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Effect of cation symmetry on the low-frequency spectra of imidazolium ionic liquids: OKE and Raman spectroscopic measurements and DFT calculations

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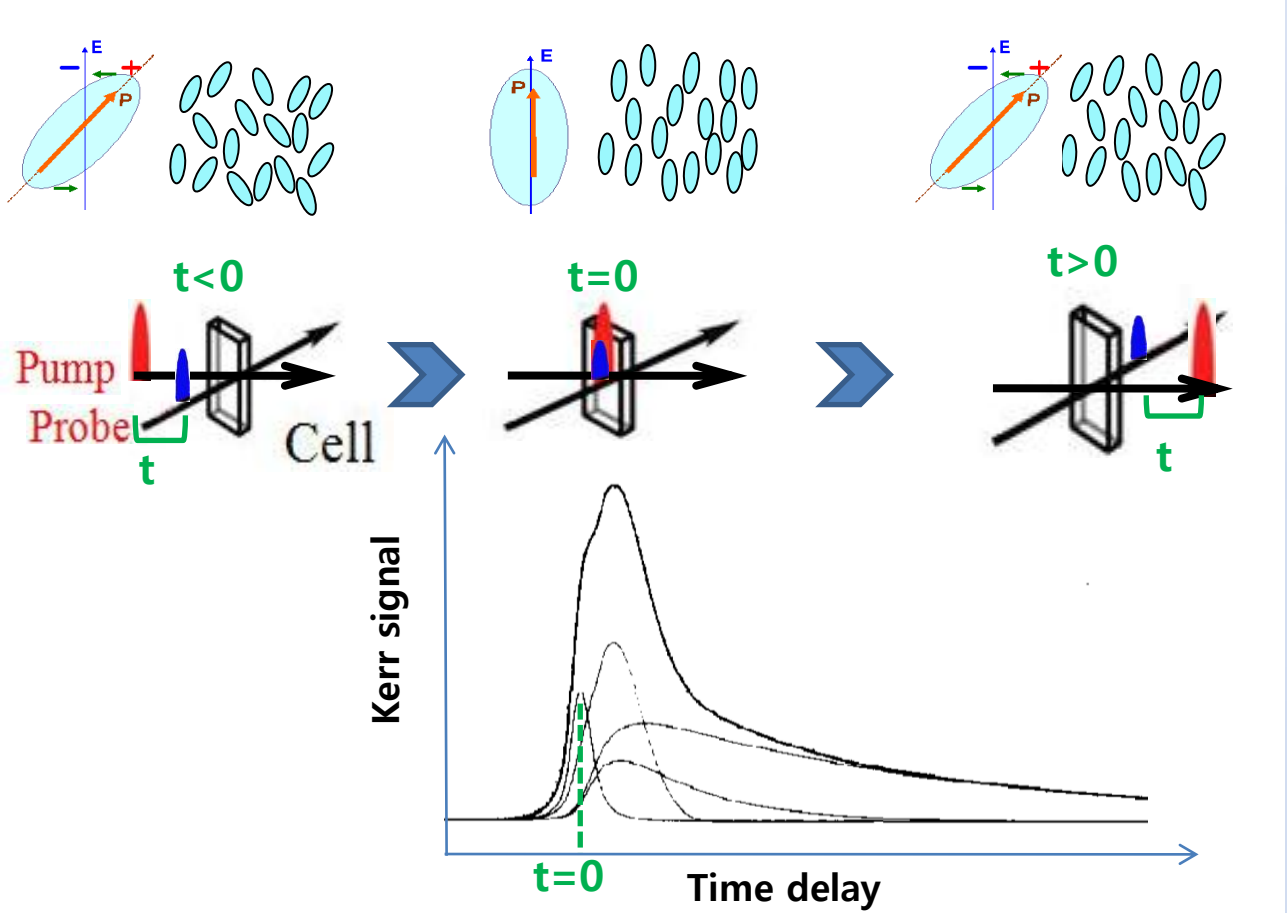
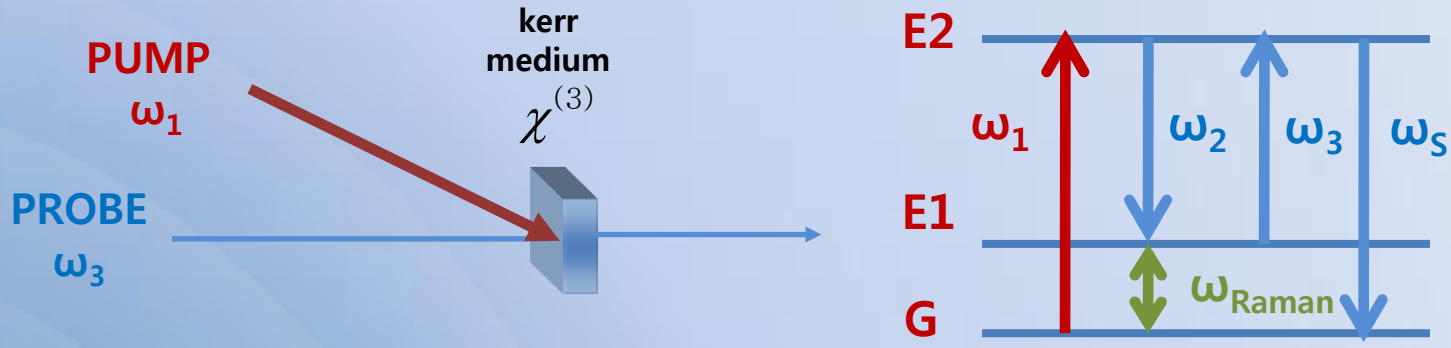
Principle of optical kerr effect



