

Exploring the Structural Features of an Octahedral Metal Ion Complex using Avogadro Software

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1. Introduction

Hexaamminecobalt (III) chloride), also known as Hexamine cobalt chloride. $\text{Co}(\text{NH}_3)_6\text{Cl}_3$ is a coordination complex composed of cobalt as the central metal ion, in +3 oxidation state, six ammonia molecules (NH_3) as ligands inside the coordination sphere, and three chloride ions (Cl) outside the coordination sphere. It is a brick red coloured solid and is used in chemical analysis, electroplating, and as a catalyst. Hexamine Cobalt(III) Chloride is a coordination complex, which means that the metal ion (cobalt in this case) is surrounded by a group of molecules or ions that are coordinated to it. These molecules or ions are called ligands, and in the case of hexamine cobalt(III) chloride, the ligands are six ammonia molecules and three chloride ions. The coordination of these ligands to the cobalt ion gives the complex its unique chemical and physical properties. Hexamine cobalt(III) chloride is typically used in chemical analysis as a reagent in the determination of chloride ions. It is also used as a catalyst in certain chemical reactions, and in electroplating, as an electrolyte to deposit cobalt metal. It is also used as an oxidizing agent in organic synthesis, particularly in oxidation of alcohols, amines and aldehydes. It is important to note that this compound should be handled with care as it can be toxic and may cause skin and eye irritation. It should be stored in a cool, dry place and kept away from heat sources and incompatible materials. Hexamine cobalt(III) chloride can also be used in the preparation of other cobalt complexes. For example, it can be used to prepare the hexamine cobalt(III) ion, $\text{Co}(\text{NH}_3)_6^{3+}$, by reacting with a strong base. It can also be used in the preparation of other coordination compounds, such as cobalt(III) chloride hexa hydrate, which is formed by adding water to hexamine cobalt(III) chloride. Hexamine cobalt(III) chloride is also used in the preparation of some biological compounds, such as vitamin B12, which is a cobalt-containing compound that is essential for human health. Vitamin B12 is prepared by reacting cobalt(II) salts with hexamine cobalt(III) chloride. Hexamine cobalt(III) chloride is a versatile coordination compound with a wide range of applications in chemical analysis, electroplating, organic synthesis, and the preparation of other coordination compounds and biological compounds. However, due to its toxicity it should be handled with care.

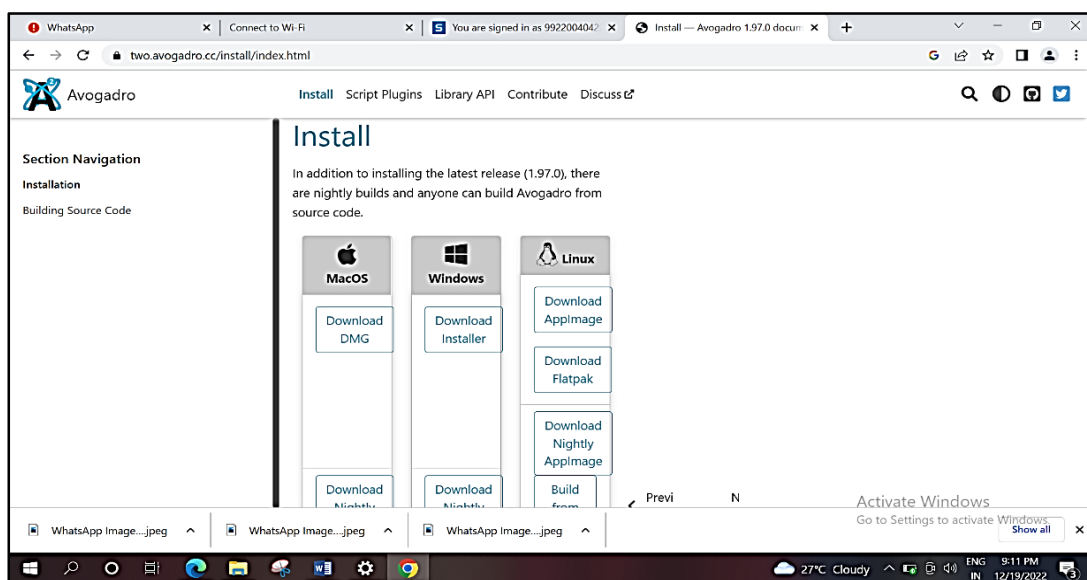
2. Objectives

- Drawing the 3D structure of the complex in Avogadro interface
- Drawing the 3D structure of the complex by replacing the amine group with aqua group
- Drawing the 3D structure of the complex by replacing the Co atom with Ni atom
- Exploring the structural properties of all the complexes in Avogadro
- Comparative analysis of all the complexes

