

NOBLE GAS ATOM AS A QUANTUM OSCILLATOR IN THE FULLERENE C₆₀: THZ STUDY

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We use THz spectroscopy to study the interaction between noble gas atoms (³He, ⁴He, Ne, Ar, Kr) and the fullerene cage. The temperature dependence of the THz absorption spectra of powdered samples were measured between 5 to 300K. The translational motion of the atom quantized by the confining potential of C₆₀ defines the THz absorption spectrum. The spectra of the He isotopes exhibit clearly resolved THz peaks at high temperatures, indicating that the potential energy function for the encapsulated atom is anharmonic.^{1,2} Other studied atoms display one broad peak at elevated temperatures, which also indicates the potential's anharmonicity. We fitted the THz absorption spectra with a three-dimensional anharmonic oscillator model including translation-induced dipole moment. We found that the harmonic potential term increases with the size of the noble gas atom, but the helium atom demonstrated the most anharmonic behavior. The empirical Lennard-Jones potentials calculated with parameters of Pang and Brisse³ are in good agreement with the experimentally derived potential functions. Our results are a testbed to verify other methods of quantum chemistry calculations.

Reference

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