

Figure S1: The analytical fit parameters for reactants (red line), products (blue line), and the combined analytically fit spectrum (black line). The infrared spectrum (violet line) is given for comparison. Left: Spectra for the PT case. Right: Spectra for the PT_R case.

Supporting Information

Analytical fits of the infrared spectra for the PT , PT_P , and PT_R cases according to Eq. 6 are given in Figs. S1 and S2.

Approximations to the spectra, as described in Sec. 4.2 are give in Fig. S3. The Condon approximation, $\phi_C(t)$, and the $\phi_{\bar{\mu}}(t)$ and $\phi_{\delta\omega}(t)$ approximations are plotted along with the full infrared spectra for the PT and P cases.

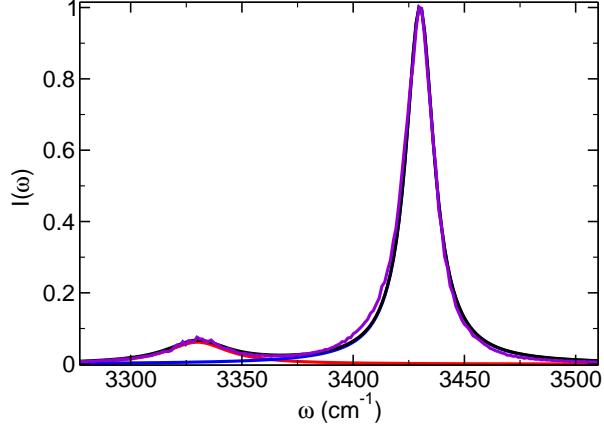


Figure S2: The analytical fit parameters for reactants (red line), products (blue line), and the combined analytically fit spectrum (black line). The infrared spectrum (violet line) is given for comparison. Spectra for the PT_P case.

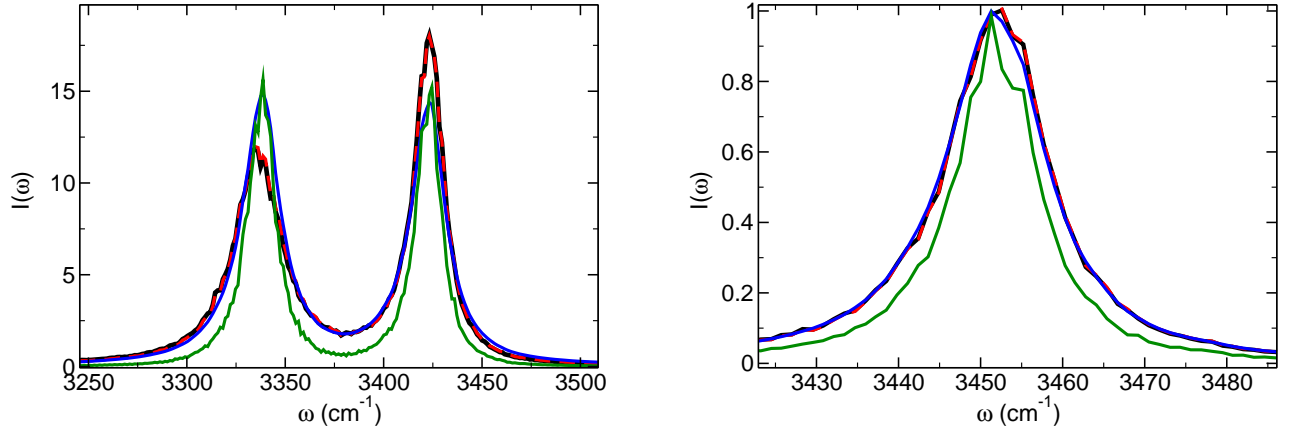


Figure S3: The full spectrum (black line), Condon approximation (dashed red line), $\phi_{\bar{\mu}}(t)$ approximation (blue line), and $\phi_{\delta\omega}(t)$ approximation (green line) for the PT and P cases. Left: Spectra for the PT case. Right: Spectra for the P case.