Inspecting various structural features of Tetraamine carbonato cobalt(III) nitrate complex with Jmol

M.Sowmya, S.Remina, A.Manasa, K.S.R.Rajeswari

School of Freshman engineering, Kalasalingam Academy of Research and Education, Anand nagar, Krishnankoil, Virudhunagar, Tamilnadu, India- 626126

1. Introduction

Tetraamine carbonato cobalt(III) nitrate is a chemical compound with the chemical formula $[Co(NH_3)_4CO_3]NO_3$. It is a blue-green solid that is soluble in water. It is also known as cobalt nitrate tetraamine carbonate or cobalt(III) tetraamine carbonate nitrate. It is typically used as a precursor in the synthesis of other cobalt compounds and as a catalytic agent in organic synthesis. Tetraamine carbonato cobalt(III) nitrate is a coordination complex, which means that the cobalt atom is bound to other atoms or molecules through coordinate covalent bonds. In this case, the cobalt atom is bound to four ammonia molecules (NH_3), one carbonate ion (CO_3), and one nitrate ion (NO_3). Coordination complexes are often useful in chemical reactions because the metal atom at the center of the complex can act as a catalyst, helping to speed up or change the direction of a chemical reaction. The complex finds its applications in ceramics, glass, and enamel industry as a colouring pigment. It is used as a raw material in the preparation of cobalt compounds, like cobalt(III) oxide and cobalt(II) carbonate. It is used as a catalyst in the organic reaction such as Diels-Alder and Friedel-Crafts alkylation. It acts as a oxidising agent and a dehumidifying agent. Tetramine carbonato cobalt (III) nitrate is a strong oxidizing agent, so it should be handled with care as it may cause burns and irration to skin or eyes. Tetraamine carbonato cobalt(III) nitrate is used in various analytical methods, such as in spectrophotometry for the determination of cobalt ions in different samples. In addition, it can also be used in the field of medicine, as it has been reported to have antimicrobial activity against bacteria and fungus. It can also be used in manufacturing of inks, dyes, and pigments. It is also important to follow the safety regulations and guidelines when working with this compound.

2. Objectives

- To create 3D structure of Tetraamine carbonato cobalt(III)nitrate using the Jmol interface.
- To label the molecule of Tetraamine carbonato cobalt(III)nitrate.
- To measure the Bond Length and Bond Angle of Tetraamine carbonato cobalt(III)nitrate.

- To evaluate the colour and structural changes of Tetraamine carbonato cobalt(III)nitrate using Jmol script console.
- To create the surface of the molecule.
- Dealing with molecular structure.

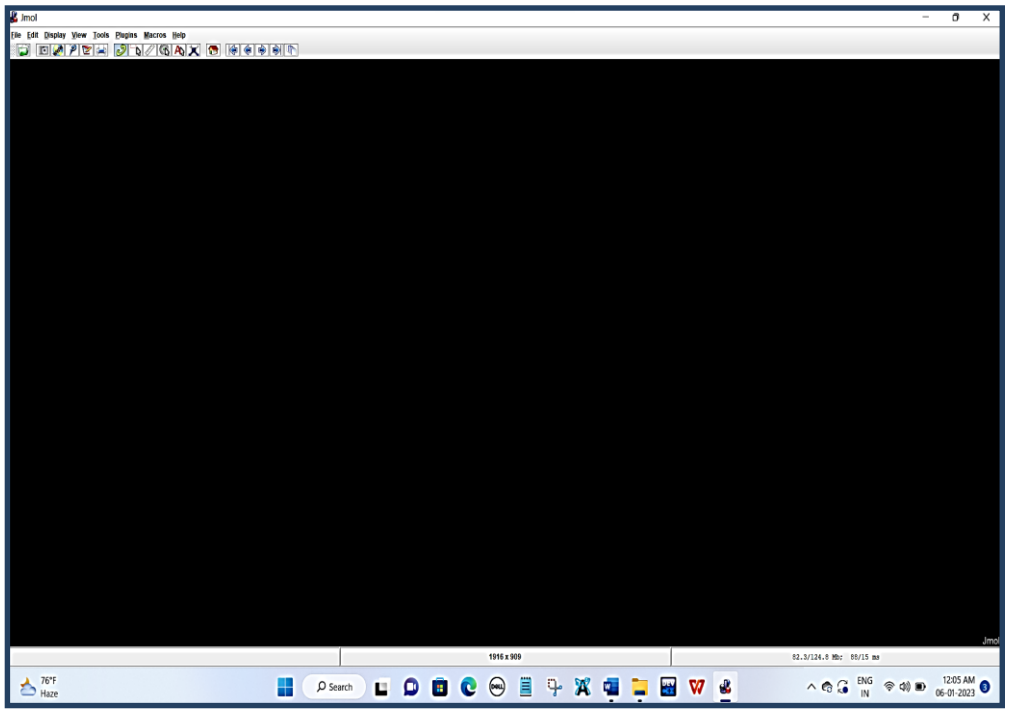
3. INSTALLATION OF Jmol

Jmol is an open-source Java viewer for chemical structures and biomolecules in 3D.

- It is free and open source software, written in Java, it runs on Windows, Mac OS X, Linux and Unix systems.

