Anharmonic DFT Study of Near-infrared Spectra of Caffeine. Vibrational Analysis of the Second Overtones and Ternary Combinations

SUPPLEMENTARY MATERIALS

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Institute of Analytical Chemistry and Radiochemistry, Leopold-Franzens University, Innrain 80/82, CCB-Center for Chemistry and Biomedicine, 6020 Innsbruck, Austria
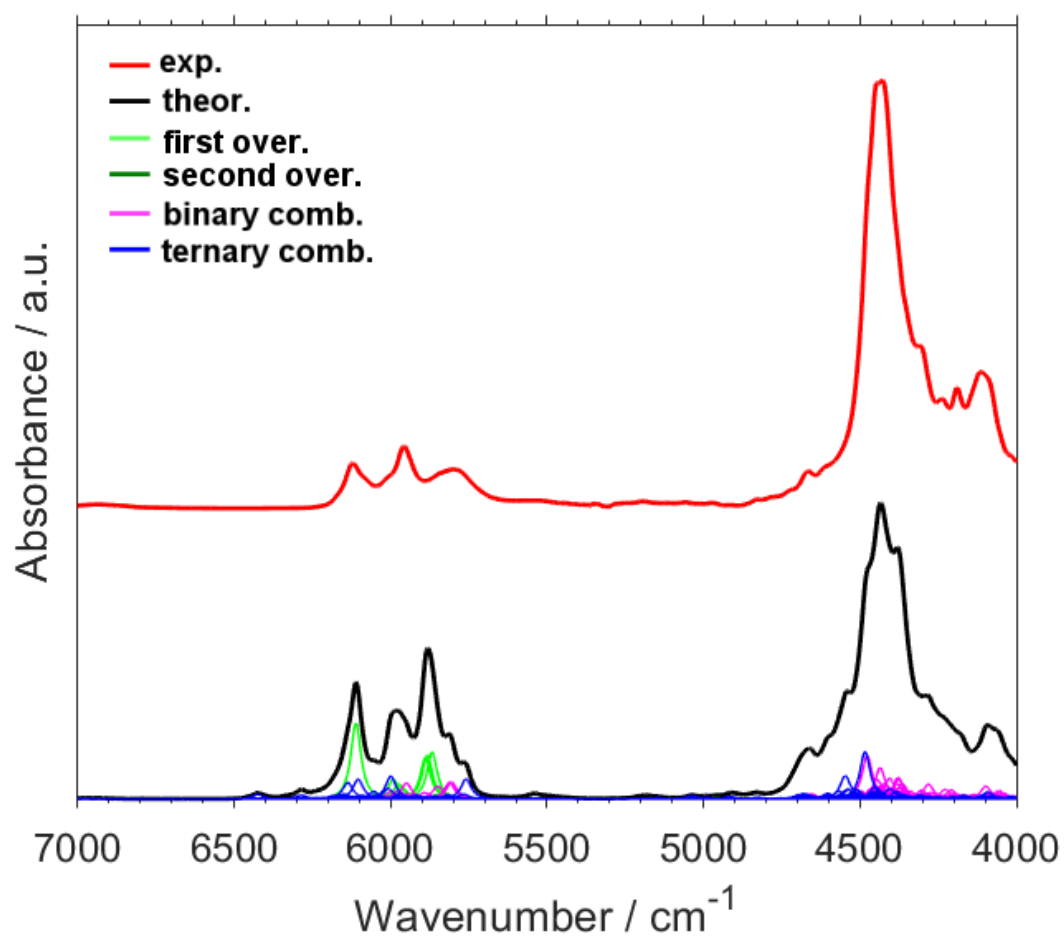
Figure S1. Experimental and calculated NIR spectra of caffeine in region 7000-4000 cm^{-1}. In addition to the theoretical lineshape, individual simulated bands are presented as well.
