

# Advanced Courses Offered by the Atomic Physics Division.

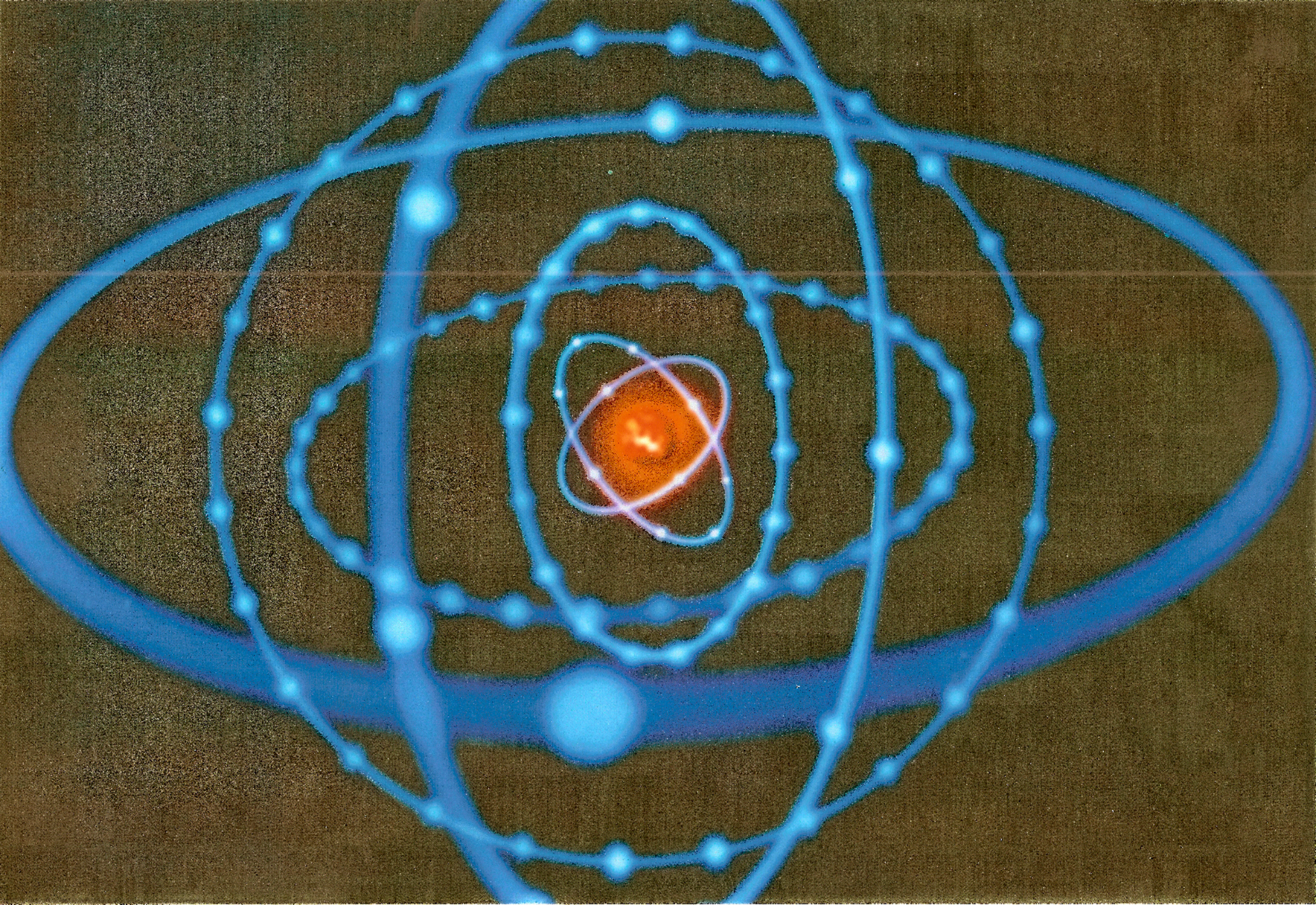
All are open for Science faculty students and given in English

Fall 1	Fall 2	Spring 1	Spring 2
<b>&gt; Engineering</b>			
<u>Optics and Optical Design</u> FAFF01, FYST43, 7.5 hp	<u>Lasers</u> FAFN01, FYSN14, 7.5 hp	<u>Optoelectronics</u>  <b>Optoelectronics</b> FFFN15 / FYST48 7.5 hp	<u>Advanced Optics and Lasers</u> FAFN10, FYST32 7.5 hp
<u>Atomic &amp; molecular spectroscopy</u> FAF080, FYST14, 7.5 hp	<u>Medical Optics</u> Will be given in 2019 for the first time, 7.5 hp	<u>Laser-based combustion diagnostics</u> FBR024, FYST28, 7.5 hp  <u>Light-Matter Interaction</u> FAFN05, FYST21, 7.5 hp	<u>Quantum Information</u> (odd years) FAFN40, FYST30 7.5 hp  Quantum Optics (even years) (no course code yet) 7.5 hp

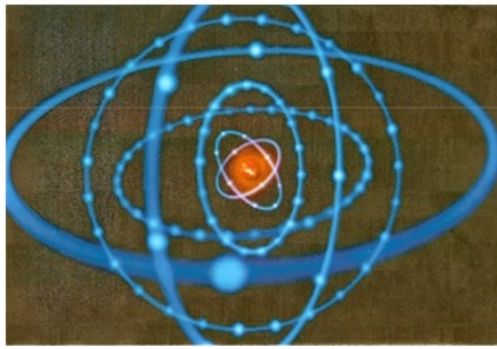
**Uses the second half of the book by Foot**

You may take individual courses or any combination up to a Masters program in Photonics. This education program is coupled to world-leading research activities in optics, lasers and their applications, performed at the [Lund Laser Centre](#) (LLC). LLC is the largest unit in the Nordic countries within the field of lasers, optics and spectroscopy, and a large scale facility of the European Union, part of [Laserlab-Europe](#). It has recently been selected as one of the 20 best research environments in Sweden, receiving a prestigious Linné grant.









- **One electron atoms, H-like.**

**Bohr model**

**Exact quantum mechanical results**

- **Hydrogenic-, Rydberg-atoms. Quantum defect**

**Accurate semi-empirical results**

- **Many electron atoms.**

**Approximations CFA + LS/jj- coupling**

- **Magnetic interactions**

**Spin-orbit, Hyperfine and**

**External mag. fields**

- **Transitions**

**Selection rules and line widths**

- **Molecules**

# The Bohr atom.

Results in a quantized one-electron (H-like) system

$$r_n = a_0 \frac{n^2}{Z}, \quad a_0 = 0,53 \text{ \AA}.$$

$$v_n = \alpha \cdot c \cdot \frac{Z}{n}, \quad \alpha \approx \frac{1}{137}.$$

$$E_n = -R \cdot \frac{Z^2}{n^2}, \quad R = 109677 \text{ cm}^{-1} \text{ for H}$$

$$\frac{1}{\lambda} = E_{n_1} - E_{n_2} = R \cdot Z^2 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right). \quad \text{Rydberg formula}$$

$$1 \text{ eV} = 8066 \text{ cm}^{-1}$$

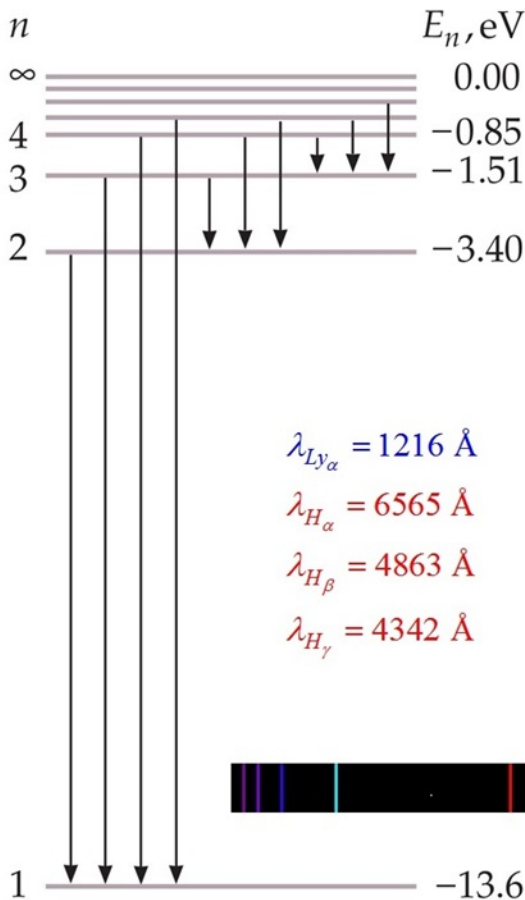
Spectral series:

Lyman, Balmer, Paschen, Brackett, Pfund, Humphreys.....