3.1. Procedure for installation of Jmol

- The open source Jmol software needs JAVA application installed in your computer. So it is better to install the latest version of Java.
- We can install JAVA application from www.java.com
- After installing JAVA go to http://www.sourceforge.net and search for Jmol and click on download.
- A zip file of Jmol will be installed.
- Now we need to extract Jmol.jar file from zip file and place it outside.
- Now to run Jmol we need to open the Jmol.jar file from the installed files.
- Now we can create and edit molecules using Jmol.



About the compound:

Compound name: Tetraamine carbonato cobalt(III)nitrate

Chemical formula: $[Co(NH_3)_4CO_3]NO_3$

3.2. Procedure for creating 3D structure of Tetraamine carbonato cobalt (III)nitrate in Jmol

Step 1: Open Jmol interface, click the model kit tool in top of the tool bar.

Step 2: Select input element as "Co", pink colour cobalt atom appears on the screen.

Step 3: Select add atoms- nitrogen atom (repeat for 4 times) by dragging from Co atom.

Step 4: Right click and select atom oxygen, then drag from Co to get oxygen atom (repeat for 2 times)

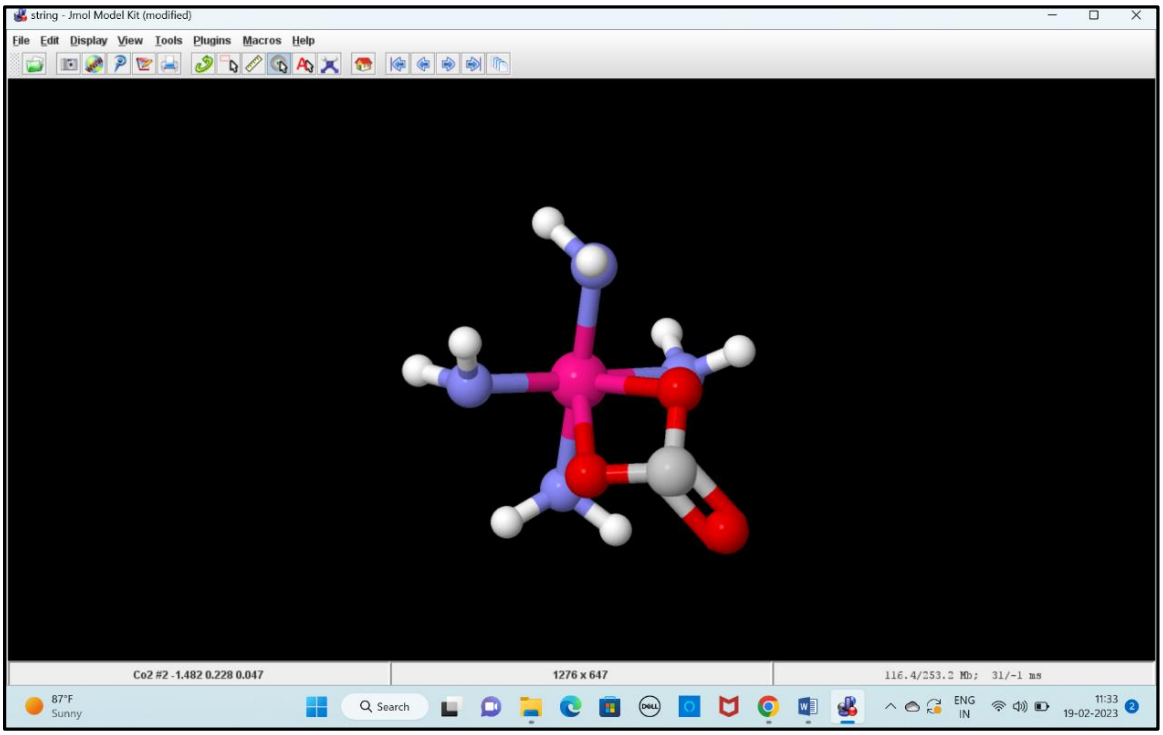
Step 5: The oxygen atoms were added along with hydrogen atom, so use delete atom option to delete the hydrogen atoms

Step 6: Click add carbon atom by dragging from both the oxygen atom

Step 7: Select add atom oxygen by dragging from carbon atom then change the bond type double

