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The intermolecular complexes of SSF$_2$ with HF, H$_2$O, NH$_3$, HCN and CH$_3$OH molecules

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ABSTRACT

Intermolecular complexes of thiothionyl-fluoride (SSF$_2$) with HY molecules (HY = HF, H$_2$O, NH$_3$, HCN and CH$_3$OH) have been studied theoretically at the MP2/aug-cc-pVTZ computational level. The SSF$_2$ can have both hydrogen and chalcogen-bond (CB) interactions with HY molecules. The central S atom of SSF$_2$ as a better electron acceptor gives stronger adducts with HY molecules. CB interactions for the central S atom correlate with red shift of the S=S band. The QTAIM and NBO analyses were carried out on SSF$_2$ complexes.

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Theoretical study; hydrogen bonding; chalcogen bonding; QTAIM; thiothionyl-fluoride; NBO

1. Introduction

Throughout the last decades, a growing amount of experimental and theoretical effort has been devoted to non-covalent interactions due to their widespread importance in many fields of chemistry and biochemistry [1–3]. Although investigations have usually focused on the most common hydrogen-bond non-covalent interaction, recently, attention for other types of intermolecular interactions, such as halogen bond [4–6] and chalcogen bond (CB), has grown [7].

Another type of the intermolecular interaction the so-called the $\sigma$-hole was first proposed by Politzer et al. [8–12] The ‘$\sigma$-hole’ concept refers to the electron-deficient outer lobe of a p orbital, which can act as an electron-pair acceptor from a Lewis base. Thus, halogen bonding is derived from $\sigma$-hole bonding [8–11]. The $\sigma$-hole interaction is also