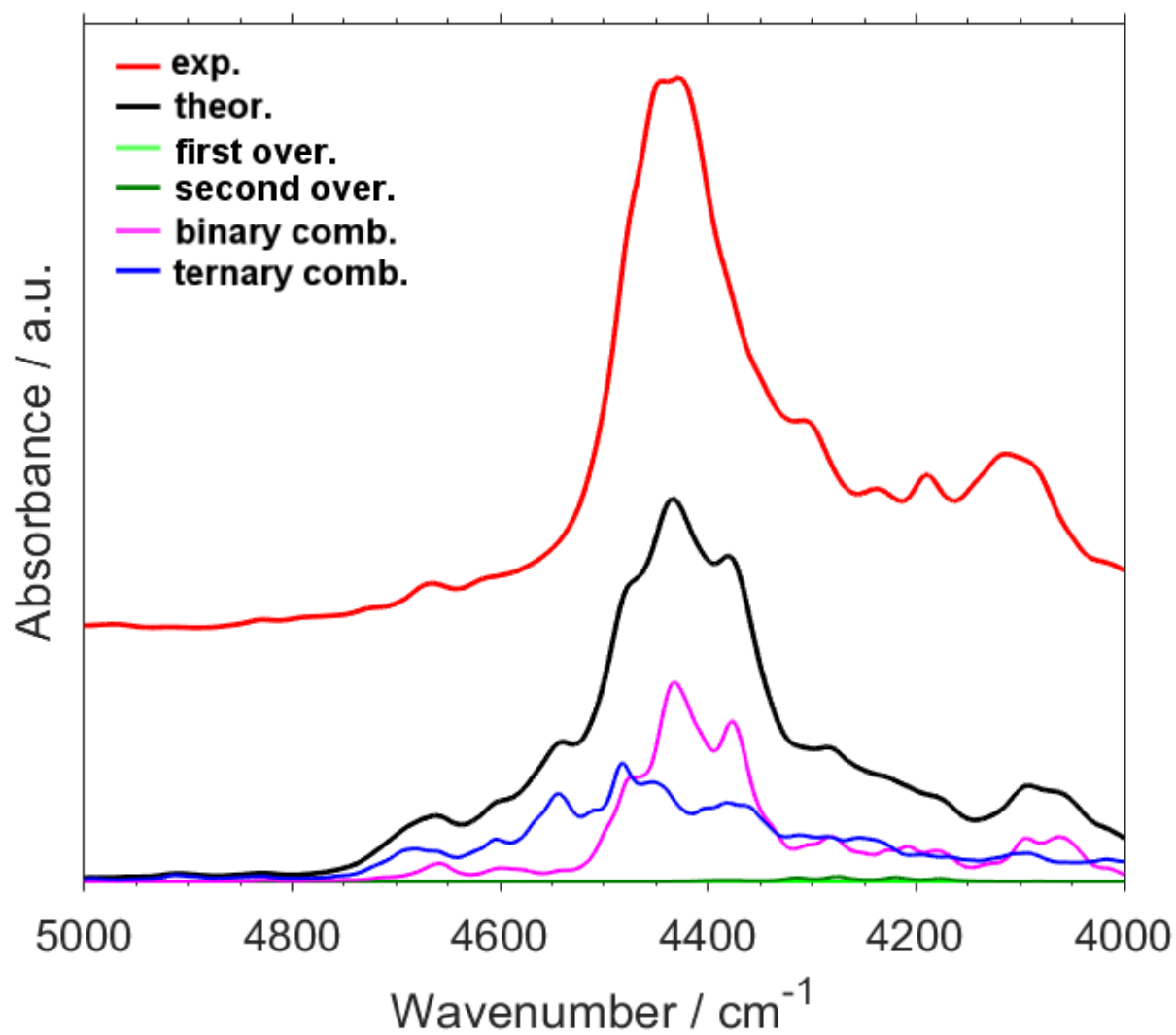
Figure S2. Experimental and calculated NIR spectra of caffeine in region 5000-4000 cm^{-1}. Theoretical lineshapes representing the summed bands of different origin are presented.
