

Spectral analysis of Ca I

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Abstract

In this project spectra of neutral calcium between 2000-30000 cm^{-1} have been recorded by the Fourier Transform Spectrometer Bruker HR IRFTS at Lund Observatory. Using 204 spectral lines, 78 energy levels in the calcium atom have been derived. Level mixing and self absorption of some transitions are discussed. The energy levels in the previously not resolved triplet $4s5g\ ^3G$ have been measured in this project.

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Introduction

Spectroscopy is a widely used and very multifaceted research method and is used in many areas in science: astrophysics, atomic physics, chemistry and geology to name a few.

In astrophysics one takes advantage of the fact that every atom and molecule has its own spectrum, which means that by studying light from e.g. a star, the elemental stellar composition can be determined. In addition, the line profiles can tell us about things such as the temperature and density of the star. In laboratory astrophysics the main questions are *What problems are encountered in astrophysics? Which of these can be solved by laboratory work?* New results in laboratory work thus help astrophysics forward, and it is therefore important to have as accurate data as possible.

An example of where spectroscopy has been used in space is the Goddard High Resolution Spectrograph (GHRS) on the Hubble Space Telescope (HST). The GHRS has high resolution in the ultraviolet region and a high signal-to-noise ratio. This has been used in e.g. a project where observations of hyperfine components and isotopic shifts in stellar spectra have been made (Leckrone et. al. 1996).

In this project spectroscopy has been used as the means of determining wavelengths and energy levels in neutral calcium. The reason calcium was chosen to be investigated is that this element has a high cosmic abundance, and is therefore often encountered in stellar spectra. In addition, there are some levels that have not been derived earlier, but with the high resolution of the Fourier Transform Spectrometer (FTS) used for the recording of the spectra, they have been derived in this analysis. The lines in the spectra give the energy of the transition between two levels, and with the definition that the energy of the lowest level is 0 cm^{-1} , the energies of the other levels have been derived.

The spectra were recorded with the Lund Observatory Bruker HR IRFTS. The FTS was chosen because it has many advantages, such as a high resolution, a high wavenumber accuracy and a wide spectral range.

Theory

LS-coupling

An electron can be collisionally excited to any level, but the deexcitation through emission of a photon is controlled by a set of rules based on the so called *LS*-coupling.

To be able to describe the origin of *LS*-coupling and what *LS*-coupling is, a brief introduction of many electron systems and the central field approximation is given below. For a more detailed description see Thorne et.al. (1999).

In an atom with charge $+Ze$ and N electrons the Hamiltonian energy operator can be written as follows:

$$H = \sum_{i=1}^N \left(\frac{-\hbar}{2m} \nabla_i^2 - \frac{Ze^2}{4\pi\epsilon_0 r_i} \right) + \sum_{i<j=1}^N \frac{e^2}{4\pi\epsilon_0 r_{ij}} + \sum_{i=1}^N \xi(r_i) (\vec{l}_i * \vec{s}_i) \quad (1)$$

where r_i is the distance between an electron and the nucleus and $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the distance between two electrons i and j .

The first sum represents the radial part of the kinetic (first term) and potential (second term) energy of all electrons in the field around the nucleus, while the second sum shows the potential energy from the repulsion between the electrons. Finally, the third sum adds the potential energy originating from the magnetic interaction between the magnetic moment (caused by the spin of the electrons) and the magnetic field (caused by the orbital motion of the electrons). \hbar is $h/2\pi$, m is the mass of the electron, ∇_i is the Laplace operator acting on the wave function for each electron in the Schrödinger equation, e is the charge of the electron, l_i is the angular momentum of the electron and s_i is its spin. The function $\xi(r_i)$ is proportional to $1/r_i$ and $dV(r_i)/dr_i$, where $V(r_i)$ is the potential (Cowan 1981).

In the central field approximation the non-central part of the electron-electron repulsion and the spin-orbit interaction are neglected, and the approximation can be described as if each electron moves independently of the other electrons in the atom in a spherically symmetric field that is created by the nucleus and the other electrons. The Hamiltonian can then be expressed in the following way:

$$H = \sum_{i=1}^N \left(\frac{-\hbar}{2m} \nabla_i^2 + V(r_i) \right) \quad (2)$$

where $V(r_i)$ is the potential energy of the electron in the central field. With this the Schrödinger equation describing the state of the system becomes:

$$\left[\sum_{i=1}^N \left(\frac{-\hbar}{2m} \nabla_i^2 + V(r_i) \right) \right] \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = E\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \quad (3)$$

This can be divided into N one electron equations:

$$\left(\frac{-\hbar}{2m} \nabla_i^2 + V(r_i) \right) \psi(\bar{r}_i) = \varepsilon_i \psi(\bar{r}_i) \quad (4)$$

A solution to equation (3) is:

$$\Psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = \psi_1(\bar{r}_1) \psi_2(\bar{r}_2) \dots \psi_N(\bar{r}_N) \quad (5)$$

The total energy is:

$$E = \sum_{i=1}^N \varepsilon_i \quad (6)$$

In *LS*-coupling the contribution to the energy due to the non-central electron-electron repulsion and the contribution from the magnetic spin-orbit interaction are included (compare with the central field approximation where these were neglected).

By adding the non-central interaction between the electrons as a perturbation to the central field energy, each configuration is split into terms (energy levels). The spin-orbit interaction is then added as a perturbation to these term energies and each term is then further split.

LS-coupling is valid when the non-central interaction is much bigger than the spin-orbit interaction (for the other way around the system is described by *jj*-coupling). It works best for the lightest elements, but is quite good for medium heavy elements as well.

With *LS*-coupling we get new quantum numbers *L*, *S* and *J* (Thorne et. al. 1999) that are related as follows:

$$\bar{J} = \bar{L} + \bar{S} \quad (7)$$

The quantum number *L* is the total orbital angular momentum, *S* represents the total spin angular momentum and *J* is the total angular momentum. *L* and *S* are given by:

$$|l_1 - l_2| \leq L \leq l_1 + l_2 \quad (8)$$

$$|s_1 - s_2| \leq S \leq s_1 + s_2 \quad (9)$$

The level of a configuration can be written as:

$${}^{2S+1}L_J \quad (10)$$

Where ${}^{2S+1}L$ is the term and $2S + 1$ is the multiplicity of the term. The multiplicity tells us the maximum number of levels a term can have, e.g. $2S + 1 = 1$ tells us that the term is a singlet while $2S + 1 = 3$ indicates that the term is a triplet.

The rules that an electron has to follow for a transition to be allowed are:

$$\left. \begin{array}{l} \Delta L = 0, \pm 1 \quad \text{where } 0 \text{ to } 0 \text{ is forbidden} \\ \Delta S = 0 \end{array} \right\} \text{These two are only valid in } LS\text{-coupling}$$

$$\Delta J = 0, \pm 1 \quad \text{where } 0 \text{ to } 0 \text{ is forbidden}$$

$\Delta\pi = \text{yes}$ π stands for parity and yes means that the parity has to change.

The parity operator is $P = -1^{\sum l_i}$, which means that the parity can be either 1 (even) or -1 (odd). For the wavefunction of a particle this means:

$$\Psi(\vec{r}) = \Psi(-\vec{r}) \quad \text{when the parity is even}$$

$$\Psi(-\vec{r}) = -\Psi(\vec{r}) \quad \text{when the parity is odd}$$

During the transition between two levels, the photon takes the parity 1 with it, and therefore this rule is necessary. Since parity depends on l , the rule can also be written:

$$\Delta l = \pm 1$$

Transitions that do not follow these rules are called forbidden lines, which does not have to mean that they are forbidden, but only less probable than the others. This holds for atoms that can be described by LS -coupling. However, this approximation does not work perfectly for all elements and sometimes the rules are broken.

Transitions that do not follow $\Delta S = 0$ are called intercombination lines.

Level mixing

As mentioned above, LS -coupling does not work impeccably for all elements. When the coupling starts to fail, energy levels get mixed and transitions that were not allowed earlier can take place. This mixing can be explained by means of perturbation theory, and will be briefly described here.

The spin-orbit energy contribution is added as a perturbation, using a time independent first order perturbation (Thorne et. al. 1999). This is written as:

$$E'_{so} = \langle \Psi_1 | H | \Psi_1 \rangle \quad (11)$$

where Ψ_1 is the unperturbed wave function and H is the perturbation operator.

The time independent second order perturbation is expressed as:

$$E''_{so} = \frac{|\langle \Psi_1 | H | \Psi_2 \rangle|^2}{E_1 - E_2} \quad (12)$$

where Ψ_1 and Ψ_2 are unperturbed wave functions, H is the perturbation operator and E_1 and E_2 are the energies for the two levels. When Ψ_1 and Ψ_2 are two different

wavefunctions they are orthogonal to each other, which means that the second order perturbation is equal to zero.

