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Modeling the liquid-solid transition in saturated triglycerides¹ C.B. HANNA, Boise State University, D.A. PINK, A.J. MACDONALD, K. THILLAINADARAJAH, St. Francis Xavier University, R. CORKERY, Ytkemiska Institute, D. ROUSSEAU, Ryerson University — Corkery et al. have proposed that the high-temperature state of the triglyceride trilaurin (TL) is a Y-conformer, in which the three hydrocarbon chains are dynamically twisted with an average angle of $\sim 120^{\circ}$ between them. Using computer simulations, we first show that the high-temperature state is indeed the Y conformation. We then develop a theory of the liquid-solid transition of this system, in which TL molecules are in a chair (h) conformation, with extended, possibly all-trans, chains at low-temperatures, and are in a Y conformation in the liquid phase at temperatures higher than the transition temperature, $T^* \approx 319 K$. We map this "h-Y model" onto an Ising model in a temperature-dependent field, perform a mean-field approximation, and calculate the transition enthalpy, which is in good agreement with experiment. We also predict the temperature-dependence of the 1132 $\rm cm^{-1}$ Raman band. Our results support the proposal that the liquid state is made up of molecules in the Y conformation.

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