NON–COVALENT INTERACTIONS IN ALCOHOL–THIOL CLUSTERS: THE 2–PHENYLETHANETHIOL AND 2–PHENYLETHANOL HETERODIMER

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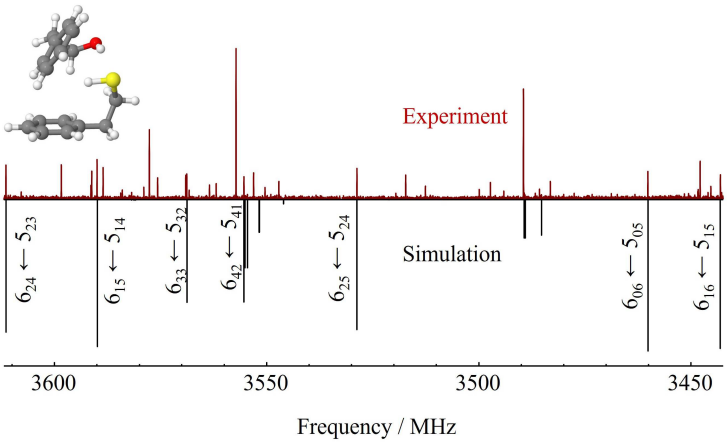
Sulfur compounds are present in multiple biologically active chemicals. The investigation of their gas phase spectra, where matrix and solvent effects are canceled, can provide detailed information on different types of intermolecular interactions and comparison with quantum mechanical calculations. We have previously reported that aromatic homodimers containing alcohol (–OH) or thiol groups (–SH) produce different interaction patterns, including either hydrogen bonding or π-stacking.[1] However, there are a few reports on aromatic heterodimers including both groups. Here we report on the heterodimer formed between 2–phenylethanethiol (2PET) and 2–phenylethanol (2PEA). The 2PET...2PEA dimer was observed in a jet expansion using chirped-pulsed microwave spectroscopy (Figure 1). Only one isomer was observed for the heterodimer, cooperatively stabilized by O–H...S, S–H...π and C–H...π interactions.[2]. The dimer avoids a stacking geometry, instead resembling the dimers of 2–phenylethanethiol or 2–phenylethanol. During the conference we will provide more details on this problem, including experimental results and supporting calculations.

[1] doi:acs.jpclett.2c03299, R. Saragi, C. Calabrese, M. Juanes, R. Pinacho, J. Rubio, C. Pérez, and A. Lesarri, *J. Phys. Chem. Lett.*, **14**(1), 207–213 (2023).

[2] doi:10.3390/sym13112022, R. Saragi, M. Juanes, R. Pinacho, J. Rubio, J. Fernández, and A. Lesarri, *Symmetry*, **13**(11), (2021).


Experiment
Simulation
$6_{24} \leftarrow 5_{23}$
$6_{15} \leftarrow 5_{14}$
$6_{33} \leftarrow 5_{32}$
$6_{42} \leftarrow 5_{41}$
$6_{25} \leftarrow 5_{24}$
$6_{06} \leftarrow 5_{05}$
$6_{16} \leftarrow 5_{15}$
3600
3550
3500
3450
Frequency / MHz