Step 8: Right click on the molecule and select minimise to optimise the geometry

3D STRUCTURE OF TETRAAMINE CARBONATO COBALT(III)NITRATE CREATED IN Jmol

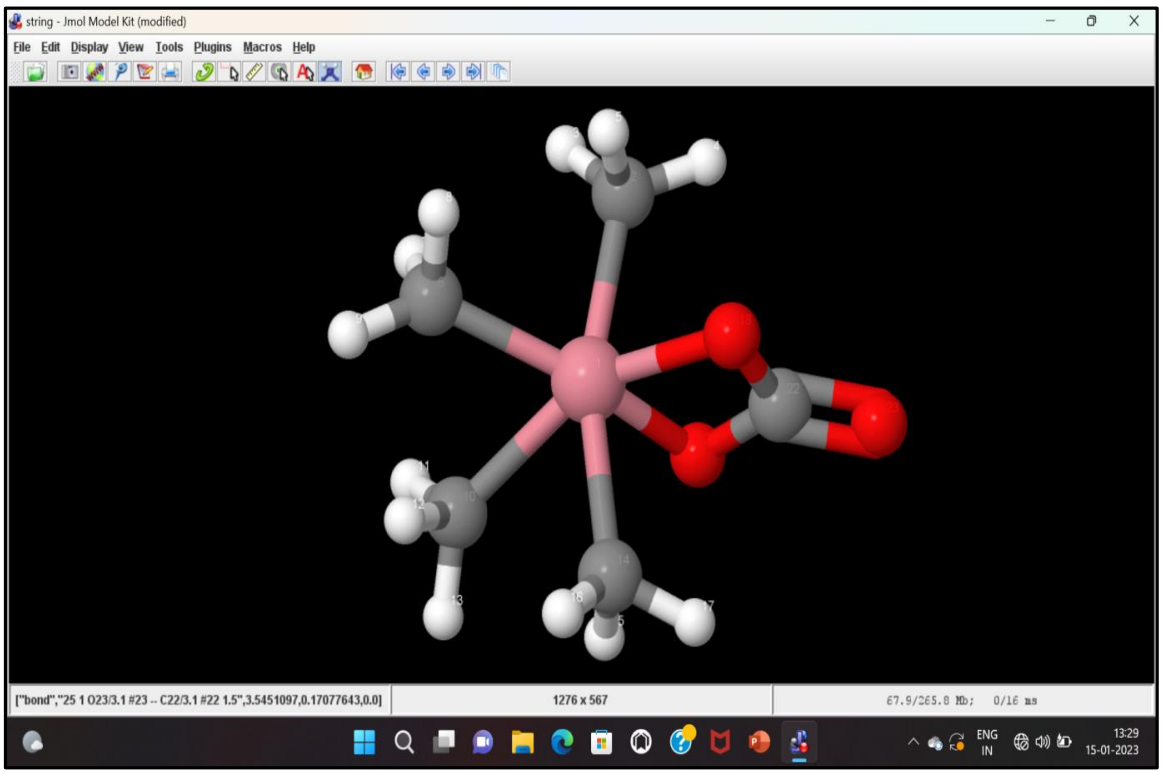


3.3. Procedure for labelling the molecule

Step 1: Open the Display menu.

Step 2: Select label from scroll down menu, under that select number.

Step 3: Now all the atoms are numbered.



3.4. Procedure for measuring the bond length and bond angle

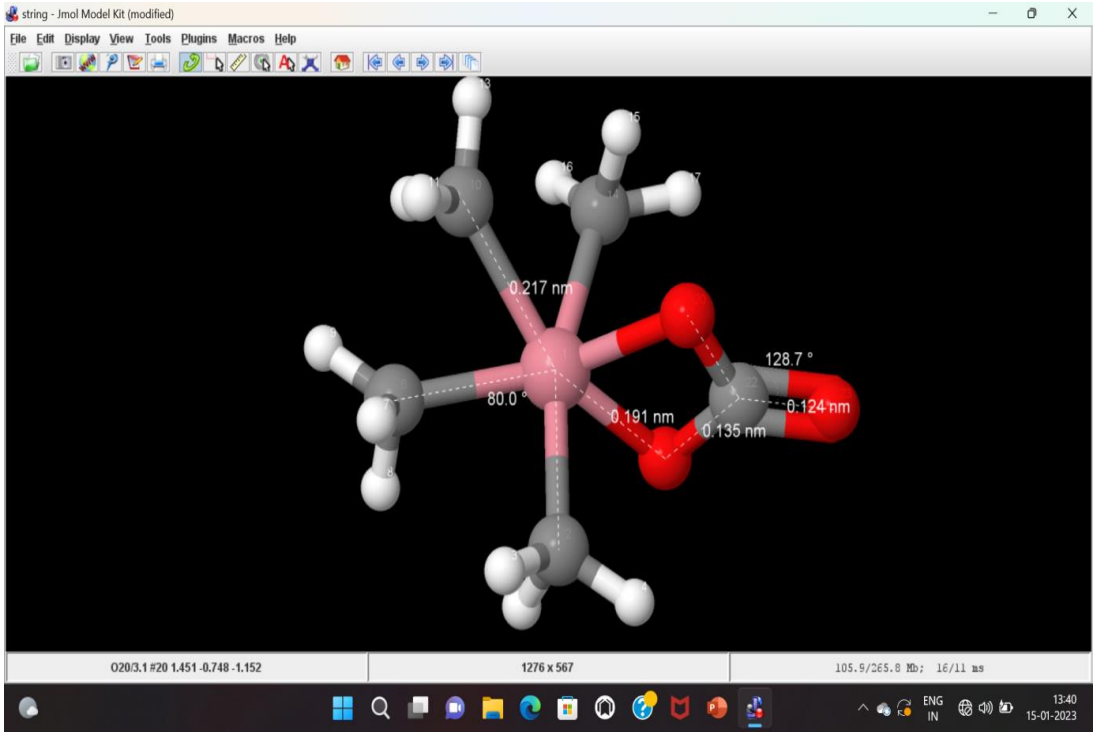
Step 1: Open the model kit menu and click on minimise. Now the model is in most stable confirmation.

Step 2: Click on 'Tools' menu select 'Distance Units .

Step 3: Now select on sub menu according to the requirement- 'Nanometers 1E-9'.

Step 4: BOND LENGTH -Double click on any atom and to fix the measurement double click on corresponding atom now the bond length will be displayed between two atoms.

