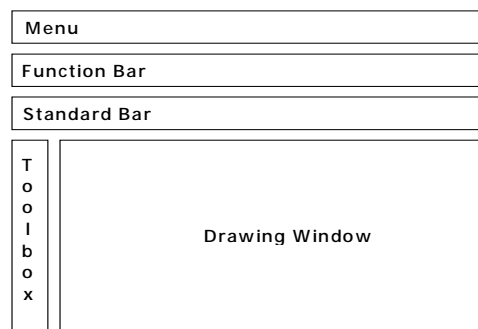
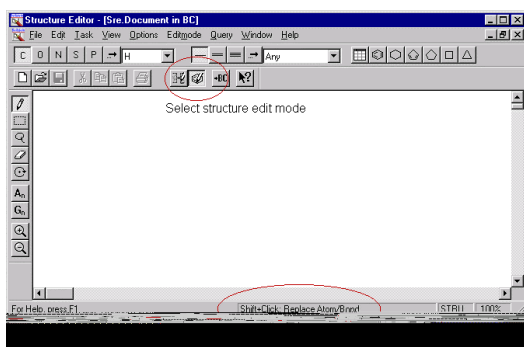




Beilstein Structure Editor

3

3 Beilstein Structure Editor

The structure editor allows the input of structure queries as well as reaction queries.




The actual *Function Bar* depends on the selected Editmode. In the Structure Editmode () you have typical atom-, bond- and template-buttons. In the Reaction Editmode () you have buttons to define a molecule role in a reaction.

The *Standard Bar* contains several buttons which provide short-cuts to menu-functions, including selecting the Editmode and switching to the Beilstein Commander.

Toolbox Keys:

-  edit
-  select
-  lasso
-  erase
-  rotate
-  magnify
-  reduce

3.1 Drawing / Editing Atoms

- Activate the edit tool  and choose one of the atom buttons (Function Bar)
- Draw the structure with the currently active atom and bond (usually the carbon skeleton)
- Click on an already existing atom to open the 'Atom Attributes' dialog box to change it (editmode)
- 'Shift+click' to change an atom to the current selected atom attribute and type


Atom buttons 


Further choice of atoms as well as generic groups:



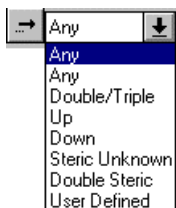
- Atoms:
H, F, Cl, Br
- Atom lists:
A (any atom), M (any metal), X (any halogen)
- User Defined
Apply user defined settings from the 'Atom Attributes' dialog box (see 3.6, p. 29)
- Elements...:
Opens periodic table from which you can choose any atom
- Generics...:
Opens table of generics from which you can choose predefined atom lists, predefined generic groups, user-defined atom lists A_x and user-defined generic groups G_x (see 3.9 and 3.10)







3.2 Drawing / Editing Bonds

- Activate the edit tool  and choose one of the bond buttons
- Draw the structure with the currently active bond (and atom)
- Click on an already existing bond to open the 'Bond Attributes' dialog box to change it (editmode) or 'shift+click' to change a bond to the current selected bond attribute and type.

Bond buttons: single, double, triple 


Further choice of bonds:

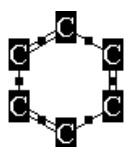


- Drawing steric bonds (up , down ) for stereogenic atoms
- Defining Z/E-isomers (double steric ) for double bonds
- Allowing groups of bonds (any , double/triple , steric unknown )
- Selecting user-defined bonds

- Stereo information is only included in the search when the 'Structure Query Options' (see section 3.7) have been set to Absolute, Relative, or Racemic. The default setting is 'stereo off'!

3.3 Drawing Rings

Clicking one of the -buttons pastes the corresponding ring into the structure window





Annelated rings: drag the square in the middle of the bond to the bond you want to fuse

Spiro-fused compounds: drag the square at the atom to merge it to another atom

3.4 Template Files

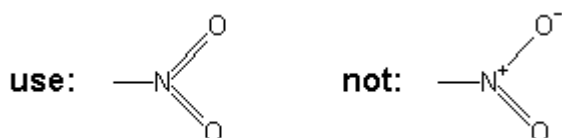
Template files contain pre-defined molecules, substructures as well as functional groups

- Use the template button  to browse the active template file and select the desired (sub)structure by 'double click'
- To change the active template file use the menu 'File: Open' in the template window or choose 'File: Template' in the structure editor menu
- To generate your own template files use the menu 'File: Save Copy As' Select the position (INO) within the template file with the  -button.

3.5 Functional Groups

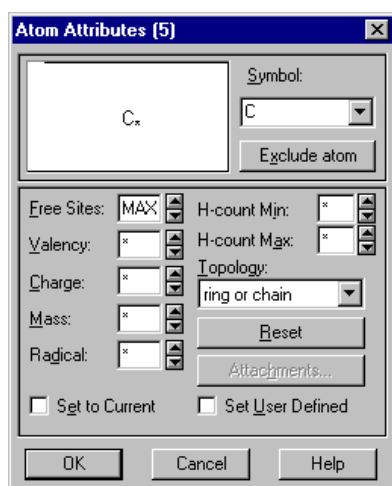
Make sure you follow the structure conventions used in the Beilstein database (see online help of the Beilstein structure editor); if you are not certain how to draw a functional group choose it from the template file "residue.bsd".



A typical pitfall:



☞ If different representations are possible, the neutral structure is preferred.

3.6 Setting Atom Attributes (individual attributes)



Click an atom in the structure editmode (/) to specify atom attributes:

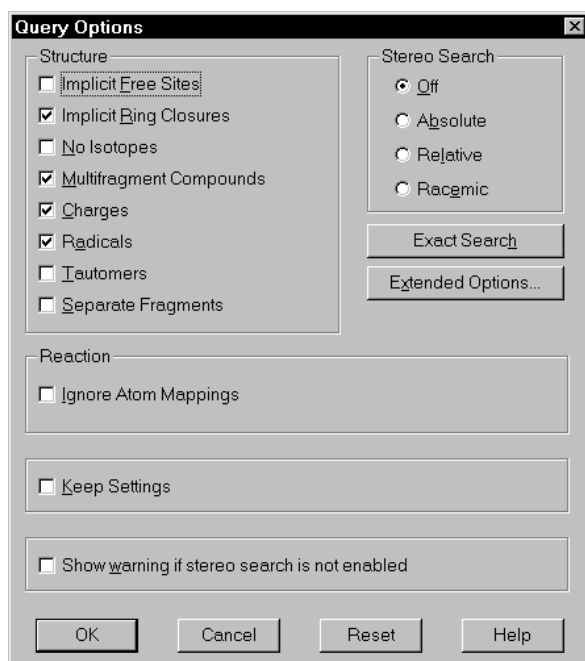
- You can enter a number of 'Free Sites' (use down arrow for MAX), the charge etc. for the selected atom
- Specify isotopes using the 'Mass' of the atom
- Specify the 'Topology' (e.g. use ring if you want the atom to be part of a ring system)
- 'Exclude atoms' which should not be retrieved in the hitset

- If you want to change several atoms in the same manner, check "Set to Current", click "OK" and use "shift+click" to place the current atom at additional sites.

