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Date: 04/11/2025
Time: 10: 00 am

III/MPHYCC10 Atomic and Molecular Physics

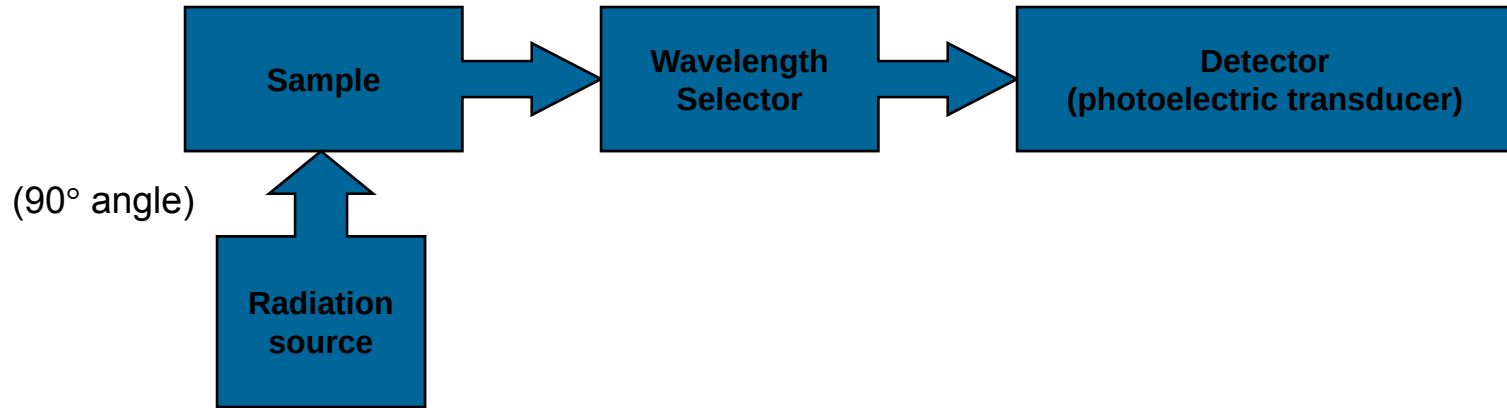
Instrumentation

Raman Lineshape



Raman Spectrometers

- The basic design dispersive Raman scattering system:

