

Supporting information for

# Matrix-isolation and cryosolution-VCD spectra of $\alpha$ -pinene as benchmark for anharmonic vibrational spectra calculations

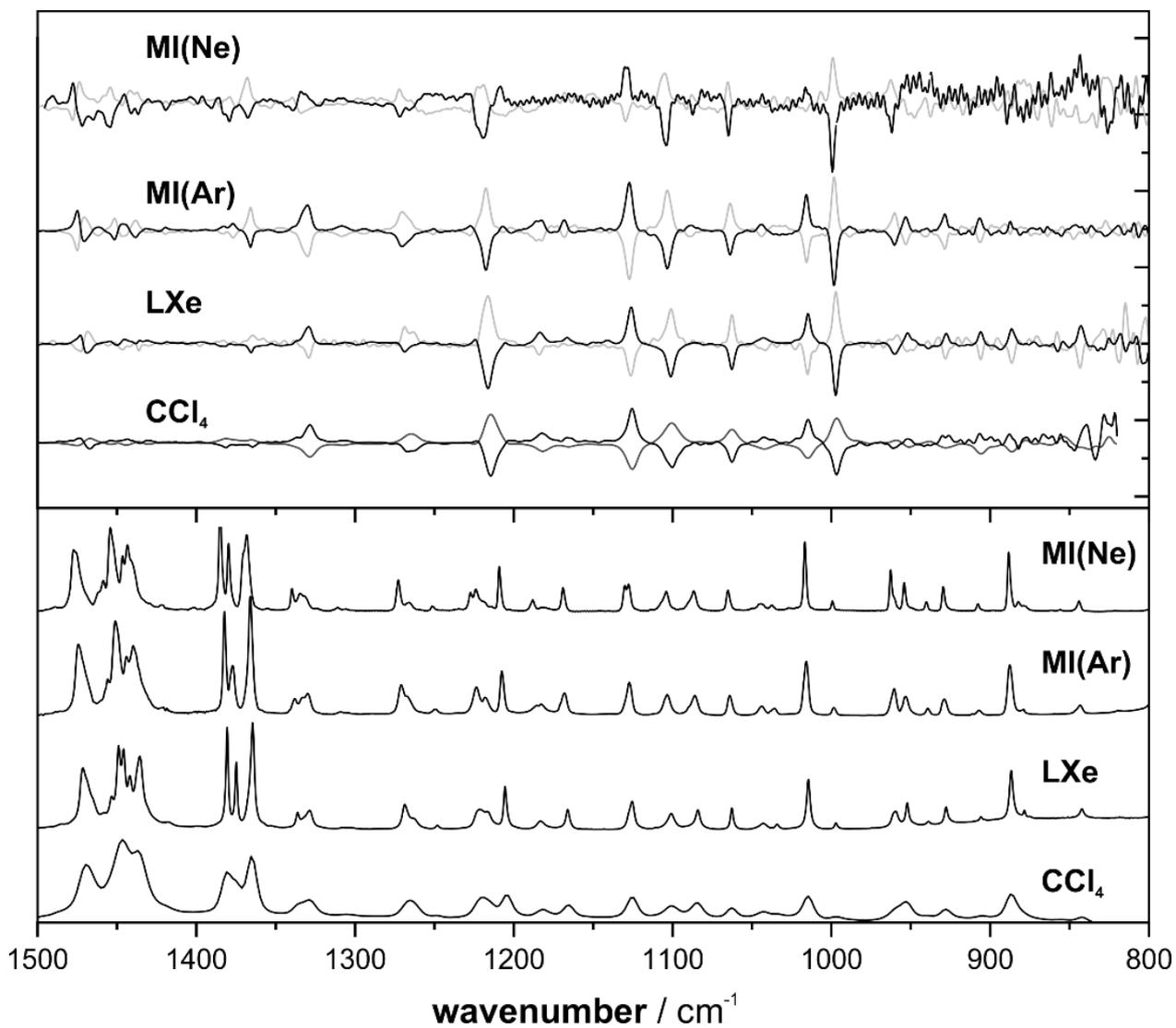
