Recommended problems and optional hand-ins in Atomic Physics spring 2019.

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The recommended problems below will help you understand the theory, train your problem-solving skills as well as giving you a very important working knowledge of atomic physics.

I strongly suggest that you do all (most of) these problems in the given order, since this will also prepare you for the hand-ins.

The problems marked as hand-in are problems that you may solve and hand in to obtain credits on the first and second examination opportunity. The exam will consist of 6 problems giving at most 4 points each, i.e. a maximum of 24. A passing grade will require 12 and "väl godkänd" 19 points. Solving perfectly all optional hand-in problems will give you 3 + 3 = 6 points on the exam. The deadline for the first hand-in is Monday 4/2 and for the second Monday 11/3.

Rules and regulations regarding the hand-ins

- The hand-ins must be solved in groups of 2 students (registered for the first time on the course), no more and no less!
- The problems give different points and you may do any number of them but at least two in each hand-in.
- Each problem must be solved on a separate paper.
- The complete hand-in should be stapled together, with a cover page containing your names, e-mail and personal identification number.
- In addition to a correct solution it is required that you write carefully in a clear and pedagogical manner. Every numerical answer must have the appropriate unit.
- All diagrams must have descriptive captions and axis labels with the appropriate units.
- It is allowed and encouraged that you discuss the physics in general with other students, but it is absolutely essential that each group individually solves the actual problems and writes the report. Note that, if you do them, the hand-ins are part of the exam and all official rules conserning plagiarism, with possible severe repercussions, applies.

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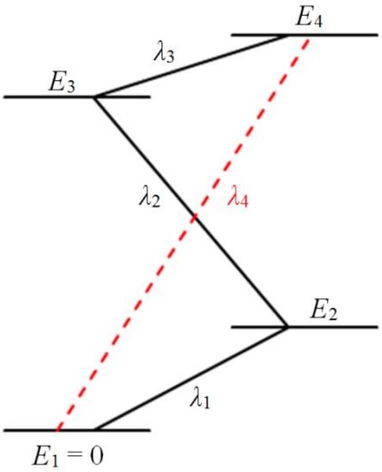
1. The wavenumber for a transition between two levels is 50000 cm^{-1}.
   a) What is the wavenumber in the unit 1 m^{-1}?
   b) What is the wavelength of the transition?
   c) What is the energy difference in the unit 1 eV?
   d) How many cm^{-1} is 1 eV?

2. Two spectral lines both have an estimated wavelength unceraintty of 0.05 Å. What is the frequency and its uncertainty if the measured wavelength is 100 and 1000 Å, respectively? What is the relative uncertainty $\Delta f / f$ at the two wavelengths?

3. **Hand-in 1 (0.5 point)**

The figure shows a 4-level system starting from the ground state. Assume the following wavelengths, in Å, and their estimated uncertainties (one standard deviation). $\lambda_1 = 3000 \pm 0.8$, $\lambda_2 = 1800 \pm 0.2$ and $\lambda_3 = 4500 \pm 5$. Derive the energy, in cm^{-1}, of all levels and the wavelength λ_4. Include an estimated one standard deviation uncertainty in all the quantities. Assume all uncertainties to be independent. (If needed, you may download from the home page a short document (in Swedish) describing the handling and propagation of uncertainties in experimental data.)



4. *Bohr's theory of the H-atom.*
   a) Show that the energy of transitions between two shells with principal quantum numbers n and $n' = n + 1$ is proportional to n^{-3}, for large values of n.
   b) Calculate the frequency of the $n = 50 - 51$ transition.
   c) What is the size of an H-atom in the $n = 50$ shell?
   d) Treat the electron as a classical particle and calculate the rotation frequency of the electron in the $n = 50$ shell. Compare your result with 4b

5. What is the shortest and longest wavelength, respectively, that can be emitted from an H-atom?

6. The table gives observed wavelength (in standard air with a refractive index of about 1.0003) from H and He$^+$, respectively. Explain the data, particularly which transitions these wavelengths correspond to?

Wavelength / nm

H	656.28	486.13	434.05	410.17	
He$^+$	656.01	541.16	485.93	454.16	433.87

7. *Commutator relations*.
   a) Prove one of these important commutator relations
   $$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z, \left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x, \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$
   b) Prove that $\left[\hat{L}^2, \hat{L}_i\right] = 0,\; i = x, y$ or z.

8. **Hand-in 1 (0.5 point)**

A particle is described by the wavefunction :

$$\Psi(\theta,\varphi) = \frac{1}{\sqrt{10}}(Y_{1,-1} + 3Y_{1,0}),\ \text{where } Y_{\ell,m}(\theta,\varphi) \text{ is an orthonormal spherical harmonics.}$$

   a) Is this an eigenfunction of $\hat{L}_z$? If so, what is the eigenvalue?
   b) Is this an eigenfunction of $\hat{L}^2$? If so, what is the eigenvalue?
   c) What is the expectation value of $\hat{L}_z$ in the state described by Ψ?
   d) What is the expectation value of $\hat{L}^2$ in the state described by Ψ ?

