

Abstract Submitted
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Systematic degeneracies as a guide to the vibrational dynamics of methanol DAVID PERRY, The University of Akron — The vibrational dynamics of the CH stretch and torsional vibrations of methanol are explored using a 4-dimensional effective Hamiltonian. The model parameters are constrained by a combination of low-resolution and high-resolution spectral data. At low excitation energies, the torsion-vibration states are at most 2-fold degenerate as expected for the combination of the E-type torsional tunneling species with the A' and A'' (in Cs) CH stretch vibrations. At high torsional energies, we find a series of approximate 4-fold degeneracies characteristic of a degenerate E-type asymmetric CH stretch in combination with the decoupled degenerate free internal rotation. When a single CH bond is excited to a high level, torsional tunneling is quenched causing all such levels to be 3-fold degenerate. When both a local CH stretch and internal rotation are highly excited, we find systematic 6-fold degeneracies characterized by free internal rotation decoupled from three equivalent local CH stretches. The transition regions between these simple limiting behaviors are explored.

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