A Carbon K-edge NEXAFS Study of the Chlorophyll Derivative Sodium Copper Chlorophyllin and its Breakdown Products

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The role of chlorophylls (Chl) in photosynthetic light-harvesting and energy transformation process has been studied extensively in order to elucidate mechanistic aspects of natural solar energy conversion. Structure-function relationships in pigment-protein complexes containing Chl molecules are in the focus of research, since efficient light-energy conversion is one of the grand challenges of our time. Model systems like porphyrins in general or chlorophyllins with comparable photo-physical properties also receive growing attention.

Using Near-Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS) the carbon backbone of sodium copper chlorophyllin (SCC), a widely used Chl derivative, and its breakdown products were analyzed to elucidate their electronic structure and physicochemical properties.

Using various sample preparation methods and complementary spectroscopic methods (including UV/VIS, X-ray Photoelectron Spectroscopy), comprehensive insight into the SCC breakdown process was obtained. Further NEXAFS investigations on the N K- and Cu L-edges confirm the complexity of the molecular structures occurring during SCC breakdown. The experimental results are supported by Density Functional Theory (DFT) calculations allowing a detailed assignment of characteristic NEXAFS-features to specific C-bonds.

The presented work provides a novel and detailed description of the electronic structure of the C backbone of SCC molecules and its breakdown products. The results also hold promise that in prospective optical pump - X-ray probe investigations dynamic processes in Chl containing photosynthetic complexes can be analyzed precisely.

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