But in the case of where Ψ_1 and Ψ_2 are linear combinations with at least one common component, the second order perturbation is not equal to zero. The second order perturbation then shifts the levels away from each other. This means that the upper level is shifted up and the lower level is shifted down. A condition for this to happen is that the levels that are mixed must have the same parity and the same J-value.

Experiment

Equipment

The Fourier Transform Spectrometer

The Fourier Transform Spectrometer (FTS) is based on a Michelson Interferometer. These two instruments are basically the same, apart from that one of the mirrors in the FTS is moveable in the direction of the light. The FTS makes use of the interference pattern that is created in the Michelson Interferometer, and the rings of this pattern will change between destructive and constructive interference as the mirror is moved. Only the inner ring is observed since if the whole pattern is studied the output signal will be constant. This is

because one ring changes from light to dark (i.e. from constructive to destructive interference), the next from dark to light and the third from light to dark and so on. This results in no changes in the total output signal, i.e. a constant signal.

The Michelson interferometer consists of two lenses, two mirrors and a beamsplitter as seen in Figure 1. Light enters the interferometer, gets

collimated by the first lens and reaches the beamsplitter where it gets partly reflected to mirror M_1 and partly transmitted to mirror M_2 . At M_1 and M_2 the light is reflected back to the beamsplitter, where half of the light from M_1 passes right through it (the other half is reflected back to the light source) and half of the light from M_2 is reflected (the other half is transmitted). The beams are recombined at the beamsplitter, and the second lens images the light on the detector.

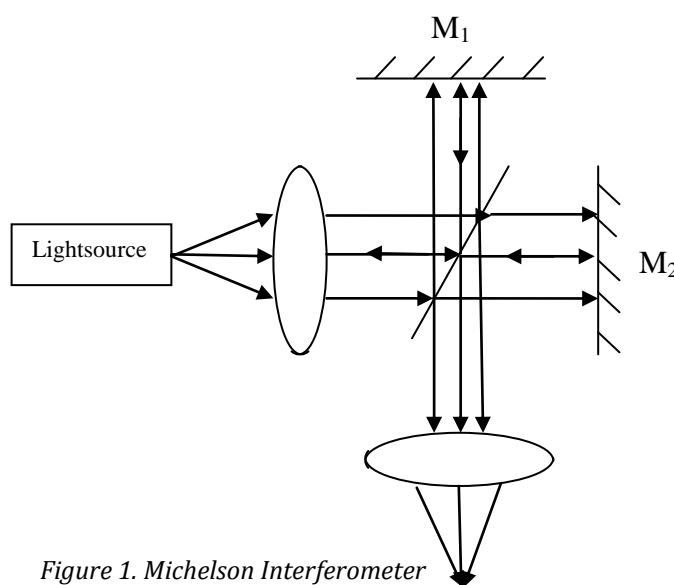


Figure 1. Michelson Interferometer

When we move one of the mirrors in the FTS the two beams create either destructive or constructive interference depending on the difference in distance the two beams

have travelled. If the light source is monochromatic, the detector will detect a cosine signal with a frequency that depends on the velocity of the mirror and the wavenumber. Having a light source with several different wavelengths will result in a signal that is a sum of cosine functions with different frequencies. The output signal will give us the intensity as a function of the position of the mirror. This is called the interferogram. By performing a Fourier transform on the interferogram we will get a spectrum with intensity as a function of the wavenumber.

The Hollow Cathode Discharge Lamp

A hollow cathode (HC) discharge lamp was used as a light source. In this discharge the cathode, as the name implies, has the shape of a cylinder with a hole through it. The hole has a diameter of about 10mm. The element that is going to be studied, in our case it is calcium, is placed in the cathode cylinder. It is in the cathode the discharge will take place and make the carrier gas and calcium glow.

The rough set-up of the hollow cathode is shown in Figure 2.

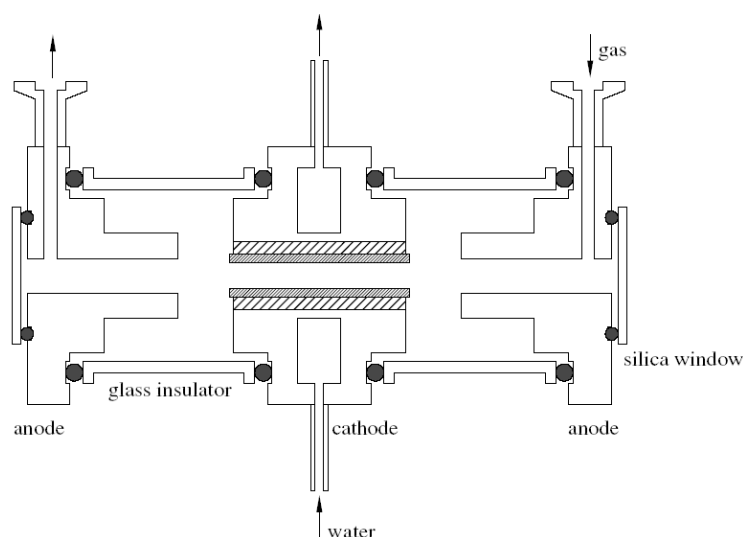


Figure 2. Hollow Cathode lamp. Figure by courtesy of Ulf Litzén

Neon was used as the carrier gas. Inside the lamp the gas is excited and ionized by free electrons, and the ions are accelerated towards the cathode where they will sputter material from the walls of the cathode. The calcium atoms will interact with the ionized gas through electron collisions, and thereby get excited. When these atoms deexcite light will be emitted, and it is this light that will be analysed.

Since it is not just the calcium atoms that will emit light, but the neon gas as well, spectral lines of both calcium and neon will be visible in the final spectrum. In addition, some lines from iron will be visible, since the cathode is made of this material.

An important thing when dealing with a HC lamp is to make sure it is cooled with water since the lamp gets very hot due to the sputtering that deposits energy into the cathode. The ion temperature in the HC lamp can be decided using the Doppler

broadening of the spectral lines:

$$\Delta\sigma_D = \sigma * 7.16 * 10^{-7} * \sqrt{T/M} \quad (13)$$

$$T = \frac{M}{(7.16 * 10^{-7})^2} * \left(\frac{\Delta\sigma_D}{\sigma}\right)^2$$

σ is the wavenumber (cm^{-1}), $\Delta\sigma_D$ is the Full Width at Half Maximum (FWHM) of the spectral line, T is the temperature (K) and M is the mass number (40 for Ca). A number of lines measured in this project (Appendix 1) was used to investigate the ion temperature in the HC lamp during this project:

σ (cm^{-1})	$\Delta\sigma_D$ (cm^{-1})	T (K)
3239.6164	0.01031	790
9664.9650	0.03049	777
15381.2022	0.05045	839
21800.0295	0.07694	972
27428.7978	0.09230	884

Table 1. Ion temperature estimated from Doppler broadening

The mean temperature is:

$$T_{mean} \approx 852 \pm 70 \text{ K}$$

Measurements

The HC lamp was evacuated by using two pumps. This is done because the purpose is to study spectral lines from calcium and not from molecules in the air, such as nitrogen. Furthermore, the molecules prevent an efficient discharge. The pumping is carried out by two vacuum pumps to get as low pressure as possible, about 10^{-3} Torr.

However, a perfect vacuum will not be reached so after letting the carrier gas in, the HC lamp is “turned on” (i.e. a power supply applies voltage and current on the lamp) and is set burning for a few hours to sputter out some of the molecules and impurities that could not be removed with the pumps. This procedure of “pumping and burning” is repeated for a few hours every day in a week to make sure that a “clean” environment as possible is obtained.

Spectra between $2000\text{-}30000 \text{ cm}^{-1}$ were recorded with the Lund Observatory Bruker HR IRFTS. Five different experimental set-ups were used:

Set-up	Detector	Beamsplitter	Approximate wavenumber range (cm^{-1})
1	InSb	CaF ₂	2000-16000
2	InGaAs	CaF ₂	6000-10000
3	Si	CaF ₂	8000-20000
4	Si	Quartz VIS	8000-26000
5	PMT VIS	Quartz VIS	10000-30000

Table 2. The five set-ups

The HC-lamp was run at a carrier gas pressure of 1 Torr. The current and voltage were adjusted until the light source was stable. In these five different set-ups the current throughout the HC lamp was between 150-500 mA. The colour of the discharge is an indication of the presence or absence of unwanted molecules. A colour mainly indicating neon in the HC-lamp is red/orange, while blue is a sign of other elements, such as nitrogen. The unwanted elements are removed (although not completely) by “pumping and burning”, and a colour check is a good way to make the final decision whether it is time to start the spectrum recording or not. This was done not only by the naked eye, but also with a spectroscope. If there are molecules present, instead of thin spectral lines one sees broad molecular bands.