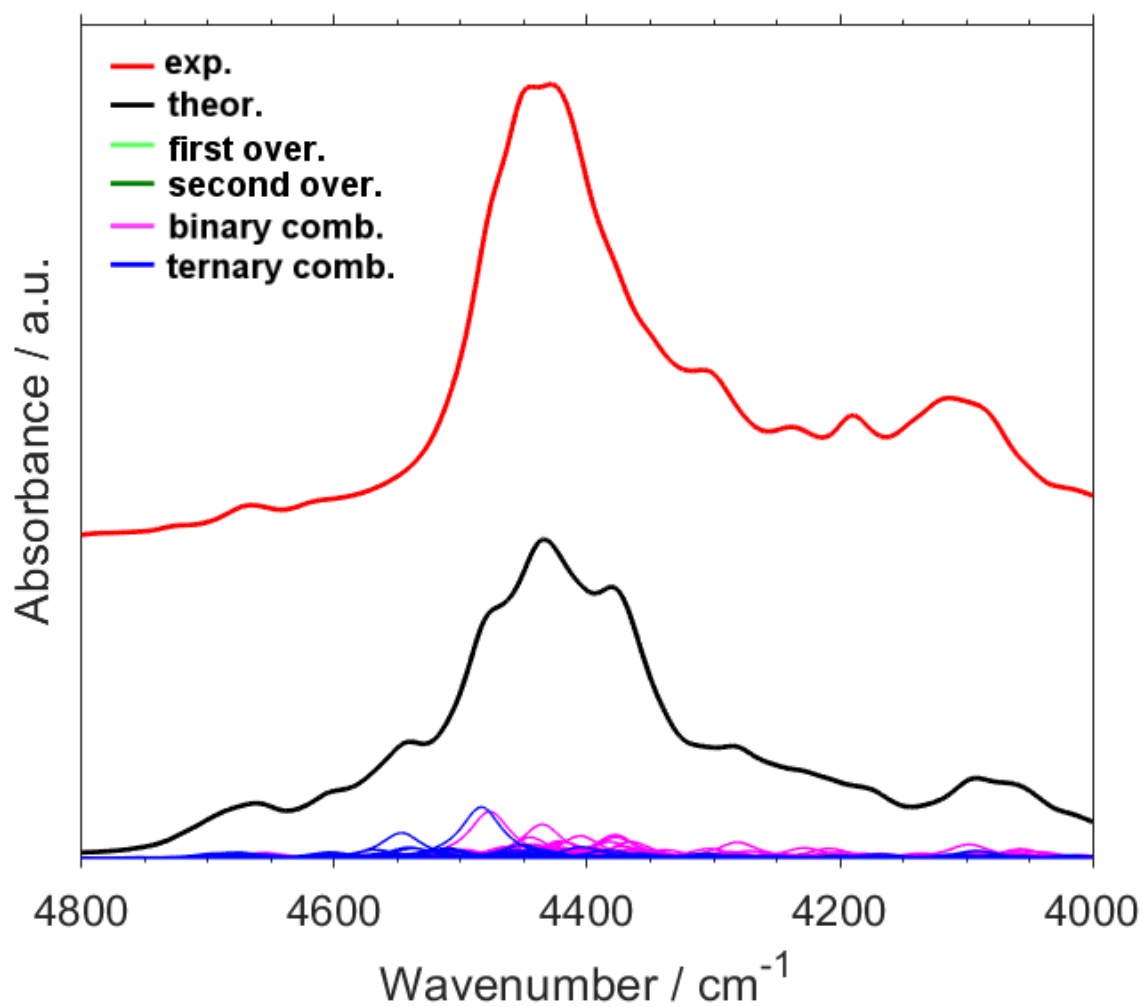
Figure S3. Experimental and calculated NIR spectra of caffeine in region 4800-4000 cm^{-1}. In addition to the theoretical lineshape, individual simulated bands are presented as well.