3. INSTALLATION OF AVOGADRO

3.1. Procedure for installation

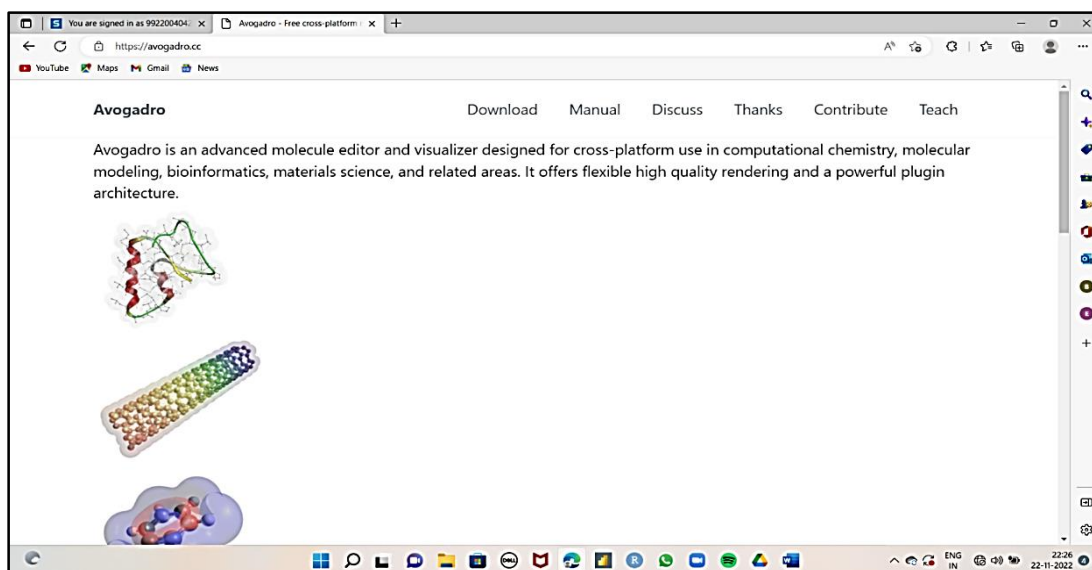
- Avogadro is an open-source software so it can be installed for free
- Go to browser and search Avogadro in search bar, a web page opens showing us the link <https://avogadro.cc>
- The download option is available at the top of the page, click on that option to download
- After completion of download install the package in the system
- At the time of installing the software click on the option saying **Add Icon to Home Screen**
- Now we can open the Avogadro software from the desktop by clicking on the icon