A number of settings are made on the FTS to make sure the correct conditions for each recording is set. One of these settings is the resolution. This has to be adjusted for every recording where a new set-up is used. The reason for this is that (13) tells us that e.g. a smaller wavenumber results in a more narrow line, which requires a higher resolution. The way of estimating the resolution needed is done with help from Doppler broadening, where (13) is used. The resolution should be chosen so that $\Delta\sigma_{FTS} < \Delta\sigma_D$ to assure that the Doppler width is the limiting factor and not the instrumental profile. The following resolutions were used for the different set-ups (σ = the lower limit of the range in each set-up, T=500K, M=40). The reason the temperature was chosen to 500 K, which is about 300-500 K lower than what was calculated under *Hollow Cathode Discharge Lamp*, is that it is better to have a higher than a lower resolution necessary to resolve the lines:

Set-up	Resolution (cm ⁻¹)	Maximum mirror movement (cm)
1	0.005	100
2	0.01	50
3	0.02	25
4	0.02	25
5	0.04	12.5

Table 3. Resolution of the FTS for the five set-ups

The third column is calculated through the relation:

$$\Delta\sigma_{FTS} = \frac{1}{2L} \quad (14)$$

where L is the maximum movement of the moveable mirror.

For each set-up about 3 spectra were recorded, and the best one among these was chosen for the analysis, i.e. one spectrum for each set-up was used. The criterion that was taken into consideration was the signal-to-noise ratio of the calcium lines.

As a starting point for the analysis the energy levels reported by J. Sugar and C. Corliss, 1985 was used. From these levels Ritz wavelengths (i.e. wavelengths derived from experimentally established energy levels) were derived.

All spectra were studied in the computer program OPUS, and the lines in our spectra were compared to the derived Ritz wavelengths. This gave a rough estimate of what the highest levels from which transitions were visible.

To be able to compare the five spectra with each other the noise has to be set to the same level in all spectra. This was done in OPUS by multiplying the spectra with different factors so that the noise had the intensity one in all of them.

The measuring of the lines was performed in the computer program GFit (written by L. Engström). Since the different detectors have different sensitivity in the wavenumber region, every spectra is measured in the interval where it is best represented. GFit fits a theoretical line profile to the experimental line and calculates the wavenumber, intensity and Full Width at Half Maximum (FWHM) of the fitted profile. All of these properties are saved for each line in all spectra.

The five spectra 1, 2, 3, 4 and 5, named after their corresponding set-ups, were measured in these intervals:

Spectra	Interval
1	2200-5650
2	5500-10300
3	10200-13500
4	10200-16200
5	16100-30000

Table 4. Spectral intervals measured

Analysis

Wavenumber calibration

The lines in the spectra have a linear shift due to the laser measuring the position of the moveable mirror in the FTS. The laser beam does not have exactly the same path through the instrument as the light from the HC lamp. The spectra therefore have to be calibrated.

The calibration was made using Ne- lines with accurate wavenumbers calibrated against Ar-lines by Norlén (1973). About 10-12 Ne-lines were chosen in each spectra, and the tabulated value (σ_{tab}) was compared with the observed value (σ_{obs}):

$$\frac{\sigma_{obs} - \sigma_{tab}}{\sigma_{tab}} = k \quad (15)$$

k is the correction factor which is used as:

$$\sigma_{corr} = \sigma_{obs}(1 - k) \quad (16)$$

where σ_{corr} is the corrected wavenumber.

For one of the spectra (1) a problem arose during the calibration. In the wavenumber interval represented by this spectrum no Ne-lines were found. Instead lines from the adjacent calibrated spectrum (2) were used to calibrate the spectrum.

Identifying Ca I-lines

The identification of the lines has been carried out in different ways. The first step was to compare the measured lines with the derived Ritz wavelengths. The lines not being identifiable through this method were identified by looking at relative intensities and Doppler broadening.

The relative intensities in a triplet transition calculated assuming LS-coupling can be used to identify the lines. The line that represents the transition between the two levels with the highest J-value is the strongest and the other transitions are certain fractions of this one. The relative intensities for different triplet transitions can be found in a table (Cowan 1981). This method for identifying the lines was used often.

In addition, measuring the Doppler broadening of a spectral line can indicate which element the line belongs to. This is done with equation (13). The fraction between the widths of a calcium line and a neon or iron line (lines from these elements are possible, since the carrier gas is Ne and the cathode is made of Fe) are:

$$\frac{\Delta\sigma_{Ca}}{\Delta\sigma_{Ne}} = \frac{\sigma_{Ca}}{\sigma_{Ne}} \sqrt{\frac{M_{Ne}}{M_{Ca}}} = \frac{\sigma_{Ca}}{\sigma_{Ne}} \sqrt{\frac{20}{40}} \approx \frac{\sigma_{Ca}}{\sigma_{Ne}} * 0.7 \quad (17)$$

Analogous for Fe:

$$\frac{\Delta\sigma_{Ca}}{\Delta\sigma_{Fe}} = \frac{\sigma_{Ca}}{\sigma_{Fe}} \sqrt{\frac{M_{Fe}}{M_{Ca}}} = \frac{\sigma_{Ca}}{\sigma_{Fe}} \sqrt{\frac{56}{40}} \approx \frac{\sigma_{Ca}}{\sigma_{Fe}} * 1.2 \quad (18)$$

By comparing an uncertain lines width with the width of a certain line (i.e. a line surely belonging to calcium), the fraction gives a hint about which element it is. If the fraction is one, this indicates that it is a calcium line.

Energy levels

The only possible level in the ground configuration ($4s^2$) is a 1S_0 with the energy 0 cm^{-1} . This is the starting point from which all the other levels, directly or indirectly, were derived. Some levels were derived by more than one spectral line, so an average value of the energy levels should be calculated. But the intensity of the lines has to be taken into consideration when calculating this average value. This is done easiest with a computer program. The result will however not differ very much from the originally calculated values, and is beyond the scope of this project.

Results and discussion

I report on 76 energy levels in Ca I derived from 194 spectral lines. The measured energy levels and the identified spectral lines are shown in the tables in Appendix 1 and 2, and an energy level diagram in Appendix 3. Compared with the energy levels reported by Sugar and Corliss (1985) my energy levels differ on generally the second or third decimal. The values have not changed much, but are probably more accurate since the measurements in this project are done with a high resolution FTS. The spectral lines measured in this project are also compared to the Ritz wavenumbers derived from the energy levels in Appendix 1 (see Appendix 2). One can see that the weak lines mostly differ on the second decimal, while the stronger lines mostly agree on all three. The deviation from the Ritz wavenumber is shown in Figure 3.

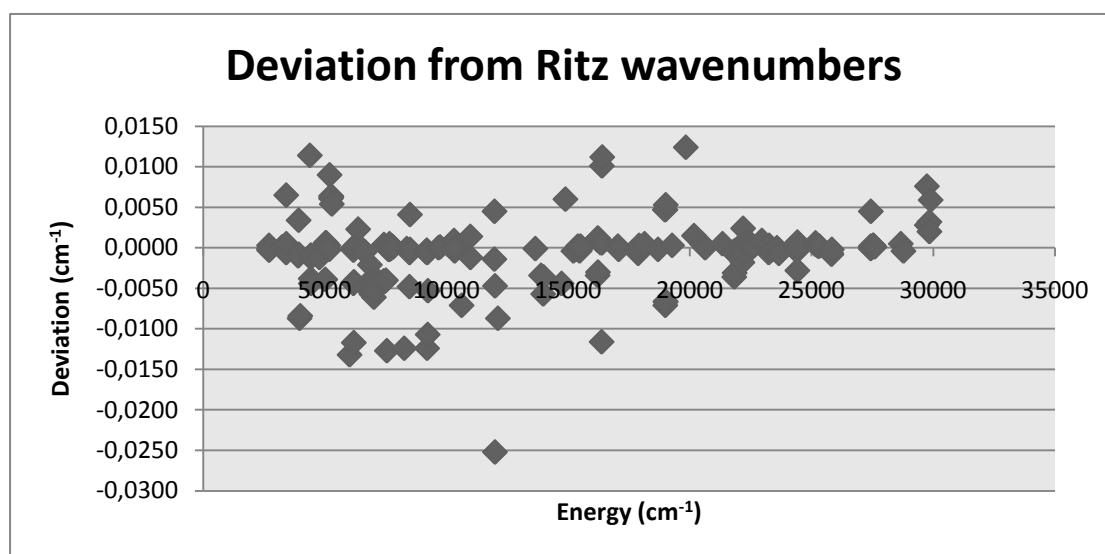


Figure 3. Deviation from Ritz wavenumber

Relative intensities and Landé interval rule

The triplet transition $3d4s\ ^3D - 4s4f\ ^3F$ is one of the transitions where relative intensities were studied:

