

## Study of Disorder in Different Phases of Tetratriacontane and a Binary Alkane Mixture, Using Vibrational Spectroscopy

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Raman spectroscopy has been used to investigate the monoclinic crystal  $\rightarrow$  rotator  $\rightarrow$  melt phase transitions in  $n$ -C<sub>34</sub>H<sub>70</sub>, for both real-time heating and cooling runs. Changes in band intensity and frequency in the CH<sub>2</sub> bending, CH<sub>2</sub> twisting, skeletal C–C stretching, and CH<sub>3</sub> rocking regions revealed both transitions, particularly when using band components related to gauche bonds. In the room temperature infrared spectrum, the CH<sub>2</sub> rocking–twisting and CH<sub>2</sub> wagging progressions were observed and indexed for  $n$ -C<sub>34</sub>H<sub>70</sub> and a 2:1 (w/w) mixture of C<sub>34</sub>H<sub>70</sub> and C<sub>36</sub>D<sub>74</sub>. This led to best estimates for the all-trans crystal core in both cases of 33 to 34 carbon atoms, indicating that the core corresponds to almost the whole of the C<sub>34</sub>H<sub>70</sub> molecule.