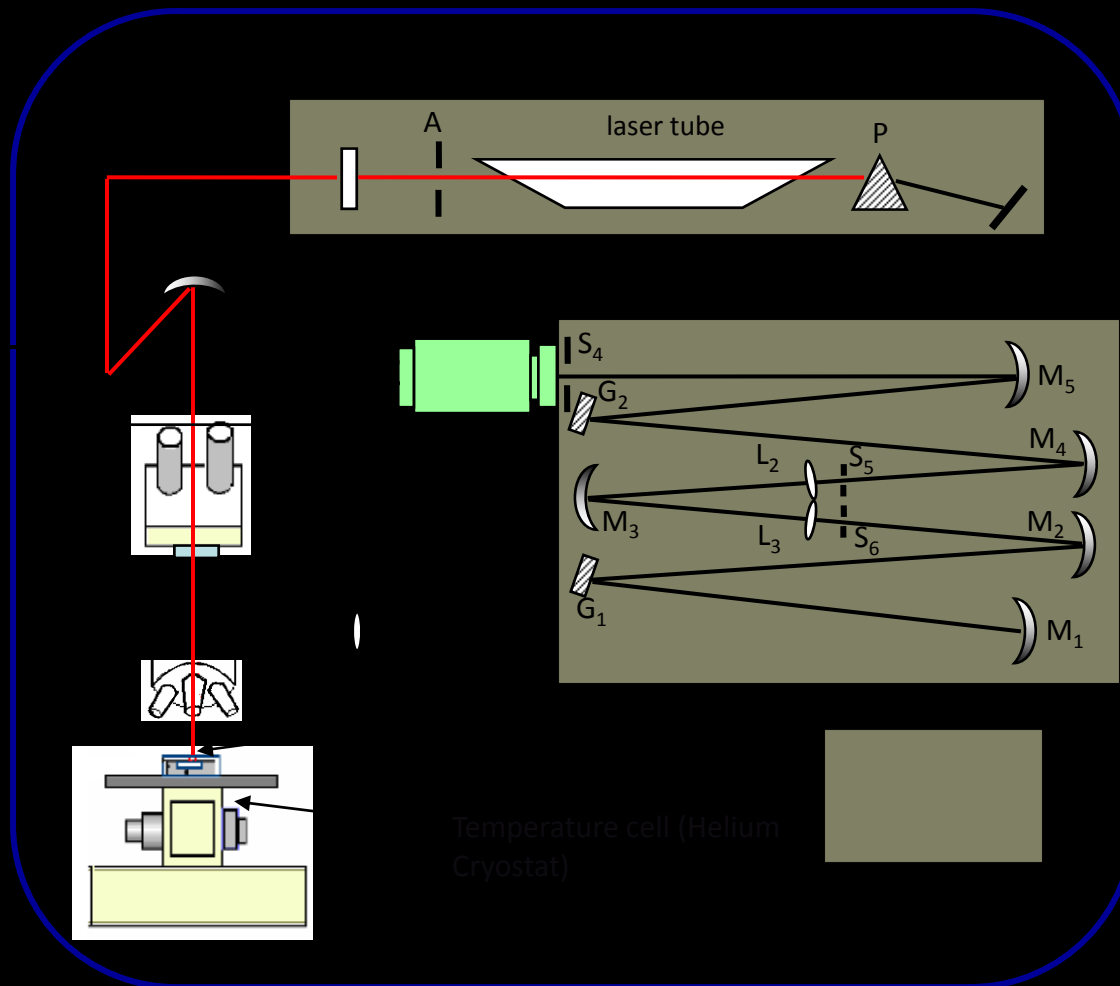


- Sources: Lasers ; Single wavelength

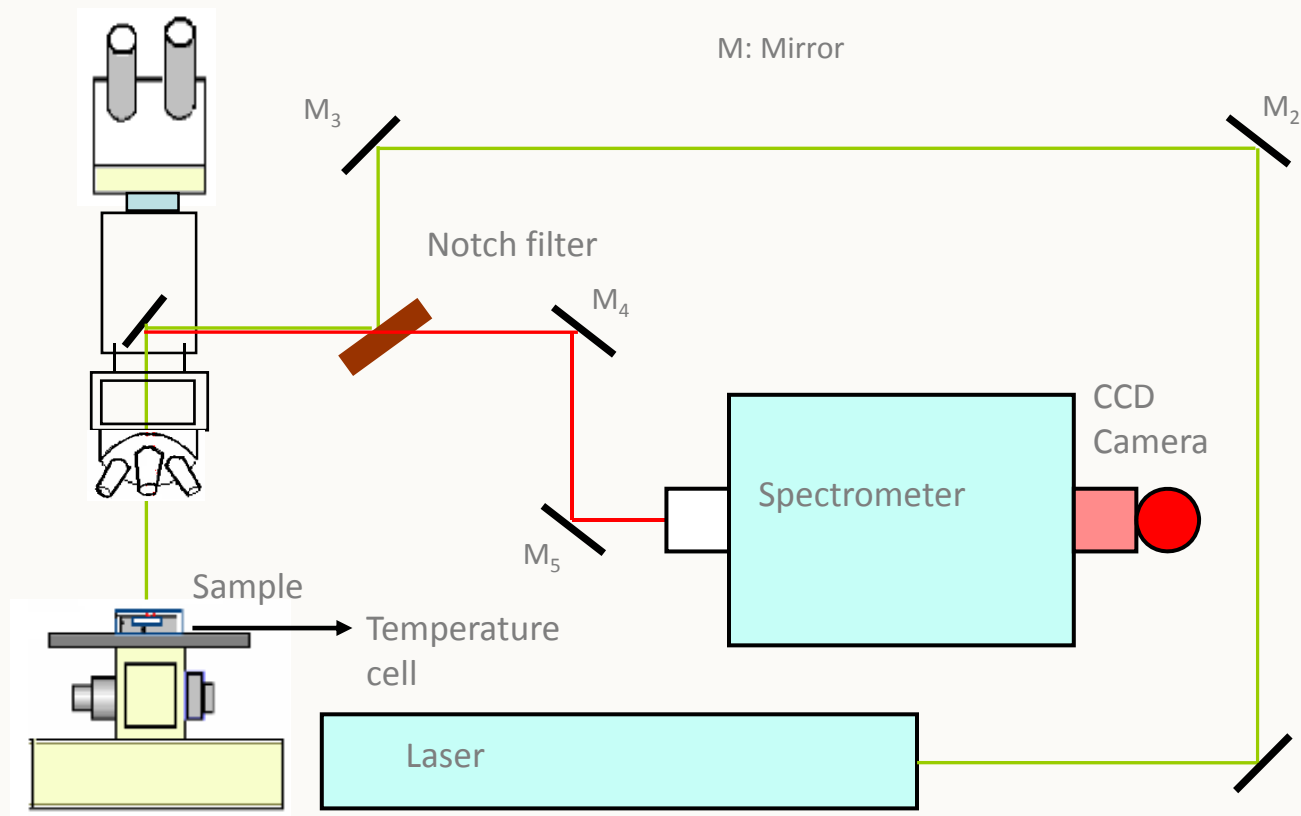
Raman scattering is a weak process

