Rovibrational Phase-Space Analysis of the $\nu_3/2\nu_4$ Polyad Band of $CF_4$: Qualitative study of high-resolution molecular spectroscopy

JUSTIN MITCHELL, WILLIAM HARTER, University of Arkansas — Advances in astronomy are driving the need for high-resolution spectroscopy of small and symmetric molecules, such as methane. These molecules have proven difficult to evaluate qualitatively for nearly a century. As other groups are providing line lists, this study strives to evaluate the spectra using the rovibrational phase-space tool of Rotational Energy Surfaces (RES). Some such analysis exists in the literature, but advances in computing hardware and computational tools have made it much easier and more practical. Previous efforts have evaluated the rotational level clustering in vibrational singlet and doublets. Here we show a more complicated RES analysis, evaluating the $\nu_3/2\nu_4$ polyad band of $CF_4$ and offer insights into possible analyses of other systems.

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