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ARTIFICIAL PHOTOSYNTHESIS: PORPHYRIN-C_{96} FULLERENE MOLECULAR COMPLEX

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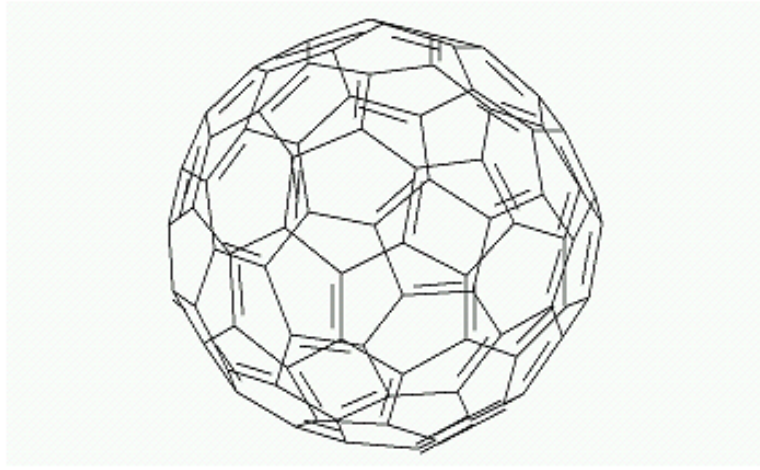
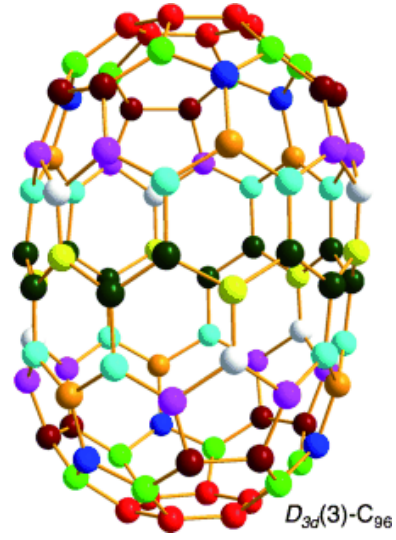
OUTLINE

- BACKGROUND
- AIM
- MATERIAL & METHOD
- RESULTS
- CONCLUSION

BACKGROUND

- C_{60} fullerene:
  - stable form (Kroto et al., 1985)
  - photo- , electro-chemical and physical properties (Bosi et al., 2003)
- C_{82} and C_{96} are members of fullerene family reported in 1992 (Kikuchi et al., 1992)





AIM

- Photodynamical studies on porphyrin and analogs-fullerene linked systems have been studied (Imahori, 2004) and some efficient photo-voltaic cells constructed on semiconductor nanoparticle have been reported (D'Souza and Ito, 2012).

- In this context, a new porphyrin-fullerene system is proposed as a new complex able to absorb better the light in the range of wavelengths of visible spectrum and was investigated.

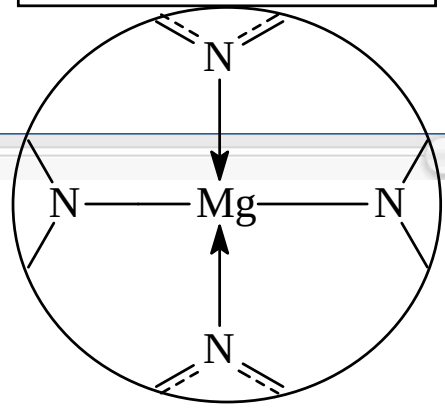
MATERIAL & METHOD

- 2 porphyrins linked together through a C_{96} fullerene ↔ minimum torsion of the bind

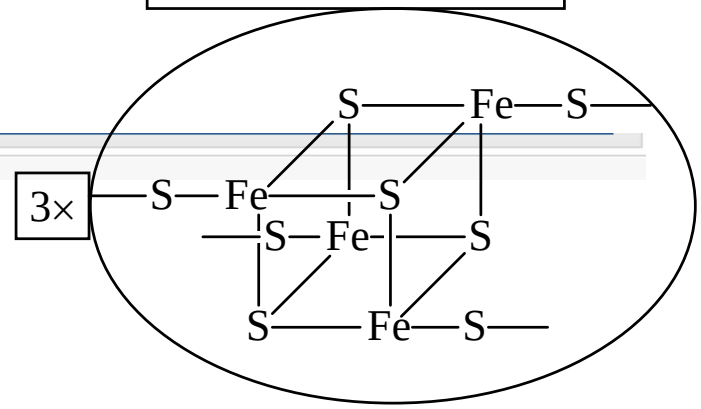
- Spartan '10: structural optimization of the investigated structures - *ab initio* package - at the restricted (post) Hartree-Fock (HF) level of theory with STO-3G refinement

