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The Raman Spectroscopy of Ionic Liquids

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Abstract

Raman and infrared spectra were recorded for the ionic liquids $[\text{CH}_3\text{N}(\text{C}_4\text{H}_8)\text{Bu}]^+[(\text{F}_3\text{CSO}_2)_2\text{N}]^-$, $[\text{Et}_3\text{NH}]^+[(\text{octyl})\text{PO}_2\text{H}]^-$, $[\text{Bu}_4\text{N}]^+[(\text{hexyl})\text{PO}_2\text{H}]^-$, and $[\text{Bu}_4\text{P}]^+[(\text{octyl})_2\text{PO}_2]^-$ and was compared to spectra calculated by Gaussian 03 using the density functional theory method B3LYP. The experimental and calculated spectra were found to be very similar, indicating that no underlying anomalous effects were perturbing the vibrational modes. The peaks of the experimental and calculated Raman and infrared spectra were found to be broad and intertwined, because of the close proximity of numerous vibrational bands.

The differential and absolute scattering cross sections of selected bands of the ionic liquids were determined using a method of comparing the area of the ionic liquid's peak to standards of known cross section (cyclohexane, carbon tetrachloride, benzene, dichloromethane, and acetonitrile). Differential and absolute cross sections were determined experimentally at wavelengths 416 nm, 487 nm, 514 nm, 532 nm and 633 nm. A-term plots were constructed with these results to obtain the coupling constant and the effective excited state energy. These parameters allowed the calculation of the differential and absolute scattering cross sections at any wavelength.

This project is the first in a series of investigations to determine the electron transfer rate of ionic liquids and determine their suitability as materials in new devices.

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