

Micellar charge induced emissive response of a bio-active 3-pyrazolyl-2-pyrazoline derivative: A Spectroscopic and Quantum Chemical analysis

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Supporting Information

Figures:

Figure S1: Binding constant plots of different PYZ-micelle systems

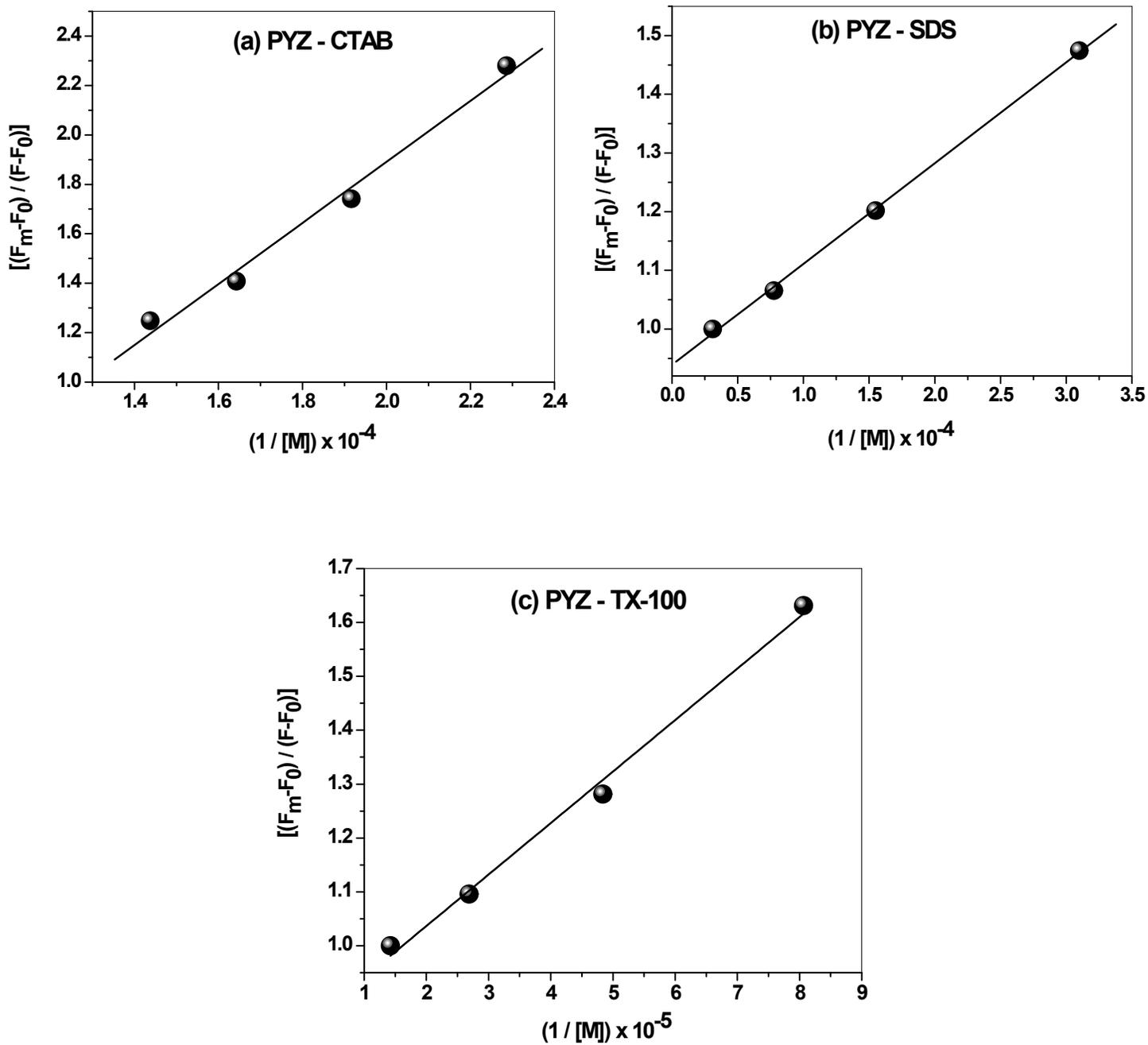


Figure S2: TD-DFT / B3LYP / 6-31G (d, p) calculated normalized absorption spectrum of PYZ in different micellar environments

