DESCRIPTION OF NON-RIGID MOLECULAR STRUCTURE THROUGH DYNAMICAL SYMMETRY BREAKING

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A novel algebraic scheme has been developed for investigating the structure and dynamics of explicitly non-rigid molecules, as manifest most simply in the spectral features of quasi-linear triatomic species. Our approach permits such "floppy" systems to be envisioned as undergoing a "shape-changing phase transition" between two dynamical symmetry limits of an encompassing algebraic framework (*e.g.*, the Lie algebra $U(3)$ for triatomic bending modes) with intermediate configurations of the nuclei corresponding to situations that break dynamical symmetries. A simple model Hamiltonian has been shown to embody appropriate effects (*i.e.*, negative or alternating positive/negative vibrational anharmonicity) for describing transformations between the "rigidly-bent" and "rigidly-linear" limiting geometries that characterize quasi-linear triatomic molecules. This theoretical treatment has been exploited successfully to interprete vibrational energy level patterns reported for the "soft" bending degree of freedom in the ground electronic states of magnesium hydroxide ($MgOH$) and its deuterated isotopomer ($MgOD$). Finally, a coherent (or intrinsic) state formalism has been shown to afford a near-direct connection between algebraic analyses and the potential energy surfaces mediating various regimes of non-rigidity, thereby furnishing valuable insight into the physical processes that govern "floppy" behavior.