UV-Vis study of 1-(2-pyridylazo)-2-naphthol (PAN) and its metal complexes with Al(III), Mn(II), Fe(III), Cu(II) and Pb(II)

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PAN is a non-selective azo dye, widely used as colorimetric reagent for metal ions spectrophotometric determination, because it forms very stable, methanol-soluble and highly colored complexes with the vast majority of transition metals [1–3]. PAN has also been used as a chelating agent for the separation and preconcentration of heavy metal traces from various media including natural waters [4].

This study reports, a Uv/Vis study on PAN (Fig.1) and its metal complexes with Al(III), Mn(II), Fe(III), Cu(II), and Pb(II). In the experimental section, Uv-vis absorption spectra were acquired at different pH values.

In the theoretical section, quantum chemical calculations based on time dependent density functional theory (TD-DFT) were performed in order to determine the geometrical, absorption characteristics of the molecules with particular the vertical absorption and emission energies, geometries of the emitting structures, adiabatic energies, 0-0 transition energies [5–7]. For this purposes, extensive TD-DFT calculations have been carried out using hybrid exchange-correlation (xc) functionals, B3LYP CAM-B3LYP and PBE0, coupled to 6-31+G(2d,2p) and 6-311G(d,p) basis sets. To account for solvent effects we used the PCM continuum model.

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References

Fig. 1 Chemical structure of PAN