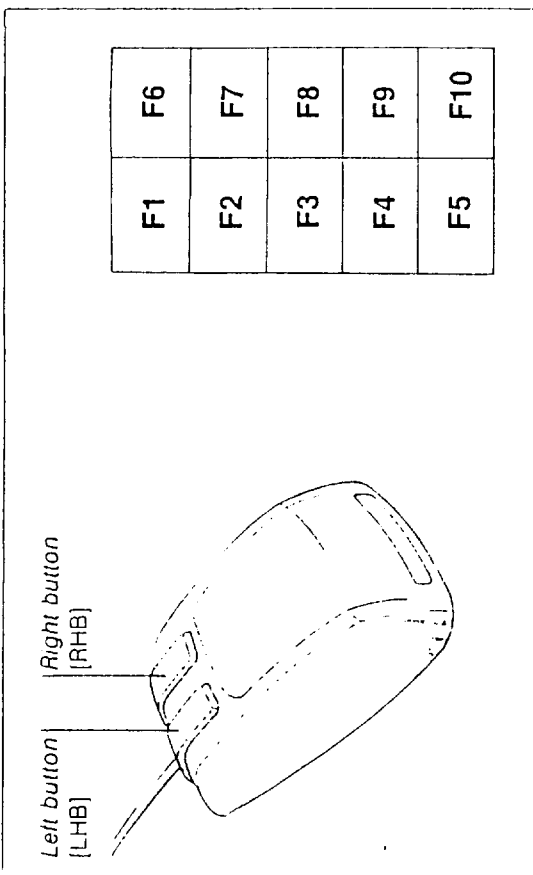


**Beilstein**

**A Brief Tutorial on the Use of Sandra**

no arrow is visible at this point, you have forgotten to install the mouse!  
Go back to Sect. 2.1.3.

In order to give you a first impression about what SANDRA actually does, we perform the following procedure to display benzene on the screen (Fig. 2):



Press

[F1]

Press

[LHB]

Then move the mouse about 1 inch (2 cm) towards you. Note that the arrow moves downwards on the screen, too (Fig. 3).

Press

[LHB]

Benzene appears on the screen (Fig. 4 →).

Type

[Q]

A message appears on the screen, asking you to touch either the 1 or the 2 on your keyboard.

Touch the number

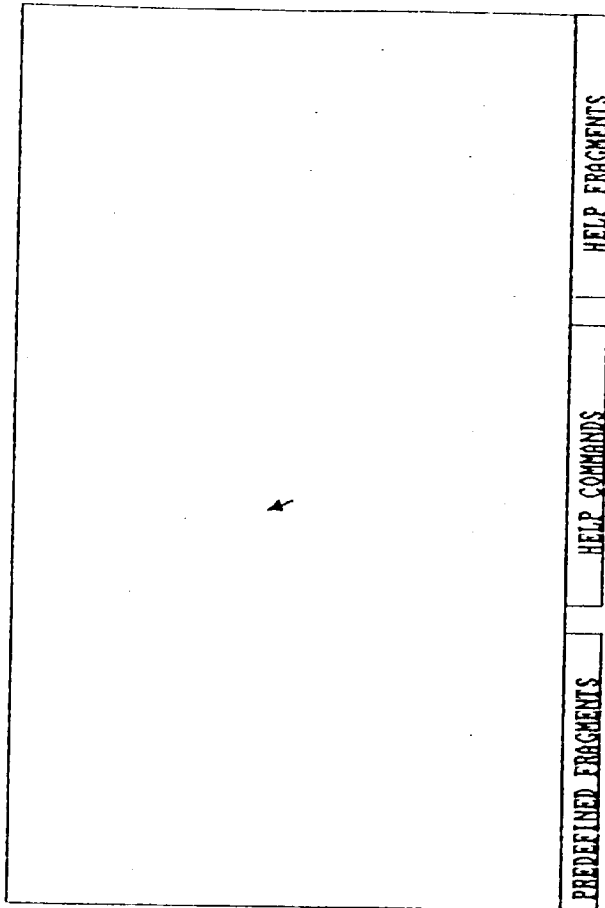
[2]

One outstanding feature of the *Beilstein* system is that the criteria for the ordering are based solely upon structural characteristics and therefore do not depend on nomenclature. Nevertheless, there is no doubt that the task of applying the rules to this monumental collection of material has dismayed and often defeated many potential users.

With SANDRA these problems have now been overcome. The program analyses the structure in terms of the *Beilstein* classification system:

- The input to the system is the structure formula of the organic compound via a graphical input (mouse). (The system itself takes care of the H atoms.)
- The output indicates to the user
  - the relevant *Handbook Series* (E III, E IV, E III/E IV, or E V) for the period 1930-1979 if the structure is in the *Handbook*
  - the relevant *volume/subvolume(s)*
  - the relevant pages within the *Basic Series* (H)
  - the relevant *system numbers*
  - additional classification characteristics of the compound (e.g., the degree of unsaturation)

Soon after you have started the system, an arrow appears in the center of the screen (Fig. 1):



