

界面の振動分光学

Vibrational spectroscopy at an interface

京都大学 化学研究所 分子環境解析化学研究領域 荒木 泰介

研究成果概要

Geometry optimization and the calculation of harmonic vibrational frequencies were conducted using density functional theory empirical dispersion corrections (DFT-D) method. Gaussian 16 program was used, and calculation was conducted on a molecular model of $n\text{-C}_{20}\text{F}_{42}$. The functional was set to $\omega\text{B97X-D}$ including the effects of dispersion interactions. For a basis, def2TZVP-P was used which is an advanced model of TZVP, and this basis was already be confirmed its suitability for conformational analysis on perfluoroalkyl chain.

As a result, I have found that the Longitudinal Acoustic Mode which is commonly known as LAM (Song et al, 1991) can be clearly observed in calculated Raman spectrum (FIG. 1), and its vibrational motion can be readily derived from the result (FIG. 2).

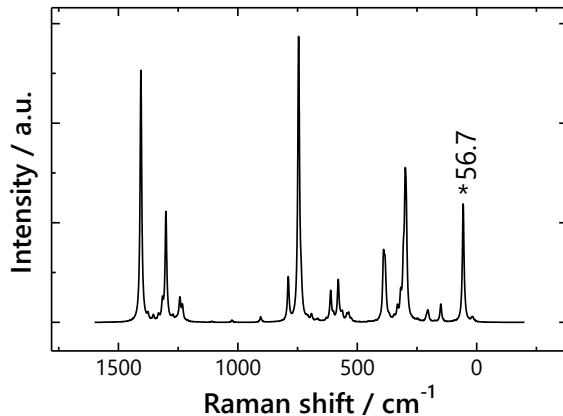


FIG. 2 Calculated Raman spectrum of $n\text{-C}_{20}\text{F}_{42}$. The labeled band appearing 56.7cm^{-1} is assigned as the LAM.

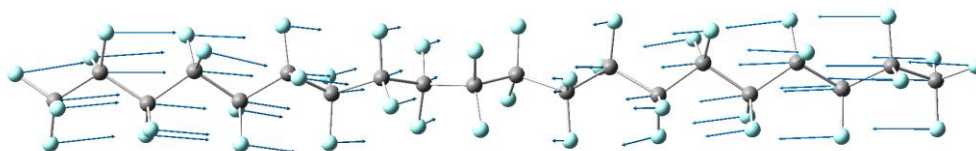


FIG. 1 Vibrational motion of LAM derived from the calculation conducted using $\omega\text{B97X-D/def2TZVP-P}$.