From Long S-S Bonds to Supramolecular Aggregates – Aspects of Chalcogen-Chalcogen Interactions

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This talk presents a series of molecules in which the distance between two bonding divalent chalcogen centers are considerably shorter than the S,S van der Waals distance (3.7Å). The examples are two-center three electron (2c-3e) bonds between divalent sulfur centers such as **1**, followed by systems with four-center six electron bonds (4c-6e) bonds (**2**) shown below.



In the case of **2** a combination of π - and σ aromaticity contributes to the bonding between both units. Experimental data are compared with high level *ab initio* calculations.¹

In a second part a number of cyclic systems containing chalcogen centers are presented which show close contacts between the chalcogen centers of neighboring rings, e.g. **3**. In the case of systems with ring size 24 to 33 the resulting tubes can include guest molecules.² By means of quantum chemical methods the forces between the chalcogen centers were analyzed.³

- ¹ R. Gleiter, G. Haberhauer, *J- Org. Chem.* **2014**, *79*, 7543.
- ² R. Gleiter, D. B. Werz, B. J. Rausch, *Chem. Eur. J.* **2003**, *9*, 2676.
- ³ C. Bleiholder, D. B. Werz, H. Köppel, R. Gleiter, J. Am. Chem. Soc. 2006, 128, 2666.