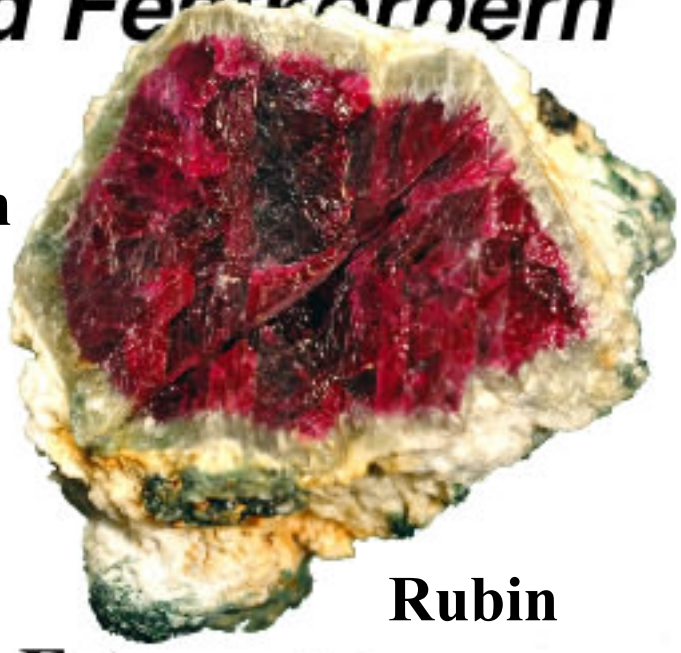
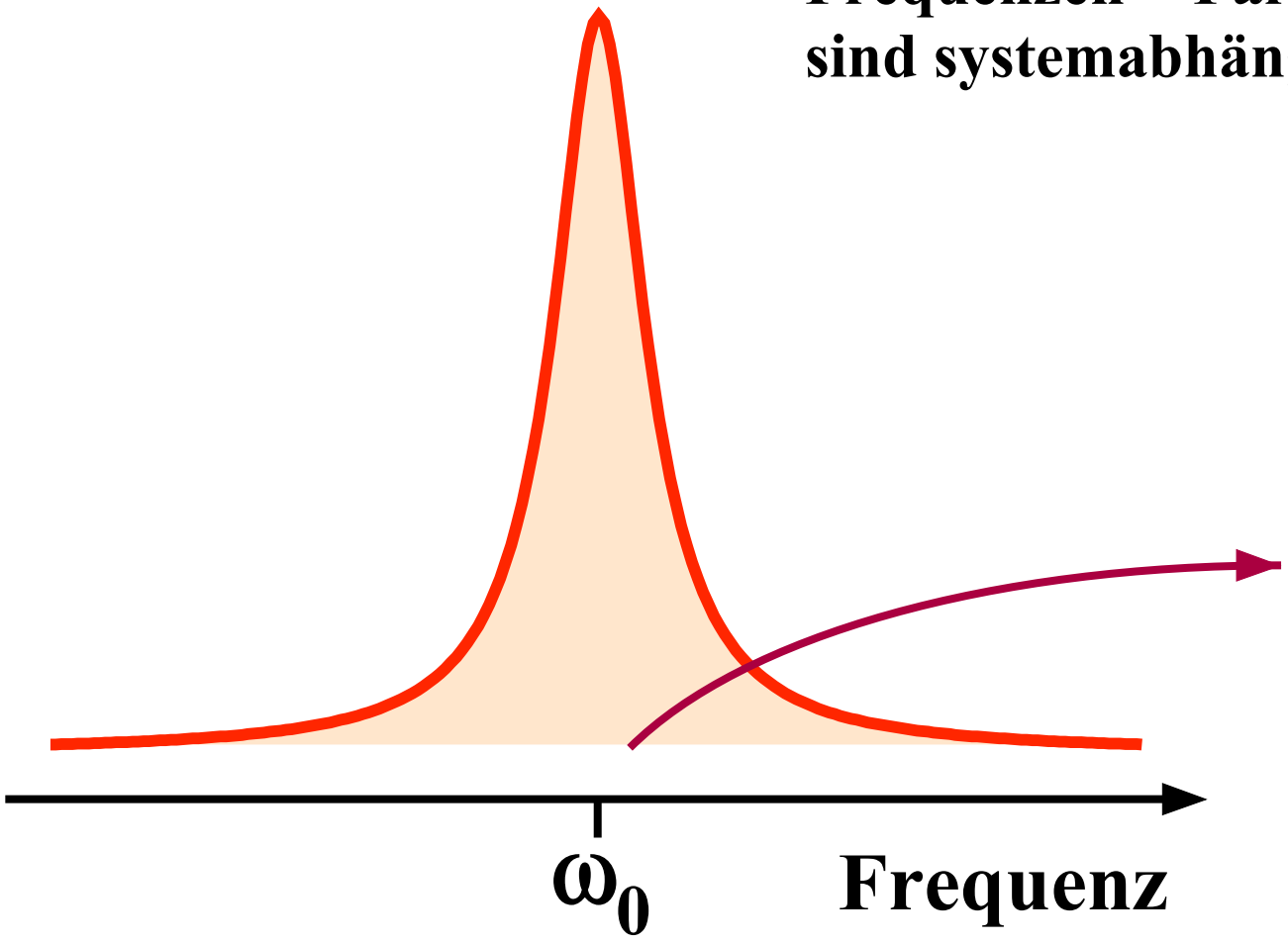
4) Optische Übergänge

