Supporting information on:

High-level rovibrational calculations on ketenimine

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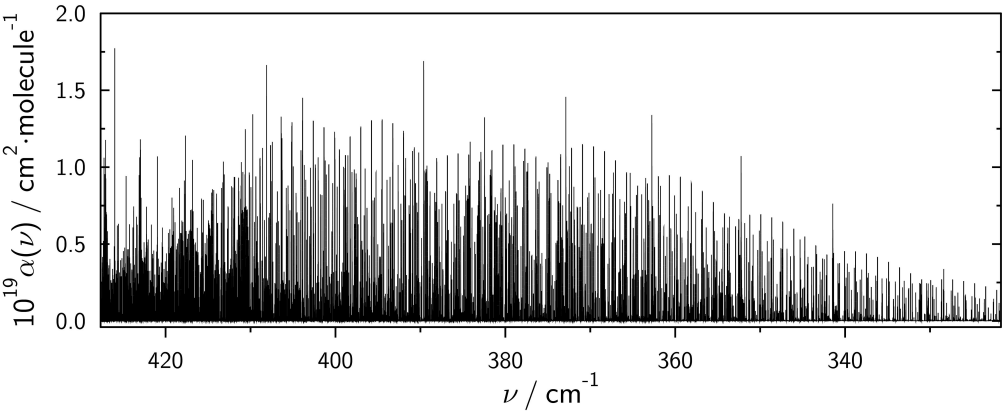

Figure S1: Calculated rovibrational spectrum of the ν_{12} band in ketenimine ($H_2C{=}C{=}NH$) at 300 K. The spectrum is obtained by convolving the calculated line intensities with a gaussian profile (FWHM = 0.002 cm).

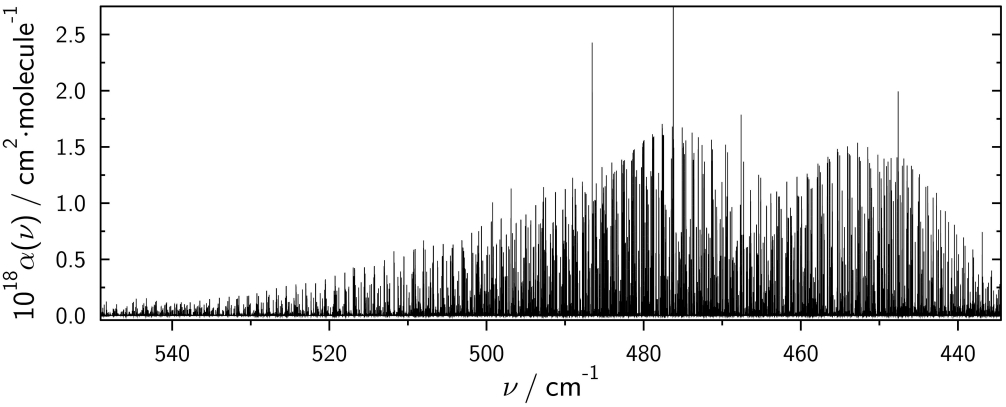

Figure S2: Calculated rovibrational spectrum of the ν_8 band in ketenimine ($H_2C{=}C{=}NH$) at 300 K. The spectrum is obtained by convolving the calculated line intensities with a gaussian profile (FWHM = 0.002 cm^{-1}).

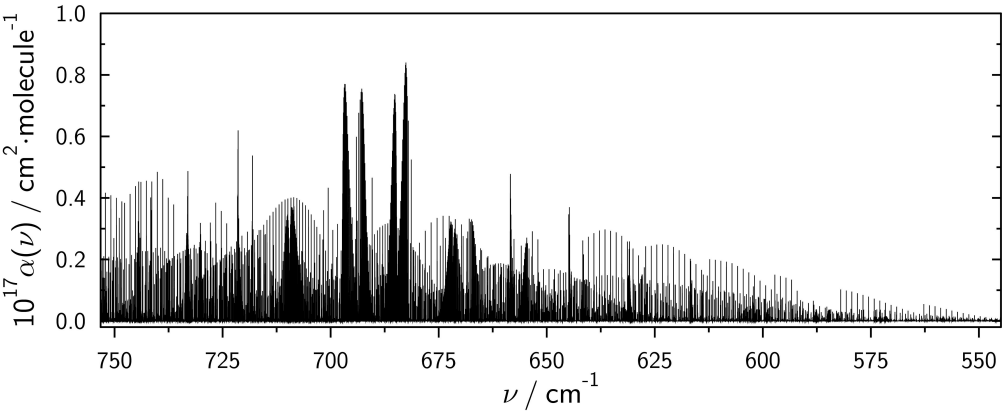

Figure S3: Calculated rovibrational spectrum of the ν_7 band in ketenimine ($H_2C{=}C{=}NH$) at 300 K. The spectrum is obtained by convolving the calculated line intensities with a gaussian profile (FWHM = 0.002 cm^{-1}).

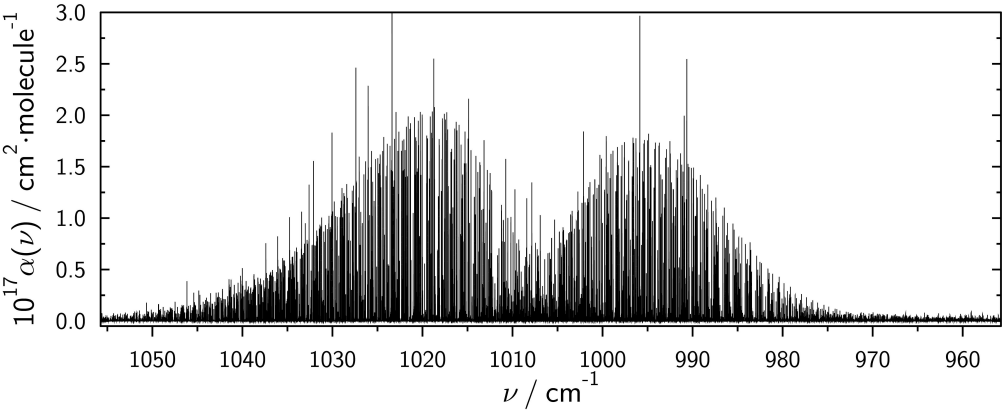

Figure S4: Calculated rovibrational spectrum of the ν_6 band in ketenimine ($H_2C{=}C{=}NH$) at 300 K. The spectrum is obtained by convolving the calculated line intensities with a gaussian profile (FWHM = 0.002 cm^{-1}).