A-3 16:30~16:45

Crystal Structure of Octahedral Cobalt(II) Complex of a Di-*N*-carboxymethylated Tetraaza Macrocycle

Ki-Young Choi, Yong-Son Kim[a], Jin-Gyu Kim[b] and Il-Hwan Suh[b]

Department of Cultural Heritage Conservation Science, Kongju National University, Koungju 314-701, Korea

[a]Department of Chemical Education, Kongju National University, Kongju 314-701, Korea

[b]Department of Physics, Chungnam National University, Taejon, 305-764 Korea

The complex $[Co(H_2L)]Cl_2 \cdot 4H_2O$ (**1**) (H_2L = 2,13-bis(2-carboxymethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16,4,$0^{1.18}$,$0^{7.12}$]docosane) has been synthesized and structurally characterized. **1** crystallizes in the triclinic space group $P\bar{1}$, a = 8.958(2) Å, b = 9.513(1) Å, c = 9.679(1) Å, α = 92.57(1)° , β = 93.47(1)° , γ = 116.33(1)° , V = 735.54(19) Å^3, Z = 1. The complex (**1**) has a centrosymmetric cation with anions and water molecules on general sites. The two pendant carboxymethyl groups of the macrocyclic ligand are *trans* to each other, and the absolute configuration is a *trans*-III in the solid state. The coordination geometry of the cobalt atom is a distorted octahedron, with an average Co-N distance of 1.999(3) Å and a Co-O(1) distance of 1.903(4) Å