INTERPLAY OF INTERMOLECULAR INTERACTIONS: COMPLEXES OF 2-DECALONE WITH WATER, BEN-ZENE, AND PHENOL

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Here we report the study on complexes between 2-decalone ($C_{10}H_{16}O$) and water, benzene, and phenol, respectively. The goal was to compare the interactions between the complex partners and the contributions of electrostatic and dispersion forces and which of them dominates when both forces are present. For that, a small hydrogen bond donor, water, was selected. Benzene is a good example for forming dispersion interactions, while in phenol both a phenyl ring and a hydrogen bond donor group are present and there could be competition between both forces. The complexes were studied in the gas phase in a cold and isolated environment generated by a supersonic expansion. The spectra were recorded using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy in the 2-8 GHz frequency region. The sample consists of cis and trans 2-decalone, and complexes with both isomers were detected. In total five water complexes were identified with dominant electrostatic interactions between the complex partners. Three complexes with benzene were assigned showing mostly dispersion interactions. Another three complexes were identified with phenol. The analysis revealed that they have a higher percentage of electrostatic than dispersion forces and display a preference for a hydrogen bond when in competition with dispersion interactions.