- Two version of the obtained structure were investigated - with and without an Mg and Fe pair. The usefulness of the Mg-Fe pair has been derived from (Jäntschi et al., 2011)

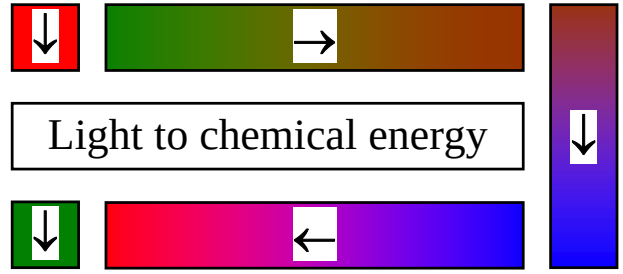
Chlorophyll

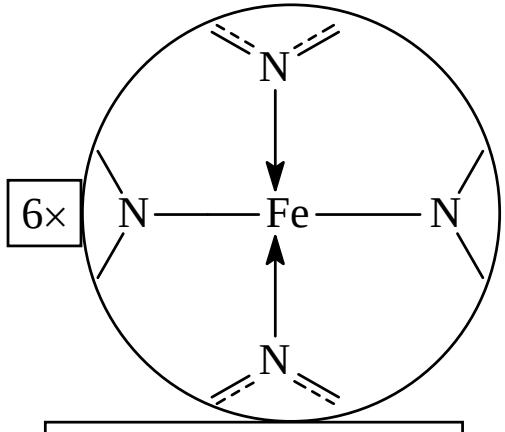


[Fe4S4]-ferredoxins

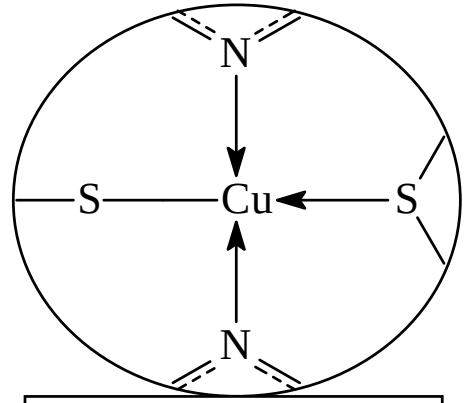


Fe, Cu, Mg – biological role





Cytochrome f

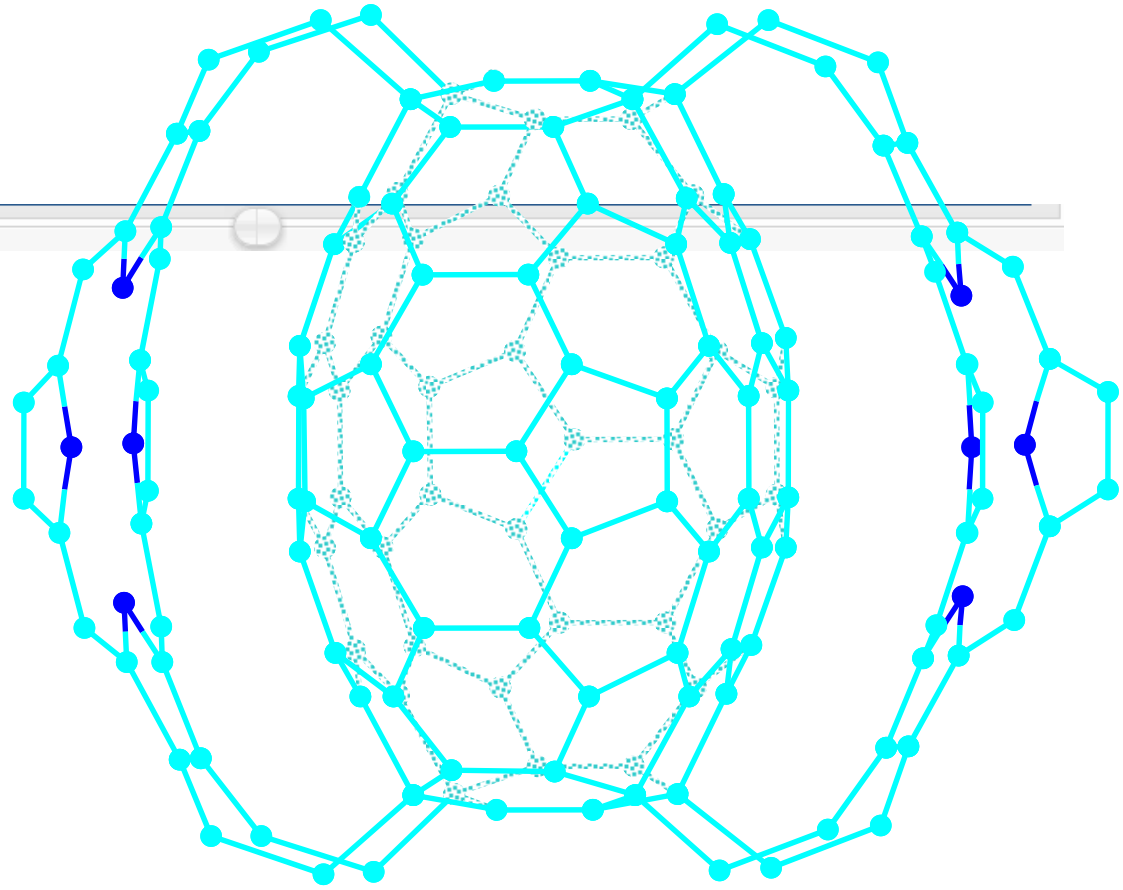


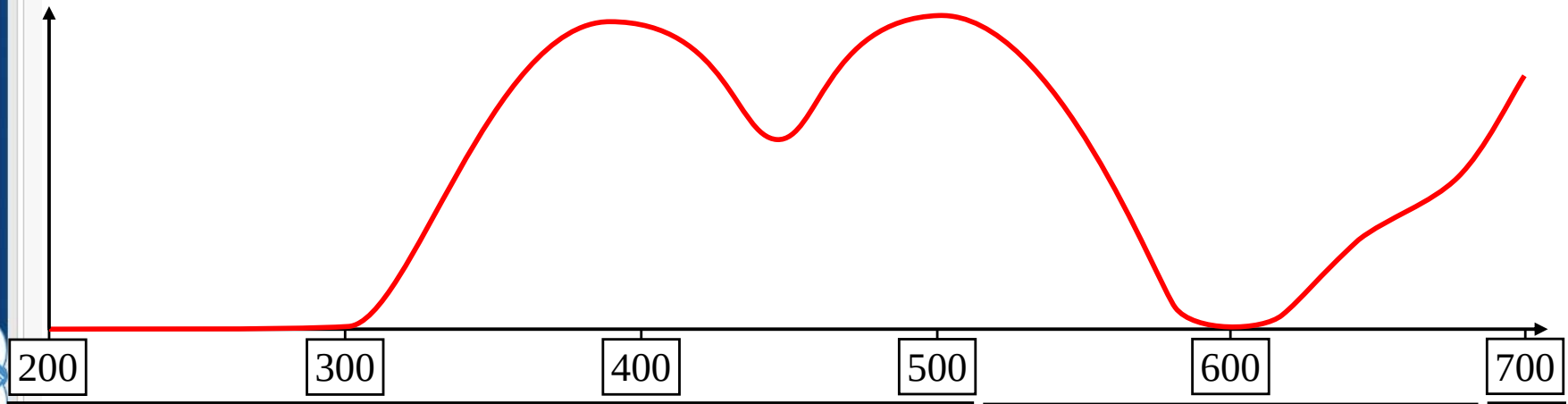