http://pchem2.s.chiba-u.ac.jp/chem/lab/shirotalab/kerr-eng.html

OHD-RIKE and DFT(density functional theory)

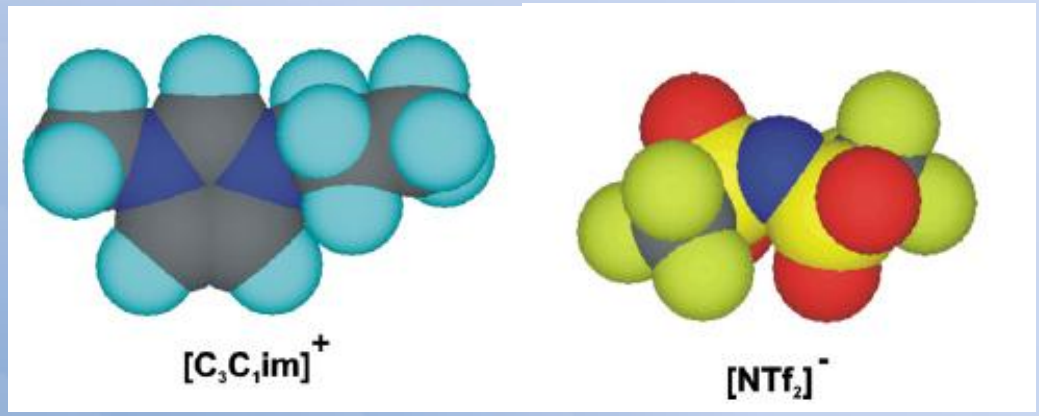
- OHD-RIKE



- DFT

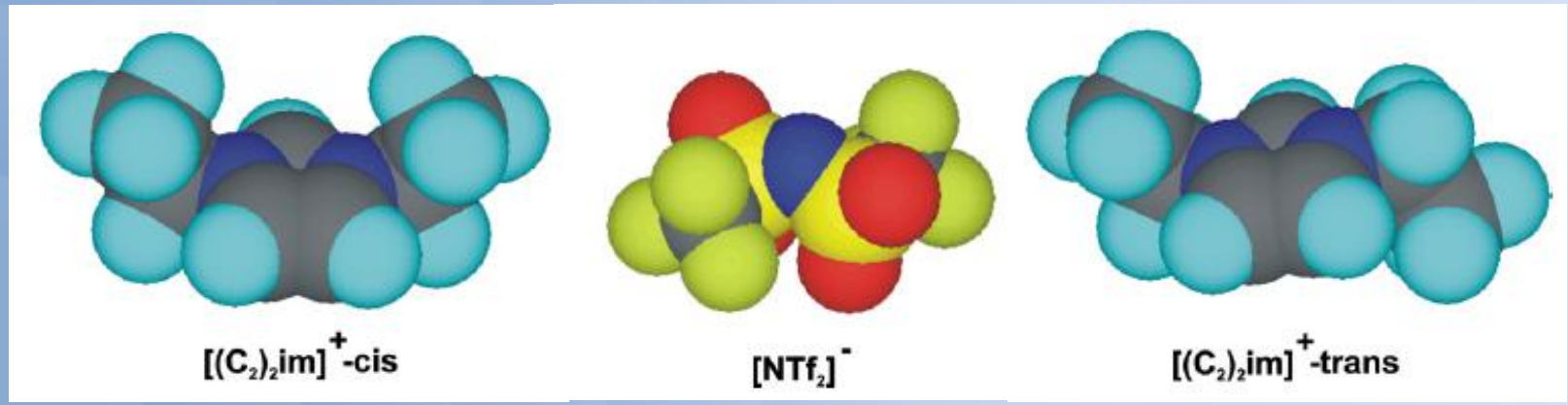
Quantum mechanical modeling method used in physics and chemistry to investigate the electronic structure (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases.

