ELECTRONIC SPECTROSCOPY OF JET-COOLED 2-METHOXYNAPHTHALENE

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The S_1 - S_0 electronic transition of jet-cooled 2-methoxynaphthalene (2MXN) has been investigated by use of laser-induced fluorescence spectroscopy. The fluorescence excitation spectrum revealed two electronic origin transitions, separated by 660 cm⁻¹. They are caused by the presence of a *cis* and a *trans* conformation of the methoxy group with respect to the naphthalene frame. Dispersed fluorescence spectra of 25 major transitions in the excitation spectrum of the *cis* conformer were recorded, employing a liquid nitrogen cooled chargecoupled device (CCD) detector. Atypical, highly structured emission indicates that extensive vibrational mixing in the S_1 electronic state of *cis*-2MXN occurs, caused by large normal coordinate (Duschinsky) rotation. Experimentally determined frequencies are compared to the predicted normal mode values of an ab-initio calculation at the HF/6-31G^{**} level. The spectrum, molecular structure, harmonic force field and vibrational coupling will be discussed.

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