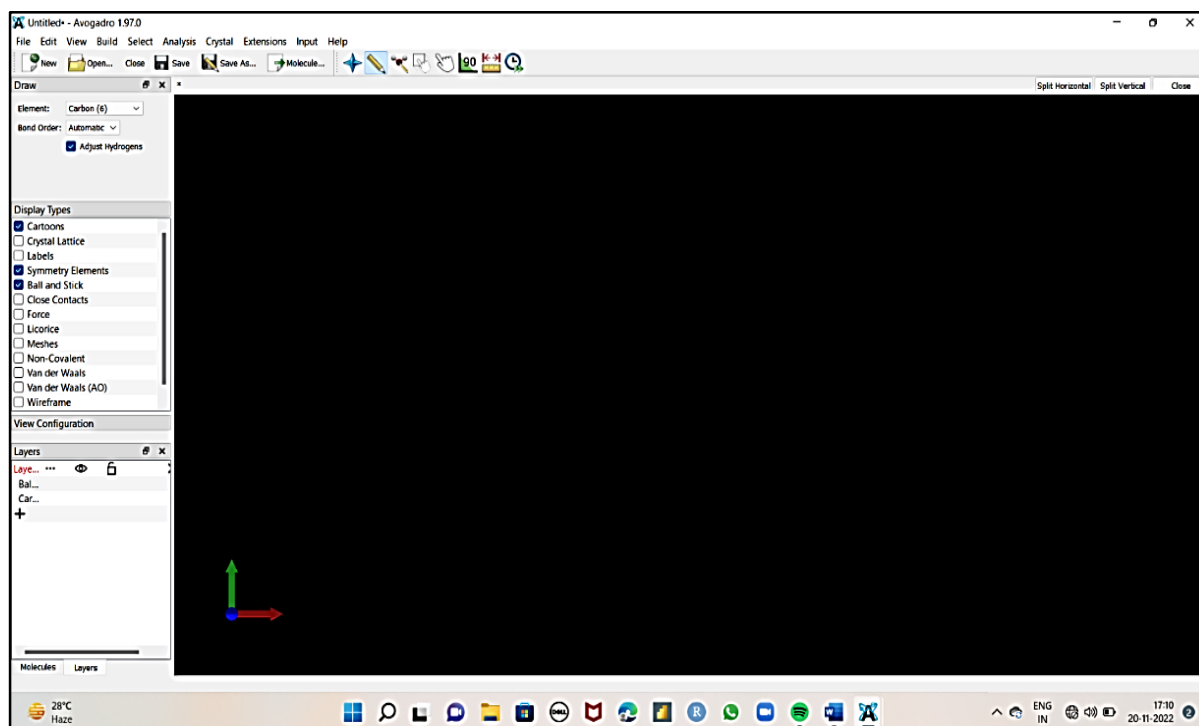
3.2. Overview of Avogadro

- Right click on the Avogadro icon on the desktop to open Avogadro software

- A window opens with different options on the top and blank space in the middle to create the structures