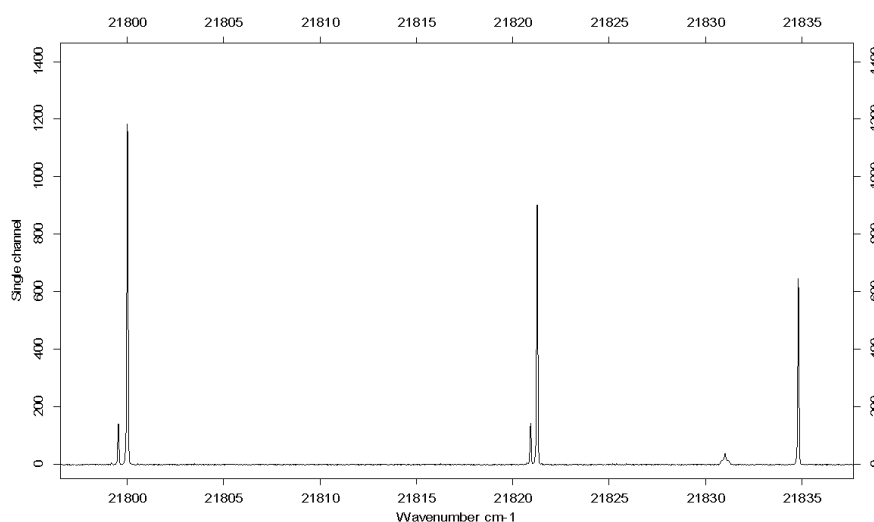


Figure 4. $3d4s\ ^3D - 4s4f\ ^3F$ transitions

4s4f ³F 3d4s ³D	4	3	2
3	100 (100)	10.96 (8.64)	0.33 (0.25)
2	-	73.81 (69.14)	10.81 (8.64)
1	-	-	52.05 (46.67)

Table 5. Relative intensities in the triplet transition $3d4s\ ^3D-4s4f\ ^3F$, the theoretical values in brackets

This is in good agreement with the line strengths calculated assuming LS-coupling (Cowan 1981). A further confirmation that these are the transitions that are studied can be given through Landés interval rule, which in LS-coupling can be described as:

$$\Delta E(J, J - 1) = A * J \leftrightarrow A = \frac{\Delta E(J, J - 1)}{J} \quad (19)$$

The rule says that the energy difference between two levels is proportional to the larger J-value. Applying the rule on the triplets mentioned above, using the tabulated values of the levels in Appendix 1, gives:

$A_{3,2} \approx 7.2\text{ cm}^{-1}$ and $A_{2,1} \approx 6.9\text{ cm}^{-1}$ for the $3d4s\ ^3D$ triplet

$A_{4,3} \approx 0.12\text{ cm}^{-1}$ and $A_{3,2} \approx 0.12\text{ cm}^{-1}$ for the $4s4f\ ^3F$ triplet

The values agree well within each triplet, which indicates that the transitions are correctly identified. Furthermore, this means that LS-coupling is a good approximation. This way of identifying the lines were used frequently in this project.

4s4f ³F-4s5g ³G transition

The $4s4f\ ^3F-4s5g\ ^3G$ triplet transitions have never been reported as experimentally measured before. Often the resolution is too low for resolving the lines. Still, the strongest transition has been measured by Litzén (1982). In this project the three strongest transitions (Figure 5) were visible thanks to the high resolution of the FTS.

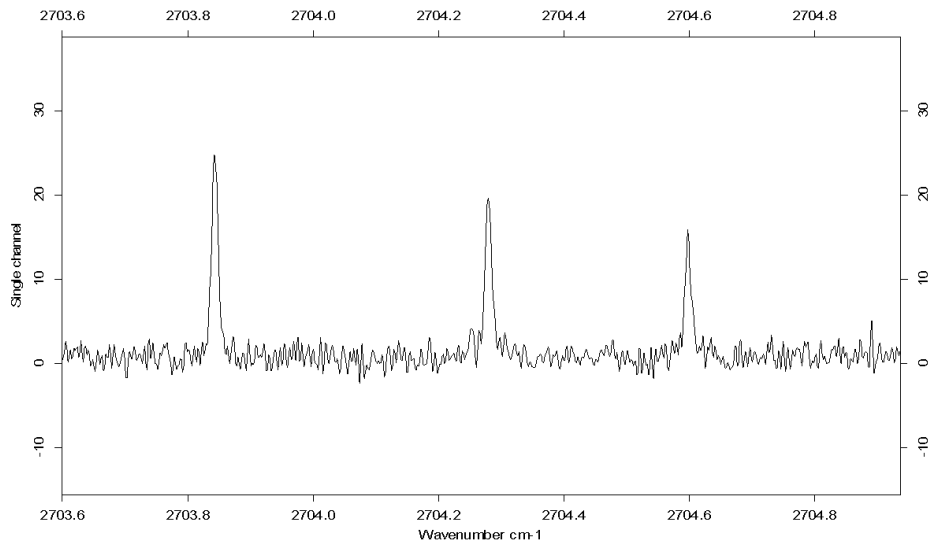


Figure 5. $4s4f\ ^3F-4s5g\ ^3G$ transitions

The three weakest transitions were not visible, since they were blended by the stronger lines. The relative intensities for the three strongest lines were measured to:

$4s4f\ ^3F$ \ $4s5g\ ^3G$	5	4	3
4	100 (100)	- (5.1)	- (0.1)
3	-	82.68 (76.7)	- (5.1)
2	-	-	56.17 (58.4)

Table 6. Relative intensities, theoretical values in brackets

These intensities agree well with the values calculated by Cowan (1981). Knowing the transitions between $4s4f\ ^3F$ and $4s5g\ ^3G$, the energy levels of $4s5g\ ^3G$ can be derived since the energy levels of $4s4f\ ^3F$ are known (see Appendix 1 for result). The levels are verified by looking on the result from the Landé interval rule:

$$A_{5,4} \approx 0.007\text{ cm}^{-1}$$

$$A_{4,3} \approx 0.008\text{ cm}^{-1}$$

Which agree well.

Worth mentioning is that the $4s4f\ ^3F$ - $4s5g\ ^3G$ triplet transitions has been measured in solar spectra by Geller (1992).

Self absorption

Self absorption occurs when a photon emitted by an atom in the HC-lamp does not reach the detector because it is absorbed by another atom. This leads to a decrease in line strength and a broadening of the spectral line. Sometimes the self absorption is so strong that the line appears as two spectral lines very close together:

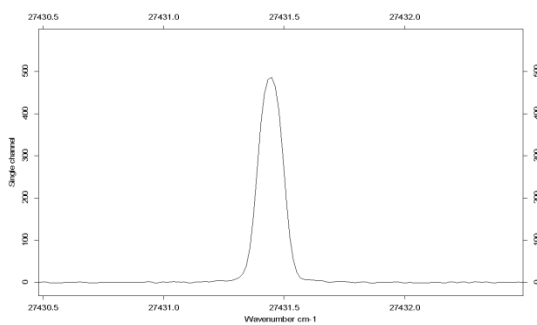


Figure 6. Self absorption of $27431.4755\text{ cm}^{-1}$

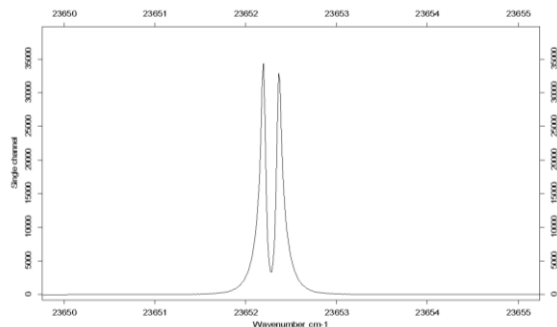


Figure 7. Self absorption of $23652.3087\text{ cm}^{-1}$

The line $27431.4755\text{ cm}^{-1}$ ($4s4p\ ^3P_2 - 4s5d\ ^3D_3$) in Figure 6 is self absorbed since it is broader than the other transitions between the two triplets and because it has a lower intensity than what it should have. The latter can be seen by looking at relative intensities:

$4s4p\ ^3P$ \ $4s5d\ ^3D$	3	2	1
2	100 (100)	28.02 (17.86)	1.97 (1.19)
1	-	67.42 (53.57)	28.61 (17.86)
0	-	-	36.80 (23.81)

Table 7. Relative intensities, theoretical values in brackets

All relative intensities lie above the theoretical value. This indicates that the strongest transition $4s4p\ ^3P_2 - 4s5d\ ^3D_3$, to whom all the other transitions are compared, is weaker than what it should be. This is a sign of self absorption.

