IT ENABLED EDUCATION

CHEMISTRY

Training Module for Teachers

2009-2010

- *G-Periodic*
- *Kalzium*
- *Chemtool*
- *Rasmol*

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PREFACE

Drastic changes have been occurring in the field of I.T. Education in Kerala. In this ever-changing world, with the advancement of Information Technology, the teaching learning process is also undergoing continuous changes. Thus it has become necessary to impart knowledge of Science subjects with the help of computer.

Learning by doing, experimentation and observation increases the flair of observation and experimentation in children. But we are unable to do certain experiments perfectly, i.e., experiments which are spontaneous as well as using dangerous materials. In such experiments we take the average as the real value gained from a number of trials. On the other hand these experiments can be done more accurately with certain sensors using computer.

We often face difficulty in making many children to do an experiment at a time. This can be rectified by using simulators and softwares. Thus the process of learning becomes interesting, interactive and worthy for the children.

Expecting the full co-operation of all the teachers to make use of the far stretching possibilities of science and technology in the field of education in this ever-changing world.

Director of Public Instruction

Thiruvananthapuram

CONTENT

1.	DAY - 1		
	Forenoon 9.30 - 10.00	-	Registration
	10.00 - 10.30	-	Introduction to the Training Program
	10.30 - 11.15	-	Introduction of Gperiodic
	11.30 - 12.00	-	Introduction of Chemtool
	12.00 - 1.00	-	Drawing structure of Molecules
	Afternoon 2.00 - 3.30	-	Inserting Templates Chemical Equations Formatting Molecular weight Installation - Chemtool
	3.30 - 4.00	-	School level implementation – Discussion & Planning
	4.00 - 4.30	-	Feedback
2	DAY 2 Forenoon 9.30 - 10.00	-	Introduction of Kalzium Window
	10.00 - 1.00	-	Customizing the window Overview Molecular weight Time line State of Matter Balancing Chemical equations Plotting graphs Glossary, Tools

	Afternoon 2.00 - 4.00	-	Introduction of Rasmol Inserting molecules Background colour Modification of the structure Ras,p; cp,,amd Installation
	4.00 - 4.30	-	Planning _ School level Feedback

Gperiodic

Gperiodic is a software which can be used to learn the classification and characteristic properties of different elements in High school classes.

To use the software, Open Gperiodic.

Application --> Education --> Gperiodic

Now opens a window with a Periodic Table. When we click on an element in this periodic table, the characteristic properties of the element is displayed.

Continue the activity with different elements.

Discuss how can we include these details in a presentation.

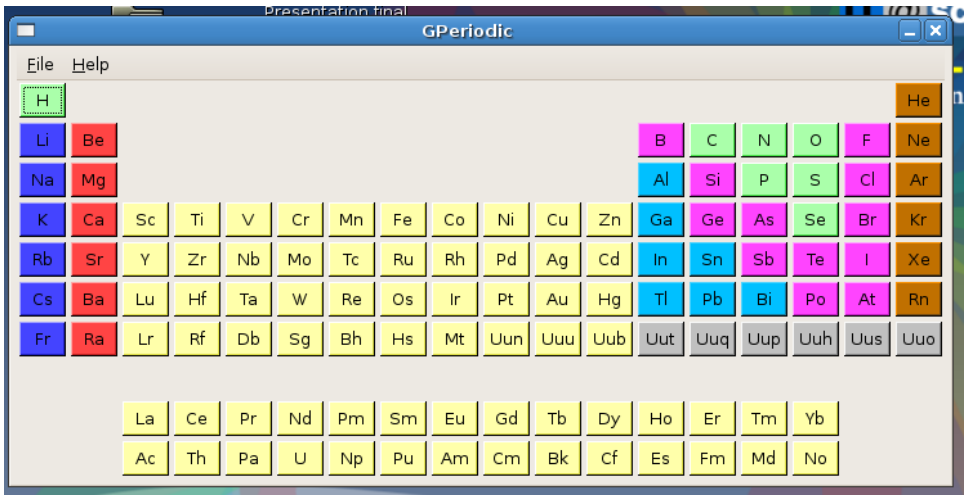
CHEMTOOL

Chemtool is another application software used to prepare two-dimensional structure of molecules of various substances. Along with the structure, chemical equations and formulae can also be included in this. Besides these we are able to calculate the molecular mass using this application.

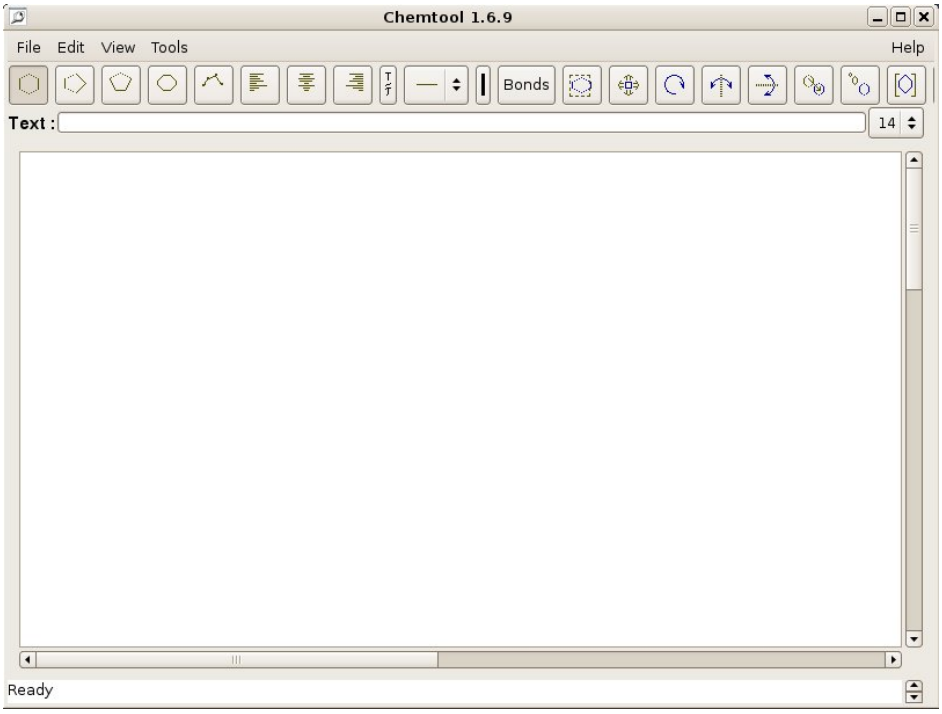
The Chemtool software is installed in our system along with IT@School Gnu Linux operating system.

To open the Chemtool window follow these steps.

