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MOLECULAR STRUCTURE AND OPTICAL PROPERTIES OF THE FREE BASE CORROLES

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Corroles represent an important group of tetrapyrrolic macrocyclic compounds which is closely related to porphyrins. The main structural difference is the direct C_a-C_a linkage between two neighboring pyrrole rings instead of a regular methine C_a-C_m-C_a bridge. The absence of one *meso*-carbon (C_m) atom changes the bond alternation pattern in the contracted tetrapyrrolic macrocycle. The free base corroles consist of three pyrrolic and one pyrrolenic ring resulting in noticeable distortions from planarity have been observed for the free base corroles, even in the absence of overcrowding peripheral substitution, due to the decreased core size and steric hindrance preventing the three inner pyrrolic NH protons to lie in the mean macrocyclic plane. These structural features result in a lower symmetry of the free base corrole macrocycle compared to porphyrins (C_s vs. D_{2h}). The different corrole NH tautomers can be identified, i.e. structurally distinct isomers depending on the location of the three pyrrolic protons. As a function of the peripheral substitution, either 2 or 4 of NH tautomers can be expected.

Two corrole NH tautomers have been identified in the solution [1-5]. These two NH tautomers have clearly distinct optical properties. The excitation energy deactivation rates and pathways of the free base corroles in solution were found to depend on the NH tautomerization process and may be tuned over a wide range by temperature and heavy atom effect. These features have been used to elucidate the characteristics of the tautomerization mechanism. In this presentation, a general overview of the optical properties of the free base *meso*-triarylcorroles tautomers is presented and discussed in detail.

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