

QUANTIZED TRANSLATIONAL MOTION OF ^3He AND ^4He ATOMS IN He@C_{60} ENDOFULLERENE

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We studied the translational motion of He atom trapped inside the molecular cage of C_{60} molecule using infrared (IR) spectroscopy. The T dependence of the IR absorption spectra of $^3\text{He@C}_{60}$ and $^4\text{He@C}_{60}$ powder samples was measured between 5 and 300K. At the lowest T, a single absorption line was observed at 81 cm^{-1} (97 cm^{-1} for ^3He), but as the T increased seven new lines appeared above the first transition (five new lines for ^3He). We fitted the IR spectra with an anharmonic spherical oscillator model and assumed a rigid C_{60} cage. The line frequencies and intensities were reproduced with the harmonic (V_2R^2), anharmonic (V_4R^4), (V_4R^6) potentials and the induced dipole moment (A_1R) terms, where R is the displacement of the He atom from the C_{60} cage center. The fit gave equal, within the error bars, potential and dipole parameters for $^3\text{He@C}_{60}$ and $^4\text{He@C}_{60}$. The translational energies will be compared to the C_{60} encapsulated translational energies of H_2 [1], HD , D_2 [2], HF [3], and H_2O [4]. Our results are the test bed of theories describing the interaction of inert gases with carbon surfaces.

References

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