Application --> Education --> Chemtool



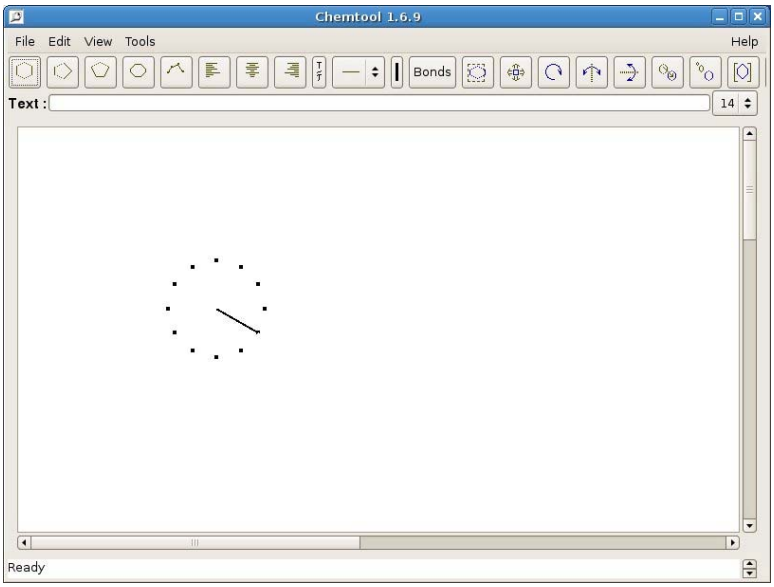
Let us see how Chemtool works.

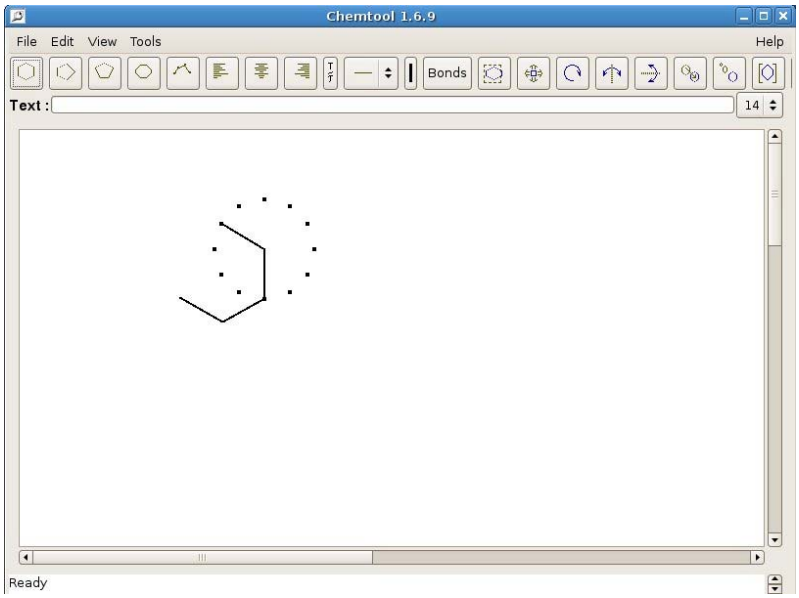


Chemtool

Chemtool window includes Menu bar, Drawing tools and Canvas.

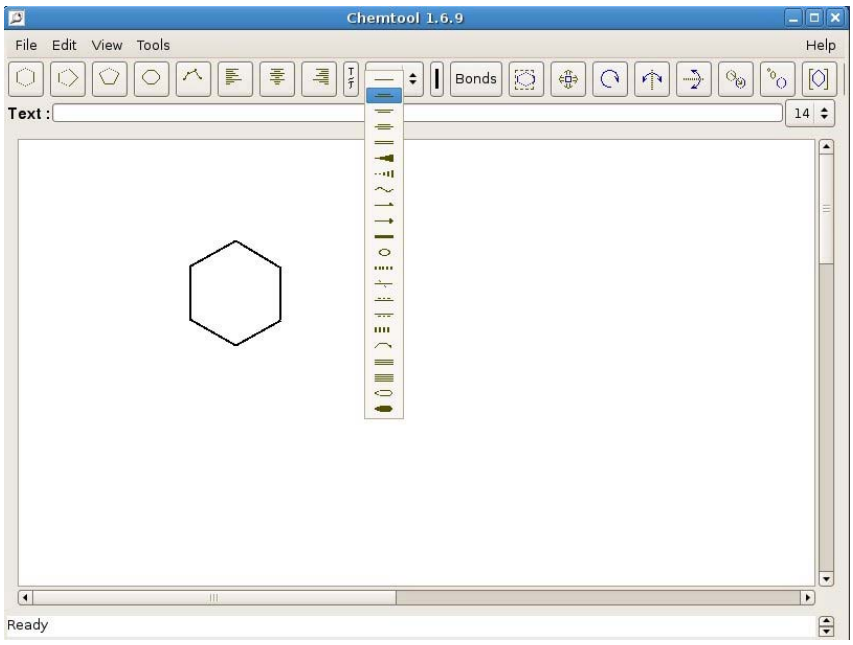
The first 4 tools among the drawing tools are used to draw the structure of molecules with different angles. For this select the tool with required angle, then click and drag inside the Canvas.