9. Use a table or the net to look up all spherical harmonics with $\ell = 0$, 1 and 2 and motivate, by direct calculation, the general result that for each ℓ-value the sum over all possible m-values is spherically symmetric, i.e. show that:

$$\sum_{m=-\ell}^{\ell} \left|Y_{\ell,m}(\theta,\varphi)\right|^2 = \frac{2\ell+1}{4\pi}, \text{ independent of the angles.}$$

This statement, called Unsöld's theorem, shows that filled orbitals are spherically symmetric, and hence contributes nothing to the angular momentum couplings.

10. **Hand-in 1 (0.5 point)**

For two electrons we have $\ell_1 = 1$ and $\ell_2 = 1$. Make a table of all possible z-components that arise when the angular momentum (vectors) $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_2$ are added. Show that this exactly corresponds to the components you would get from a quantized momentum $\boldsymbol{L} = \boldsymbol{\ell}_1 + \boldsymbol{\ell}_2$ with the quantum number $L = 0$, 1 and 2.

11. Let Y_{ℓ_i,m_i} be an eigenfunction of $\hat{\ell}_i^2$ and $\hat{\ell}_{z_i}$ for $i = 1,2$ in a two electron atom. The total orbital angular momentum is given by $\hat{L} = \hat{\ell}_1 + \hat{\ell}_2$ and the eigenfunction of $\hat{L}^2$ and $\hat{L}_z$, $\psi_{\ell_1,\ell_2,L,M}$, can be expressed as linear combinations of those for the individual angular momenta, Y_{ℓ_i,m_i}, using the Clebsch-Gordan coefficients, C.

$$\psi_{\ell_1,\ell_2,L,M} = \sum_{m_1} C(\ell_1,m_1,\ell_2,M-m_1 : L,M)\cdot Y_{\ell_1,m_1}\cdot Y_{\ell_2,M-m_1}$$

a) Make a table of all possible combinations of m_{ℓ_1}, m_{ℓ_2} and the resulting $M_L = m_{\ell_1} + m_{\ell_2}$ when we couple a p and a d-electron. How many combinations give $M_L = 1$ and how many give $M_L = 2$? Which L-values are involved in these states?

b) Write down the complete wavefunctions corresponding to these L-values and $M_L = 1$ and 2. For clarity, use the notation $\left|\ell_1,\ell_2,L,M_L\right\rangle$. A Clebsch-Gordan calculator may be found at: http://personal.ph.surrey.ac.uk/~phs3ps/cgjava.html to obtain the analytical values of the Clebsch-Gordan coefficients. For clarity, use the notation $Y_{\ell_i,m_i} \equiv \left|\ell,m\right\rangle$ to denote the spherical harmonics, do not write them out explicitly

c) Chose one of the $M_L = 1$ functions and show that it is normalized and orthogonal to all the others with $M_L = 1$. Use the relation $\left\langle Y_{\ell,m}\middle|Y_{\ell',m'}\right\rangle = \delta_{\ell,\ell'}\cdot\delta_{m,m'}$

12. The radial wavefunctions, $R_{n\ell}(r)$, for a one-electron system with nuclear charge Z and $n = 3$ are:

$$R_{30}(r) = 2(Z/3)^{3/2}\cdot\left(1-\frac{2Zr}{3}+\frac{2(Zr)^2}{27}\right)\cdot e^{-Zr/3}$$

$$R_{31}(r) = \frac{4\sqrt{2}}{9}(Z/3)^{3/2}\cdot\left(1-\frac{Zr}{6}\right)\cdot Zre^{-Zr/3}$$

$$R_{32}(r) = \frac{4}{27\sqrt{10}}(Z/3)^{3/2}\cdot(Zr)^2\cdot e^{-Zr/3}$$

where the distance, r, from the nucleus is measured in the unit 1 a_0.

a) Use e.g. MatLab and plot the functions for $Z = 1$ and $Z = 2$. What happens as Z increases?

b) Which orbital ($n\ell$) is ≠ 0 at the nucleus, $r = 0$?

c) Verify that the number of nodes, i.e. zero-crossings, for $r > 0$ is given by $n - l - 1$.

13. **Hand-in 1 (0.5 point)**

The probability of finding the electron at a distance *r*, independent of the angles θ and φ, is given by the radial distribution function $D_{n\ell}(r)$.

$$D_{n\ell}(r) = r^2 \left|R_{n\ell}(r)\right|^2$$

a) Plot $D_{n\ell}(r)$ for $Z = 2$ for the 3s, 3p and 3d orbitals above.

b) Use the figures to estimate the distance corresponding to the maximum probability for 3d and compare with the value calculated using the Bohr formalism.