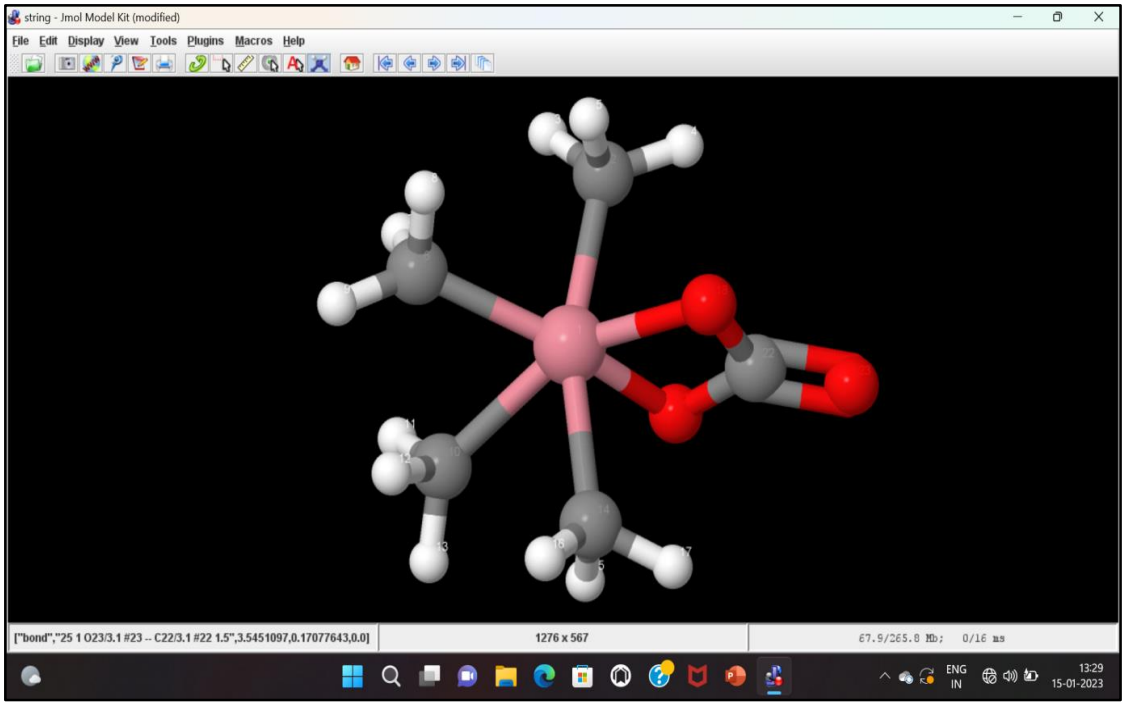
Step 5: BOND ANGLE -Double click on a particular atom and click on corresponding atom and double click on third atom now the angle will be formed.