3.7 Structure Query Options (global attributes)

Options that will be taken into account for the whole structure query can be set

- in the Structure Editor from the menu 'Query' or
- in the Commander by opening the dialog box with the 'Options'-button (hereby you can use those options for drawings imported from other structure editors such as ISIS)



- Check 'Implicit Free Sites' if you want to perform a unspecified substructure search

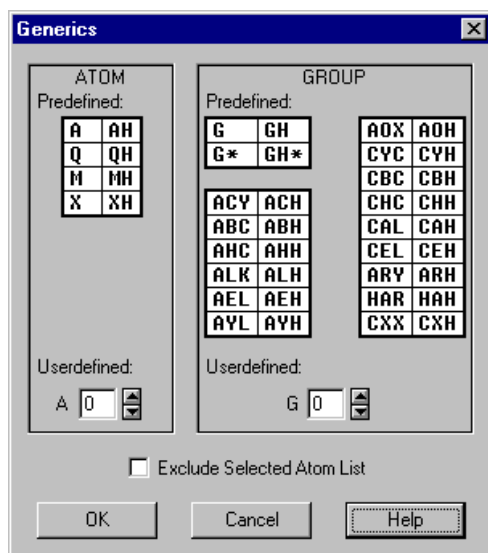
- If you are interested in stereochemistry use the appropriate switch (i.e. 'Absolute' if you are searching for exactly the drawn stereochemistry)

Note: Click the button 'Extended Options' to get a new dialog box, in which you can specify the number range of charges, unpaired electrons, components etc.




- You can also allow or exclude charged or multifragment compounds, isotopes, radicals, tautomers etc.

3.8 Generic Groups and Atom Lists

The predefined generics allow you to enter groups of atoms (*Predefined Atom Lists*) or structural elements with certain basic tautologic features (*Predefined Generic Groups*) without the need to specify them completely.





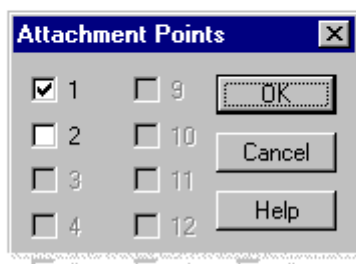
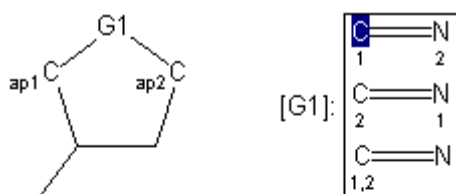
To enter an atom list or a generic group you can:

- choose from the atom box  H : 'Generics', select the desired atom list or group and place it in the structure you are drawing or
- click an atom in the editmode () and select 'Symbol; Generics' in the Atom Attributes dialog (see 3.6, p. 29)

- To see the definitions of the predefined generic groups look at the tool tip or use the help button to view the hierarchical order
- The predefined generic groups except G and G* can only have one bond to the parent structure. User-defined generic groups and atom lists can have more than one bond.

3.9 Creating User-defined Generic Groups

1. Place the G_n-atom symbol (G 0 ) as shown in the previous section in the structure you are drawing
2. Draw the desired fragments for the generic group
3. Select the fragments to be part of the generic group and press the -button; choose the same number as in step 1



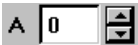



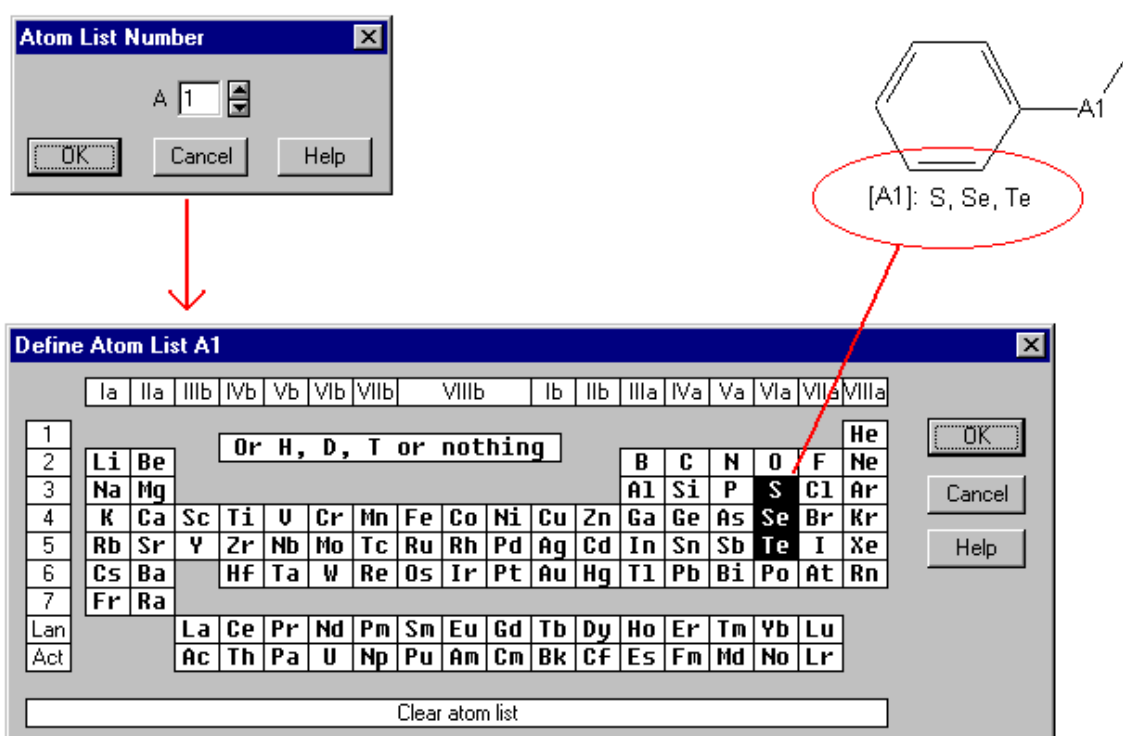
For fragments containing more than one atom you have to set attachment points:

1. Click the atom of the fragment where it is to be attached to the parent structure
2. Press the 'Attachments'-button in the atom dialog box
3. Click the appropriate number(s)

- You can define a frequency for any generic group via the menu 'Query; Generic Frequency'; this feature allows you to restrict the occurrences of generic groups at the defined positions (e.g. group 1 may occur up to two times at 3 possible positions)

3.10 Creating User-defined Atom Lists


1. Choose 'Generics' from the atom menu  H  and select a number  A 0
2. Place the A_n-atom symbol in the structure you are drawing using 'Shift+click'
3. Press the  button and select the number of the atom group
4. Choose the desired atoms from the periodic table appearing on the screen



The image illustrates the process of creating a user-defined atom list. It shows three main components:

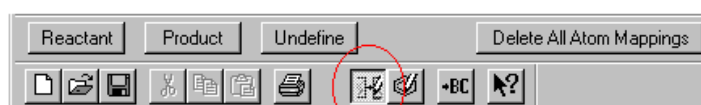
- Atom List Number Dialog:** A small window with a title bar 'Atom List Number'. It contains a text field 'A' with the value '1' and a dropdown arrow. Below the field are three buttons: 'OK', 'Cancel', and 'Help'.
- Chemical Structure:** A skeletal structure of a benzene ring with a substituent atom labeled 'A1' attached to one of the carbons. A red oval highlights the 'A1' label, and a red arrow points from this oval to the 'Define Atom List A1' dialog.
- Define Atom List A1 Dialog:** A larger window with a title bar 'Define Atom List A1'. It features a periodic table of elements. Above the table is a text input field containing 'Or H, D, T or nothing'. The element 'S' (Sulfur) is highlighted in the table. To the right of the table are three buttons: 'OK', 'Cancel', and 'Help'. Below the table is a text input field labeled 'Clear atom list'.

