# CRYSTAL STRUCTURES OF METAL COMPLEXES OF 2-HYDRAZINO-4-HYDROXY-6-METHYLPYRIMIDINE (ISOCYTOSINE DERIV.)

Hiroshi Sakaguchi, Hiroshi Anzai,* Kimio Furuhata, Haruo Ogura,** and Yoichi Iitaka***

*School of Hygienic Sciences, Kitasato University,* School of Pharmaceutical Sciences, Kitasato University,***
*and Faculty of Pharmaceutical Sciences, University of Tokyo,**** *Sagamihara-shi, Kanagawa, 228, Japan**

The compound of 2-hydrazino-4-hydroxy-6-methylpyrimidine (LH) is an interesting ligand, worthy of study because of its multifaceted coordination possibilities with metal ions. We prepaired $[Zn^{II}(LH)_2(H_2O)_2]Cl_2 \cdot 2H_2O$, $[Ni^{II}(LH)_2(H_2O)_2]Cl_2 \cdot 2H_2O$, $[Co^{II}(LH)_2(H_2O)_2]Cl_2 \cdot 2H_2O$, $[Fe^{II}(LH)_2(H_2O)_2]Cl_2 \cdot 2H_2O$, $[Cu^{II}(LH)_2(H_2O)]Cl_2 \cdot 2H_2O$, $[Pt^{IV}Cl_6](LH)_2$, $[Hg^{II}Cl_4](LH)_2 \cdot 2H_2O$, and $[Hg^{II}(LH)Cl_2]Cl_2 \cdot 2H_2O$, which were analysed with IR, NMR, and ESR spectra. And it was assumed that the ligand molecules of LH were coordinated to keto form of isocytosine ring, and $H^+$ of the hydroxyl group were protonated at N1 or N3 of pyrimidine ring. Then, we carried out X-ray analysis of the LH complexes except $[Fe(LH)_2(H_2O)_2]Cl_2 \cdot 2H_2O$ and $[Hg(LH)Cl_2]Cl_2 \cdot 2H_2O$.

In the Zn complex, LH is coordinated to Zn(II) through N3 and also through the amino nitrogen atom of hydrazino group. The two LH residues are coordinated *trans* to each other forming a square planar coordination. The fifth and sixth coordination sites are occupied by the two water oxygen atoms. The hydroxyl group at C4 takes the keto form, since the hydrogen atom of the hydroxyl group transfers to N1. And also the structure of Ni and Co complexes was the same as of Zn complex. In the Cu complex, There are two mirror-image complex molecules in a unit cell. Each Cu complex has five coordinated bonds and assumes a distorted square pyramid structure. LH is coordinated to Cu(II) through N3 and also through the amino nitrogen atom. In each LH-Cu(II), the one apical coordination site is occupied by the water oxgen atom. The hydroxyl group at C4 takes the keto form. The chloride ions are not directly hydrogen-bonded to the N1 atoms of the rings, but are bound to the apical water oxygen atoms. $[HgCl_4](LH)_2 \cdot 2H_2O$ and $[Pt^{IV}Cl_6](LH)_2$ not had the metal coordination, but are bound LH to metal ions through the hydrogen bonds. In the all LH-metal complexes, the pyrimidine rings are stacked.

The structure of $[Fe(LH)_2(H_2O)_2]Cl_2 \cdot 2H_2O$ was the same as of LH complexes of Zn(II), Ni(II), and Co(II) by IR spectra.