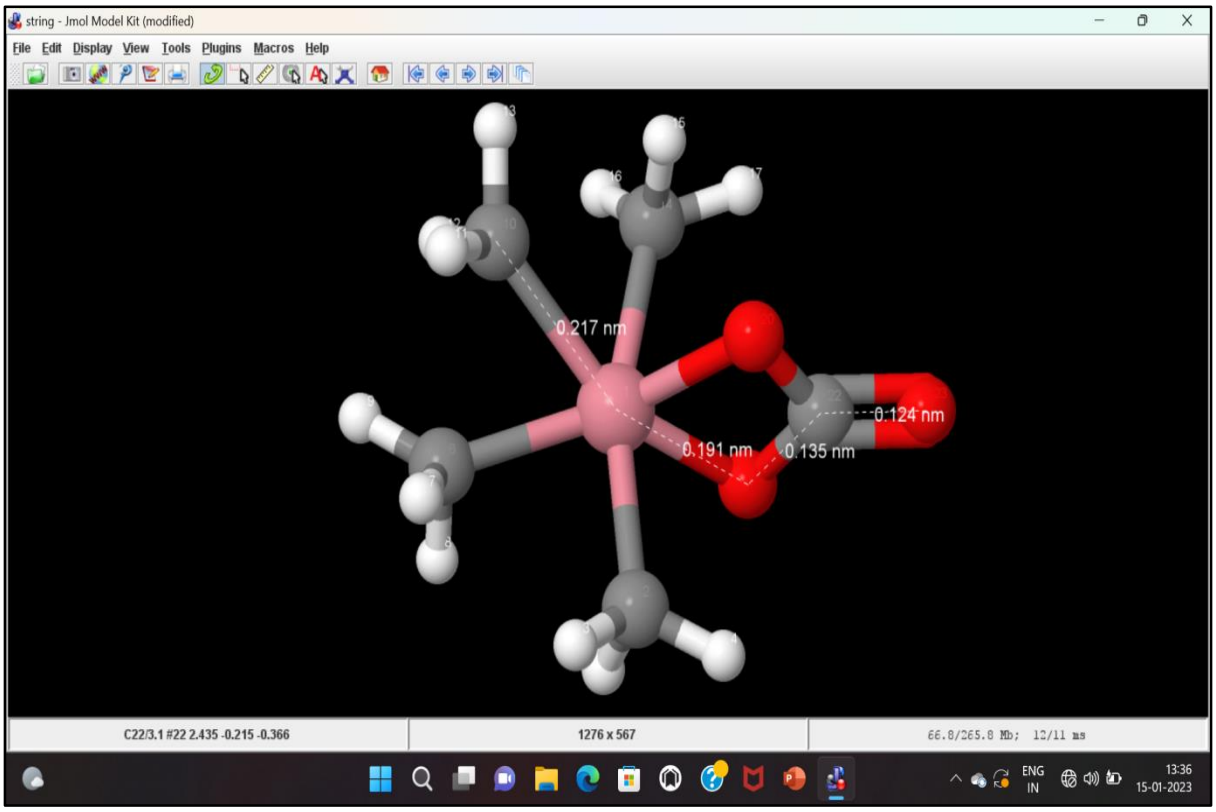


3.5. Procedure for tabulation of measurements

Step 1: Click on 'click atoms to measure distance 'icon in the tool bar.

Step 2: Measurements dialogue box opens on the panel





3.6. Procedure for editing in 'SCRIPT CONSOLE'

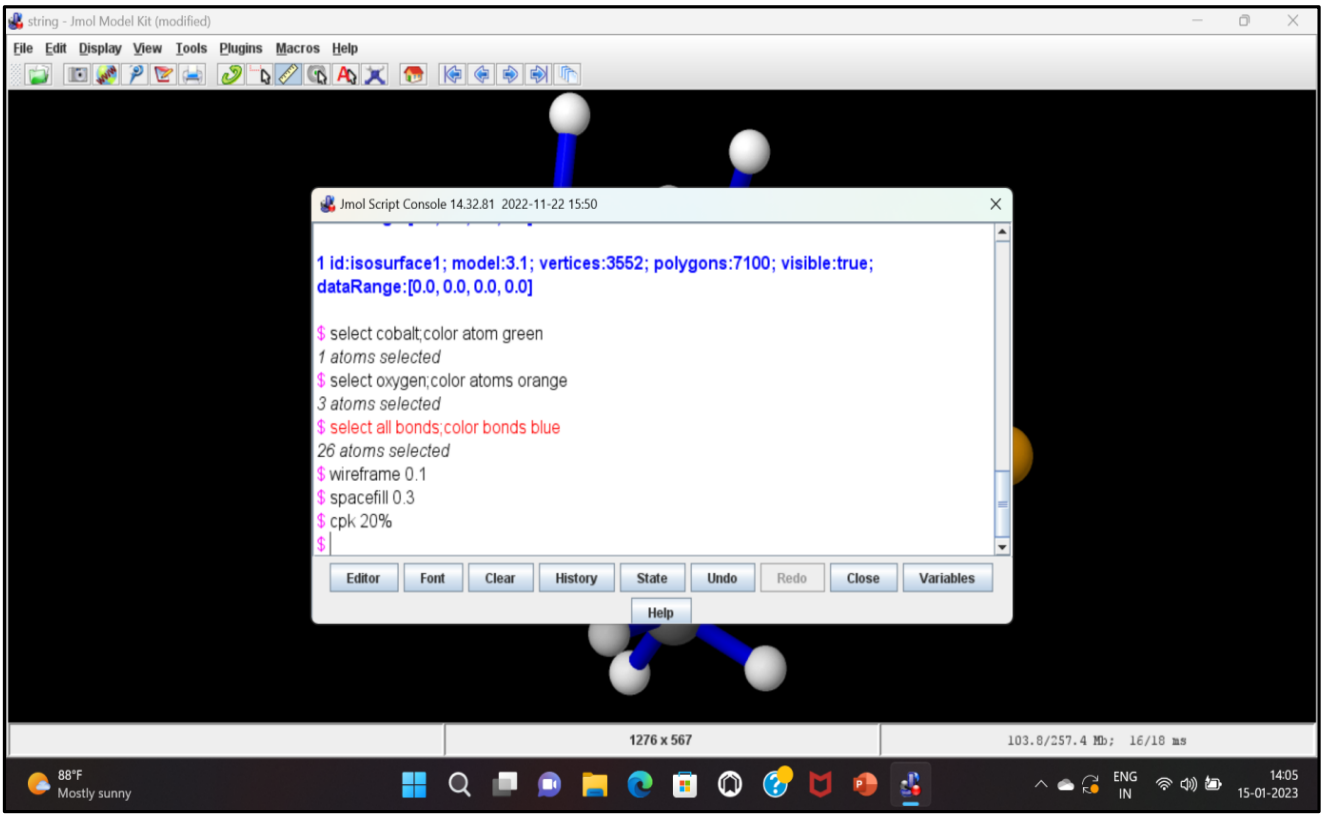
Step1: Click on 'file menu' in menu bar.

