

Supporting Information for

**Differences in the IR Methylene Rocking Bands between the Crystalline Fatty Acids  
and n-Alkanes: Frequencies, Intensities, and Correlation Splitting**

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Figures 1S, 2S and 3S

Figure Captions: (1S) Observed IR intensities of the rocking mode bands for the C-form fatty acids and the orthorhombic n-alkane n-C<sub>21</sub> at 10 K plotted against the phase difference. The *k*-odd and *k*-even bands are represented by open and filled symbols, respectively. The values of the intensities are on a common scale. The methods used to scale the spectra are described in the text.

(2S) The rocking fraction of the vibrational eigenfunction based on the fraction of potential energy from methylene rocking plotted against phase difference.

(3S) Observed and calculated dipole moment derivatives for the rocking bands of n-C<sub>21</sub> at 10 K, plotted against phase difference. ○ represents observed values; ■ and ● represent respectively values calculated with  $M_0$ ,  $M_1$ , and  $M_m$  equal to 1, and with  $M_0 = 1$  and  $M_1 = M_m = 1.63$ .