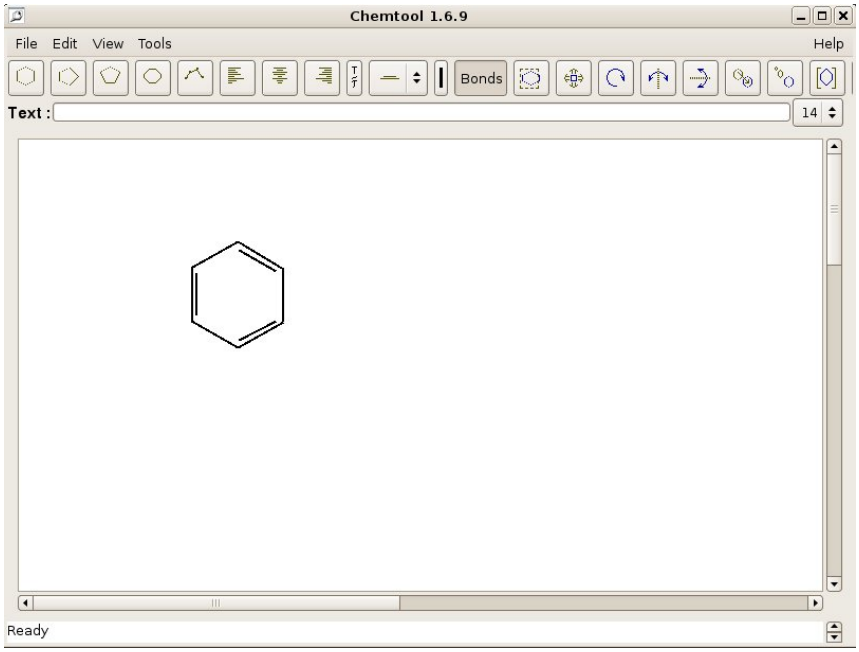


Chemtool

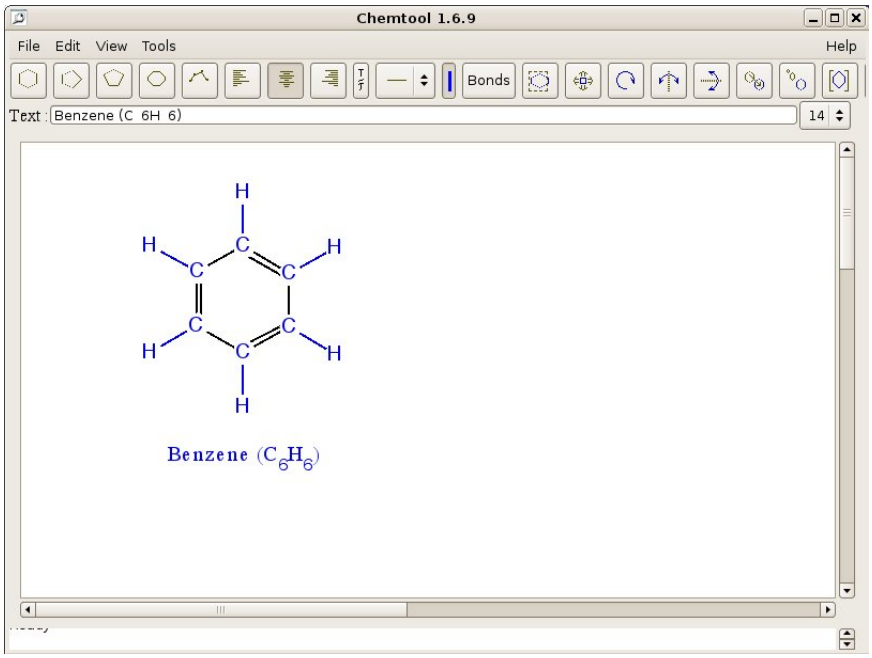
Double bonds are to be included to make the picture that can be seen in the structure of Benzene. To do this click on the drawing tool 'bond type' and select double bond from that. Then click and select the tool 'Bonds', after that click on the point where we need a double bond. We can see a double bond there.



Chemtool

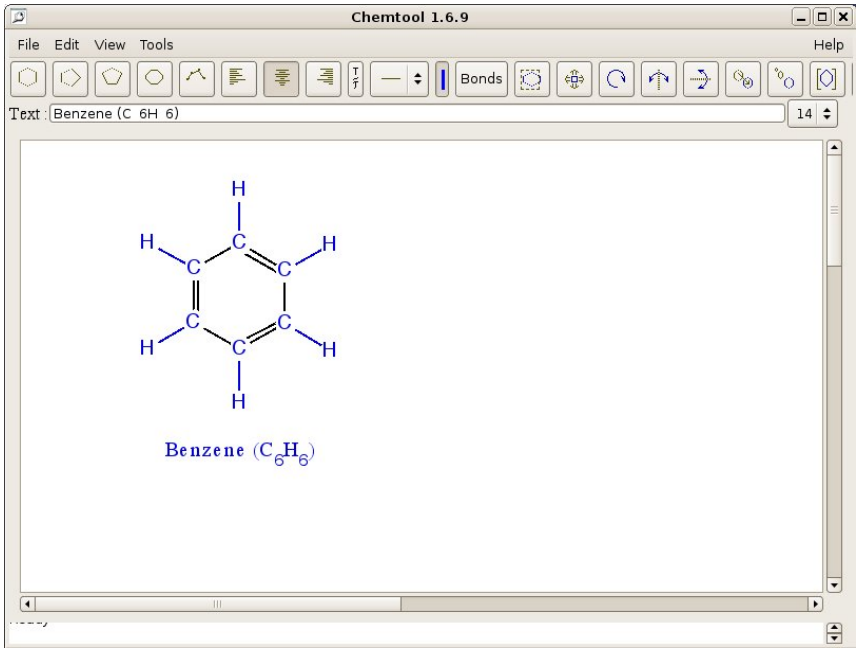


Chemtool - Benzene



Chemtool Benzene

Now we can include the symbols of elements. For that click on the 'current text' and type the symbol of the element in the space provided for text. Now this can be positioned with the cursor by clicking on the drawing canvas where we want to include/place the symbol.



Draw the structure of the following and save them i n your folder

- Methane
- Ethane
- Ethanol
- Cyclopropane
- Cyclobutane
- Cyclohexane

Templates

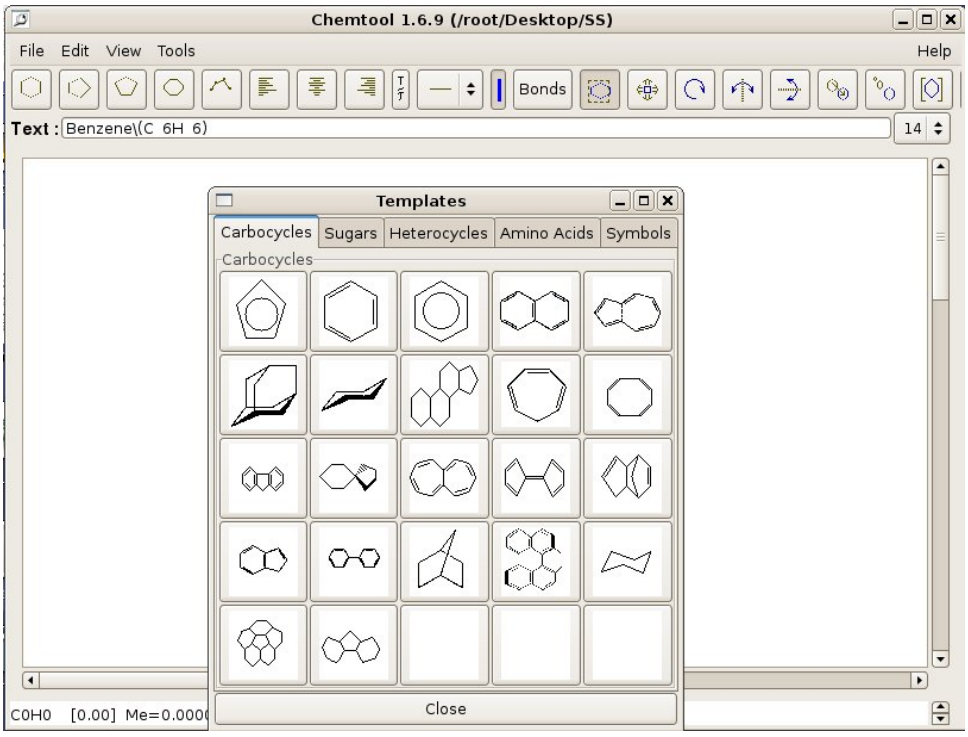
Molecular structure of so me substances are included in the Chemtool as Templates. To open the Template window click as follows

Tool --> Templates

We can include the necessary items from this. Try to include the structure of following from Template.