14. In quantum mechanics the mean radius (in units of 1 a_0) is calculated as the expectation value:

$$< r >_{n\ell} = \int_0^\infty R^*_{n\ell} \cdot r \cdot R_{n\ell} \cdot r^2 dr$$

Use e.g. MatLab to numerically calculate $< r >$ for the 3 orbitals above for $Z = 2$ and compare with the general quantum mechanical expression. $< r >_{n\ell} = \frac{1}{2Z}[3n^2 - \ell(\ell+1)]$

15. **Hand-in 1 (0.5 point)**

In Hydrogen the complete wavefunction for the ground state is:

$$\Psi_{1s}(r,\theta,\varphi) = \sqrt{\frac{1}{\pi a_0^3}} \cdot e^{-r/a_0}$$

Calculate analytically the probability of finding the electron inside a sphere of radius r_b centered on the nucleus. Assume $r_b << a_0$ so that you may make convenient approximations.

16. Calculate the internal magnetic field experienced by a 2s and a 2p-electron in He$^+$ and in F^{8+}. Use the general quantum mechanical result for a one-electron system

$$< \frac{1}{r^3} >_{n\ell} = \frac{1}{\ell(\ell+1/2)(\ell+1)} \cdot (\frac{Z}{na_0})^3, \quad \ell > 0$$

17. Motivate the selection rule $\Delta j = 0, \pm 1$, not $0 \rightarrow 0$. Assume that the atom makes a transition from a level with $j = 3/2$ to a lower level j' through the emission of a photon with spin $s_\gamma = 1$. Calculate all possible *z*-components that arise when the angular momenta (vectors) $\boldsymbol{j}$ and $\boldsymbol{s}_\gamma$ are subtracted. Show that this exactly corresponds to the components from a quantized momentum (vector) $\boldsymbol{j}'$ with the quantum number $j = 1/2$, 3/2 or 5/2.

18. Calculate the wavelengths for 1s $^2S_{1/2}$ – 2p $^2P_{1/2,3/2}$ in He II including the 3 relativistic corrections (mass, spin-orbit and Darwin). Compare with the accurate experimental results available in the data base at NIST (National Institute of Standards and Technology) in Washington, USA https://physics.nist.gov/PhysRefData/Elements/index.html (*Click on the element symbol in the periodic table, then choose "Lines" among the database icons that appear*.) Which effect is responsible for the small, but significant, remaining discrepancy in the absolute energies?

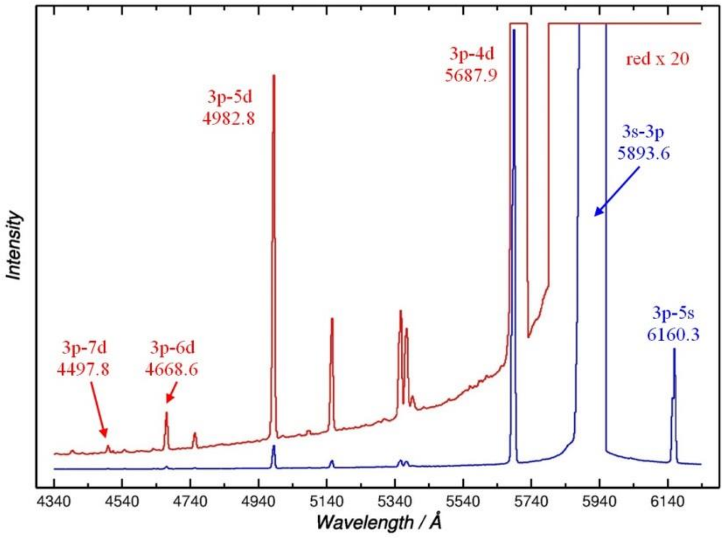
19. The configuration $1s^2 3d$ in Li I has the (*excitation*) *energy* 31283.10 cm^{-1}. The *ionization energy* in Li is 43487.19 cm^{-1}.
    a) What is the *term value* of the ground state $1s^2 2s$?
    b) What is the *binding energy* of $1s^2 2s$?
    c) What is the term value of $1s^2 3d$?
    d) What is the term value of 3d in H?

20. In He I there is a state with the energy 166271 cm^{-1} and the term value 32034 cm^{-1}. What is the ionization energy?

21. Use the database at NIST (National Institute of Standards and Technology) in Washington, USA https://physics.nist.gov/PhysRefData/Elements/index.html to obtain level energies in F VII and the ionization limit for F^{+6}
    (*Click on the element symbol in the periodic table, then choose "Levels" among the database icons that appear*. *For the ionization limit, scroll down the NIST table!*)
    a) Calculate the term value of $1s^2 3s$.
    b) Calculate the quantum defect for the 4s, 4p, 4d and 4f states. Use the center-of-gravity energies ($2j+1$ weighted mean) for the 4p ^2P and 4d ^2D terms.

22. In He-like Carbon, C V, the excitation energy of 1s3s ^1S is 2851180 cm^{-1} and for 1s4s ^1S it is 2988246 cm^{-1}. Estimate the ionization energy. Compare with the value in the NIST database!

