Rovibrational Phase-Space Surfaces for High Resolution Analysis of Polyad Bands

JUSTIN MITCHELL, WILLIAM HARTER, University of Arkansas — After nearly a century of scientific effort the spectra of spherical top molecules, such as methane, are notoriously problematic to evaluate both experimentally and theoretically. At the same time, astronomical applications require ever higher resolution data of exactly these molecules. Several theoretical and computational tools exist to predict these spectra quantitatively, but Rovibrational Phase-Space analyses, such as the Rotational Energy Surface (RES) serve as qualitative tools. Some such analysis exists in the literature, but advances in computing hardware and computational tools has 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 $CF_4$. 

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