- Naphthalene
- Cytosine

- Maltose



Chemtool

Let us type the chemical equations

Click on the tool Current textfont T/T, then appears a text box, type the equation in the text box. To type subscript use 'underscore' and for superscript ^ (rise to). Then click on the canvas where we need the equation.

Formatting

Colour :- Colour of bonds and texts in the structure/fragment can be altered. To change the colour use 'select pen colour' tool.

Selection:- To move and change the size of the fragment it has to be selected. ' Mark Object ' tool is used for selecting an object in the canvas.

Move : - Drawn pictures can be moved to another place on the canvas using 'move marked object' tool.

Changing the size :- We can increase or decrease the size of a drawn picture using ' Resize marked object' tool.

Molecular Mass :-

Type the molecular formula and place it in the canvas. Select it and then select 'Calculate formula weight' in the Tools menu. The molecular weight is displayed on the bottom portion of the Chemtool window.

Deleting :- To delete a marked fragment click on the right button after highlighting it. To high light it click and drag through the required area.

KALZIUM

Kalzium provides you with a lot of information about the Periodic Table and the Elements in it. Using Kalzium visualizations of the elements is also possible. We can visualize the Periodic Table of the Elements by groups, period, acidic behavior, families etc.

We can easily plot graphs using different properties of elements. Kalzium can also be used to know the Changes in the states of matter according to the changes in the molecular mass, temperature etc. of molecules.

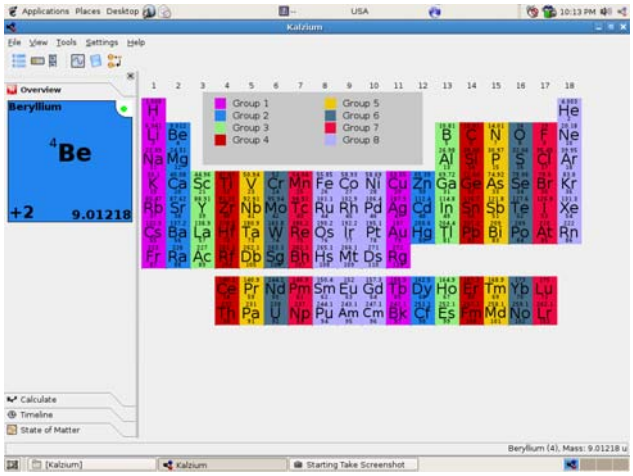
Let us see the Kalzium Window

To open the Kalzium window try the following methods

1. Application --> Education --> Kalzium

   OR

2. Press Alt + F2 and type Kalzium (in the Run Application window) then press Enter key



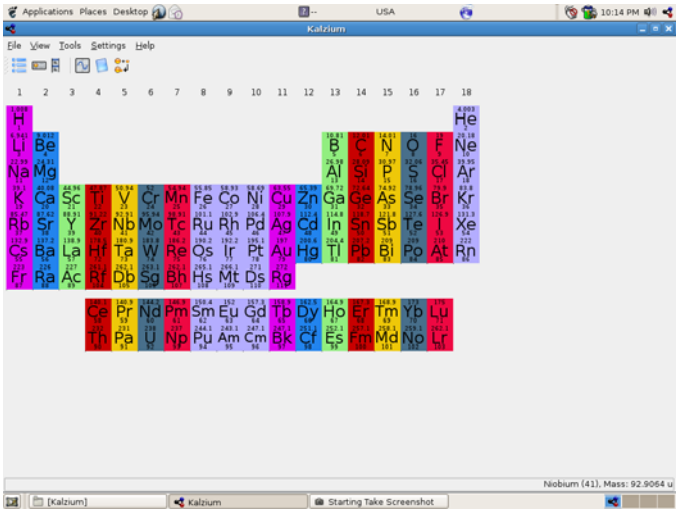
Activity – 1

Let us familiarize the sidebar, table view, standard menu bar, status bar etc. in the Kalzium window.

Now let us arrange the Window :

Activity – 2

Take the screenshot of the Kalzium window after removing the sidebar, tooltip and legend. Now paste it in the folder named Kalzium in your folder.



Kalzium Window

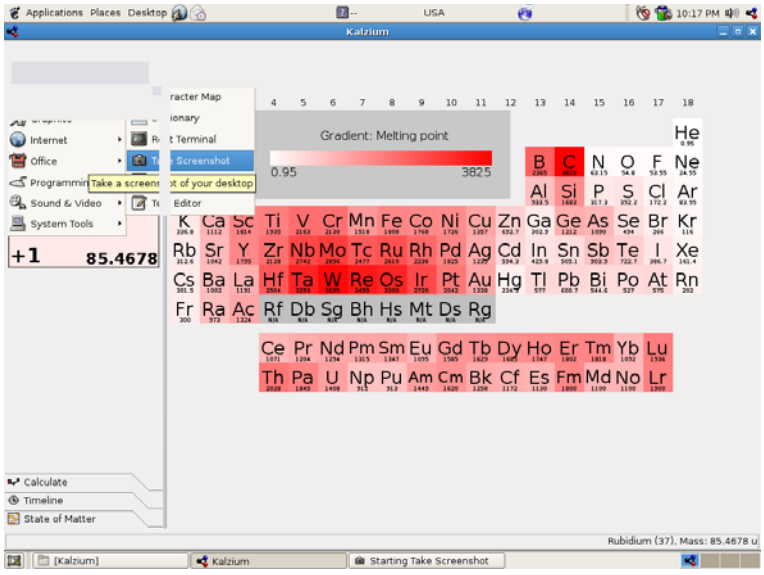
View --> Hide sidebar

Now include sidebar, tool tip and legend into the window.

Activity – 3

Display the periodic table with different colour schemes according to the variation in the properties like melting point, electro negativity etc. of the elements.

View --> Look --> Gradient --> Melting Point

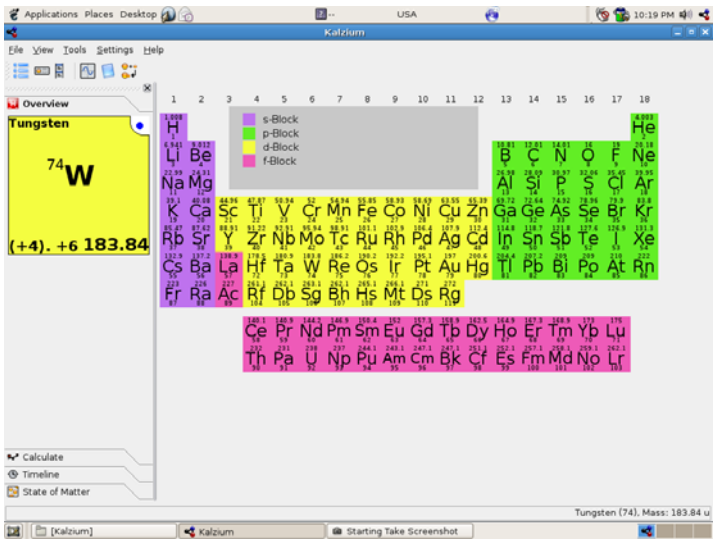


Kalzium Window

Activity – 4

Arrange the Table view to display the Blocks, Crystal Structure, Acidic nature etc.