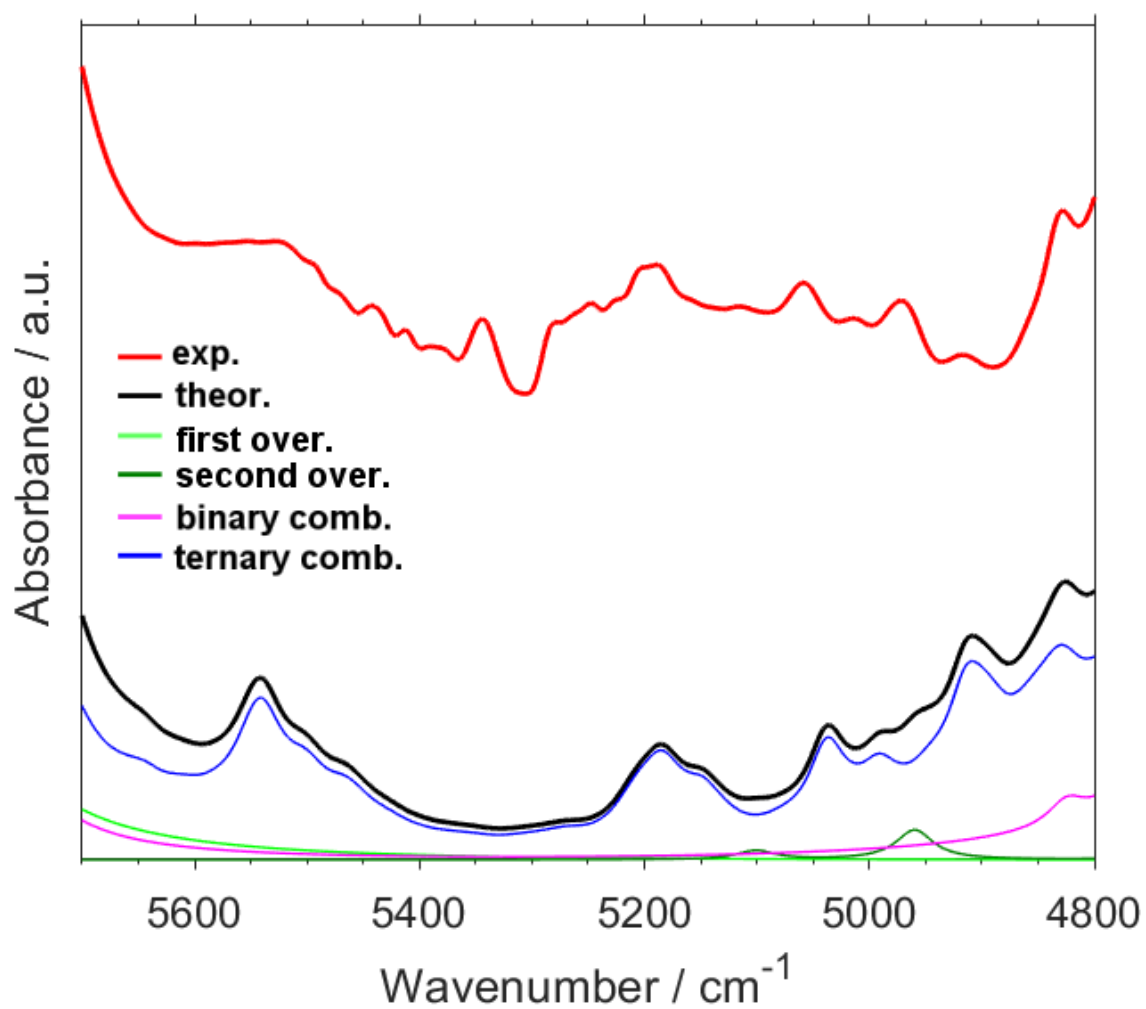
Figure S4. Experimental and calculated NIR spectra of caffeine in region 5700-4800 cm^{-1}. Theoretical lineshapes representing the summed bands of different origin are presented.