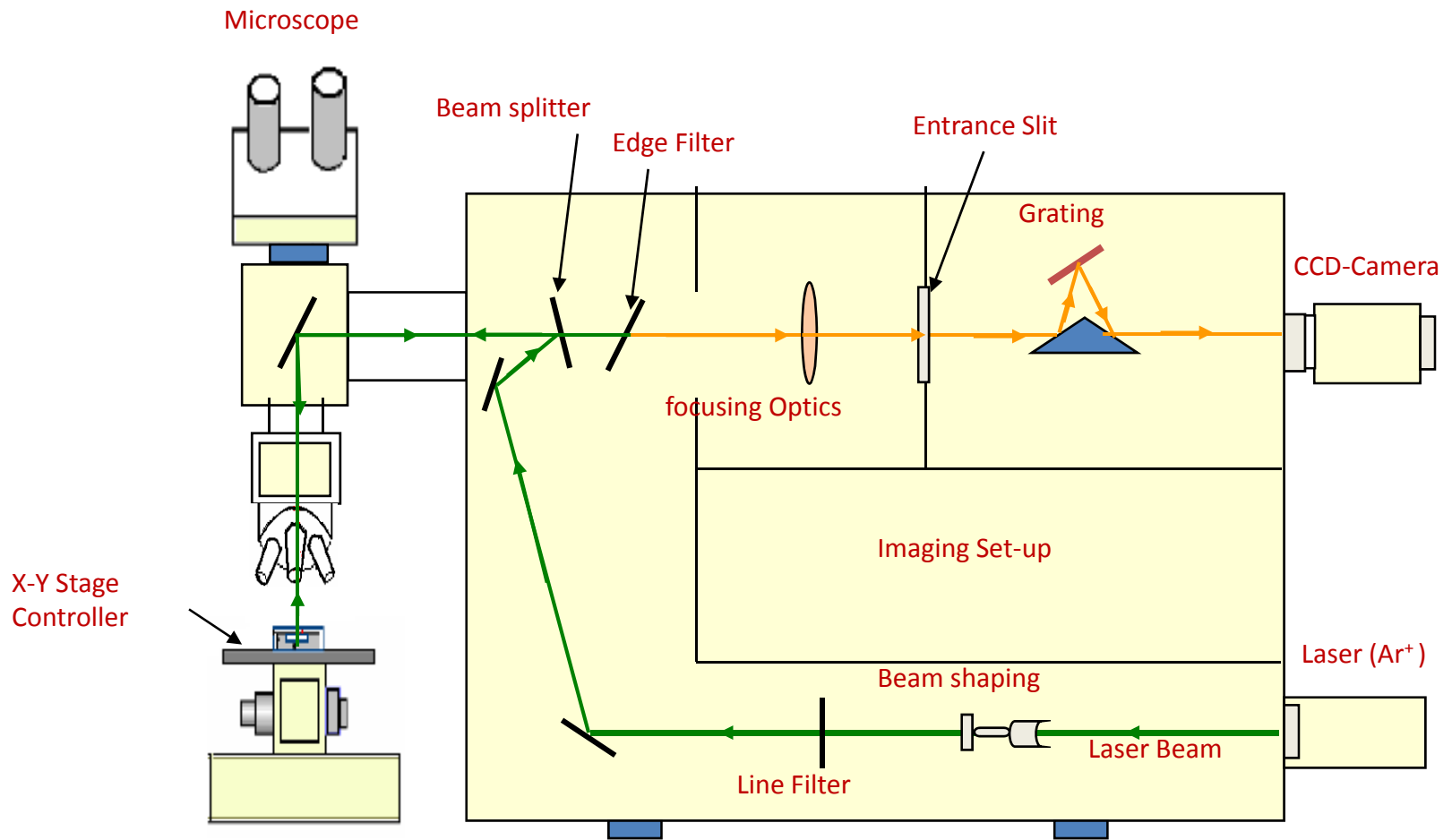
He-Cd (441.6 nm), Ar⁺ (488.0 nm, 514.5 nm), He-Ne (632.8),
Diode (782 or 830), Nd/YAG (1064)

