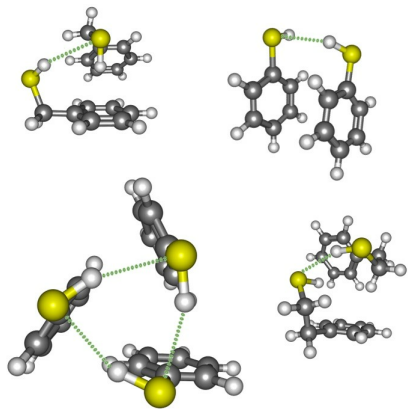


SULFUR HYDROGEN BONDING IN THE OLIGOMERS OF AROMATIC THIOLS

RIZALINA TAMA SARAGI, MARCOS JUANES, ALBERTO LESARRI, *Departamento de Química Física y Química Inorgánica, Universidad de Valladolid, Valladolid, Spain*; JOSÉ A. FERNÁNDEZ, *Departamento de Química Física, Universidad del País Vasco (UPV-EHU), Bilbao, Spain*.



Following previous experiments on sulfur hydrogen bonding^a we have observed several oligomers of the aromatic thiols thiophenol, phenylmethanethiol and 2-phenylethanethiol in a jet-cooled expansion using broadband (chirped-pulsed) microwave spectroscopy (2-8 GHz). The homodimers of the three aromatic thiols are primarily stabilized by S-H ... S hydrogen bonds and other weak interactions. The phenylmethanethiol and 2-phenylethanethiol dimers exhibit additional combinations of S-H ... π , C-H ... π or C-H ... S interactions, while the two phenyl rings in the thiophenol dimer are stacked, displaying a π - π interaction. A single symmetric-top isomer of the thiophenol trimer has been observed, characterized by a C_3 symmetry topologically equivalent to that observed in the phenol^b and aniline^c trimers. The trimer structure combines S-H ... S hydrogen bonds and C-H ... π interactions. Accurate rotational parameters and supporting ab initio and DFT calculations will be reported at the symposium.

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