3.11 Reaction Attributes


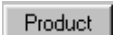
First draw the molecules in the structure editmode, then switch to reaction editmode by using the -button or choose from the menu 'Editmode: Reaction'.



Structure Edit Mode




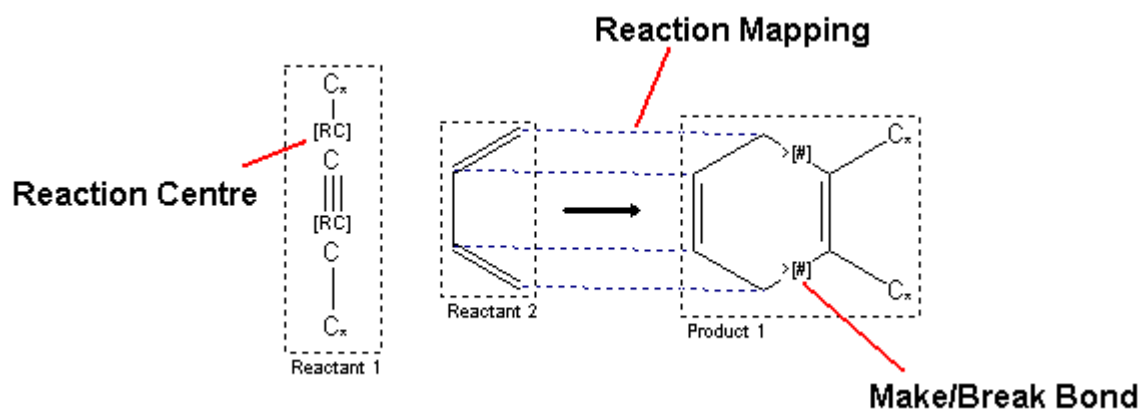
Reaction Edit Mode

The function bar changes to allow reaction role setting and the selectmode is activated. Now select a molecule and press the  /  -buttons to define its role as starting material or product.

	<ul style="list-style-type: none"> • You can define one or more reactants <i>and</i> one or more products • You can also define only reactant(s) or product(s), so-called "half-reactions"
--	--

3.12 Further Reaction Attributes (optional)

In the reaction editmode the function of the -button is altered. If you click on an atom you get the 'Atom Attributes in Reaction' dialog box; if you click on a bond you enter the 'Bond Change by Reaction' dialog.



Mapping: links corresponding atoms in the reactant(s) and product(s) respectively by drawing a dashed line between them in the same way a chemical bond usually is drawn

Reaction center: defines that a reaction must take place (or must not take place) at a particular atom

Bond change

3.13 Special Hot Keys (Structure Editor)

'Ctrl + D'	Delete all	'N'	reset average bond length to standard
'Ctrl + E'	Copy all	'F'	fit structure into whole window

Easy Data Search (EDS) - Form

4

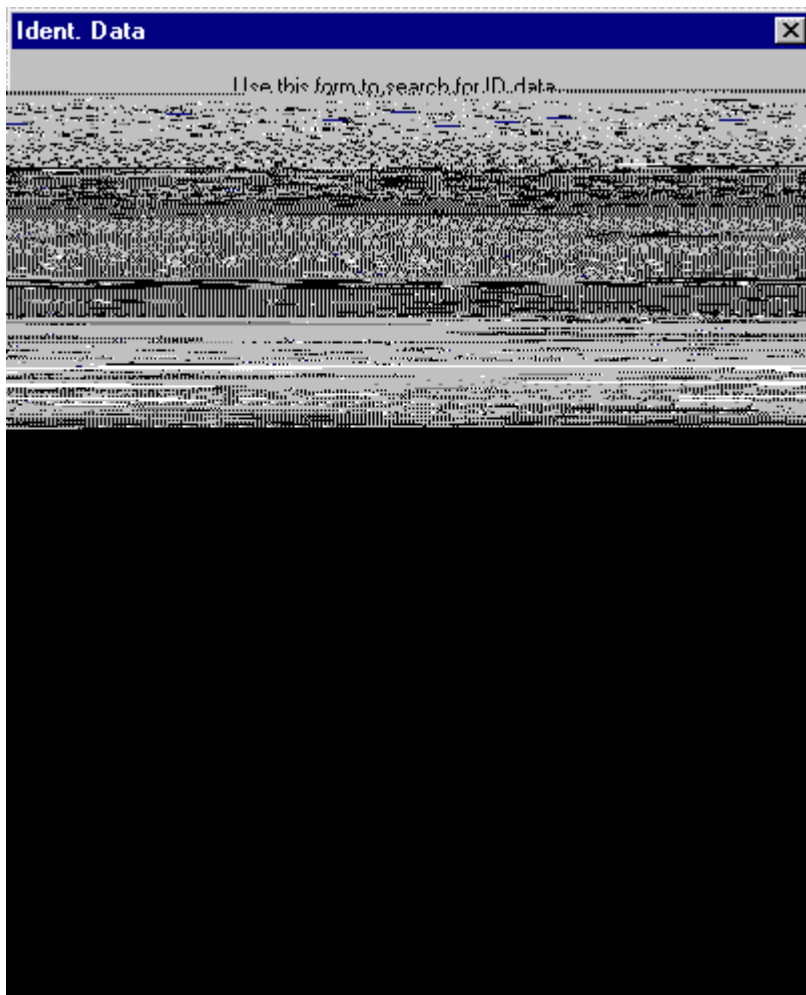
4 Easy Data Search (EDS) Forms

There is a list of predefined EDS-Forms available. The list of EDS-Forms depends on the selected database. There are specific Beilstein EDS Forms and Gmelin EDS Forms, well adapted for the convenient search in these databases.


Some examples are described in the following sections.