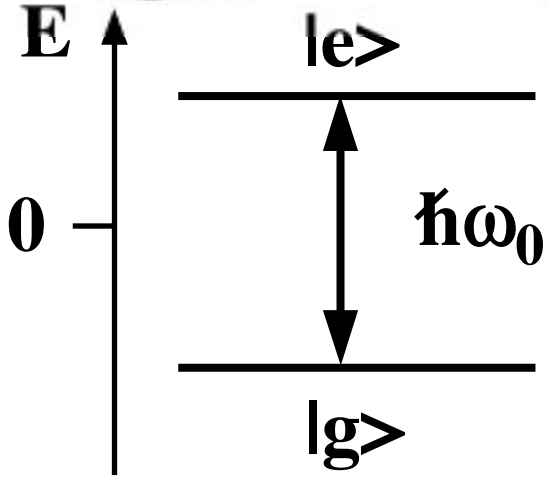
in Atomen, Molekülen und Festkörpern

Frequenzen = Farben
sind systemabhängig

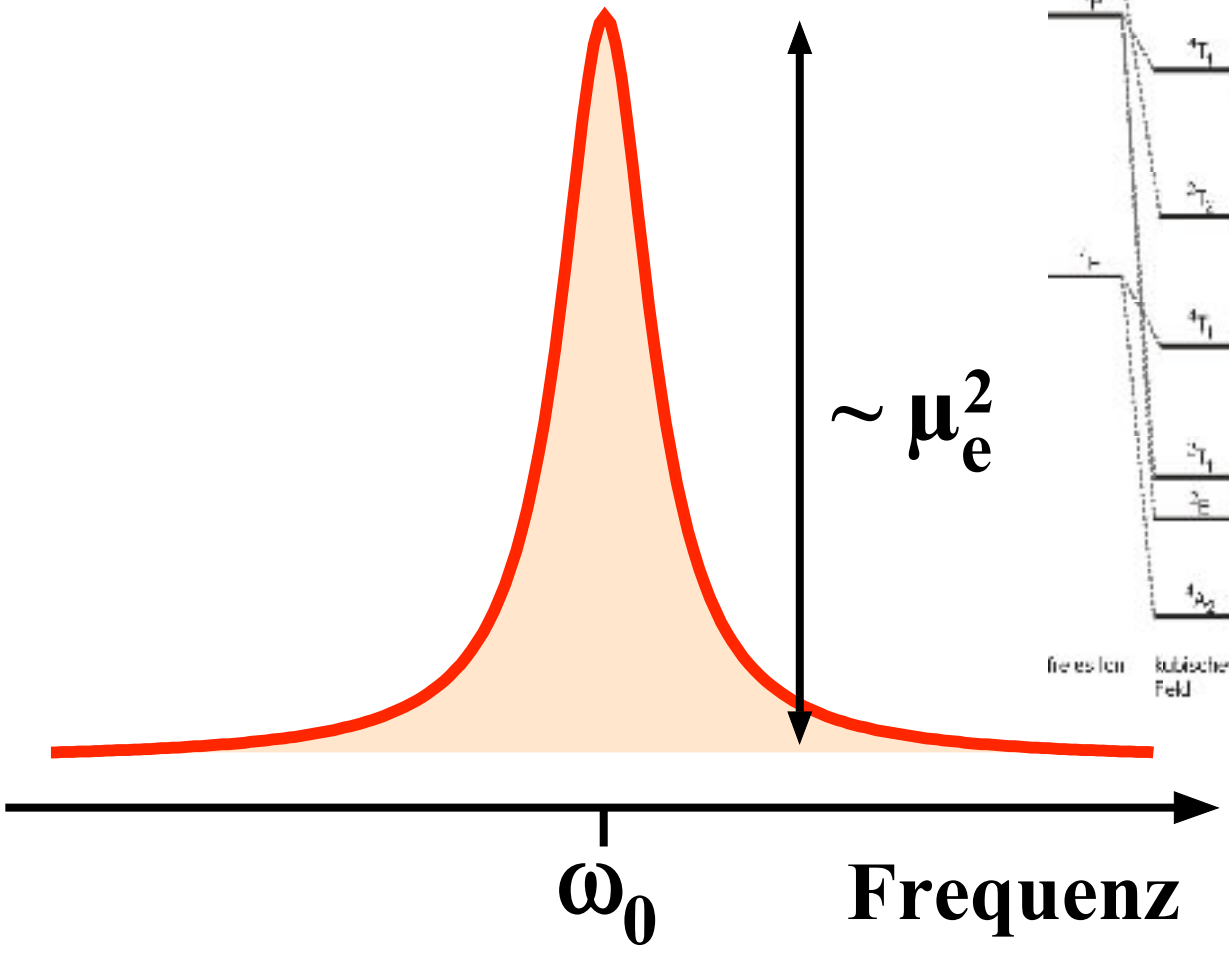


Rubin

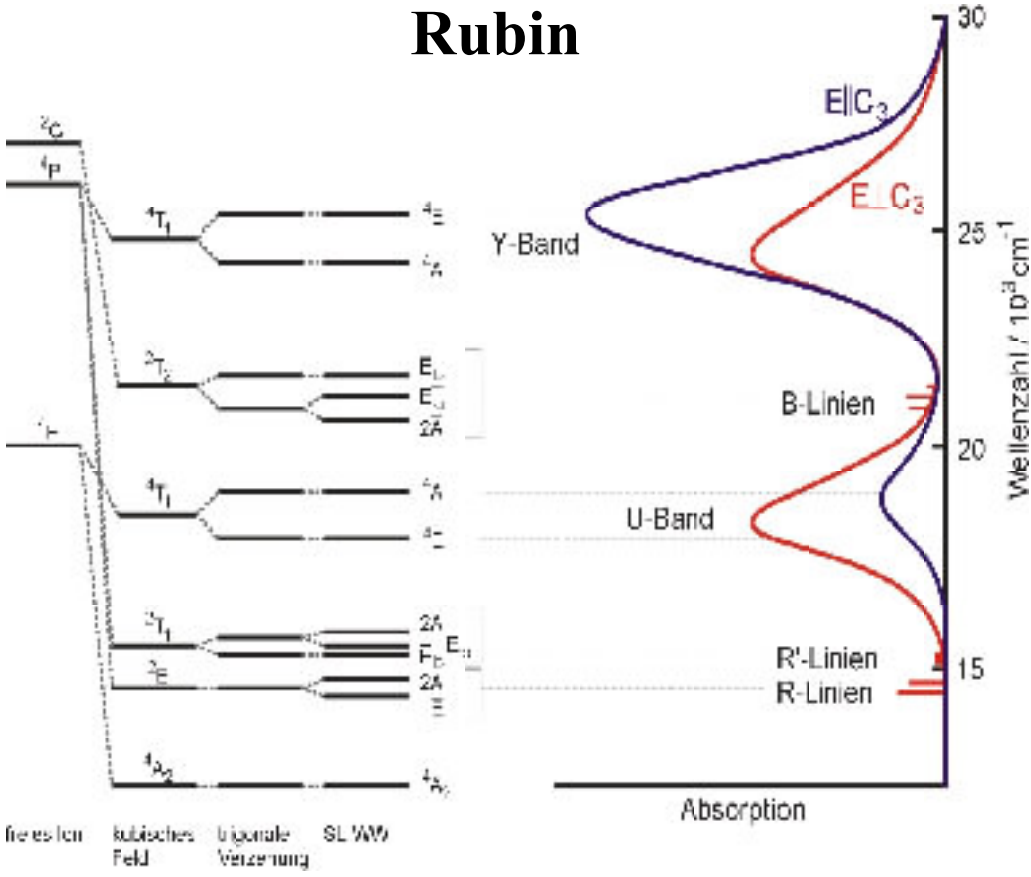




Amplituden

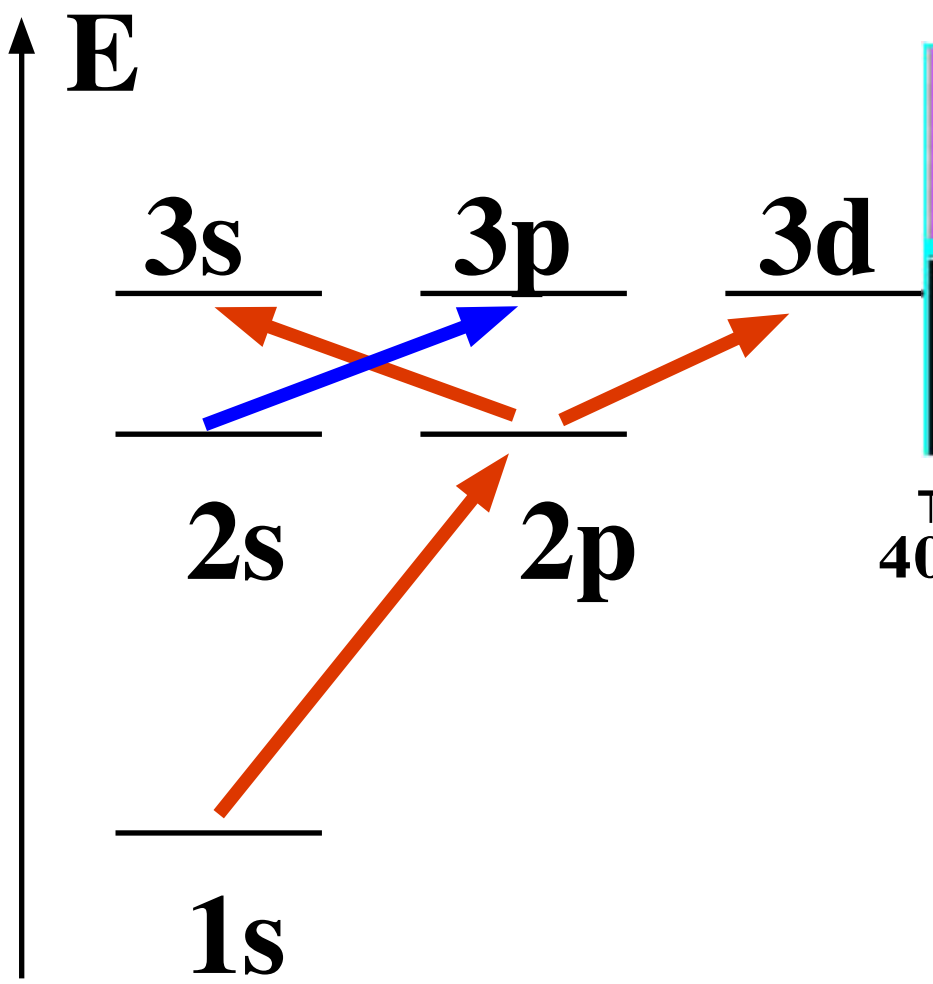


Rubin

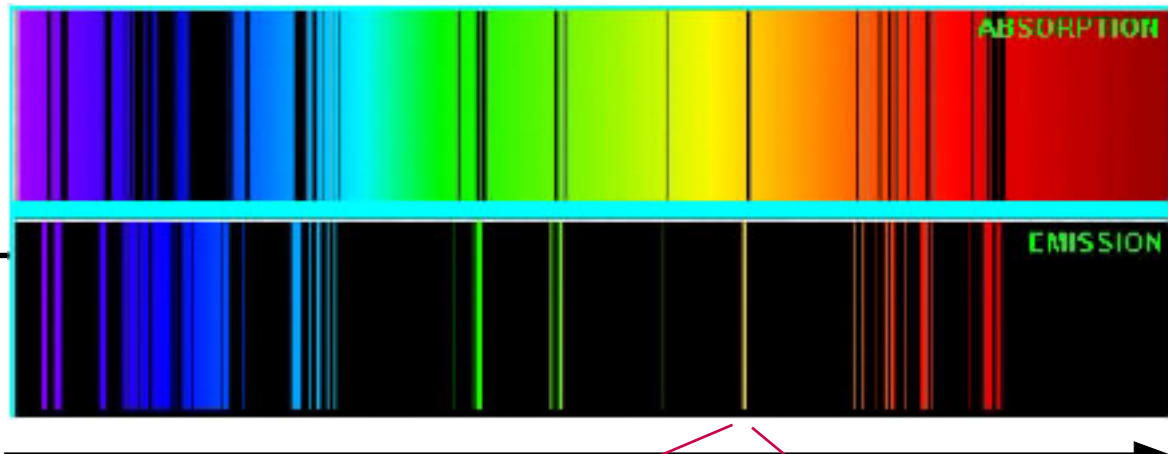


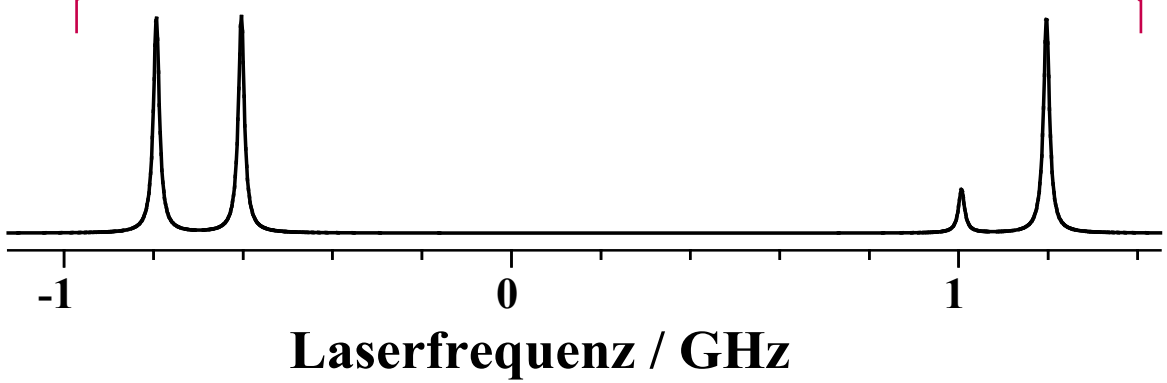
Atome

typische atomare
Niveaustruktur

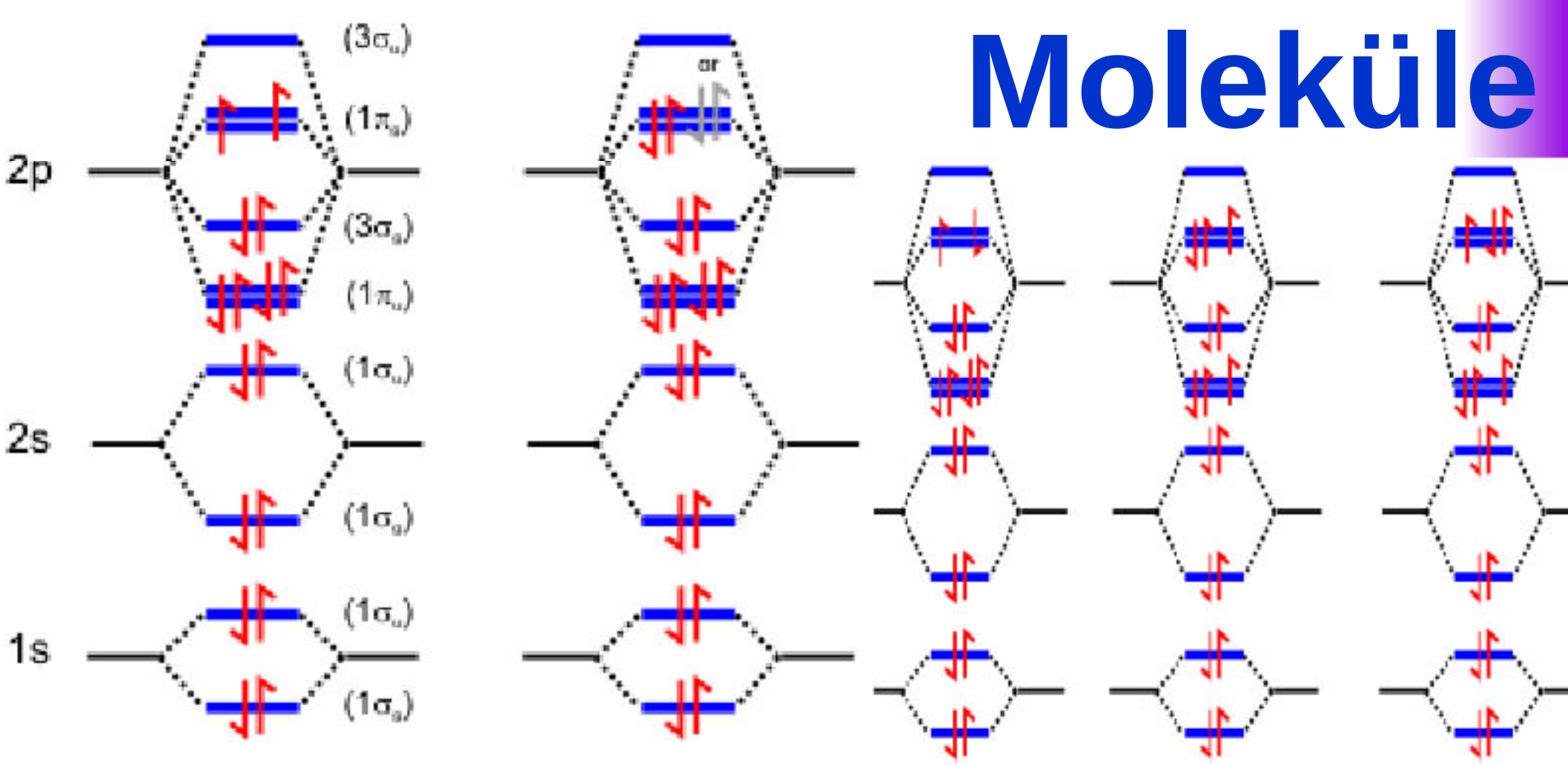


Na Spektrum





Moleküle



Ground State

$(^3\Sigma_g^-)$

0 eV

Excited State

$(^1\Delta_g)$

1268 nm

(0.9772 eV)

Excited State

$(^1\Sigma_g^+)$

762 nm

(1.6266 eV)

Excited State

$(^3\Sigma_u^+)$

280 nm

(4.4278 eV)

Excited State

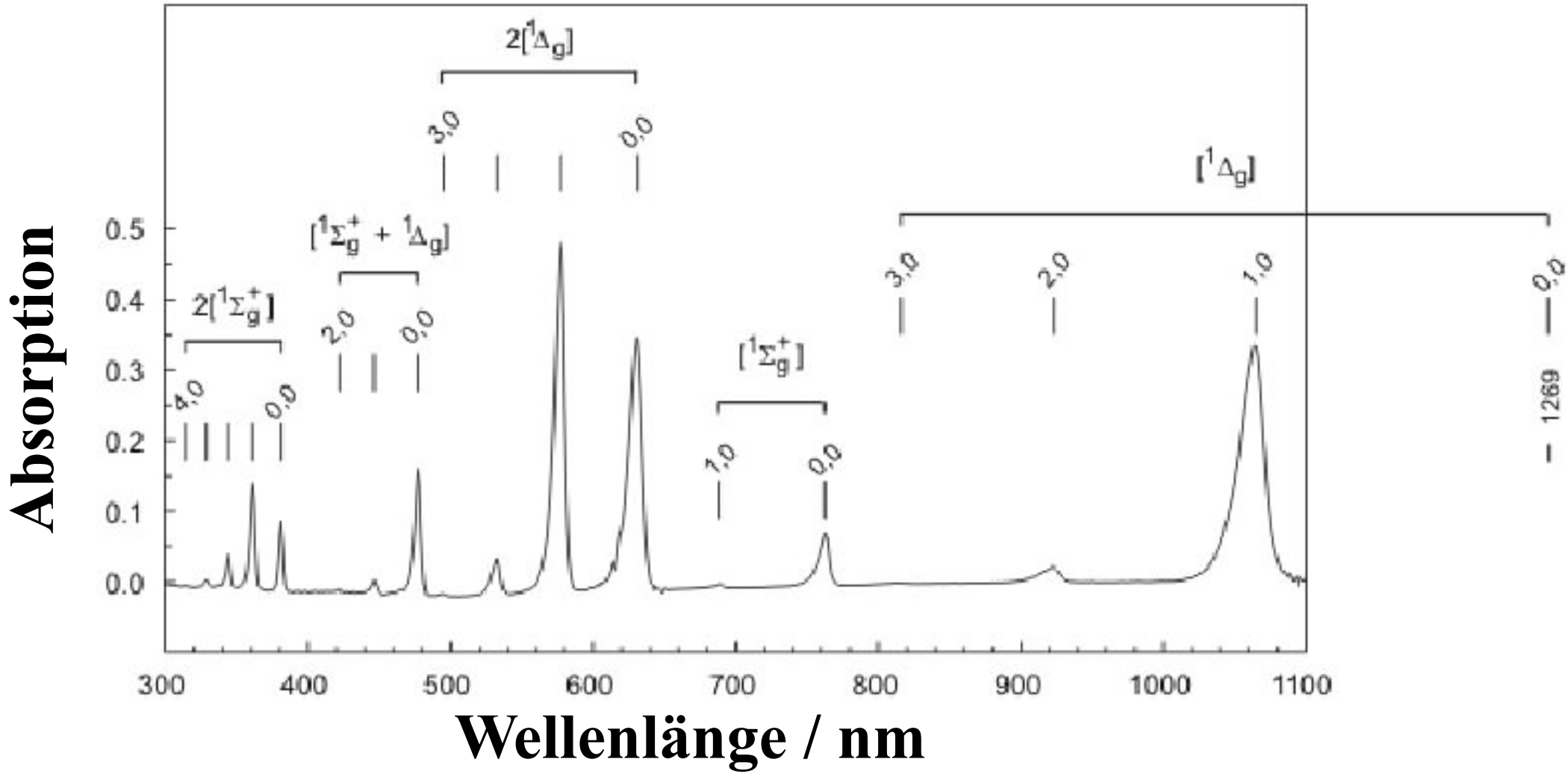
$(^3\Sigma_u^-)$

202 nm

(6.1202 eV)

