

NON-RESONANT RAMAN SPECTRA OF THE METHYL RADICAL $^{12}\text{CH}_3$ SIMULATED IN VARIATIONAL CALCULATIONS

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We report first-principles variational simulation of the non-resonant Raman spectrum for methyl radical ($^{12}\text{CH}_3$) in the electronic ground state. Calculations are based on a high level *ab initio* potential energy and polarizability tensor surfaces of CH_3 and employ accurate variational treatment of the ro-vibrational dynamics implemented in the general code TROVE [S. N. Yurchenko, W. Thiel, and P. Jensen, *J. Mol. Spectrosc.* **245**, 126–140 (2007); A. Yachmenev and S. N. Yurchenko, *J. Chem. Phys.* **143**, 014105 (2015)]. We extend the capabilities of TROVE towards simulations of the Raman spectra, which can in be applied to arbitrary molecule of moderate size. The simulations for CH_3 are found to be in a good agreement with the available experimental data.