# ES 290R Topics in Physics and Chemistry of the Earth

## Vibrational Spectroscopy, Symmetry, Crystals and You

An overview of the underlying physics of vibrational spectroscopy (especially infrared and Raman spectroscopy, but extendable to Brillouin spectroscopy, as well) and crystal symmetry. Emphasis will be on symmetry and spectroscopy of crystals, including: symmetry constraints; constraints on bonding properties/force constants; group theory's influence on allowing or disallowing vibrations (factor group and normal mode analysis); introduction to lattice dynamics; origin of absorption and reflectivity of crystals; Kramers-Kronig analyses and the role of polarizability and dielectric constants; origin of line-shapes and relative intensities of bands; origin of high order phenomena, such as overtones, resonances, and LO-TO splitting; and role of vibrational spectra in determining thermochemical properties

Format: 7 2-3 hour lectures by the instructor (Q. Williams)
Weekly Readings
Occasional Problem Sets (probably 1 over the course of the quarter)
Last two meetings will incorporate class presentations--
these will either involve relevant projects (either class project(s) or general research) or recent notable literature contributions.

Schedule:

Introduction, Logistics and Overview

Dynamics of a Linear Chain; Dispersion relations/Brillouin Zones; Boundary conditions

Crystal Symmetry; Character Tables and Introductory Group Theory

Infrared and Raman selection rules: What's active and why.

Factor Group, Site group Analyses: Worked Examples

Dielectric constants, Kramers-Kronig analyses, Relation between reflection and absorption spectroscopy, Polarization of Raman and IR spectra

Miscellaneous spectroscopic phenomena: Why vibrations aren't (or are almost never) δ-functions; What happens when vibrations meet and greet; What structural disorder does to spectra.

Thermodynamic implications of spectroscopic data

Student Presentations

Student Presentations

Source Books (or just old fashioned good reading)

M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford, 1954.
A classic!

P. Bruesch, Phonons: Theory and Experiment I, Springer-Verlag, 1982.
The nicest treatment of dispersion around.

P.F. Choquard, The Anharmonic Crystal, Benjamin, 1967.
No index, and not too many words, either.

K. Nakamoto, Infrared and Raman Spectra of Molecules (in lab)
A bit of a data table, but the first 60 pages are nice.

G. Venkataraman, L.A. Felkdamp, and V.C. Sahni, Dynamics of Perfect Crystals, MIT Press, 1975.
A nice treatment, with good explanations.

G. Turrell, Infrared and Raman Spectra of Crystals, Academic, 1972.
A lousy translation of a good book.

J.C. Decius and R.M. Hexter, Molecular Vibrations in Crystals, McGraw-Hill, 1977.
Maybe the best book on crystals of the lot---much reading will come from here.

W.G. Fateley et al., Factor Group Analysis, Academic, 1965 (?).
The title says it all.