# Automated Resonance Identification Schemes for Vibrational Perturbation Theory's Variational Subspaces

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We present the results of various schemes to automate recognition of Fermi/Darling-Dennison resonances in VPT2+FK methodology. Identifying such *a priori* resonances is analogous to identifying strongly correlated orbitals in the electronic Schrodinger equation to select the proper configurations in MR-CI or CAS. We consider recognition via the Bloino-Barone methodology, our own independent thresholds for resonance identification based on different numerical cutoffs, and iterative schemes based on changes in line strengths. This is a true optimization problem, as excessive CI character results in much lower quality in estimating the total spectrum. We compare to our test set of experimentally broadened IR spectra at STP conditions, a database consisting of ~300 peaks over 23 molecules. We emphasize that we are comparing against broadened conditions, such that there is implicit aggregation of the peak data as a result of the broadening. We discuss the relative merits of various resonance identification schemes in balancing resonance removal vs. variational imbalance compared to experimental spectra.