STRUCTURE AND SPECTRA OF A COMPLEX BIOCHROMOPHORE - DEPROTONATED BILIVERDIN IX

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Biliverdin (BV) is an attractive candidate for use in fluorescence microscopy applications, because it can be genetically encoded (and engineered) as a red fluorescent biomarker by binding to cysteine and including it in fluorescent proteins. An important step towards rational design of a biomarker with specific desired properties is to study the intrinsic properties of the molecule, i.e., in the absence of any chemical environment. In the present work, we focus on the singly and doubly deprotonated forms of the position isomer biliverdin IX (see Figure). The structural flexibility of this molecule makes structural identification of its conformation in vacuo rather challenging. Ion mobility and cryogenic infrared spectroscopy allow us to obtain structural information. The electronic spectrum depends strongly on the deprotonation state of the molecule. We interpret the data with density functional theory calculations.