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Book of Abstracts

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Relationship between geometry and energy of interactions in S_8 dimers

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Elemental sulfur exists in several allotropes, including α-S_8, β-S_8, and γ-S_8, wherein the arrangement of cyclic S_8 molecules varies according to the specific allotrope [1]. Intermolecular interactions among S_8 molecules have been detected within crystal structures extracted from the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD). Within these structures, S_8 molecules assume a parallel-displaced alignment, as illustrated in Figure 1a.

Quantum chemical calculations confirm that the parallel-displaced orientation represents the most stable geometry for two S_8 molecules. The interaction energy for the most stable geometry is calculated to be $\Delta E_{CCSD(T)/CBS}$= -8.70 kcal/mol (Figure 1b). According to the energy decomposition analysis performed using the SAPT 2+(3) method, the dominant attractive force between two S_8 molecules arises from dispersion interactions with the significant contribution of electrostatics.

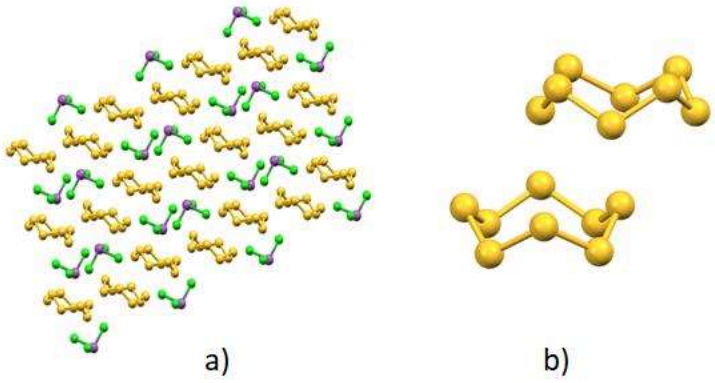

Figure 1. Parallel-displaced interactions between S_8 rings in a) Cl_3S_8Sb compound (ICSD ID: 35741) and the most stable geometry of S_8 dimer obtained by quantum chemical calculations.

References

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