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A new series of heterocyclic N-oxides as promising drug candidates

Recognition of type of interactions and binding mechanism between receptor and an introduced bioactive agent (drug), requires the knowledge of several components. Of which primary importance are: lipophilic (hydrophobic) factor, electronic (substituent) parameter, steric factor, ability to form hydrogen bonds as well as charge transfer (CT) or proton transfer (PT) nature of the drug. Aromatic heterocyclic compounds, such as derivatives of pyridine N-oxides, due to their practical impact on pronounced biological activity, occupy in this field a very particular place. They exhibit antifungal, antiviral or antibiotic properties and many of their derivatives show herbicidal activity. Furthermore, they are also able to inhibit electron transport across cell membranes or mediate proton transfer across the mitochondrial membrane. N-oxides and many of their derivatives are characteristic of CT interactions resulting from a partial transfer of electron density from the HOMO orbital of the electron-rich functional group to the LUMO orbital of electron-poor substituent. Their electron donating or proton accepting abilities can be easily varied by appropriate substitution at certain position of the π-electron system. In this presentation, X-ray structures and spectral properties in the gas phase and solution of nitraminopyridine N-oxides containing the –NH-NO2 substituent in position 2 with respect to the –NO group and methyl group in different positions of the pyridine ring [3, 4, 5 or 6, e.g. 3-methyl-2-nitraminopyridine N-oxide (3M)] are demonstrated. In the solid state, two centrosymmetric crystals form a dimer where a mutually parallel or perpendicular location of the two monomers in the crystal lattice results in the corresponding molecular (H) or proton transferred (PT) form. In the (H) form, the amino hydrogen is at the –NH-NO2 group while in the PT form, it is located at the NO group. Between both molecules in dimer, the N-H...O or O-H...N intermolecular hydrogen bonds of different strength are formed. Interestingly, both forms exhibit favourable for drug-receptor CT interactions. Theoretical TD DFT calculations show that the S0→S1 electronic transition in these compounds is of the ππ* type in the (H) forms and a mixed ππ* + n, π* type in the PT forms. Additionally, contrary to the solid, the monomeric forms are present in the solution and prototropic equilibria of amino (H) <-> imino (PT) type should be taken into consideration.

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), KU Leuven (Belgium) and Centre of Nuclear Researches (Strasburg, France). She occupies with Organic Molecular Photo physics, 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 on "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 "Photo physics of Electron and Proton Transfer" in the framework of ICCMSE- 2014 conference, in Athens (Greece) and presented the Keynote lecture on "Behaviour of styryl derivatives under the light irradiation" during 4th-Annual European Pharma Congress-2015 in Valencia (Spain).

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