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

Abstract

The 3D structure of the complex Tetraamine carbonato cobalt(III) nitrate was created in Jmol interface. The various structural features were analysed using the Jmol interface. The complex $[Co(CO_3)(NH_3)_4]NO_3$ 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···O hydrogen bonds involving both the chelating and the non-chelating O atoms of the carbonate ligand as hydrogen-bond acceptors of the amine H atoms, which are also involved in hydrogen-bonding inter-actions with the nitrate O atoms. Using various options in the Jmol we labelled the atoms, measured the bond length and angles, tabulated the measured parameters, created surfaces over 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,