View --> Look --> Show group



Kalzium Window

Activity – 5

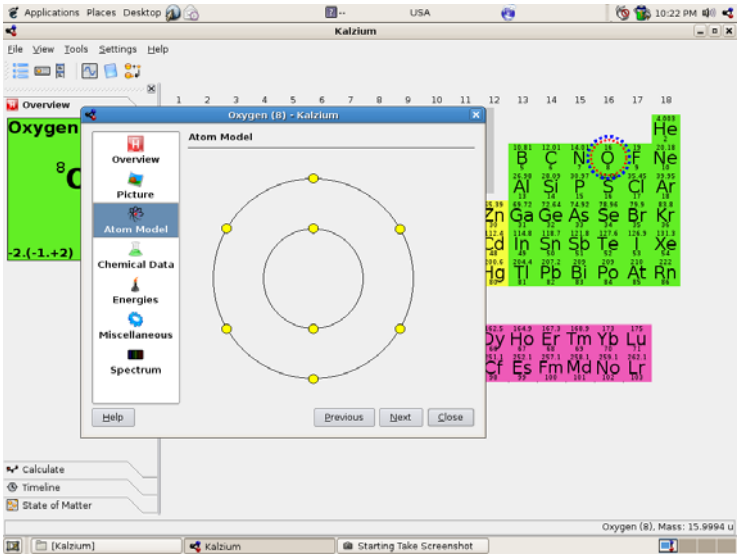
Display the periodic table with the numbers used by IUPAC, CAS (Chemical Abstract Service), Old IUPAC etc to represent different periods in the periodic table.

View --> Look --> Show group

We have learnt to arrange the periodic table according to the contents in the Text Book. Now let us familiarize different uses of Kalzium.

Overview

Click on Overview seen on the sidebar and then click on an element in the table view. We can see the most important information about the element.



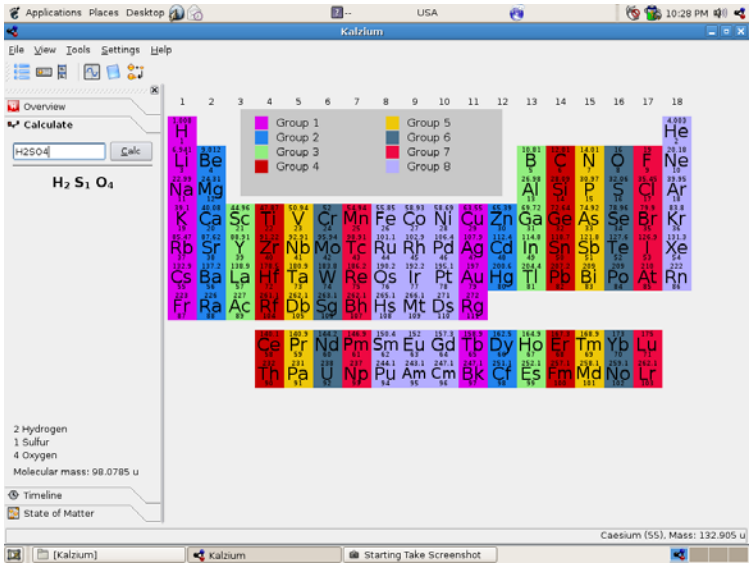
Activity – 6

Draw the Bohr model and note down the oxidation stage, isotopes, half life period, ionization energy, origin of name etc. of any two elements from their overview.

Kalzium – to calculate the Molecular mass

We can calculate the molecular mass of different substances using Kalzium. To calculate this click 'calculate ' on the side bar. Type the moleculare formula of the substance in the text box appears. Now click on the button 'calc' on the right side.

For example to find the molecular mass of Sulphuric acid, type H2SO4 in the text box and click 'calc' button.



Kalzium Window

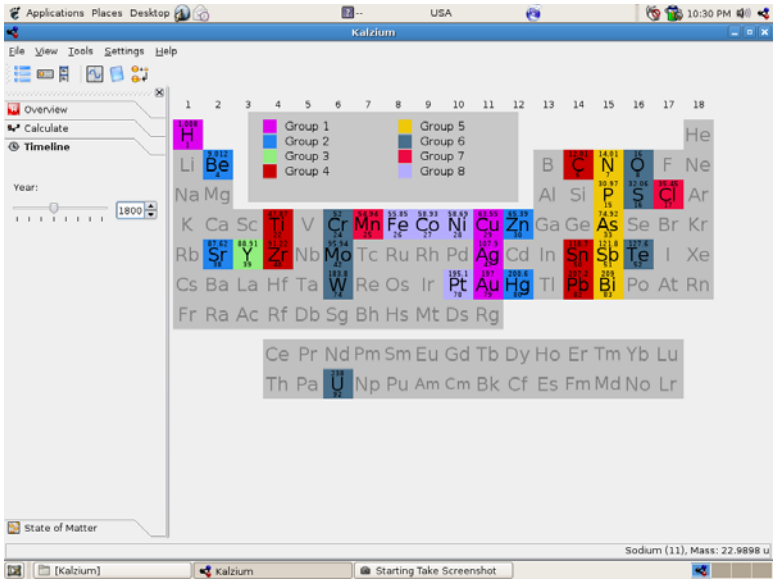
Activity – 7

Find the molecular mass of the molecules of

HNO_3	$C_{24}H_{42}O_{21}$
$C_{12}H_{22}O_{11}$	$CH_3(CH_2)_2\ COOH$
$Ca_3(PO_4)_2$	Na_3AlF_6

Timeline

The Timeline feature allows us to explore the elements discovered in a particular time period. Click 'Timeline' on the sidebar, then move the slidebar below year and place it on the required year. Watch the changes in the table view as the slider moves.



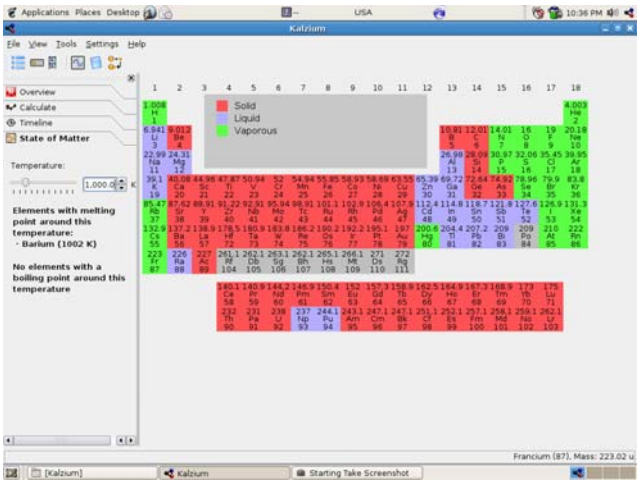
Kalzium Window

Activity – 8

Take a screen shot of the Kalzium Window with the elements discovered till 1800 and keep this in your folder.