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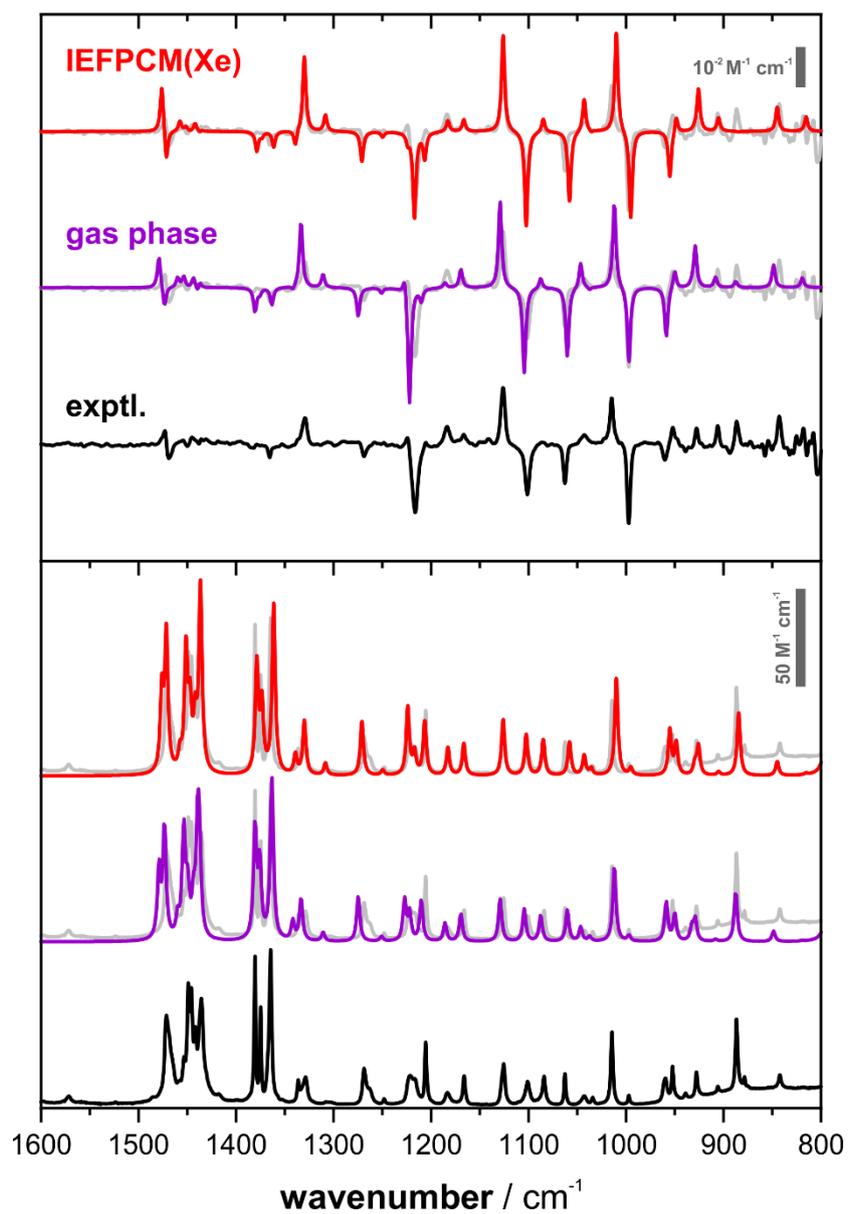
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## 1. Additional Figures