Mass dependence of the Rydberg constant for an element with nuclear mass  $M$  and massnumber  $A$ :

$$R_M = \frac{1}{1 + \frac{m}{M}} R_\infty = \frac{1}{1 + \frac{1}{1836 \cdot A}} R_\infty, \quad R_\infty = 109737 \text{ cm}^{-1}$$

# Spectral series in H



## Quantum mechanical treatment of one-electron systems

$$H\Psi = E\Psi$$

$$H = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{Ze^2}{4\pi\epsilon_0 r}$$

The Hamilton operator in spherical polar coordinates:

$$\hat{H} = -\frac{\hbar^2}{2\mu} \left[ \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2 \sin(\theta)} \left( \frac{\partial}{\partial \theta} \sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right] - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$L^2$  in spherical polar coordinates

$$\hat{L}^2 = -\hbar^2 \left[ \frac{1}{\sin(\theta)} \left( \frac{\partial}{\partial \theta} \sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right]$$

thus

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{\hat{L}^2}{2\mu r^2} - \frac{Ze^2}{4\pi\epsilon_0 r}$$

Spherically symmetric

Used again in the central-field approximation

Since  $L^2$  only contains angular coordinates  $[H, L^2] = 0$ , i.e.  $H$  and  $L^2$  have common eigenfunctions that we may write as:

$$\Psi_{n,\ell,m_\ell}(r, \theta, \phi) = R_{n,\ell}(r) \cdot Y_{\ell,m_\ell}(\theta, \phi)$$

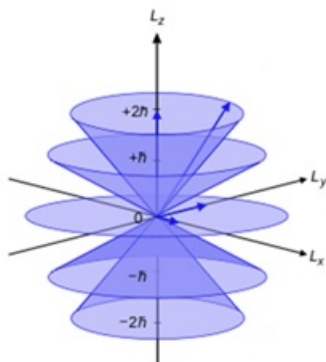
where

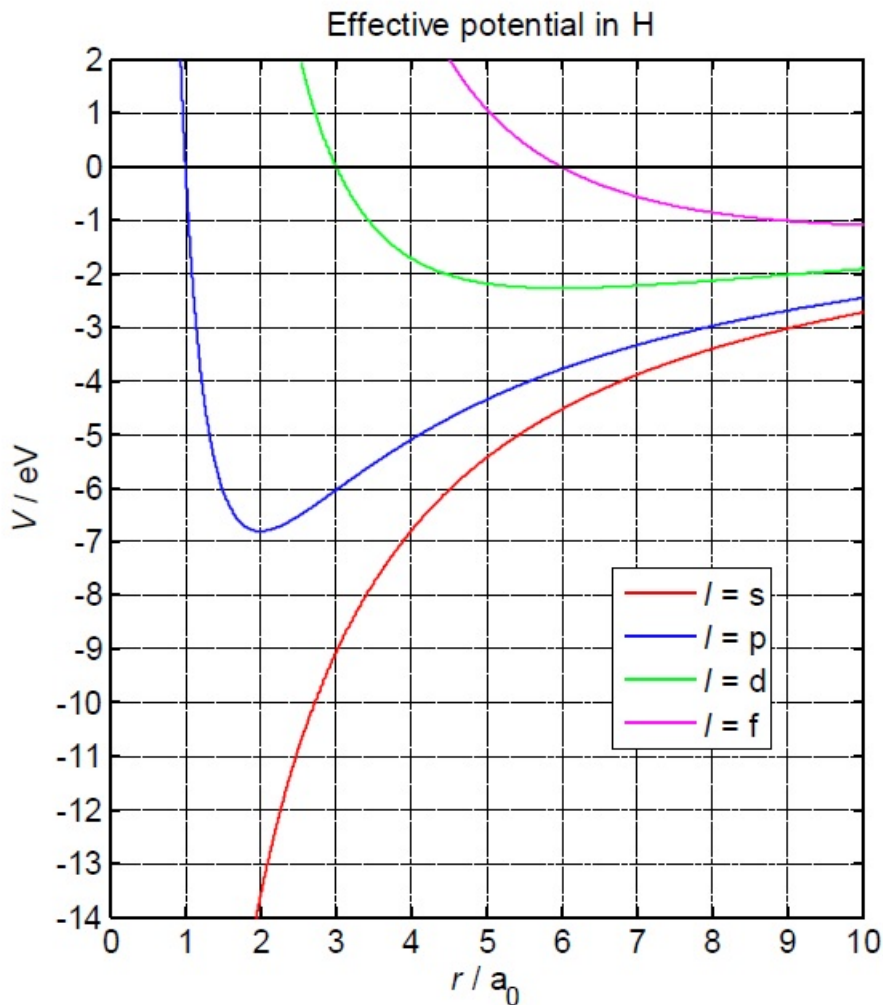
$$L^2 Y_{\ell,m_\ell}(\theta, \phi) = \hbar^2 \ell(\ell+1) \cdot Y_{\ell,m_\ell}(\theta, \phi)$$

$$L_z Y_{\ell,m_\ell}(\theta, \phi) = \hbar m_\ell \cdot Y_{\ell,m_\ell}(\theta, \phi)$$

and  $\ell$  is an integer,  $\ell = 0, 1, 2, \dots, n-1$

and  $m_\ell = -\ell, -\ell+1, \dots, \ell-1, \ell$



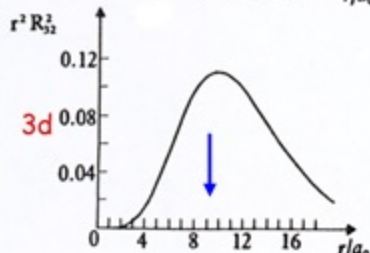
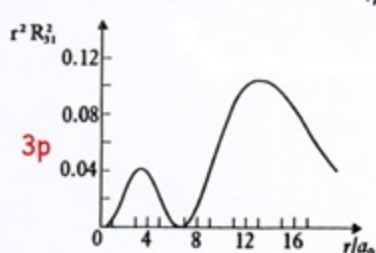
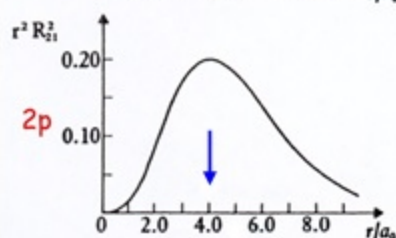
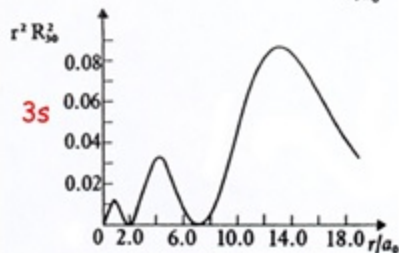
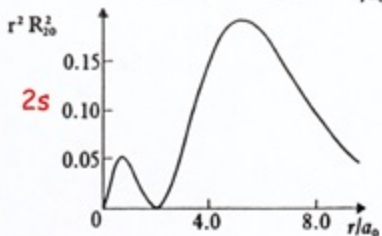
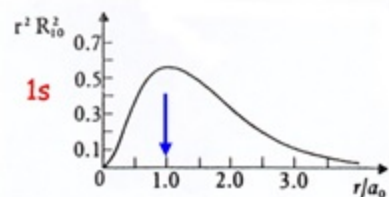


$$V_{\text{eff}} = \frac{\hbar^2 \ell \cdot (\ell + 1)}{2\mu \cdot r^2} - \frac{Ze^2}{4\pi\epsilon_0 \cdot r}$$

**Note, only s-electrons can move close or into the nucleus.**

- ⇒ Large quantum defect for s-electrons
- ⇒ Large hyperfine structure for unpaired s-electrons
- ⇒ Only s-electrons experience the charge distribution inside the nucleus giving rise to the so-called volume shift.

# Radial probability distribution in H.



For 1s, 2p, 3d,... i.e.

$$n, \ell = n - 1$$

the most probable distance  $r_n$  is given by:

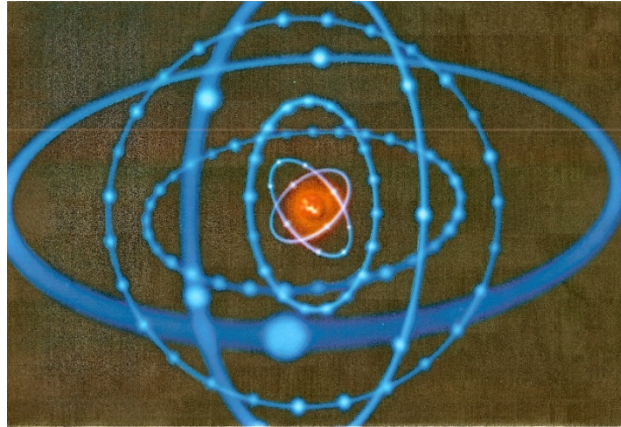
$$r_n = a_0 \frac{n^2}{Z}$$

i.e. the same result as in the Bohr model!