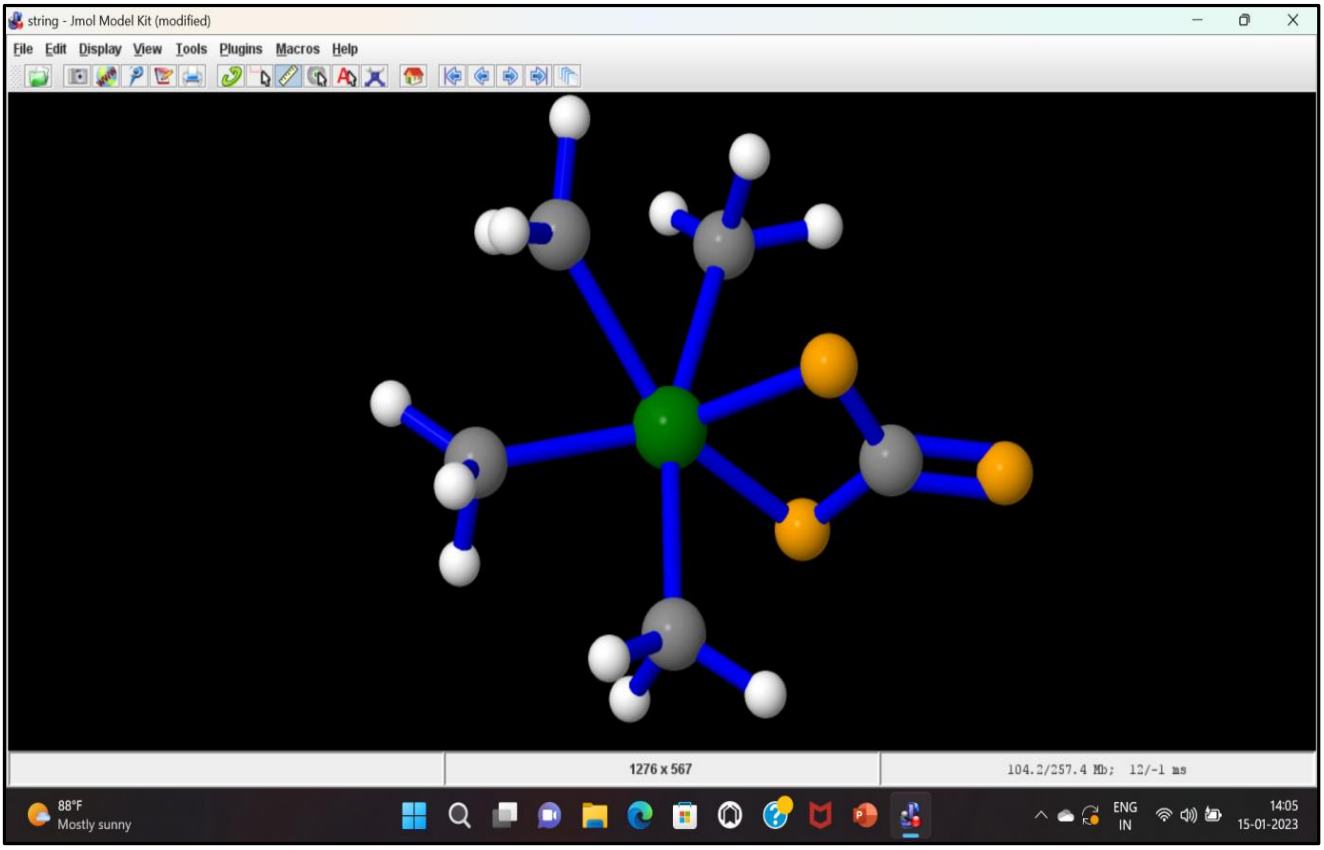
Step 2: In drop down click on console option.

Step 3: Jmol scrip Console window opens on the screen.

Step 4: Console window has a text area to type the command.

Step 5: Type the commands which you want to modify.