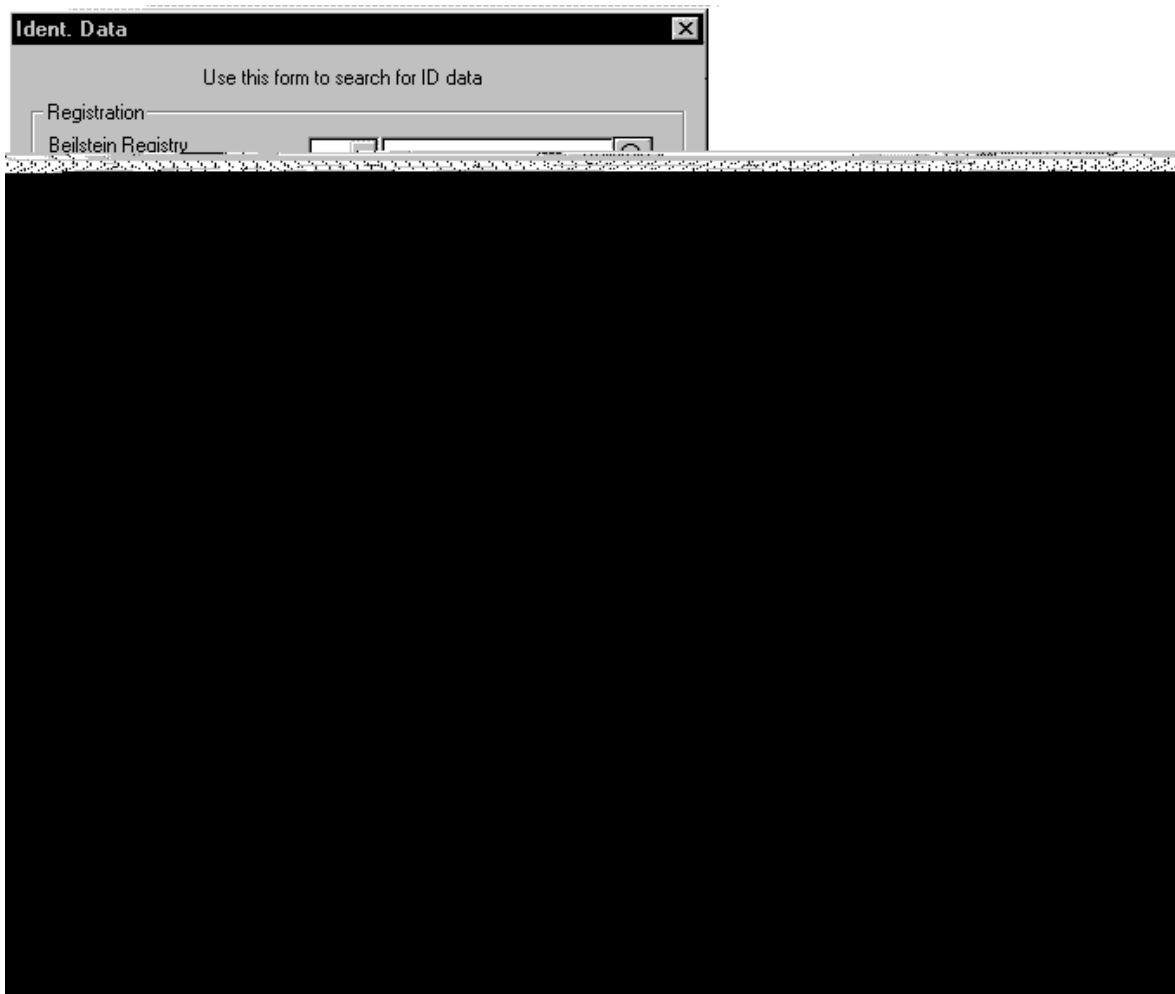
4.1 Identification Data (for the Beilstein Database)

The EDS-form 'Identification Data' for the Beilstein database looks like:



In the case of numeric fields (e.g. number of fragments) there is the option to use the following operators: "=", "<", "<=", ">" or ">=".

- Fill in the search term you are looking for, e.g. chemical name = nifedipine
- Press the  -button and you will see a list of field values (index of all entries in this field).



- Select a data entry and click 'OK'.
- Click 'OK' again and you will get back to the Commander.
- Start the Search by clicking the **Start Search** -button or 'F7' key.

4.2 Bibliographic Data

This form allows to search for authors, journal titles and publication year.

In addition there is the search field 'basic index search', which allows searching the abstracts including titles and keywords.

The screenshot shows a dialog box titled "Bibliographic Data" with a close button (X) in the top right corner. It is divided into two main sections: "Find all citations, where" and "Basic Index Search".

Find all citations, where

- Author:** A dropdown menu is set to "is" and a text box contains "paulsen". A search icon is to the right.
- Journal Title:** A dropdown menu is open, showing options: "is", "starts with", "ends with", and "contains". Below the dropdown is the text "e.g. tetrahedron". A search icon is to the right.
- Publication Year:** A dropdown menu is set to "=", and a text box is empty. Below the dropdown is the text "e.g. 1994-1996". A search icon is to the right.

Basic Index Search

- Search for any word in Titles or Abstracts or Keywords, which** A dropdown menu is set to "is" and a text box is empty. Below the dropdown is the text "e.g. force near constant (check Help for more details)". A search icon is to the right.

At the bottom of the dialog box are three buttons: "OK", "Help", and "Cancel".

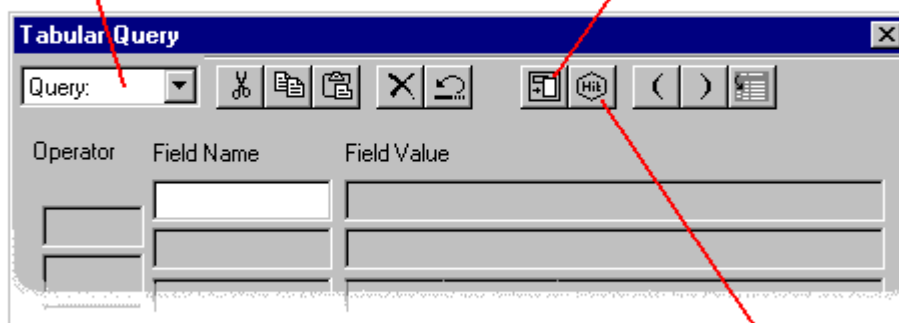
- Looking for an author: If you enter only the last name of the author, you should select the option „starts with“.
- The feature „Basic Index Search“ is only available, if CrossFire Abstracts or CrossFire EcoPharm is licensed.

5 Tabular Query Editor

The Tabular Query or Fact Editor allows you to search for properties of substances or reactions or for bibliographic information. You can perform factual queries either directly in the Fact Editor window (experts) or in the Tabular Query Editor (see below).

Selection Area


Expand Field/List Values



Select Hitset

5.1 Field Name

Fill in the code of the field you want to search for:


- Type the codes directly into the field **or**
- Pick them from the data structure, which can be opened by the -button, double-clicking the cell or 'F2'-key. Select the appropriate field code by 'double click' in the 'Available Fields' dialog box.
- You can search for a specific field name by using the '*Find*'-button and typing the name of the desired property or attribute in the 'Available Fields' dialog box ('F2'-key).

5.2 Field Value

Fill in the search term(s) (e.g. values, keywords, phrases) you are looking for:

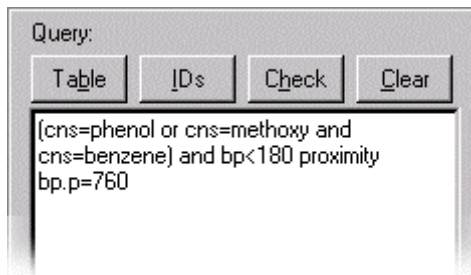
Operator	Field Name	Field Value
	cns	phenol
+or	cns	methoxy
+and	cns	benzene
and	bp	<180
proximity	bp.p	760

- You can fill in ranges using a dash ("-") or use "<" and ">"-operators when looking for numerical values
- You can use truncation when you look for text ("*" for any number of letters, "?" for exactly one letter); you can truncate at the beginning, middle or end of the word

You can see a list of field values (index of all entries in this field) by the  -button or 'F2'-key

5.3 Operators

Use the logical operators **proximity**, **and**, **not**, **or**, **near**, **next** to combine fact queries (hierarchy: proximity > and, not > or):



Query:






Table	IDs	Check	Clear
-------	-----	-------	-------


(cns=phenol or cns=methoxy and
cns=benzene) and bp<180 proximity
bp.p=760

- Proximity requires that the search terms have to appear in the same subrecord and belong to the same occurrence of the fact (in this example boiling points measured at 760 Torr).
- If you want to combine fact queries in a different order than the default order, use parentheses **()** or type a "+" in front of the operator in the fact editor table.

