Advanced Physical Chemistry

Summer term 2018

Prof. Dr. Ulrich K. Deiters

A Spectroscopy

1. Interaction of matter and radiation
   1.1. Principles of spectroscopy
   1.2. Conservation laws (energy, rotational momentum, spin)
   1.3. Selection rules (transition dipole moment, symmetry)
   1.4. Special transition types (stimulated emission, two-photon processes, magnetic transitions)
   1.5. Line widths (Doppler and collision broadening)
2. Rotation and vibration spectroscopy
   2.1. Rotation spectra
   2.2. Vibration spectra (anharmonicity, polyatomic molecules)
   2.3. Combined rotation-vibration spectroscopy (IR, Raman, NIR)
3. Electronic transitions
   3.1. Electronic transition spectroscopy of atoms
   3.2. Electronic transition spectroscopy of molecules (Franck–Condon principle, UV absorption, fluorescence, phosphorescence)
   3.3. Laser
4. NMR spectroscopy and related techniques
   4.1. Principles: spins in a magnetic field (Larmor frequency)
   4.2. Continuous vs. relaxation measurement, relaxation pathways
   4.3. Chemical shift (screening), spin–spin coupling

B Statistical Thermodynamics

1. Theory of probability
   1.1. Probability distributions (binomial, Poisson, Gauss)
   1.2. Means and standard deviations
   1.3. Autocorrelation functions
2. Principles of statistical thermodynamics
   2.1. Concepts and axioms
   2.2. Isolated systems, microcanonical ensemble

2.3. Entropy
2.4. Isothermal systems, canonical ensemble (partition function, Boltzmann statistics)
2.5. Indistinguishable particles, quantum statistics (Fermi–Dirac, Bose–Einstein)
2.6. Open systems, grand canonical ensemble
2.7. Fluctuations

3. Applications
    3.1. Monoatomic ideal gas (translational partition function)
    3.2. Polyatomic ideal gas (rotational, vibrational, electronic partition function)
    3.3. Relevance for spectroscopy
    3.4. Real gas (pair distribution function, virial equation)
    3.5. Electron gas
    3.6. Equilibrium constants of chemical reactions
    3.7. Monoatomic crystals (models of Einstein and Debye)
    3.8. Lattice models (adsorption isotherms: Langmuir and BET models, phase transitions: Bragg–Williams and Ising models)
    3.9. Polymer solutions (Flory–Huggins model)

4. Electrical properties of matter
    4.1. Matter in an electric field (electric polarization, dielectric constant)
    4.2. Orientation of dipols (Langevin)
    4.3. Relaxation phenomena

5. Thermodynamics of irreversible processes
    5.1. Concepts: fluxes and forces
    5.2. Coupled fluxes, entropy production
    5.3. Onsager's reciprocity relations

Recommended literature:

1. P. W. Atkins, J. de Paula, and J. Keeler*Physical Chemistry*, 11th ed., Oxford University Press, Oxford 2018.
   in addition: J. Bolgar and H. Lloyd, *Students' Solution Manual to Accompany Atkins' Physical Chemistry*, 11th ed., Oxford University Press, Oxford 2018.
2. P. W. Atkins, J. de Paula, *Physikalische Chemie*, 5. Aufl., Wiley-VCH, Weinheim 2013 [Do not confuse this with the "Kurzlehrbuch Physikalische Chemie!].
   in addition: Ch. A. Trapp, M. P. Cady, and C. Giunta, *Arbeitsbuch Physikalische Chemie*, 5. Aufl., Wiley-VCH, Weinheim 2013.
3. G. Wedler and H.-J. Freund, *Lehrbuch der Physikalischen Chemie*, 6. Aufl., Wiley-VCH, Weinheim 2012.
   in addition: G. Wedler and H. J. Freund, *Arbeitsbuch Physikalische Chemie*, 6. Aufl., Wiley-VCH, Weinheim 2012.
4. W. Göpel and H.-D. Wiemhöfer, *Statistische Thermodynamik*, Spectrum-Verlag, Berlin 2000.
5. G. H. Findenegg and T. Hellweg, *Statistische Thermodynamik*, 2. Aufl., Springer, Berlin 2015.
6. T. L. Hill, *Statistical Thermodynamics*, Addison-Wesley, Reading 1960 [ancient, but still good].