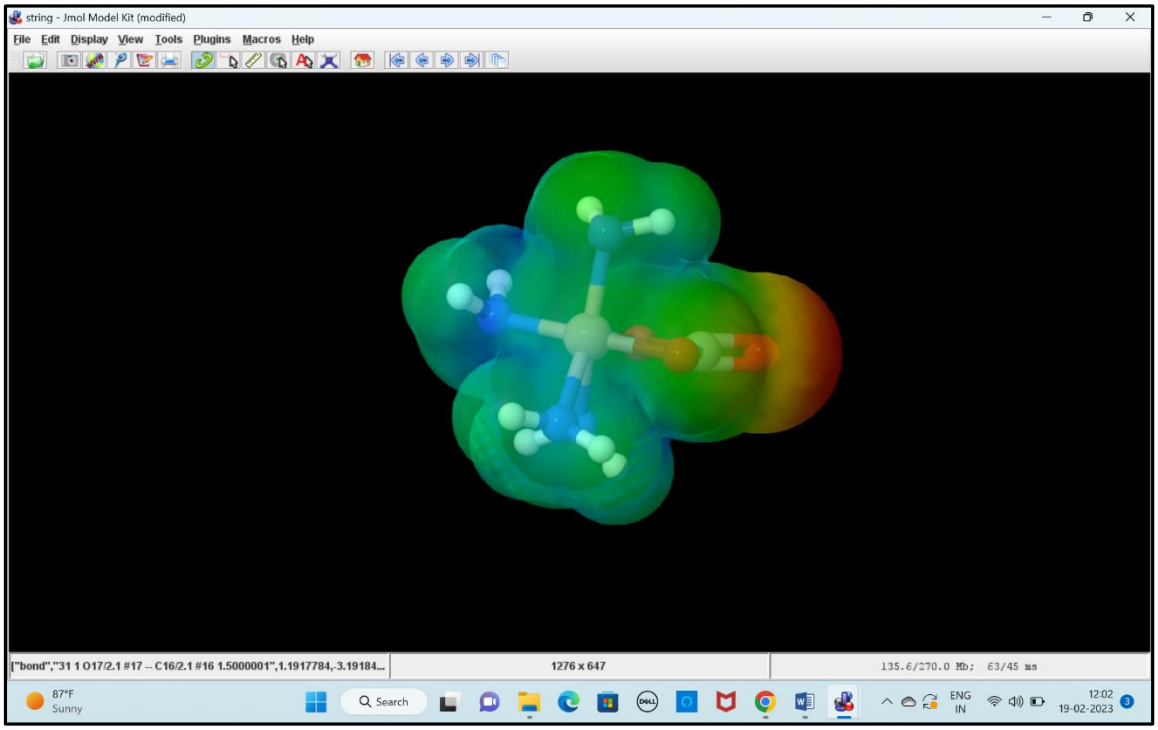

string - Jmol Model Kit (modified)
File Edit Display View Tools Plugins Macros Help
Jmol Script Console 14.32.81 2022-11-22 15:50
1 id:isosurface1; model:3.1; vertices:3552; polygons:7100; visible:true;
dataRange:[0.0, 0.0, 0.0, 0.0]
$ select cobalt;color atom green
1 atoms selected
$ select oxygen;color atoms orange
3 atoms selected
$ select all bonds;color bonds blue
26 atoms selected
$ wireframe 0.1
$ spacefill 0.3
$ cpk 20%
$
Editor Font Clear History State Undo Redo Close Variables
Help
1276 x 567
103.8/257.4 Mb; 16/18 ms
88°F
Mostly sunny
ENG
IN
14:05
15-01-2023


string - Jmol Model Kit (modified)
File Edit Display View Tools Plugins Macros Help
1276 x 567
104.2/257.4 Mb; 12/-1 ms
88°F
Mostly sunny
ENG
IN
14:05
15-01-2023

3.7. Procedure for creating the surface of the molecule

Step 1: Right click on the molecule, if model kit was open –close it.

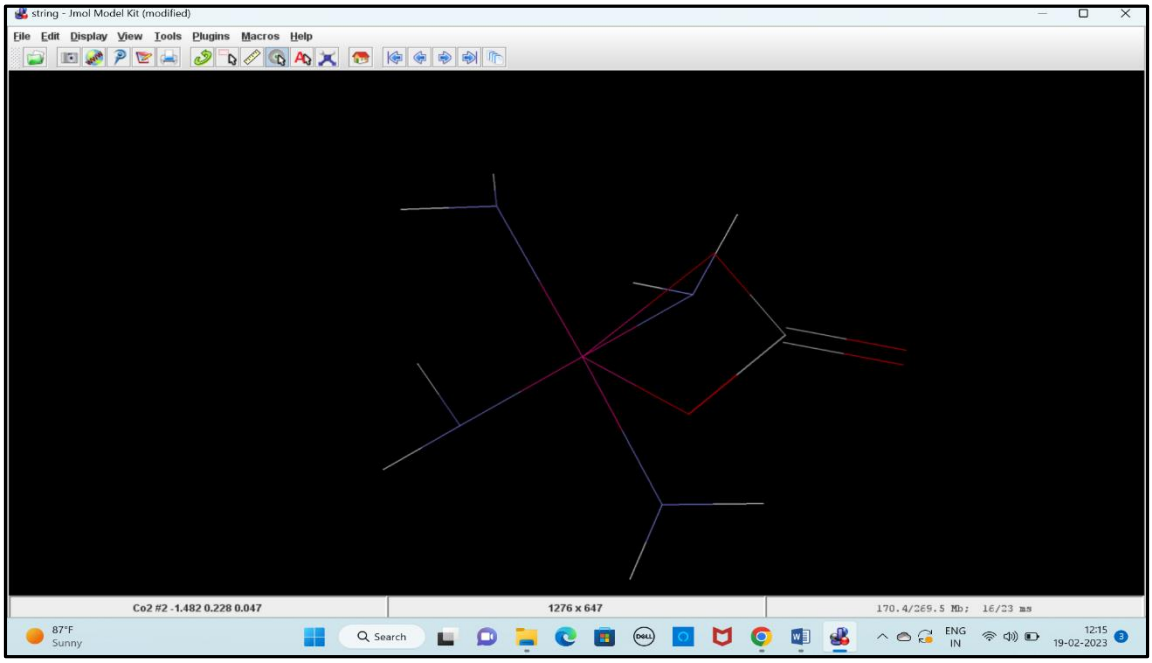
Step 2: Right click on the molecule and select surface option within that select Electrode potential (All ranges)



3.8. Procedure for creating various types of molecular representations

Step 1: Right click on the molecule, if model kit was open –close it.