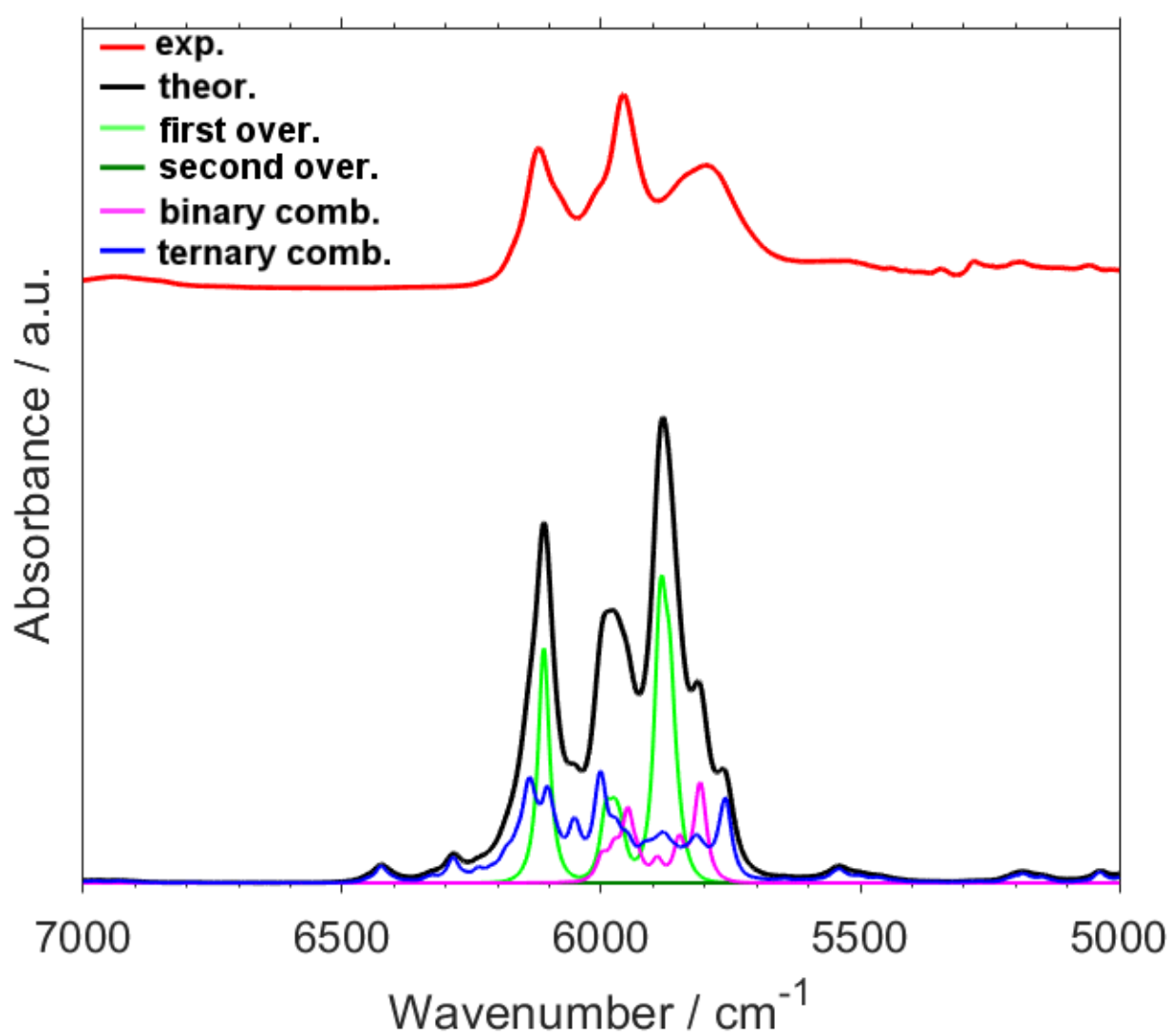
Figure S5. Experimental and calculated NIR spectra of caffeine in region 7000-5000 cm^{-1}. Theoretical lineshapes representing the summed bands of different origin are presented.