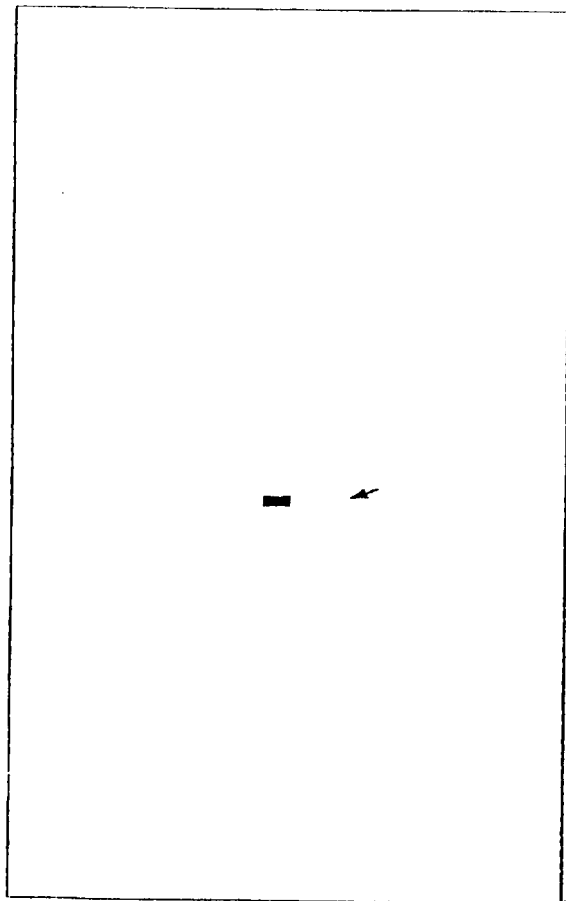


Fig. 3

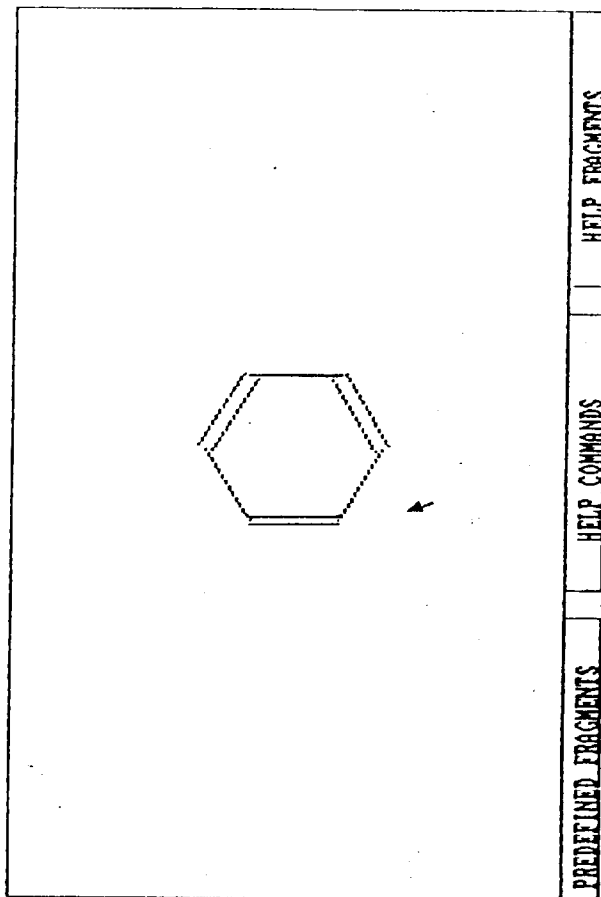


Fig. 4

After a few seconds, the references relevant to benzene appear on the screen (Fig. 5 →).

Another molecule? (y/n)

H-PAGE 173 to 280   Syst-No 463 to 465  
 STAMMVERBINDUNG, 2n-6, C: 6

E IV subvolume(s) : 5/2,  
 E III subvolume(s) : 5/2,  
 C 6 H 6

Fig. 5

Thus you have entered a structure via the graphical input and you have received the references of your structure.

### 2.3 Interpreting the Output

The great advantage of SANDRA is that you no longer have to know all the details of the *Beilstein* system. All the classification operations are carried out automatically and the results are displayed on the screen with the structure. Let's examine this particular example more closely.

Message [5] (Fig. 6) gives the particular volume/subvolumes in the distinct series (E III, E IV, E III/IV, E V). In this example, message [5] indicates that benzene will be found in

E IV (Fourth Suppl. Series), Vol. 5, Subvol. 2  
 E III (Third Suppl. Series), Vol. 5, Subvol. 2.

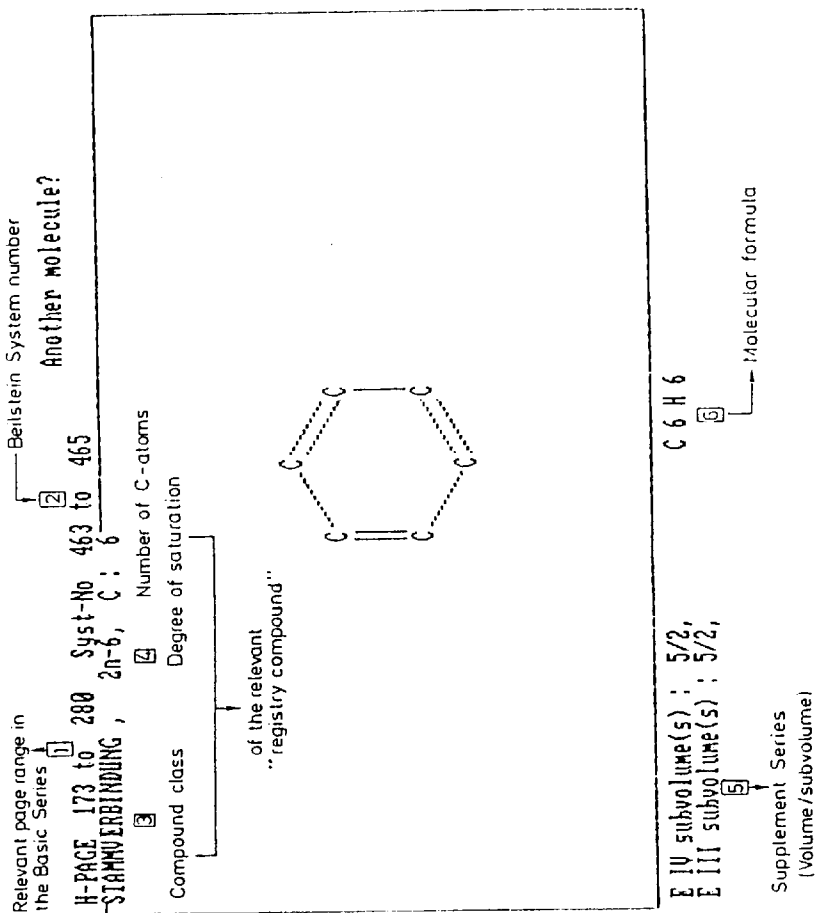


Fig. 6

Note: The fact that SANDRA gives you a reference does not necessarily imply that the compound is actually in the *Beilstein Handbook*, but rather that if it is, then it is to be found at the quoted place. SANDRA will always give a reference, sometimes two.

The messages [1] + [2] + [3] + [4] are pointers to specific pages in the indicated subvolumes. They are also useful for browsing and similarity searching. You will find these pointers printed at the top of each page in the *Handbook* (page headers), e.g.,

[2] right-hand page (odd numbered): [1]  
 Syst.No. 462-463 / H 173-179

[3] left-hand page (even numbered): [4]  
 Isocyclische Kohlenwasserstoffe  $C_n H_{2n-6} C_6$

for the given example in E IV, Vol. 5/2, on pages 583-584. In most cases this is enough to determine the location of the compound to within a few pages of the appropriate volume and subvolume. Messages [3] and [4] are also useful for searching with the help of the table of contents at the beginning of each subvolume, e.g., E IV 5/2 (Fig. 7).

