Anomalous X-Ray Scattering Studies of Supermolecules and Aggre-	V71
gates in Organic Solution	ΛίΑ

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Anomalous X-ray scattering (AXS) study has been conducted on a covalently linked modified chlorophyll dimer, and its corresponding monomer with zinc as the central metal ions. The molecule under AXS studies is a chlorophyll dimer cyclophane, where two covalent linkages connect two macrocycles side-by-side. The ester linkages will make the two chlorophyll rings to fold into a "clam shell" like conformation. Our AXS experiment intends to probe the metal-metal distance in this "clam shell" like molecule in solid and in solution. Based on a preliminary molecular mechanical calculation, the metal-to-metal distance in bis-Zn-chlorophyllide cyclophane is 4.9, a distance is beyond the probing range for EXAFS in disordered system. The coordination number of the metal ions is also an important struc-tural factor in predicting the function of the molecule. We have found temperature dependence of the coordination state in these cyclophanes by EXAFS experiment, where the ligands bind to the metal at temperature below 200K, but not at room temperature. The coordination of the ligands requires the "clam shell" to open up, thus this is related also to metal-to-metal distance in the molecules. The covalently linked chlorophylls function as either electron donor or acceptor. The electron transport processes in these supermolecules are normally triggered by light. Thus, these supermolecules have potential applications as molecular devices. Structural parameters of these supermolecules are very important information in predicting their electron transfer properties. We have obtained AXS data for powder and solution of the dimer as well as the corresponding monomer. Significant differences in the spectral features have been observed between the dimer and monomer. However, in order to obtain Zn-Zn distance in this molecule, a correct method of background subtraction and data normalization is very crucial. We are in a process of completing the analysis of the AXS data.