Novel U-Shaped D-A-D $\pi$-conjugated Systems with Mechanochromic Properties: An Experimental and Theoretical Vibrational Spectroscopic Investigation

S. Fernández-Palacios, a Y. Takeda, b S. Minakata, b J. T. López Navarrete, a M. Moreno Oliva, a M. C. Ruiz Delgado a

$\pi$-conjugated compounds have been widely studied in the last few decades due to their huge field of application in organic electronics. Specifically, stimuli-responsive $\pi$-conjugated materials which are sensitive to external stimulus (i.e., temperature, pressure, etc) have several uses like sensors, probes and security inks, for example.1 In this work, we study two U-shape Donor-Acceptor-Donor (D-A-D) systems that are found to exhibit interesting thermal- and pressure-dependent properties.2 They consist on two different conformers of phenothiazine-dibenzo[a,j]phenazine-phenothiazine which differs from the position of the phenothiazine respect to the dibenzophenazine central core. Compound 1R is the equatorial-equatorial conformer and 1Y is the axial-axial conformer (Figure 1). The dibenzophenazine group acts as an electron acceptor whereas the phenothiazine unit acts as an electron-donor. It has been reported that this U-shape D-A-D compound shows a multi-active color changing in 3 steps and their luminescence changes with temperature, pressure and acid exposition.2 In this work, we aim to elucidate how the external stimuli (i.e. temperature, pressure, acid ambient) affects the molecular structure at both intra- and intermolecular level. To this end, we use UV-Vis absorption, Raman (Figure 1) and Infrared spectroscopy experiments in combination with DFT calculations.

Figure 1. Chemical structure of 1R and 1Y compounds and their corresponding experimental Raman spectra.

References