Moleküle

Absorptionsspektrum von O_2



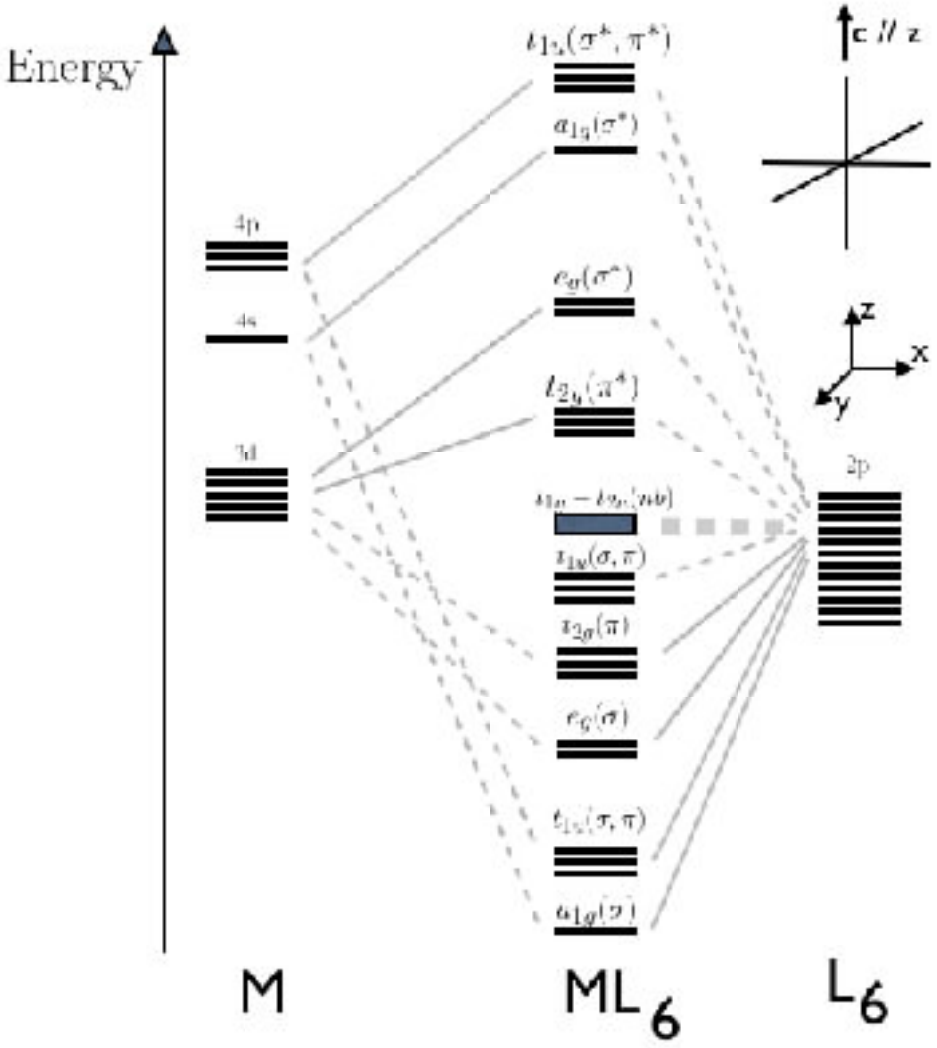
Moleküle

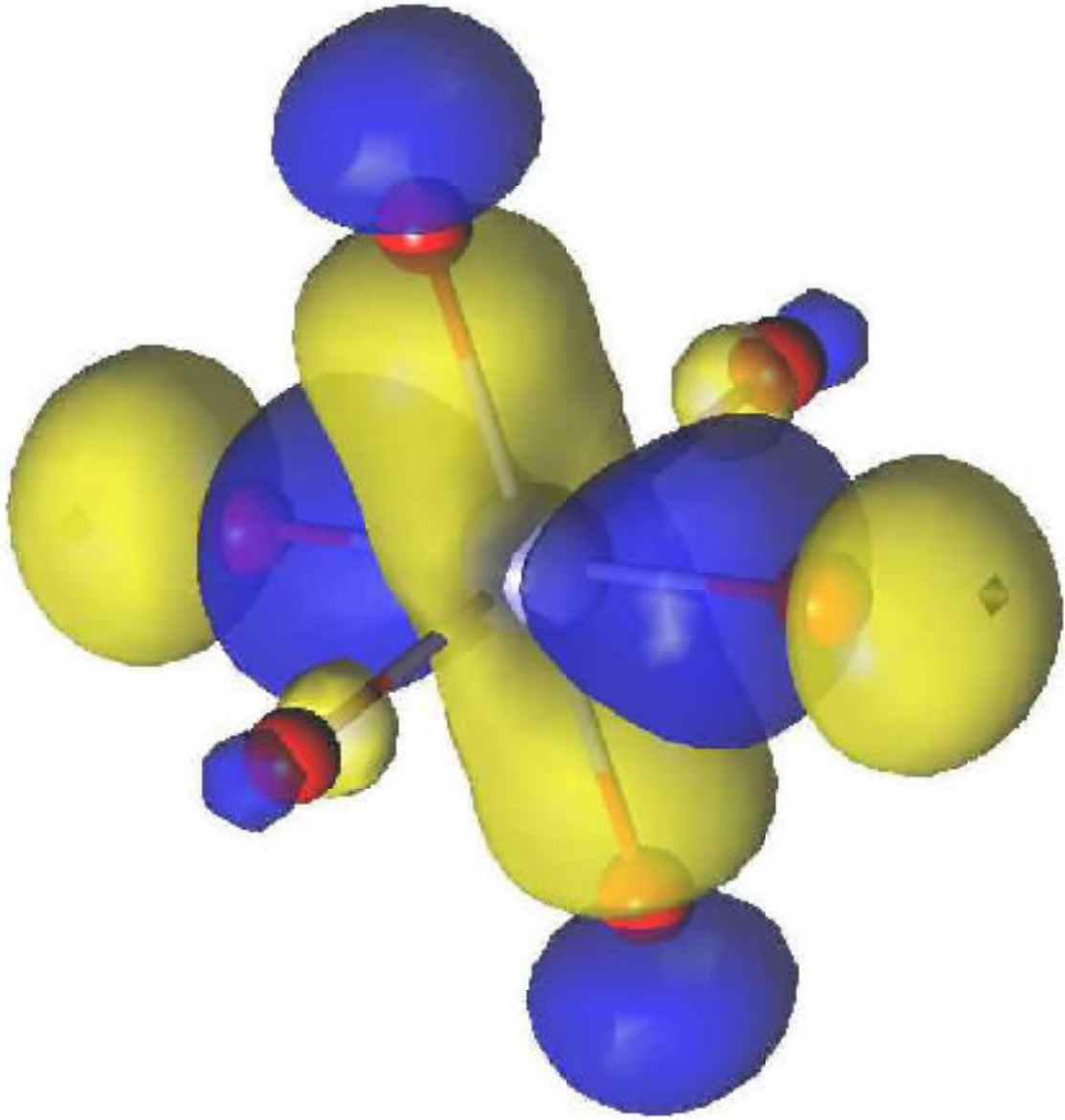
Aurora Emission Lines

Emission (nm)	type	
630.0	OI	Intense red band in aurora (photo above)
557.7	OI	Intense green band in aurora (photo above)
777.4	OI	Airglow emission
844.6+ 436.8	OI	Airglow and seen in twilight emission (weak)
732.0 + 372.8	OII	Twilight emission (weak)
500.7 + 495.9	OIII	Astronomical nebula

