

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.

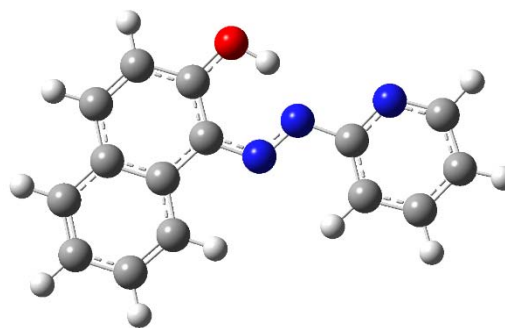


Fig. 1 Chemical structure of PAN

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References

- [1] K.L. Cheng, K. Ueno, T. Imamura, O,N-donating chelating reagents, in: Handbook of Organic Analytical Reagents, CRC Press Inc., Florida, 1982.
- [2] P. Sett, N. Paul, S.K. Brahma, S. Chattopadhyay, J. Raman Spectrosc. 30 (1999) 611.
- [3] L. Szabo, K. Hermana, N. E. Mircescu, A. Falamas, L. F. Leopold, N. Leopold, C. Buzumurg, V. Chiş, Spectrochim. Acta A 93 (2012) 266–273
- [4] M. Soy lak, Y.E. Unsal, N. Kizil, A. Aydin, Food Chem. Toxicol. 48 (2010) 517.
- [5] D. Jacquemin, A. Planchat, C. Adamo, B. Mennucci, J. Chem. Theory Comput., 8 (2012) 2359–2372.
- [6] N. De Mitri, S. Monti, G. Prampolini, V. Barone, J. Chem. Theory Comput., 9 (2013) 4507–4516.
- [7] M. Oltean, A. Calborean, G. Mile, M. Vidrighin, M. Iosin, L. Leopold, D. Maniu, N. Leopold, V. Chiş, Spectrochim. Acta A, 97 (2012) 703-710.