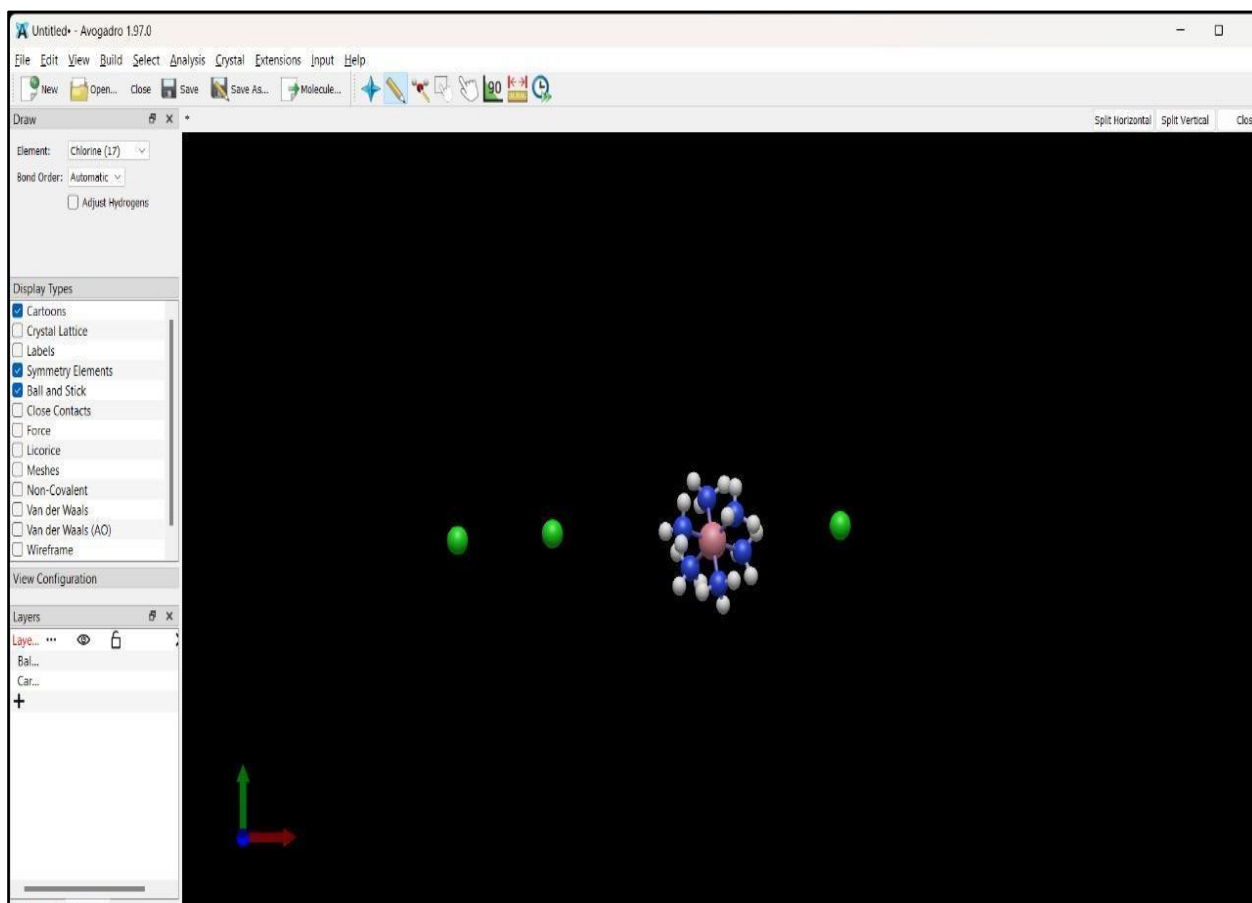


- Learnt the basic commands and tools in Avogadro by watching tutorials from Spoken Tutorial website
- Link for the Spoken Tutorial is provided here <https://spoken-tutorial.org>
- Practicing the software by building some structures and analysing their properties using different options in the software
- Learnt how to save the files in the Avogadro software and we should save the files by using .cml



4. Procedure for drawing the 3D structure of Hexamine Cobalt III Chloride complex

- From the toolbar on the top of the screen, select the **Draw** tool and a menu appears on the left side of the screen named **Draw Settings**.
- Select cobalt atom **Co** from the element selector option where we can see whole periodic table.
- Now attach six chlorine atoms to the co atom and also attach two chlorines atoms to Cobalt atom.
- Now for each nitrogen atom attach three hydrogens
- Now our structure is built, go to **Auto Optimization Tool** which is in the tool bar present at the top.
- The **Auto Optimization Settings** menu appears on the left side of the screen.
- Select Force field as **UFF** and click on the **start** button.
- Wait for few seconds to optimize and now our structure is optimized.



3D structure of Hexamine Cobalt III Chloride complex

4.1 Procedure for measuring the distance and bond angle

- There is an option known as **Click to Measure** on the toolbar, select that option.
- First click on an atom and then on other one to measure the distance between them.
- The parameters we measured were displayed at the bottom of the screen (arrow mark represents them)

	Type	Atom 1	Vertex	Atom 3	Angle (°)
1	NCoN	2	1	3	90.019
2	NCoN	2	1	4	89.438
3	NCoN	2	1	5	89.750
4	NCoN	2	1	6	90.920
5	NCoN	2	1	7	178.706
6	NCoN	3	1	4	90.348
7	NCoN	3	1	5	90.758
8	NCoN	3	1	6	179.013
9	NCoN	3	1	7	88.743
10	NCoN	4	1	5	178.628
11	NCoN	4	1	6	89.966
12	NCoN	4	1	7	90.194
13	NCoN	5	1	6	88.941
14	NCoN	5	1	7	90.641
15	NCoN	6	1	7	90.320
16	CoNH	1	2	10	113.491
17	HNH	9	2	10	108.283
18	CoNH	1	3	11	111.840
19	CoNH	1	3	12	112.461
20	CoNH	1	3	13	110.450
21	HNH	11	3	12	108.069
22	HNH	11	3	13	105.999
23	HNH	12	3	13	107.726
24	CoNH	1	4	14	112.527
25	CoNH	1	4	15	109.919

	Type	Atom 1	Vertex	Atom 3	Angle (°)
18	CoNH	1	3	11	111.840
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23	HNH	12	3	13	107.726
24	CoNH	1	4	14	112.527
25	CoNH	1	4	15	109.919
26	CoNH	1	4	16	111.374
27	HNH	14	4	15	107.457
28	HNH	14	4	16	108.362
29	HNH	15	4	16	106.972
30	CoNH	1	5	22	112.359
31	HNH	21	5	22	106.933
32	CoNH	1	6	23	113.035
33	CoNH	1	6	24	110.274
34	CoNH	1	6	25	111.665
35	HNH	23	6	24	105.678
36	HNH	23	6	25	108.227
37	HNH	24	6	25	107.651
38	CoNH	1	7	17	110.801
39	CoNH	1	7	18	110.672
40	CoNH	1	7	19	113.035
41	HNH	17	7	18	106.127
42	HNH	17	7	19	108.325