According to the derived Ritz wavelengths from the energy levels by Sugar and Corliss (1985) the line should be located at 27431.444 cm^{-1} , which differs about 0.03 cm^{-1} from what I have measured. This difference can possibly be due to the self absorption

In Figure 7 the resonance line of calcium is shown ($4s^2\ ^1S_0 - 4s4p\ ^1P_1$). The resonance line is the spectral line representing the transition from the lowest excited state to the ground configuration. The resonance line is very strong since an excitation to the lowest state does not require so much energy, i.e. lots of atoms get excited to this state. The only way to deexcite is to the ground state and lots of photons with the energy $23652.3087\text{ cm}^{-1}$ are sent out. A high number of photons mean a higher probability for self absorption, and that is why the resonance line so clearly is self absorbed. This kind of self absorption, where a line has an absorption feature, is called self reversal.

Level mixing

Deviation from LS -coupling was encountered several times during this project. This resulted in a number of intercombination lines, which should not be possible in pure LS -coupling, i.e. LS -coupling does not work perfectly for all levels in the calcium atom.

One example of level mixing is the levels $3d4p\ ^3F_2$ and $3d4p\ ^1D_2$. If $3d4p\ ^3F_2$ and $3d4p\ ^1D_2$ are mixed, $3d4p\ ^1D_2$ should have transitions to $3d4s\ ^3D$ since $3d4p\ ^3F_2$ has it. The spectral line $15464.4154\text{ cm}^{-1}$ representing $3d4s\ ^3D_3 - 3d4p\ ^1D_2$ is one example. Furthermore $3d4s\ ^1D_2$ should have transitions to $3d4p\ ^3F_2$. We find the spectral line at $13880.8364\text{ cm}^{-1}$ representing this transition. As a further verification that these levels are mixed, the Landé interval rule is investigated for the triplet $3d4p\ ^3F$. If it does not agree well, it is indicating that the levels are mixed:

$$A_{4,3} \approx 19.5\text{ cm}^{-1}$$

$$A_{3,2} \approx 29.4\text{ cm}^{-1}$$

Finally the relative intensities for the transitions $3d4s\ ^3D - 3d4p\ ^3F$ are studied. If they do not agree well with the theoretical values, another sign of level mixing is presented:

$3d4s\ ^3D \backslash 3d4p\ ^3F$	4	3	2
3	100 (100)	21.30 (8.64)	0.34 (0.25)
2	-	78.35 (69.14)	15.01 (8.64)
1	-	-	49.26 (46.67)

Table 8. Relative intensities for the transitions $3d4s\ ^3D-3d4p\ ^3F$, theoretical values in brackets

In table 8 one can see that the experimental intensities do not differ much from the theoretical values (except for the transition $3d4s\ ^3D_3-3d4p\ ^3F_3$). The level is however still mixed. The reason the values agree well is self absorption in the transitions. The strongest transition is most self absorbed. This means that the other relative intensities become stronger than what they should be compared to this. If the transitions were not self absorbed the relative intensities would be weaker and many of them would be smaller than the theoretical values. The intensities would then not agree well with the theoretical values and this indicates level mixing.

Another example of level mixing is the levels $4s5p\ ^1P_1$ and $4s5p\ ^3P_1$. Since $4s5p\ ^1P_1$ has transitions to $4s5d\ ^1D$ (6187.4457 cm^{-1}), $4s5p\ ^3P_1$ should have it as well. One spectral line that was found is 6364.2927 cm^{-1} identified as $4s5p\ ^3P_1-4s5d\ ^1D_2$. A transition between $4s5p\ ^1P_1 - 4s5d\ ^3D_2$ at 6013.1282 cm^{-1} is seen as well because of this mixing. The Landé interval rule for the triplet $4s5p\ ^3P_1$ gives:

$$A_{2,1} \approx 10.2\text{ cm}^{-1}$$

$$A_{1,0} \approx 7.1\text{ cm}^{-1}$$

Appendix 1

Presentation of the 78 derived energy levels in Ca I. * indicates an energy level with odd parity. The first level column represents the energy levels derived in this project. The second level column is the energy levels reported by Sugar and Corliss (1985).

Configuration	Term	J	Level (cm ⁻¹)	Level (cm ⁻¹)
4s ²	¹ S	0	0,0000	0,000
4s4p	³ P*	0	15157,8933	15157,901
		1	15210,0624	15210,063
		2	15315,9416	15315,943
3d4s	³ D	1	20335,3615	20335,360
		2	20349,2601	20349,260
		3	20370,9970	20371,000
3d4s	¹ D	2	21849,6299	21849,634
4s4p	¹ P*	1	23652,3087	23652,304
4s5s	³ S	1	31539,4999	31539,495
4s5s	¹ S	0	33317,2737	33317,264
3d4p	³ F	2	35730,4623	35730,454
		3	35818,7181	35818,713
		4	35896,8940	35896,889
3d4p	¹ D*	2	35835,4123	35835,413
4s5p	³ P*	0	36547,7044	36547,688
		1	36554,7631	36554,749
		2	36575,1372	36575,119
4s5p	¹ P*	1	36731,6242	36731,615
4s4d	¹ D	2	37298,2838	37298,287
4s4d	³ D	1	37748,1951	37748,197
		2	37751,8664	37751,867
		3	37757,4682	37757,449
3d4p	³ D*	1	38192,3935	38192,392
		2	38219,1195	38219,118
		3	38259,1143	38259,124
4p ²	³ P	0	38417,5572	38417,543
		1	38464,8171	38464,808

		2	38551,5627	38551,558
3d4p	³ P*	0	39333,3900	39333,382
		1	39335,3296	39335,322
		2	39340,0948	39340,080
4s6s	³ S	1	40474,2512	40474,241
3d4p	¹ F*	3	40537,9002	40537,893
4s6s	¹ S	0	40690,4405	40690,435
4p²	¹ D	2	40719,8529	40719,847
4s6p	¹ P*	1	41679,0258	41679,008
4p²	¹ S	0	41786,2772	41786,276
4s4f	³ F*	2	42170,2046	42170,214
		3	42170,5555	42170,558
		4	42171,0265	42171,026
4s4f	¹ F*	3	42343,5858	42343,587
4s6p	³ P*	0	42514,8478	42514,845
		1	42518,7125	42518,708
		2	42526,5788	42526,591
4s5d	³ D	1	42743,0121	42743,002
		2	42744,7391	42744,716
		3	42747,4215	42747,387
4s5d	¹ D	2	42919,0584	42919,053
3d²	³ F	2	43474,8353	43474,827
		3	43489,1281	43489,119
		4	43508,1012	43508,088
3d4p	¹ P*	1	43933,4756	43933,477
4s7s	³ S	1	43980,7658	43980,767
4s7s	¹ S	0	44276,5317	44276,538
4s5f	³ F*	2	44762,6294	44762,620
		3	44762,8394	44762,839
		4	44763,1203	44763,118
4s5f	¹ F*	3	44804,8660	44804,878

4s5g	³ G	3	44874,8069	-
		4	44874,8392	-
		5	44874,8736	44874,86
4s6d	¹ D	2	44989,8312	44989,830
4s6d	³ D	1	45049,0088	45049,073
		2	45050,3603	45050,419
		3	45052,2828	45052,374
4s7p	¹ P	1	45425,3709	45425,358
4s8s	³ S	1	45738,7026	45738,684
4s8s	¹ S	0	45887,1912	45887,200
4s6f	³ F	2	46164,6407	46164,644
		3	46164,7889	46164,785
		4	46164,9736	46164,971
4s6f	¹ F	3	46182,3936	46182,399
4s7d	³ D	3	46306,0781	46306,059
4s7f	¹ F	3	47015,1385	47015,141
3d²	³ P	0	48524,0979	48524,093
		1	48537,6265	48537,623
		2	48563,5194	48563,522

Appendix 2

Presentation of the 204 spectral lines that were used in the derivation of the 78 energy levels. * indicates an energy level with odd parity and ^s indicates that the line is self absorbed.

