HIGH RESOLUTION SPECTROSCOPIC STUDIES OF 1-(1-NAPHTHYL)ETHYLAMINE IN S_0 AND S_1: EXPLORING THE DEPENDENCE OF CIRCULAR DICHROISM ON CONFORMATIONAL STRUCTURE

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Classical and/or quantum mechanical models developed for isolated molecules are commonly used to extract structural information from optical activity measurements dispite the lack of experimental data for validation of these models. Rotationally-resolved gas phase spectra of the prototypical chiral molecule, 1-(1-Naphthyl)ethylamine (NEA), and its amine deuterated forms have been obtained in the microwave and ultraviolet regions to provide such data. The results of the microwave study indicate that only one conformational form exists under jet-cooled conditions. The substituted atom positions and dipole moment orientation are used to identify the structural configuration of the attached chiral group from amoung nine possible ab initio forms (B3LYP/6-31G*). The S_1 inertial parameters and transition moment orientation from the UV data of the band origin at 314 nm have been used to test excited state predictions from ab initio models. CD spectra have also been calculated for the four lowest energy conformations and compared with the observed CD spectrum of (S)-NEA in cyclohexane. These results provide rigorous benchmark data and further elucidate the importance of conformational structure for determinations of absolute stereochemistry from CD spectra. The current progress on gas phase CD measurements will also be discussed.