

**Supplementary Information to
Vibrational infrared and Raman spectrum of HCOOH from variational
computations**

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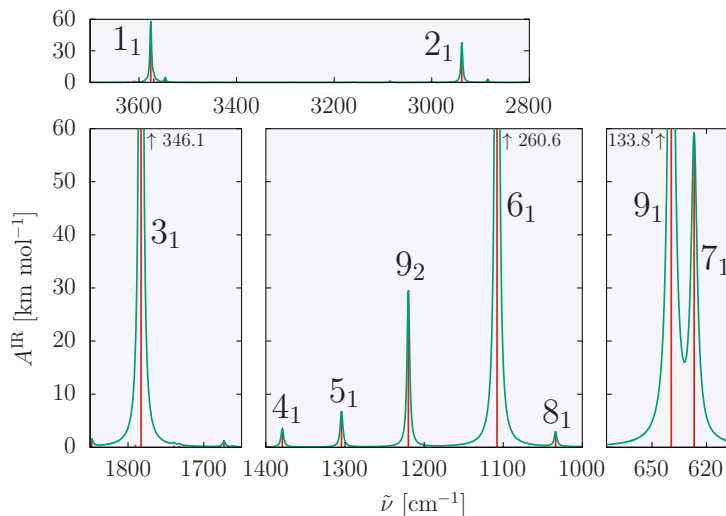


FIG. S1. Simulated vibrational infrared spectrum of HCOOH (transitions from the vibrational ground state) corresponding to the body-fixed frame of Fig. 1. The stick spectrum (in red) has been convoluted (in green) using a Lorentz distribution with full-width-at-half-maximum (FWHM) of 5 cm^{-1} . It is worth comparing this figure with Fig. 8 of the manuscript, which corresponds to the Eckart frame of the *trans* equilibrium structure, small differences in the vibrational intensity values can be observed.

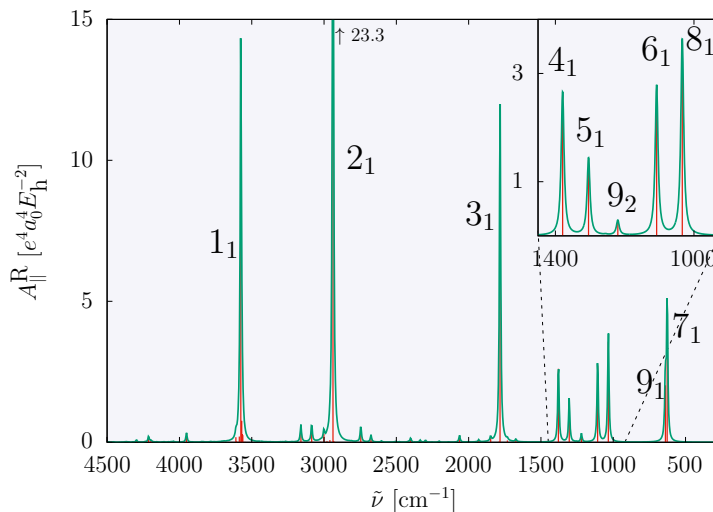


FIG. S2. Parallel Raman spectrum of HCOOH (including transitions from the vibrational ground state) corresponding to the body-fixed frame of Fig. 1 of the manuscript. The stick spectrum (in red) is convoluted (in green) with a Lorentz distribution with FWHM of 10 cm^{-1} . It is worth comparing this figure with Fig. 9 of the manuscript, which corresponds to the Eckart frame of the *trans* equilibrium structure. Major (ca. an order-of-magnitude) difference in the 8_1 (A'') and 9_1 (A') activities can be observed, which is discussed in Sec. 5.

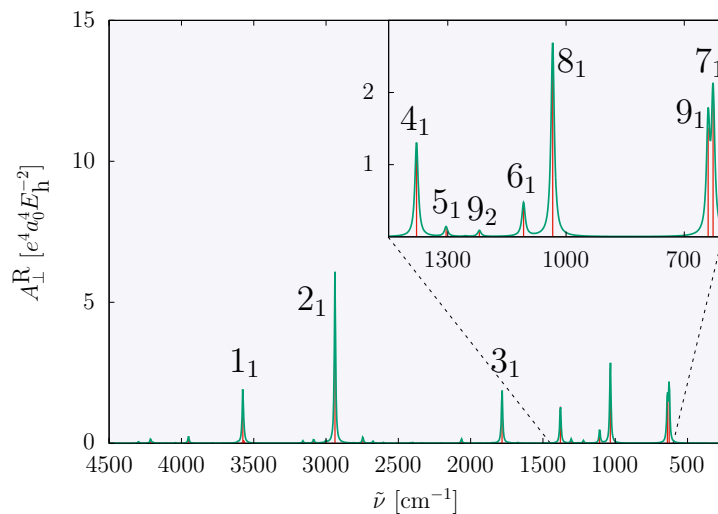


FIG. S3. Perpendicular Raman spectrum of HCOOH (including transitions from the vibrational ground state) corresponding to the body-fixed frame of Fig. 1 of the manuscript. The stick spectrum (in red) is convoluted (in green) with a Lorentz distribution with FWHM of 10 cm^{-1} . It is worth comparing this figure with Fig. 10 of the manuscript, which corresponds to the Eckart frame of the *trans* equilibrium structure. Major (ca. an order-of-magnitude) difference in the 8_1 (A') and 9_1 (A'') activities can be observed, which is discussed in Sec. 5.