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Experimental and Theoretical Study of Raman Spectra of Polyisobutylene¹ PRADEEP KUMAR, JAMIE MESSMAN, BRIAN ANNIS, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, BOBBY SUMPTER, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, CHARLES FEIGERLE, Department of Chemistry, University of Tennessee, Knoxville TN 37996 — The effects of strain induced partial crystallization, partial deuteration, molecular weight and temperature on the Raman spectra of polyisobutylene (PIB) are determined. The Raman spectra of stretched PIB are correlated with the development of crystallinity as found by X-ray diffraction. One of the spectral regions altered by the stretching is in the vicinity of 200 cm^{-1} which is often attributed to disordered longitudinal modes. The results are compared with spectra computed from 1st principles electronic structure calculations using Density Functional Theory and Hartree-Fock approaches on model PIB systems.

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