Title

Is it possible to alter hydrogen bond in H2S by the presence of cation?

Abstract structure

Hydrogen sulfide (H2S) is a colorless gas known for its unpleasant rotten egg odor and its corrosive capacity on metals. It is generated by various industrial activities and results in a negative environmental impact. While sharing a similar structure with water it is interesting to note that their state in normal conditions differ, gas and liquid, originating from the presence or not of hydrogen bonds.

This study focuses on investigating whether the presence of a cation has an effect on the hydrogen bonds of H2S molecules. To address this question, we employed the DFT quantum technique as implemented within the ORCA program. This methodology is valuable for assessing how a cation influences hydrogen bonds in H2S, as it provides accurate information about the structure, bond energy and electronic distribution. Crucially, it allows the analysis of the alterations in hydrogen bond geometry and stability due to interaction with the cation, as well as providing a detailed view of the spectroscopic properties, fundamental to interpret the changes in hydrogen bonds occurring in the presence of a cation.

In conclusion, the incorporation of a cation, such as lithium (Li), into an H2S molecule leads to a significant impact on the molecular geometry and charge distribution, generating new hydrogen bonds as a result of the interaction between hydrogen atoms and lithium. This theoretical prediction could pave the way towards a new approach of H2S treatment.

Key words:

Hydrogen bond, Hydrogen sulfide, DFT, NOn covalent interaction (NCI), H2S Treatment