STRUCTURE AND NON-COVALENT INTERACTIONS OF THE BENZOFURAN-DIETHYL DISULFIDE COMPLEX CHARACTERIZED BY ROTATIONAL SPECTROSCOPY

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The complex of benzofuran and diethyl disulfide has been investigated using Fourier transform microwave spectroscopy complemented by theoretical calculations. Two isomers have been observed, in which diethyl disulfide configures as gauche-gauche-gauche conformation sitting on the face of the benzofuran ring. The lone pair electrons of the sulfur atom points to the π-electron cloud of the benzofuran with a distance of about 3.6 Å, thus indicating a direct interaction between S and aromatic ring. NCIplot analysis suggests both observed isomers are stabilized by cooperative S$\cdots\pi$, CH$\cdots\pi$, and CH$\cdots$O weak intermolecular interactions with total interaction energies of about 26 kJmol^{-1} and is dominated by dispersion. Detailed spectroscopic and computational results will be presented.