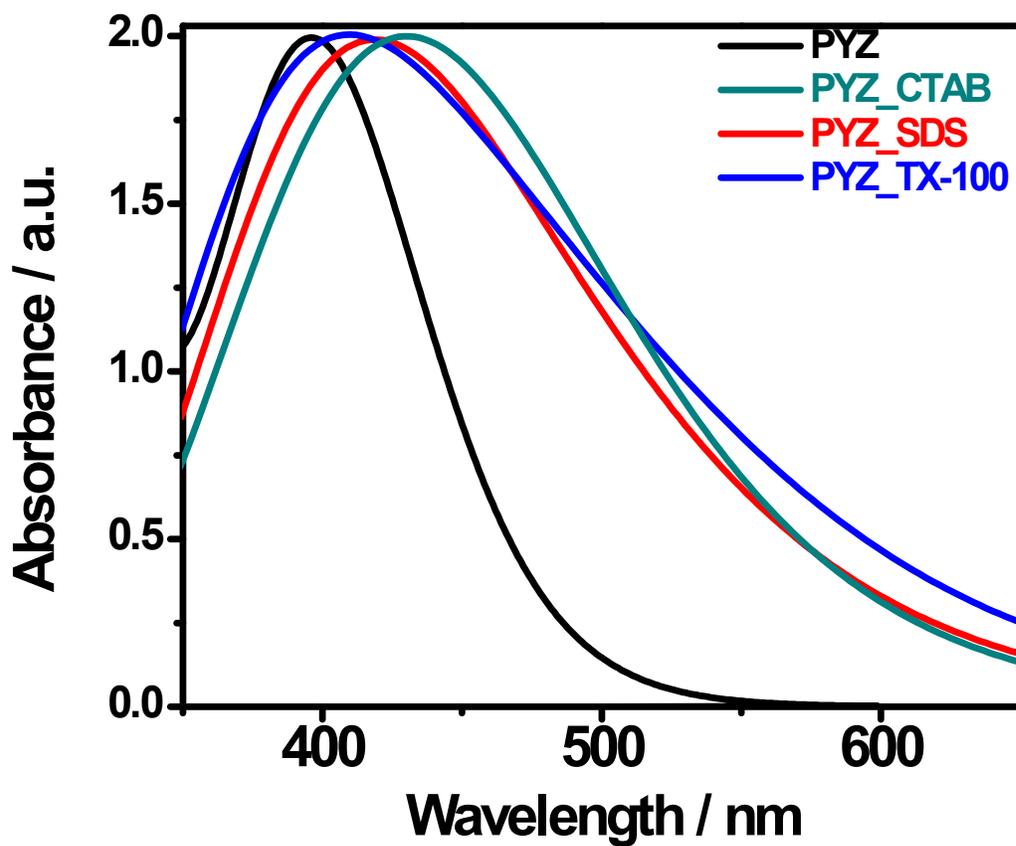


Figure S3(a): MO diagrams of PYZ (ground state), PYZ*(excited state) in CTAB micellar media along with their corresponding energy values calculated by

TD-DFT / B3LYP / 6-31G (d, p) method

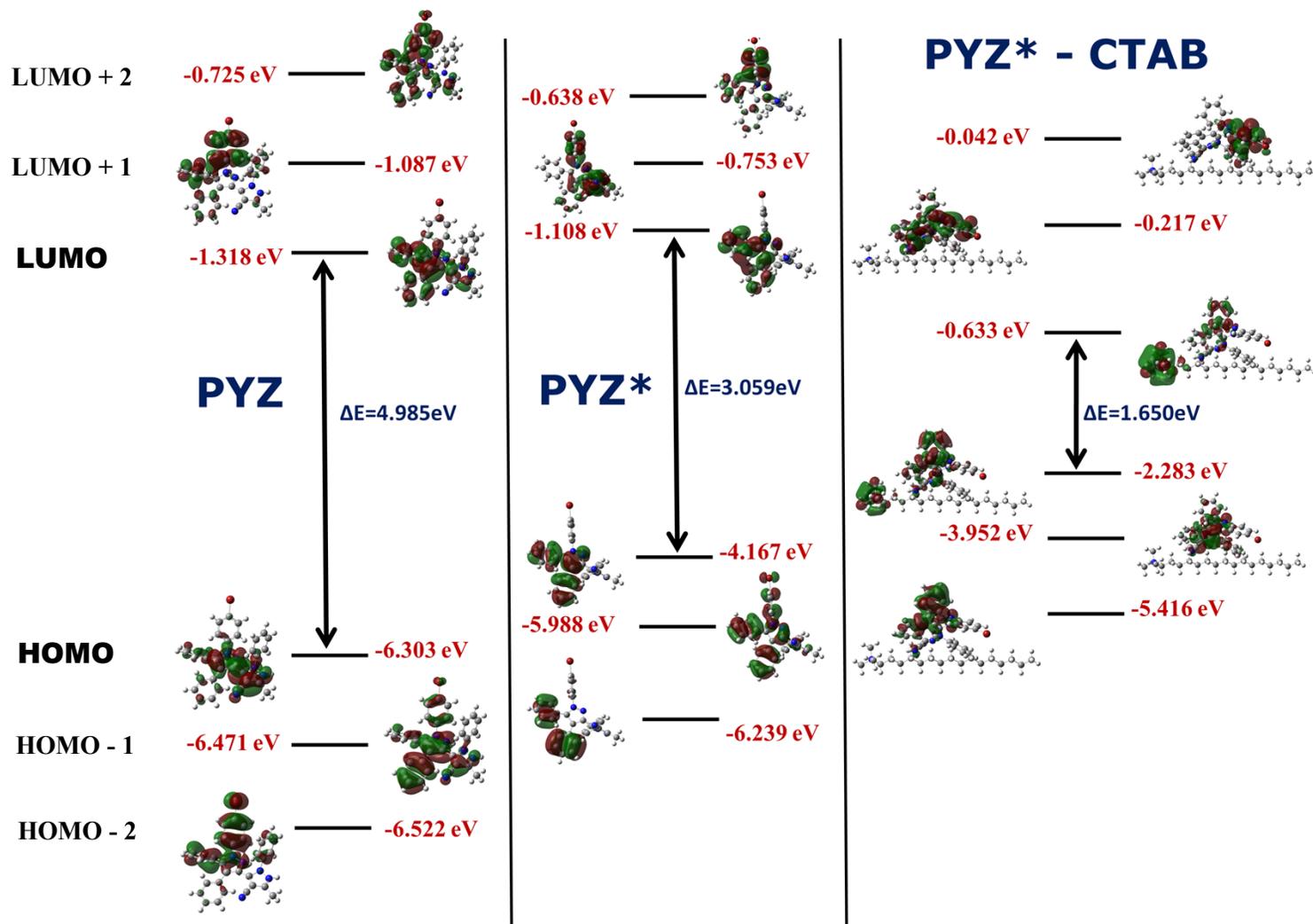


Figure S3(b): MO diagrams of PYZ* in TX-100 and TX-100-CpCl media along with their corresponding energy values calculated by

TD-DFT / B3LYP / 6-31G (d, p) method