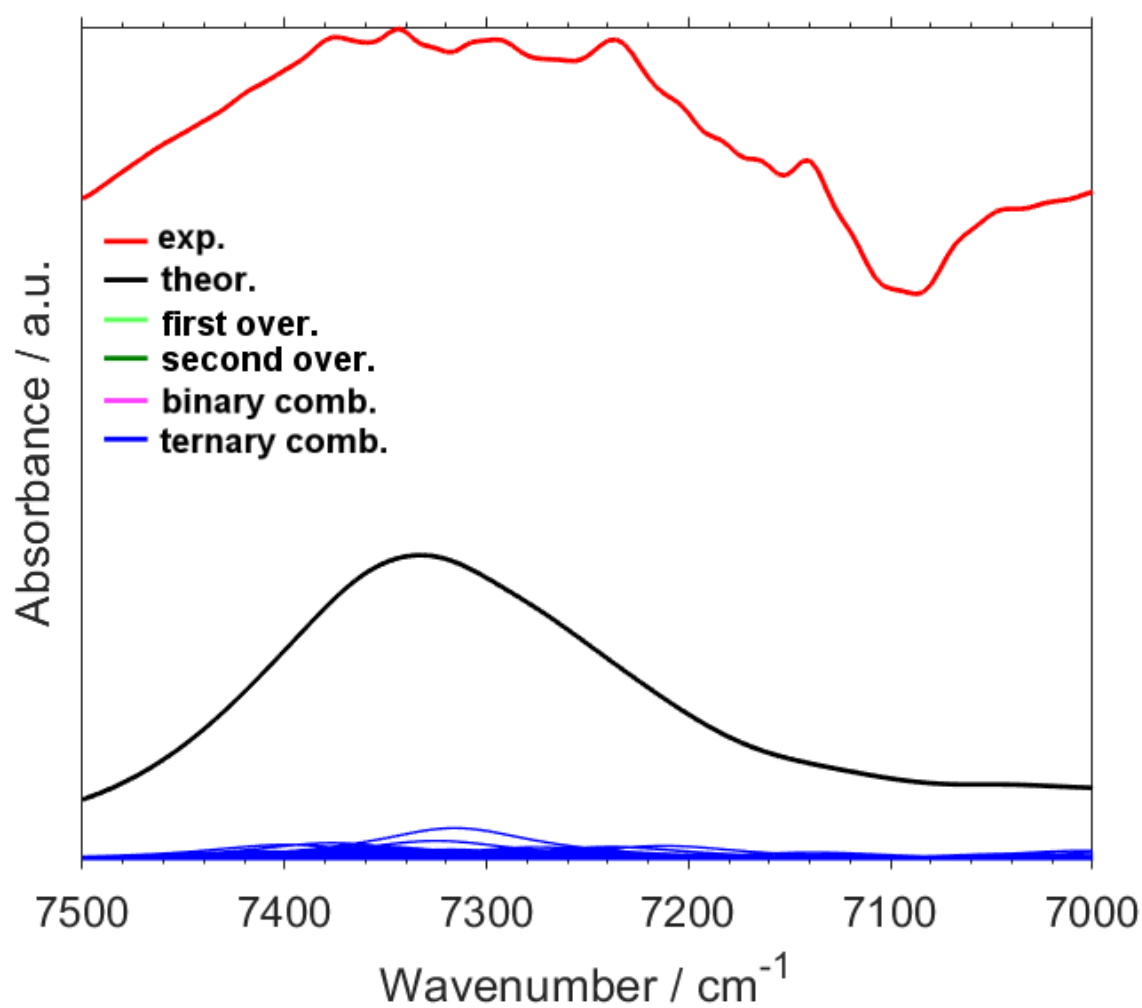
Figure S6. Experimental and calculated NIR spectra of caffeine in region 7000-5000 cm^{-1}. In addition to the theoretical lineshape, individual simulated bands are presented as well.