Temperature and the State of Matter

Which are the elements in solid state at 3630K ? Which are the elements in gaseous state at this Temperature ? - To get the answers we can make use of Kalzium. Click 'State of Matter' on the Sidebar. Type 3630 under the Temperature and enter. Then the table view shows us which elements are solid/liquid/vaporous at this given temperature. We can also change the temperature by moving the slider.



Kalzium Window

Activity – 9

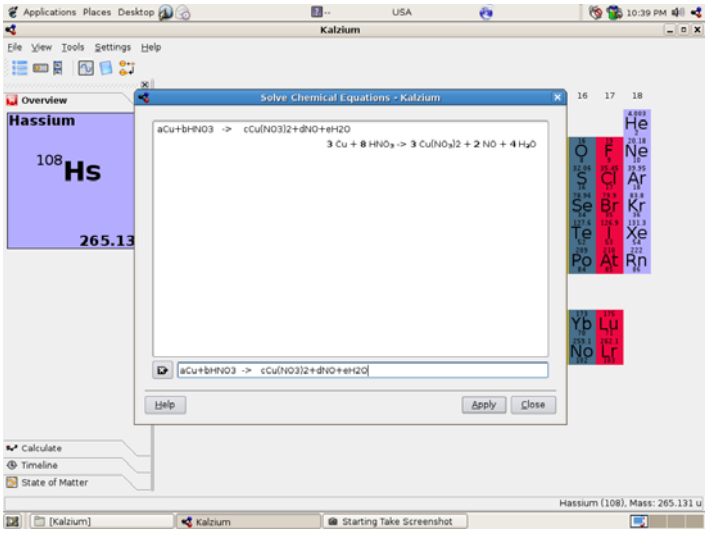
Take a screen shot of Kalzium Window which shows the State of Matter of the elements at 2000K and keep that in your folder.

Chemical equations can be Balanced

We can easily balance the chemical equation H_2 + I_2 --> HI , but sometimes we may find it difficult to balance Cu + HNO_3 --> $Cu(NO_3)_2$ + NO + H_2O. To balance an equation click 'Equation solver' on Tools menu. Then type the equation to the right side of the symbol " and click 'Apply' button. While typing the equation instead of digits use variables like a,b,c,d.... and the symbol --> can be included using '--' and '>' .

Example :

aCu + bHNO3 --> cCu (NO3)2 + dNO + CH2O



Kalzium Window

Activity – 10

Balance the given equations using Kalzium, then take the screen shot of the Kalzium window which shows these and keep that in your folder.

$CH_4 + C_2H_6 + O_2 + HNO_3 \text{ ---> } H_2O + CO_2 + NO_2$

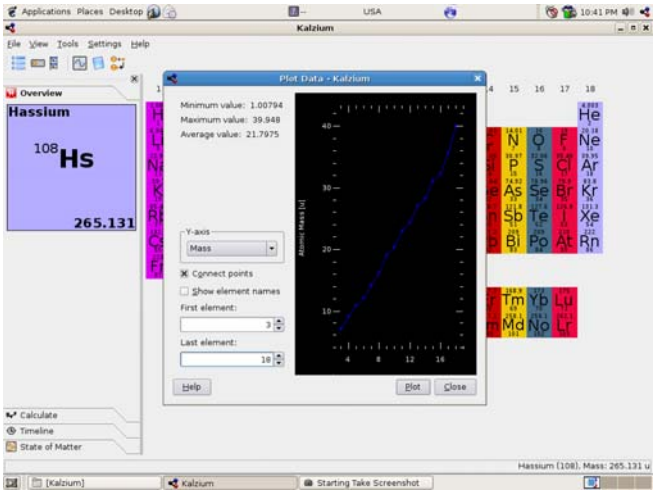
$CH_3 (CH_2)_3 COOH + O_2 \text{ ---> } H_2O + CO_2$

$C_{24}H_{42}O_{21} + H_2O \text{ ---> } C_6H_{12}O_6$

$Fe^{[2+]} + MnO_4^{[-]} + H_3O^{[+]} \text{ ---> } Mn^{[2+]} + H_2O + Fe^{[3+]}$

Graphs can be drawn

To plot graphs click 'plotdata' in the Tools menu. Then appears a window in which X-axis represents a range of elements (from one number to a higher number). Click on the ▽ in the text box below 'Y axis' and then select mass or electro negativity from the options. Then check in the box against 'Connect points'. Enter the numbers representing the first element and last element and click on the 'Plot' button.



Kalzium Window

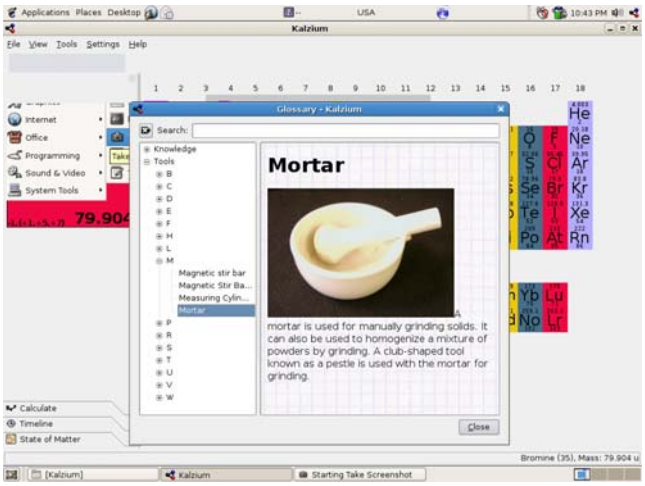
Activity – 11

Prepare a graph, which shows the differences in the Electro negativity, Mass and the Melting point of the elements in the 3rd group.

Glossary and Tools

The Glossary we get when we click

Tools --> Glossary --> Knowledge/Tools includes the definitions of the most used chemical terms and diagrams. For example it contains the explanations of terms such as Covalent Radius, Vander Waal's radius, Isobar etc and the diagrams of Water Jet Pump, Mortar etc.



Kalzium Window

We have identified the peculiarities of this application. Now discuss in which all topics we can make use of this.

