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DFT study of tetracationic 5,10,15,20-tetrakis(1-methyl4-pyridyl)-21H,23H porphyrin[1] HELENA PETRILLI, EDUARDO SUREZ, Universidade de So Paulo, Instituto de Fisica, DANILO PEREIRA, Universidade de So Paulo, Instituto de Quimica, FILIPE LIMA, Instituto Federal de Educao,Campus Mato, ARLES REBAZA, Universidade Nacional de La Plata, Instituto de Fisica, VERA CONSTANTINO, Universidade de So Paulo, Instituto de Quimica — Porphyrins are heterocyclic macrocycle organic compounds with many applications such as photosensitizers for light harvesting and chemical reactions, molecular electronics and enzymatic catalysis. They can be found in biological systems like photosynthesis of light, enzymes, and transport proteins. The porphyrins optical spectra can be characterized by the presence of a dominant so called Soret band plus a Q-band structure, whose positions and shapes offer a method to characterize porphyrins in various environments. Here the electronic and spectroscopic properties of tetracationic 5,10,15,20-tetrakis(1-methyl4-pyridyl)-21H,23H-porphyrin (TMPyP) is investigated in the framework of the DFT. The IR and UV-vis spectra are compared with experimental results. The influence of the environment and functional on the UV-vis spectra is investigated. These results are further discussed to tentative address the TMPyP/Clay interaction.

[1]Fapesp,Cnpq, Capes

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