The influence of transition metal atoms and solvents on the absorption spectrum of Phthalocyanine

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Phthalocyanines (Pc) are conjugated macrocycles and can form compounds with transition metals. At room temperature they form crystals with different possible crystalline arrangements. These arrangements exert a high influence on their properties. In addition, they exhibit intense absorption in the visible range, between 600 and 700 nm. The conjugated benzoic groups to the central Porphyrin structure are fundamental to give them thermal stability and low reactivity. A large number of applications for Pc have been investigated, such as gas detection, catalytic action, photodynamic therapy and solar cells[]. The large number of applications, associated with a low manufacturing cost, have generated high interest in the scientific and industrial community. Since the 90s the optoelectronic and electrochemical properties of the Pcs began to be exploited for the construction of photovoltaic cells, electronic devices such as diodes and transistors, as well as electrodes modified in electrochemistry for chemical and biological sensors. Photodynamic Therapy is an alternative treatment for some types of cancer and other diseases. The molecular excitation of the drug injected into the sick tissue through radiation, in the most diverse possible wavelength ranges, allows efficient treatment with low side effects and considerable action specificity. Pcs are currently one of the most promising compounds used in Photodynamic Therapy. In this work we used the time-dependent density-functional theory to study the absorption spectrum of Pc molecules with different metal atoms (Co, Cu, Fe, Ni, Zn) adsorbed at its central Porphyrin ring. Further, the polarizable continuum model (PCM) was used to simulate the effect of different solvent environments, as acetonitrile and dichloromethane. Our results show that there will be three different general behaviors: (i) one for Co and Cu, (ii) another for Ni and Zn, and (iii) a third one for Fe. In general, the presence of a metal atom causes a blue shift of the main absorption peak at 600 nm, with an exception for Fe where a split of the main peak is observed. For Co and Cu, the high energy peaks appearing from 300 - 400 nm in the pure Pc disappear, while for Ni and Zn these high energy peaks are preserved. The solvent environment causes a red shift in the absorption peaks, with a split in main peak at 600 nm being observed for the cases of Ni and Zn metal atoms.