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H-S... π interactions

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Abstract: The hydrogen sulfide gas has an intense relationship with environmental chemistry and astrophysics. The alteration of the composition of atmosphere has as main factor from the human activities, by the increase of the concentration of some of its components and by the inclusion of other chemical species. These aspects make this gas of interest to various areas of science. [1] H₂S events can be found in the oil and natural gas deposits, in the extraction of salt (sodium chloride), in groundwater, in sanitary sewers, and others. In industries, H₂S comes from acid gas removal processes, effluent treatment, and also fermentation. The effects of this atmospheric pollution on the environment are observed in several regions of the Earth and, therefore, it is a subject of global relevance [2]. Therefore, it is extremely important to carry out studies of interaction processes between the chemical species that can be found in the atmosphere involving H₂S.

To verify the interactions between dimers, especially the hydrogen bonding, computational calculations was carried out. More specifically, we studied the interactions of type HS ... π , and HS ... X, among which, H₂S ... H₂S, H₂S ... NO, H₂S ... CO, H₂S ... CO₂, H₂S ... Benzene, H₂S ... Phenol, H₂S ... Chlorobenzene, H₂S ... Nitrobenzene, H₂S ... C₂H₂ and H₂S ... C₂H₄. For this purpose, the electronic structure program GAUSSIAN09 was used. Calculations were performed using the Density Functional Theory (DFT), using the B3PW91 functional, and the second-order Møller-Plesset perturbation theory (MP2). Allied to each method, we used the aug-cc-pVTZ basis function, and will be verified the influence of the base function when in the analysis of the hydrogen bond and other cooperative interactions. The Discrete Variable Representation (DVR) method was used to find the spectroscopic constants using the systems rovibrational energies.

Results and Discussion

In order to investigate and understand how the interaction of the dimers occurs, their interaction energies were calculated at DFT and MP2 level. With this, the energies found showed a good correlation between the density functional B3PW91 and the MP2 reference. In addition, one of the significant properties in characterizing the formation of a hydrogen bond relates to the changing of the frequency of the vibrational stretching mode. The frequency calculation of the MP2 method obtained higher stretching frequencies, symmetrical and asymmetrical, when compared to the frequencies of the same complexes calculated with DFT. Different analyzes were used for the interaction energy, including basis size superposition error (BSSE) and zero point energy (ZPE). The highest interaction energy was found for the H₂S-H₂S dimer, with both methods.

Final Remarks



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It was concluded that the calculations of interaction energies of different complexes involving H₂S showed that the most stable is H₂S-H₂S dimer and that the B3PW91 density functional, in general, showed a good correlation with the MP2 reference. As for the spectroscopic constants, the DVR method calculations are not yet complete.

Key-words: H₂S, ab initio, dimers.

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References:

- [1] L. Remuzgo, G. Truelba, J. M. Sarabia, *Physica A*, 2016, 444, 146-157.
- [2] F. D. Meylan, V. Moreau, S. Erkman, *J. CO2 Utilization*, 2015, 12, 101-108