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Spectroscopically Deciphering the Difference in Stabilizing Interactions of Poly(lactic acid) Polymorphs KAORU AOU, XIGUO ZENG, SHAW LING HSU, University of Massachusetts Amherst — Poly(lactic acid), or PLA, crystals have been difficult to analyze, owing to uncertainties in the actual atomic placements. Our previous studies indicate that the stereocomplex has a melting enthalpy of 129 J/g in comparison to 99 J/g for the alpha crystal. The enthalpic interaction is thus responsible for the stereocomplex thermal stability. Here we use spectroscopy to complement published atomic coordinate information to better understand the origins of PLA crystal stability. Spectroscopic analysis shows that methyl-related vibrations change dramatically as the alpha crystal unit cell thermally shrink, whereas the stereocomplex vibrations were almost unchanged. Indeed the closest $(CH_2)H...H(H_2C)$ distances in the alpha crystals are shorter than that in the stereocomplex crystal indicating that methyl-methyl interactions have a larger impact on alpha crystal stability. We also performed energy calculations on the alpha and stereocomplex structures from which we find the relative contribution of van der Waals and electrostatic interactions in the two crystals.

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