23. **Hand-in 1 (0.5 point)**
    The spectrum shows the series 3p - *n*d, *n* = 4 - 7 in Na as well as the resonance line 3s - 3p, with the experimental vacuum wavelengths in Å.



    a) Why does the 3p - 5s transition (6160 Å) occur at a much longer wavelength than 3p-5d?
    b) Calculate the quantum defect for the nd ^2D *n* = 4-7 terms. Estimate, as accurately as possible, the wavelength for 3p - 8d. The ionization energy in Na I is 41449.6 cm^{-1}. Neglect all finestructure.

24. *Ionization energy in He-like C, C V.*
    An accurate experimental value is (3162408 ± 20) cm^{-1}.
    a) Estimate the ionization energy by completely neglecting the repulsion between the electrons.
    b) Now refine your value by making a semi-classical estimate of the repulsion energy by simply assuming that the two electrons always are on the opposite side of the nucleus from each other, i.e. separated by the diameter of the first Bohr orbital.
    c) Use first order perturbation theory to calculate the ionization energy in C^{+4}. Note that the repulsion energy, to first order, is a linear function of *Z* given by $E_{\mathrm{rep}} = 1.25 \cdot R \cdot Z$ for $1s^2$ in a two electron system, see e.g. AP eq. 3.24.

25. **Hand-in 2 (1 point)**

Derive the electrostatic repulsion potential felt by an outer electron in Li, e.g. a 4f electron being attracted to the nucleus and repelled by the two inner 1s electrons. This calculation gives an indication of how a self-consistent-field solution in the central field approximation is obtained.

a) Write down the total charge density of the two 1s electrons, i.e.

$$\rho(r) = -2 \cdot e \cdot \left|\phi_{100}(r,\theta,\varphi)\right|^2$$

Here we rather crudely assume that both electrons move independently and feel the full charge, +3e, from the nucleus.

b) To obtain the corresponding electrostatic potential you have to solve Poisson's equation:

$$\nabla^2 V(r) = -\rho(r)/\varepsilon_0 \Leftrightarrow \frac{1}{r}\frac{d^2}{dr^2}(rV(r)) = -\rho(r)/\varepsilon_0.$$

Where we have used the radial part of ∇^2 in polar coordinates, as we did when solving the one-electron problem. Derive $V(r)$ by direct integration. This requires some partial integrations and a bit of work!

Hint: Introduce new help variables to get nice looking equations without any explicit fundamental constants and do not forget the integration constants. Use reasonable boundary conditions (at $r = 0$ and $r = \infty$) to determine the integration constants.

c) Plot the final repulsion energy $U(r) = -e \cdot V(r)$, the Coulomb energy from the nucleus, and the sum in the same plot frame. Use eV as the energy unit and a_0 as the unit for distance.

26. The table gives the energies in the 3s3p configuration in Mg I and in Mg-like Fe XV.

a) Give the *LSJ*-designations for the levels.

b) Is the Landé interval rule valid in the two atoms?

c) A line at 417.26 Å in the solar spectrum has been identified as emanating from the 3s3p configuration in Fe XV. Which transition is it? Would you expect an analogous line in Mg I?

E / cm^{-1}	
Mg I	**Fe XV**
21850.405	233842
21870.464	239660
21911.178	253820
35051.264	351911

27. Prove that the number of fine structure levels in an *LS*-term is $\mathrm{Min}(2S+1, 2L+1)$.

28. *sp – pp' transitions.*

a) What *LSJ*-levels do these configurations give rise to?

b) Which transitions are (*LS*) allowed between these configurations?

29 *p^2 – pd transitions.*

a) What *LSJ*-levels do these configurations give rise to?

b) Which transitions are allowed between these configurations in *LS*-coupling?

30. The table below gives J-values and energies for the levels in the 3p4s and 3p7s configurations of Si I.

E / cm^{-1}

J	**3p4s**	**3p7s**
0	39683.163	61538.05
1	39760.285	61595.43
2	39955.053	61823.55
1	40991.884	61881.60

a) Give the LSJ-designation for the levels.

b) Why do the two configurations have nearly the same ΔE (2 - 0) but quite different ΔE (1 - 1)?

c) Give the jj-designation for the levels in 3p7s.

31. Hand-in 2 (0.5 point)

A 125 cm^3 gas cell contains lithium vapor with a pressure of 135 Pa at a temperature of 970 K. The total radiated power from the 2s-2p transition at 760.8 nm is 34.7 mW.

a) What is the ratio of the population in 2s and 2p, i.e. $\frac{N_{2p}}{N_{2s}}$.

b) Calculate the lifetime of the 2p term in Li I.

32. We are investigating hydrogen in a plasma with the temperature 4500 ºC. Calculate the probability per atom and second for stimulated emission from 2p to 1s if the lifetime of 2p is 1.6 ns

33. Hand-in 2 (0.5 point)

The table gives the theoretical relative intensities in LS-coupling for all possible ^3F – ^3F transitions.

a) Use this data to verify the sum rules for LS-intensities in a multiplet.

b) Use the sum rules to derive the relative intensities in a ^2D – ^2F multiplet.
Hint: denote the intensities a, b and c and solve a system of equations.