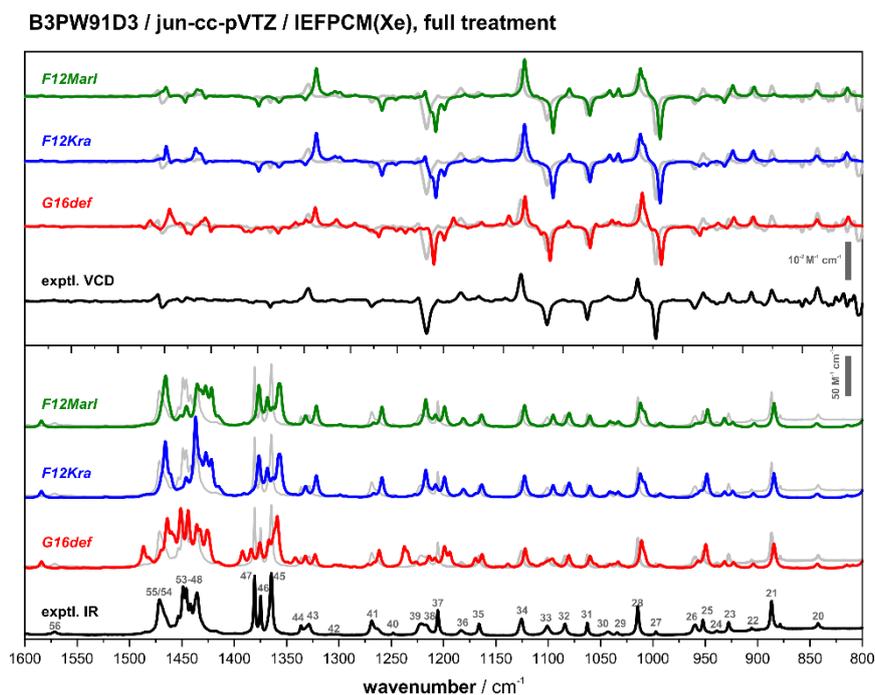


**Figure S1.** Enlarged view of the fingerprint range of the experimental spectra of  $\alpha$ -pinene.

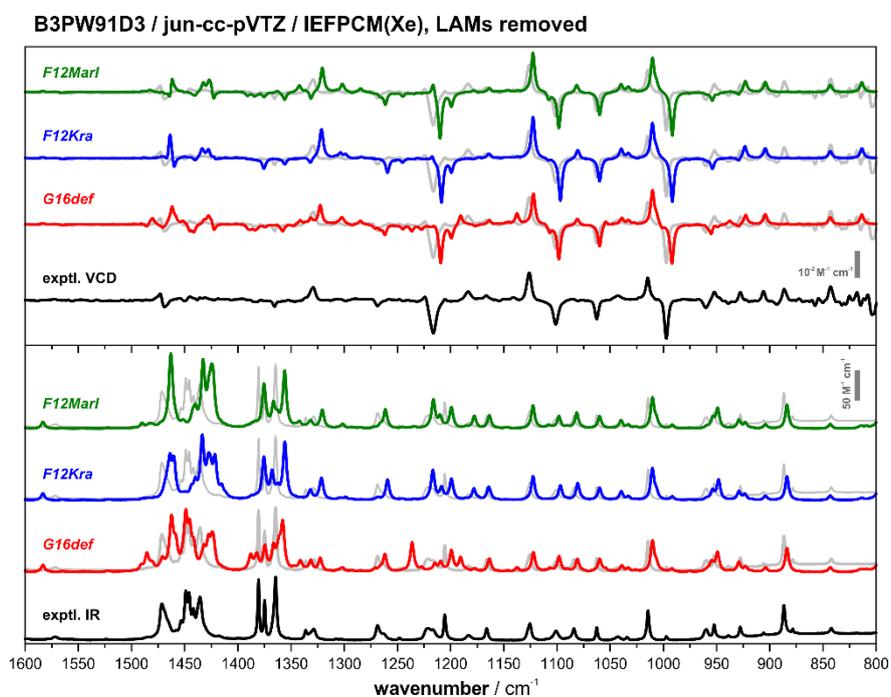


**Figure S2.** Solvent effect on the IR and VCD spectra of  $\alpha$ -pinene (B3PW91D3)

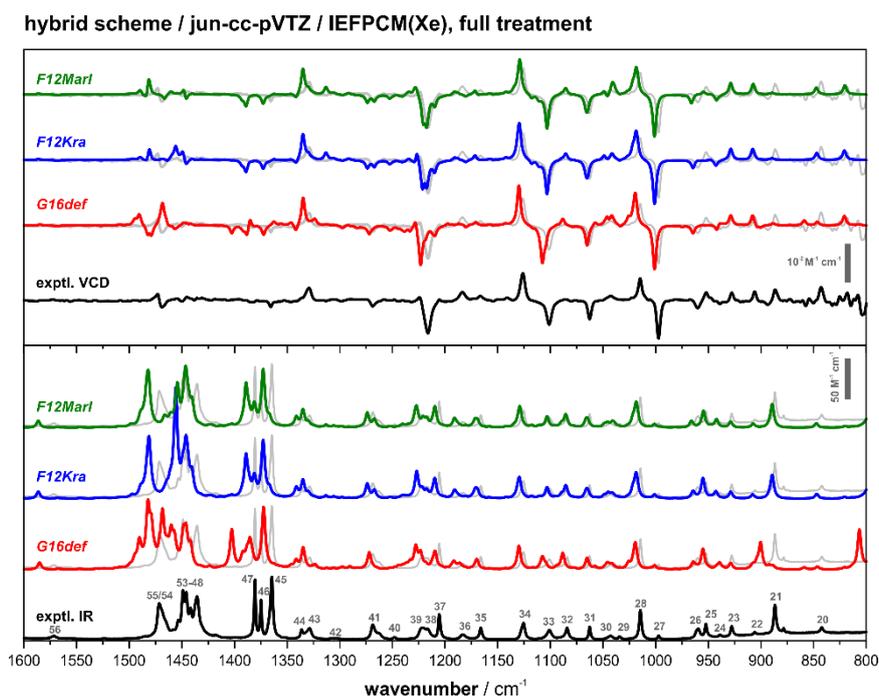
