Intermolecular Forces and their effect on Complex, a Theoretical Study

Pedro Heitor Rodrigues Fernandes¹, Ricardo Gargano², João Batista Lopes Martins¹

¹- Universidade de Brasília, Instituto de Química, CP 4478, 70904970
²- Universidade de Brasília, Instituto de Física, 70919-970

Abstract: The development of new technologies has an impact on a better understanding of the components present in inter/circumstellar space and also of the interactions of different species.[1] That is one of Astrochemistry focus, and it is a challenge for the scientists, even more due to the limited access and knowledge on that characteristic environment. [2,3] Therefore, the study of interactions between molecules, using Theoretical Chemistry, is of great importance for a better understanding of such interactions. Molecules as H₂O, CH₄, N₂ and CO are commonly found in the composition of spatial ices.[4] Another important task for this investigation lies on the fact that some of these molecules, in many studies, are related to the origin of life.[5,6] In another hand, one of the complex produced on this essay involving the molecules of N₂ and CO, was known as dizirinone. [7] This complex has not well established its detection. Therefore, the existence of this molecule has been speculated in the literature.[8]

This work is a theoretical study of the intermolecular forces and their effect on complex, such as: CH₄ - CO; N₂ - CH₄; and N₂ - CO. Geometry Optimizations calculations followed by characterization of minimum by vibrational frequency were carried out for these dimers. We have used the DFT method (functionals: B3LYP, CAMB3LYP, B3PW91, HCTH, HSEH1PBE, MPW1PW91, PBEPBE, TPSSTPSS e WB97XD) and the MP2 method as well. The basis set used for all calculations was the “aug-cc-pVQZ”. The Spectroscopic Constants were also determined. Table 1 shows the results of the interactions.
Table 1 – Interaction Energy (kJ/mol), distance between centers (Å), Spectroscopic Constant $\omega$ e (cm$^{-1}$)

<table>
<thead>
<tr>
<th></th>
<th>$E_i$</th>
<th>R(A-B)</th>
<th>$\omega$ e (DUNHAM/DVR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_4$-CO</td>
<td>HCTH</td>
<td>-3.00</td>
<td>3.96</td>
</tr>
<tr>
<td></td>
<td>MP2</td>
<td>-2.37</td>
<td>3.62</td>
</tr>
<tr>
<td>N$_2$-CH$_4$</td>
<td>HCTH</td>
<td>-2.93</td>
<td>3.84</td>
</tr>
<tr>
<td></td>
<td>MP2</td>
<td>-2.62</td>
<td>3.55</td>
</tr>
<tr>
<td>N$_2$-CO</td>
<td>HCTH</td>
<td>-2.64</td>
<td>4.94</td>
</tr>
<tr>
<td></td>
<td>MP2</td>
<td>-1.85</td>
<td>3.86</td>
</tr>
</tbody>
</table>

Table 1 shows us the results of the DFT HCTH calculation in comparison with the MP2 calculation. In general, the DFTs calculations behaved in the same way, higher values of Interaction Energy when compared to the values obtained by the MP2 calculations, which was observed in all of the three dimers. It is observed that in the N$_2$-CO dimer, the interaction is not so effective.

**Key-Words:** Dimers; DFT; MP2; Spectroscopic Constants; Astrochemistry; aug-cc-pVQZ.

**Support:** LQC (Laboratório de Química Computacional); CNPq; CAPES; FAPDF

**References:**