Raman Spectrometer: Spex 1404 double monochromator with
647 nm laser line from Kr⁺ laser.



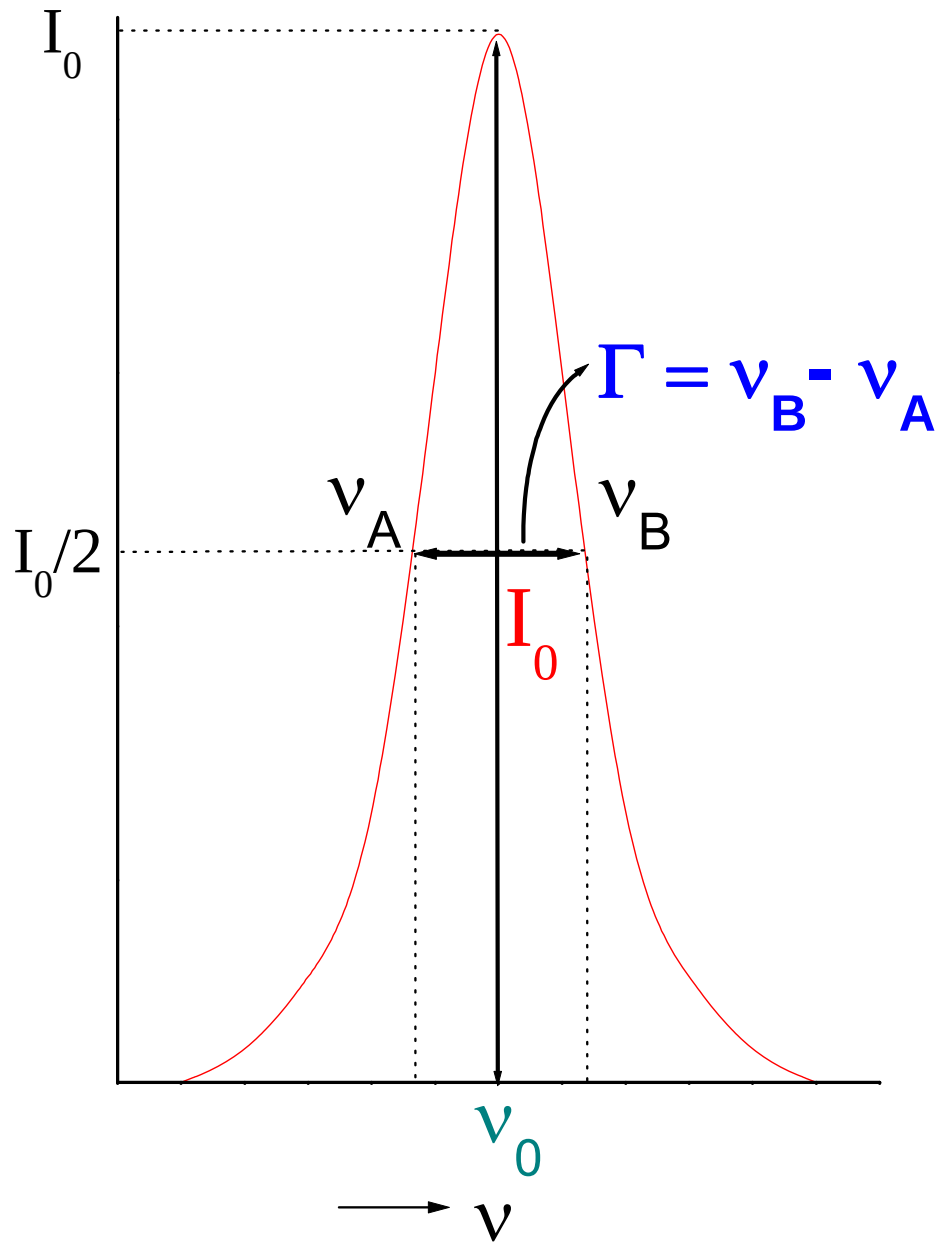
Micro-Raman set-up from LabRam with 532 nm line
of frequency-doubled Nd:YAG laser.



