

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

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π -conjugated compounds have been widely studied in the last few decades due to their huge field of application in organic electronics. Specifically, stimuli-responsive π -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.

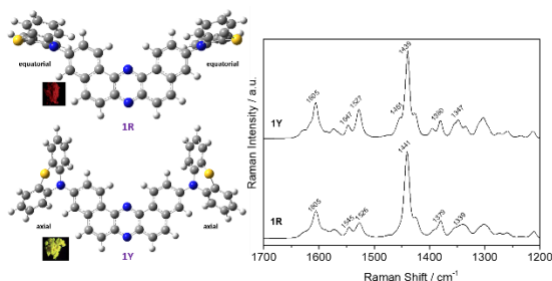


Figure 1. Chemical structure of 1R and 1Y compounds and their corresponding experimental Raman spectra.

References

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2. M. Okazaki Y. Takeda, P. Data, P. Pander, H. Higginbotham, A.P. Monkman and S. Minakata, *Chemical Science.* 2017, **8**, 2677