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CHARACTERIZATION OF ADAMANTYL THIOETHERS BY ROTATIONAL SPECTROSCOPY

Marina Šekutor,[a] Pablo Pinacho,[b,c] Donatella Loru,[b] Tatjana Šumanovac,[a] Melanie Schnell[b,d]

[a] Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia, [b] Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany, [c] Physical Chemistry Department, University of the Basque Country (UPV/EHU), B° Sarriena, S/N, 48940, Leioa, Spain, [d] Christian-Albrechts-Universität zu Kiel, Institute of Physical Chemistry, Max-Eyth-Str. 1, 24118 Kiel, Germany

* msekutor@irb.hr

The thioether group (R–S–R´) is a common motif in the structures of bioactive molecules and is often a starting point in the formation of higher oxidation state sulfur derivatives.[1] Despite a vast number of known thioether containing derivatives, a compound class incorporating the adamantyl group remains scarcely described in the literature. However, such alkyl adamantyl thioethers could have pharmaceutical applications due to a combination of properties emerging from these functional subunits. We therefore studied the fundamental properties of a prepared series of alkyl adamantyl thioethers using a combination of high-resolution rotational spectroscopy and computational tools.[2] Here it should be noted that the studied 1,1'-diadamantyl thioether is one of the largest molecules studied to date by high-resolution rotational spectroscopy. We also compared the obtained findings with a structurally analogous 1,1'-diadamantyl ether that we explored previously[3,4] in order to assess the influence of the sulfur atom on the intermolecular cluster formation with solvents molecules, especially water (Figure 1). Investigation of such microsolvated clusters provides valuable insights into the preference of water to establish sulfur-centered hydrogen bonds with thioethers.

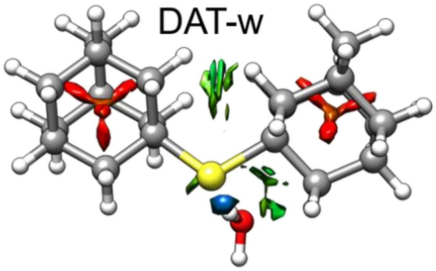

Figure 1. Structure of the monohydrated complex of 1,1'-diadamantyl thioether with depicted non-covalent interaction surfaces, blue (strong attraction *via* hydrogen bonds), green (weak dispersion interactions) and red (repulsion inside the adamantyl cages).

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