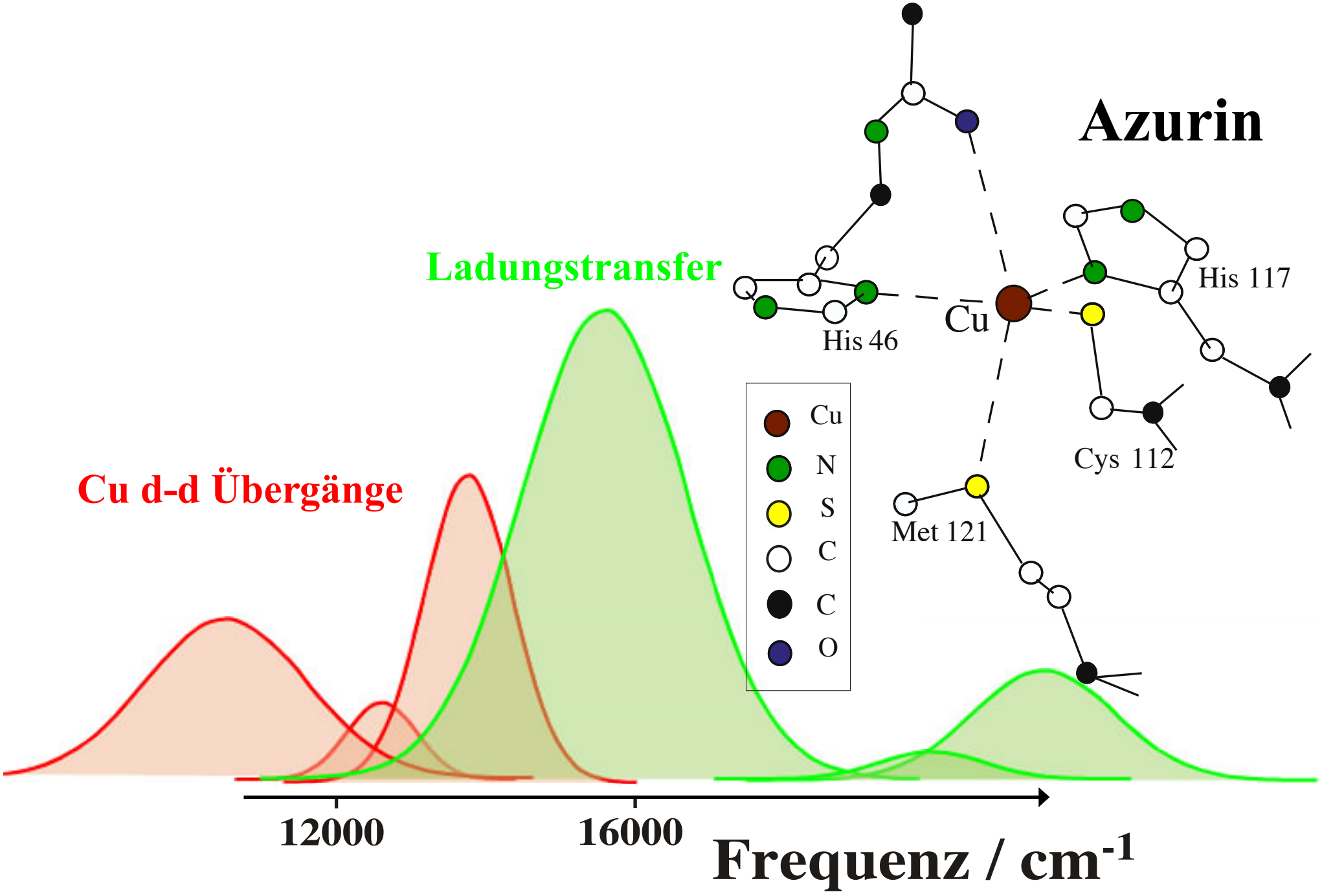
Moleküle

FeO_6

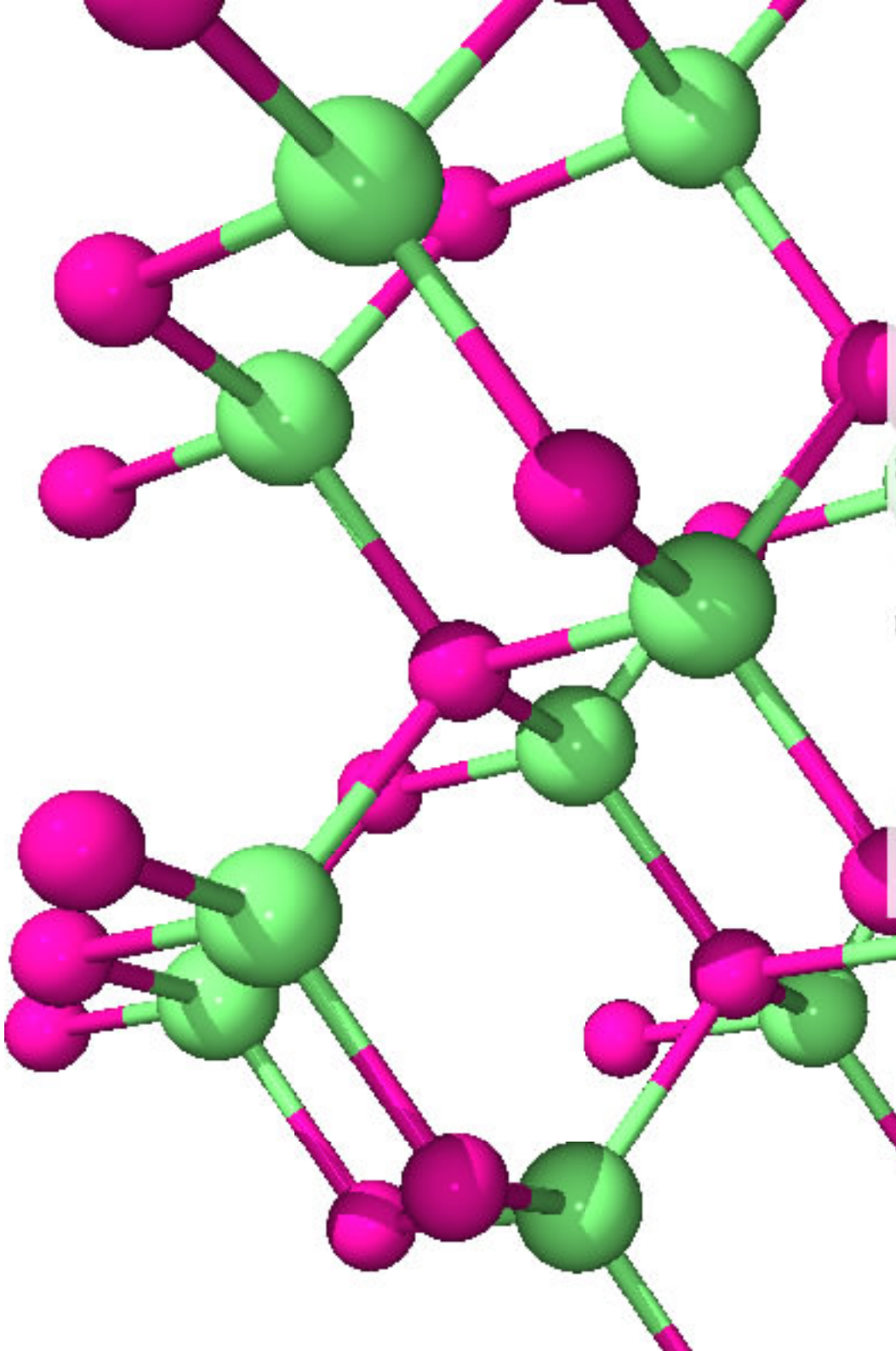


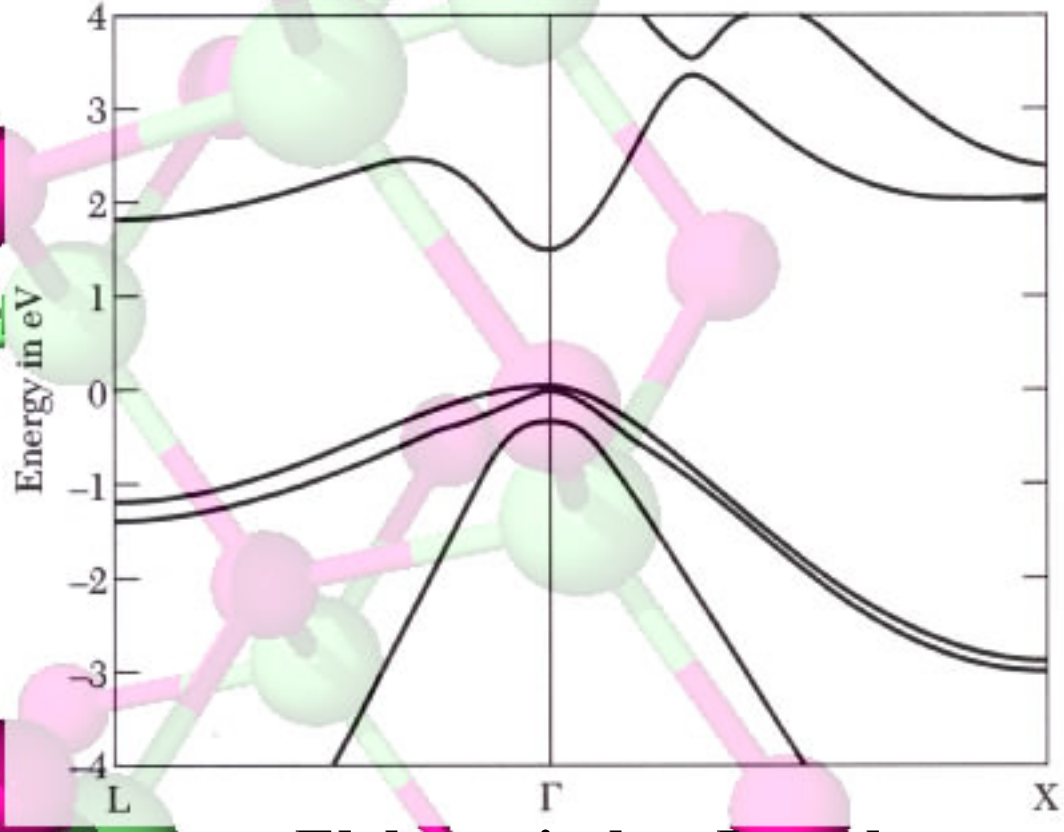


Polyatomare Moleküle



Festkörper

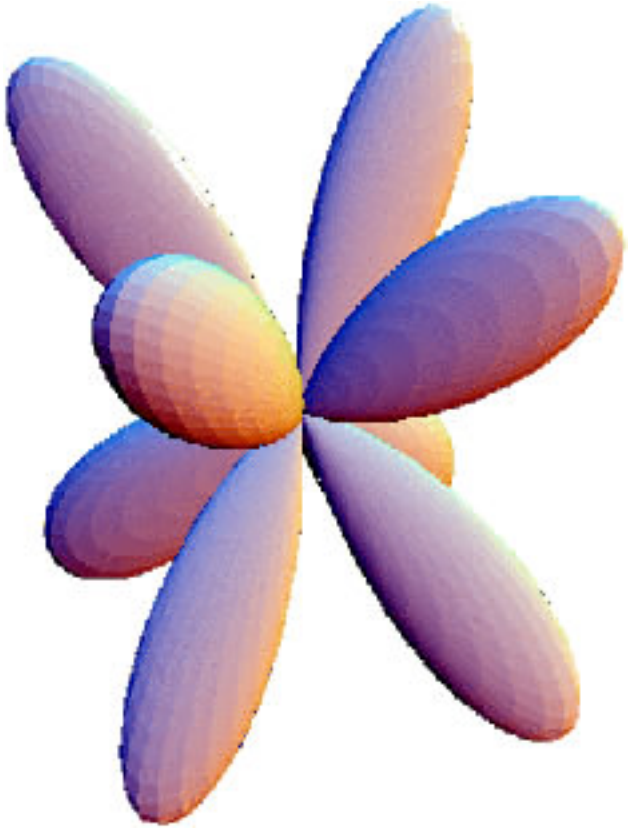




Elektronischer Impuls

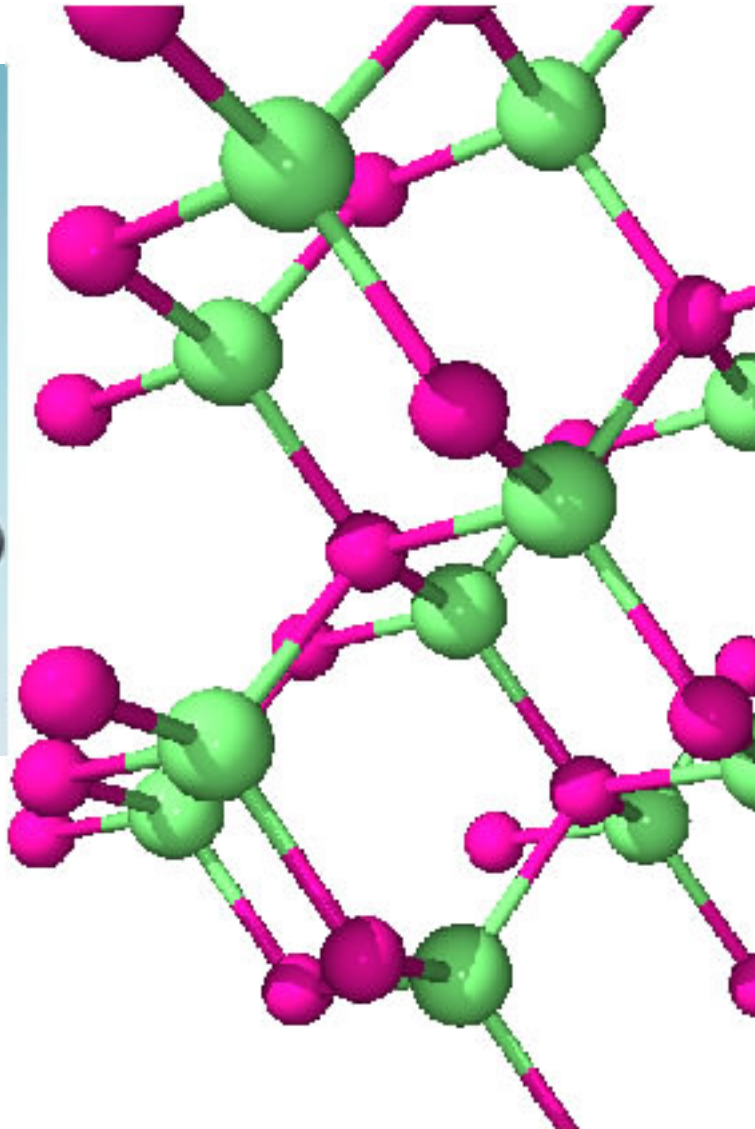
4.2 Symmetrie

Atome



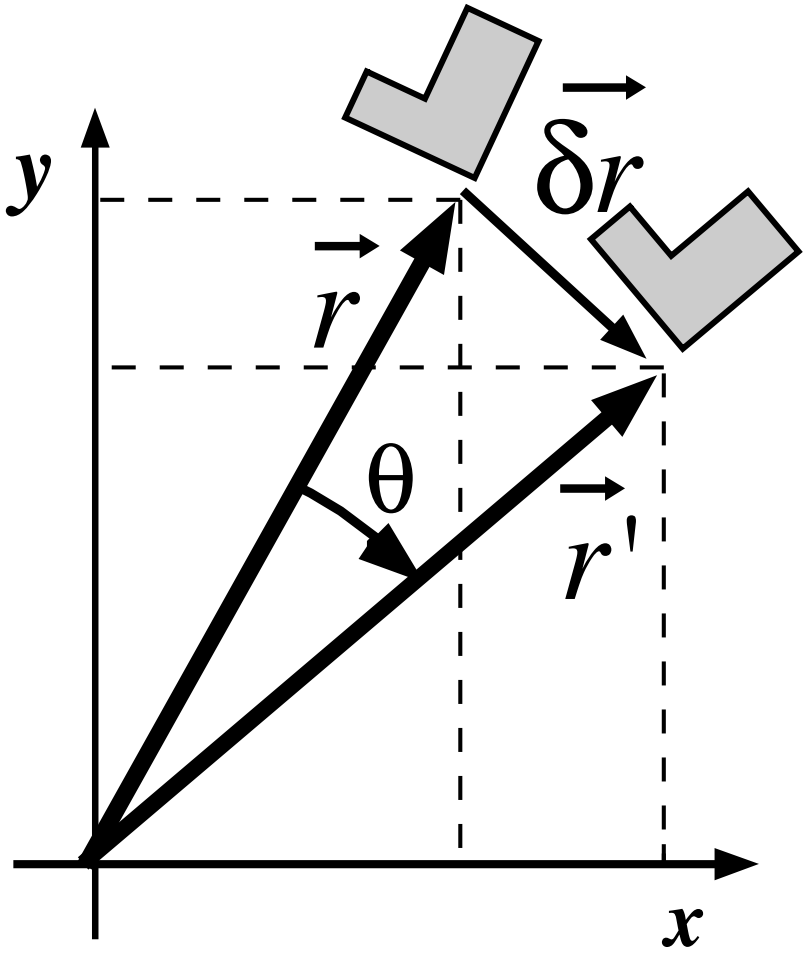
Moleküle

Festkörper

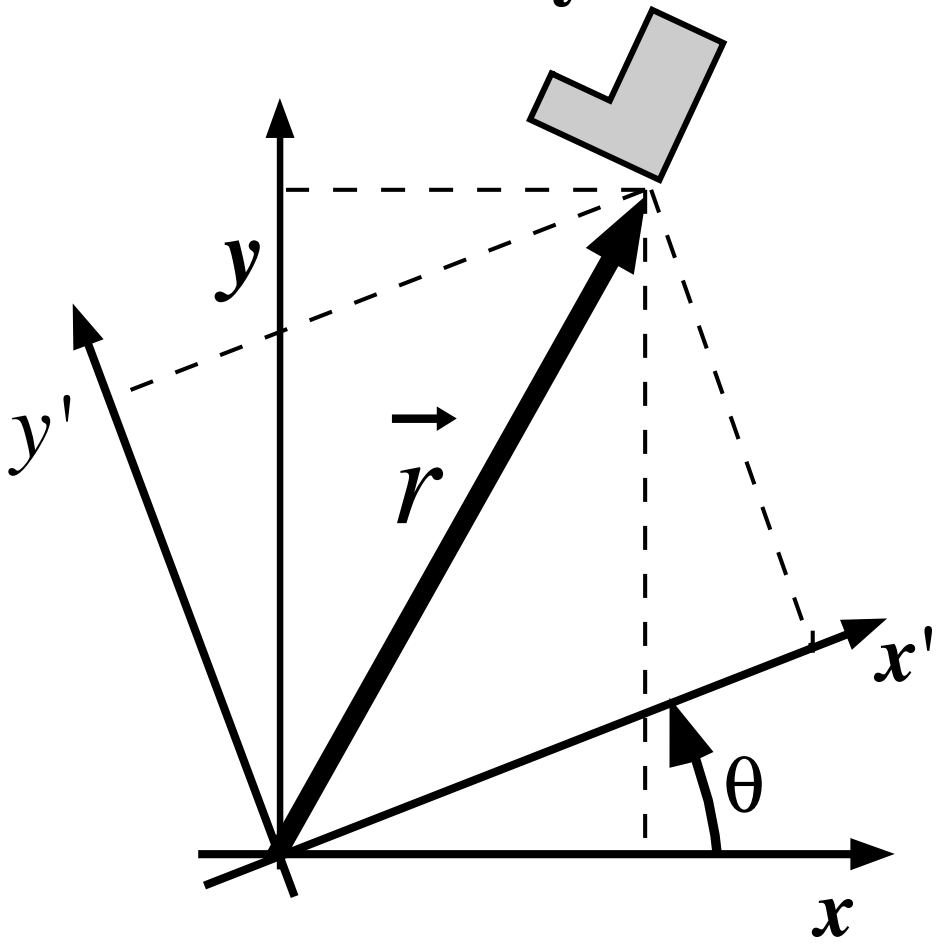


Rotationen

Rotation des Objekts

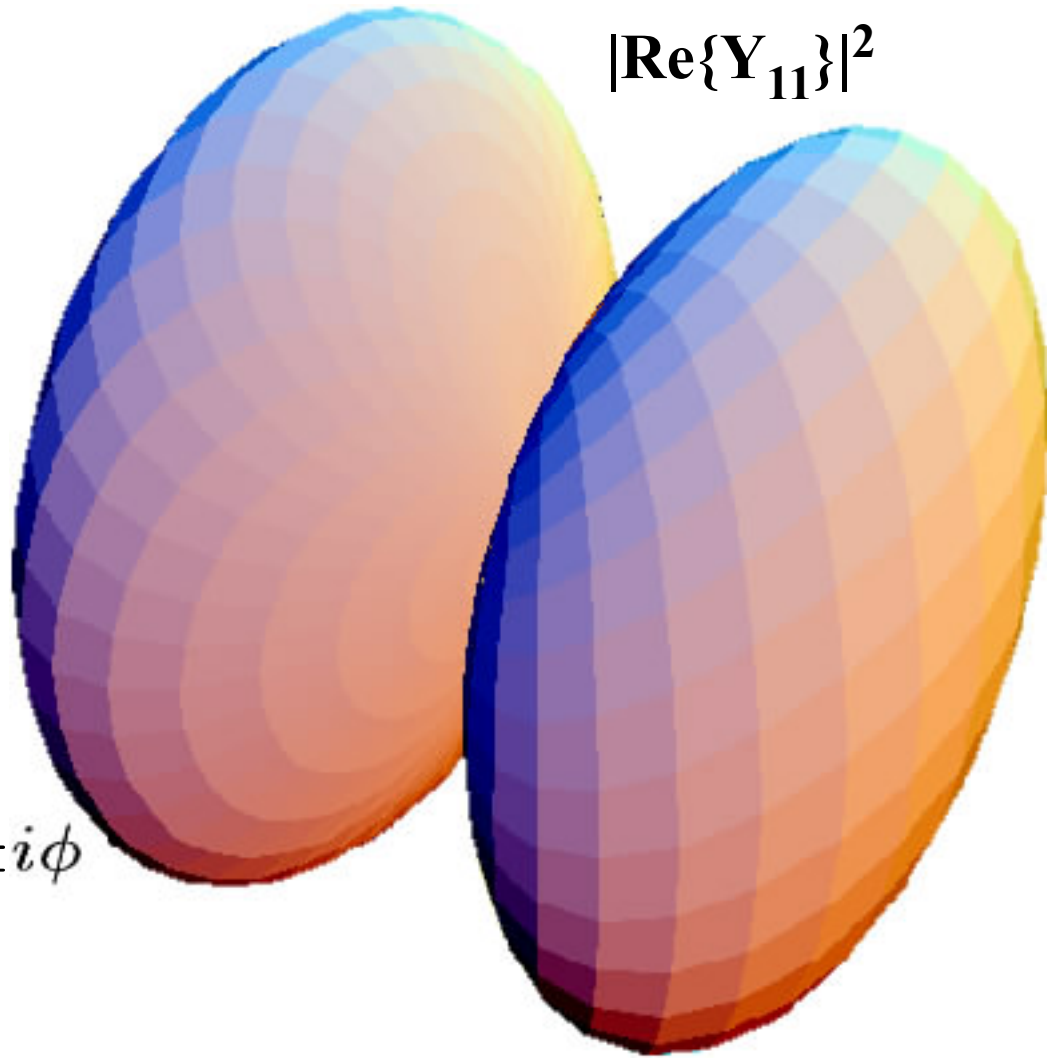


Rotation des Koordinatensystems

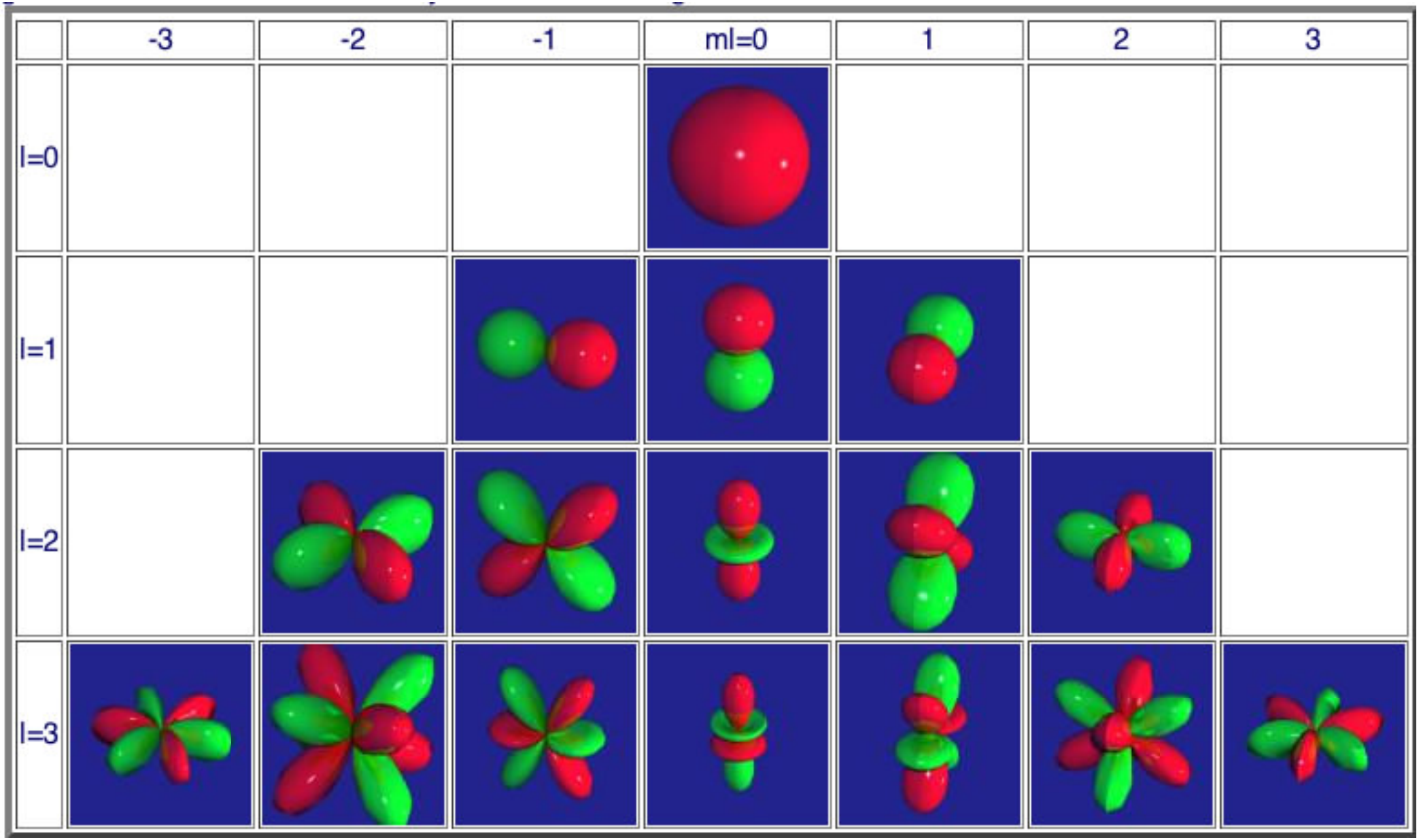


Kugelflächenfunktionen

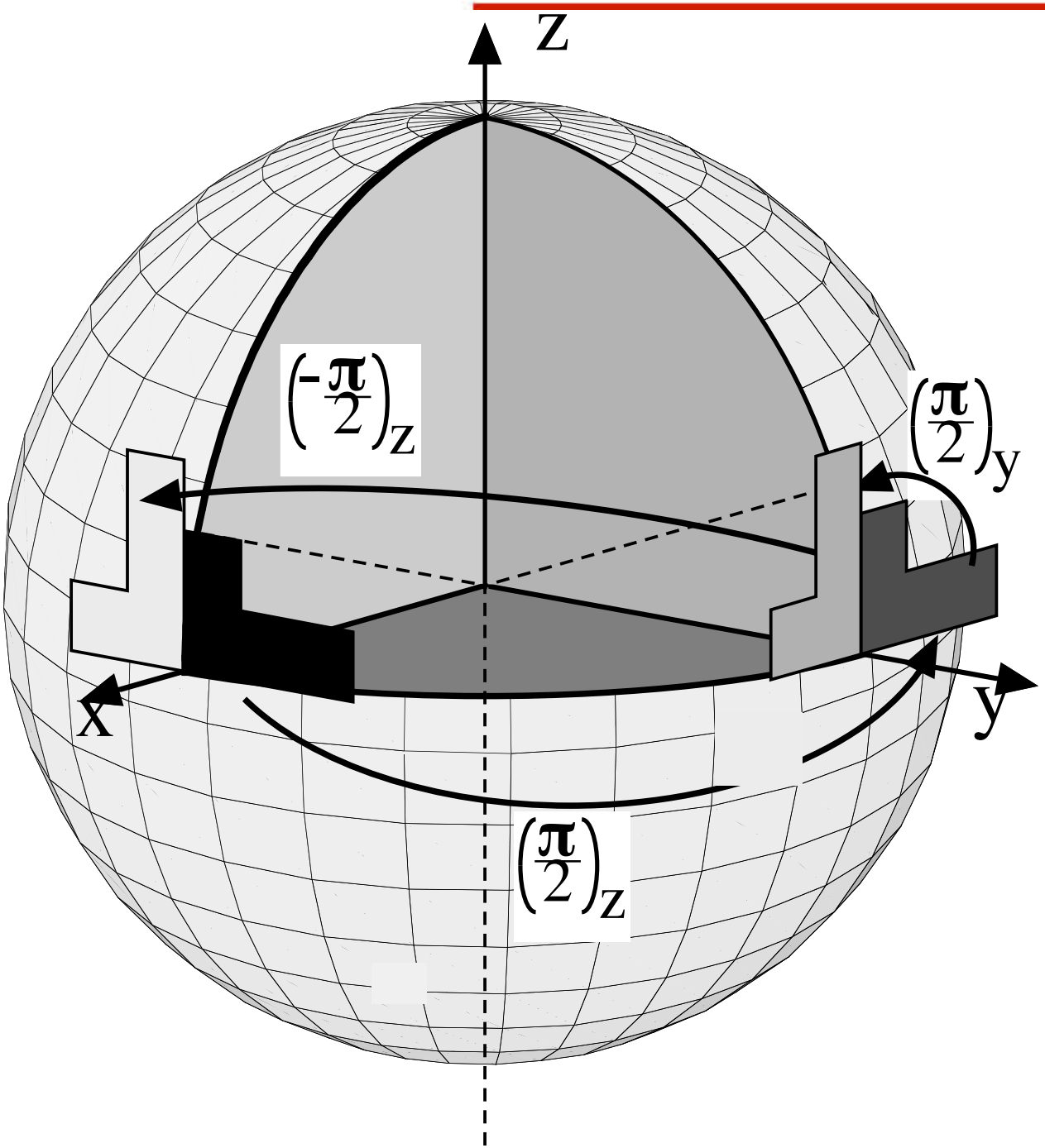
l	m	Y_{lm}
0	0	$\sqrt{\frac{1}{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}}\cos\theta$
1	± 1	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$
2	0	$\sqrt{\frac{5}{4\pi}}\frac{1}{2}(3\cos^2\theta - 1)$



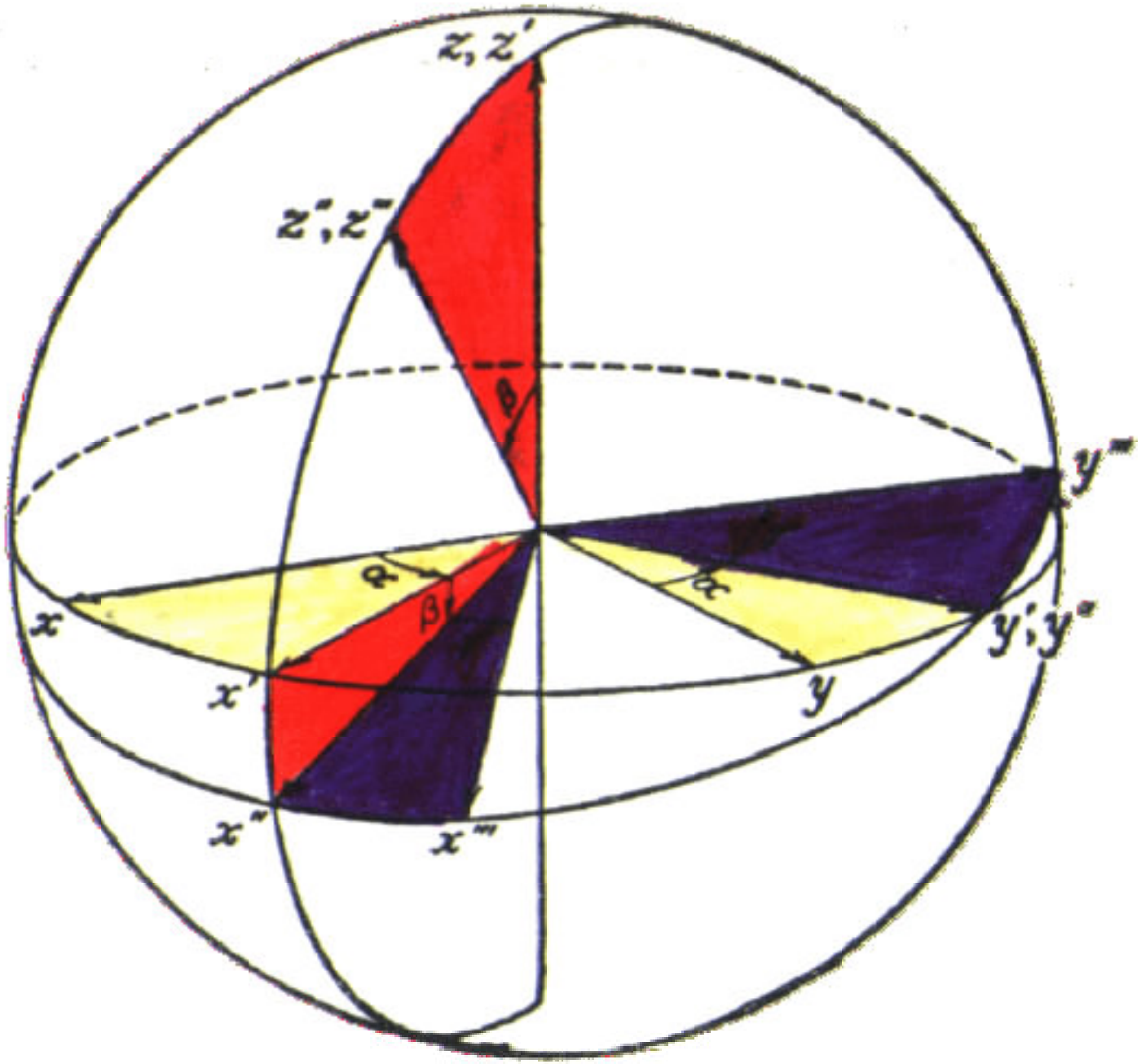
Kugelflächenfunktionen



Rotation in 3D



Euler Winkel



Kugelflächenfunktionen

l	m	Y_{lm}
0	0	$\sqrt{\frac{1}{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}}\cos\theta$
1	± 1	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$

sind orthonormiert

$$\boxed{\iint \sin\theta \, d\theta \, d\phi Y_{lm} = \delta_{l0}\delta_{m0}\sqrt{4\pi}}$$

Matrixelemente

irreduzibler Tensoroperator

$$\langle \alpha, L, m | T_q^{(k)} | \alpha\prime, L\prime, m\prime \rangle$$

$$= (-1)^{L-m} \begin{pmatrix} L & k & L\prime \\ -m & q & m\prime \end{pmatrix} \langle \alpha, L || T^{(k)} || \alpha\prime, L\prime \rangle \, .$$

3J-Symbole

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = 0 \qquad \text{if} \quad j_1 + j_2 + j_3 \text{ is odd}$$

