THE HIDDEN KERNEL OF MOLECULAR QUASI-LINEARITY: QUANTUM MONODROMY

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Chain molecules with one single low-lying bending mode provide a set of model species for the exploration of quantum monodromy in quasi-linear molecules. Recent work on water[a] and NCNCS[b] have shown that the topology of the energy-momentum maps of such molecules follows closely predictions based on the mathematical concept of non-trivial monodromy. From experimental data and new general semi-rigid bender (GSRB) calculations which extrapolate beyond the existing data for various species, we can now present the topological properties of the bending-rotation energy-momentum maps of a wide range of molecules, from rigidly linear to rigidly bent. It will also be shown that the energy-momentum map for the end-over-end rotational energy, represented by the effective rotational constant $\bar{B}$, has unexpected properties which, like the bending-rotation energy-momentum map, are robust across the whole set of molecules studied. The molecules discussed are OCCCS, NCCNO, HCNO, OCCCO, ClCNO and BrCNO, NCNCS, HCCNCO, NCNCO and NCSCN.

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