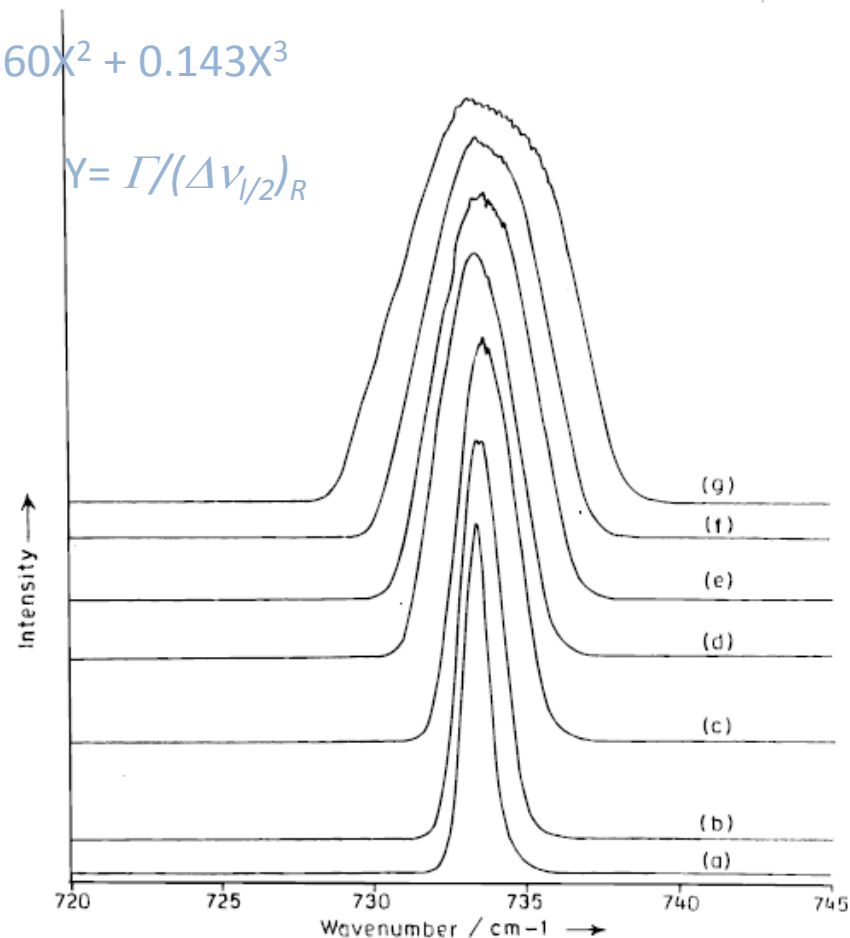
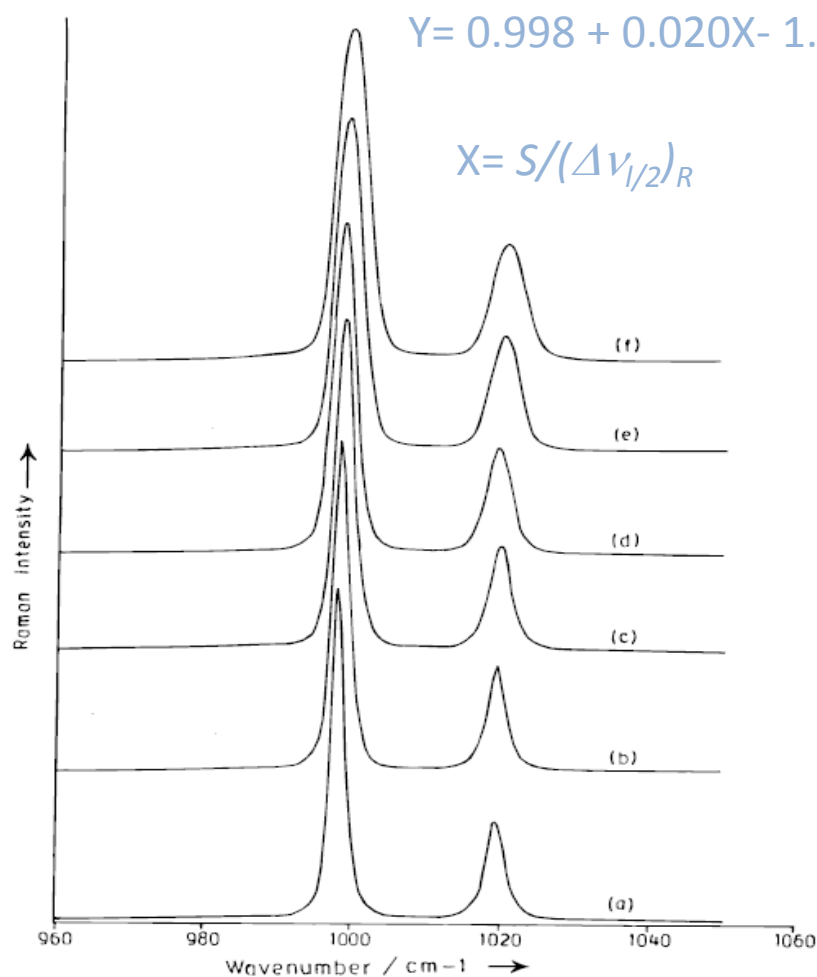


Schematic of Micro Raman Set-up

LINE SHAPE PARAMETERS



Effect of Slit Width

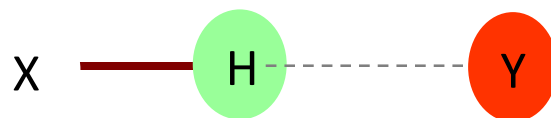


Plasma lines at 734 cm⁻¹ for the 488.0 nm line of the Ar⁺-laser at seven slit openings: (a) 50; (b) 100; (c) 150; (d) 200; (e) 250; (f) 300; (g) 400 mm.

Raman spectra of two bands at 999 and 1024 cm⁻¹ of chlorobenzene at six slit openings: (a) 50; (b) 100; (c) 150; (d) 200; (e) 250; (f) 300 mm.

