09. STRUCTURES OF ORGANIC, ORGANO METALLIC AND COORDINATION COMPOUNDS


Thio- and seleno semicarbazones derived from 2-acetylpyridine, such as 3-aza-bicyclo[3.2.2]nonane-3-thiocarboxylic acid 2-{1-[2-pyridyl]ethylidene} hydrazide (A), have shown significant antioxidant and cytostatic properties. These complexes are also efficient transition metal chelators, with a metal to ligand ratio of 1:2. Antimalarial and cytostatic properties are enhanced. The metal ions coordinate with up to 2 organic ligands. The coordination of the metal ions in these compounds has been found to be square planar (Cu(II), Ni(II)), square-pyramidal (Fe(III)) and octahedral (Fe(II), Ni(II), Co(III)). The structures of several of these chelates are being studied as part of a project comparing the biological activities of this class of compounds. This paper will report on the structures of the coordination compounds of A with Fe, Cu and Co and on the structure of a non-thiol derivative of A. The Fe complex is octahedral and crystallizes in space group R3c along with [FeCl4]4-. The Cu complex is square planar, complexing with one molecule of A and one thiocyanate anion in space group Pt. The Co complex is octahedral and crystallizes with [Co(NCS)4]2- in space group P1 with a ratio of 2 Co complexes to 1 Co(NCS)4 molecule. Solvent molecules were also found in this system. The organic ligand crystallizes in the space group P21/c. Samples were provided by Major John Scovill of the Walter Reed Army Institute of Research.

09.4-7 CRYSTAL STRUCTURE OF Bis(3,5-DIMETHYL-1-PYRROLYL)-NITRATO IRIDIUM(V). By Alok Poddar, J.K. Datta Gupta, Saha Institute of Nuclear Physics, Sectors-I,-II, Block-JA, Bidhan Nagar, Calcutta-700054, India and N. Saha, Department of Chemistry, University College of Science, Calcutta-700009, India.

Pyrazole derivatives are well known for their medicinal values. The crystal structure analysis of pyrazole derivatives of Cu has been undertaken in order to investigate the coordination properties of pyrazole derivatives with transition metal ions. Bis[3,5-dimethyl-1-pyrazolyl]Cu(II)nitrate crystallizes in triclinic space group P with one molecule per unit cell. The cell dimensions are a=708(1), b=664(2), c=937(3)Å, α=92.39(1), β=90.41(2), γ=108.54(3). The structure has been solved by heavy atom method and was refined by block-diagonal least-squares method to a R value of 0.055. The structure is centrosymmetric about the Cu-atom. The two tertiary ring nitrogens of the pyrazole ring and the two nitrogens of the guanyl moiety are the binding sites and these constitute the square plane around the Cu atom. The two apical sites of the octahedron are occupied by the two nitrogens of the centrosymmetrically related nitrate groups. The structure is stabilized by hydrogen bonds of the type N···H.O.

09.4-8 NEW ADDITION COMPOUNDS OF GALLIUM. By K. Anton (a,b), A. L. Beauchamp (a) and H. Whitt (b); (a): Université de Montréal, Département de Chimie, Montréal, Québec, H3C 3V1, CANADA; (b): Institut für Anorganische Chemie, Universität München 2, Weisstr. 1, F.R.G.

To gain information about the relative basicity of donor atoms in multifunctional heterocyclic molecules such as aminoborane, purine and imidazole, the ligands (1)-(4) were reacted with GaCl3, which is known to be a very strong and sensitive Lewis acid.