	$^3F_2$	$^3F_3$	$^3F_4$
$^3F_2$	640	80	--
$^3F_3$	80	847	81
$^3F_4$	--	81	1215

34. Hand-in 2 (0.5 point)

Line widths in wavelength units.

a) The 3p level in Na I has a lifetime of about 16 ns. Calculate the natural line width (in Å) of the 3s – 3p transition at 5890 Å.

b) If the Na-atoms are created in an oven with a temperature of 700 K what is the Doppler width of the 5890 Å transition.

c) Assume the spectrum is analyzed in the first spectral order using a 5 cm wide grating with 2400 lines/mm. What is the smallest possible observed line width? (In practice it will most likely be much larger!)

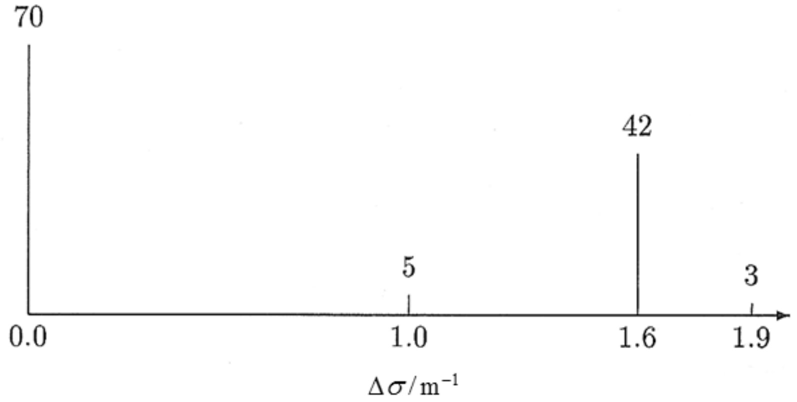
d) In the spectrum of He there is a line at 2578 Å that corresponds to the transition 2s2p ^3P – 2p3p ^3D, i.e. a transition between two doubly excited configurations. The excitation of both electrons in He requires so much energy that these configurations are situated above the first ionization limit. This also means that the states have a probability to decay through the emission of an electron, so called autoionization. If possible, this process is very probable and leads to very short lifetimes. Assume that *both* terms have a lifetime of 1 ps and calculate the natural line width of the 2578 Å transition.

35. *Zeeman effect in Na.*
    a) Calculate the g_J-value for the levels $^2S_{1/2}$, $^2P_{1/2}$, $^2P_{3/2}$.
    b) Derive the splitting of the $^2S_{1/2}$ - $^2P_{3/2}$ line in a weak magnetic field when viewed perpendicular to the field.
    c) What is the polarization of the different components?
    d) What is the spacing, in units of 1 cm^{-1} and in 1 eV, between the closest-lying components if the magnetic field is 1 T?
    e) Look up the wavelengths of the two fine structure lines 3s – 3p in Na I. What magnetic field would produce a Zeeman splitting, as in 32d), equal to the energy difference between these lines?

36. *Zeeman vs. Paschen-Back effect.*
    With a weak magnetic field we first couple ***L*** and ***S*** to ***J*** and use $|LSJM_J\rangle$ coupled wavefunctions to calculate the magnetic contribution as a perturbation. If, on the other hand, the external magnetic field becomes sufficiently strong (e.g. in a white dwarf star) the order should be reversed, i.e. we first evaluate the magnetic interaction using the wavefunctions $|LM_LSM_S\rangle$ (which is much easier) and then take the spin-orbit interaction $<\beta \boldsymbol{L}\cdot\boldsymbol{S}> = \beta\cdot<L_z\cdot S_z>$ into account. Make a clear and easily understandable table of the energies, and draw an energy diagram showing the splittings of a ^3P term in the 2 cases: Zeeman: $\mu_B B = \frac{1}{10}\beta$, and Paschen-Back: $\mu_B B = 10\beta$. (Strictly, the factor should be larger than 10 for the perfect extreme cases, but then it will be difficult to draw nice diagrams!)

37. The figure below shows the hyperfine structure in the transition 6s $^2S_{1/2}$ - 8p $^2P_{3/2}$ in ^{115}In (I = 9/2). The measurement is made using a narrow-band tunable laser and a collimated atomic beam; hence the Doppler width is greatly reduced. The 6 components shown have the following frequencies 31, 112, 210, 8450, 8515 and 8596 MHz. Draw a schematic figure of the energy levels with the appropriate quantum numbers and show the allowed transitions. Determine the hyperfine constants, in MHz, for the two fine structure levels

38. A high-resolution scan over the resonance line 4s $^2S_{1/2}$ - 4p $^2P_{1/2}$ in K I is shown in the figure below, where the relative positions and intensities of the observed hyperfine components are given. Naturally-occurring potassium is a mixture of the isotopes ^{39}K and ^{41}K in the ratio 14:1. Identify the lines in the figure and deduce the nuclear spin of the two isotopes.