Number of minima:

$$N = n - \ell - 1$$





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**Exact quantum mechanical results**

- ➔ • Hydrogenic-, Rydberg-atoms. Quantum defect

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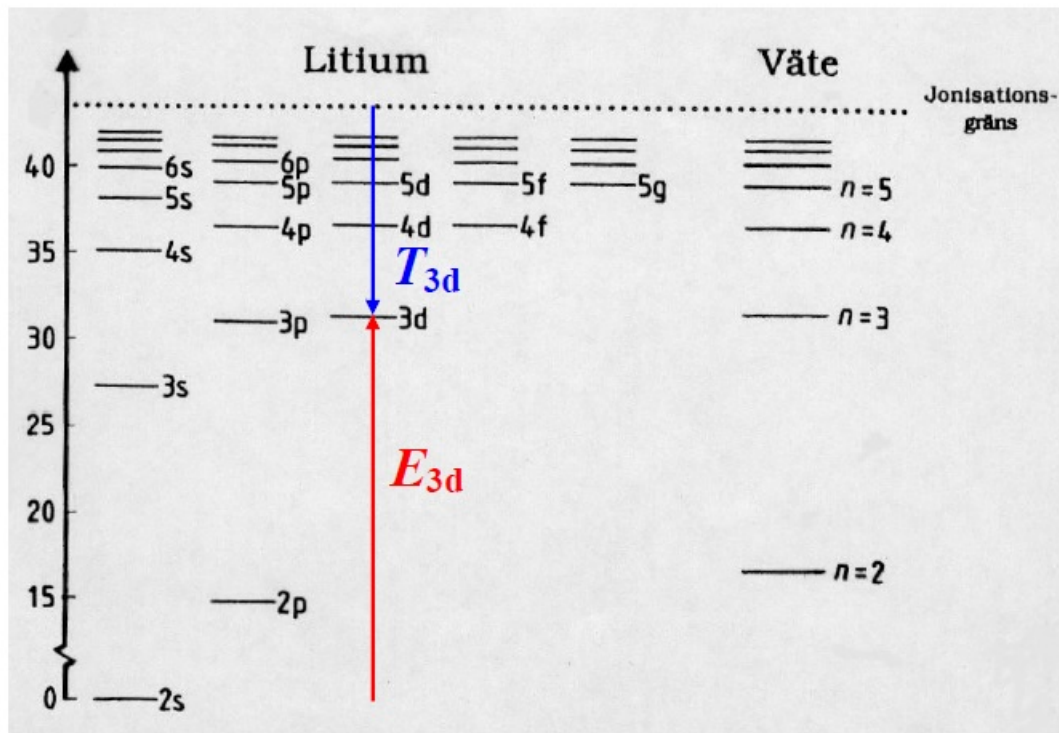
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# Term values in Li and H.

$$T = E_{jon} - E$$



	$T_{\text{exp}} / \text{cm}^{-1}$	$T_{\text{H}} = R_{\text{Li}}/9 / \text{cm}^{-1}$	% fel
$1s^2 3s$	16281	12192	33
$1s^2 3p$	12562	-"	3
$1s^2 3d$	12204	-"	0.1

## Quantum defect in F VII

$$T = R \cdot \frac{Z^2}{n^2} \quad \text{H-like}$$

$$T = R \cdot \frac{\zeta^2}{n^2} \quad \text{Completely screened nucleus}$$
$$\zeta = Z - N_{\text{iner}}$$

$$T = R \cdot \frac{\zeta^2}{(n - \delta)^2} \quad \delta = \text{quantum defect}$$

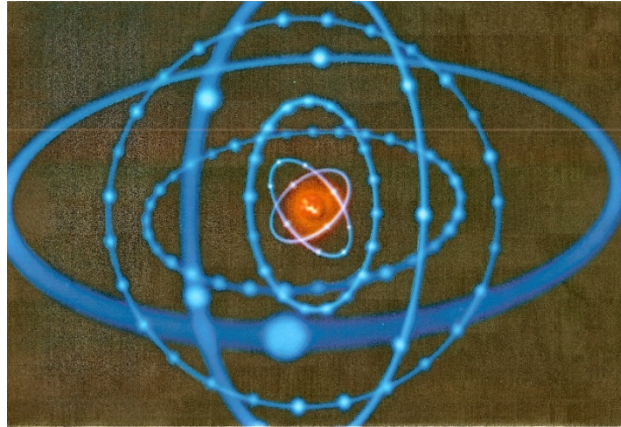
$\delta$  is:

- experimentally determined
- strongly dependent of  $\ell$
- approximately independent of  $n$ .

## Quantum defect in F VII (Li-like)

$n$	$s$	$p$	$d$	$f$	$g$
2	0.1026	0.02660			
3	0.0992	0.02693	0.001295		
4	0.0983	0.02711	0.001794	0.000262	
5	0.0979	0.02718	0.002030	0.000466	0.000181
6	0.0976	0.02782	0.002016	0.000529	0.000266
7	0.0975		0.002147	0.000455	-
8			0.002665	0.000528	0.000304
9				0.000530	





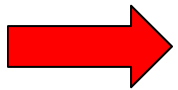
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## The central field approximation

- Each electron moves independently of the other in the electrostatic field from the nucleus and the other  $N - 1$  electrons.
- This field is assumed to be spherically symmetric.

**Independent**

$$H\Psi = E\Psi$$
$$H = \sum_{i=1}^N H_i = \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_i(r_i) \right)$$

**Unknown but spherically symmetric**

$$\Psi = \prod_{i=1}^N \phi_i \quad E = \sum_{i=1}^N \varepsilon_i \quad H_i \phi_i = \varepsilon_i \phi_i$$
$$\phi_i = R_{n_i l_i}(r_i) \cdot Y_{l_i, m_{l_i}}(\theta_i, \varphi_i) \cdot \chi_{m_{s_i}}(s_{z_i})$$

**Determined numerically**

# Configurations in Ne I

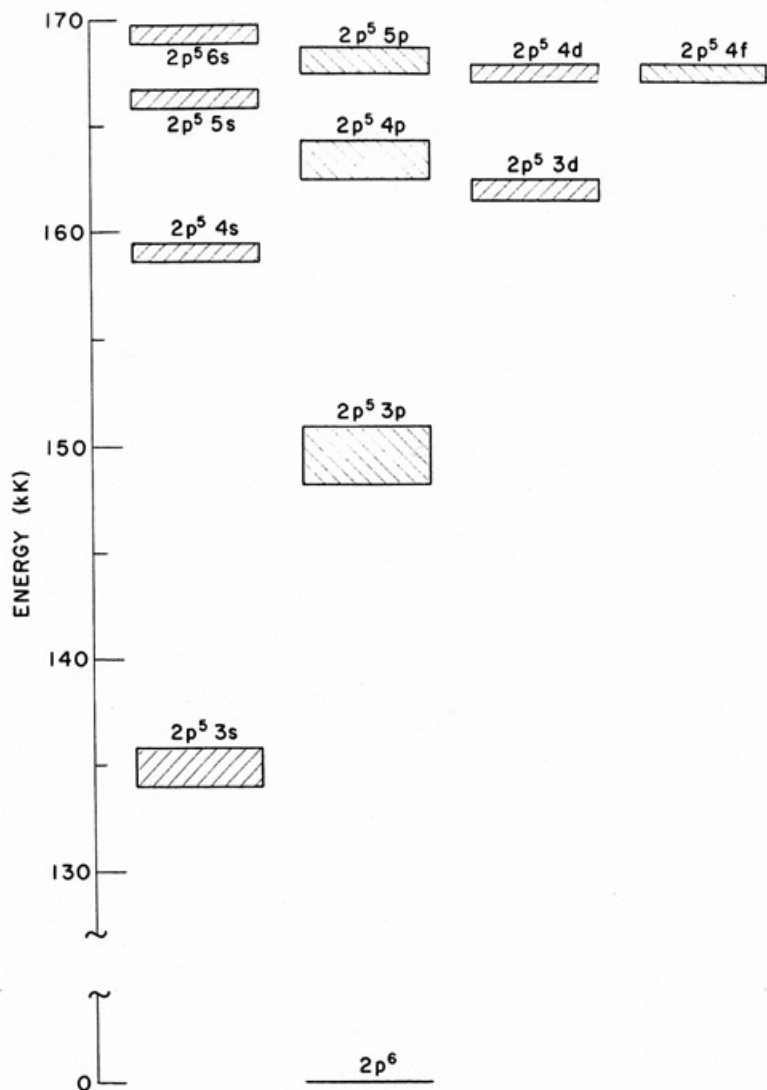


Fig. 4-1. Block diagram of the lowest configurations of Ne I. The levels of each configuration lie within the limited energy range shown by the corresponding shaded block. (There is one level in  $2p^6$ , and there are four levels in each  $p^5s$  configuration, ten levels in each  $p^5p$ , and twelve levels in each  $p^5d$  or  $p^5f$  configuration.)



