

NON COVALENT INTERACTIONS IN LARGE DIAMONDOID DIMERS IN THE GAS PHASE - A MICROWAVE STUDY

CRISTOBAL PEREZ, *CoCoMol, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany*; MARINA SEKUTOR, ANDREY A. FOKIN, *Institute for Organic Chemistry, Justus Liebig University of Giessen, Giessen, Germany*; SEBASTIAN BLOMEYER, YURY V. VISHNEVSKIY, NORBERT W. MITZEL, *Lehrstuhl für Anorganische Chemie und Strukturchemie, Institut für Anorganische Chemie, Bielefeld, Germany*; PETER R. SCHREINER, *Institute for Organic Chemistry, Justus Liebig University of Giessen, Giessen, Germany*; MELANIE SCHNELL, *MPSD, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*.

Accurate structure determination of large molecules still represents an ambitious challenge. Interesting benchmark systems for structure determination are large diamondoid dimers, whose structures are governed by strong intramolecular interactions. Recently, diamondoid dimers with unusually long central C–C bonds (up to 1.71 Å) were synthesized. This long central C–C bond was rationalized by numerous CH \cdots HC-type dispersion attractions between the two halves of the molecule. The thermodynamic stabilization of molecules equipped with bulky groups has provided a conceptually new rationale, since until then it had been assumed that such molecules are highly unstable. We performed a broadband CP-FTMW spectroscopy study in the 2-8 GHz frequency range on oxygen-substituted diamondoid dimers (C₂₆H₃₄O₂, 28 heavy atoms) as well as diadamantyl ether to provide further insight into their structures. The experimental data are compared with results from quantum-chemical calculations and gas-phase electron diffraction. For the ether, we even obtained ¹³C and ¹⁸O isotopologues to generate the full heavy-atom substitution structure.