$$\begin{pmatrix} j+\frac{1}{2} & j & \frac{1}{2} \\ m & -m-\frac{1}{2} & \frac{1}{2} \end{pmatrix} = (-1)^{j-m-\frac{1}{2}} \sqrt{\frac{j-m+\frac{1}{2}}{(2j+2)(2j+1)}}$$

$$\begin{pmatrix} j+1 & j & 1 \\ m & -m-1 & 1 \end{pmatrix} = (-1)^{j-m-1} \sqrt{\frac{(j-m)(j-m+1)}{(2j+3)(2j+2)(2j+1)}}$$

$$\begin{pmatrix} j+1 & j & 1 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m-1} \sqrt{\frac{(j+m+1)(j-m+1)}{(2j+3)(j+1)(2j+1)}}$$

3J-Symbole

M. Weissbluth,
'*Atoms and molecules*',
Academic Press,
San Diego (1978).

$$\begin{pmatrix} j & j & 1 \\ m & -m-1 & 1 \end{pmatrix} = (-1)^{j-m} \sqrt{\frac{(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}$$

$$\begin{pmatrix} j & j & 1 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m} \frac{m}{\sqrt{(2j+1)(j+1)j}}$$

$$\begin{pmatrix} j & j & 0 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m} \frac{1}{\sqrt{2j+1}}$$

$$\begin{pmatrix} j & j & 2 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m} \frac{3m^2 - j(j+1)}{\sqrt{(2j+3)(j+1)(2j+1)2j(2j-1)}}$$

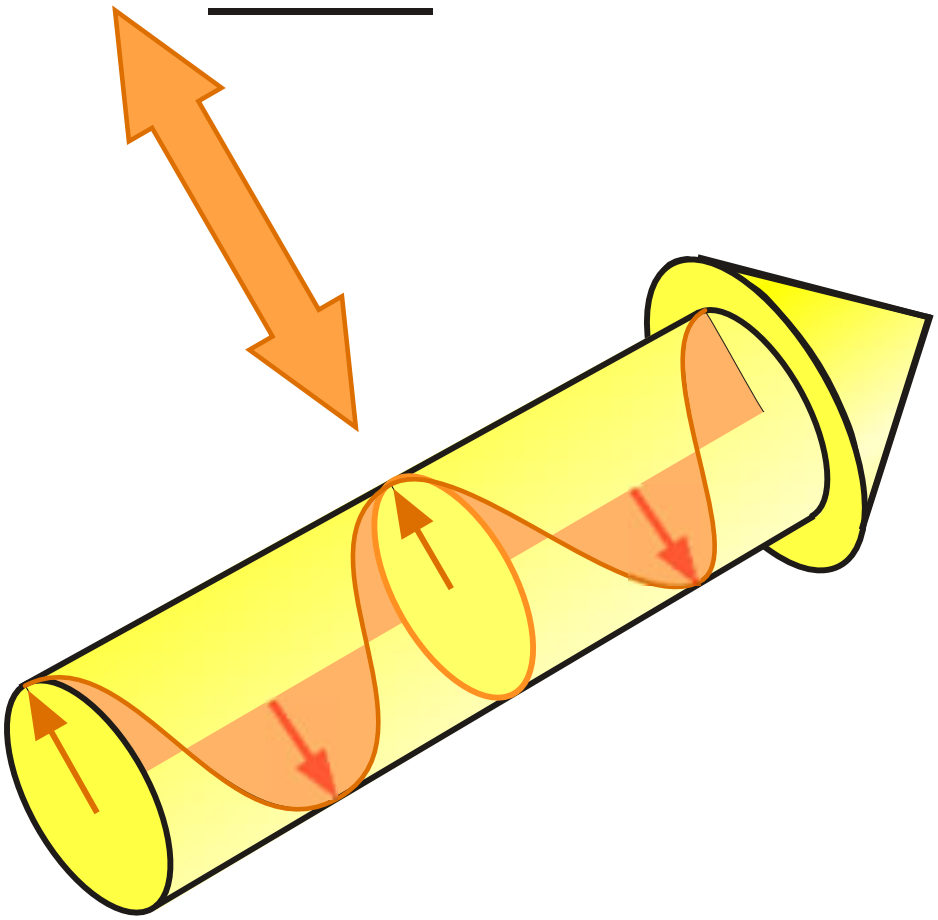
3J Werte

j_1	j_2	j_3	m_1	m_2	m_3	
1	1	0	0	0	0	*01
2	1	1	0	0	0	111
2	2	0	0	0	0	001
2	2	2	0	0	0	*1011,
3	2	1	0	0	0	*0111,
3	3	0	0	0	0	*0001,
3	3	2	0	0	0	2111,
4	2	2	0	0	0	1011,
4	3	1	0	0	0	2201,
4	3	3	0	0	0	*1001,1
4	4	0	0	0	0	02
4	4	2	0	0	0	*2211,1
4	4	4	0	0	0	1201,11
1/2	1/2	0	1/2	-1/2	0	1

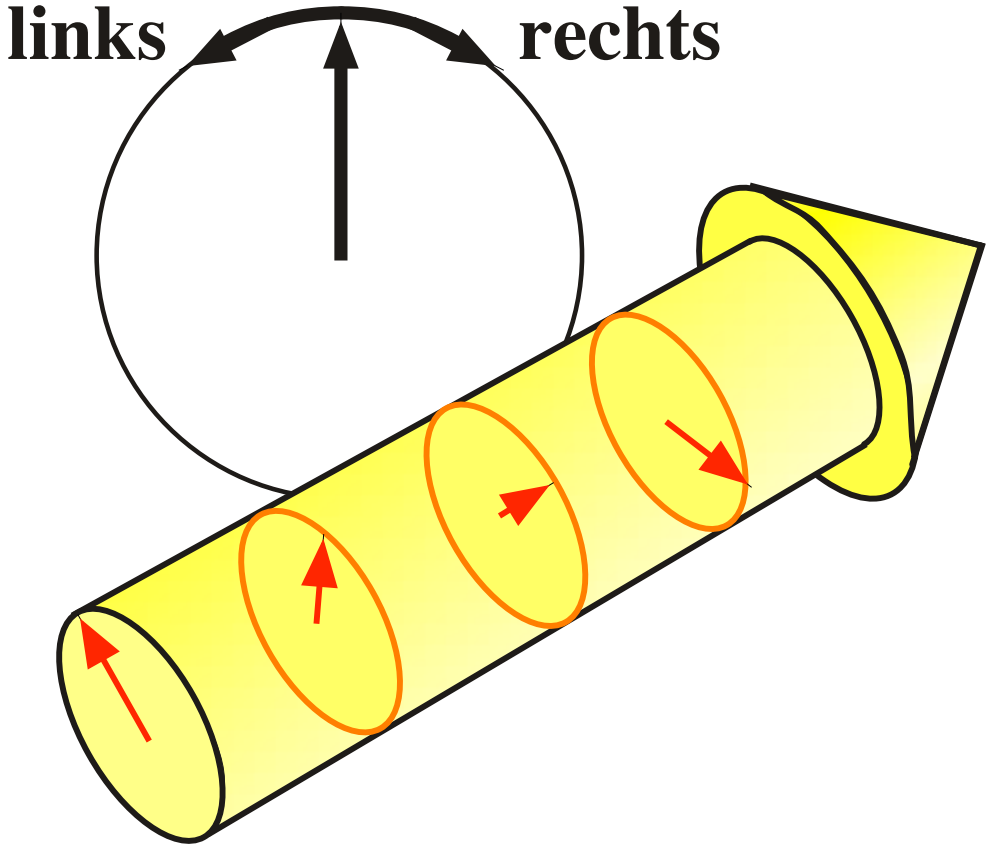
j_1	j_2	j_3	m_1	m_2	m_3	
3/2	3/2	1	1/2	-3/2	1	*101
3/2	3/2	1	1/2	-1/2	0	*211
3/2	3/2	1	3/2	-3/2	0	211
3/2	3/2	1	3/2	-1/2	-1	*101
2	1	1	-1	0	1	*101
2	1	1	0	-1	1	111
2	1	1	0	0	0	111
2	1	1	1	-1	0	*101
2	1	1	1	0	-1	*101
2	1	1	2	-1	-1	001
2	3/2	1/2	0	-1/2	1/2	*101
2	3/2	1/2	1	-3/2	1/2	201
2	3/2	1/2	1	-1/2	-1/2	211
2	3/2	1/2	2	-3/2	-1/2	*001