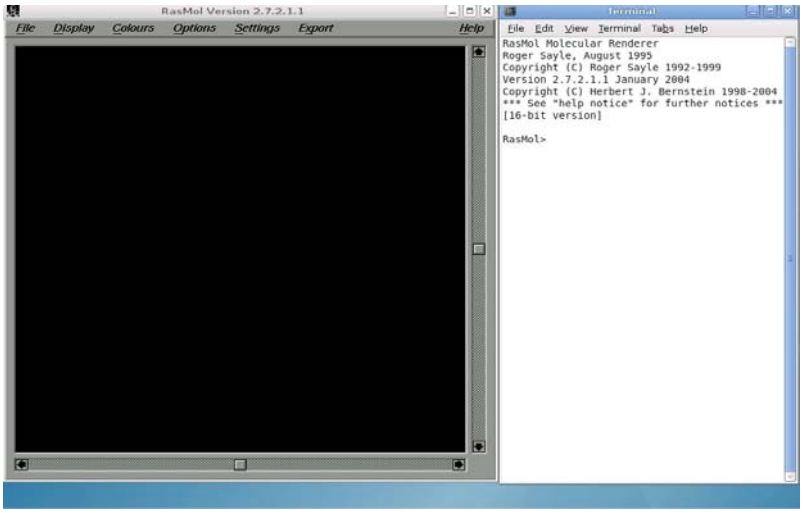
Rasmol

Rasmol is a software which can be used to view and analyse the three dimensional diagrams of different molecules. A file with the basic details of the molecule is given as input in this software and a three dimensional figure of the molecule is displayed in the screen. We can make use of different types of file formats for input. Commonly used file format is PDB (Protene Data Bank).

How to open Rasmol

Application --> Education --> Rasmol Molecular Graphics. Visualization.

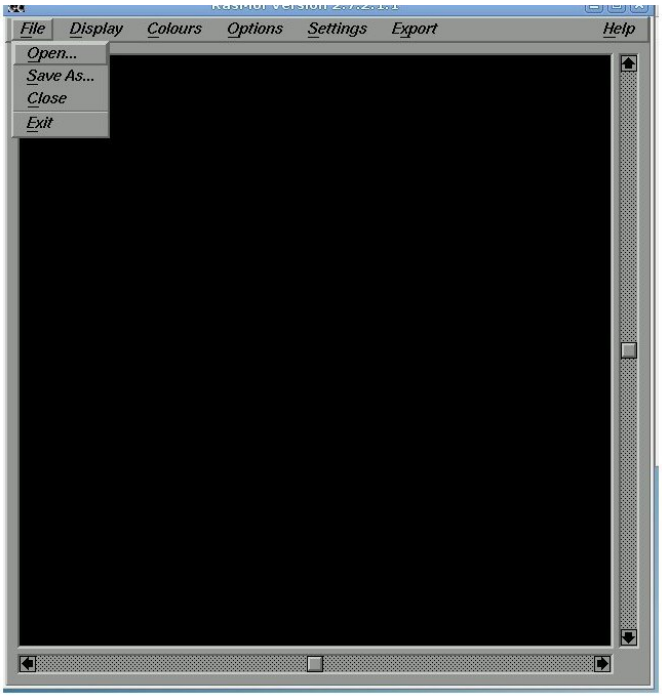
When we open this application two windows are opened. Graphics or Canvas Window (Diagram Ras.1.jpg) and the second one, Command line or terminal window.



Ras 1.jpg

Here we go through the steps to draw the structure of ethanol using Rasmol. For this Copy the file named ethanol.PDB to home directory from the CD. [We can copy more pdb files from the website ftp://ftp.wwpdb.org/pub/pdb/data.]

1. Open Rasmol Molecular Graphics Visualization

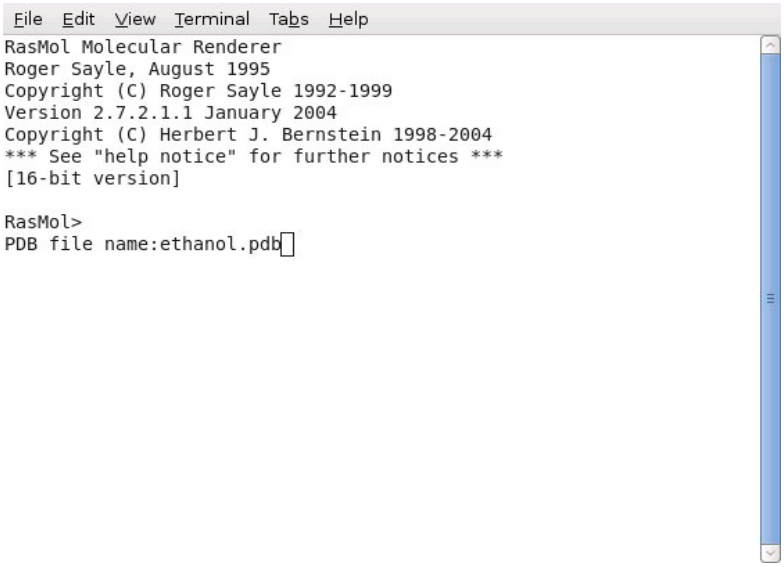


Ras.2.jpg

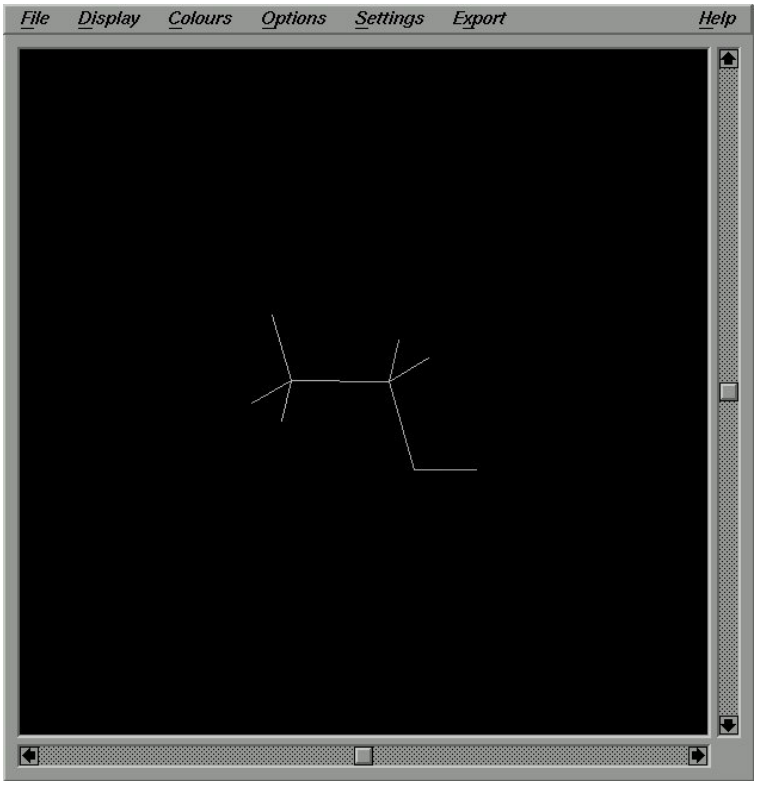
2. In the canvas window click as follows

   File --> Open --> (Ras.2n) then in the terminal window we can see a request for file name.