Intensity (arbitrary units)	Measured wavenumber (cm ⁻¹)	Ritz wavenumber (cm ⁻¹)	Lower level	Upper level
169	2703,8471	2703,847	4s4f ³ F ₄ *	4s5g ³ G ₅
140	2704,2837	2704,284	4s4f ³ F ₃ *	4s5g ³ G ₄
98	2704,6023	2704,602	4s4f ³ F ₂ *	4s5g ³ G ₃
1037	3239,6169	3239,617	4s4d ¹ D ₂	3d4p ¹ F ₃ *
65	3407,3276	3407,327	3d4p ³ P ₂ *	4s5d ³ D ₃
35	3409,4035	3409,410	3d4p ³ P ₁ *	4s5d ³ D ₂
2263	3414,3505	3414,351	4s5s ¹ S ₀	4s5p ¹ P ₁ *
440	3899,1150	3899,114	4s5p ³ P ₂ *	4s6s ³ S ₁
383	3919,4846	3919,488	4s5p ³ P ₁ *	4s6s ³ S ₁
129	3926,5478	3926,547	4s5p ³ P ₀ *	4s6s ³ S ₁
338	3958,8247	3958,816	4s5p ¹ P ₁ *	4s6s ¹ S ₀
366	3988,2364	3988,228	4s5p ¹ P ₁ *	4p2 ¹ D ₂
160	4380,7306	4380,742	4s4d ¹ D ₂	4s6p ¹ P ₁ *
1574	4413,5592	4413,558	4s4d ³ D ₃	4s4f ³ F ₄ *
137	4418,3418	4418,338	4s4d ³ D ₂	4s4f ³ F ₂ *
1071	4418,6899	4418,689	4s4d ³ D ₂	4s4f ³ F ₃ *
714	4422,0134	4422,009	4s4d ³ D ₁	4s4f ³ F ₂ *
56	4769,1112	4769,110	4s4d ³ D ₃	4s6p ³ P ₂ *
1288	5008,2045	5008,205	4s5s ³ S ₁	4s5p ³ P ₀ *
3909	5015,2679	5015,264	4s5s ³ S ₁	4s5p ³ P ₁ *
6962	5019,4199	5019,420	4s4p ³ P ₂ *	3d4s ³ D ₁
84739	5033,3184	5033,319	4s4p ³ P ₂ *	3d4s ³ D ₂
6474	5035,6374	5035,638	4s5s ³ S ₁	4s5p ³ P ₂ *
1261	5045,3020	5045,302	4s4d ¹ D ₂	4s4f ¹ F ₃ *
237674	5055,0554	5055,056	4s4p ³ P ₂ *	3d4s ³ D ₃
86760	5125,2991	5125,299	4s4p ³ P ₁ *	3d4s ³ D ₁
172769	5139,1977	5139,198	4s4p ³ P ₁ *	3d4s ³ D ₂
108246	5177,4682	5177,468	4s4p ³ P ₀ *	3d4s ³ D ₁
89	5192,1160	5192,125	4s5s ³ S ₁	4s5p ¹ P ₁ *
2076	5248,9809	5248,987	3d4p ³ D ₃ *	3d ² ³ F ₄
178	5255,7096	5255,716	3d4p ³ D ₂ *	3d ² ³ F ₂
1488	5270,0027	5270,009	3d4p ³ D ₂ *	3d ² ³ F ₃
1001	5282,4366	5282,442	3d4p ³ D ₁ *	3d ² ³ F ₂
24	6013,1282	6013,115	4s5p ¹ P ₁ *	4s5d ³ D ₂
76	6167,8793	6167,875	4s5p ³ P ₂ *	4s5d ³ D ₁
1190	6169,6064	6169,602	4s5p ³ P ₂ *	4s5d ³ D ₂
6572	6172,2843	6172,284	4s5p ³ P ₂ *	4s5d ³ D ₃
4951	6187,4457	6187,434	4s5p ¹ P ₁ *	4s5d ¹ D ₂
1168	6188,2490	6188,249	4s5p ³ P ₁ *	4s5d ³ D ₁

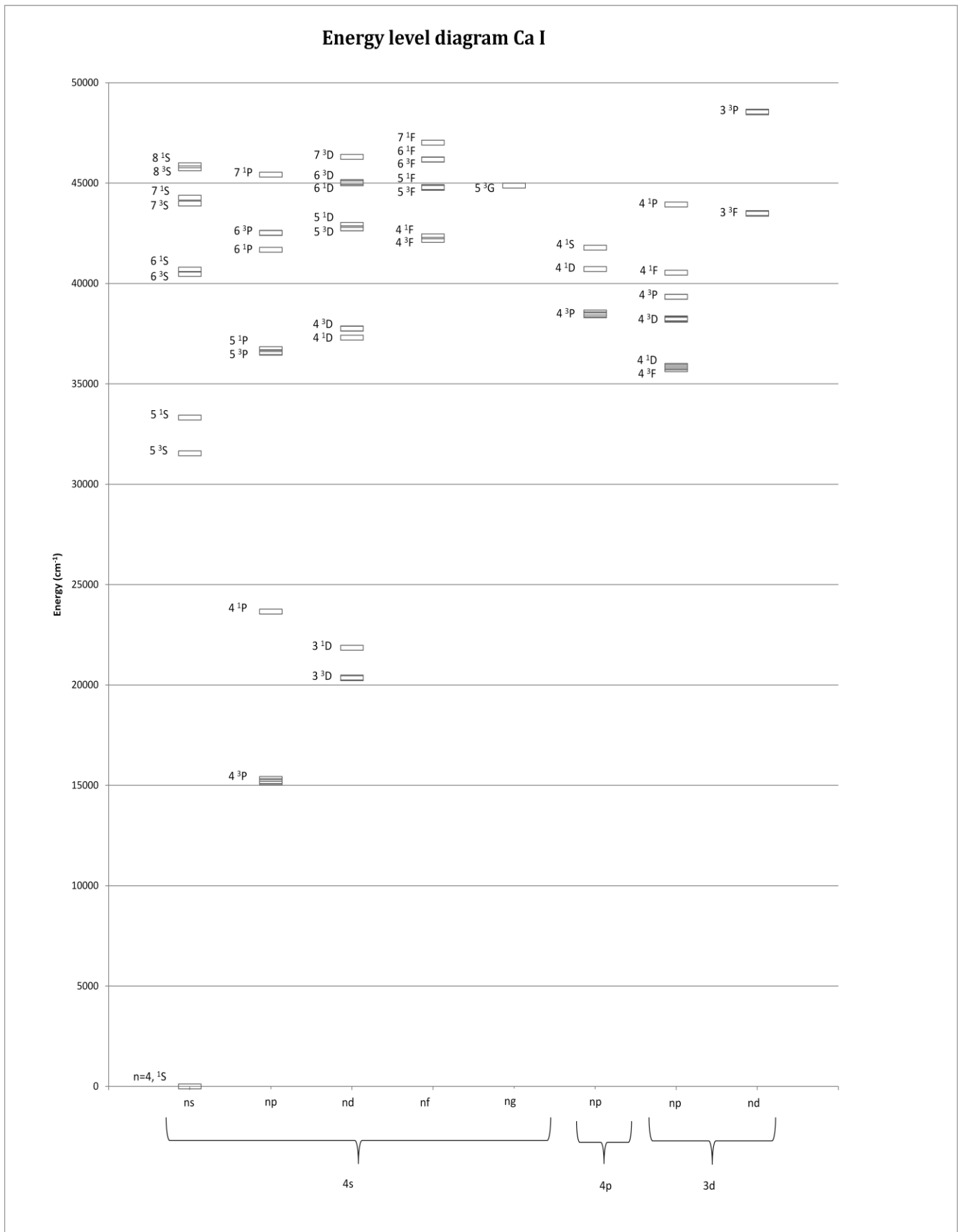
3526	6189,9759	6189,976	4s5p ³ P ₁ *	4s5d ³ D ₂
1594	6195,3122	6195,308	4s5p ³ P ₀ *	4s5d ³ D ₁
42	6364,2927	6364,295	4s5p ³ P ₁ *	4s5d ¹ D ₂
277	6533,6882	6533,688	4s4p ³ P ₂ *	3d4s ¹ D ₂
462	6635,1967	6635,192	4s4d ¹ D ₂	4snp ¹ P ₁ *
1488	6639,5675	6639,567	4s4p ³ P ₁ *	3d4s ¹ D ₂
128	6850,5291	6850,527	3d4p ³ F ₄ *	4s5d ³ D ₃
18	6907,6057	6907,600	3d4p ¹ D ₂ *	4s5d ³ D ₁
96	6926,0263	6926,021	3d4p ³ F ₃ *	4s5d ³ D ₂
47	7005,3751	7005,371	4s4d ³ D ₃	4s5f ³ F ₃ *
537	7005,6573	7005,652	4s4d ³ D ₃	4s5f ³ F ₄ *
36	7010,7679	7010,763	4s4d ³ D ₂	4s5f ³ F ₂ *
367	7010,9773	7010,973	4s4d ³ D ₂	4s5f ³ F ₃ *
39	7012,5561	7012,550	3d4p ³ F ₂ *	4s5d ³ D ₁
244	7014,4393	7014,434	4s4d ³ D ₁	4s5f ³ F ₂ *
80	7083,6498	7083,646	3d4p ¹ D ₂ *	4s5d ¹ D ₂
40	7188,6002	7188,596	3d4p ³ F ₂ *	4s5d ¹ D ₂
485	7405,6321	7405,628	4s5p ³ P ₂ *	4s7s ³ S ₁
262	7426,0016	7426,002	4s5p ³ P ₁ *	4s7s ³ S ₁
88	7433,0652	7433,061	4s5p ³ P ₀ *	4s7s ³ S ₁
711	7506,5870	7506,583	4s4d ¹ D ₂	4s5f ¹ F ₃ *
375	7544,9197	7544,907	4s5p ¹ P ₁ *	4s7s ¹ S ₀
2815	7592,2341	7592,234	3d4p ³ F ₄ *	3d ² ³ F ₃
41289	7611,2072	7611,207	3d4p ³ F ₄ *	3d ² ³ F ₄
6607	7639,4229	7639,423	3d4p ¹ D ₂ *	3d ² ³ F ₂
816	7653,7155	7653,716	3d4p ¹ D ₂ *	3d ² ³ F ₃
2875	7656,1172	7656,117	3d4p ³ F ₃ *	3d ² ³ F ₂
30020	7670,4100	7670,410	3d4p ³ F ₃ *	3d ² ³ F ₃
2576	7689,3831	7689,383	3d4p ³ F ₃ *	3d ² ³ F ₄
16835	7744,3730	7744,373	3d4p ³ F ₂ *	3d ² ³ F ₂
1885	7758,6658	7758,666	3d4p ³ F ₂ *	3d ² ³ F ₃
5454	7800,5949	7800,595	4s5s ³ S ₁	3d4p ³ P ₂ *
952	8258,2194	8258,207	4s5p ¹ P ₁ *	4s6d ¹ D ₂
2251	8361,7521	8361,752	4s5s ¹ S ₀	4s6p ¹ P ₁ *
130	8475,2278	8475,223	4s5p ³ P ₂ *	4s6d ³ D ₂
740	8477,1456	8477,145	4s5p ³ P ₂ *	4s6d ³ D ₃
136	8494,2409	8494,245	4s5p ³ P ₁ *	4s6d ³ D ₁
409	8495,5972	8495,597	4s5p ³ P ₁ *	4s6d ³ D ₂
180	8501,3044	8501,304	4s5p ³ P ₀ *	4s6d ³ D ₁
48	9155,3885	9155,388	3d4p ³ F ₄ *	4s6d ³ D ₃
33	9163,5654	9163,565	4s5p ³ P ₂ *	4s8s ³ S ₁
548	9188,7683	9188,768	3d4p ³ P ₁ *	3d ² ³ P ₀
456	9197,5444	9197,532	3d4p ³ P ₂ *	3d ² ³ P ₁
293	9202,2976	9202,297	3d4p ³ P ₁ *	3d ² ³ P ₁
390	9204,2365	9204,236	3d4p ³ P ₀ *	3d ² ³ P ₁
336	9223,4357	9223,425	3d4p ³ P ₂ *	3d ² ³ P ₂
37	9231,6473	9231,642	3d4p ³ F ₃ *	4s6d ³ D ₂
112139	9664,9650	9664,965	4s4p ¹ P ₁ *	4s5s ¹ S ₀
109	9730,9409	9730,941	4s5p ³ P ₂ *	4s7d ³ D ₃
367	10304,4041	10304,405	3d4p ³ D ₃ *	3d ² ³ P ₂