**Zweite Abteilung**

**Isocyclische Verbindungen**

**I. Kohlenwasserstoffe**  
 (Fortsetzung)

4. Kohlenwasserstoffe  $C_n H_{2n-6}$  . . . . . 583  
 Kohlenwasserstoffe  $C_n H_{2n-6}$   
 Benzol . . . . .

Message [6], the molecular formula of the target compound, will help you to use the *Formula Indexes*, in particular, the formula index of the subvolume indicated.

There are three kinds of indexes:

- (a) the *Cumulative Index*,
- (b) the *Subvolume Indexes*, and
- (c) the *General Indexes* (H-E II) (*Generalregister*)

(a) The *Cumulative Index* is provided for individual volumes (e.g., Vol. 5) or groups of volumes (e.g., Vols. 17 and 18). These indexes cover the contents of all series of the volumes in question (Basic Series to E IV). The names conform to the latest nomenclature.

(b) If the corresponding *Cumulative Index* is not available, use the indicated *Subvolume Index* (at the rear of the book). This index contains only the compounds described in that subvolume, but the entry for the compound will contain the back references to the preceding *Beilstein* series.

(c) If the required compound was only described before 1930 then the entry can always be found by using the *General Index* (H-E II) (*Generalregister*). For this reason, SANDRA does not give any specific references

mands. Note that some stereochemical descriptors are available. In addition you can manipulate the structure in the following ways: introduce hetero atoms, change bond orders, delete any bond or atom and even the whole molecule, change the size, and move the structure. It is important to stress that the results you receive from the program are not in any way dependent on the way in which you arrive at your final structure: you can draw your rings freehand, use function keys, make new joins or delete bonds, move atoms about, redefine them as heteroatoms, etc. — the answers you get are based on the final connection table of the structure on the screen at the moment you leave the input mode by using the quit [Q] command. Thus cyclohexane can be drawn as chair, boat, or simple hexagon; the answer is always the same.

to the Series H-E II in field [5]. However, the volume number given (e.g. 5 in the case of E IV 5/2) naturally also applies to the single volume in the series H to E II.

*Summary.* You will have observed that the program produces a series of pointers which are also used as page headers in the printed Handbook. The ranges given should always overlap (for H page and Syst. No. and be identical for the "fine tuning" of the degree of unsaturation ("2 n-x") and carbon number given in the field [4].

Thus for the given example:

Book headers	SANDF
H page	173-174
Syst. No.	462-463
unsaturation	2n-6
C number	6

#### 2.4 What You Need to Know First

As mentioned above, SANDRA presents a rapid and flexible way of drawing chemical structures. We will differentiate between three different modes of input. As you will see later, however, the distinctions are somewhat arbitrary because these input modes can often be combined:

1. Using predefined fragments (templates).  
Figure 10 (Table 2) shows the predefined fragments available on the system. Instructions on how to use them will be given in detail in Sect. 3.3.
2. Freehand drawing.  
Moving the mouse and using the LHB (left-hand mouse button) or RHB (right-hand mouse button) you can draw single, double, triple and conjugated bonds. This drawing mode will be explained in Sect. 3.4.
3. Using user-defined fragments (self-defined templates).  
Using the [Fx], [CTRL-Fx], and the [ALT-Fx] keys you can define your own fragments. This feature will be explained in detail in Sect. 3.5.

In every input mode (note that all possible combinations can be made several manipulations can be performed using one-letter keyboard commands. Figure 9 (Table 1) provides an overview of the keyboard commands.

## 3 Working with the Program

*Summary.* In this section you have learned how to use the [K] (kill) command to clear the screen.

### 3.2 The Screen Boxes

In this section you will learn:

1. How to use the [LHB] to release the cursor
2. How to use the [RHB] to call up
  - (a) help commands
  - (b) predefined fragments
  - (c) user-defined fragments

This section should take about 5 minutes to read.

The mouse has two buttons on the top, the [LHB] and the [RHB] (Fig. 2). The cursor is moved around the screen by sliding the mouse around the table.

Pressing the [LHB] once locates a C atom (not normally visible on the screen, see below); you can now draw bonds by moving the mouse. By pressing the [LHB] twice releases the cursor (arrow). You can now move the cursor without creating bonds (see Sect. 3.4).

**Note:** To move the cursor without drawing on the screen, it is necessary to release the cursor, i.e., make the arrow visible!

Move the cursor into the "HELP COMMANDS" box at the bottom of the screen (Fig. 8 →).

Press

[RHB]

The screen displays Fig. 9 (→).

which shows you a list of all available keyboard commands. This list is reproduced in Appendix A (Sect. 4.2.1). A message appears on the screen:

**Press any key to continue**

Press

[space bar] or either of the mouse buttons.

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### 3.1 How to Clear the Screen

In this section you will learn:

How to use the [K] (kill) command.

This section will take about 3 minutes to read.

First of all, do not be afraid of experimenting with SANDRA: the worst thing that can happen to you when inputting your structure is that you have to draw the structure again. This may, for example, be necessary if you made a mistake drawing your structure and you do not see any possibility of correcting it.

If that happens, you can use the [K] (kill) command, described below.

Let us assume that you have benzene on the screen if you performed the procedure described in Sect. 2.2. Your screen looks like Fig. 5 and the system displays (right-hand side at the top of the screen):

**Another molecule (Y/N)?**

Now press

[Y]

The screen now looks like Fig. 4. (Sandra always returns the last structure used in your session as a possible starting point for possible derivatives.)

Type in

[K]

The system displays a message:

**Are you sure Y/N?**

Type in

[Y]

The screen is cleared. You can now draw another structure.