5.4 Special Hot Keys (Fact Editor)

The 'Selection Area' list box determines the working area of most functions in the Tabular Query Editor. Possible Selections are the *whole query*, a *single line* or only the *marked text*.

'Ctrl + X'		CUT selection
'Ctrl + C'		COPY selection
'Ctrl + V'		PASTE selection
'Ctrl + D'		DELETE Selection
'Ctrl + Z'		UNDO

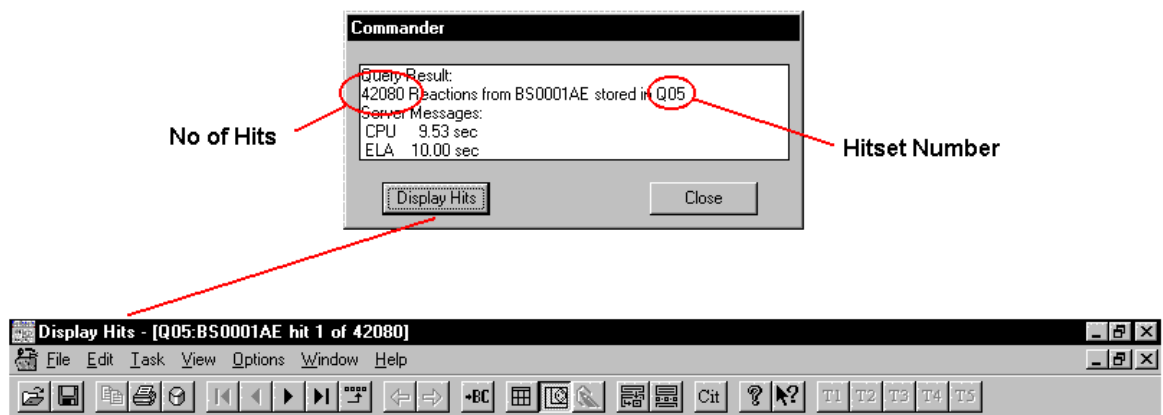
- If you use the "expand"-function by double clicking the field, clicking the -button or the 'F2'-key, make sure the cursor is placed in the field you want to expand
- The 'F3'-key opens a window where you can type in the query

Display Hit

6


6 Display Hits

After performing a search you will get a message indicating how many hits are in your hit set. To open the 'Display Hits'-Window click the **Display Hits**-button.



- You can customise the way hits are displayed via the 'View' menu (6.3, p.56), the 'Options' menu (6.4, p.61) and the Function Bar!

6.1 Browsing the Hitset

Hot Key	Button	Menu 'Edit: Goto Hit'
'Ctrl + Home'		First Hit
'Ctrl + PgUp'		Previous Hit
'Ctrl + PgDown'		Next Hit
'Ctrl + End'		Last Hit
'Alt + S'		Select Hit Number

- You can select and copy both structures and facts from the Display Hits Window and paste them into the Structure or Fact Editor where you can change and modify them to submit a new query. You can also paste it into any other application.

6.2 The File Menu



Open Hitset:

A hitset is loaded from the server side.

Close Hitset:

The current hitset will be closed.

Save Hitset as:

The current hitset will be saved on the server side.

Delete Hitset:

Deletes a saved hitset from the server side.

View Communication:

A separate window shows the communication with the server (former application: CrossLink)

Select Registry Number:

Entering a registry number retrieves the appropriate substance, reaction or citation

Get All References for a Hit:

Retrieves a list of references for a given substance or reaction (same as CIT-button).

Get Citation from LitLink:

A selected citation is sent to the LitLink server.

Export:

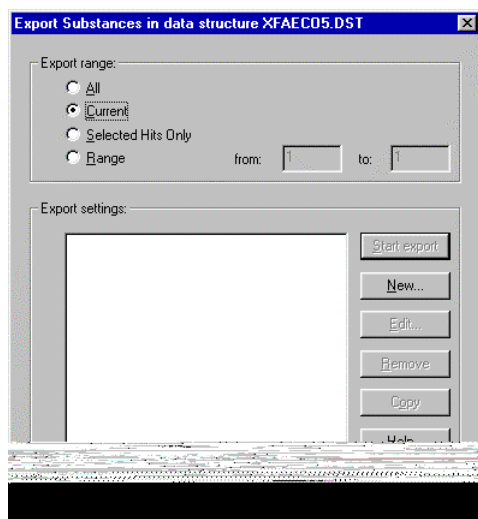
Exports data from the current hit or hitset. (See following section).

Print:

You can print the current hit, a range of hits or the complete hitset.

6.2.1 The Export Function

The menu item **File > Export** opens the following Export Dialog Box:



This dialog box is divided into two areas: “Export range” and “Export settings”.

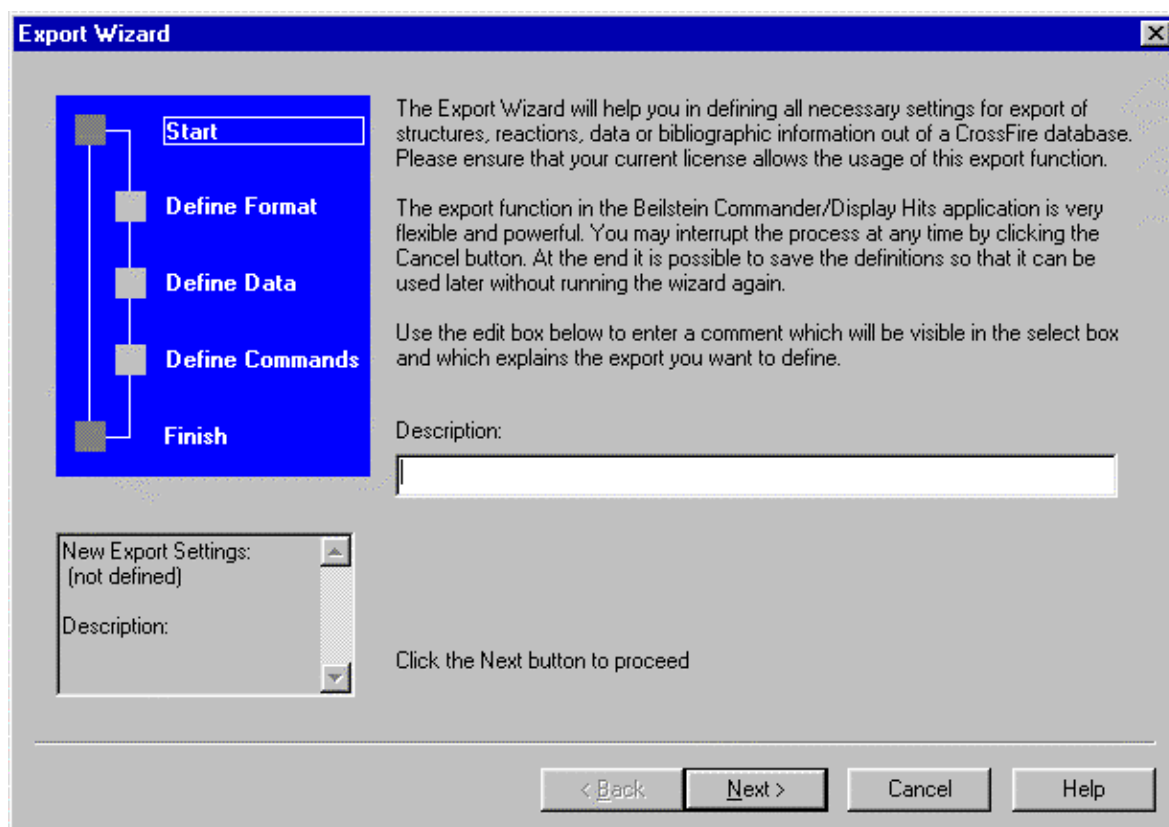
- **Export range**

Within this area you can decide whether you would like to export “All” hits, the “Current” hit, “Selected Hits Only” or a “Range” of hits from a given hitset.