## 2. Effect of Large Amplitude Motions on Spectra of $\alpha$ -Pinene



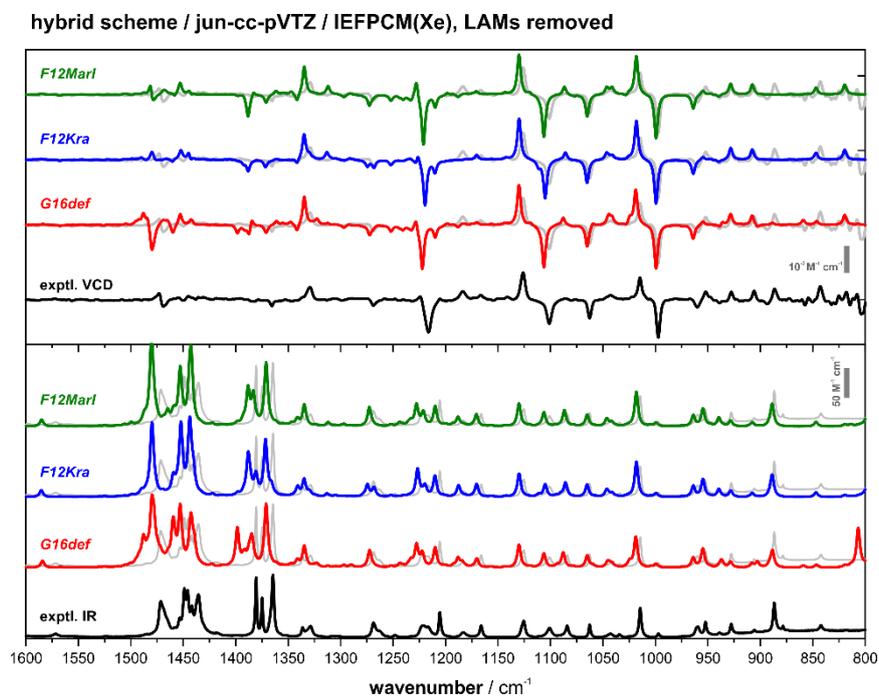
**Figure. S3.** Comparison of the experimental and calculated spectra obtained at the B3PW91D3 / jun-cc-pVTZ / IEFPCM(Xe) level of theory and considering all modes.