# The physical background to the periodic table of the elements.

1. Number of quantum states  $N$ :

a) Given  $n$  and  $\ell$ . Orbital / subshell

$N = 2 \cdot (2\ell + 1)$  due to  $m_s$  and  $m_\ell$ .

b) Given  $n$ . Shell

$$N = 2n^2$$

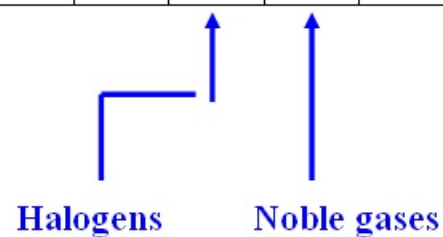
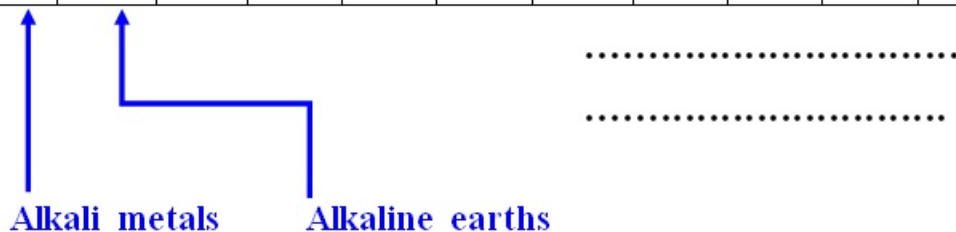
$$N = \sum_{\ell=0}^{n-1} 2(2\ell+1) = \sum_{\ell=0}^{n-1} 4\ell + \sum_{\ell=0}^{n-1} 2 = 4 \frac{n(n-1)}{2} + 2n = 2n^2$$

2. Highest binding energy for low  $n$  and  $\ell$  due to the quantum defect

3. Pauli principle, i.e. antisymmetric wavefunctions, demanding that no 2 electrons have all 4 quantum numbers identical

## Periodic System (first four rows)

<b>H</b> <b>1s</b>																	<b>He</b> <b>1s<sup>2</sup></b>	Filled K-shell
<b>Li</b> <b>2s</b>	<b>Be</b> <b>2s<sup>2</sup></b>											<b>B</b> <b>2p</b>	<b>C</b> <b>2p<sup>2</sup></b>	<b>N</b> <b>2p<sup>3</sup></b>	<b>O</b> <b>2p<sup>4</sup></b>	<b>F</b> <b>2p<sup>5</sup></b>	<b>Ne</b> <b>2p<sup>6</sup></b>	Filled L-shell
<b>Na</b> <b>3s</b>	<b>Mg</b> <b>3s<sup>2</sup></b>											<b>Al</b> <b>3p</b>	<b>Si</b> <b>3p<sup>2</sup></b>	<b>P</b> <b>3p<sup>3</sup></b>	<b>S</b> <b>3p<sup>4</sup></b>	<b>Cl</b> <b>3p<sup>5</sup></b>	<b>Ar</b> <b>3p<sup>6</sup></b>	8 outer electrons 3s <sup>2</sup> 3p <sup>6</sup>
<b>K</b> <b>4s</b>	<b>Ca</b> <b>4s<sup>2</sup></b>	<b>Sc</b> <b>3d</b>	<b>Ti</b> <b>3d<sup>2</sup></b>	<b>V</b> <b>3d<sup>3</sup></b>	<b>Cr</b> <b>3d<sup>4</sup></b>	<b>Mn</b> <b>3d<sup>5</sup></b>	<b>Fe</b> <b>3d<sup>6</sup></b>	<b>Co</b> <b>3d<sup>7</sup></b>	<b>Ni</b> <b>3d<sup>8</sup></b>	<b>Cu</b> <b>3d<sup>9</sup></b>	<b>Zn</b> <b>3d<sup>10</sup></b>	<b>Ga</b> <b>4p</b>	<b>Ge</b> <b>4p<sup>2</sup></b>	<b>As</b> <b>4p<sup>3</sup></b>	<b>Se</b> <b>4p<sup>4</sup></b>	<b>Br</b> <b>4p<sup>5</sup></b>	<b>Xe</b> <b>4p<sup>6</sup></b>	8 outer electrons 4s <sup>2</sup> 4p <sup>6</sup>



# Configurations in Ne I

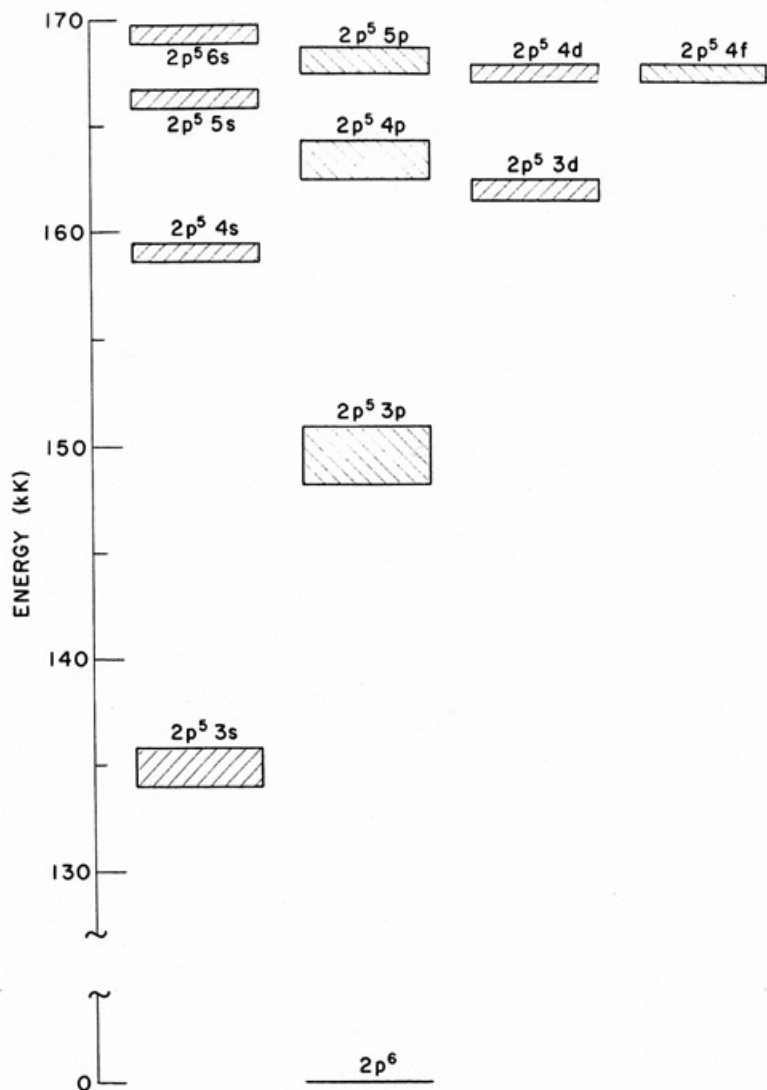


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## ***LS-coupling***

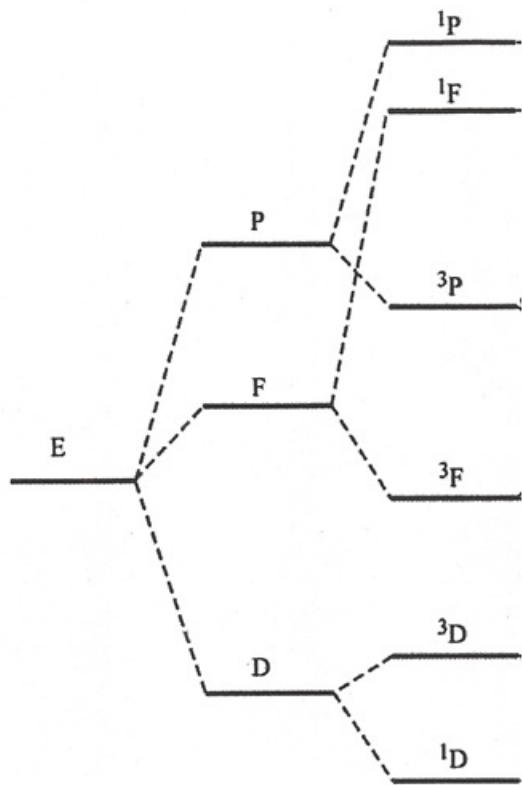
$$\hat{L} = \sum_{i=1}^N \hat{\ell}_i, \quad \hat{S} = \sum_{i=1}^N \hat{s}_i$$

(Note NOT  $\hat{J} = \hat{L} + \hat{S}$ !!)

Assume no spin-dependent terms in  $\hat{H}$  i.e. no spin-orbit interaction, then  $[\hat{H}, \hat{J}] = [\hat{H}, \hat{S}] = [\hat{H}, \hat{L}] = 0$ . Thus all energy levels must be characterized by the quantum numbers,  $L$ ,  $S$  and  $J$ .

