

Optical characterization of phthalocyanine compounds at different pH

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Phthalocyanines were discovered at the beginning of the XX century by Brown and Tchernic; they are macrocyclic compounds with alternating nitrogen and carbon atoms forming a ring. The structure is constituted by eight azoto and carbon atoms linked by a double conjugated structure [1]. Between the most important properties of phthalocyanines are the high thermal and chemical stability and interesting optical properties [2]. The spectroscopic characteristics are provided by the high electron density, due to the 18 π electrons, of the macrocyclic ring of these compounds. The UV-Vis of the spectrum has characteristic features, with high intensity absorption, resulting in colored compounds. Conformational changes may result in spectral modifications, like shift of the bands, resulting in color changes of these compounds [2]. This work focuses on the optical properties of the nickel tetrasulphonated phthalocyanine at different pH. Figure 1 show the UV-Vis spectrum of NiTsPc at different pH. The UV-vis optical absorption bands between 550 and 700 nm with a shoulder are related to the Q bands. The features between 400 and 200 nm are related with the B band and it is mixed with the absorption of the lateral substituents. The literature [2] still discusses the correct attribution of the bands in this last region. Apparently, there are no substantial changes of the spectral behavior with pH changes. Nevertheless, Lambert Beer analysis on the different bands produces different coefficients; in other words, the linear coefficient changes with pH. Table 1 have the linear coefficient (b) obtained fitting the maxim absorbance in function of concentration for different pH. This linear coefficient is related to the absorption cross section, the spring constant and the transition probability. Modifying the conditions of the solution alter the parameters that characterize the transition. In general, nominal values of the linear coefficient have a tendency to increase with the OH concentration. $\pi \rightarrow \pi^*$ transitions, where the electron cloud is open, are more susceptible to interact with the solvent. However, it is not clear this interaction, since just the relative concentration of OH and H is changing.

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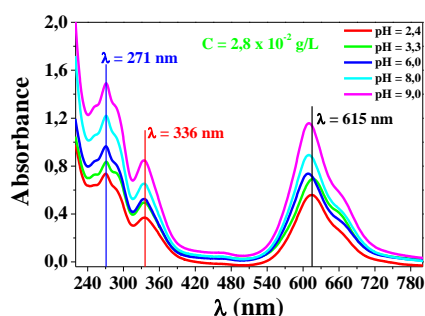


Figure 1: UV-Vis spectrum of NiTsPc in different pH.

$\lambda = 615 \text{ nm}$	$\lambda = 336 \text{ nm}$	$\lambda = 270 \text{ nm}$
$b_{pH=2}$	$b_{pH=2}$	$b_{pH=2}$
$= 25,3 \pm 0,3$	$= 17,7 \pm 0,2$	$= 32,6 \pm 0,3$
$b_{pH=3}$	$b_{pH=3}$	$b_{pH=3}$
$= 26,6 \pm 0,2$	$= 19,4 \pm 0,2$	$= 32,8 \pm 0,2$
$b_{pH=6}$	$b_{pH=6}$	$b_{pH=6}$
$= 25,5 \pm 0,1$	$= 19,9 \pm 0,1$	$= 36,4 \pm 0,5$
$b_{pH=8}$	$b_{pH=8}$	$b_{pH=8}$
$= 31,5 \pm 0,2$	$= 24,2 \pm 0,2$	$= 45,1 \pm 0,5$
$b_{pH=9}$	$b_{pH=9}$	$b_{pH=9}$
$= 39,8 \pm 0,2$	$= 30,0 \pm 0,2$	$= 54,8 \pm 0,8$

Table 1: The linear coefficient (b)

References

- [1] Frank Hans Moser, Arthur Louis Thomas - Phthalocyanine Compounds, publicado por Reinhold Pub. Co., 1963
[2] Leznoff, C.C.; Lever, A.B.P. Phthalocyanines: Properties and Applications. Vol. 1, VCH Publishers, New York, p. 139-247 1993