

5th Annual European Pharma Congress

July 18-20, 2016 Berlin, Germany

**Anna Szemik-Hojniak**

University of Wroclaw, Poland

Favorable for drug candidates the CT properties of Alkylamino pyridine N-oxides in solution

The spectrum of therapeutic activities of heterocyclic N-oxides and specifically those of pyridine N-oxides is rather broad. Since their discovery about twenty years ago, they were broadly recognized as antibacterial, antihypertensive, anti-inflammatory, antiparasitic, as well as anti-HIV, anti-inflammatory, and neuroprotective agents. The heterocyclic N-oxides form a new class of bioreductive drugs with favorable drug-receptor interactions of the charge transfer (CT) type. Different N-oxides have been detected in animals, plants, and microorganisms, and therefore it is an utmost important issue to recognize their physico-chemical and physiological properties. The former (CT) interactions in N-oxides are strongly enhanced under the light irradiation and the excited electronic CT state results from electron transfer (ET) between electron donor /acceptor (electron-donating/withdrawing) functional groups. When additionally, the N-oxide contains the hydrogen donor and hydrogen acceptor substituents, the compound enhances its reactivity and may exhibit also the proton transfer process that may occur as a concerted or sequential combined Proton Coupled Electron Transfer (PCET) process. The PCET is pivotal both in biological systems and in bioenergetic conversion. Example of the former is the reduction of protons to hydrogen by hydrogenase and for the latter is the energy storage process. A series of new alkylamino- (NHR-) type hydrogen bonding compounds including 2-aminobutyl and 2-aminomethyl (4 nitro)-5-or 6 methyl pyridine N-oxides were designed and synthesized. This makes feasible the comprehensive spectroscopy and dynamics studies of amino-nitro excited state electron transfer (ET) and excited-state intramolecular proton transfer (ESIPT) along the N-H...O hydrogen bonding in the systems under investigations. In this talk, the PCET process in the electronic excited state of targeted pyridine N-oxides in solution where the normal HB form and the PT form exhibit the CT nature will be discussed both from experimental (absorption, steady state and time-resolved fluorescence) and theoretical [TD DFT B3LYP/6-31G(d,p) calculations] point of view.

Biography

Anna Szemik-Hojniak has completed her PhD in Radiochemistry from the University of Wroclaw and Post-doctoral studies in Physical Chemistry and Radiochemistry from Solvay Foundation (Belgium), KULeuven (Belgium) and Centre of Nuclear Researches (Strasbourg, France). She occupies with Organic Molecular Photophysics, and published more than 45 papers and serves as a reviewer in scientific journals. In the years (2002-2011) she served as the INWES Board director (2002-2011) for INWES corporation- the operational partner of UNESCO. In 2007, at the University of Wroclaw, (Poland), she organized international workshop "Strategies for the Highly Skilled Global Workforce". In 2011, she was awarded with Distinguished Service Award. Presently she is INWES-ERI General Secretary and the Board Director (headquarters-Ottawa, Canada). In 2014 and 2015, she organized Mini Symposium "Photophysics of Electron and Proton Transfer" in the framework of ICCMSE- 2014 conference, in Athens (Greece) and presented the Keynote lecture on "Behavior of styryl derivatives under the light irradiation" during 4th-Annual European Pharma Congress-2015 in Valencia (Spain).

anna.szemik@chem.uni.wroc.pl