Step 2: Right click on the molecule and select Style –Scheme – Wire frame



4. Result and Discussion

4.1. Reaction for Tetramine carbonato cobalt(III) nitrate

The synthesis of $[Co(NH_3)_4CO_3]NO_3$ involves the following unbalanced equation,

$$Co(NO_3)_2 + NH_3(aq) + (NH_4)_2CO_3 + H_2O_2 \longrightarrow [Co(NH_3)_4 CO_3]NO_3 + NH_4 NO_3 + H_2O$$

4.2. Structure of Tetramine carbonato cobalt(III) nitrate

The complex is '**Tetrahedral**"

BOND ANGLE

The angle between the atoms 7,1 and 2 is 80°

The angle between the atoms 20, 22 and 23 is 128.7°

BOND LENGTH

The length between atoms 1 and 10 is 0.217 nm

The length between atoms 1 and 21 is 0.191 nm

The length between atoms 21 and 22 is 0.135 nm

The length between atoms 22 and 23 is 0.124 nm

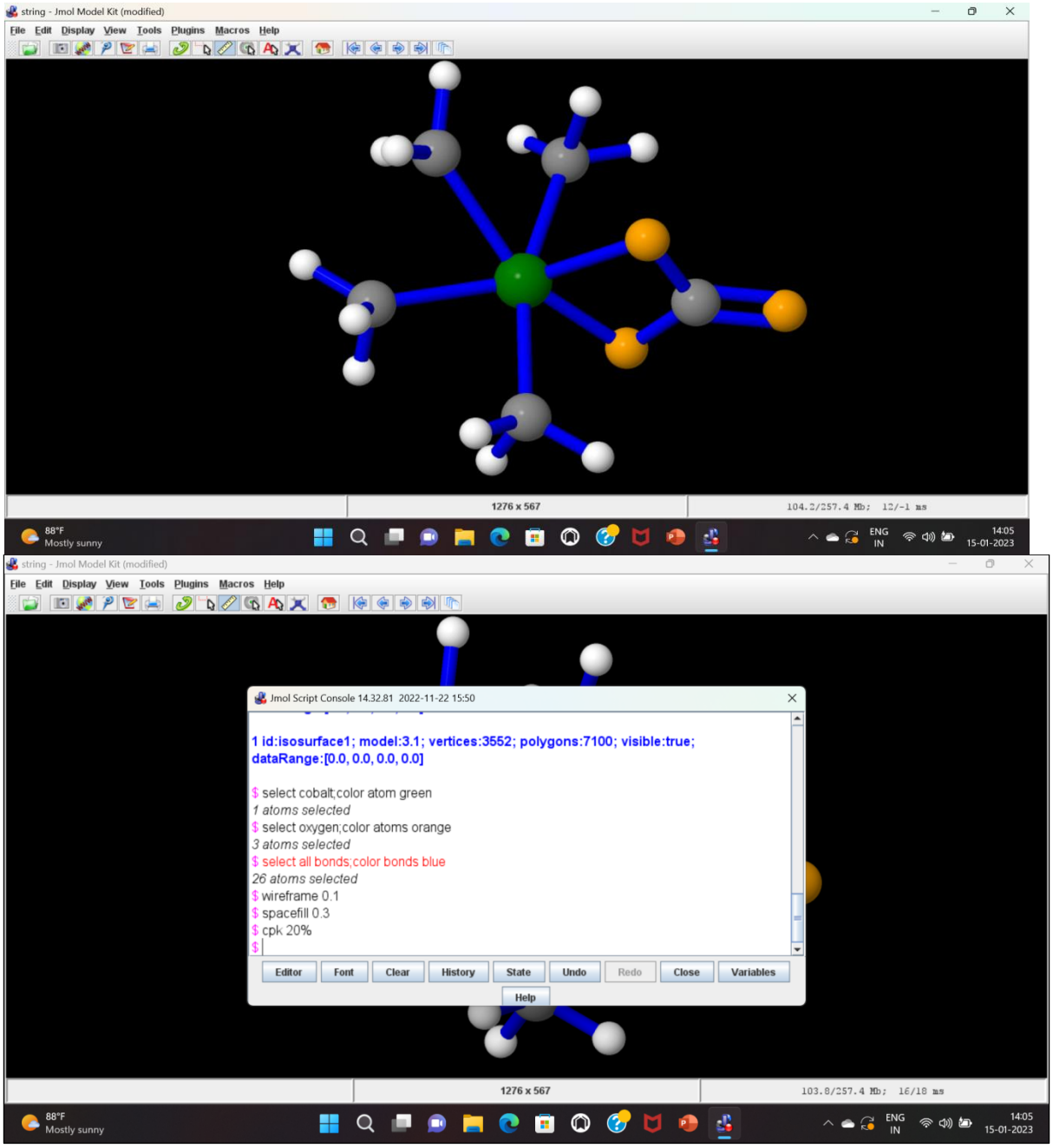
4.3. Script console

We use some specific commands in script console

For changing the colour of the atom use the command '$select atom colour'

For changing the colour of the bond use the command '$select bonds; colour'

For size of the bond use the command '$wireframes size'



After using the console script, the final molecule

Conclusion:

The Tetramine carbonato cobalt (III) nitrate synthesised in laboratory was observed to be in Pinkish violet colour. The 3D model of the complex was created in Jmol interface and various properties of the complex were explored in Jmol. The atoms of the complex were labelled, the bond length and angles were predicted. Using the **Script console,** we had changed the colour of the atoms as well as bonds. We also changed the size (width) of the bond in the 3D model using Jmol application. We also explored the electrostatic potential of the molecule in surface menu of the Jmol interface.

Acknowledgement

We wish to express our gratitude to our KARE Management for providing the facilities for fabrication. We also wish to express our heartfelt thanks to Dr. Koteswara Rao Anne, Director Academics, Dr.N.Rajini, Dean Freshman Engineering and Dr. P. Sivaranjana project guide for their encouragement and support.