777	10318,5072	10318,507	3d4p ³ D ₂ *	3d ² ³ P ₁
487	10331,7044	10331,704	3d4p ³ D ₁ *	3d ² ³ P ₀
69	10344,3999	10344,400	3d4p ³ D ₂ *	3d ² ³ P ₂
255	10345,2330	10345,233	3d4p ³ D ₁ *	3d ² ³ P ₁
884	10616,2091	10616,202	4s5s ¹ S ₀	4snp ¹ P ₁ *
93	10975,3466	10975,348	4s5s ³ S ₁	4s6p ³ P ₀ *
298	10979,2142	10979,213	4s5s ³ S ₁	4s6p ³ P ₁ *
79	11962,4904	11962,489	4s5p ³ P ₂ *	3d ² ³ P ₁
83	11969,3295	11969,334	4s5p ³ P ₁ *	3d ² ³ P ₀
118	11988,4072	11988,382	4s5p ³ P ₂ *	3d ² ³ P ₂
63	11989,9267	11989,922	4s5p ³ P ₀ *	3d ² ³ P ₁
75	12108,1057	12108,097	4s5s ¹ S ₀	4s7p ¹ P ₁ *
110400	13645,9751	13645,975	4s4p ¹ P ₁ *	4s4d ¹ D ₂
101997	13880,8364	13880,833	3d4s ¹ D ₂	3d4p ³ F ₂ *
84	13969,0947	13969,089	3d4s ¹ D ₂	3d4p ³ F ₃ *
195082	13985,7866	13985,783	3d4s ¹ D ₂	3d4p ¹ D ₂ *
128	14725,5124	14725,508	3d4s ¹ D ₂	4s5p ³ P ₂ *
76393	14881,9890	14881,995	3d4s ¹ D ₂	4s5p ¹ P ₁ *
19330	15210,0624	15210,062	4s2 ¹ S ₀	4s4p ³ P ₁ *
1225	15359,4652	15359,465	3d4s ³ D ₃	3d4p ³ F ₂ *
53638	15381,2022	15381,202	3d4s ³ D ₂	3d4p ³ F ₂ *
175974	15395,1008	15395,101	3d4s ³ D ₁	3d4p ³ F ₂ *
7609	15447,7209	15447,721	3d4s ³ D ₃	3d4p ³ F ₃ *
147	15464,4154	15464,415	3d4s ³ D ₃	3d4p ¹ D ₂ *
279928	15469,4581	15469,458	3d4s ³ D ₂	3d4p ³ F ₃ *
18153	15486,1522	15486,152	3d4s ³ D ₂	3d4p ¹ D ₂ *
99519	15500,0508	15500,051	3d4s ³ D ₁	3d4p ¹ D ₂ *
357261	15525,8969	15525,897	3d4s ³ D ₃	3d4p ³ F ₄ *
20092	16204,1389	16204,140	3d4s ³ D ₃	4s5p ³ P ₂ *
12024	16205,5064	16205,503	3d4s ³ D ₂	4s5p ³ P ₁ *
5832	16212,3418	16212,343	3d4s ³ D ₁	4s5p ³ P ₀ *
4557	16219,4050	16219,402	3d4s ³ D ₁	4s5p ³ P ₁ *
72385	16223,5571	16223,558	4s4p ³ P ₂ *	4s5s ³ S ₁
4610	16225,8760	16225,877	3d4s ³ D ₂	4s5p ³ P ₂ *
301	16239,7749	16239,776	3d4s ³ D ₁	4s5p ³ P ₂ *
58066	16329,4364	16329,437	4s4p ³ P ₁ *	4s5s ³ S ₁
20	16369,5016	16369,490	3d4s ¹ D ₂	3d4p ³ D ₂ *
34437	16381,6054	16381,606	4s4p ³ P ₀ *	4s5s ³ S ₁
92	16382,3539	16382,364	3d4s ³ D ₂	4s5p ¹ P ₁ *
160	16396,2518	16396,263	3d4s ³ D ₁	4s5p ¹ P ₁ *
1005	17038,1318	17038,132	4s4p ¹ P ₁ *	4s6s ¹ S ₀
37130	17067,5442	17067,544	4s4p ¹ P ₁ *	4p ² ¹ D ₂
16706	17843,1334	17843,133	3d4s ³ D ₂	3d4p ³ D ₁ *
18203	17848,1225	17848,122	3d4s ³ D ₃	3d4p ³ D ₂ *
34762	17857,0321	17857,032	3d4s ³ D ₁	3d4p ³ D ₁ *
45012	17869,8597	17869,859	3d4s ³ D ₂	3d4p ³ D ₂ *
17344	17883,7579	17883,758	3d4s ³ D ₁	3d4p ³ D ₂ *
65386	17888,1173	17888,117	3d4s ³ D ₃	3d4p ³ D ₃ *
20831	17909,8537	17909,854	3d4s ³ D ₂	3d4p ³ D ₃ *
6889	18133,9685	18133,969	4s4p ¹ P ₁ *	4p ² ¹ S ₀