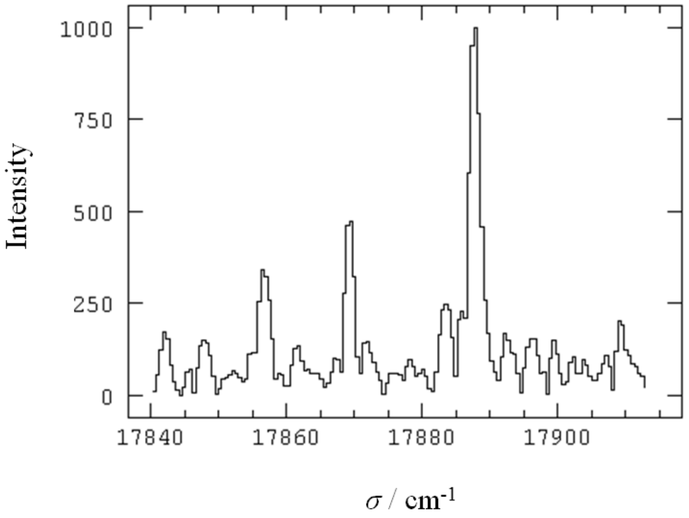
39. The observed spectrum of F^{6+} (F VII) contains, among many other lines, the following wavelengths with their estimated relative intensities corresponding to transitions among levels with $n \leq 3$. The intensities are not calibrated, and can hence only be compared between closely spaced lines. Use this data to derive the energies (in cm^{-1}) for all observed levels with $n \leq 3$ in F VII.

λ_{vac} / Å	***Rel. Int.***
112.941	806
112.977	410
127.653	950
127.799	1600
134.707	430
134.882	870
883.11	1700
890.79	800
3247.48	130
3277.90	60

Hint: Start by drawing a term diagram with roughly the correct relative energies of all the possible terms $1s^2nl$ with $n \leq 3$ and indicate their fine structure levels. Then solve the "puzzle", making good use of the relative intensities. The better your relative energies are the easier it will be to solve the problem. Check as much as you can that the solution is consistent.

40. The Ca spectrum below, recorded using a Fourier Transform Spectrometer (FTS), shows the resolved 3d4s ^{3}D - 3d4p ^{3}D multiplet. The wavenumbers and their relative intensities are given in the table. Identify all the lines and determine the fine structure constants in the two triplets (both are positive).

σ / cm^{-1}	***Rel. Int.***
17841.88	106
17847.70	101
17856.50	353
17869.12	414
17883.32	250
17887.54	1074
17909.46	160



41. A classical model for the vibration of the Oxygen- and Carbon-atom in a CO molecule can be obtained as follows. The potential energy of the binding force between the atoms, as a function of their separation, r, is quite accurately given by the Morse potential:

$$U(r) = D\cdot(e^{-2a\cdot(r-r_0)} - 2e^{-a\cdot(r-r_0)}).$$

Here D = 11.36 eV is the binding energy. The equilibrium distance between the atoms is r_0 = 1.15 Å and the empirical constant a = 2.29 Å^{-1} for CO.

a) Draw a diagram of the Morse potential between e.g. $0.8 \le r \le 5$ Å.

b) Assume that the kinetic energy due to the vibration is 9.36 eV. What is then the smallest and largest possible separation between the atoms in a classical picture?

c) To simplify the calculations we approximate the Morse potential by a harmonic oscillator. This approximation should be quite accurate if we are close to the minimum in the real potential ($r \approx r_0$). Calculate a number of values for the Morse potential very close to r_0 and fit a second order polynomial to the data. Draw the polynomial in the same figure as in a). In what range would you say that the approximation is reasonable?

d) Use the general expression

$$F = -\frac{dU}{dr}$$

to show that the ”spring constant” [k in the expression for the force in a harmonic oscillator $F = -k\cdot(r - r_0)$] is twice the coefficient for the second order term in the polynomial approximation.

e) Use your value of k together with the reduced mass μ of the CO-molecule to calculate the vibrational frequency from the harmonic oscillator model:

$$\omega_0 = \sqrt{\frac{k}{\mu}}.$$

Compare with the experimental result $\omega_0 = 3.97\cdot10^{14}$ rad/s => $f = 6.32\cdot10^{13}$ Hz.

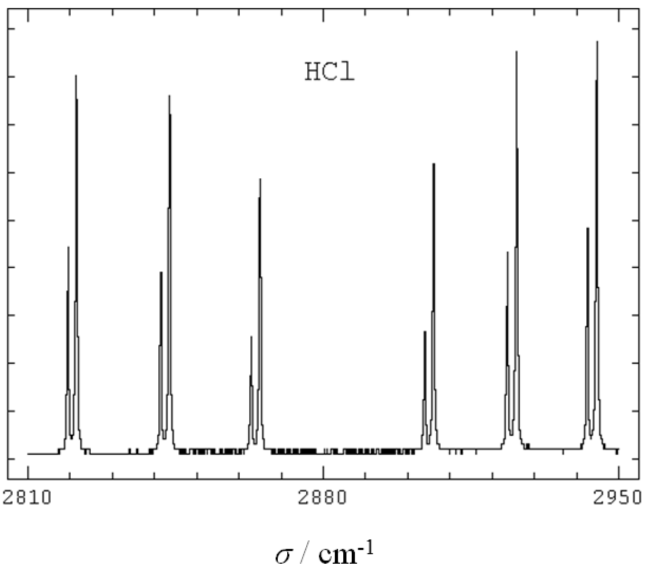
Hint: make sure that you get the unit of k correct for this calculation.