Observed Bond angles of the Hexamine Cobalt III Chloride complex

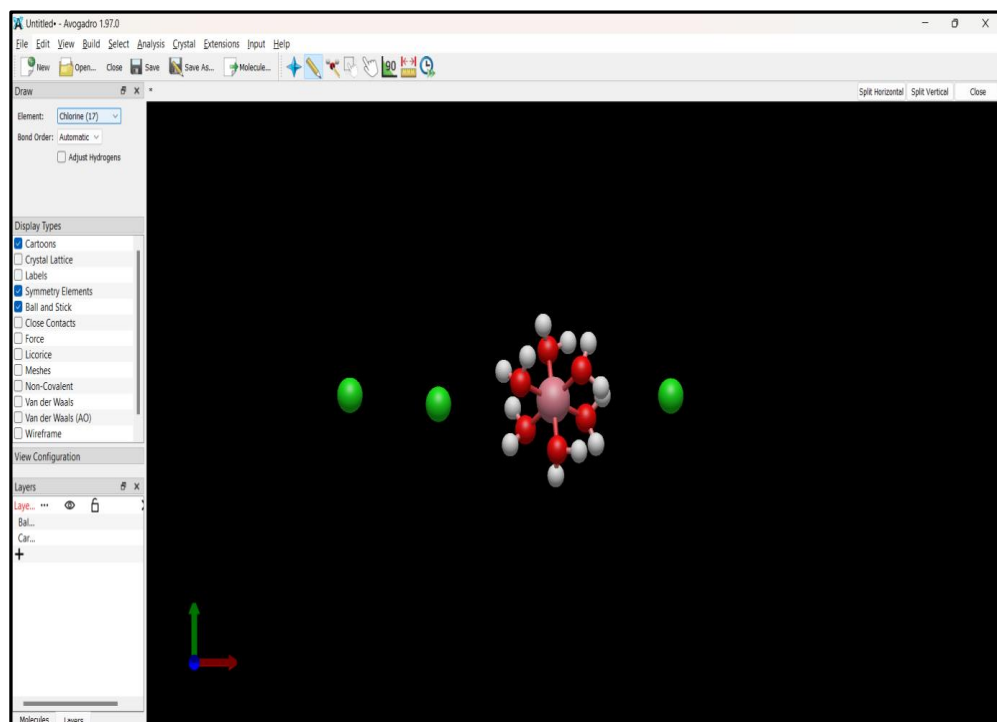
4.2 Procedure for measuring the bond length

- To measure bond length, go to **View** option available on the taskbar.
- In view menu there are different options available, select the **Properties** option.
- In **Properties** box select the bond properties and by selecting it, a table displays showing the bond properties.
- We can find the different properties by using the various options.

- Here are some reference pictures of various properties options mentioned below.

Bond Properties					
	Type	Start Atom	End Atom	Bond Order	Length (Å)
Bond 1	N-H	2	3	1	1.044
Bond 2	N-H	2	4	1	1.044
Bond 3	N-H	2	5	1	1.044
Bond 4	N-H	6	7	1	1.044
Bond 5	N-H	6	8	1	1.043
Bond 6	N-H	6	9	1	1.044
Bond 7	N-H	10	11	1	1.044
Bond 8	N-H	10	12	1	1.044
Bond 9	N-H	10	13	1	1.044
Bond 10	N-H	14	15	1	1.044
Bond 11	N-H	14	16	1	1.044
Bond 12	N-H	14	17	1	1.043
Bond 13	N-H	18	19	1	1.044
Bond 14	N-H	18	20	1	1.043
Bond 15	N-H	18	21	1	1.045
Bond 16	N-H	22	23	1	1.043
Bond 17	N-H	22	24	1	1.043
Bond 18	N-H	22	25	1	1.045
Bond 19	Co-N	1	2	1	1.946
Bond 20	Co-N	1	6	1	1.948
Bond 21	Co-N	1	10	1	1.943
Bond 22	Co-N	1	14	1	1.945
Bond 23	Co-N	1	18	1	1.946

