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Synthesis and Characterisation of 2-Chlorobenzoyl Thiourea and 4-Chlorobenzoyl Thiourea and Its Manganese(II) and Cobalt(II) Complexes

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Structured Abstract

Background: Thiourea possesses great potential in biological and industrial applications. Acylthiourea, thanks to donor atoms N, S and O, can coordinate with multiple metals to form metal complexes, with most having enhanced properties as compared to the thiourea derivatives. The synthesis of thiourea derivatives however have presented with varying yields, which also affects the yields of its metal complexes. As such, the synthesis of thiourea derivatives must be focused on.

Methods: A two-step reaction was used for the synthesis of the ligand. Potassium thiocyanate was added into 2-chlorobenzoyl chloride or 4-chlorobenzoyl chloride then refluxed with stirring before being filtered. Then, the filtrate was used to react with diphenylamine in reflux for 4 hours. The synthesis pathway proposed that there may be 2 possible structures formed, between N-((2-aminophenyl)carbamothioyl)-2-chlorobenzamide and N,N'((1,2-phenylenebis(azanediyl))bis(carbanothioyl))bis(2-chlorobenzamide) for ligand 1 and between N-((2-aminophenyl)carbamothioyl)-4-chlorobenzamide and N,N'((1,2-phenylenebis(azanediyl))bis(carbanothioyl))bis(4-chlorobenzamide) for ligand 2. To synthesise the metal complex, metal chloride was added with the diphenylamine before undergoing reflux. Characterisation was done to determine the structure via ¹H NMR, FTIR and elemental analysis.

Results: ¹H NMR showed that aromatic protons were present between 7-8ppm, and three peaks were present at 10-13ppm for first ligand, 2 peaks for the second ligand. The IR spectra showed that the N-H stretching was seen at ranges 3300-3000cm⁻¹, with the peaks for C=O at 1700-1600cm⁻¹. C-N peaks were determined between 1350-1200cm⁻¹, while a C=S peak was seen at 1200-1100cm⁻¹. The manganese metal complex was coordinated via N and O atoms, while the cobalt metal complex was formed via bondings with S and O atoms for ligand 1; manganese complex for ligand 2 was coordinated via S and O atoms with cobalt attached to S and N atoms. The shifting of peaks in the IR spectroscopy showed the formation of metal complexes.

Conclusion: The ligands formed were N-((2-aminophenyl)carbamothioyl)-2-chlorobenzamide and N,N-((1,2-phenylenebis(azanediyl))bis(carbanothioyl))bis(4-chlorobenzamide). This is determined by looking at the N-H region for the 1H NMR, in which showed that there are 3 peaks present for ligand 1, and two peaks for ligand 2.

Keywords: Benzoyl thiourea, Synthesis, Characterisation, Manganese, Cobalt

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