Notation:  $^{2S+1}L_J$

# pd-configuration LS-coupling



**Configuration**

**Central field**

**Term**

**Repulsion**

Numerical example for 2p3d in O V, energies in  $\text{cm}^{-1}$

$$E(2p3d) = 701810$$

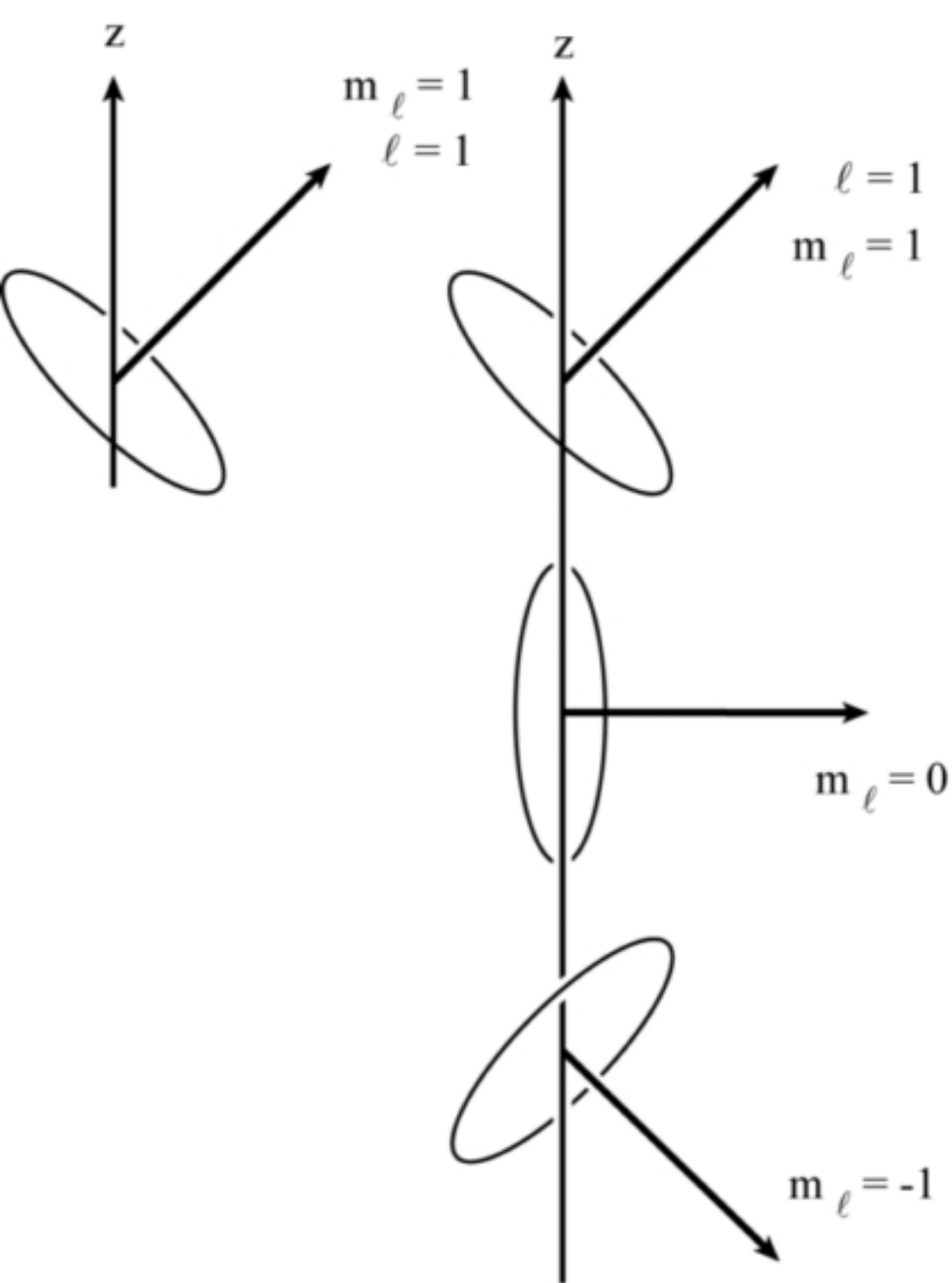
$$\Delta E (P - D) = 8980$$

$$\Delta E ({}^1F - {}^3F) = 15074$$

Kinetic and central part of electrostatic

Direct part of electrostatic repulsion

Exchange part of electrostatic repulsion



**Direct electrostatic interaction in a  $pp'$  config.**  
 $pp'$  contains a S, P and D term ( $\ell_1 = \ell_2 = 1 \Rightarrow L = 0, 1, 2$ )

**D;  $L = 2$ :**  $M_L$   $\ell$   $m_\ell$

$$|1\ 1\ 2\ 2\rangle = |1\ 1\rangle \cdot |1\ 1\rangle$$

$$|1\ 1\ 2\ 1\rangle = \frac{1}{\sqrt{2}}|1\ 1\rangle|1\ 0\rangle + \frac{1}{\sqrt{2}}|1\ 0\rangle|1\ 1\rangle$$

$$|1\ 1\ 2\ 0\rangle = \frac{1}{\sqrt{6}}|1\ 1\rangle|1\ -1\rangle + \sqrt{\frac{2}{3}}|1\ 0\rangle|1\ 0\rangle + \frac{1}{\sqrt{6}}|1\ -1\rangle|1\ 1\rangle$$

$$|1\ 1\ 2\ -1\rangle = \frac{1}{\sqrt{2}}|1\ 0\rangle|1\ -1\rangle + \frac{1}{\sqrt{2}}|1\ -1\rangle|1\ 0\rangle$$

$$|1\ 1\ 2\ -2\rangle = |1\ -1\rangle \cdot |1\ -1\rangle$$

**P;  $L = 1$ :**

$$|1\ 1\ 1\ 1\rangle = \frac{1}{\sqrt{2}}|1\ 1\rangle|1\ 0\rangle - \frac{1}{\sqrt{2}}|1\ 0\rangle|1\ 1\rangle$$

$$|1\ 1\ 1\ 0\rangle = \frac{1}{\sqrt{2}}|1\ 1\rangle|1\ -1\rangle - \frac{1}{\sqrt{2}}|1\ -1\rangle|1\ 1\rangle + 0 \cdot |1\ 0\rangle|1\ 0\rangle$$

$$|1\ 1\ 1\ -1\rangle = \frac{1}{\sqrt{2}}|1\ 0\rangle|1\ -1\rangle - \frac{1}{\sqrt{2}}|1\ -1\rangle|1\ 0\rangle$$

**Note!!**

**S;  $L = 0$ :**

$$|1\ 1\ 0\ 0\rangle = \frac{1}{\sqrt{3}}|1\ 1\rangle|1\ -1\rangle - \frac{1}{\sqrt{3}}|1\ 0\rangle|1\ 0\rangle + \frac{1}{\sqrt{3}}|1\ -1\rangle|1\ 1\rangle$$

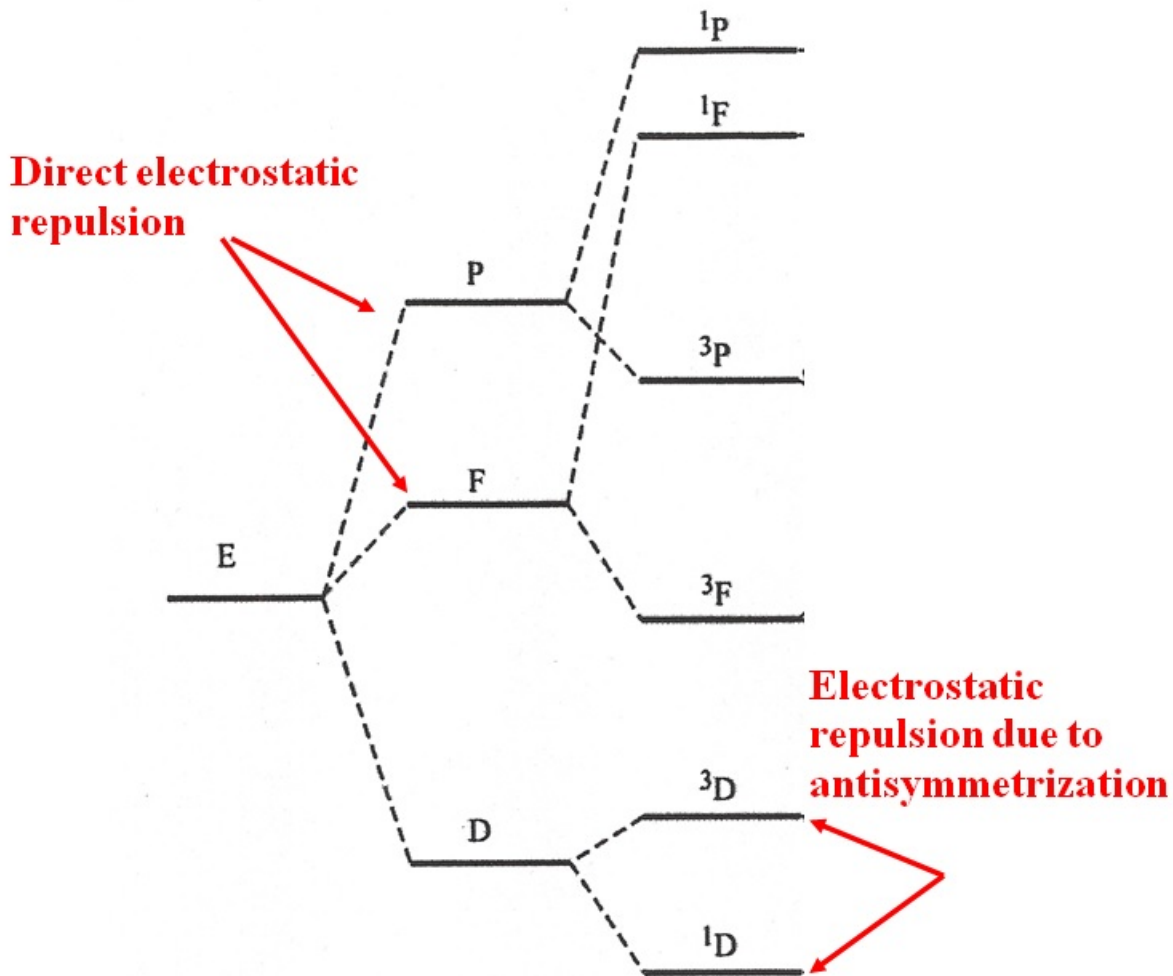
Combinations with maximum overlap between the charge distributions are marked in **blue**. Max overlap means max repulsion means less binding energy means higher excitation energy.