42. The rotation fine structure in the *n* = 0 - *n* = 1 vibration transition in HCl is shown in the figure. The wavenumbers for the 4 central lines are given in the table. Chlorine has two isotopes ^{35}Cl (76%) and ^{37}Cl (24%), with mass 34.968852 and 36.965903 u, respectively. Use the data in the table to:

a) Determine the equilibrium distance between the H and Cl atoms in the two isotopes.

b) Determine the resonance frequency for the vibration of the atoms in the two isotopes.

σ / cm^{-1}	***Rel. Int.***
2862.8404	216
2864.9120	511
2903.9340	231
2906.0693	532



43. Hand-in 2 (0.5 point)

The wavenumbers for the first 3 members of the *R* and *P* branch in the 0 - 2 vibrational transition in CO are given in the Table below.

Wavenumbers of the *R* and *P* branch in CO

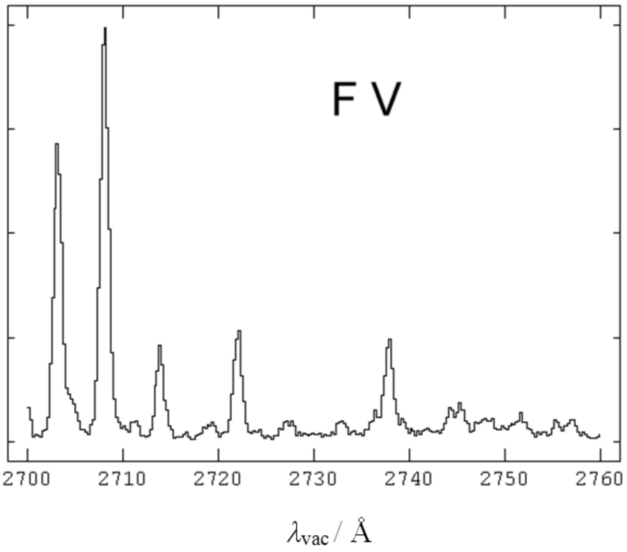
σ / cm-1
4248.13
4252.13
4256.06
4263.65
4267.37
4271.01

a) Determine the energy difference between the vibrational levels 0 and 2 and the rotation constant, *B*, (in the unit 1 cm^{-1}) assuming that the moment of inertia is the same in both states.

b) Repeat the analysis but this time take into account that the rotation constants, *B*" (*v* = 0) and *B*' (*v* = 2) are not exactly equal.

44. The lines in the table below are identified as transitions to a quartet P from two higher-lying quartets (S and D) in F V. ^{4}P - ^{4}S have wavelengths around 2250 Å while the ^{4}P - ^{4}D transitions occur around 2700 Å. All possible transitions in the latter multiplet, shown in the figure, could not be resolved in the experiment. Identify all the lines!

λ_{vac} / Å	***Rel. Int.***
2241.14	320
2253.75	610
2277.73	820
2703.10	710
2707.97	990
2713.68	200
2721.87	270
2737.72	240
2756.99	50



Hint: All the terms involved have a positive fine-structure constant. Furthermore, in pure *LS*-coupling the relative intensities in a ^{4}P - ^{4}D multiplet is given in the table below. Even if a real term system is not perfectly described in *LS*-coupling these relative intensities is often of great qualitative help.

		^{4}D			
		7/2	5/2	3/2	1/2
^{4}P	5/2	120	27	3	
	3/2		63	32	5
	1/2			25	25

45. In the Zeeman laboratory exercise you study the multiplet 5s5p ^{3}P - 5s6s ^{3}S in Cd I in a magnetic field. Here we investigate another multiplet in Cd, with no external field. The figure below shows the observed 5s5p ^{3}P - 5s5d ^{3}D multiplet, where the inset gives a magnified picture of the three rightmost lines.