- **Export settings**

The “Export Settings” window presents you all known export settings files for a given database. You can select various export settings files, which you can define by yourself, or create new ones. Once a settings file has been selected a click on “Start export” will perform the export.

Click the ‘New’-Button to define new export settings. The Export Wizard starts:



Export Wizard

The Export Wizard is a combination of five dialog boxes which will be presented one after the other and which will guide you in a logical order through the process of defining export settings.

The five steps for defining export settings are:

1. **Start:**
this is the first of the export wizards dialog boxes in which it is possible to enter a short description of the export settings to be defined.
2. **Define Format :**
here it is possible to define the export target format and the target itself.
3. **Define Data :**
define here the "Export View", i.e. which data Display Hits should export. If "ASCII" has been selected in step 2. then "Structures" will be grayed out.
4. **Define Commands :**
in this dialog box you can define whether you want to execute a command after the export has been performed. It is also possible to force Display Hits

to show a dialog box, before the actual export starts (default), and to define a Task menu item / Task button for the use of the defined export settings.

5. **Finish :**

Before the export settings can be saved this dialog box will display any errors and the final settings in an overview. If an error occurs during the definition then the 'Finish' button will be not available but a 'Next' button will show up. A click on this button will open the Wizard dialog box in which the error was observed.

6.3 The View Menu



Short Display ():

toggles between Short- and Full-Display mode. The Short display allows several hits within one window for a quick overview (specify the number of rows and columns in the 'Options' menu). Select individual hits by 'clicking' them. Double-click to view the full display for a record.

Identification:

shows only Identification (IDE)-data of each hit

All Fields:

displays all available fields for each hit

Hit only:

displays IDE-fields and only the data for the facts that have been searched

User View:

shows only those fields that have been selected by the user (customise within the menu 'Options > Define User View...')

Field Availability ():

opens an additional window which shows the names and codes of all available fields (see section 6.3.1).

Hitset Navigator:

The navigator dialog box allows navigating in hitsets and hyperlinks (see section 6.3.2).

Highlight Hits:

Highlights the data or (sub)structures that have been searched (the default colour is red)

Include Structures ():

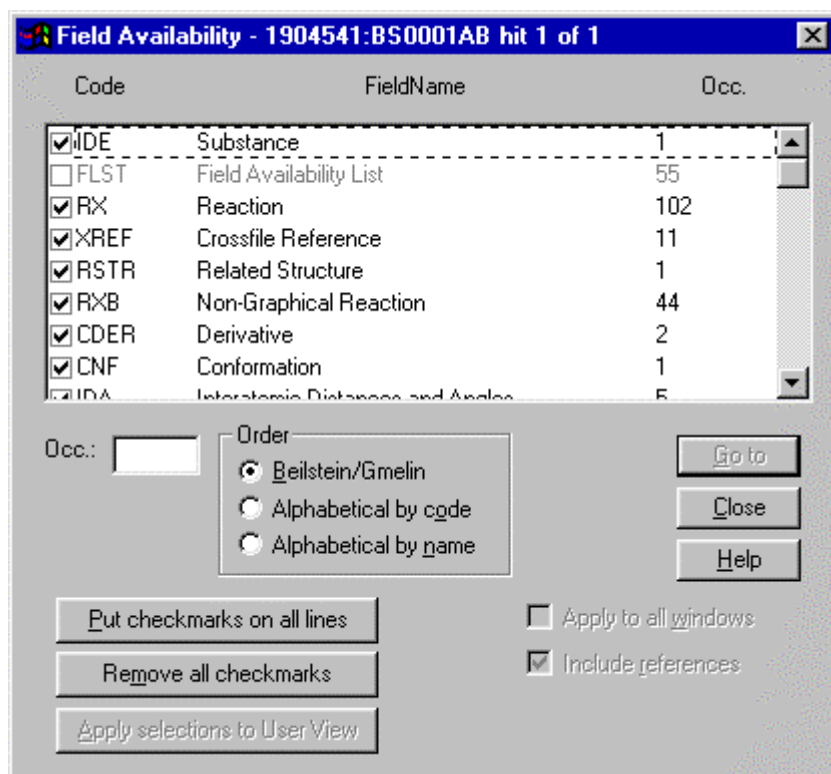
shows the structures associated with the hit in the data display (not recommended in the case of large hitsets or slow machines)

Include Field Availability:

displays a table of all available fields after the IDE-data for each hit

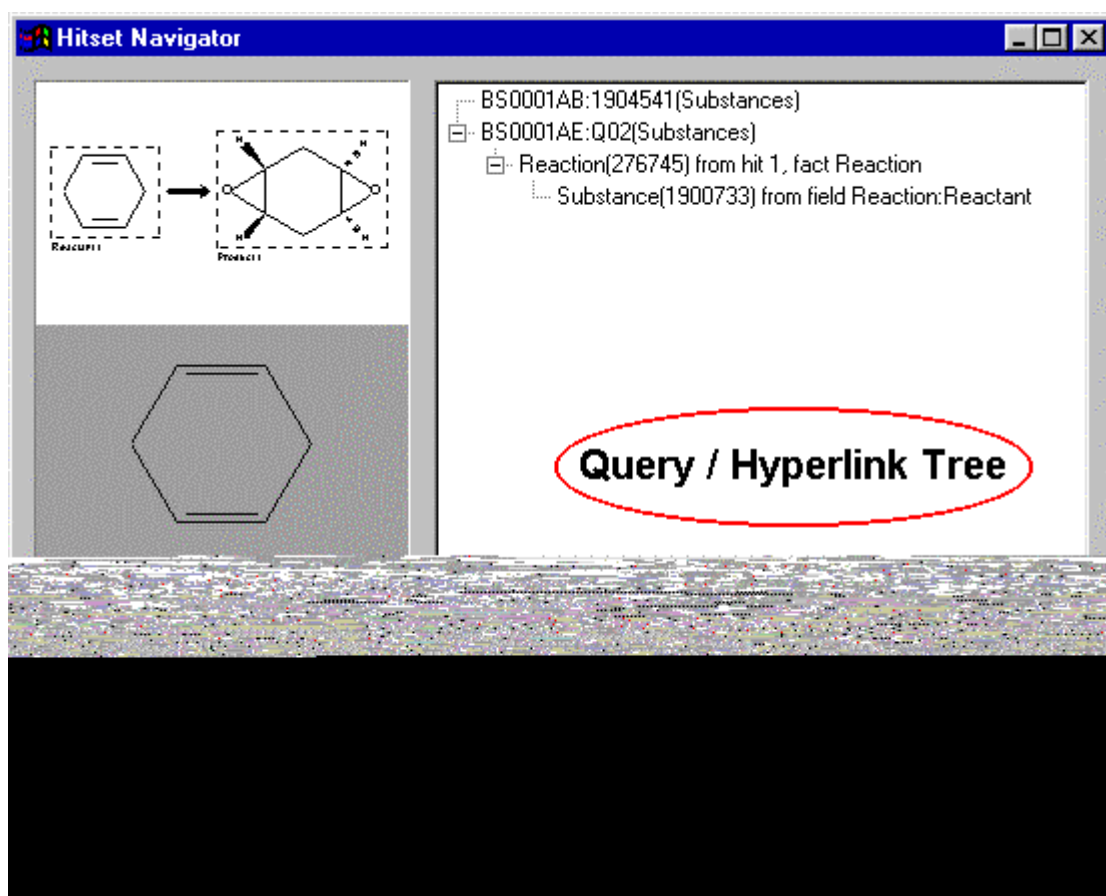
6.3.1 Field Availability Dialog Box

The Field Availability dialog box displays the name of each fact and number of occurrences for each fact respectively, thus providing an overview of the information present.