**Thus, S and D terms tend to lay higher than P in  $pp'$ -configurations**

**Generally highest and lowest  $L$  terms tend to lay higher.**



# Details of the electrostatic interactions in a $pd$ -configuration in LS-coupling



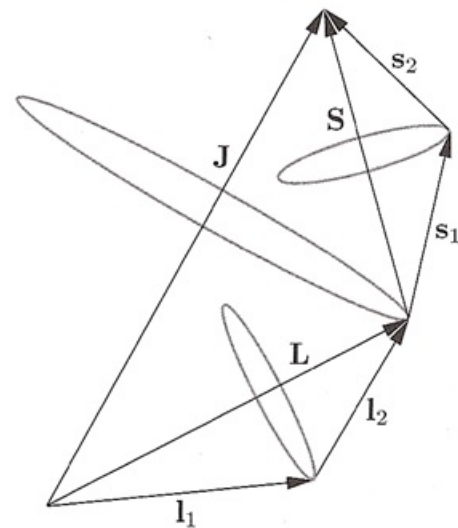
## Angular momentum couplings of two electrons in open subshells

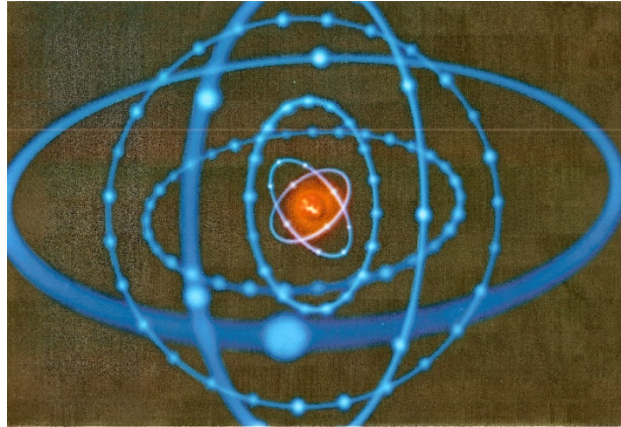
Energy structure	Angular momentum coupling	Wavefunctions	Eigenfunctions to
Configuration	-	$ \ell_i, m_{\ell_i}\rangle \cdot  s_i, m_{s_i}\rangle$	$\hat{\ell}_i^2, \hat{\ell}_{iz}, \hat{S}_i^2, \hat{S}_{iz}$
Term $2S+1L$	$\hat{L} = \hat{\ell}_1 + \hat{\ell}_2, \hat{S} = \hat{s}_1 + \hat{s}_2$	$ L, M_L, S, M_S\rangle$	$\hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z$
Level $2S+1L_J$	$\hat{J} = \hat{L} + \hat{S}$	$ L, S, J, M_J\rangle$	$\hat{L}^2, \hat{S}^2, \hat{J}^2, \hat{J}_z$

$$|\ell_i, m_{\ell_i}\rangle \cdot |s_i, m_{s_i}\rangle = R_{n_i \ell_i}(r_i) \cdot Y_{\ell_i m_{\ell_i}}(\theta_i, \varphi_i) \cdot \chi_{m_{s_i}}(s z_i)$$

Example of  $\hat{L} = \hat{\ell}_1 + \hat{\ell}_2$  coupling using Clebsch-Gordan coeff.

$$|\ell_1, \ell_2, L, M_L\rangle = \sum_{m_{\ell_1}} C(\ell_1, m_{\ell_1}, \ell_2, M_L - m_{\ell_1} : L, M_L) |\ell_1, m_{\ell_1}\rangle |\ell_2, M_L - m_{\ell_1}\rangle$$





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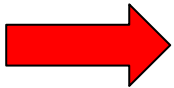
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## Magnetic interactions - internal

$$E = \langle -\hat{\mu} \cdot \hat{B} \rangle_{\Psi}$$

### Spin-Orbit interaction

$$\left. \begin{array}{l} \hat{\mu} = \hat{\mu}_s = -2 \frac{e}{2m} \hat{S} \\ \hat{B} \sim \hat{L} \\ \Psi = |L, S, J, M_J\rangle \end{array} \right\} \Rightarrow E_{SO} \approx \langle \hat{L} \cdot \hat{S} \rangle_{\Psi} = \beta \cdot \frac{1}{2} [J(J+1) - L(L+1) - S(S+1)]$$

Landé:  $E_{SO}(J) - E_{SO}(J-1) = \beta \cdot J$

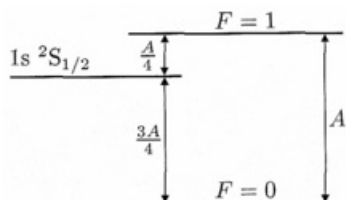
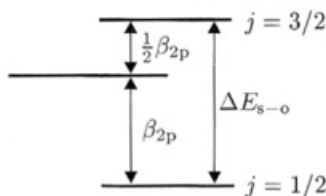
### Hyperfine interaction (Note $m_p \approx 2000 \cdot m_e$ )

$$\left. \begin{array}{l} \hat{\mu} = \hat{\mu}_I = +g_I \frac{e}{2m_p} \hat{I} \\ \hat{B} \sim \hat{J} \\ \Psi = |J, I, F, M_F\rangle \end{array} \right\} \Rightarrow E_{\text{hfs}} \approx \langle \hat{J} \cdot \hat{I} \rangle_{\Psi} = A \cdot \frac{1}{2} [F(F+1) - J(J+1) - I(I+1)]$$

Landé:  $E_{\text{hfs}}(F) - E_{\text{hfs}}(F-1) = A \cdot F$

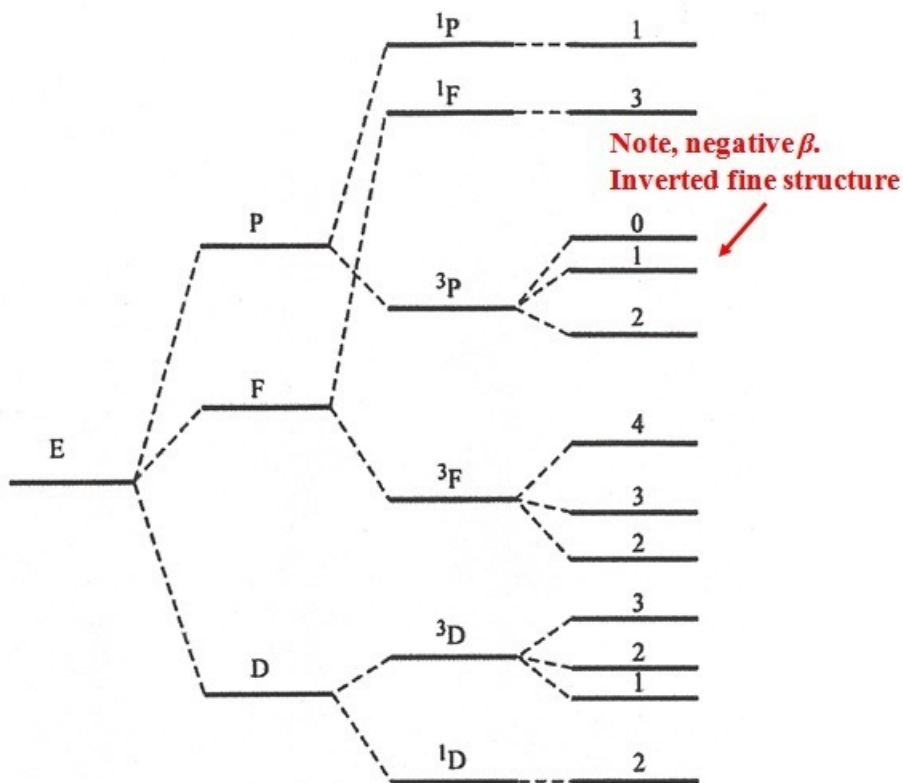
**Scaling:**  $\beta_H \sim \frac{Z^4}{n^3 \cdot \ell^3} \rightarrow \frac{\zeta^4}{(n^*)^3 \cdot \ell^3}, \quad n^* = n - \delta, \quad \zeta = Z - N_{\text{core}}$

$$A_H(s) \sim \frac{Z^3}{n^3} \rightarrow \frac{\zeta^3}{(n^*)^3}$$





# pd-configuration LSJ-coupling



Configuration	Term	Level
Central field	Repulsion	Spin-orbit

Numerical example for 2p3d in O V, energies in  $\text{cm}^{-1}$

$E(2p3d) = 701810$	Kinetic and central part of electrostatic
$\Delta E (P - D) = 8980$	Direct part of electrostatic repulsion
$\Delta E ({}^1F - {}^3F) = 15074$	Exchange part of electrostatic repulsion
$\Delta E ({}^3F_4 - {}^3F_3) = 235$	Spin-orbit magnetic energy

