

MS32-P14 | HYPERVALENT CHALCOGEN-CHALCOGEN HETEROPENTALENES AND THEIR CHARGE TRANSFER ADDUCTS

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The bonding or nonbonding interactions between atoms in molecules are one of the most central concepts in chemistry. In this paper, we consider two types of nonbonding interactions; hypervalent chalcogen---chalcogen and charge-transfer interactions.

For the interaction between sulfur atoms a wide range of S---S distances has been observed. These range from covalent disulfide bonds (2.03(2) Å), hypervalent bonds between sulfur atoms in thiathiophthenes or in bicyclic heteropentalenes (2.42 (5) Å, which we report here), so-called pancake bonds (3.02 (5) Å, for example in dithiadiazolyls) as well as Van der Waals S---S interactions (many shorter than the sum of the Van der Waals radii, 3.60 Å).

Charge-transfer complexes (CTs) have been known for decades. In this work we also investigate the use of substituted heteropentalenes, such as dithia-6-azapentalene, together with strong aromatic donors, such as trinitrobenzene, to generate a new class of charge-transfer adducts showing electrostatic potential complementarity.

Here we report the structures of five new 1,6a-dithia- or diseleno -6-azapentalenes containing hypervalent bonds between two chalcogen atoms, charge-transfer adducts of two of them with 1,3,5-trinitrobenzene and an analysis of the intra- and inter-nonbonding interactions. DFT calculations of different conformers of the heteropentalenes show that the *cis* form is more stable than the *trans* form by about 60 kJ/mol due to the hypervalent S---S interaction.

Keywords: charge-transfer complex, heteropentalene, hypervalent bond