42418	18688,2712	18688,271	3d4s ¹ D ₂	3d4p ¹ F ₃ *
36967	18969,0923	18969,097	3d4s ³ D ₃	3d4p ³ P ₂ *
25027	18986,0761	18986,069	3d4s ³ D ₂	3d4p ³ P ₁ *
12892	18990,8293	18990,834	3d4s ³ D ₂	3d4p ³ P ₂ *
13848	18998,0357	18998,029	3d4s ³ D ₁	3d4p ³ P ₀ *
11902	18999,9746	18999,968	3d4s ³ D ₁	3d4p ³ P ₁ *
1093	19004,7277	19004,733	3d4s ³ D ₁	3d4p ³ P ₂ *
12479	19266,7497	19266,750	4s4p ¹ P ₁ *	4s5d ¹ D ₂
8799	19829,3836	19829,396	3d4s ¹ D ₂	4s6p ¹ P ₁ *
49	20166,9015	20166,903	3d4s ³ D ₃	3d4p ¹ F ₃ *
11120	20493,9555	20493,956	3d4s ¹ D ₂	4s4f ¹ F ₃ *
378	20624,2230	20624,223	4s4p ¹ P ₁ *	4s7s ¹ S ₀
809	21337,5225	21337,523	4s4p ¹ P ₁ *	4s6d ¹ D ₂
21	21799,2076	21799,207	3d4s ³ D ₃	4s4f ³ F ₂ *
714	21799,5585	21799,558	3d4s ³ D ₃	4s4f ³ F ₃ *
6516	21800,0295	21800,029	3d4s ³ D ₃	4s4f ³ F ₄ *
704	21820,9476	21820,944	3d4s ³ D ₂	4s4f ³ F ₂ *
4809	21821,2954	21821,295	3d4s ³ D ₂	4s4f ³ F ₂ *
3392	21834,8461	21834,843	3d4s ³ D ₁	4s4f ³ F ₂ *
3002	22083,8457	22083,846	3d4s ¹ D ₂	4snp ¹ P ₁ *
253	22155,5828	22155,581	3d4s ³ D ₃	4s6p ³ P ₂ *
132	22169,4524	22169,452	3d4s ³ D ₂	4s6p ³ P ₁ *
49	22177,3187	22177,318	3d4s ³ D ₂	4s6p ³ P ₂ *
59	22179,4863	22179,486	3d4s ³ D ₁	4s6p ³ P ₀ *
48	22183,3486	22183,351	3d4s ³ D ₁	4s6p ³ P ₁ *
43	22234,8825	22234,883	4s4p ¹ P ₁ *	4s8s ¹ S ₀
2036	22432,2533	22432,254	4s4p ³ P ₂ *	4s4d ³ D ₁
22352	22435,9248	22435,925	4s4p ³ P ₂ *	4s4d ³ D ₂
45102	22441,5266 ^s	22441,527	4s4p ³ P ₂ *	4s4d ³ D ₃
19828	22538,1327	22538,133	4s4p ³ P ₁ *	4s4d ³ D ₁
33505	22541,8040	22541,804	4s4p ³ P ₁ *	4s4d ³ D ₂
22937	22590,3018	22590,302	4s4p ³ P ₀ *	4s4d ³ D ₁
1621	22955,2361	22955,237	3d4s ¹ D ₂	4s5f ¹ F ₃ *
14973	23207,4948	23207,495	4s4p ³ P ₁ *	4p ² ³ P ₀
29704	23235,6216 ^s	23235,621	4s4p ³ P ₂	4p ² ³ P ₂
12791	23254,7547	23254,755	4s4p ³ P ₁	4p ² ³ P ₁
21852	23341,5003	23341,500	4s4p ³ P ₁	4p ² ³ P ₂
517	23575,7410	23575,741	3d4s ¹ D ₂	4s7p ¹ P ₁ *
507406	23652,3087 ^s	23652,308	4s ² ¹ S ₀	4s4p ¹ P ₁ *
294	24332,7637	24332,764	3d4s ¹ D ₂	4s6f ¹ F ₃ *
105	24391,8424	24391,842	3d4s ³ D ₃	4s5f ³ F ₃ *
1041	24392,1233	24392,123	3d4s ³ D ₃	4s5f ³ F ₄ *
125	24413,3718	24413,369	3d4s ³ D ₂	4s5f ³ F ₂ *
746	24413,5783	24413,579	3d4s ³ D ₂	4s5f ³ F ₃ *
511	24427,2679	24427,268	3d4s ³ D ₁	4s5f ³ F ₂ *
5139	25158,3094	25158,310	4s4p ³ P ₂ *	4s6s ³ S ₁
60	25165,5086	25165,509	3d4s ¹ D ₂	4s7f ¹ F ₃ *
3101	25264,1888	25264,189	4s4p ³ P ₁ *	4s6s ³ S ₁
1077	25316,3578	25316,358	4s4p ³ P ₀ *	4s6s ³ S ₁
135	25793,9766	25793,976	3d4s ³ D ₃	4s6f ³ F ₄ *

91	25815,5288	25815,528	3d4s ³ D ₂	4s6f ³ F ₃ *
67	25829,2792	25829,279	3d4s ³ D ₁	4s6f ³ F ₂ *
78	27427,0711	27427,071	4s4p ³ P ₂ *	4s5d ³ D ₁
1116	27428,7978	27428,798	4s4p ³ P ₂ *	4s5d ³ D ₂
3983	27431,4755 ^s	27431,480	4s4p ³ P ₂ *	4s5d ³ D ₃
1140	27532,9497	27532,950	4s4p ³ P ₁ *	4s5d ³ D ₁
2686	27534,6767	27534,677	4s4p ³ P ₁ *	4s5d ³ D ₂
1466	27585,1189	27585,119	4s4p ³ P ₀ *	4s5d ³ D ₁
205	28664,8235	28664,824	4s4p ³ P ₂ *	4s7s ³ S ₁
114	28770,7034	28770,703	4s4p ³ P ₁ *	4s7s ³ S ₁
85	29734,4162	29734,419	4s4p ³ P ₂ *	4s6d ³ D ₂
352	29736,3334	29736,341	4s4p ³ P ₂ *	4s6d ³ D ₃
78	29838,9428	29838,946	4s4p ³ P ₁ *	4s6d ³ D ₁
226	29840,2960	29840,298	4s4p ³ P ₁ *	4s6d ³ D ₂
108	29891,1091	29891,115	4s4p ³ P ₀ *	4s6d ³ D ₁

Appendix 3



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Kalciumatomens energinivåer

I alla år har människan tittat upp på natthimlen och funderat över det som finns där uppe: "Vad består stjärnor av? Hur varma är de?" är kanske frågor som dykt upp. Idag kan man genom att studera ljuset som kommer från stjärnorna få svar på dessa frågor. Detta kräver dock att man kan tolka det ljus som kommer till oss. I detta arbete har ljuset från grundämnet kalcium undersökts i laboratorium.

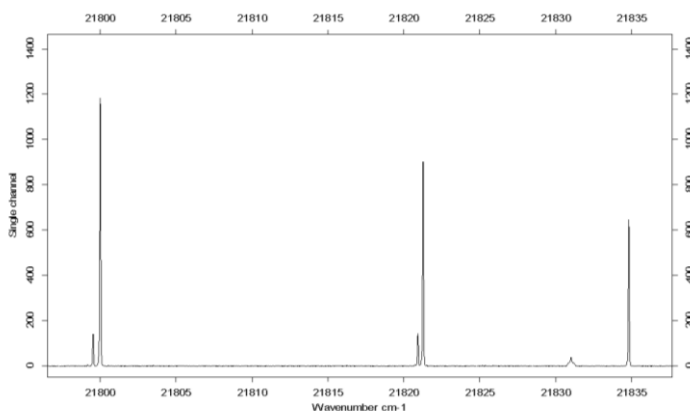
Varje atom har minst en elektron. Elektronen/elektronerna hos en atom kan hoppa mellan olika energinivåer i atomen. Detta kan ske när atomen absorberar energi, dvs. om det är den rätta mängden energi som kommer in. Processen kallas excitation och kan ske på olika sätt, till exempel genom kollisioner med andra partiklar eller genom absorption av en foton. I det första exemplet räcker det att energin hos den inkommande partikeln är lika med eller större än excitationenergin (energin mellan de nivåer som elektronen ska hoppa mellan), medan det i det sistnämnda exemplet är viktigt att fotonens energi är exakt lika med excitationenergin.

Deexcitation är motsatsen till excitation. Det innebär alltså att elektronen faller ner till en lägre nivå, och därmed minskar sin energi. Energiförhållningen säger att ingen energi kan förstöras utan endast omvandlas mellan olika former. I det här fallet sänds minskningen av energi ut i form av ljus. Det utsända ljuset kan registreras med en spektrometer och man får ett spektrum. Ett spektrum är ett diagram där varje övergång som elektronerna gör i atomerna registrerats som en spektrallinje.

Inom astrofysiken utnyttjar man det faktum att varje atom och molekyl har sitt eget karakteristiska spektrum, vilket innebär att om man tittar på ljuset från en stjärna kan man ta reda på bl.a. dess innehåll, temperatur och densitet.

I detta arbete har ljuset som sänds ut från kalcium studerats i form av ett spektrum registrerat av en fouriertransformspektrometer (FTS). Linjerna som tillhörde kalcium mättes och analyserades.

Då man vet att den lägsta nivån i atomen har energin 0 cm^{-1} räknades andra energinivåer ut med hjälp av de mätta spektrallinjerna.



Spektrallinjer från kalcium i vågtalsområdet kring 21800 cm^{-1}