Molecular Association

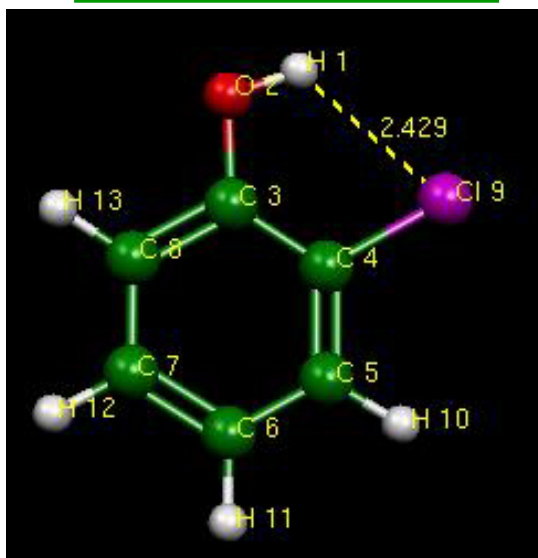
Hydrogen Bonding



2 – 4 Å⁰

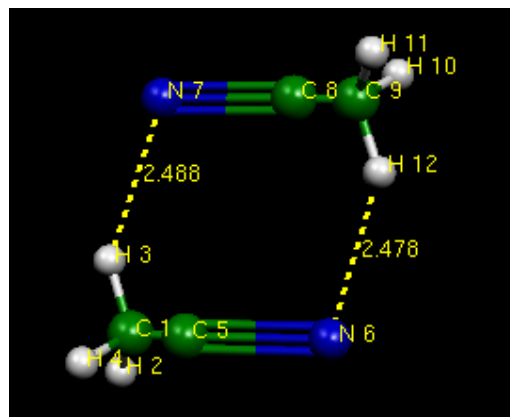
X & Y are the electronegative atoms

Intra-Molecular

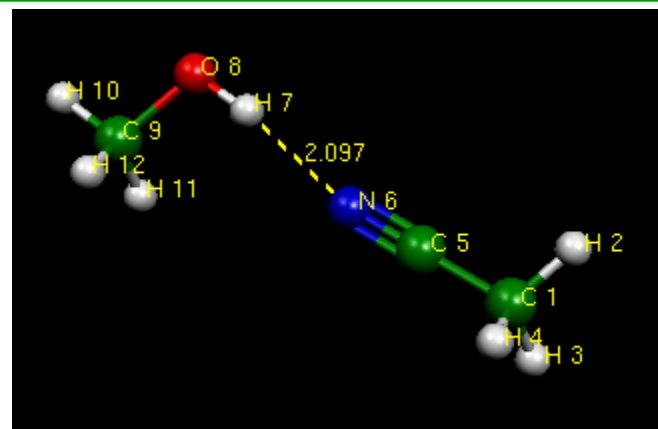


Inter-Molecular

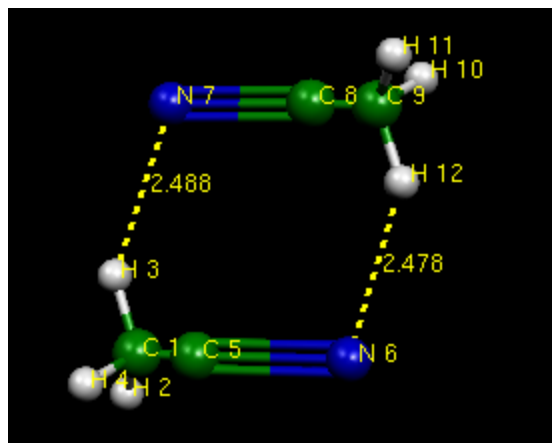
Self-Association



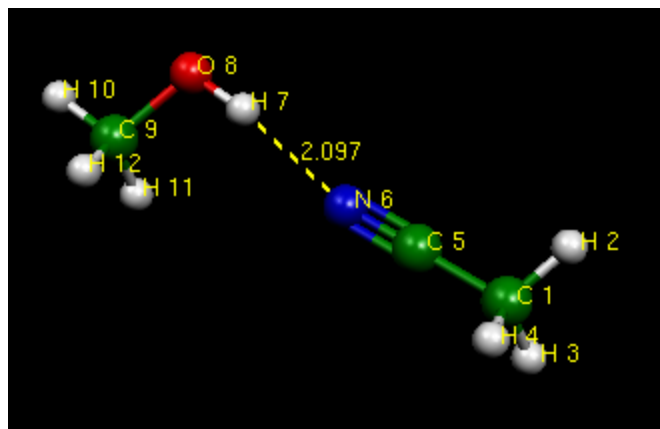
Hydrogen Bonded Complex



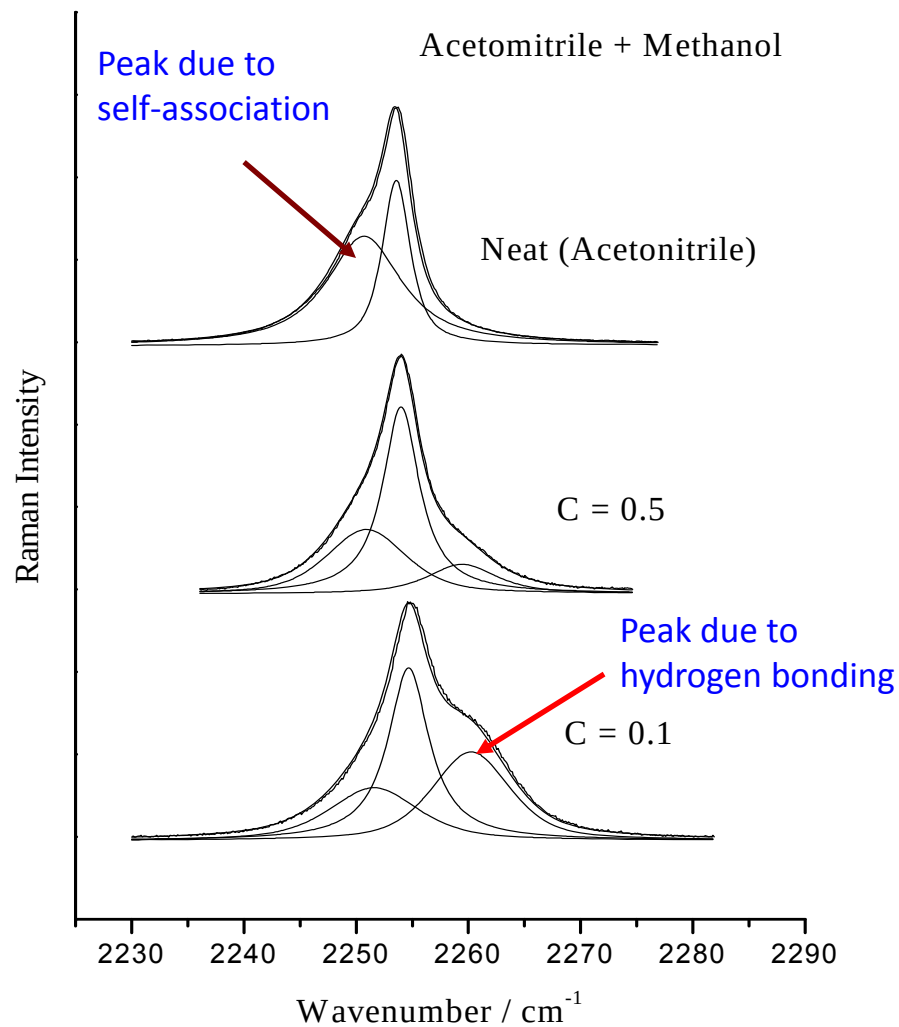
