

## NON-COVALENT INTERACTIONS FROM THE POINT OF VIEW OF QUADRUPOLEAR NUCLEUS: THE ENERGETICALLY SIMILAR STRUCTURES OF BROMOBENZENE · · · STYRENE OXIDE

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Rotational spectroscopy is often used to determine the gas-phase structures of weakly bonded complexes. When combined with the power of quantum chemical calculations, relative stabilities of various conformations can be confirmed. Occasionally, complexes with more than one structure are observed, and experimentally the relative intensities of the rotational transitions lead to a nearly 50/50 estimation of the conformational population in the measurement. If it happens that the relative energies predicted computationally are nearly identical for two conformers, the question of which structure is favored is left unanswered.

To this end, we present a rotational spectroscopic study on two conformations of a bromobenzene-styrene oxide complex that are nearly equivalent in energy, but structurally different. In the 2-8 GHz region, the observed nuclear hyperfine structure from the  $^{79}\text{Br}$  and  $^{81}\text{Br}$  nuclei ( $I=3/2$ ) are used to fit the nuclear quadrupole coupling tensor. For each bromine isotope, the diagonalized nuclear quadrupole tensor is used to confirm the favored structure. Results are presented along with symmetry-adapted perturbation theory (SAPT) calculations of the interaction energies. A brief comparison to similar halogenated analogs is also presented.