Polarisation und Drehimpuls

Linear



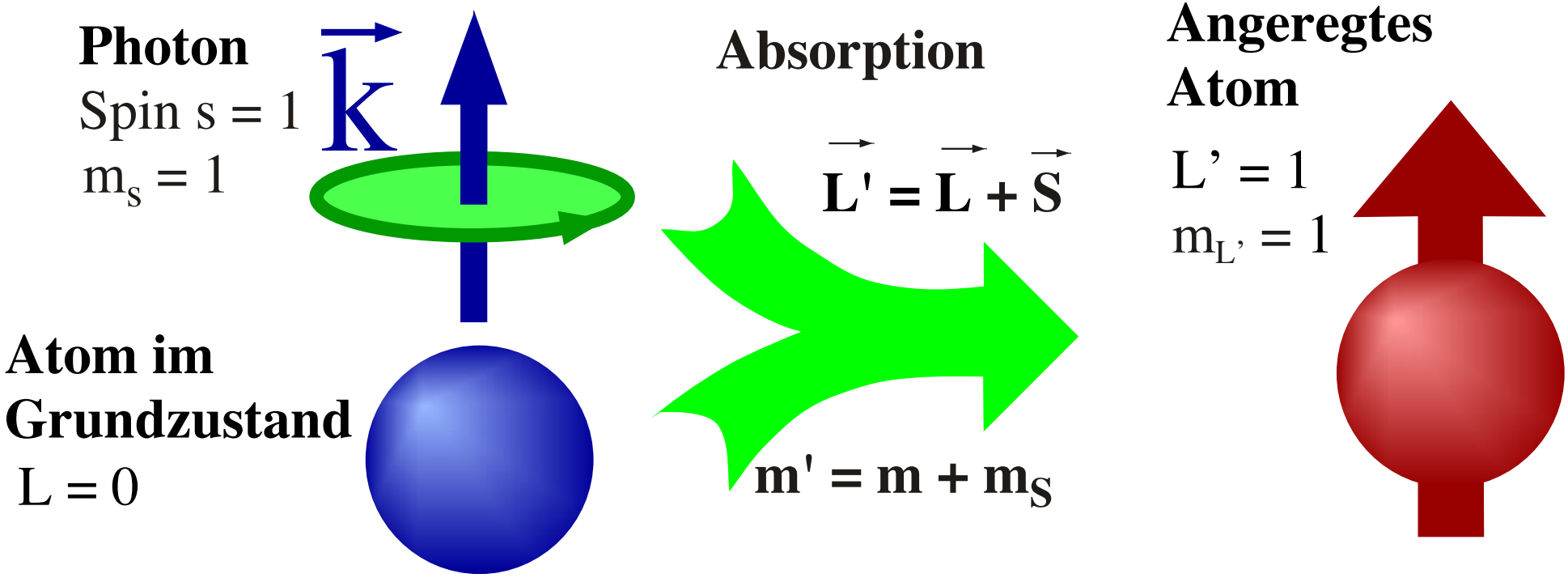
Zirkular

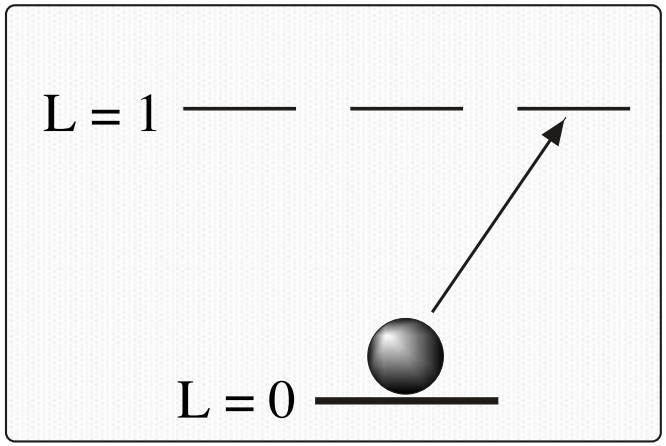


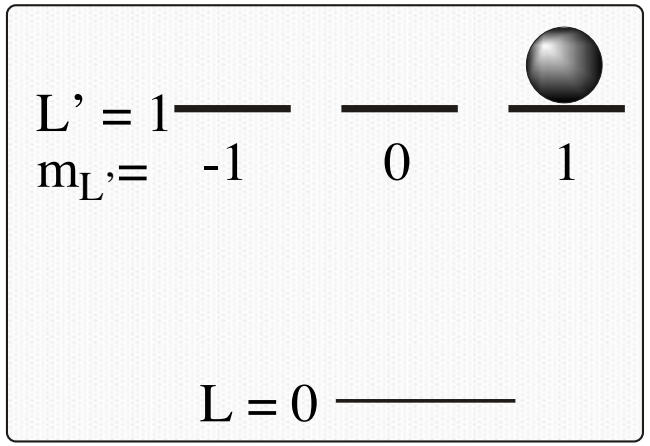
$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = E_0 \begin{pmatrix} \cos(\omega t - kz) \\ 0 \end{pmatrix}$$

$$E_0 \begin{pmatrix} \cos(\omega t - kz) \\ \sin(\omega t - kz) \end{pmatrix}$$

Drehimpulserhaltung



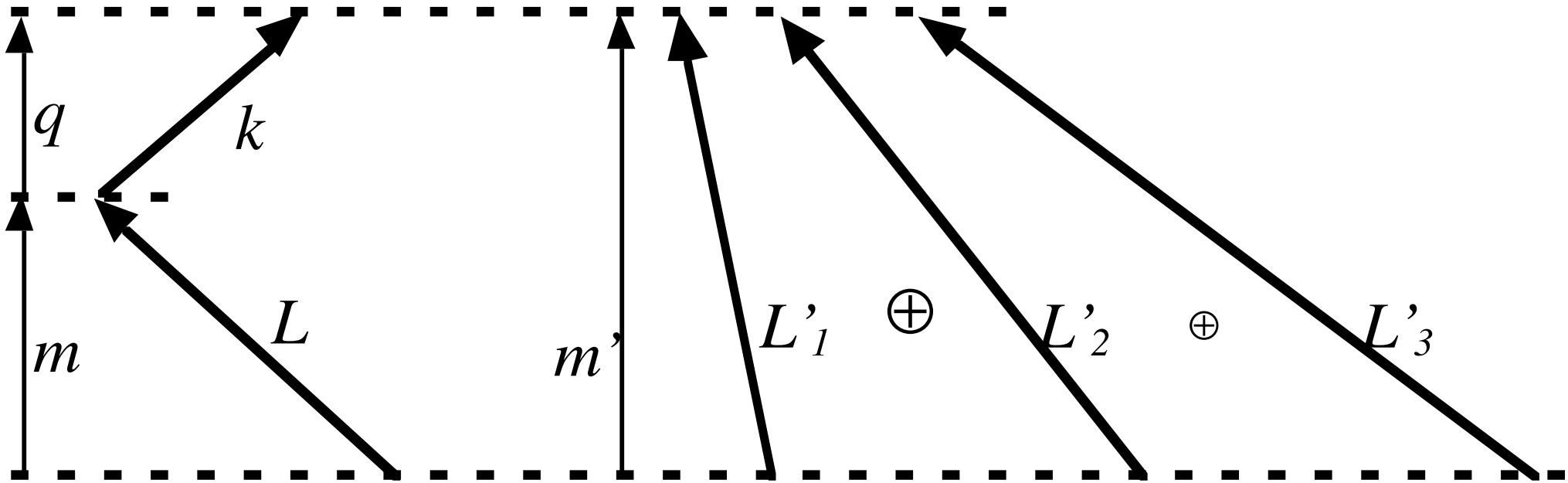




Auswahlregeln

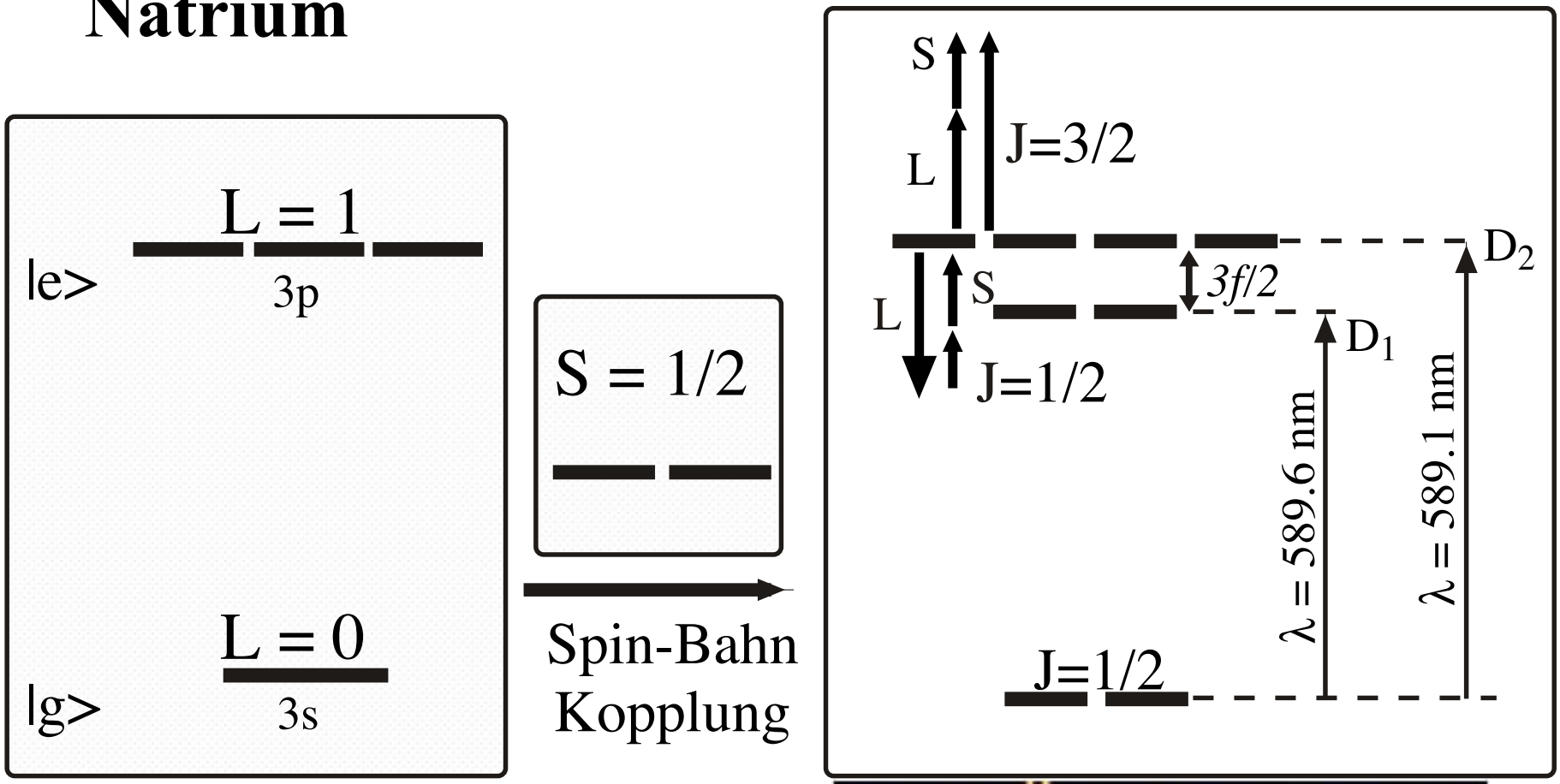
$$\langle e; L', m_{L'} | T_q^{(k)} | g; L, m_L \rangle$$