4.3 The 3D structure of the Hexaaqua Cobalt(III) Chloride Complex

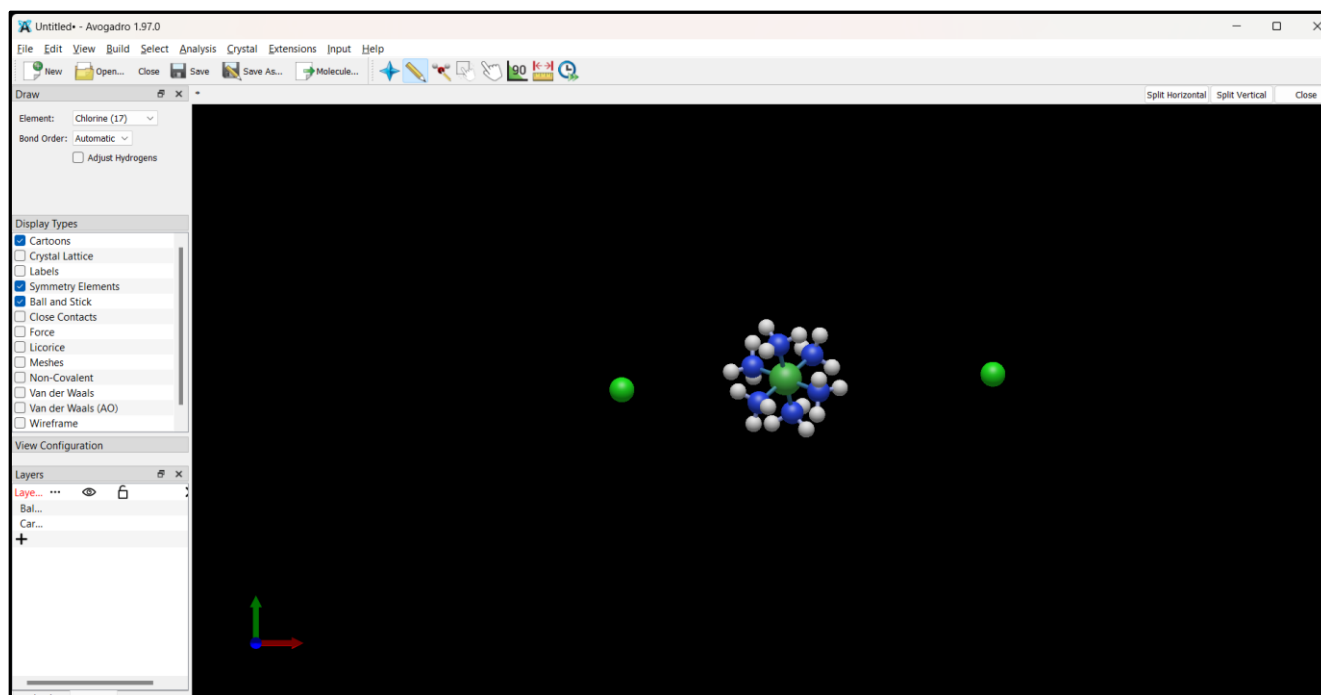


4.3.1. Bond length and Bond Angle measurements of Hexaaqua Cobalt(III) Chloride complex

	Type	Start Atom	End Atom	Bond Order	Length (Å)
Bond 1	Co-O	1	2	1	1.860
Bond 2	Co-O	1	3	1	1.869
Bond 3	Co-O	1	4	1	1.872
Bond 4	Co-O	1	5	1	1.871
Bond 5	Co-O	1	7	1	1.869
Bond 6	Co-O	1	6	1	1.861
Bond 7	O-H	5	19	1	0.989
Bond 8	O-H	5	18	1	0.991
Bond 9	O-H	7	17	1	0.989
Bond 10	O-H	7	16	1	0.989
Bond 11	O-H	6	15	1	0.990
Bond 12	O-H	6	14	1	0.990
Bond 13	O-H	4	12	1	0.991
Bond 14	O-H	4	13	1	0.989
Bond 15	O-H	3	10	1	0.990
Bond 16	O-H	3	11	1	0.989
Bond 17	O-H	2	9	1	0.991
Bond 18	O-H	2	8	1	0.990

