

## Inspecting various structural features of Tetraammine carbonato cobalt(III) nitrate complex using Jmol

### Abstract

The 3D model of the complex Tetraamminecarbonatocobalt(III) nitrate,  $[\text{Co}(\text{CO}_3)(\text{NH}_3)_4]\text{NO}_3$  was created using the **Jmol** interface. The various structural features were analysed using the tools available in the Jmol interface. The complex  $[\text{Co}(\text{CO}_3)(\text{NH}_3)_4]\text{NO}_3$  exists in a tetrahedral geometry. The central metal ion Co(III) ion is in a tetrahedral coordination by a chelating carbonate group and four amine ligands. The structure reveals an intricate array of N—H $\cdots$ O hydrogen bonds involving both the chelating and the non-chelating oxygen atoms of the carbonate ligand as hydrogen-bond acceptors of the amine hydrogen atoms. The carbonyl oxygens are also involved in hydrogen-bonding interactions with the oxygen atoms of the nitrate group. Using various tools in the Jmol we labelled the atoms, measured the bond length and angles. We have tabulated the measured parameters, created surfaces of the molecule, and also created various molecular representations. We have also explored the Script Console option in Jmol to change the colour of the atoms.

### Keywords:

Jmol, script console, hydrogen, bonding, chelating ligands, tetrahedral complex, cobalt complex,