Photoinduced electron transfer in pentacoordinated complex of zinc tetraphenylporphyrin and isoquinoline N-oxide : crystal structure, spectroscopy and DFT studies.

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Streszczenie

A novel, pentacoordinated complex of (1:1) zinc tetraphenylporphyrin and isoquinoline N-oxide (ZnTPP–IQNO) was synthesized and its crystal structure along with photophysical properties by experimental methods (absorption, steady state and time-resolved emission) in conjunction with DFT and TD DFT calculations were investigated. In ZnTPP–IQNO complex, the isoquinoline N-oxide ligand (IQNO) is directly coordinated to the central zinc atom of the ZnTPP unit through the oxygen atom of the NO group and crystallizes in centrosymmetric triclinic unit, in the space group . Particular contacts between the two monomeric units (hydrogen bonds, OH–C interactions, …etc.) lead to a supramolecular dimer which forms the layers propagating both along the *a* and the *b*-axis. The electronic locally excited and the charge-transfer states of the complex were calculated by TDDFT CAM-B3LYP/6-31G(d,p) method. A surprising presence of the charge transfer states between the Soret and the Q bands leads to excitation energy dissipation processes involving the opening of the radiationless channels of excited ZnTPP–IQNO complex. Emission from the S_1 state (Q band) in ethyl acetate decays accordingly to monoexponential function (1.92 ns) while a bi-exponential decay is found in *n*-propanol [(2.5 ns (87%); 14.4 ns (13%)] and in the solid state [1.36 ns (67.5%), 7.31 ns (32.5%)].

Słowa kluczowe

crystal structure, Zinc tetraphenylporphyrin, Isoquinoline N-oxide, Excited states, electron transfer, lifetimes

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