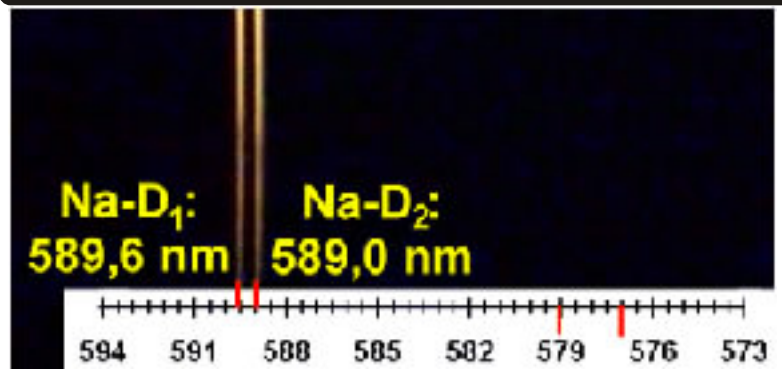
Werte ≠ 0 für



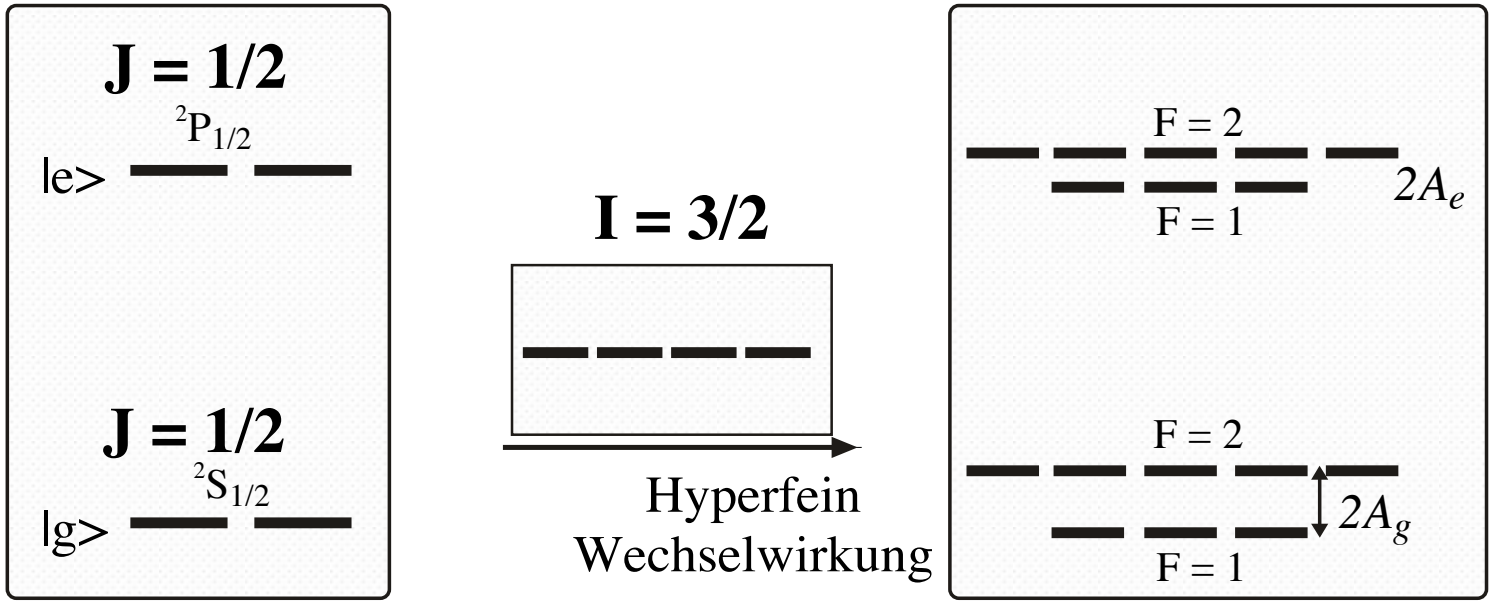
Spin-Bahn Kopplung

Natrium

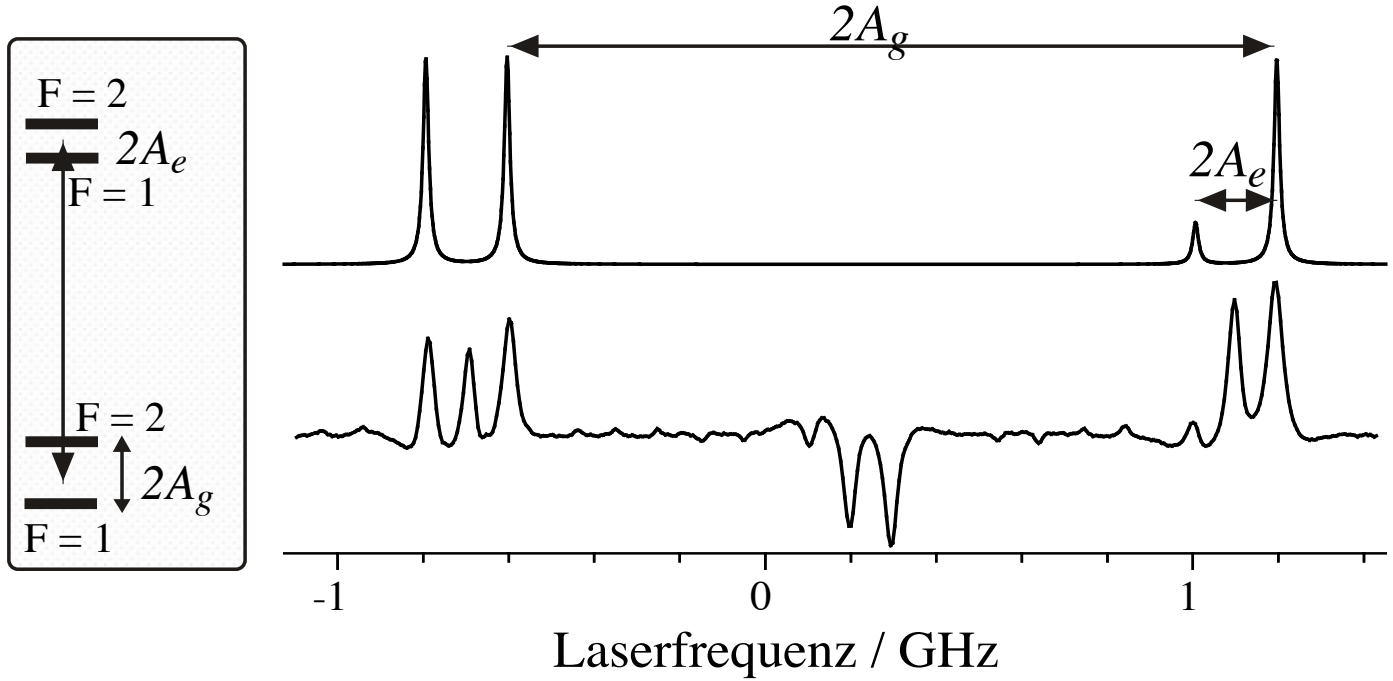




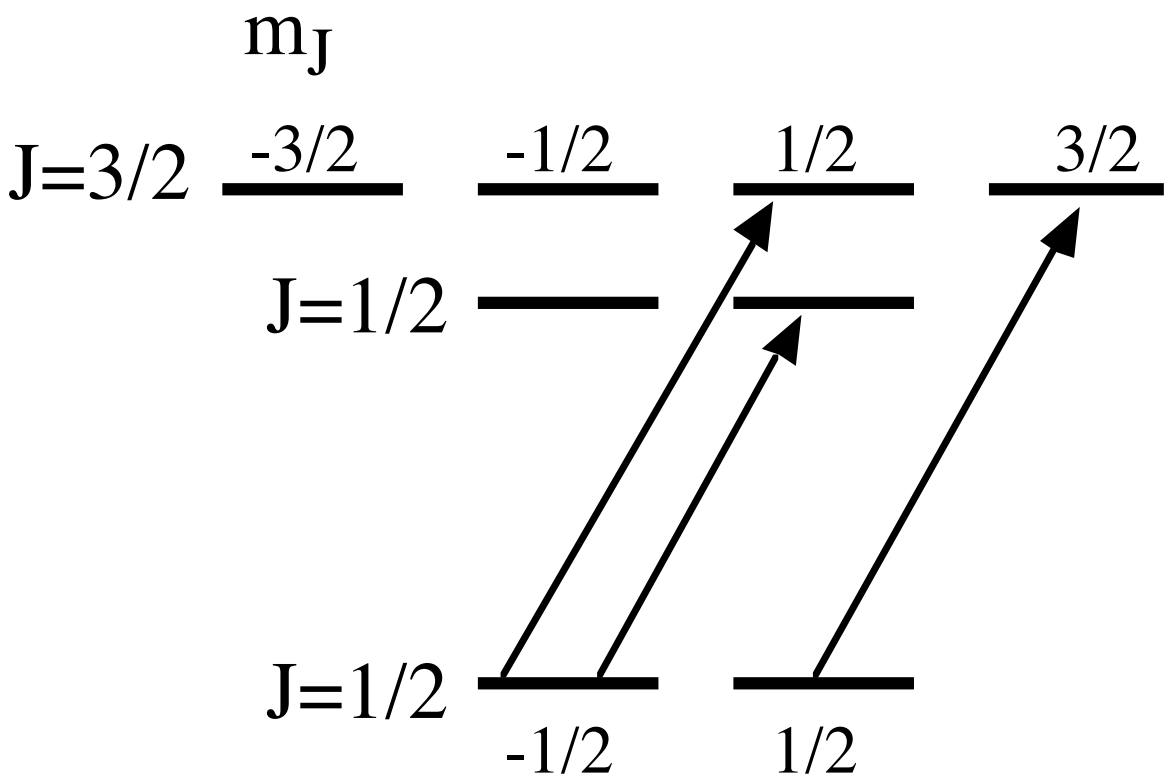
Hyperfein Wechselwirkung



experimentelles Spektrum



Matrixelemente



$$|\langle e; J_e||r_q||g; J_g\rangle|^2 = (2J_g+1)(2J_e+1)$$
$$\left\{ \begin{array}{ccc} J_g & 1 & J_e \\ L_e & S & L_g \end{array} \right\}^2 |\langle e; L_e||r||g; L_g\rangle|^2$$

Numerische Werte für 6J Symbole 6J Symbole

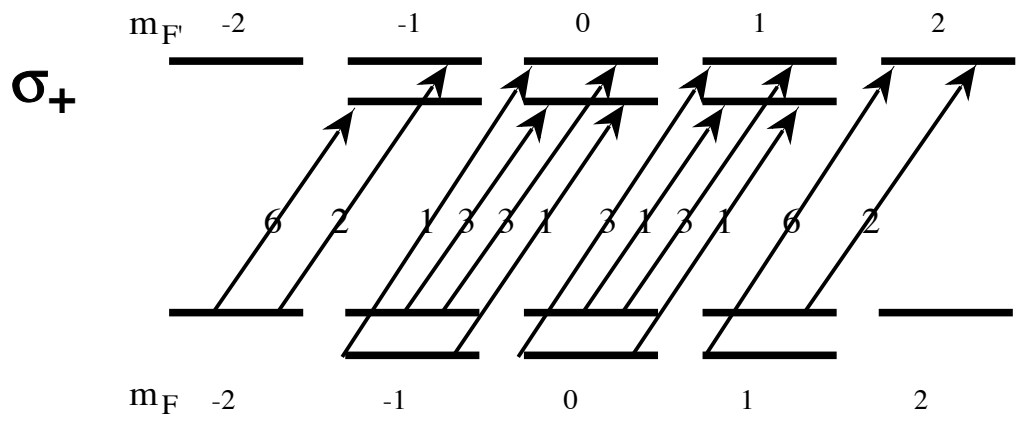
j_1	j_2	j_3	l_1	l_2	l_3	
1/2	1/2	0	0	0	1/2	*1
1/2	1/2	0	1/2	1/2	0	*2
1	1/2	1/2	0	1/2	1/2	2
1	1/2	1/2	1	1/2	1/2	22
1	1	0	0	0	1	01
1	1	0	1/2	1/2	1/2	11
1	1	0	1	1	0	02
1	1	0	1	1	1	*02
1	1	1	1/2	1/2	1/2	*12
1	1	1	1	0	1	*02
1	1	1	1	1	0	*02
1	1	1	1	1	1	22
3/2	1	1/2	0	1/2	1	*11
3/2	1	1/2	1/2	1	1/2	*02
3/2	1	1/2	1	1/2	1	*22
3/2	1	1/2	1	1	1/2	*12

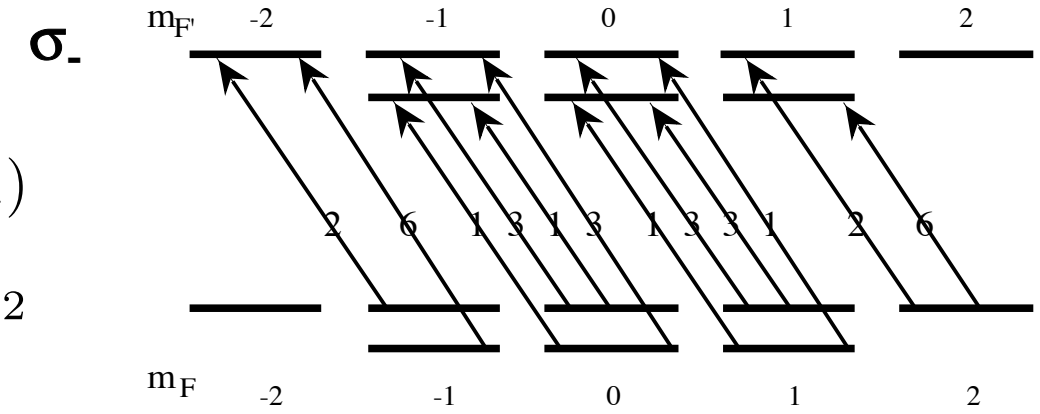
j_1	j_2	j_3	l_1	l_2	l_3	
2	1	1	1	1	1	22
2	1	1	2	1	1	222
2	3/2	1/2	0	1/2	3/2	3
2	3/2	1/2	1/2	1	1	21
2	3/2	1/2	1	1/2	3/2	301
2	3/2	1/2	1	3/2	1/2	4
2	3/2	1/2	1	3/2	3/2	*201
2	3/2	1/2	3/2	1	1	311
2	3/2	1/2	2	3/2	1/2	402
2	3/2	1/2	2	3/2	3/2	*212
2	3/2	3/2	0	3/2	3/2	*4
2	3/2	3/2	1/2	1	1	*31
2	3/2	3/2	1	1/2	3/2	*231
2	3/2	3/2	1	3/2	1/2	*231
2	3/2	3/2	1	3/2	3/2	402
2	3/2	3/2	3/2	1	1	*112

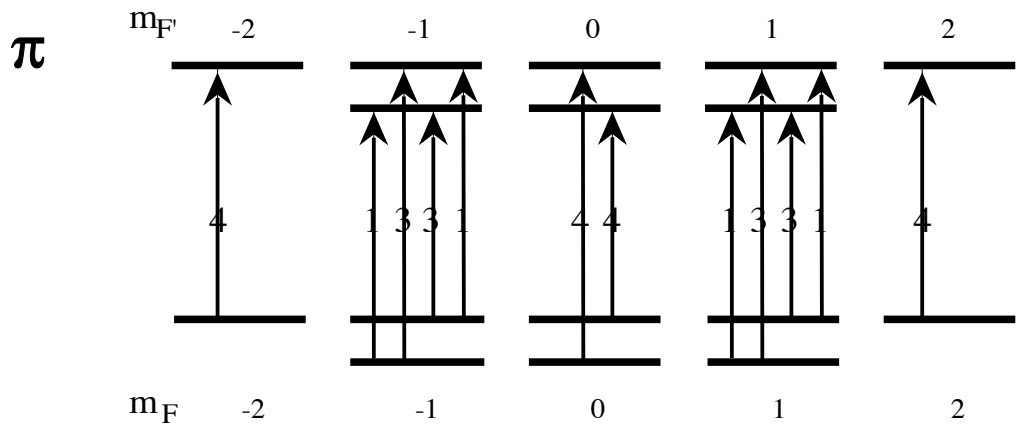
Matrixelemente

Übergangsstärke mit Kernspin

$$|\langle e; F_e||r||g; F_g\rangle|^2 = (2F_g+1)(2F_e+1) \begin{Bmatrix} F_g & 1 & F_e \\ J_e & I & J_g \end{Bmatrix}^2 |\langle e; J_e||r||g; J_g\rangle|^2$$



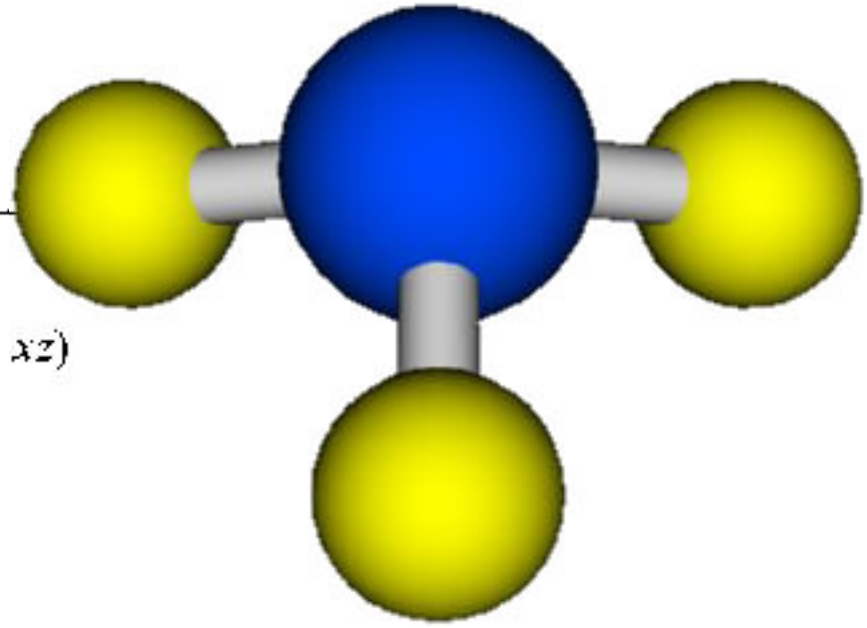




Irreduzible Darstellungen

Charaktertabelle für Gruppe C_3

C_3 (3)	E	C_3	C_3^2	$\epsilon = \exp(2\pi i/3)$	
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E	$\begin{cases} 1 \\ 1 \end{cases}$	$\begin{matrix} \epsilon \\ \epsilon^* \end{matrix}$	$\begin{matrix} \epsilon^* \\ \epsilon \end{matrix}$	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(yz, xz)$



