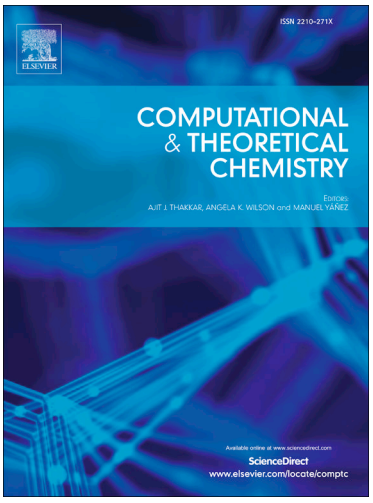

Theoretical Investigation on the Electronic Properties and UV-Vis Absorption Spectra of Expanded Porphyrin Mono-Cu(II) Complexes

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PII: S2210-271X(17)30423-1
DOI: https://doi.org/10.1016/j.comptc.2017.09.018
Reference: COMPTC 2633

To appear in: *Computational & Theoretical Chemistry*

Received Date: 5 August 2017
Revised Date: 20 September 2017
Accepted Date: 21 September 2017

Please cite this article as: G. Sun, X-S. Liu, E. Lei, C-G. Liu, Theoretical Investigation on the Electronic Properties and UV-Vis Absorption Spectra of Expanded Porphyrin Mono-Cu(II) Complexes, *Computational & Theoretical Chemistry* (2017), doi: https://doi.org/10.1016/j.comptc.2017.09.018

Theoretical Investigation on the Electronic Properties and UV-Vis Absorption Spectra of Expanded Porphyrin Mono-Cu(II) Complexes

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Abstract: The metalation chemistry of expanded porphyrins exhibits wide-ranging applications in numerous fields. In the work, we have investigated the electron spin density, charge transfer, frontier molecular orbitals and UV-Vis absorption spectra of four expanded porphyrin mono-Cu(II) complexes (Cu(II)@P, Cu(II)@HP, Cu(II)@OP and Cu(II)@*d*-OP) using density functional theory (DFT) method and time-dependent DFT. The results show that Cu(II)@HP has different electronic properties and absorption spectra compared with other complexes. What is more interesting is that the single electrons of Cu(II)@HP are not only distributed on the Cu atom and the four coordination N atoms, but also on the uncooridnation conjugated pyrroles. However, the single electrons of other complexes are mainly distributed on the Cu atom and the four coordination N atoms. This phenomenon can be successfully explained by the specific mechanism of Cu(II)@HP unlike the Zn(II)@HP. Meanwhile, the calculated values of extended charge decomposition analysis indicate that beta electrons of Cu(II)@HP have more transfer, and its frontier molecular orbitals demonstrate greater involvement of Cu(II) ion compared