Spectra-Structure correlation



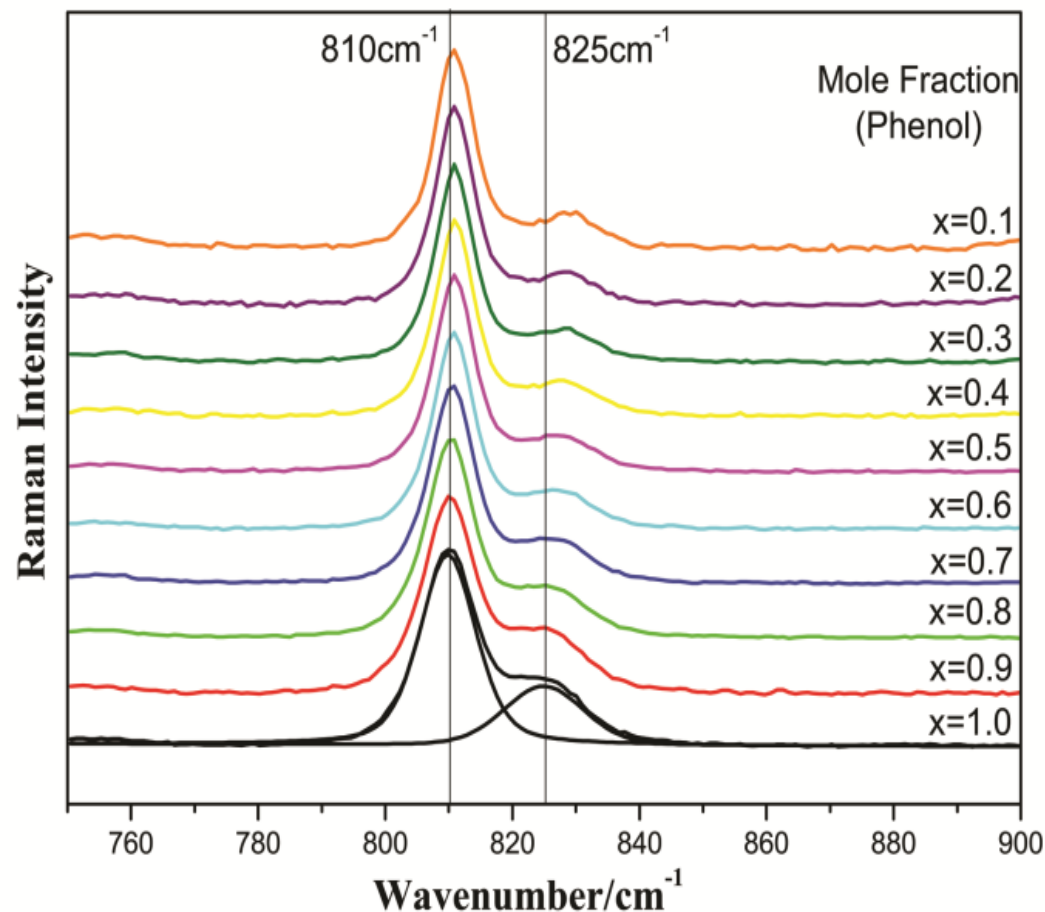
Self associated structure



Hydrogen bonded structure



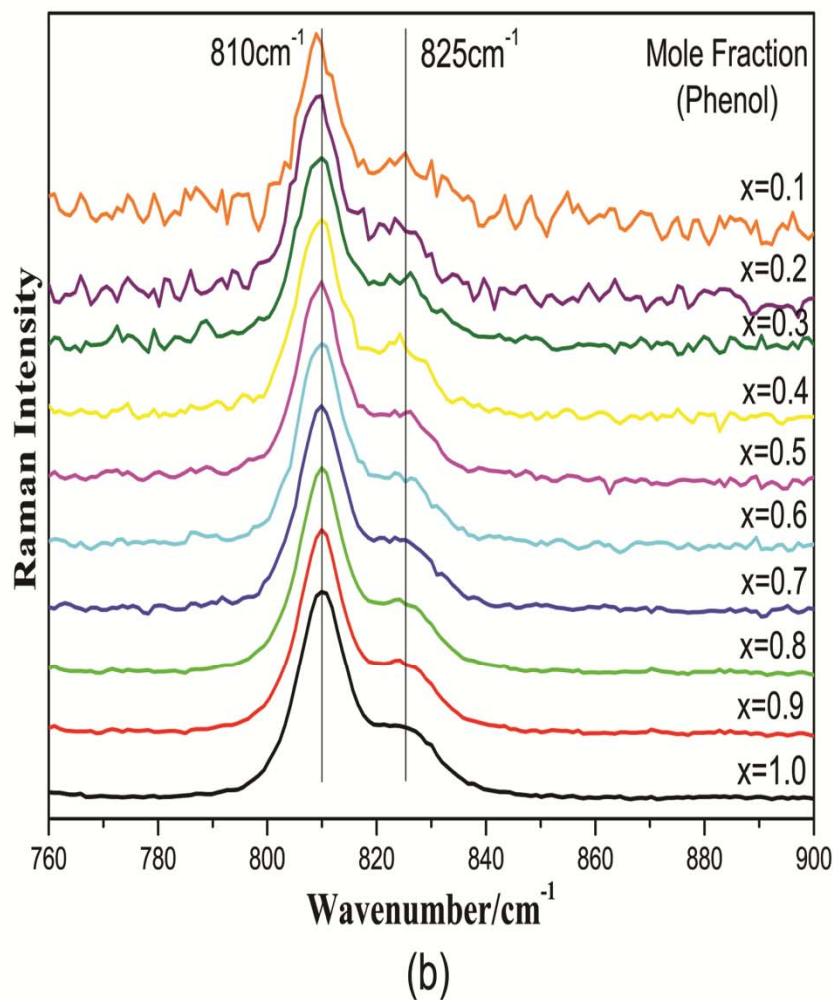
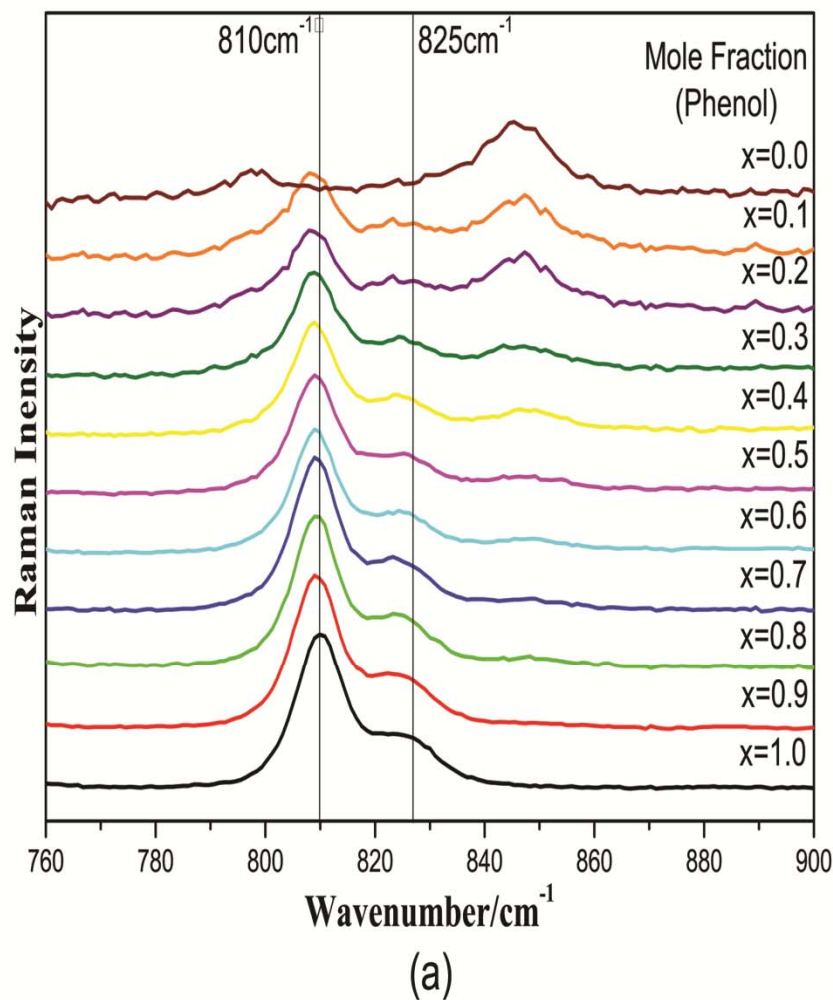
Ring deformation in phenol



- 810 cm⁻¹ Ring deformation of monomer phenol
- 825 cm⁻¹ Ring deformation of dimer/oligomer phenol decreases.
- 829 cm⁻¹ Ring deformation of phenol +ACN

