THE QUANTITATIVE ANALYSIS OF THE ROTATIONAL SPECTRUM OF NCNCS

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The analysis of the rotational data which were the basis of our two previous publications[a] [b]about NCNCS as an example of quantum monodromy has been completed, and the data extended to include the 6th excited state of the quasilinear bending mode. This talk will present the results of fitting the data with the GSRB Hamiltonian, which provides structural and potential parameters. Ab initio calculations contributed some parameters that could not be determined from the data. The predicted variation of the expectation value of ρ, which is the complement of the CNC angle, and of the electric dipole transition moment, upon rovibrational excitation indicate the mapping of monodromy in the potential function into these properties of the molecule.

[a]B. P. Winnewisser, M. Winnewisser, I. R. Medvedev, M. Behnke, F. C. De Lucia, S. C. Ross and J. Koput *Phys. Rev. Lett.* **95** (243002), 2005.
[b]M. Winnewisser, B. P. Winnewisser, I. R. Medvedev, F. C. De Lucia, S. C. Ross and L. M. Bates *J. Mol. Struct.* **798** (1-26), 2006.