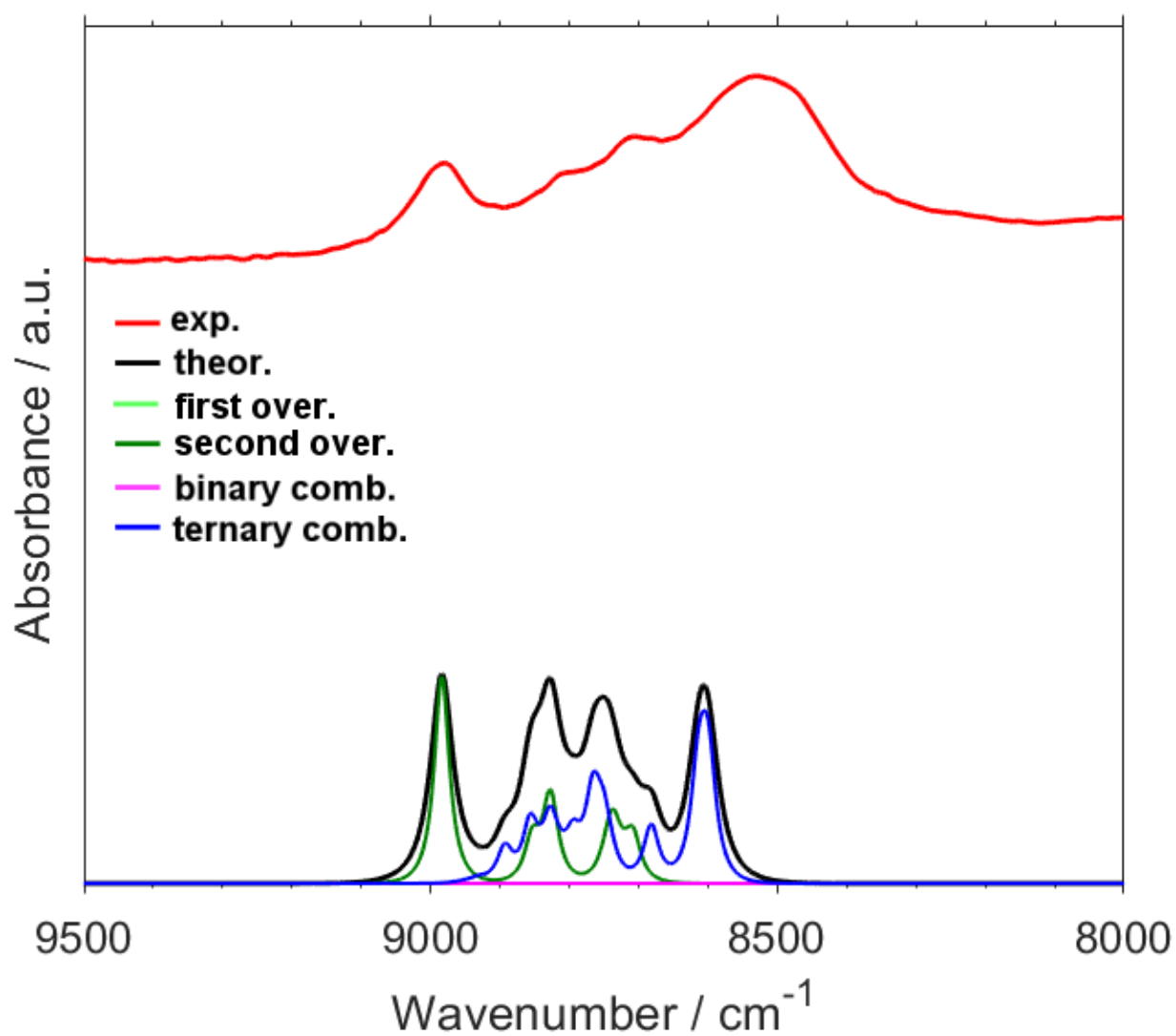
Figure S7. Experimental and calculated NIR spectra of caffeine in region 9500-8000 cm^{-1}. Theoretical lineshapes representing the summed bands of different origin are presented.