## Magnetic interactions - external

### Zeeman effect. ( $B \sim 1 \text{ T}$ )

Weak field, i.e. much less energy than that of the SO-interaction

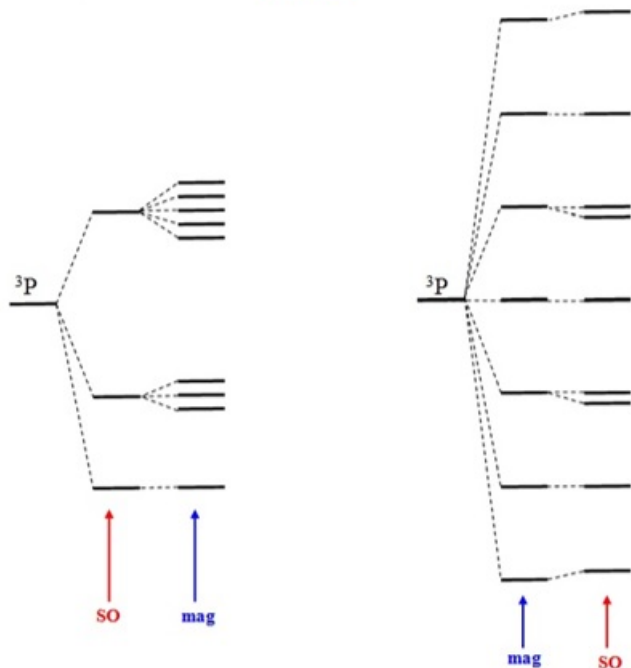
$$\left. \begin{aligned} \hat{\mu} &= \hat{\mu}_L + \hat{\mu}_S = -\frac{e}{2m}(\hat{L} + 2\hat{S}) \\ \hat{B} &= B_{\text{ext}} \cdot \hat{e}_z, \Psi = |L, S, J, M_J\rangle \end{aligned} \right\} \Rightarrow E(L, S, J, M_J) = E(L, S, J) + \mu_B \cdot B \cdot g_J \cdot M_J$$

### Paschen-Back effect. ( $B \sim 1000 \text{ T}$ )

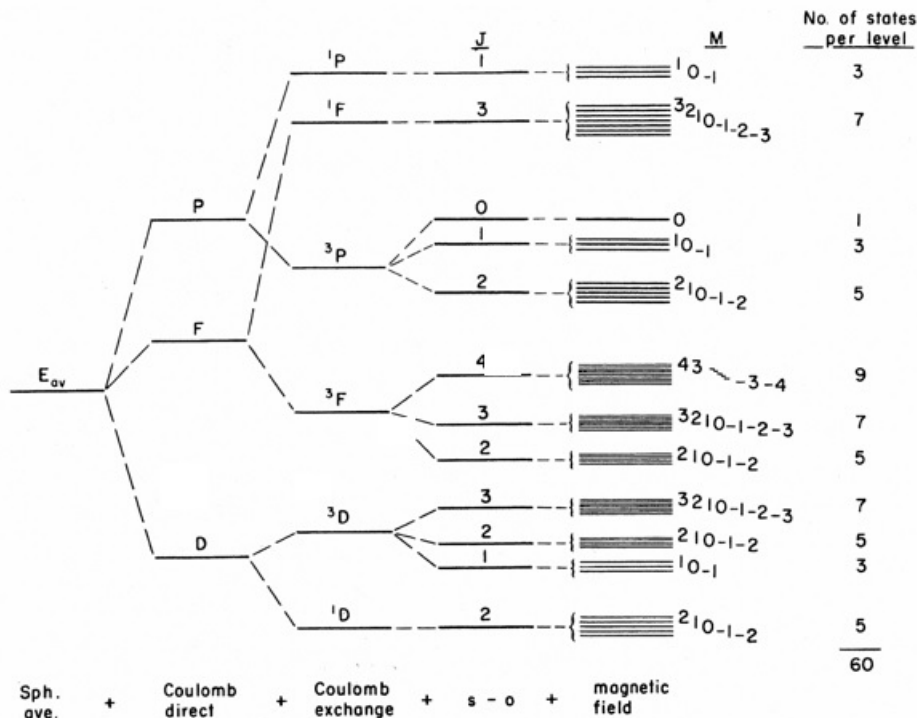
Strong field, i.e. much more energy than that of the SO-interaction.

$$\left. \begin{aligned} \hat{\mu} &= \hat{\mu}_L + \hat{\mu}_S = -\frac{e}{2m}(\hat{L} + 2\hat{S}) \\ \hat{B} &= B_{\text{ext}} \cdot \hat{e}_z, \Psi = |L, M_L, S, M_S\rangle \end{aligned} \right\} \Rightarrow E(L, M_L, S, M_S) = E(L, S) + \mu_B \cdot B \cdot (M_L + 2M_S)$$

Then SO as the next perturbation,  $\beta \cdot M_L M_S$



# pd-configuration with external magnetic field



Configuration      Term      Level      State  
 Central field      Repulsion      Spin-orbit      External B-field

## Numerical example for 2p3d in O V, energies in cm<sup>-1</sup>

$$E(2p3d) = 701810$$

$$\Delta E (P - D) = 8980$$

$$\Delta E ({}^1F - {}^3F) = 15074$$

$$\Delta E ({}^3F_4 - {}^3F_3) = 235$$

$$\Delta E_{\text{mag}} = g_J \cdot \mu_B \cdot B = 0.5$$

Kinetic and central part of electrostatic

Direct part of electrostatic repulsion

Exchange part of electrostatic repulsion

Spin-orbit magnetic energy

$B = 1 \text{ T}$ ,  $g_J = 1$ ,  $\Delta M_J = 1$ . Indep. of atom

## Magnetic interactions

General:  $E = \langle -\boldsymbol{\mu} \cdot \mathbf{B} \rangle_{\Psi}$

Where  $\boldsymbol{\mu}$  is a magnetic moment and  $\mathbf{B}$  the magnetic field strength

### Spin-Orbit interaction. $\mathbf{J} = \mathbf{L} + \mathbf{S}$

$$\left. \begin{array}{l} \boldsymbol{\mu} = \boldsymbol{\mu}_S = -2 \frac{e}{2m} \mathbf{S} \\ \mathbf{B} \sim \mathbf{L} \end{array} \right\} \Rightarrow E_{SO} \sim \langle \mathbf{L} \cdot \mathbf{S} \rangle = \beta \cdot \frac{1}{2} [J(J+1) - L(L+1) - S(S+1)]$$

### Hyperfine interaction (Note $m_p \approx 2000 \cdot m_e$ ). $\mathbf{F} = \mathbf{J} + \mathbf{I}$

$$\left. \begin{array}{l} \boldsymbol{\mu} = \boldsymbol{\mu}_I = +g_I \frac{e}{2m_p} \mathbf{I} \\ \mathbf{B} \sim \mathbf{J} \end{array} \right\} \Rightarrow E_{hfs} \sim \langle \mathbf{J} \cdot \mathbf{I} \rangle = A \cdot \frac{1}{2} [F(F+1) - J(J+1) - I(I+1)]$$

### Zeeman effect. ( $\mathbf{B} \sim 1 \text{ T}$ )

Weak field, i.e. much less energy than that of the SO-interaction

$$\left. \begin{array}{l} \boldsymbol{\mu} = \boldsymbol{\mu}_L + \boldsymbol{\mu}_S = -\frac{e}{2m} (\mathbf{L} + 2\mathbf{S}) \\ \mathbf{B} = \mathbf{B}_{\text{ext}}, \Psi = |L, S, J, M_J\rangle \end{array} \right\} \Rightarrow E(L, S, J, M_J) = E(L, S, J) + \mu_B \cdot B \cdot g_J \cdot M_J$$

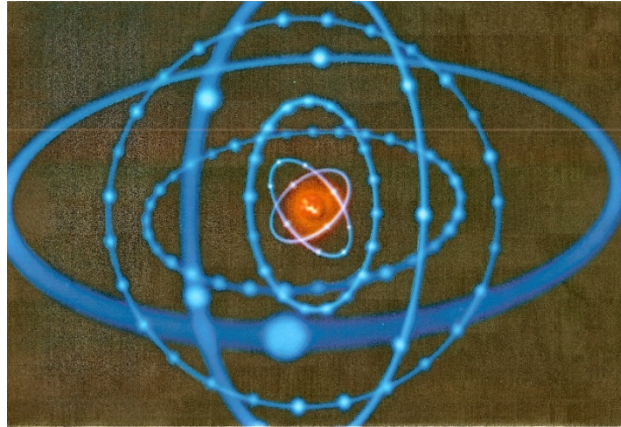
### Paschen-Back effect. ( $\mathbf{B} \sim 1000 \text{ T}$ )

Strong field, i.e. much more energy than that of the SO-interaction.

$$\left. \begin{array}{l} \boldsymbol{\mu} = \boldsymbol{\mu}_L + \boldsymbol{\mu}_S = -\frac{e}{2m} (\mathbf{L} + 2\mathbf{S}) \\ \mathbf{B} = \mathbf{B}_{\text{ext}}, \Psi = |L, M_L, S, M_S\rangle \end{array} \right\} \Rightarrow E(L, M_L, S, M_S) = E(L, S) + \mu_B \cdot B \cdot (M_L + 2M_S)$$

Then SO as the next perturbation,  $\beta \cdot M_L M_S$





- One electron atoms, H-like.

**Bohr model**

**Exact quantum mechanical results**

- Hydrogenic-, Rydberg-atoms. Quantum defect

**Accurate semi-empirical results**

- Many electron atoms.

