

## SUPPLEMENTAL INFORMATION

### THz to far-infrared spectra of the known crystal polymorphs of Phenylalanine

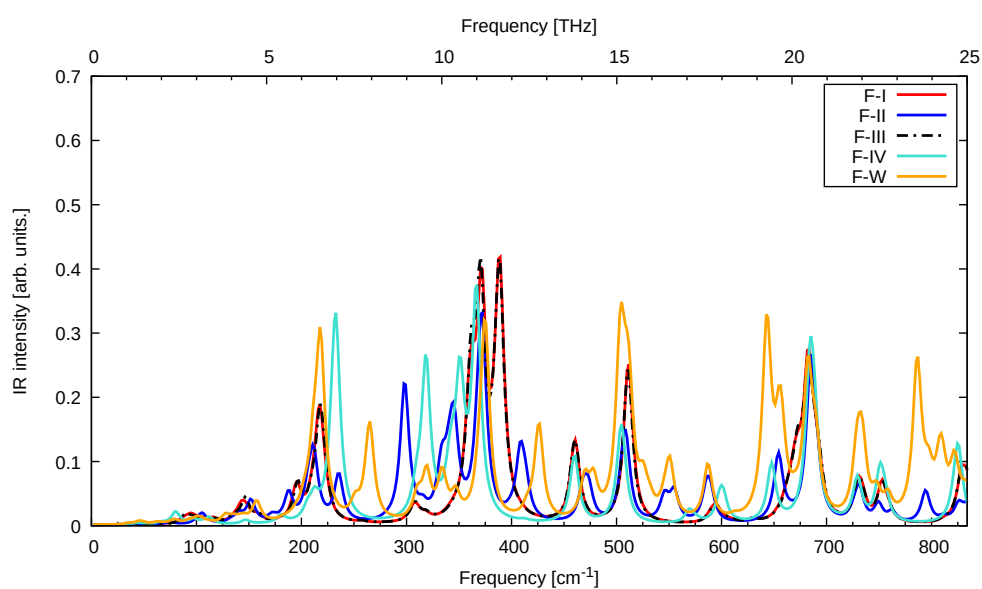
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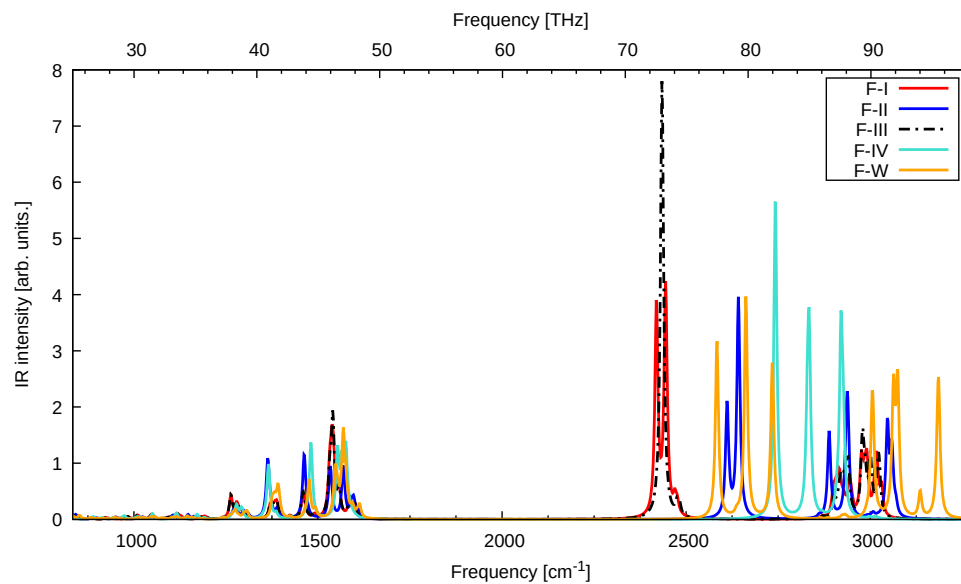
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SI Figure 1. Calculated absorption spectrum of all considered polymorphs **F-I** to **F-IV** together with the monohydrate **F-W** up to 25 THz. The intensity is normalized for the number of molecules in the simulation cell.

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SI Figure 2. Calculated absorption spectrum of all considered polymorphs **F-I** to **F-IV** together with the monohydrate **F-W** between 25 and 100 THz. The intensity is normalized for the number of molecules in the simulation cell.

theory ( <b>F-III</b> )	experiment (THz-TDS)	experiment (FTIR)	mode description
90			$\omega$ (Phe)
146			$\tau$ (Phe)
158			$\rho$ (Phe)
197			$\rho$ (Phe)
218	200		$\nu$ (O-NH <sub>3</sub> )
308			$\rho$ (CH <sub>2</sub> )
371	370	366	$\rho$ (NH <sub>3</sub> )
388		374	$\rho$ (NH <sub>3</sub> )
461	470	470	$\gamma$ (Ph)
512	526	526	$\gamma$ (Ph)
595	606	606	$\tau$ (NH <sub>3</sub> )
683	700	700	$\gamma$ (Ph)
731	747	747	$\omega$ (H-Ph)
753	780	780	$\gamma$ (CO <sub>2</sub> )
830	853	850	$\omega$ (H-Ph)
886	914	914	$\tau$ (H-Ph)
923		951	$\delta$ (CH-NH <sub>3</sub> )
983		1005	$\omega$ (NH <sub>3</sub> )
1010		1026	$\nu$ (Ph)
1049		1076	$\nu$ (Ph)
1096		1131	$\nu$ (C-N)
1117		1155	$\omega$ (NH <sub>3</sub> )
1192		1227	$\nu$ (C-C)
1263		1309	$\nu$ (C-O)
1280		1322	$\nu$ (C-C)

SI Table I. Vibrational frequencies of Phenylalanine up to 1300 cm<sup>-1</sup> from the DFT calculations for conformer **F-III** and the two experimental techniques (THz-TDS, FTIR) used in this article in units of wavenumbers (cm<sup>-1</sup>). The abbreviations in the approximate mode description stand for:  $\tau$ : twisting,  $\rho$ : rocking,  $\omega$ : wagging,  $\nu$ : stretching,  $\delta$ : scissoring,  $\gamma$ : out-of-plane motion, Ph: phenyl ring, Phe: Phenylalanine.