3. Type the file name (ethanol.PDB) in the terminal window and enter. (Diagram Ras.3.jpg). Wireframe model of the ethane molecule appears in the canvas window (Diagram Ras.4.jpg)



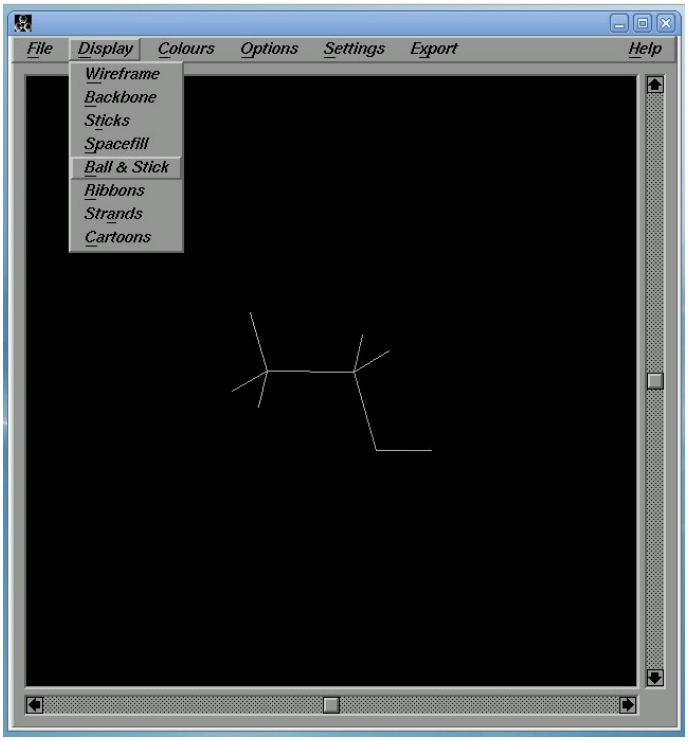
Ras.3.jpg



Ras 4.jpg

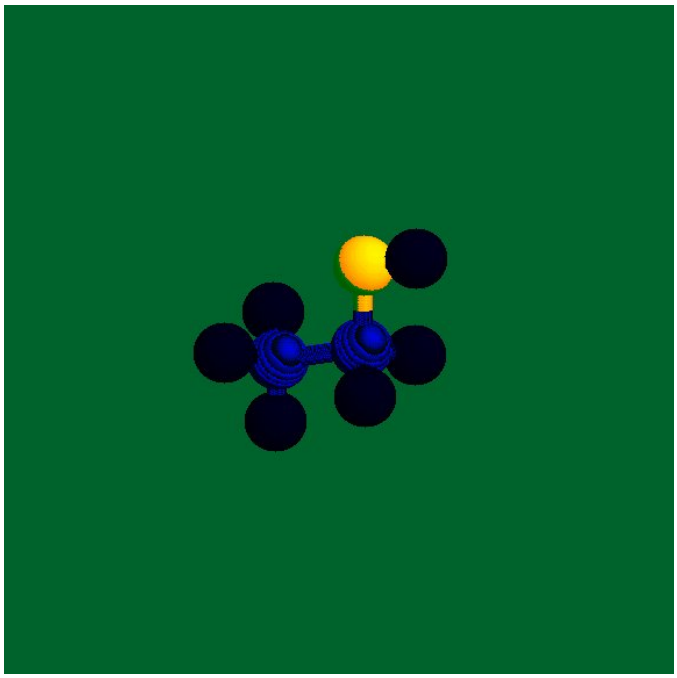
4. Now we can convert this wireframe model into the Ball and Stick model. For this click as follows

Display ---> Ball & Stick (Diagram Ras.5.jpg)



Ras 5.jpg

Ball and Stick model of Ethane is displayed in the Canvas window (Ras.6.jpg).



Ras 6.jpg

Now we can modify this structure.

1. To rotate the molecule with respect to X axis or Y axis use scroll bar or drag from X axis or Y axis using mouse.
2. To display the molecule in different models

   Display --> select the required model

3. To give different colours of our choice

   colors --> select the required mode

4. To label the molecules

   Settings --> pick label

   then click on the atom which has to be labeled

5. To measure the angles and distances between the atoms

   Settings --> Pick Angle

   Settings --> Pick distance

   then click on the required atoms.

6. To export (into PPM format)

   Export --> PPM

   then give the file name in the terminal window. To export into other formats select that item instead of PPM.

7. To save the file

   File --> Save as (give the file name in the terminal window)

8. To close the file

   File --> Close

   <u>We can change the back ground of the display window</u>

   In the terminal window type the command

   background < colour >

   We can use either colour name or Colour code here.

For example, to give blue colour to the background the command is as follows

background (0,0,255)

To change the Text size

In the terminal window give the command

Set fontsize <Size>

eg: Set fontsize 12

To change Font stroke

In the terminal window give the command

Set fontstroke <num>

eg: Set fontstroke 1

To change the colour of the atom

We can change the colour of an atomin two steps

1. Select the atom.
2. Change the colour of the selected atom.

For example, we have to change the colour of Caron atoms into blue

In the terminal window give the following commands

Select Carbon
Colour blue or Colour (0,0,255)

ACTIVITY

1. Export the following molecules into PPM format

Diamond, graphite, fallarine

2. Take a screen shot which shows the distance between the atoms H and O in H_2O molecule.
3. Give red colour to Carbon and blue colour to the Hydrogen atom in Methane Molecule. Take a screen shot of this methane molecule.
4. Rotate Ethane molecule in different angles and take screen shot in each case.

Installation of Rasmol

1. Copy the deb file rasmol_2.7.2.1.1-5.i386.deb into the home directory.
2. Right click on the file and select " Open with GDebi Package Installer".
3. Package installer window opens. Click on the button ' Install Package'.

OR

Run the following command in the Root Terminal Window

dpkg -i rasmol_2.7.2.1.1-5_i386.deb

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Kalzium

I Std. VIII

1. *Chapter - 5 - Molecular Atom*
2. *Chapter - 6 - Chemical bonding*
3. *Chapter - 7 - Stability*

II Std. IX

1. *Chapter - 1 - Periodic table*
2. *Chapter - 2 - Chemical bonding*
3. *Chapter - 5 - Carbob - Equation balancing*
4. *Chapter - 7 - Non-metals*
5. *Chapter - 8 - Metals*

III Std. X

1. *Chapter - 1 - Language of chemistry*
2. *Chapter - 2 - Structure of atom and periodic table*
3. *Chapter - 7 - Organic compounds chemical reaction - Equation balancing*
4. *Chapter - 10 - Acids - Equation balancing*

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