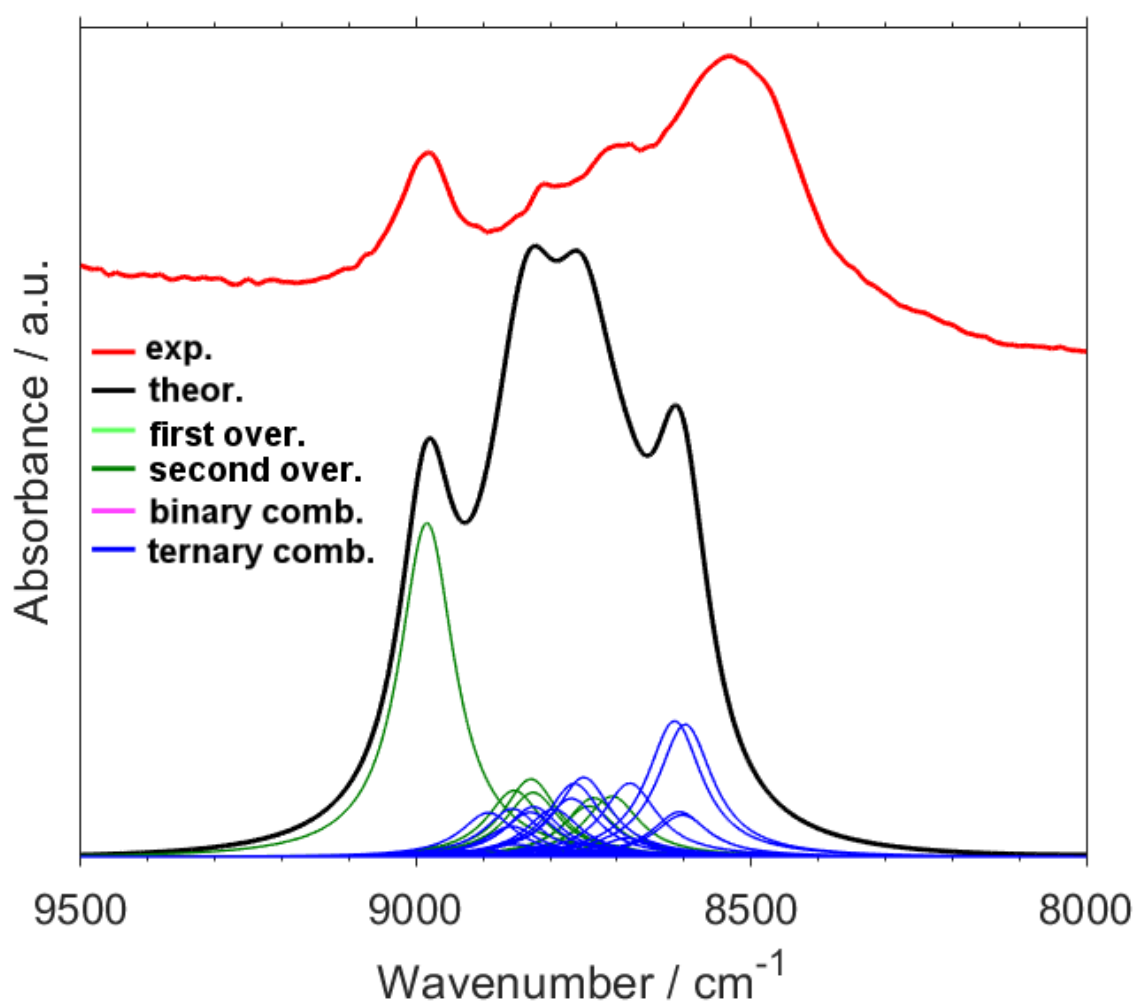**Figure S8.** Experimental and calculated NIR spectra of caffeine in region 9500-8000cm⁻¹. In addition to the theoretical lineshape, individual simulated bands are presented as well.
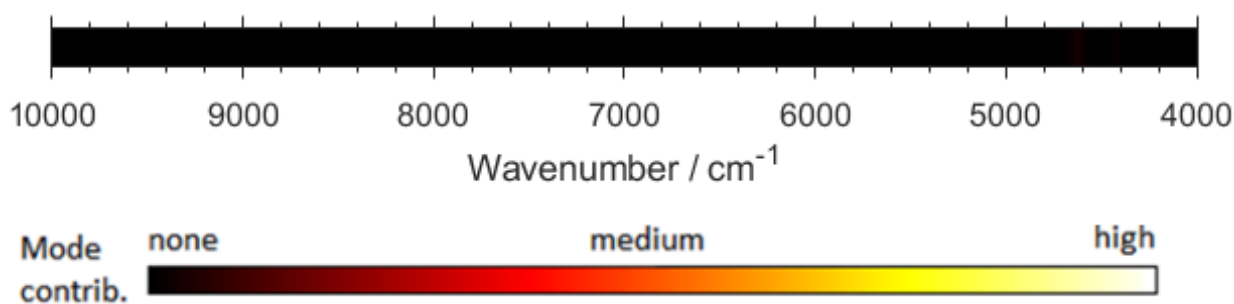

Figure S9. The calculated contributions to NIR spectrum of caffeine of C=O stretching transitions.

Funding

Acknowledgement