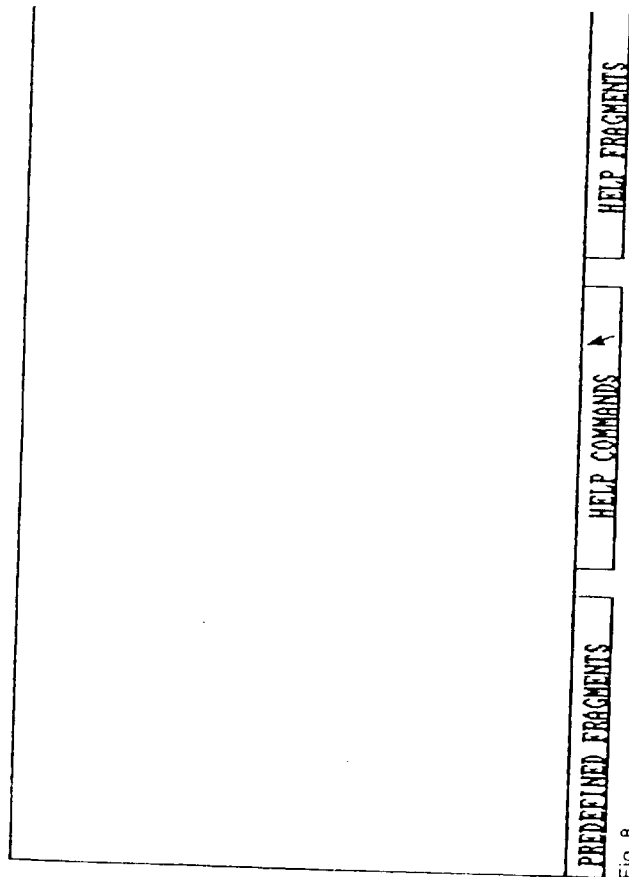


Fig 8

The screen displays Fig 10.

Table of PREDEFINED FRAGMENTS

F1	6-Ring (unsat.)	F2	n-Ring (unsat.)
F3	6-Ring (sat.)	F4	n-Ring (sat.)
F5	C-COOH	F6	C-CH
F7	C-SO3H	F8	O-6O3H
F9	O-SiMe3	F10	O-PUGHZ
CTRL-F1	C-nitro	CTRL-F2	C-diazo
CTRL-F3	C-azido	CTRL-F4	benzoyl
CTRL-F5	benzyl	CTRL-F6	trityl
CTRL-F7	t-butoxycarbonyl (Boc)	CTRL-F8	benzyloxycarbonyl (Z, Bzo, Cbo)
CTRL-F9	toluyl-4-sulfonyl (tosyl)	CTRL-F10	trifluoroacetyl
ALT-F1	Gly	ALT-F2	L-Ala
ALT-F3	L-Val	ALT-F4	L-Leu
ALT-F5	L-Asp	ALT-F6	L-Glu
ALT-F7	L-Phe	ALT-F8	L-Phe
ALT-F9	L-His	ALT-F10	L-Try

Press any key to Continue

which shows a list of all available predefined fragments. You will learn how to use these in the next section. This list is reproduced in Appendix B (Sect. 4.2.2). At the bottom of the list, a message is displayed:

**Press any key to continue**

Press

**[space bar]**

or either of the mouse buttons. The list disappears. Finally, move the cursor into the "PREDEFINED FRAGMENTS" box at the left-hand side.

Press

**[RHB]**

This box now changes to "USER-DEFINED FRAGMENTS." Move the cursor into the "HELP FRAGMENTS" box and press

**[RHB]**

The screen displays Fig. 11 (→),

which shows you a list of user-defined fragments. Only four function keys are reserved for the system. You can use all other function keys to define your own fragments. (See Sects. 3.5 and 3.7.)

Press

**[space bar]**

Press any key to Continue

Fig 9

Table 1 (Appendix A) disappears. Now, move the cursor into the "HELP FRAGMENTS" box. Note that the box at the left-hand side of the bottom line displays "PREDEFINED FRAGMENTS."

Press

**[RHB]**

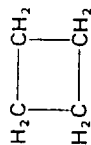
### 3.3 SANDRA at Work: Using Predefined Fragments

In this section you will perform a structure search comprising the following features:

1. How to move the mouse.
2. How to manipulate your structure.
  - (a) How to center the structure.
  - (b) How to decrease the size of the structure.
  - (c) How to enlarge the size of the structure.

It will take about 5 minutes to read.

#### 3.3.1 First Example: Cyclobutane



The first structure and reference analysis in this section is of cyclobutane. You need not bother about the H atoms; the system itself takes them into account. If you make a mistake, the worst thing that can happen is that you have to draw your structure again (see Sect. 3.1). If the cursor is not visible before you start release it by pressing

[LHB]

and clear the screen, if necessary, by using the kill command.) If the arrow is visible on the screen, press

[F4]

[F4] is the function key of the predefined n-membered, saturated ring. A message appears on the screen:

**Ring size:**

Type

[4] [return]

and another message appears on the screen:

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Table of USER-DEFINED FRAGMENTS

F1	6-Ring (unsat.)
F2	6-Ring (sat.)
F3	
F4	n-Ring (unsat.)
F5	n-Ring (sat.)
F6	
F7	
F8	
F9	
F10	
CTRL-F1	
CTRL-F2	
CTRL-F3	
CTRL-F4	
CTRL-F5	
CTRL-F6	
CTRL-F7	
CTRL-F8	
CTRL-F9	
CTRL-F10	
ALT-F1	
ALT-F2	
ALT-F3	
ALT-F4	
ALT-F5	
ALT-F6	
ALT-F7	
ALT-F8	
ALT-F9	
ALT-F10	

Press any key to continue

Fig. 11

or either of the mouse buttons to continue. You return to the input mode. The cursor is again visible on the screen.

#### Summary

1. By pressing [LHB] twice sets an atom and then releases the cursor. You can now move the cursor without drawing on the screen.
2. By pressing [RHB] when the cursor is in the right-hand box, you display predefined fragments.
3. By pressing [RHB] when the cursor is in the box in the middle of the bottom line, you display a list of the keyboard commands.
4. By pressing [RHB] when the cursor is in the left-hand box, moving into the right-hand box and pressing [RHB] again, you display user-defined fragments.

released, you can decrease ([D]), enlarge ([E]), center ([C]), or even move ([M]) the structure.  
Type in

[E]

The structure is enlarged.

Type in

[D]

and the structure decreases its size. If you type in

[C]

the structure is centered.

