OBSERVING QUANTUM MONODROMY: AN ENERGY-MOMENTUM MAP BUILT FROM EXPERIMENTALLY-DETERMINED LEVEL ENERGIES OBTAINED FROM THE ν_7 FAR-INFRARED BAND SYSTEM OF NCNCS

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The concept of Quantum Monodromy (QM) provides a fresh insight into the structure of rovibrational levels in those flexible molecules for which a bending mode can carry the molecule through the linear configuration. To confirm the existence of QM in a molecule required the fruits of several strands of development: the formulation of the abstract mathematical concept of monodromy, including the exploration of its relevance to systems described by classical mechanics and its manifestation in quantum molecular applications; the development of the required spectroscopic technology and computer-aided assignment; and the development of a theoretical model to apply in fitting to the observed data. We present a timeline for each of these strands, converging in our initial confirmation of QM in NCNCS from pure rotational data alone.[a] In that work a Generalised SemiRigid Bender (GSRB) Hamiltonian was fitted to the experimental rotational structure. Rovibrational energies calculated from the fitted GSRB parameters allowed us to construct an "Energy-Momentum" map and confirm the presence of QM in NCNCS. In further experimental work at the Canadian Light Source Synchrotron we have identified a network of transitions directly connecting the relevant energy levels and thereby have produced a refined Energy Momentum map for NCNCS from experimental measurements alone. This map extends from the ground vibrational level to well above the potential energy barrier, beautifully illustrating the characteristic signature of QM in a system uncomplicated by interaction with other vibrational modes.

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[a]B. P. Winnewisser *et al.*, Phys. Rev. Lett. **95**, 243002 (2005).