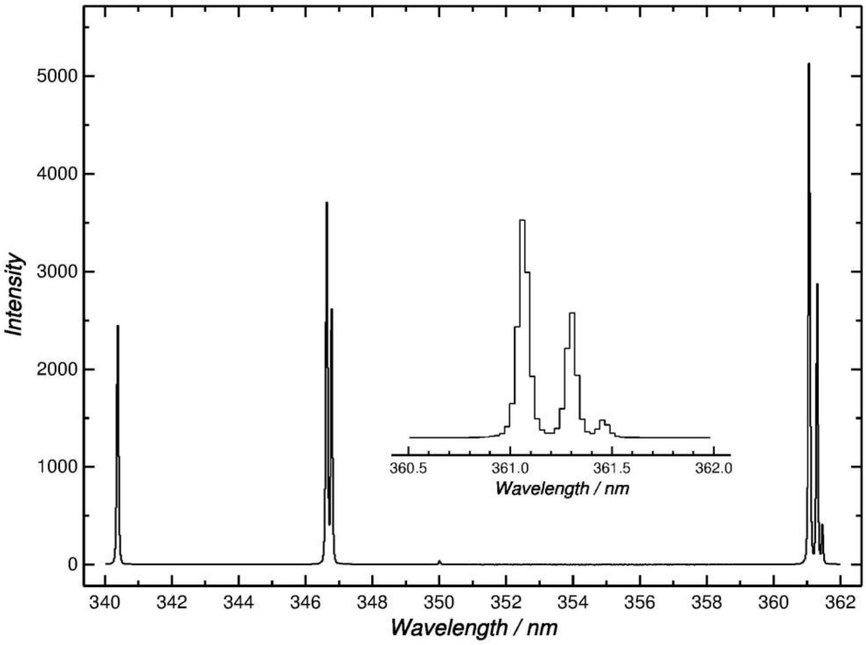


Table 1 list the wavelengths and relative intensities obtained in the spectrum and Table 2 gives the experimental energies for the ^{3}P levels.

Table 1.

λ_{vac} / nm	**Relative Intensity**
340.4629	2183
346.7193	3363
346.8648	2566
361.1538	4824
361.3903	2615
361.5484	389

Table 2

5s5p^{3}P$_J$	***E* / cm^{-1}**
0	30113.99
1	30656.09
2	31826.95

a) Identify the six transitions.

b) Derive the energies of the ^{3}D levels, as accurately as possible from the given data.

c) Check the Landé interval rule in both ^{3}P and ^{3}D. Is this consistent with *LS*-coupling? If not, what could be the reason(s)?

d) Check the sum rules using the experimental intensities. Is this consistent with *LS*-coupling? If not, what could be the reason(s)?

e) The barely noticeable peak at 350 nm is the so-called forbidden transition 5s5p ^{3}P$_1$ - 5s5d ^{1}D$_2$. How does such a line arise?

46. Neutral indium has atomic number 49 and the ground configuration [Kr]$4d^{10}\,5s^2\,5p$ (or just 5p), and nuclear spin $I = 9/2$. Figure 1 shows the spectral lines between 6p $^2P_{1/2}$ and 7s $^2S_{1/2}$ and Figure 2 those between 6p $^2P_{3/2}$ and 7s $^2S_{1/2}$. Both Figures shows (parially) resolved hyperfine structure, and are produced in a hollow cathode and measured with the Lund FTS. The table gives all observed wavenumbers.

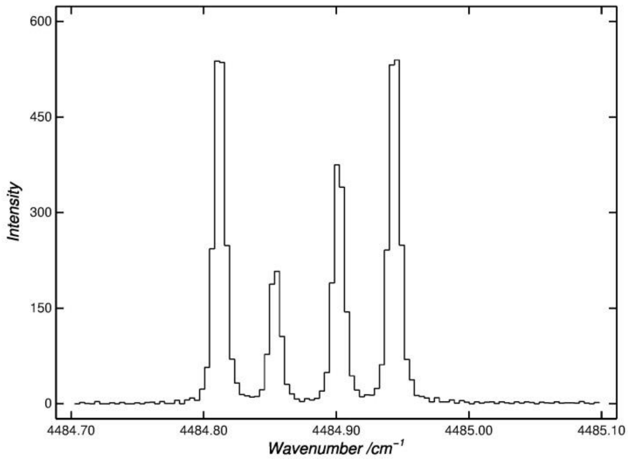


Figure 1. 6p $^2P_{1/2}$ - 7s $^2S_{1/2}$

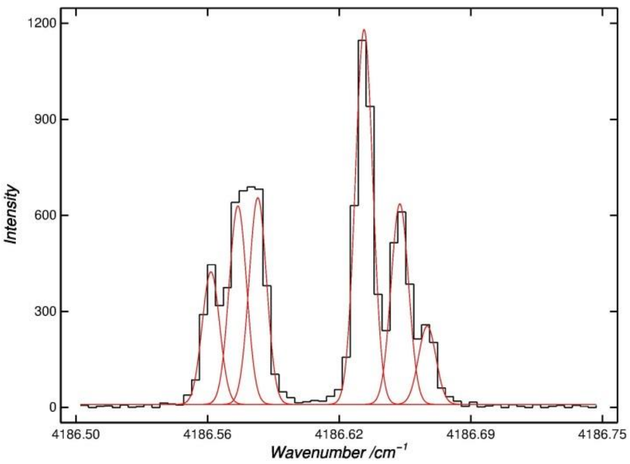


Figure 2. 6p $^2P_{3/2}$ - 7s $^2S_{1/2}$

Wavenumber / cm^{-1}	Intensity / a.u.
4484.810	585
4484.852	214
4484.900	390
4484.942	583
4186.562	417
4186.575	622
4186.585	647
4186.635	1173
4186.652	629
4186.665	248

a) Identify the lines and draw an energy diagram of the hfs structure in all levels involved.

b) Derive the hyperfine constants for the levels (all are positive).