ROVIBRATIONAL PHASE-SPACE SURFACES FOR ANALYSIS OF $\nu_3/2\nu_4$ POLYAD BAND OF CF_4

JUSTIN MITCHELL, WILLIAM HARTER, *University of Arkansas, Department of Physics, Fayetteville, AR 72701*; VINCENT BOUDON, *Institut Carnot de Bourgogne, UMR 5209 CNRS–Université de Bourgogne, 9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France*.

Even 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. These are molecules that show complex interactions, strongly coupling rotations to vibrations, if not electronics. Theoretical and computational tools exist[a] to predict these spectra, but they could be greatly aided by Rovibrational Phase-Space analysis, such as the Rotational Energy Surface (RES). Some such analysis exists in the literature[b] [c], but advances in computing hardware and computational tools have made it much easier. This talk will show a more complicated RES analysis than has been done before, evaluating the $\nu_3/2\nu_4$ polyad band of CF_4.

[a] Ch. Wenger, J.P. Champion, J. Quant. Spect. and Rad. Trans. 59, 471 (1998)
[b] W.G. Harter, C.W. Patterson and H.W. Gailbraith, J Chem Phys 69, 4896 (1978)
[c] Dhont et al, J Mol Spect, 201, 95 (2000)