Raman spectra of binary mixtures of phenol + ACN at different mole fractions

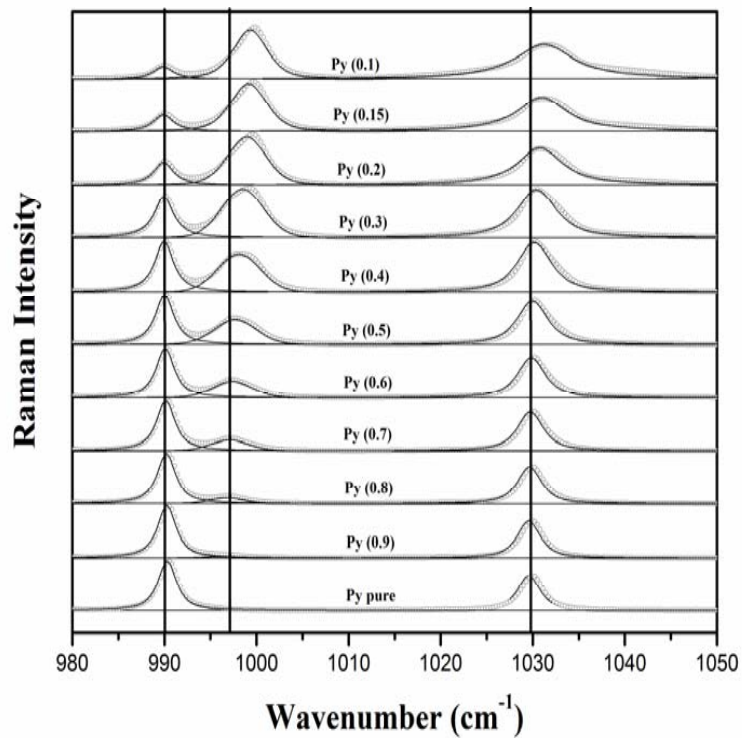
Ring deformation in phenol



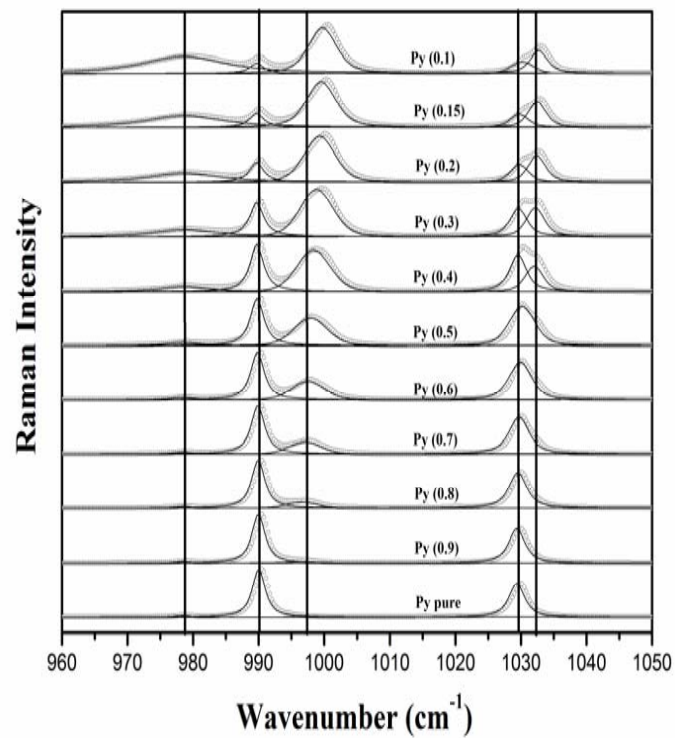
Raman spectra of binary mixtures of (a) phenol + benzene and (b) phenol + ODCB at different mole fractions of phenol (x)



Pyridine+CH₃OH/CD₃OD



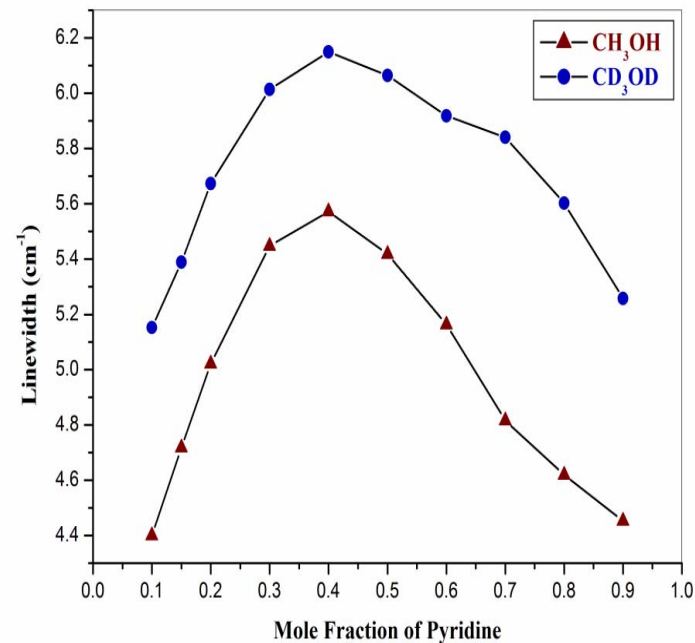
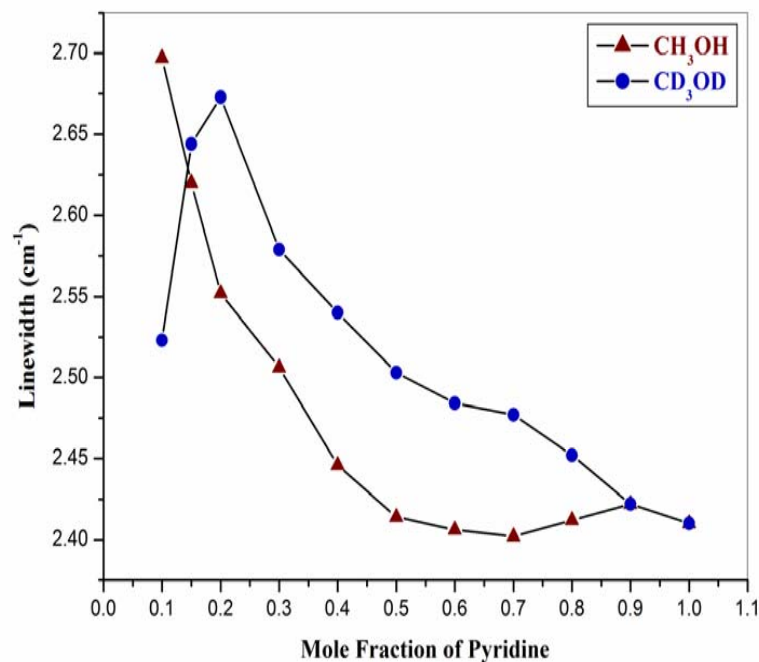
Raman Spectra for Pyridine+CH₃OH complex



Raman Spectra for Pyridine+CD₃OD complex



Variation of linewidth



Variation of linewidth of 990 cm⁻¹ band of pyridine+CH₃OH (▲) and pyridine+ CD₃OD (●).

Variation of linewidth of 996 cm⁻¹ band of pyridine+CH₃OH (▲) and pyridine+CD₃OD (●).

The diffusion coefficient of CH₃OH is 1.58X10⁻⁹ m²/s and of CD₃OD is 2.23X10⁻⁹ m²/s. Motional narrowing and caging effect, Concentration fluctuation.