

**DIFFERENT NON-COVALENT INTERACTION TYPES AND
GEOMETRIES FOR SIMILAR COMPLEXES OF
PHENYLACETALDEHYDE–H₂O AND PHENYLACETALDEHYDE–H₂S**

M. LI, W. LI, J.-U. GRABOW, A. LESARRI, *Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, Hannover 30167, (Germany); M. Li: meng.li@pci.uni-hannover.de*

Molecules with aromatic rings are extremely versatile in exercising non-covalent interactions (NCIs), making them prototype systems to study π – π stacking,¹ lone pair... π –hole interactions,² and H... π interactions,³ etc. Phenylacetaldehyde (PAA) is the derivative of the simplest aromatic aldehyde (benzaldehyde) towards a longer carbon chain. Thus, there are more probabilities for its bonding with other molecules by different NCI sites due to its increased flexibility.

The chalcogens O and S, being homologues next to each other in their main group of the periodic system, show some similar but indeed varying physical and chemical properties. Therefore, H₂O and H₂S can serve as simple model molecules to study how such property changes effect NCI types and, consequently, the geometries of their respective complexes formed between them and identical partner molecules.

E.g., it had been reported that the geometry is similar in the case of benzene–H₂O⁴ and benzene–H₂S complexes,⁵ but very different in phenylacetylene–H₂O⁶ and phenylacetylene–H₂S complexes.⁷ This raises the question if trends for different functionalizatin can be established: E.g., how will the aldehyde complexes of PAA–H₂O and PAA–H₂S behave? At this purpose, the two title complexes have been investigated using broadband rotational spectroscopy in frequency range of 2–8 GHz.

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