Type in

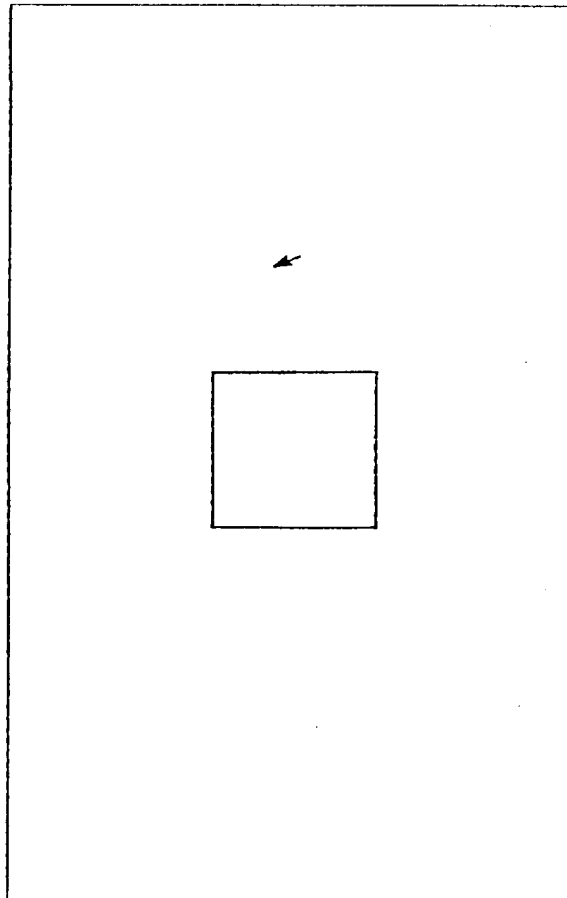
[M]

and a message appears on the screen:

**Press left mouse button to enter old reference point**

Move the cursor to any point of your choice (Fig. 13) and press

[LHB]



**Press left mouse button to enter old reference point**

Fig. 13

20

**Press left mouse button to enter first reference point**

**Fragment name is 4-Ring (sat.)**

The program requires two reference points to locate the fragment. The distance between the two reference points defines the side length of the ring. In Appendix C (Sect. 4.2.2) you will find the structures of all predefined fragments with two reference points indicated by 1 (first) and 2 (second).

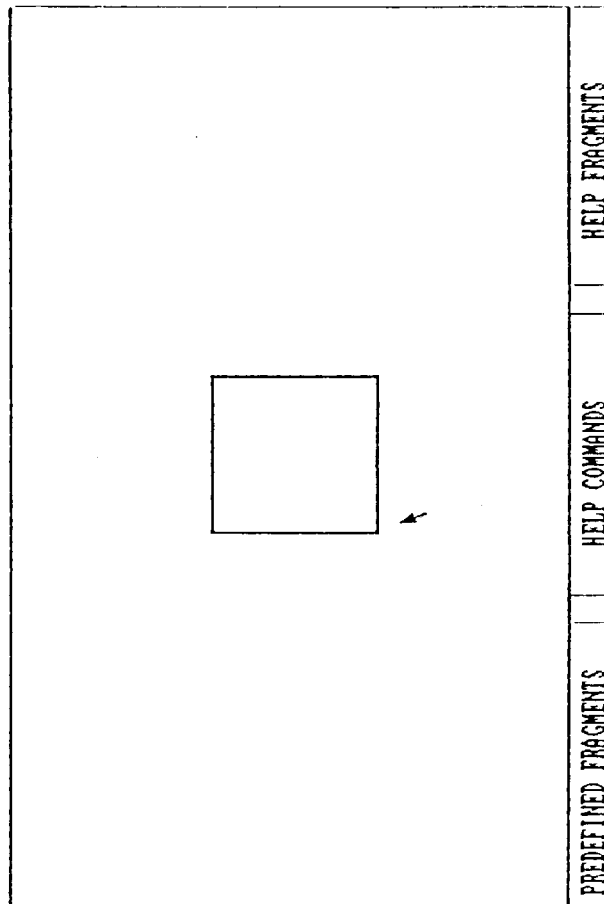
Now, move the mouse to the center of the screen and press

[LHB]

to define your first reference point. A **■** appears on the screen. The second reference point is defined in the same way. Move the mouse to a second reference point and press

[LHB]

again. Cyclobutane appears on the screen. Note that no atomic symbols are displayed. The screen looks like Fig. 12.



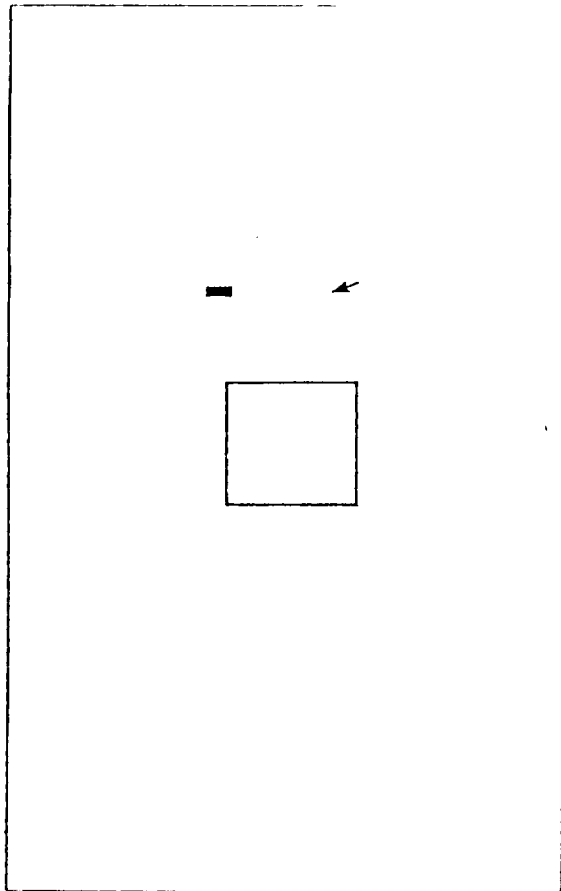
It may be that the structure is partly off the screen, depending on the distance between the reference points you have used. If the cursor is

After a few seconds, the reference pointers for cyclobutane are displayed (Fig. 15).

Another message demands the new reference point. Move the cursor to a new reference point on the screen and press

[LHB]

to define the new reference point. Your structure is now in the new position (Fig. 14).



