TOWARDS UNDERSTANDING QUANTUM MONODROMY IN QUASI-SYMMETRIC MOLECULES: FASSST ROTATIONAL SPECTRA OF CH_3NCO AND CH_3NCS

ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; SARAH FORTMAN, IVAN R. MEDVEDEV, MANFRED WINNEWISSER, FRANK C. DE LUCIA, Department of Physics, The Ohio State University, Columbus, OH 43210; JACEK KOPUT, Department of Chemistry, Adam Mickiewicz University, 60-780 Poznań, Poland.

The recent studies of the rotational spectrum of the NCNCS molecule^{*a,b,c*} demonstrated the success of quantum monodromy in describing the quasilinear behavior of this molecule, inclusive of the abrupt transition of spectroscopic behavior from the bent to the linear molecule regime. Similar, quasisymmetric behaviour, is known to be present in symmetric top molecules, and has been studied at lowest-*J* transitions for two such molecules, CH_3NCO^d and CH_3NCS .^{*e*}

Further progress requires more experimental data and presently we report FASSST rotational spectra of CH_3NCO and CH_3NCS . The spectra provide practically continuous 117-376 GHz coverage and are very rich, since the ladder of excited vibrational states associated with the qualinear bending coordinate is multiplied by the nearly free internal rotation of the methyl group. Initial stages of the analysis leading up to an analysis in an extension of the framework used for NCNCS are described.

^aB.P.Winnewisser, et al., Phys. Rev. Lett. 95. 243002 (2005).

^bM.Winnewisser, et al., J. Mol. Struct. 798, 1 2006.

^cB.P.Winnewisser, et al., *Phys. Chem. Chem. Phys.* DOI:10.1039/B922023B (2010).

^dJ.Koput, J. Mol. Spectrosc. **115**, 131 (1986).

^eJ.Koput, J. Mol. Spectrosc. 118, 189 (1986).