QUANTUM MONODROMY IN REAL QUASILINEAR MOLECULES

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The top of the barrier to linearity in the two dimensional anharmonic potential well for one bending mode of an otherwise linear molecule forms the critical monodromy point of, in topological terms, a gross obstruction, leading to a catastrophic discontinuity in the mathematical description of the eigenstates of such systems in the spaces below and above this point. Previously, only model calculations had been made showing the relevance of this concept to quasilinear and bent molecules.[a] We show that the molecules BrCNO, ClCNO and NCNCS exhibit precisely the predicted behavior above and below the critical point. Furthermore, a pragmatic application of this perspective is shown to be revealing and useful in the assignment of the rotational structure of the bending vibrational states of these systems.

[a] M. S. Child, T. Weston and J. Tennyson, Mol. Phys. 96, 371–379 (1999)