Press left mouse button to enter new reference point

Finally to enter the analysis mode, type

[Q]

The atomic symbols are now visible, to facilitate a final check. A message appears on the screen:

**1 = correction ; 2 = start analysis**

In our example, type

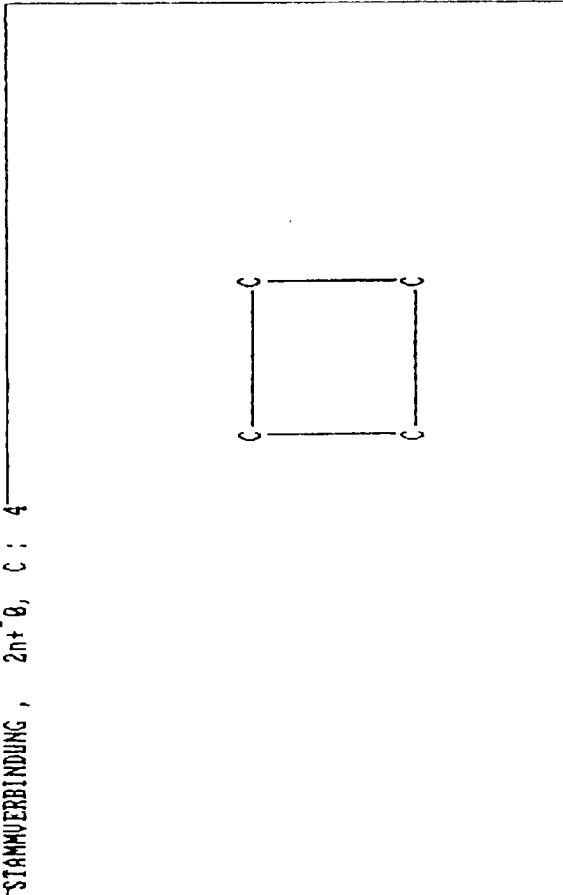
[2]

Another message appears on the screen :

\*\*\*\*\* please wait a few seconds \*\*\*\*\*

Another molecule?

H-PAGE 17 to 19 Syst-No 452  
STAMMVERBINDUNG, 2n+0, C: 4



E IV subvolum(s) : 5/1,  
E III subvolum(s) : 5/1,  
C 4 H 8

The program is now waiting for input. Look at the top right-hand corner of the screen. If you type "[N]" you exit the program and go back to DOS. In order to continue, type

[Y]

The references disappear and the structure is displayed without the atomic symbols. In the next section you will introduce a functional group.

Summary: You learned how to use:

1. The [E] (enlarge), the [D] (decrease), the [C] (center), and the [M] (move) commands
2. The command [Q] (quit structure input, start analysis)
3. The function keys for standard rings

### 3.3.2 Second Example: Introducing a Carboxyl Group

We continue by adding a carboxyl group to cyclobutane, again by using predefined fragments.

Which function key calls up the carboxyl group (C-COOH)? If you do not remember, move the cursor into the box on the right and press [RHB]. [F5] is the correct one. Press [RHB] to return to the draw mode and press

[F5]

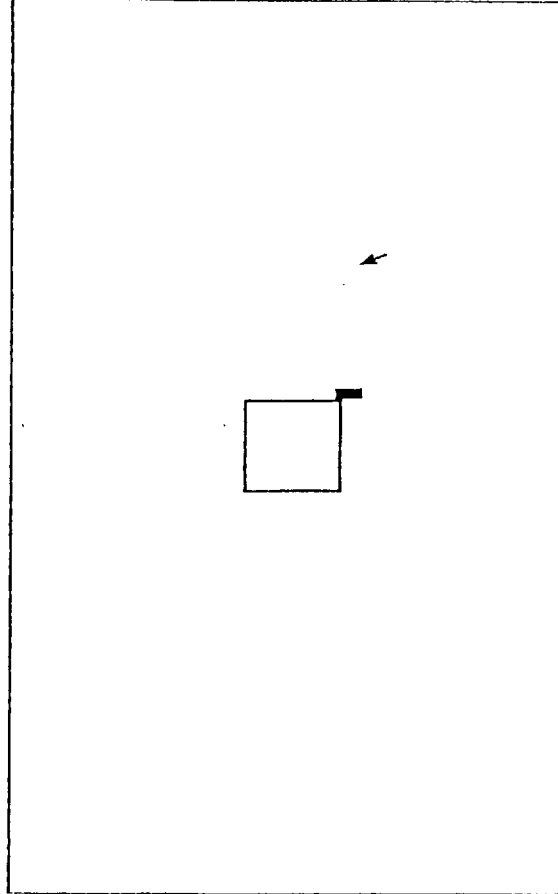
A message is displayed on the screen:

**Press left mouse button to enter first reference point**  
**Fragment name is C-COOH**

Move the cursor to the C atom where you want to insert the C-COOH group. Press

[LHB]

once to enter the first reference point. A ■ appears at this point (Fig. 16).



**Press left mouse button to enter second reference point**  
**Fragment name is C-COOH**

Move the cursor to the desired second reference point; the distance between the two reference points equals the carboxyl C-C bond length. Press

[LHB]

again to enter the reference point. Cyclobutane carboxylic acid appears on the screen with implied H atoms.

Press

[Q]

to enter the analysis mode. The bottom line looks like this:

**1 = correction; 2 = start analysis**

Type

[2]

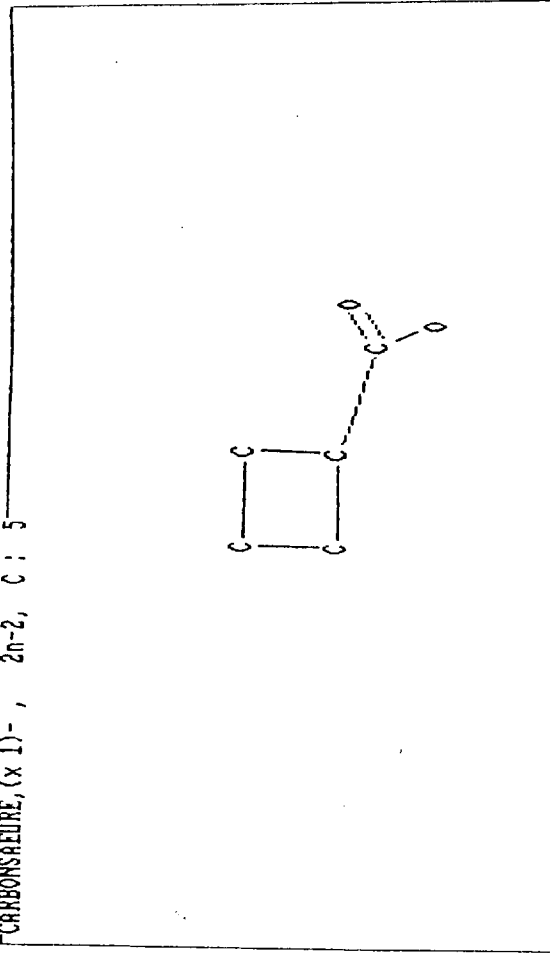
A message appears on the screen:

**\*\*\*\*\* please wait a few seconds \*\*\*\*\***

Cyclobutane carboxylic acid is then displayed together with the references (Fig. 17).

