THEORETICAL DFT INSIGHTS INTO THE NATURE OF CHALCOGEN BONDING BETWEEN SO_2, SO_3 AND DIAZINE: NONCOVALENT INTERACTIONS INVOLVING π HOLES

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The irritant gases SO_2 and SO_3 can be the cause of certain health problems, especially in sensitive people such as children. Short exposures can cause bronchial spasms, coughing spells, impaired respiratory function and eye irritation. By attaching to fine particles, a small part of this pollutant can even penetrate to the lower respiratory tract. Too high concentrations of SO_2 and SO_3 can cause acidification of the environment. Once emitted into the air and in the presence of water, SO_2 and SO_3 are transformed into sulfuric acid H_2SO_4 which contributes to the phenomenon of acid rain. The consequences of such rains are acid deposits on building materials which can cause damage to the architectural and cultural heritage, the acidification of surface waters leading to the death of fish and soil deterioration which can have harmful effects on the vegetation and plants. DFT calculation of the capture of SO_2 and SO_3 viaπholes is performed with diazine molecules. The charge transfer interactions is highlighted by the wiberg indices calculation and the NBO analysis. The IRC calculation is performed to connect the reactants SO_2 and SO_3 with the H_2SO_4 product via the transition states.