

Synthesis, characterization and DFT calculations of Schiff base Co(III) complexes

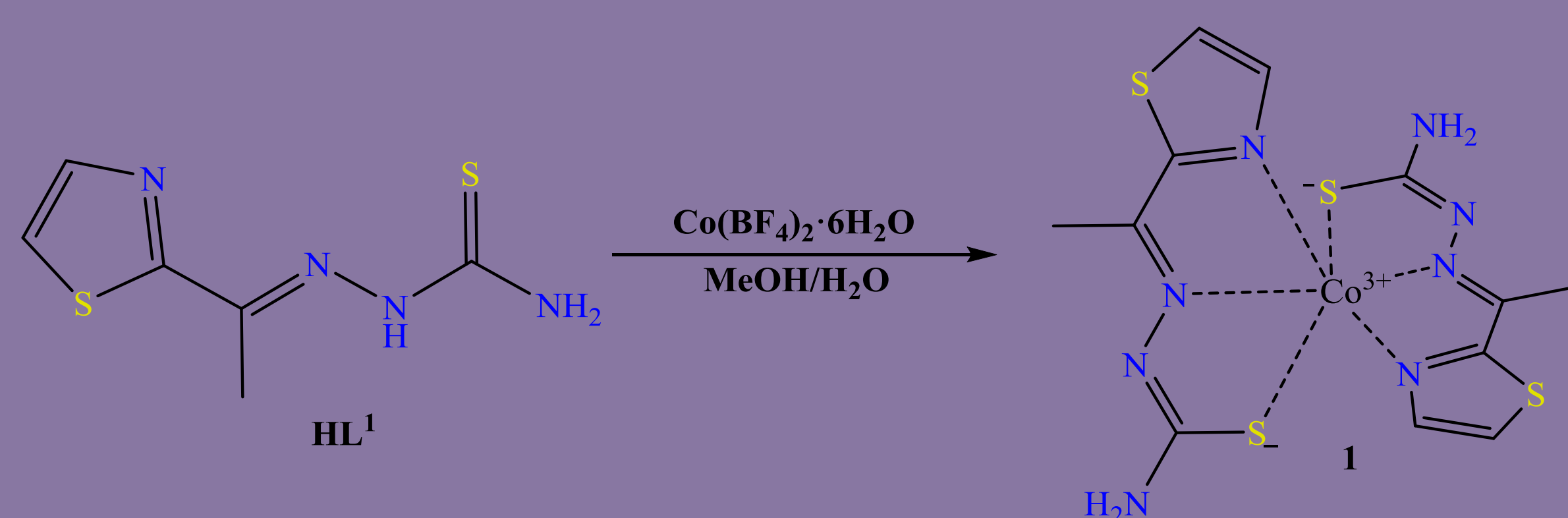
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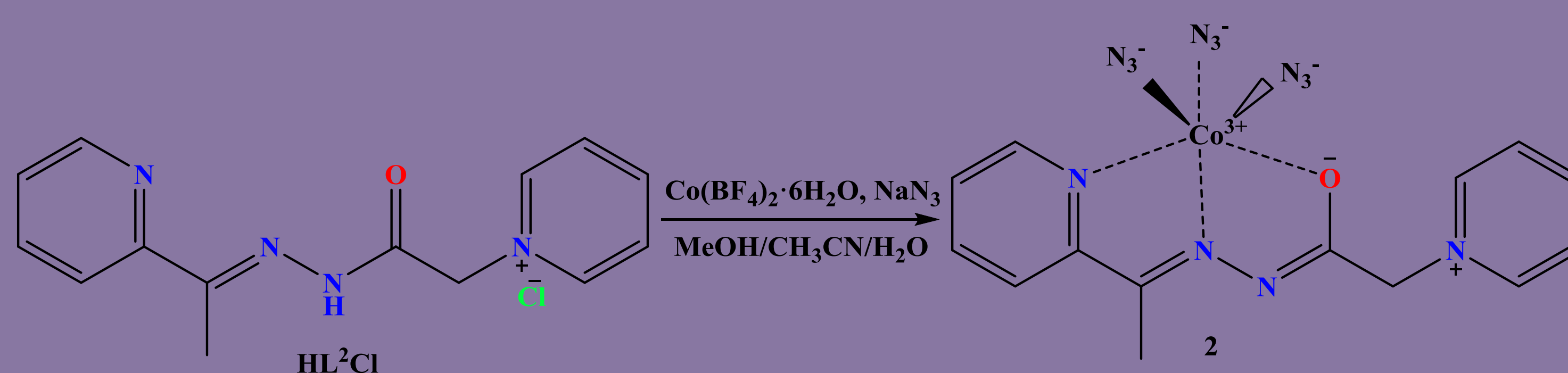


Two Co(III) complexes $[\text{Co}(\text{L}^1)_2]\text{BF}_4 \cdot \text{H}_2\text{O}$ (**1**), and $[\text{Co}(\text{L}^2)(\text{N}_3)_3]$ (**2**) with condensation product of thiosemicarbazide and 2-acetylthiazole (HL^1) and the condensation product of 2-acetylpyridine and Girard's P reagent (HL^2Cl) and $\text{Co}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$ have been synthesized **Scheme 1** and **2**. Complexes were characterized by elemental analysis, IR and NMR spectroscopy and X-ray crystallographic analysis.