H-PAGE 5 to 6 Syst-No 893  
CARBOXYACIDE, (x 1)-, 2n-2, C ; 5

Another molecule? (y/n)



E IV subvolume(s) : 9/1,  
E III subvolume(s) : 9/1,

C 5 H 8 O 2

### 3.4 Using Freehand Drawing

In this section you will learn how to

1. Use the mouse to draw
  - (a) single (default);
  - (b) double, and
  - (c) triple bonds
2. Delete a bond
3. Introduce a hetero atom
4. Display symbols on atoms

This section will take about 10 minutes to read.

In the previous sections you learned that predefined fragments are a powerful tool. However, it is not always possible to divide the desired structure into components so that you can use predefined fragments. Therefore, it is often necessary to draw certain components of your structure using the freehand drawing mode.

Until now, we have carefully avoided the freehand drawing mode. What you do when you release the cursor is that you actually leave the freehand drawing mode. If the cursor is not released, i.e., if it is not visible on the screen, you always draw a bond when you move the mouse. Pressing [LHB] creates a single C atom; the cursor is not released. At this point you can continue drawing bonds. If you press [LHB] a second time before moving the mouse, you release the cursor while locating a single C atom. To draw a double or triple bond you must press [2] or [3] while moving the mouse. After having drawn a double or triple bond, you must explicitly press [1] while moving the mouse to reinstall the single bond mode.

Before you start, clear the screen with the kill command.

*To Repeat:*

1. Each time you press [LHB], move the mouse, press [LHB], move the mouse, press ... you create a CH<sub>2</sub> group. Each time you press [LHB] you draw a bond and at the same time move the mouse.
2. Each time you press [LHB] twice and you release the cursor you create a single C atom. You can now move the mouse without drawing a bond.

The program waits for input. If you want to continue, press

[Y]

otherwise type [N].

If you continue, then clear the screen by typing

[K]

A message appears:

**Are you sure Y/N?**

Type

[Y]

The screen is cleared.

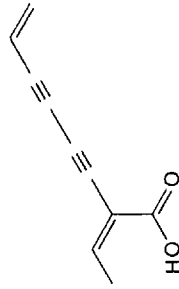
Now you have performed the second analysis using predefined fragments.

*Summary:* You practiced how to:

1. Incorporate a predefined fragment into your structure
2. Leave the structure input and enter the analysis mode

### 3.4.1 First Example: Carbon Chains

Our first example is a carbon chain with 10 C atoms and single, double, and triple bonds. The structure looks like this:



Note that the commands [1] (single bond), [2] (double bond), and [3] (triple bond) should be used only if the cursor is not released, i.e., if you are in the "rubber bond" mode.

Move the cursor to the left-hand side of the screen. To locate the chain, press

[LHB]

A bottom line appears on the screen:

**Atom number 1 Atomic symbol: C Charge: Radical: Abnormal mass:**

Now move the mouse. A single bond is drawn on the screen.

Press

[LHB]

to locate the second C atom. Note, however, that no atomic symbols are displayed. The bottom line appears indicating that you have now located the atom number 2. To draw a double bond between the second and the third atom move the mouse to atom number 3 and press

[2]

Press

[LHB]

to locate the third C atom. The bottom line appears again. In order to draw the next single bond move the mouse and press

[1]

Press

[LHB]

to locate the fourth C atom. Move the mouse and type

[3]

to draw a triple bond.

Continue in this fashion until you end up at the C atom number 9. Release the cursor by pressing

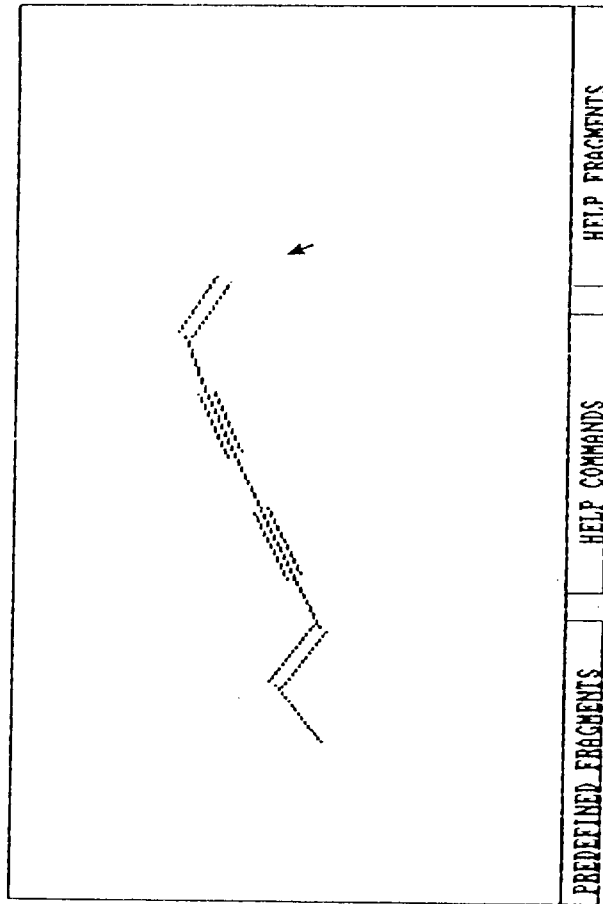
[LHB]

a second time without moving the mouse.

Note: Sometimes it happens that you draw over several parts of your structure unintentionally in the rubber bond mode, whereupon they may then appear somewhat worse-of-wear or even disappear.

However, they are not really deleted; you can display them again by typing [P] (for paint), which restores your screen.

The screen looks like Fig. 18.



Type

[1]

Remember: You can use function keys and command keys ([C], [E], [D], [K], [P] etc.) only when the cursor is released.

