MODELING of CIDNP FIELD DEPENDENCE for MOLECULAR DONOR-ACCEPTOR COMPOUNDS

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The study of magnetic and spin effects in a reversible photoinduced intramolecular electron transfer reaction establishes a connection between the exchange interaction and the spatial and electronic structure of the biradical. However, the interpretation of such experimental data is not necessarily straightforward. Careful modelling is required in order to obtain quantitative data on the exchange interaction and the biradical electronic structure. It creates a basis for the development of new approaches to the directed design of organic materials with specified electronic properties for practical applications in photovoltaics or spintronics.

In this presentation, we will examine the examples of numerical modeling of CIDNP field profiles derived from two distinct types of molecular donor-acceptor compounds (see Figure 1): A rigid triad (D-Ir-A) has been utilized in the study of electron transfer, with D (triarylamine) serving as the e-donor, Ir (cyclometallated iridium complex) as the bridge, and A (naphthalene diimide) as the e-acceptor; the bridge complex Ir has been identified as a crucial component in this research [1]. A flexible tetrapeptide/photosensitizer conjugate, His-Gln(BP)-Tyr-Gly, with tyrosine or histidine residues serving as the e-donor and 4-aminobenzophenone serving as the e-acceptor [2]. In both cases, the same numerical approach initially outlined in [1] was employed, with modifications described in [3] that significantly enhance the calculation speed and convenience of the simulation procedure.

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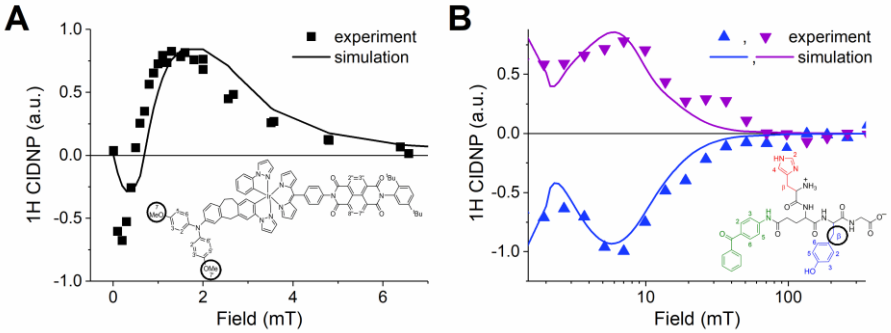

Fig. 1. Experimental (dots) and simulated (lines) 1H CIDNP field dependences of: **A -** six equivalent methyl protons of D–Ir–A; **B -** two β-protons of tyrosine residue of conjugate His-Gln(BP)-Tyr-Gly.