Plastocyanin

RESULTS

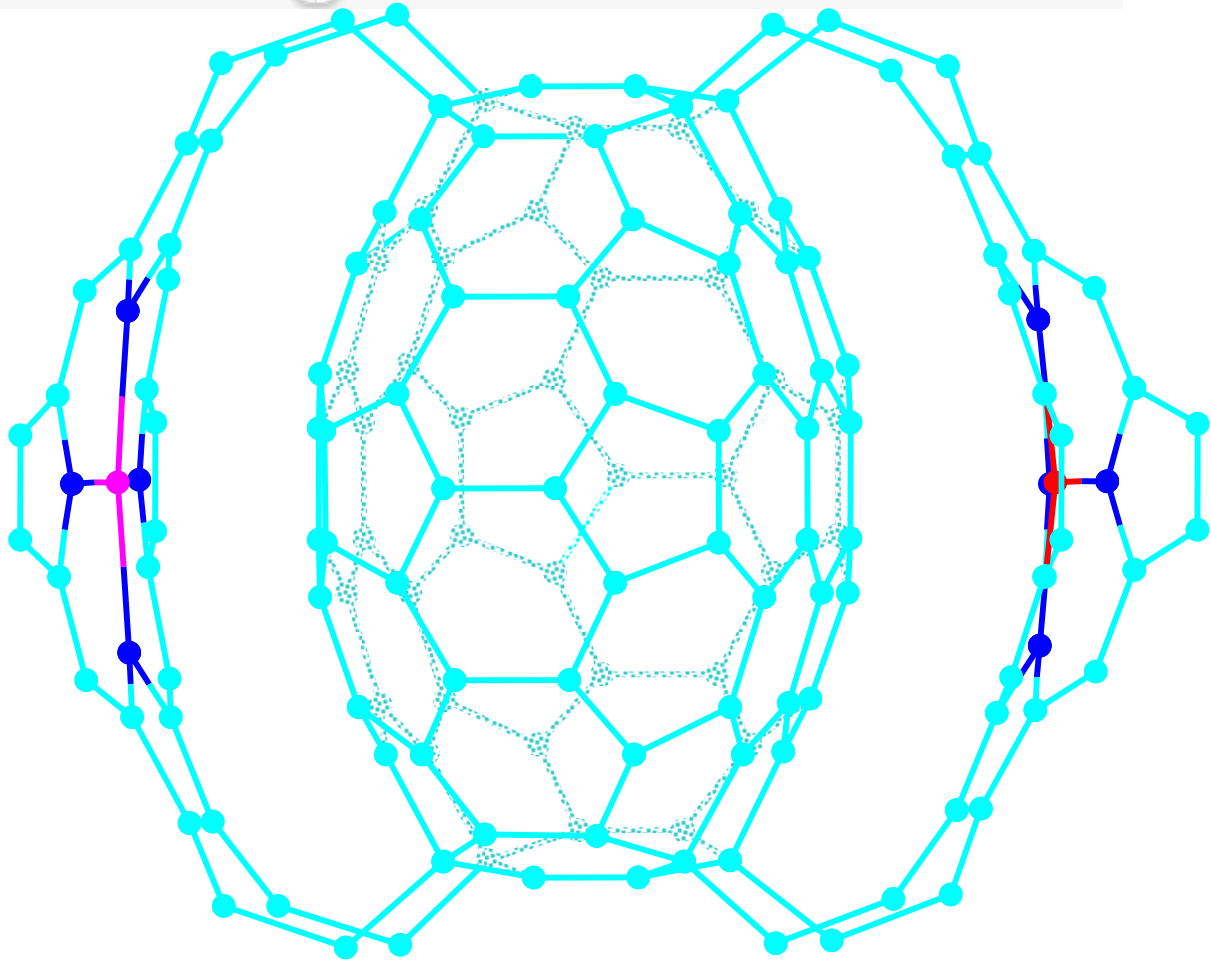
Formula	**$C_{28}H_{52}N_4$**	**$C_{152}H_{48}FeMgN_8$**
Weight (amu)	444.752	2066.264
Area ($Å^2$)	1134.04	1104.75
Volume ($Å^3$)	1731.94	1715.47
PSA ($Å^2$)	65.508	23.094
Ovality	1.63	1.59
E-HOMO (eV)	-2.49	-2.68
E-LUMO (eV)	2.11	1.90
Dipole moment (debye)	2.55	2.99
Polarizability	40.29	40.29

RESULTS




200
300
400
500
600
700
Spartan '10 Hartree-Fock STO-G +UV-VIS (excited state)
Calculated UV-VIS spectrum
nm

RESULTS



- too huge to perform accurate calculations for UV-VIS spectrum

CONCLUSIONS

- The obtained results provide important information regarding the possibilities of these new complexes
- The results obtained open a gate for the development of photo-initiated molecular devices

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Thank you for your attention!

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