Sample



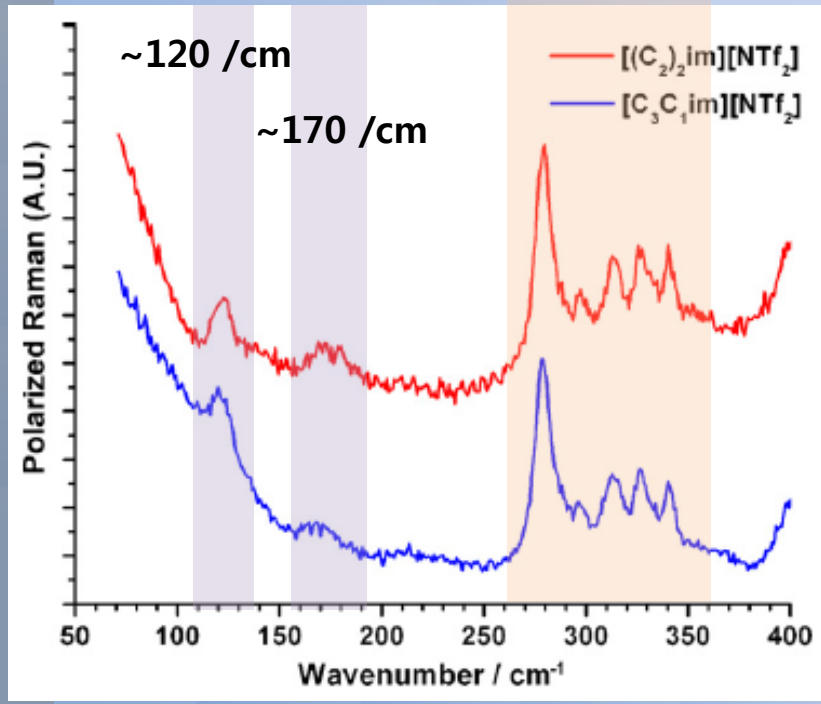
$[C_3C_1im]^+[NTf_2]$

$[(C_2)_2im]^+$ (-trans and -cis) $[NTf_2]$

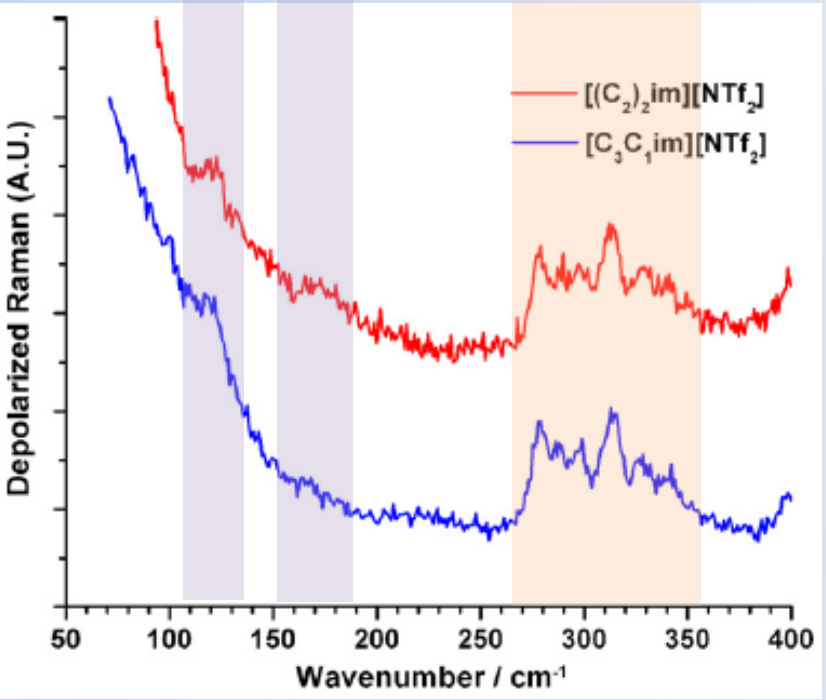


Raman Spectra

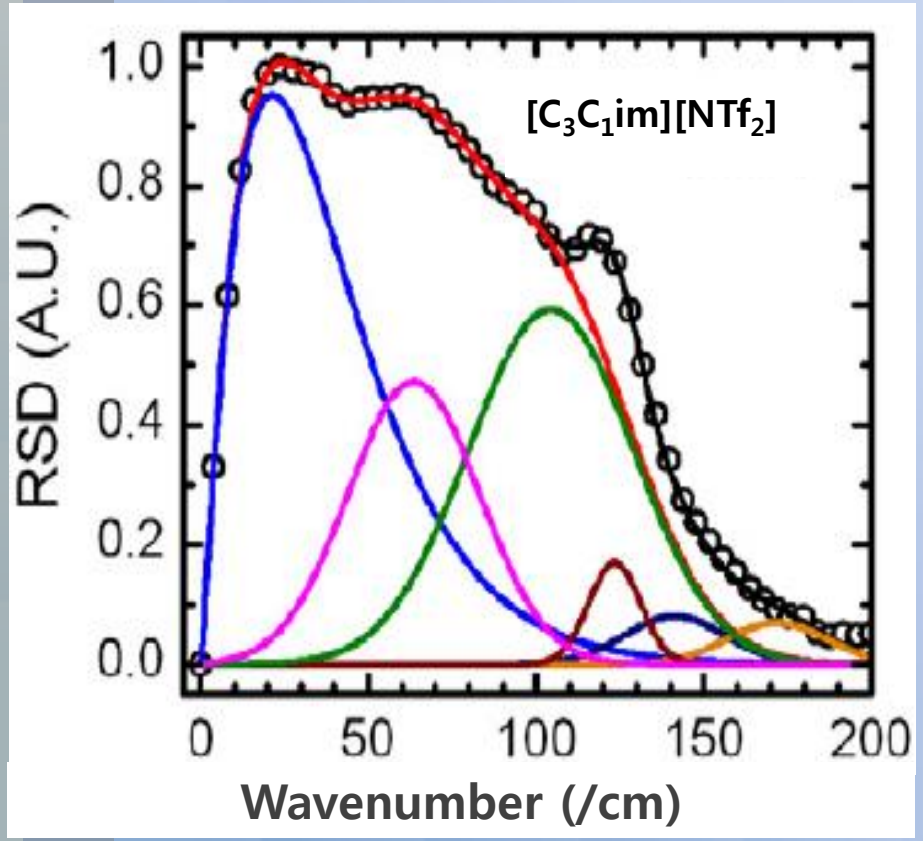
- Polarized Raman spectra

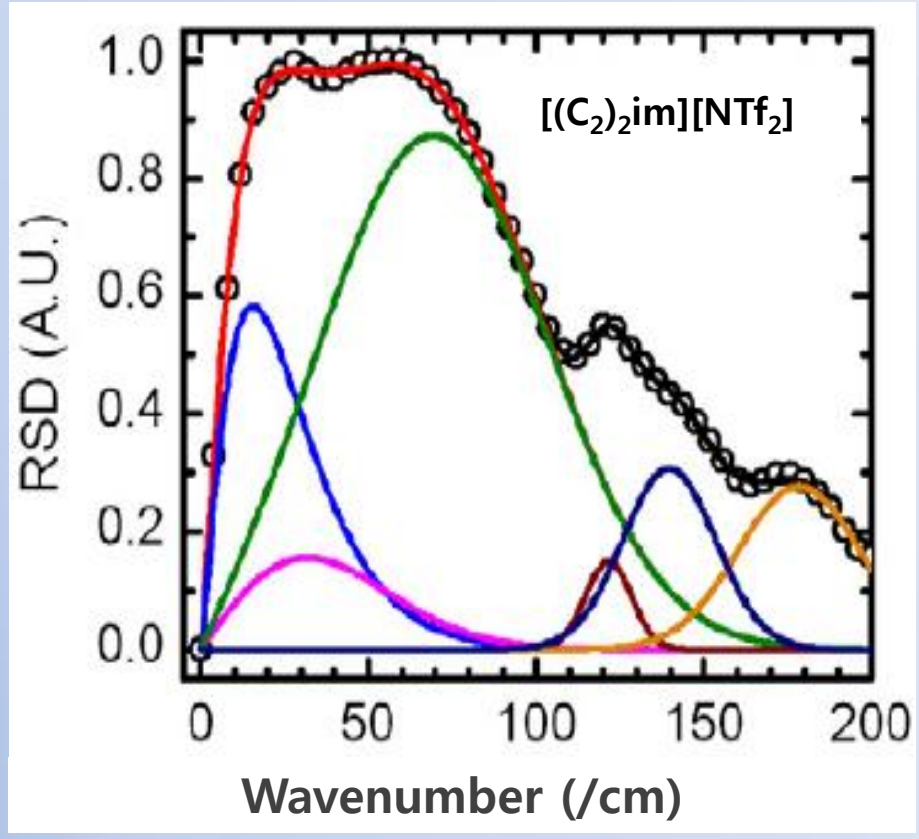


