IN PURSUIT OF THE FAR-INFRARED SPECTRUM OF CYANOGEN ISO-THIOCYANATE, NCNCS, UNDER THE INFLUENCE OF THE ENERGY LEVEL DISLOCATION DUE TO QUANTUM MONODROMY

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Quantum Monodromy has a strong impact on the ro-vibrational energy levels of chain molecules whose bending potential energy function has the form of the bottom of a champagne bottle (i.e. with a hump or punt) around the linear configuration. NCNCS is a particularly good example of such a molecule and clearly exhibits a distinctive monodromy-induced dislocation of the energy level pattern at the top of the potential energy hump[a]. The generalized semi-rigid bender (GSRB) wave functions are used to show that the expectation values of any physical quantity which varies with the large amplitude bending coordinate will also have monodromy-induced dislocations. This includes the electric dipole moment components. High level ab initio calculations not only provided the molecular equilibrium structure of NCNCS, but also the electric dipole moment components μ_{a} and μ_{b} as functions of the large-amplitude bending coordinate. The calculated expectation values of these quantities indicate large ro-vibrational transition moments that will be discussed in pursuit of possible far-infrared bands. To our knowledge there is no NCNCS infrared spectrum reported in the literature.

[a]B. P. Winnewisser, M. Winnewisser, I. R. Medvedev, F. C. De Lucia, S. C. Ross and J. Koput, Phys. Chem. Chem. Phys., 2010, DOI:10.1039/B922023B