

“Acidochromic Spiropyran-Merocyanine stabilization in the solid-state”

Vanessa Kristina Seiler^a, Kevin Callebaut^a, Koen Robeyns^a, Nikolay Tumanov^b, Johan Wouters^b, Benoît Champagne^b, Tom Leysens^a

a) *Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, 1, Place Louis Pasteur, B-1348, Louvain-la-Neuve, Belgium.*

E-mail: Tom.Leyssens@uclouvain.be

b) *Unité de Chimie Physique, Théorique et Structurale, UNamur, 61, Rue de Bruxelles, B-5000 Namur, Belgium*

In this work, we present an innovative approach to stabilize the open-ring Merocyanine form of a Spiropyran compound. At the solid state the Merocyanine form is only rarely observed, highlighting the importance of this contribution. Our concept is based on a co-crystallization approach of the open form with an inorganic acid. This way we identified a reliable technique of stabilizing the colored Merocyanine form and in one specific case we even obtained crystals with increased stability towards photodegradation. 15 novel crystal structures of Spiropyran derivatives with several inorganic acids were determined by single crystal X-ray diffraction. Solvent evaporation of Spiropyran compounds, i.e. 1,3,3-Trimethylindolinobenzopyrylospiran (**SPH**), 1,3,3-Trimethylindolino-beta-naphthopyrylospiran (**SPBenz**), 1,3,3-Trimethylindolino-8'-methoxybenzopyrylospiran (**SPOMe**) and 1,3,3-Trimethylindolino-6'-nitrobenzopyrylospiran (**SPNO2**), in presence of inorganic acids, namely hydrochloric acid, hydrobromic acid, nitric acid, sulphuric acid and phosphoric acid, yielded the rare open-ring Merocyanine form stabilized by protonation of the primary oxygen atom unfolded by the ring-opening isomerization and compensating the charge with a hydrogen bonded anion. Analysis of the solid state properties was performed by thermal gravimetric analysis and diffuse reflectance spectroscopy.