Computer simulation of Raman spectra and mode assignment: Application to methane

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Abstract

This work uses driven molecular dynamics (DMD) method, in conjunction with an analytic PES calculated using MP2/aug-cc-pVDZ energies to identify and assign Raman vibrational modes of methane. Recently, a new linearized approach was proposed for the Polarizability Tensor Surfaces (PTS) that yields a unique solution to the least-squares fitting problem and provides a competitive level of accuracy compared to the non-linear PTS model. We used the previously reported B3LYP/6-31+G(d) molecular geometries for CH_4 and generated a new PTS at the MP2/aug-cc-pVDZ level of theory. The performance of the linearly parametrized functional form for the CH_4 PTS is examined. DMD trajectories were run up to 10 ps with 0.5 fs time step and absorbed energy was monitored for each resonant frequency. Atomic coordinates, driving forces, and polarizability tensors collected along the trajectory provide rich source of information that assists mode assignment. This computational work will provide an efficient yet accurate method to simulate Raman vibrational spectra of medium-sized molecules.