	Type	Atom 1	Vertex	Atom 3	Angle (°)
1	OCoo	2	1	3	91.283
2	OCoo	2	1	4	88.891
3	OCoo	2	1	5	91.053
4	OCoo	2	1	7	88.780
5	OCoo	3	1	4	89.666
6	OCoo	3	1	5	90.253
7	OCoo	3	1	7	179.911
8	OCoo	4	1	5	179.901
9	OCoo	4	1	7	90.399
10	OCoo	5	1	7	89.682
11	OCoo	6	1	7	91.200
12	CoOH	1	2	9	107.061
13	HOH	8	2	9	104.133
14	CoOH	1	3	10	108.815
15	CoOH	1	3	11	108.693
16	HOH	10	3	11	103.432
17	CoOH	1	4	12	108.411
18	CoOH	1	4	13	109.989
19	HOH	12	4	13	104.827
20	CoOH	1	5	19	109.702
21	HOH	18	5	19	104.605
22	CoOH	1	6	15	107.088
23	HOH	14	6	15	104.079
24	CoOH	1	7	17	108.581
25	HOH	16	7	17	103.243

4.4. The 3D structure of Hexamine Nickle(II) chloride complex



4.4.1. The measurement of bond angle and bond length in Hexamine Nickle(II) chloride complex

	Type	Start Atom	End Atom	Bond Order	Length (Å)
Bond 1	Ni-N	1	2	1	1.892
Bond 2	Ni-N	1	3	1	1.891
Bond 3	Ni-N	1	4	1	1.889
Bond 4	Ni-N	1	5	1	1.891
Bond 5	N-H	7	19	1	1.045
Bond 6	Ni-N	1	7	1	1.891
Bond 7	N-H	2	9	1	1.044
Bond 8	N-H	2	8	1	1.043
Bond 9	N-H	2	10	1	1.044
Bond 10	N-H	3	11	1	1.044
Bond 11	N-H	3	12	1	1.043
Bond 12	N-H	3	13	1	1.044
Bond 13	N-H	4	14	1	1.044
Bond 14	N-H	4	15	1	1.043
Bond 15	N-H	4	16	1	1.044
Bond 16	N-H	7	17	1	1.043
Bond 17	N-H	7	18	1	1.043
Bond 18	Ni-N	1	22	1	1.889
Bond 19	H-N	20	22	1	1.045
Bond 20	H-N	21	22	1	1.043
Bond 21	N-H	22	6	1	1.044
Bond 22	N-H	5	23	1	1.044
Bond 23	N-H	5	24	1	1.043
Bond 24	N-H	5	25	1	1.044

	Type	Atom 1	Vertex	Atom 3	Angle (°)
1	NNiN	2	1	3	90.307
2	NNiN	2	1	4	89.703
3	NNiN	2	1	5	90.580
4	NNiN	2	1	7	179.721
5	NNiN	2	1	22	89.554
6	NNiN	3	1	4	90.089
7	NNiN	3	1	5	89.721
8	NNiN	3	1	7	89.970
9	NNiN	3	1	22	179.857
10	NNiN	4	1	5	179.660
11	NNiN	4	1	7	90.264
12	NNiN	4	1	22	89.875
13	NNiN	5	1	7	89.454
14	NNiN	5	1	22	90.315
15	NNiN	7	1	22	90.169
16	NiNH	1	2	9	111.992
17	NiNH	1	2	10	111.523
18	HNH	9	2	10	105.510
19	NiNH	1	3	11	112.201
20	NiNH	1	3	12	112.816
21	NiNH	1	3	13	111.782
22	HNH	11	3	12	107.182
23	HNH	11	3	13	106.337
24	HNH	12	3	13	106.082
25	NiNH	1	4	14	112.108

5. RESULT AND DISCUSSION

The percentage (%) yield of Hexamine Cobalt (III) Chloride is 82%

Information regarding the Hexamine Cobalt (III) Chloride complex

- The chemical formula of Hexamine Cobalt (III) Chloride $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
- The molecular weight of Hexamine Cobalt(III) Chloride is 237.9g/mol
- IUPAC Name of the complex is Hexamine cobalt(III) chloride, some old literature it is mentioned as Hexaamminecobalt(III) chloride.
- It is a dark purple or red solid that is typically used in chemical analysis, electroplating and as a catalyst
- It can also be dissolved in water or other solvents to form solutions

