

CHAPTER VII

CONCLUSIONS

The present work declared supramolecular structure of *N,N*-bis(2-hydroxybenzyl)alkylamine. In solution state, (i) the 2:1 host-guest ratio of *N,N*-bis(2-hydroxybenzyl)alkylamine derivatives with CuCl_2 as characterized by Job's plot, (ii) the inclusion formation as the molecular assembly of *N,N*-bis(2-hydroxybenzyl)alkylamines as studied by ESIMS, and (iii) the interaction at the hydroxyl and aza-methylene group as determined by ^1H NMR and ^1H - ^1H NOESY suggested that *N,N*-bis(2-hydroxybenzyl)alkylamines performed as a host in accepting Cu^{2+} guests. In solid state, the single crystal X-ray analysis proved that *N,N*-bis(2-hydroxy-5-methylbenzyl)cyclohexylamine and copper ion formed a unit cell $P2_1/n$ of inclusion compound with the host-guest ratio of 1:1. The dimeric system of *N,N*-bis(2-hydroxybenzyl)alkylamine with no guest was stabilized under hydrogen bond network whereas the supramolecular structured dimeric system of *N,N*-bis(2-hydroxybenzyl)alkylamine-copper with Cu^{2+} was formed under charge transfer system as evidenced by Cerius² program calculation and MS modeling.

The unique simultaneous inclusion of copper and neutral molecules within a single host-guest system was identified. *N,N*-Bis(2-hydroxy-3,5-dimethylbenzyl)methylamine provided the simultaneous inclusion of guest species in a host showing the interactions of coordination via the lone pair electrons and the hydrogen bonds based on phenyl groups as determined from the single crystal analysis. In this case, the neutral molecules functioned as a linkage between the copper complexes of *N,N*-bis(2-hydroxy-3,5-dimethylbenzyl)methylamine to result highly stabilized packing crystal structures.

The original plan of this work aims to generalize the inclusion phenomena between *N,N*-bis(2-hydroxybenzyl)alkylamine and transition metal ions. However, there were some limitations in the studies for both in solution and solid state of inclusion complexes. In solution, the inclusion phenomena of *N,N*-bis(2-hydroxybenzyl)alkylamine with Cu^{2+} , Cd^{2+} , and Zn^{2+} were studied to find that in the cases of Cd^{2+} and Zn^{2+} , the solutions were colorless to limit the basic observation by

UV spectrophotometry technique. In addition, the peak shift or new peaks referring to the formation of host-guest compound in FTIR spectra of *N,N*-bis(2-hydroxybenzyl)alkylamine with Cd^{2+} and Zn^{2+} were hardly identified. However, the analysis by ^1H NMR showed the peak shift for Cu^{2+} , Cd^{2+} , and Zn^{2+} . This limited us to study only on the case of Cu^{2+} which all information from various analytical techniques were relevant. In the solid state, the crystal formation was not accomplished except for the copper ion. As a result, the work was focused on only host-copper inclusion. Although the work ended up with only copper ion inclusion, it is for the first time that *N,N*-bis(2-hydroxybenzyl)alkylamine is proven for the host molecules to accept copper ion.

In the macrocyclic synthesis, the present work originally succeeded in showing a [1+1] selective and effective macrocyclization of *N,N*-bis(2-hydroxybenzyl)alkylamine with 1,3-bis(tosyloxy)propane.