Press

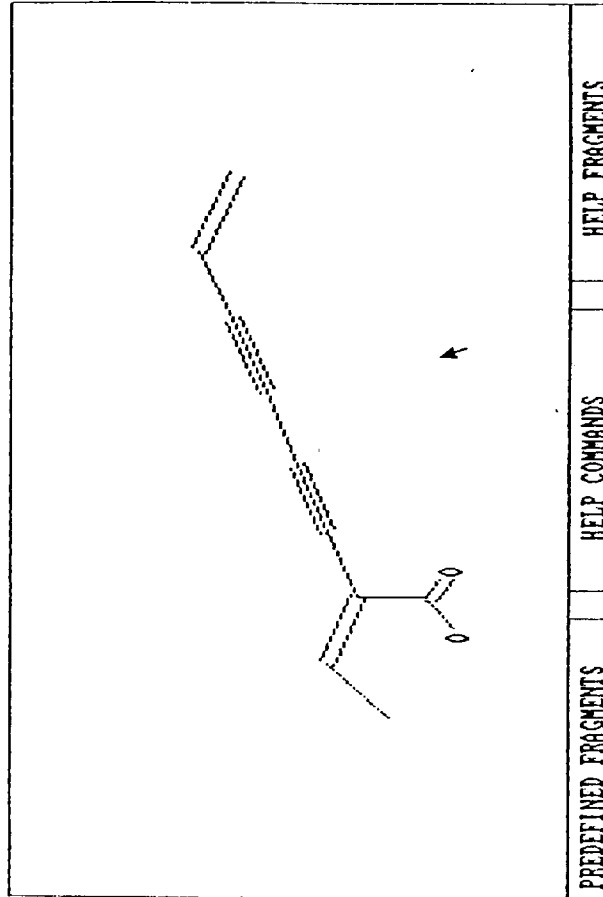
[F5]

Move the cursor to the third C atom and press

[LHB]

to enter the first reference point. Move the mouse and enter the second reference point (Fig. 19) by pressing

[LHB]



Type

[Q]

to enter the search mode. A message appears on the screen:

**1 = correction; 2 = start analysis**

Suppose that you see a mistake in your structure at this point. For instance, you might want to convert the acid into the corresponding aldehyde. To delete the single bonded O atom of the COOH group,

Note: Routine for deleting single atoms now follows:

You are back again in the input mode. Move the cursor to the O atom and press

[RHB] [RHB]

The atom and all bonds connecting it to other atoms are deleted. Press

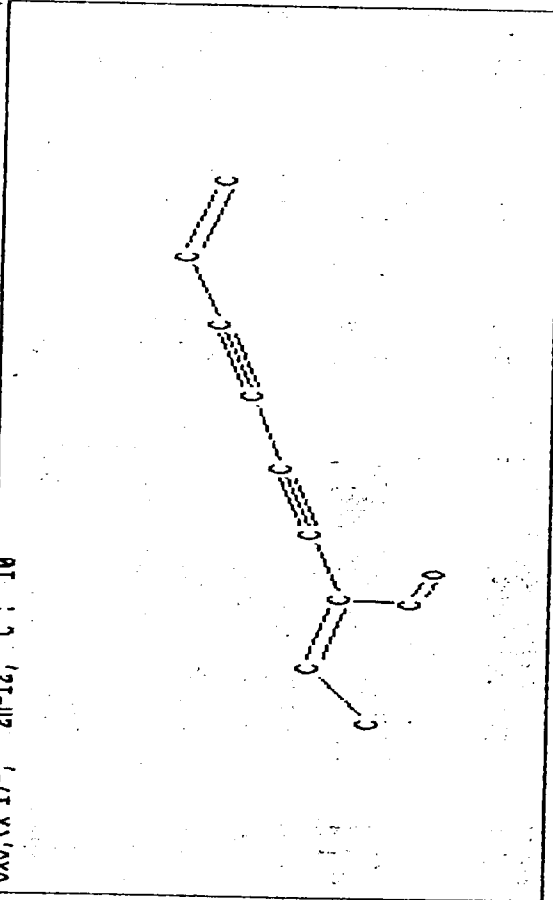
[Q]

to enter again the search mode. After the message appears on the screen, type

[2]

and wait a few seconds. The structure references are then displayed. The screen looks like Fig. 20.

H-PAGE 758 to 759 Syst-No 93 to 95 Another molecule?  
COXO, (X 1)-, 2m-12, C: 10



E IV subvolume(s) : 1/5,  
E III subvolume(s) : 1/3,  
C 10 H 8 O 1

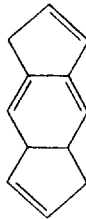
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### 3.4.2 Second Example: Condensed Rings

Repeat the procedure described in Sect. 2.2 to get benzene on the screen:

1. Press **[F1]**
2. Press **[LHB]** to enter the first reference point
3. Move the mouse
4. Press **[LHB]** to enter the second reference point
5. Benzene is displayed on the screen
6. Number the atoms using **[N]**

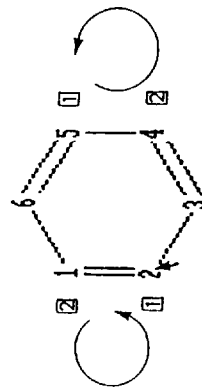
Use the **[C]**, **[D]**, or **[E]** command if necessary. Suppose we are interested in the following molecule:



To obtain this molecule, we must add two five-membered rings to benzene. The double bonds will be inserted later. We want to draw the ring on the right so that it is outside the benzene ring.

Note: The new ring atoms generated by the function keys F1 to F4 are always introduced in a counterclockwise sequence through the two reference atoms, in the order in which you specify these.

Thus to append a ring to the right, the first reference point must be at atom 5, and the second at atom 4 (Fig. 21).



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The program is waiting for input.

Type

**[Y]**

and you are back in the input mode.

Note: Routine for moving single atoms now follows:

You can move any specified atom and the bonds connecting it with other atoms by locating the cursor at the atom and pressing (once!)

**[RHB]**

Now you can move the atom as if it were tied to the mouse with rubber bands. To release the cursor, press

**[LHB]**

Note: It is good practice to "clean up" the screen using the command **[P]** (paint) after using this procedure.

Clear the screen by typing

**[K]**

A message appears on the screen:

**Are you sure Y/N?**

Type

**[Y]**

You are back in the input mode.

Summary: You learned:

1. How to draw bonds by moving the mouse and pressing **[LHB]** alternately
2. That by pressing **[1]**, **[2]**, or **[3]** while moving the mouse you can draw single, double, or triple bonds
3. How to use **[RHB]** to delete atoms
4. How to use the **[RHB]** to move individual atoms