Solid-state spiro-rhodamines: rational design of photoactive materials

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The system of study is a family of Spiro-Rhodamines (SRA), which are a derivative from the commercial Rhodamine dye with an aliphatic or aromatic amine. During the derivatization, a cyclization takes place, with loss of aromaticity, leading to a colourless and non-fluorescent CLOSE isomer (SF), which is thermally stable. Irradiation in the absorption band of this Isomer (around 350 nm) promotes the rupture of the C-N bond formed, recovering the Rhodamine´s chromophore and fluorophore in the OPEN isomer (OF). The change is thermally reversible, and the equilibria involves a protonation of the colourful isomer for stabilization.

The system was characterized in solid state, by reflection, absorption and emission spectroscopy and X-ray diffraction, evaluating the changes produced after irradiating the corresponding SF with ultraviolet light for different derivatives. These characterizations have been performed in single crystal and thin films. Moreover, computational calculations were performed in order to explore the initial step of the light-induced opening mechanism.

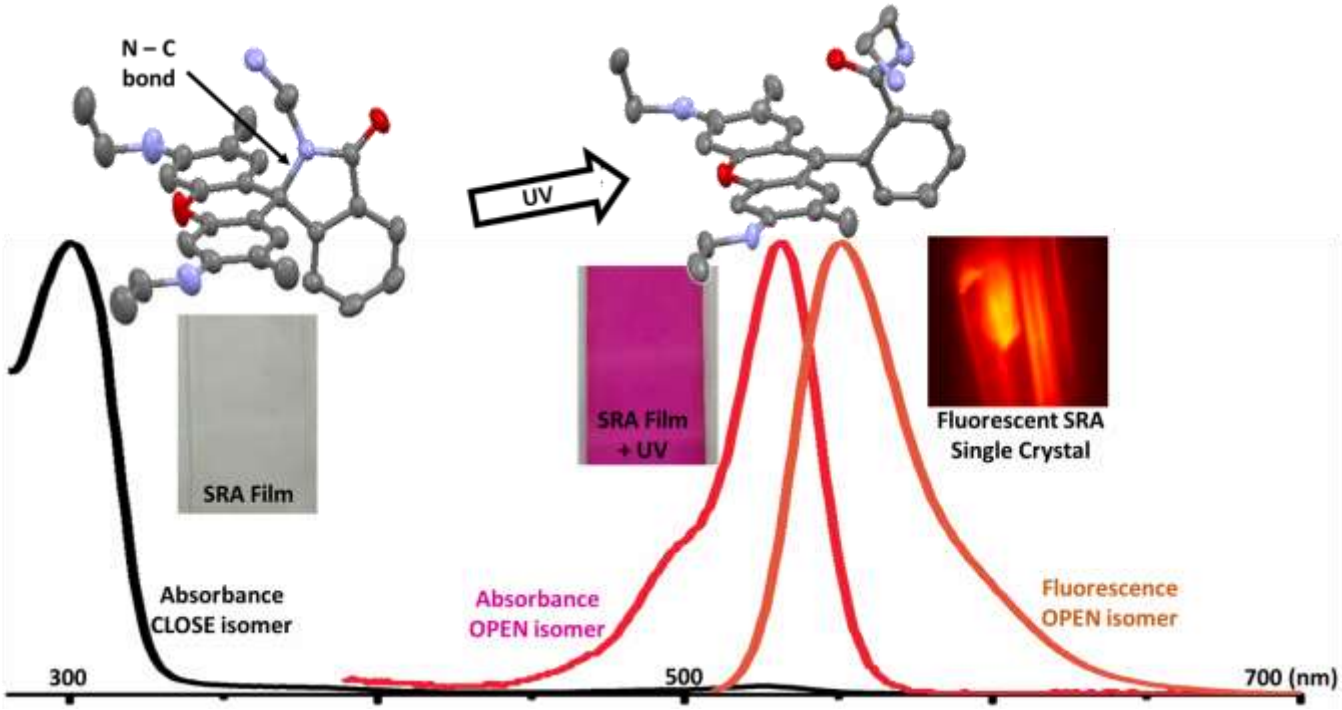

Figure 1. This is a figure caption (Heading 6 style, Times New Roman 9 pt).

The structures of seven different derivatives have been solved and differences in the absorption and emission spectrum have been found depending on the amine used in the synthesis. Moreover, different isomerization times have been found in solid state also depending on the amine used. This were very promising results for the use of this family as rational designed compounds to develop materials and coats with spectral memory to sense pH and light changes.

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