5.1. Structure of Hexamine Cobalt (III) Chloride complex

- The molecule consists of a cobalt atom in the centre, surrounded by six ammonia (NH_3) ligands, forming a coordination complex
- The cobalt atom is in the +3 oxidation state and is bonded to the six ammonia ligands through coordination bonds
- The molecule also has three chloride (Cl^-) ions that are not coordinated to the cobalt atom but are instead ionically bonded to it
- The overall charge on the molecule is neutral
- The coordination bonds in hexamine cobalt(III) chloride are formed through the nitrogen atoms of the ammonia ligands and the cobalt atom
- In terms of the arrangement of the ligands around the cobalt atom, hexamine cobalt(III) chloride is an octahedral complex
- The six ammonia ligands are arranged around the cobalt atom in an octahedral shape, with each ammonia ligand occupying one vertex of the octahedron.
- The three chloride ions are not coordinated to the cobalt atom and are situated in the axial positions of the octahedron
- Overall, the structure of hexamine cobalt(III) chloride is a complex coordination compound that features a central cobalt atom, six coordinating ammonia molecules and three chloride anions

5.2. Structure of Hexaaqua Cobalt (III) Chloride complex

- The cobalt ion is surrounded by six aqua molecules inside the coordination sphere and three chloride ions outside the coordination sphere forming a coordination complex with an octahedral molecular geometry
- The cobalt ion is in +3 oxidation state

5.3. Structure of Hexamine Nickel (II) Chloride complex

- The Nickel ion is surrounded by six amine molecules inside the coordination sphere and two chloride ions outside the coordination sphere forming a coordination complex with an octahedral molecular geometry
- The Nickel ion is in +2 oxidation state

5.4. Comparison of bond length and bond angle of complexes with changing the ligand

- In case of Hexamine Cobalt(III) Chloride complex the central metal atom Co is bonded to amine molecule through N atom
- The bond length between Co-N was around 1.9 \AA
- In case of Hexaaqua Cobalt(III) Chloride complex the central metal atom Co is bonded to aqua molecule through O atom
- The bond length between Co-O was around 1.8 \AA
- The Metal to ligand bond length of Co-N is greater than Co-O
- In case of Hexamine Nickel(II) Chloride complex, the central metal ion Ni was bonded to amine molecule through N atom
- The bond length between Ni-N was around 1.8 \AA
- The change in metal atom shows difference in bond length even with same ligand
- Since all the three above mentioned complexes are in octahedral geometry, the bond angle is 90°
- Though there is a change in ligand and metal still the geometry is octahedral the bond angle remains same

5.5. Applications of the complexes

- It is commonly used in the synthesis of organic compounds, such as in the preparation of aldehydes and ketones from alcohols

- It is also used in the production of pigments and dyes, as well as in the electroplating of metals
- Additionally, hexamine cobalt(III) chloride has been investigated for its potential use in medical imaging and as a contrast agent for magnetic resonance imaging (MRI)

5.6. Catalytic Activity

- Hexamine cobalt(III) chloride is an active catalyst in a wide range of chemical reactions, including oxidation, reduction, and ligand substitution reactions.
- In oxidation reactions, hexamine cobalt(III) chloride can be used to convert primary alcohols to aldehydes and secondary alcohols to ketones. This is achieved through the transfer of an oxygen atom from cobalt(III) to the alcohol, resulting in the formation of the corresponding carbonyl compound.
- In ligand substitution reactions, hexamine cobalt(III) chloride can be used to replace one or more of the ligands bound to the cobalt ion with other ligands. This can be done under mild conditions and with high selectivity, making it an attractive catalyst for organic synthesis.
- Hexamine cobalt(III) chloride is a versatile and active catalyst in a wide range of chemical reactions and has been widely used in organic synthesis, electroplating, and medical imaging.

6. Conclusion

The synthesised complex hexamine cobalt(III)chloride is light orange in colour. The bond length decreases when amine ligands were replaced with aqua ligands. The colour of the hexamine cobalt III chloride is due to d-d transition. $[\text{Co}(\text{NH}_3)_6]^{3+}$ is diamagnetic, with a low-spin $3d^6$ octahedral Co(III) centre. The NH_3 is so tightly bound to the Co(III) centres that it does not dissociate to allow its protonation. Upon heating, hexamine cobalt(III) begins to lose some of its amine ligands, eventually producing a stronger oxidant. The replacement of amine ligands with aqua ligand changes the bond length. The replacement of Co atom by Nickel atom also results in the change of bond length. As all these complexes are in octahedral geometry the bond angle remains same.

Acknowledgement

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