Scheme 1. Synthesis of complex $[\text{Co}(\text{L}^1)_2]\text{BF}_4 \cdot \text{H}_2\text{O}$ (**1**).

Cobalt(III) complex (**1**) with HL^1 ligand is bis octahedral complex in which two deprotonated ligand molecules coordinate in a *mer* arrangement through two NNS sets of donor atoms, while with HL^2Cl , the ligand is coordinated to Co(III) ion in tridentate fashion through NNO set of donor atoms, and the other three coordination sites of a monokis octahedron are occupied by meridionally coordinated azide anions (**2**).



Scheme 2. Synthesis of complex $[\text{Co}(\text{L}^2)(\text{N}_3)_3]$ (**2**).

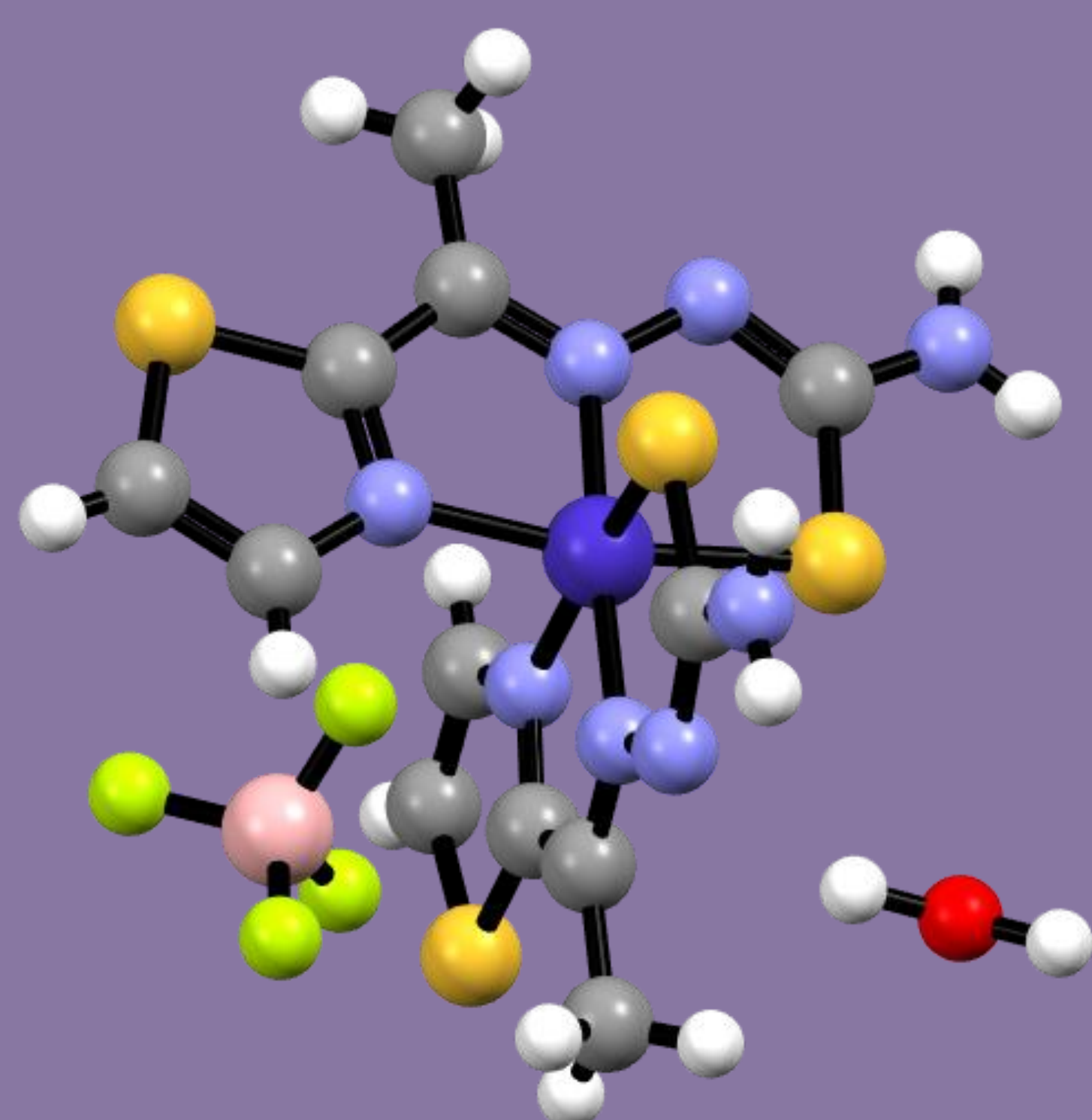


Fig 1. The drawing of $[\text{Co}(\text{L}^1)_2]\text{BF}_4 \cdot \text{H}_2\text{O}$ complex

Fig 1. The complex **1** crystallizes in the orthorhombic space group $Pbca$.

