ARTIFICIAL PHOTOSYNTHESIS:
PORPHYRIN-C$_{96}$ FULLERENE MOLECULAR COMPLEX

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OUTLINE

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

- **C₆₀ fullerene:**
  - stable form (Kroto et al., 1985)
  - photo-, electro-chemical and physical properties (Bosi et al., 2003)

- C₈₂ and C₉₆ 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 $\text{C}_{96}$ 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)
Fe, Cu, Mg – biological role

Light to chemical energy
## RESULTS

<table>
<thead>
<tr>
<th>Formula</th>
<th>( C_{28}H_{52}N_4 )</th>
<th>( C_{152}H_{48}FeMgN_8 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight (amu)</td>
<td>444.752</td>
<td>2066.264</td>
</tr>
<tr>
<td>Area (Å²)</td>
<td>1134.04</td>
<td>1104.75</td>
</tr>
<tr>
<td>Volume (Å³)</td>
<td>1731.94</td>
<td>1715.47</td>
</tr>
<tr>
<td>PSA (Å²)</td>
<td>65.508</td>
<td>23.094</td>
</tr>
<tr>
<td>Ovality</td>
<td>1.63</td>
<td>1.59</td>
</tr>
<tr>
<td>E-HOMO (eV)</td>
<td>-2.49</td>
<td>-2.68</td>
</tr>
<tr>
<td>E-LUMO (eV)</td>
<td>2.11</td>
<td>1.90</td>
</tr>
<tr>
<td>Dipole moment (debye)</td>
<td>2.55</td>
<td>2.99</td>
</tr>
<tr>
<td>Polarizability</td>
<td>40.29</td>
<td>40.29</td>
</tr>
</tbody>
</table>
RESULTS

Calculated UV-VIS spectrum

Spartan ’10 Hartree-Fock STO-G +UV-VIS (excited state)

Calculated UV-VIS spectrum
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
REFERENCES


Thank you for your attention!

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