6.3.2 Hitset Navigator Dialog Box

This is the dialog box for navigating in hitsets and hyperlinks. It will always stay in front of the Display Hits until the Close-button has been clicked or the menu item **View > Hitset Navigator** has been unchecked.



The Hitset navigator is divided into a Structure / Query Display Window and a Query / Hyperlink Tree.

- **Query / Hyperlink Tree**

This window will display all open windows of the Display Hits (the same list can be seen under the Windows menu of the Display Hits, but only as a plain list). It usually starts with a hitset identified by its name, typically a Q-number, together with a database name. From this every hyperlink will open a new branch. A single click on an entry of a branch will update the “Structure / Query Display” window.

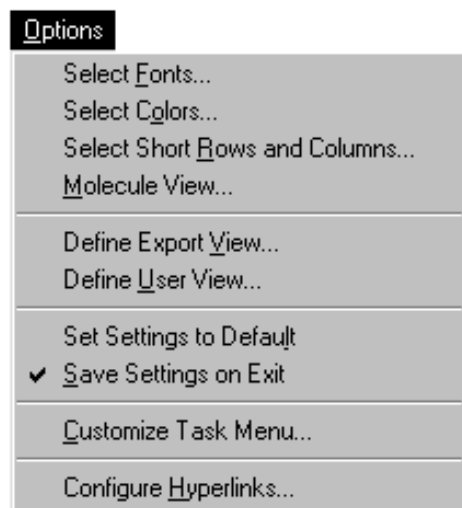
A double click on an entry will update the “Structure / Query Display” window and the Display Hits itself and will bring the corresponding hitset/hyperlink window to the front. The button “Go To” will do the same.

- **Structure / Query Display window**

This window will always show three pictures. The grey area in the middle corresponds to the selected entry in the tree display to the right. If the selected entry is a hitset, then it will display the query. If it is a hyperlink then it will display the entire structure or reaction. The area on top of the grey area displays the structure/reaction of the previous hyperlink. The area below the grey area will show the structure/reaction of the following hyperlink. It will only display structures or reactions if the hyperlink has been performed manually in the Display Hits.

6.4 The Options Menu

You can customise the appearance of the individual applications to a great extent using the 'Options' menu. In the display hits application you may want to specify the display or export layout:



Select Colors:

changes the colours of hyperlinks and highlighting

Select Short Rows and Columns:

changes the layout within the short display; up to 15 rows and columns can be used independently (this should scale with your screen resolution); in the citation context only the definition of rows is utilised (that is, you can only have one column).

Molecule View:

Specify bond length, atom font etc....

Define Export View:

You can define the extent of information to be extracted.

- For defining the specific export format and the destination of the data please use the menu item **File > Export** (section 6.2.1.)

Define User View:

Sets a user-defined filter for the display of hits; the fields can be selected and combined freely from the data structure of the selected database. Of course you can save or load individual user views.

- *'Define User View'* does not automatically activate it! You can do this in the *'View'* menu (see 6.3, p.56)

Customize Task Menu:

Within this dialog box you can define tasks, which could be started directly from the Display Hits. The defined tasks can be started from the **Task** menu or via button (T1, T2 etc.).

Configure Hyperlinks:

Within this dialog box you may define additional hyperlinks.

- A hyperlink may start a Commander query.
- A hyperlink may link to a web page using URL.



AutoNom

7

7 AutoNom

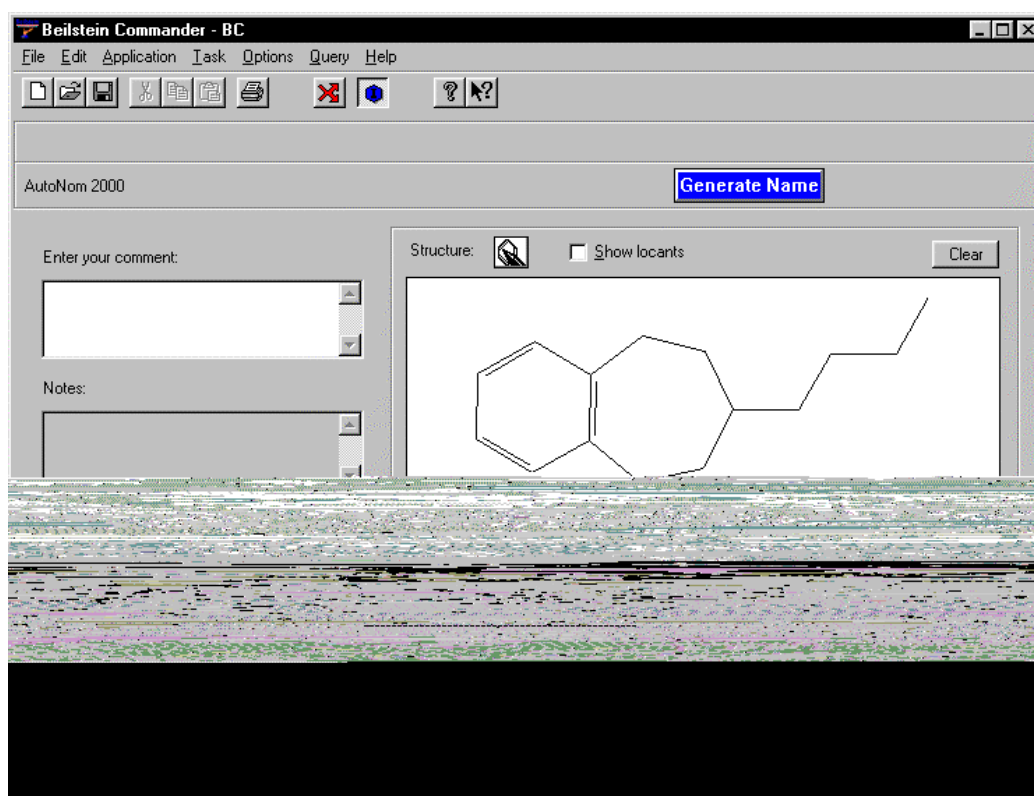
7.1 Starting AutoNom

AutoNom (Automatic Nomenclature) is a fully automatic and practical computerized system for the generation of IUPAC systematic nomenclature directly from the structure diagrams of organic compounds.

- Please start the structure editor (see section 2.2.4) and draw a structure (see section 3).
- Transfer the structure to the Commander using the -button or the 'F7'-key.
- Click the -button.

You will get the appropriate IUPAC name.