The asymmetric unit of **1** consists of $[\text{Co}(\text{L}^1)_2]^+$ complex cation, BF_4^- counter anion, and one solvent water molecule.

Fig 2. The complex **2** crystallizes in the triclinic space group $P-1$.

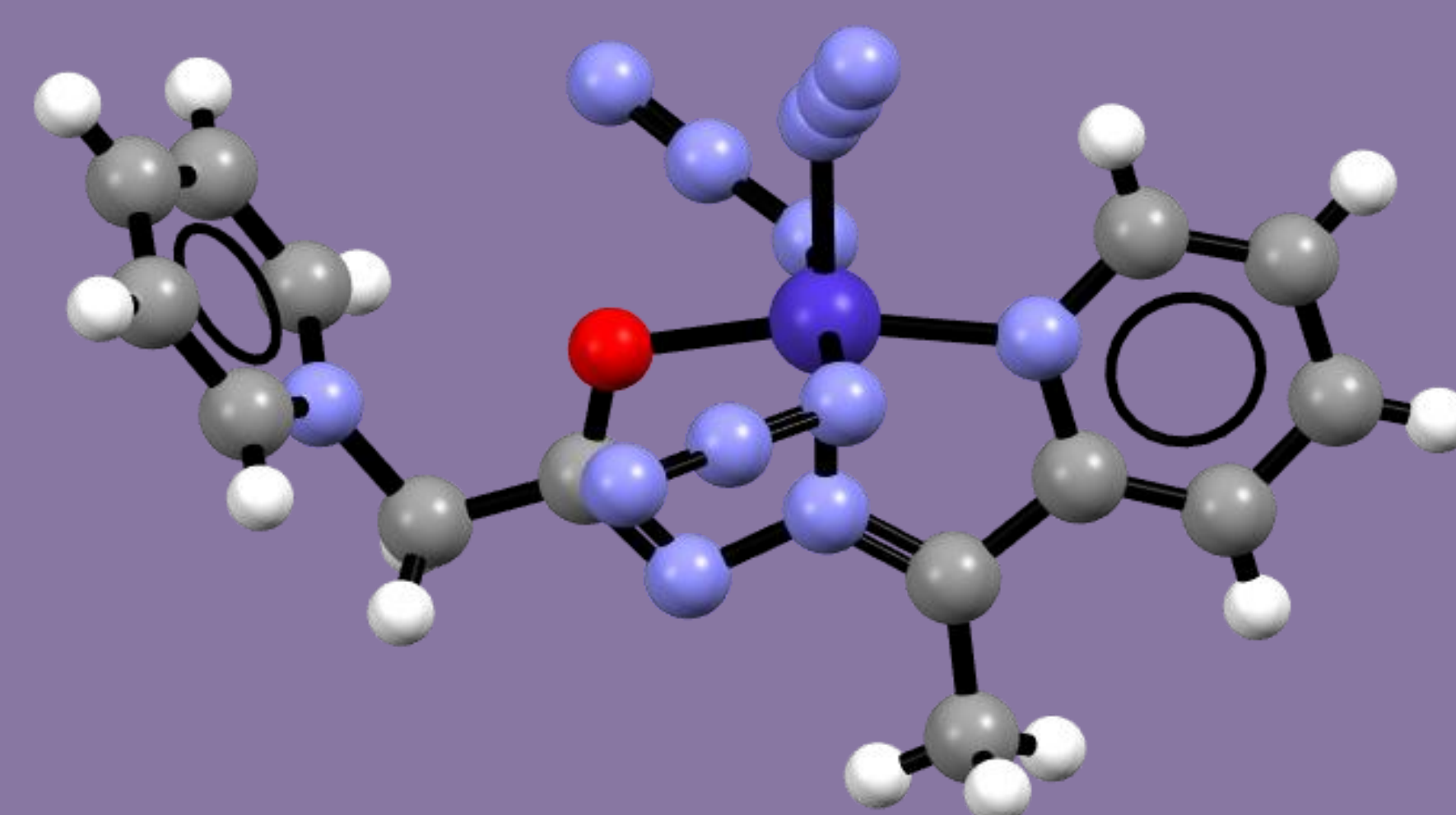


Fig 2. The drawing of the $[\text{Co}(\text{L}^2)(\text{N}_3)_3]$ (**2**) complex