Study of the Impact of the Central Atom on the Geometrical Parameters of Phthalocyanines

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INTRODUCTION

In recent years, studies of phthalocyanines (Pcs) and its derivatives have attracted great interest because of their unique properties of this class of molecules. By varyng the central atom (usually a metal), a variety of molecules have been designed for different applications in organic electronics. For example, Pc and its derivatives have been used in electrochromic display devices, organic light emitting diodes (OLEDs), organic photovoltaics (OPVs) and organic field effect transistors (OFETs). In this study, we analyzed the impact of the central atom on the geometrical properties of phthalocyanines. This study should shed light into the suitability of specific derivatives for a given technological application.

METHODS

We start by extracting the X-Ray geometries metallophthalocyanine (MePcs) molecules from Cambridge Structural Database (CSD). In order to speed up the theoretical calculations, we removed long alkyl chains by -CH_3groups.. We then use the Gaussian 09 program suite with the B3LYP/6-31G ** method to compute the energy and optimize the geometry of such molecules.

RESULTS AND DISCUSSION

We show that the distance between the center metal atom of the molecule (Figure 1), taking the average between the inner four nitrogen atoms indicated that there was little or no change of this distance by optimization. This distance has been analyzed for a set of molecules before and after optimization. A careful analysis has also been performed to understand the impact of each atom on the structure of the Pc cage.

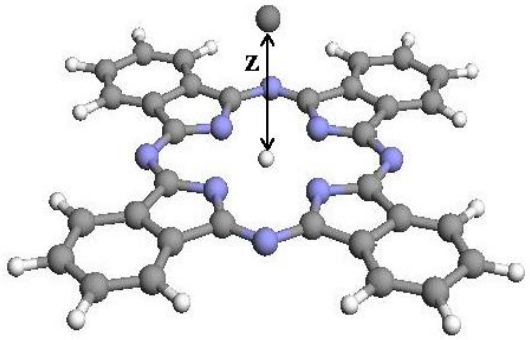

Figure 1. Distance central metal atom at the center of the phthalocyanine molecule.

CONCLUSIONS

In this work, we analyze the impact of the central atom of the geometry on the structural properties of phthalocyanines and its derivatives. Our preliminary results indicated that some central atoms deform quite drastically the geometry of the Pc molecule whereas others only mildly change its properties.

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