Example:

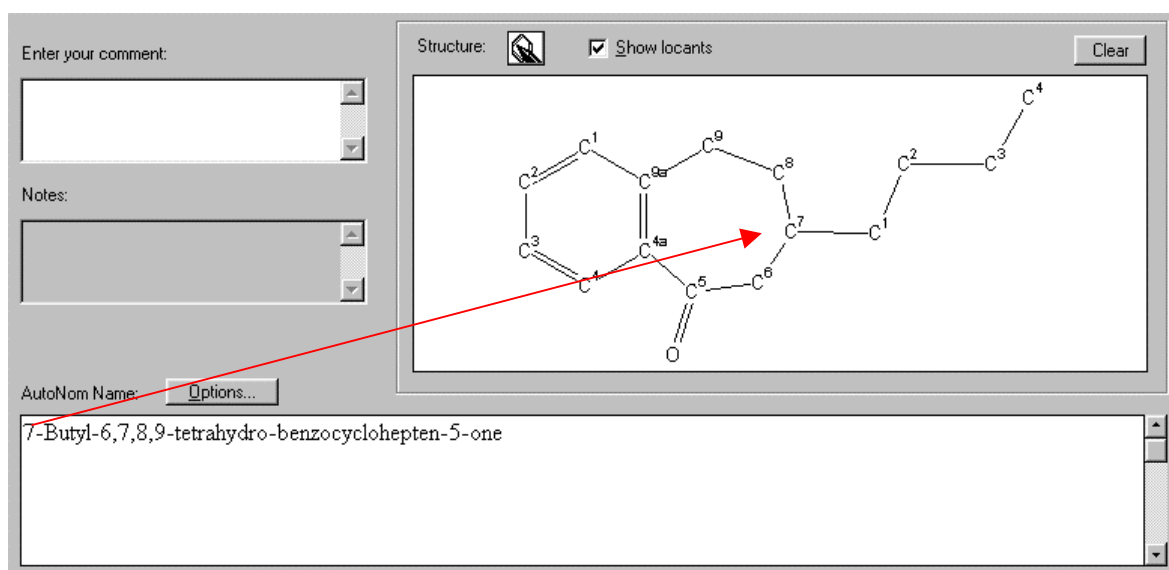


7.2 AutoNom 2000: Additional Features

7.2.1 Show Locants

Switch on “Show locants” and you will get the structure display with the nomenclature locants.

Example:

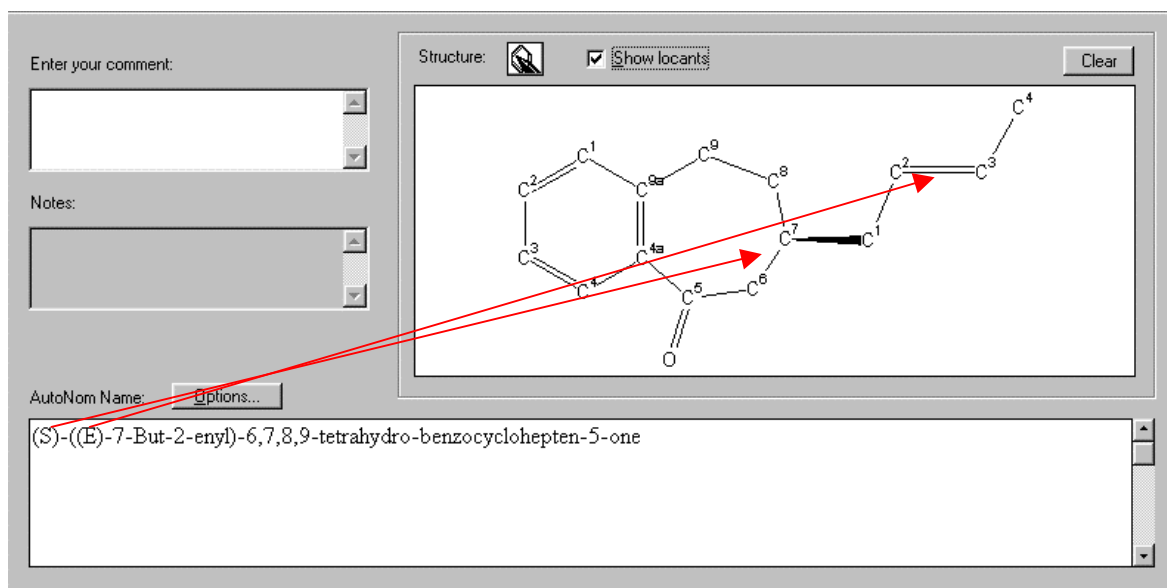


7.2.2 Stereochemistry

Autonom 2000 can process stereochemical information:

- Description of the absolute configuration on chirality centers (R,S)
- Description of the topological stereochemistry on double bonds (E,Z).

Example:

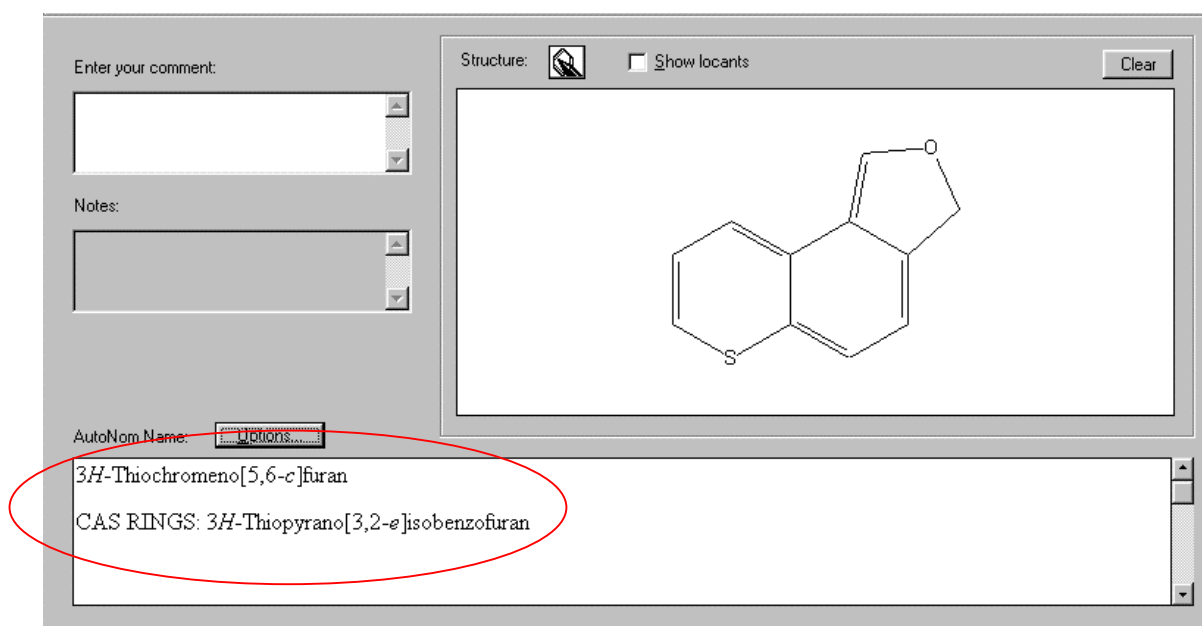


7.2.3 CAS ring naming convention

Autonom 2000 supports CAS naming convention in the nomenclature of rings as alternative (or addition) to the Beilstein ring system nomenclature.

Click on the AutoNom Name 'Options' button. Select the option: 'Both'.

Example:



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8 Index

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