**Approximations CFA + LS/jj- coupling**

- Magnetic interactions

**Spin-orbit, Hyperfine and**

**External mag. fields**



- Transitions

**Selection rules and line widths**

- Molecules

# E1 Selection Rules

Only one electron may change  $n$  and  $\ell$  quantum numbers, i.e. orbital.

$$\Delta\ell = \pm 1$$

$$\Delta J = 0, \pm 1 \text{ not } 0 \text{ to } 0$$

LS-coupling

$$\Delta S = 0$$

$$\Delta L = 0, \pm 1 \text{ not } 0 \text{ to } 0$$

jj-coupling

$$\Delta j_1 = 0$$

$$\Delta j_2 = 0, \pm 1 \text{ not } 0 \text{ to } 0$$

With hyperfine structure also

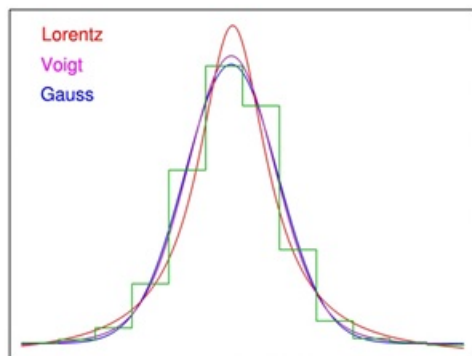
$$\Delta F = 0, \pm 1 \text{ not } 0 \text{ to } 0$$

In an external magnetic field

$$\Delta M_J = 0, \pm 1 \text{ not } 0 \text{ to } 0 \text{ if } \Delta J = 0$$

# Line widths and profiles

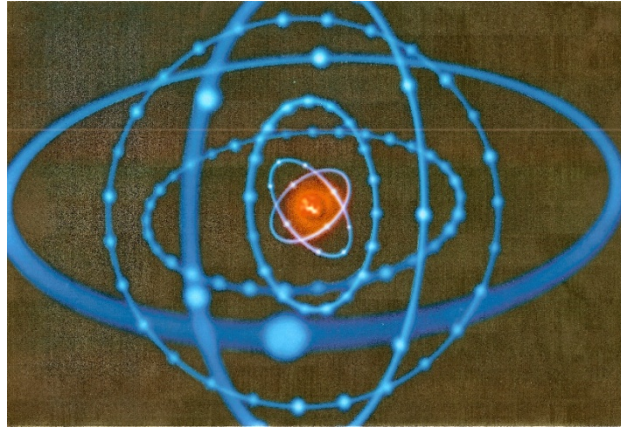
In the atom	Natural	Lorentz
In the light source	Collisional	Lorentz
	Power	Lorentz
	Self absorption	---
	Doppler	Gauss
In the detector	Instrumental	Approx. Gauss



Voigt = convolution of Lorentz and Gauss

Na-example  
(3s - 3p 5890 Å, lifetime 16 ns)

Broadening	$\Delta f / \text{GHz}$	$\Delta \lambda / \text{\AA}$
Natural	0.01	0.0001
Power, $I = 170 \text{ mW/cm}^2$	0.054	0.0006
Pressure, $p = 0.1 \text{ atm}$	0.084	0.0009
Doppler (600 K)	1.86	0.022
Instrument. Fabry Perot: $d = 1 \text{ cm}$ , $R = 0.9$	0.25	0.003
Instrument. Grating 1200 $\ell/\text{mm}$ , 50 $\mu\text{m}$ slit	30	0.35



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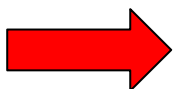
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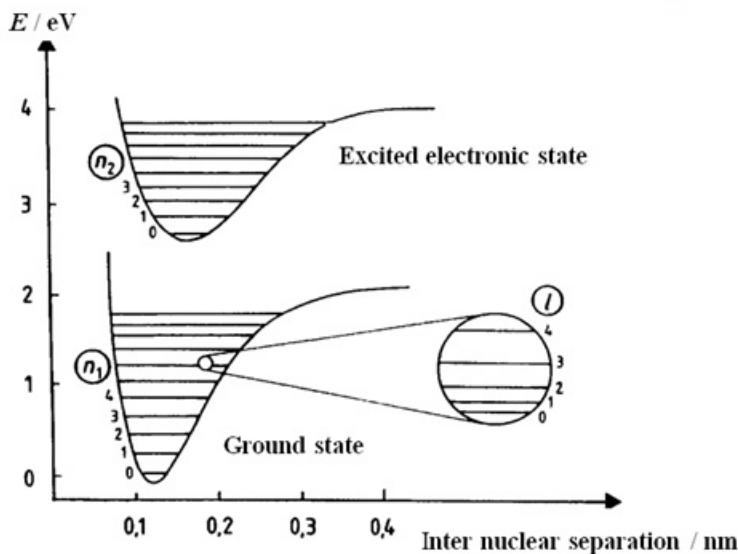


- Molecules



## Energies in a Diatomic Molecule - Summary.

$$E = E_{elektron} + E_{vib} + E_{rot} = E_{elektron} + \hbar\omega_0\left(\nu + \frac{1}{2}\right) + \frac{\hbar^2}{2\mu r^2} \cdot \ell(\ell+1)$$

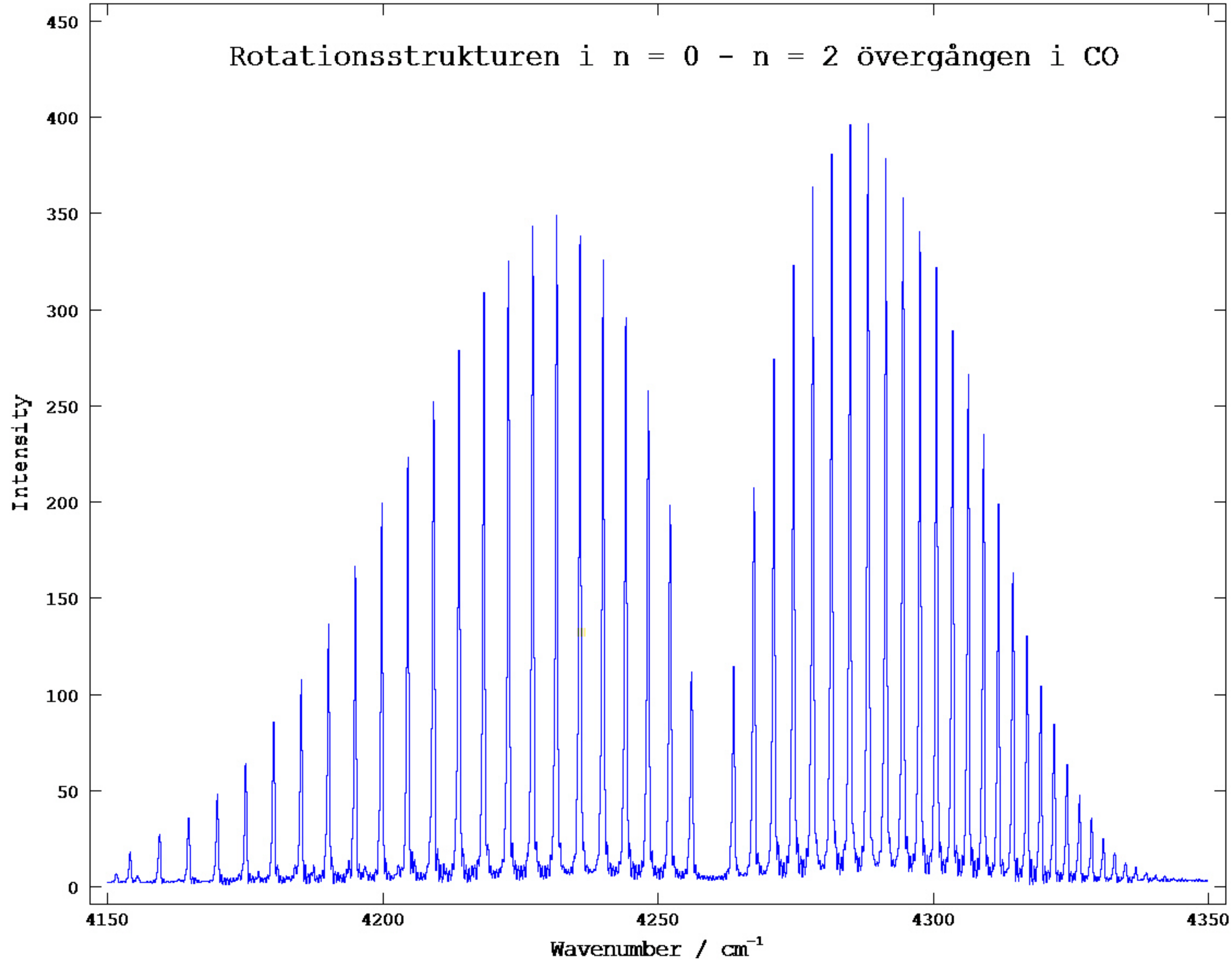


### Orders of magnitude

	Electron	Vibration	Rotation
$E / \text{cm}^{-1}$	40000	1500	10
$E / \text{eV}$	5	0.2	0.001
$\lambda / \mu\text{m}$	0.3	6	1000
$T / \text{K}$	40000	1500	10

(Note the coincidence that energies expressed in  $\text{cm}^{-1}$  and as a temperature in K has almost the same numerical value, i.e.  $1/(100 \cdot h \cdot c) = 5.035 \cdot 10^{22} \approx 2/(3 \cdot k) = 4.83 \cdot 10^{22}$ !)

# Rotationsstrukturen i $n = 0 - n = 2$ övergången i CO



# The Greenhouse Effect.

The black-body radiation from the Sun (5500 °C) and the Earth (18 °C) and the absorption in the atmosphere in different wavelength regions