**Figure. S4.** Comparison of the experimental and calculated spectra obtained at the B3PW91D3 / jun-cc-pVTZ / IEF-PCM(Xe) level of theory after removal of contributions from large amplitude motions (modes 2, 4, 5).

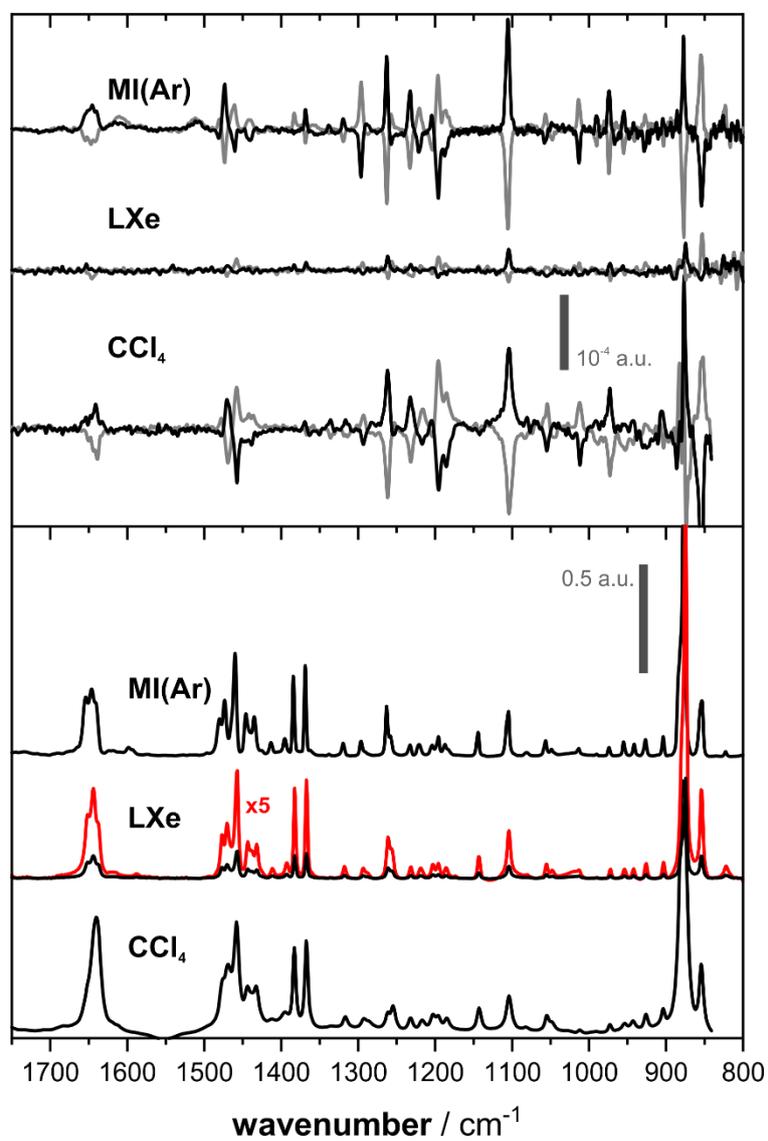


**Figure. S5.** Comparison of the experimental and calculated spectra obtained with the hybrid scheme and jun-cc-pVTZ/IEF-PCM(Xe), considering all modes.