- Depolarized Raman spectra

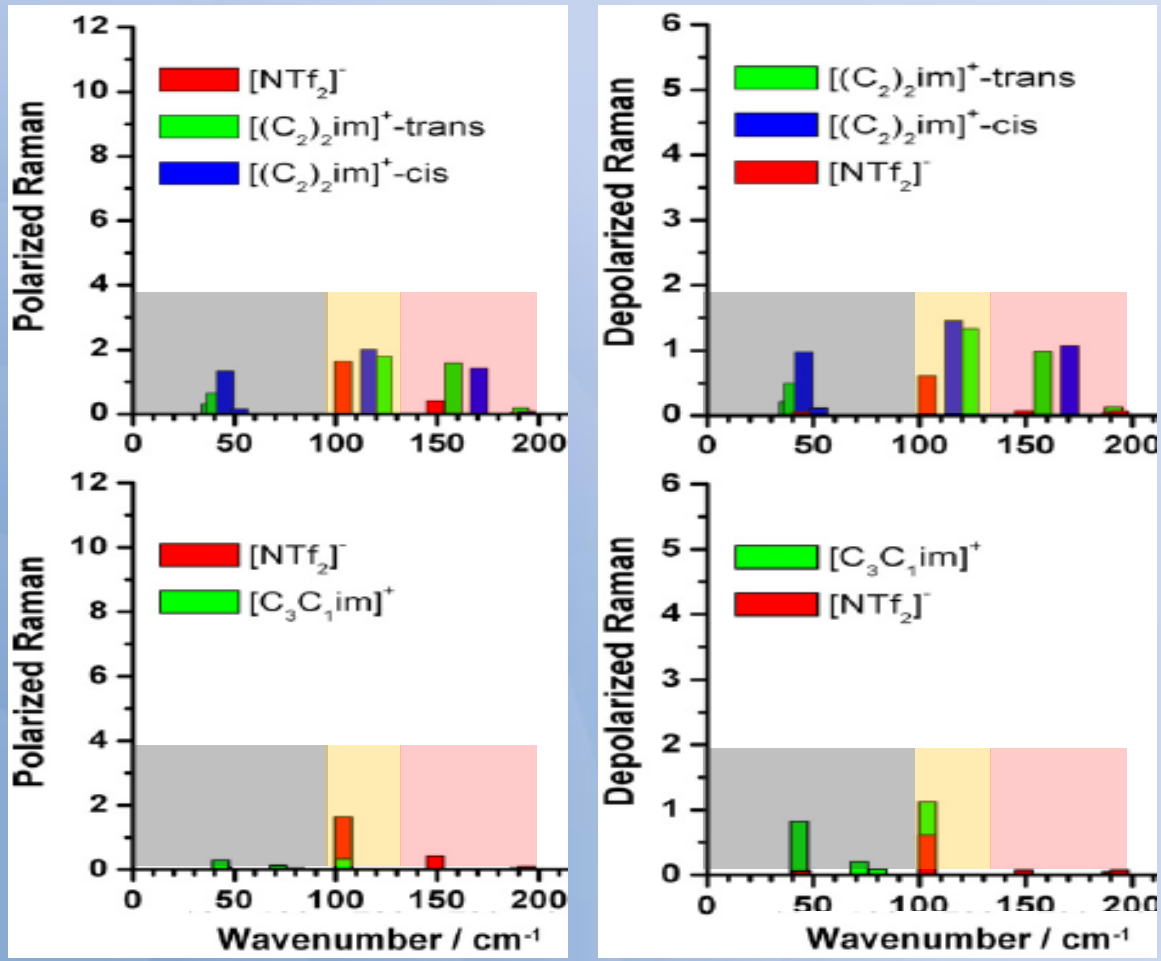


Reduced Spectral Density by Kerr signal





Calculated Raman spectra



region A1: 0<w≤100 /cm

region A2: 100<w≤125 /cm

region A3: 125<w≤200 /cm

Concluding remarks

- According to Kerr experiment on two kinds of ionic liquids, the intermolecular motion could be determined by symmetry of cation.

- In the range from 100 to 200 /cm, a weak peak originate from the anion.

- The intramolecular motion should be considered besides the intermolecular motion when you do peak assignment.