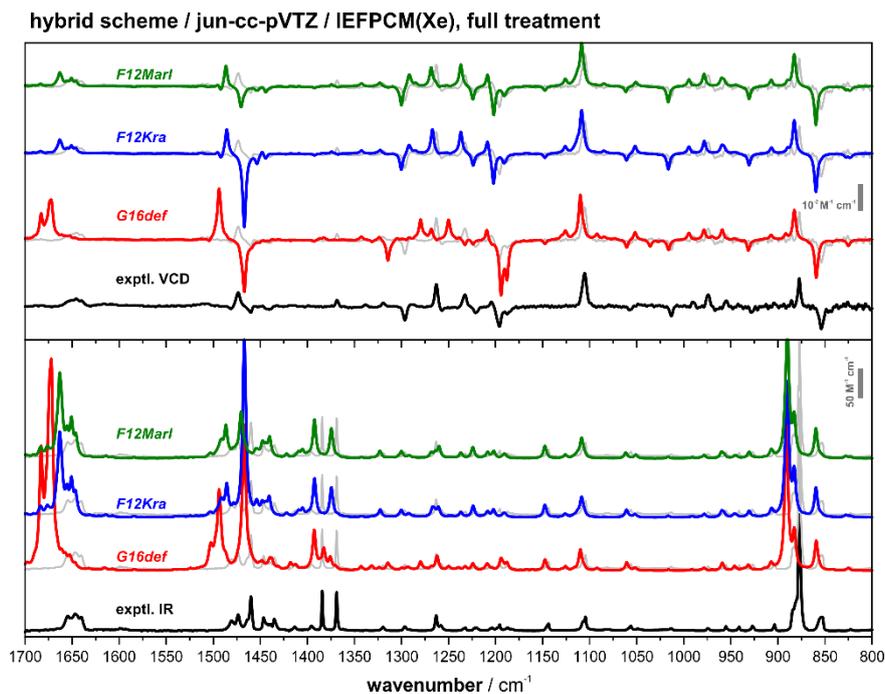


**Figure. S6.** Comparison of the experimental and calculated spectra obtained with the hybrid scheme and jun-cc-pVTZ/IEF-PCM(Xe) after removal of contributions from large amplitude motions (modes 2, 4, 5).

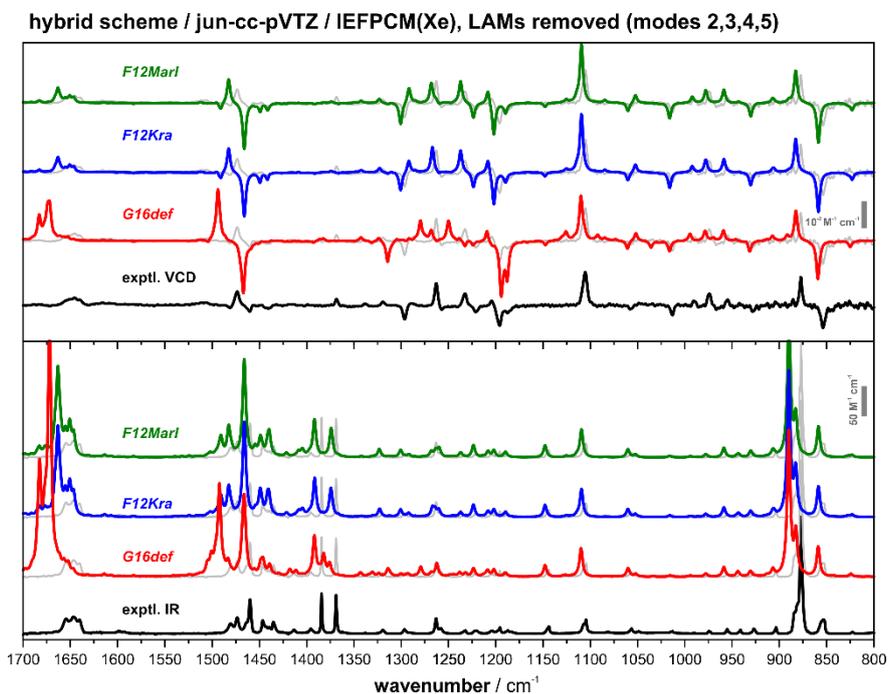
### 3. Additional Figures for $\beta$ -Pinene



**Figure S7.** Comparison of the experimental spectra of  $\beta$ -pinene in different environments.



**Figure. S8.** Comparison of the experimental and calculated spectra of  $\beta$ -pinene obtained with the hybrid scheme and jun-cc-pVTZ/IEF-PCM(Xe), considering all modes.



**Figure. S9.** Comparison of the experimental and calculated spectra of  $\beta$ -pinene obtained with the hybrid scheme and jun-cc-pVTZ/IEF-PCM(Xe) after removal of contributions from large amplitude motions (modes 2, 3, 4, 5).