Produktregeln

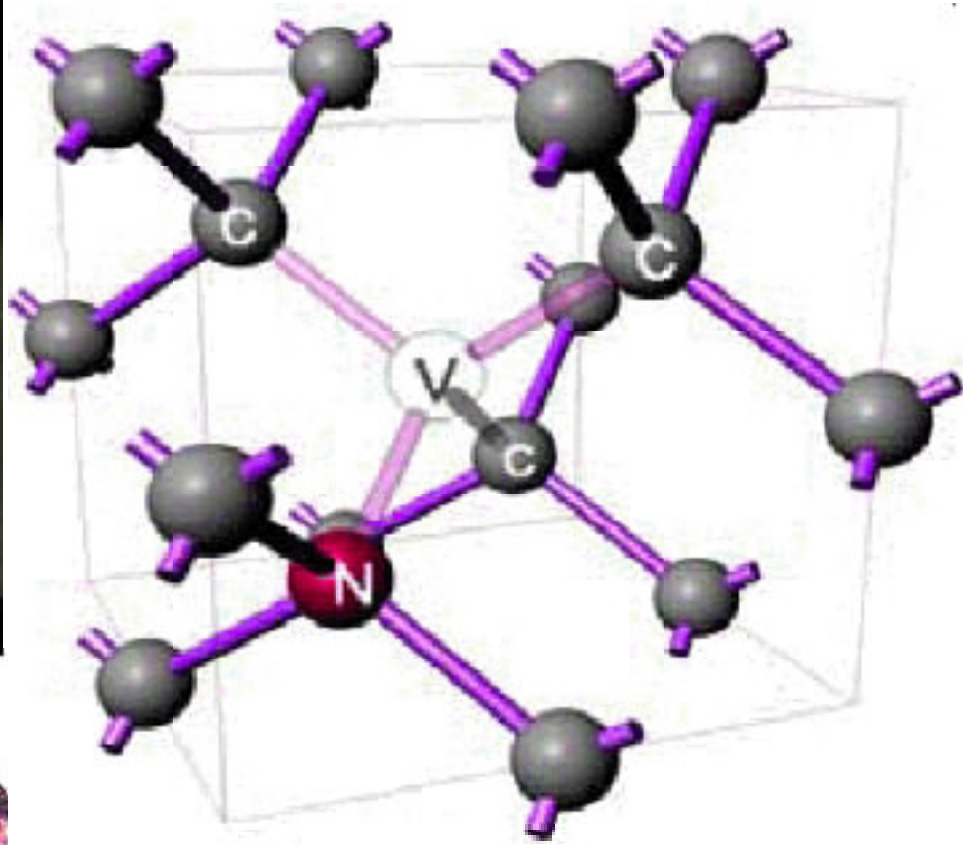
2. For C_2, C_3, C_6, D_3, D_6, C_{2v}, C_{3v}, C_{6v}, C_{2h}, C_{3h}, C_{6h}, D_{3h}, D_{6h}, D_{3d}, S_6

	A_1	A_2	B_1	B_2	E_1	E_2
A_1	A_1	A_2	B_1	B_2	E_1	E_2
A_2		A_1	B_2	B_1	E_1	E_2
B_1			A_1	A_2	E_2	E_1
B_2				A_1	E_2	E_1
E_1					$A_1 + [A_2] + E_2$	$B_1 + B_2 + E_1$
E_2						$A_1 + [A_2] + E_2$

P.W. Atkins, M.S. Child, and C.S.G. Phillips, '*Tables for group theory*', Oxford University Press, Oxford (1970).

Farbige Diamanten

N/V Zentrum in rosa Diamanten



Cr^{3+} Zentren

Rubin

$Cr^{3+}:Al_2O_3$

$\Delta E = 2.23$ eV

$\lambda_0 = 556$ nm

Alexandrit

$Cr^{3+}:BeAl_2O_4$

$\Delta E = 2.17$ eV

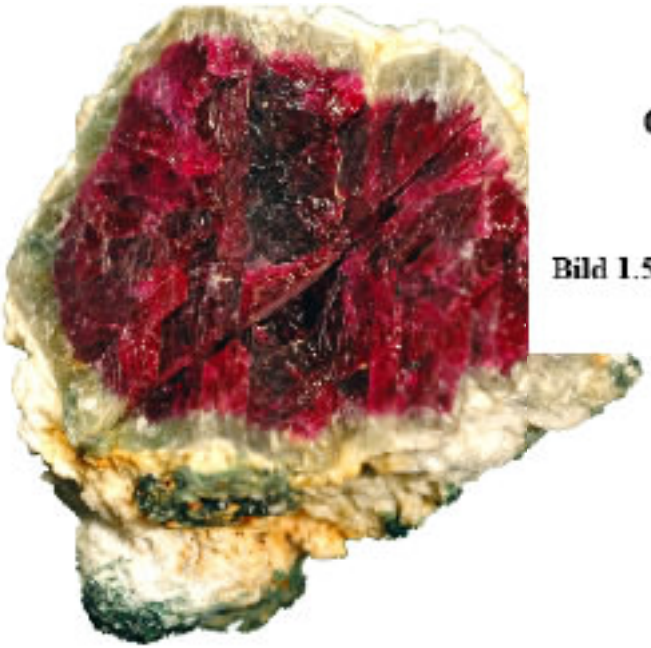
$\lambda_0 = 571$ nm

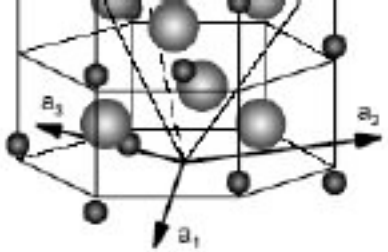
Smaragd

$Cr^{3+}:Be_2Al_2Si_6O_{18}$

$\Delta E = 2.05$ eV

$\lambda_0 = 605$ nm

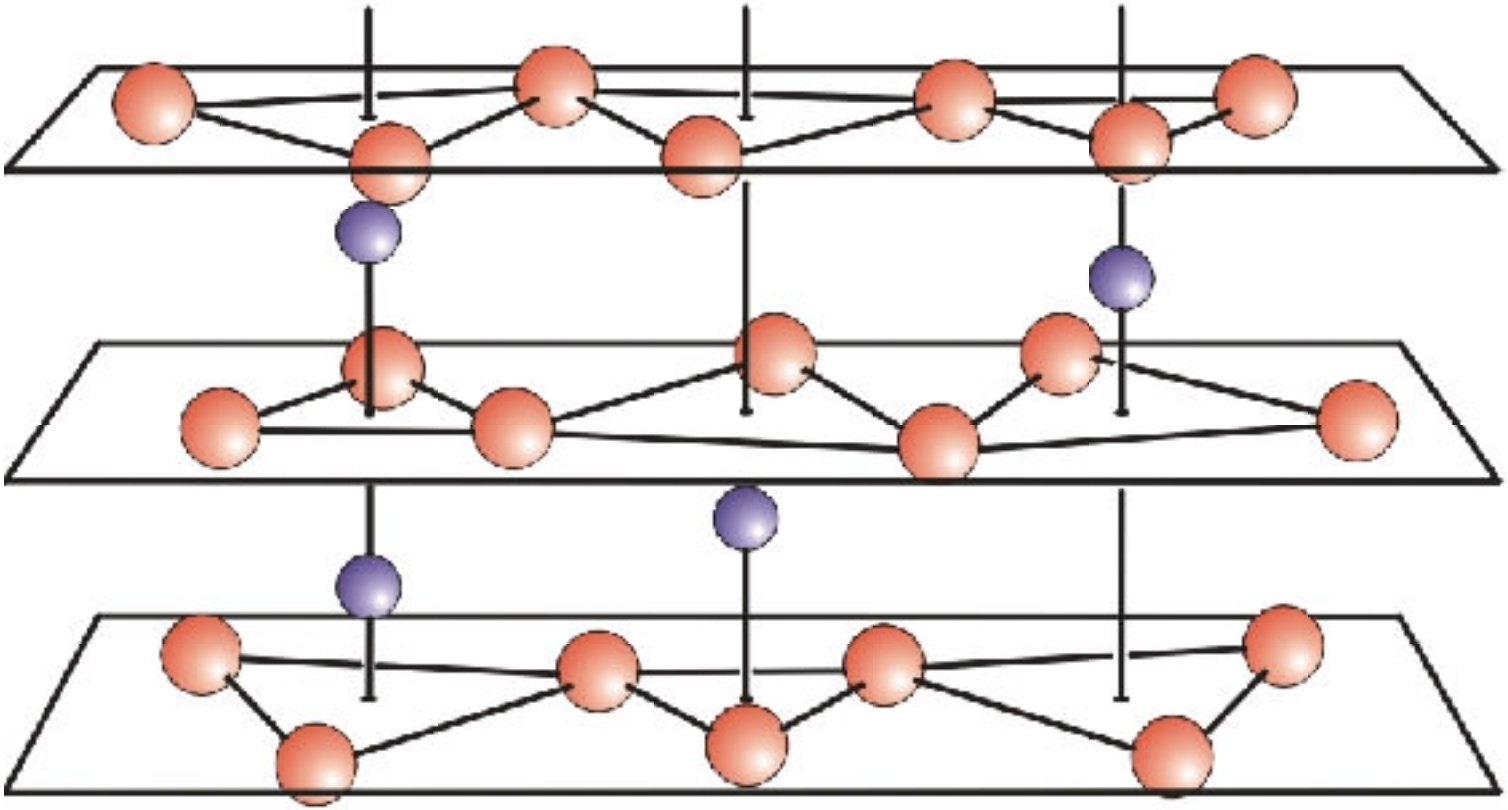




Sauerstoff Aluminium

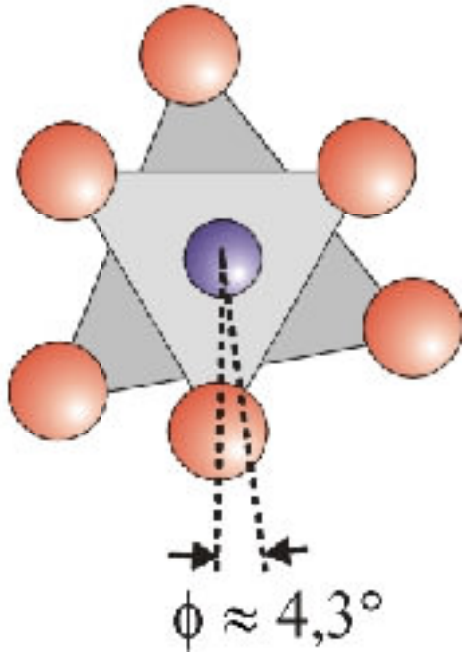
Bild 1.5: Hexagonal-rhomboedrische Gitterstruktur des α-Al_2O_3 (nach [84-86]). Eingezeichnet ist ebenfalls der Umriß der trigonalen Einheitszelle.

Struktur

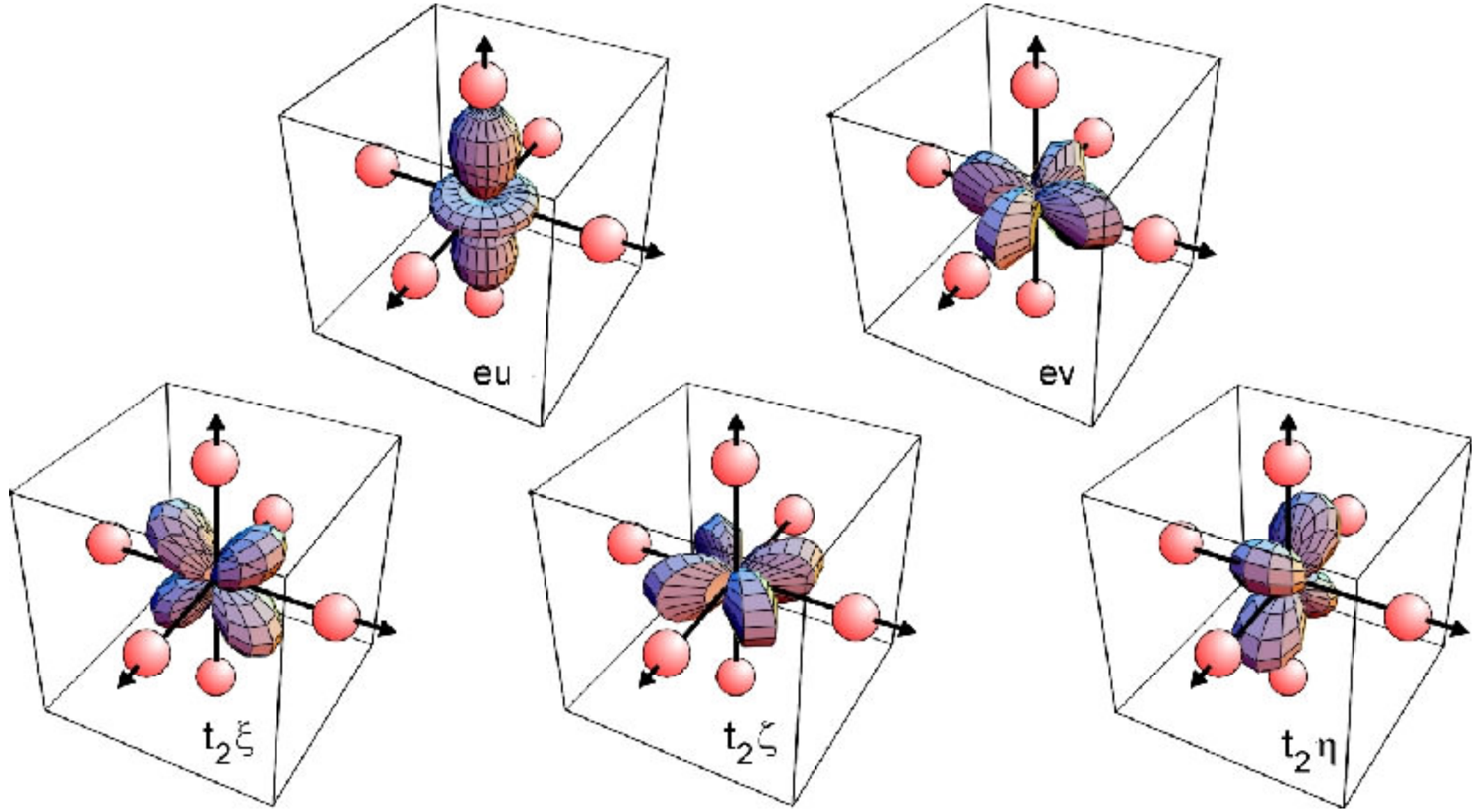


O^{2-}

Al^{3+} / Cr^{3+}

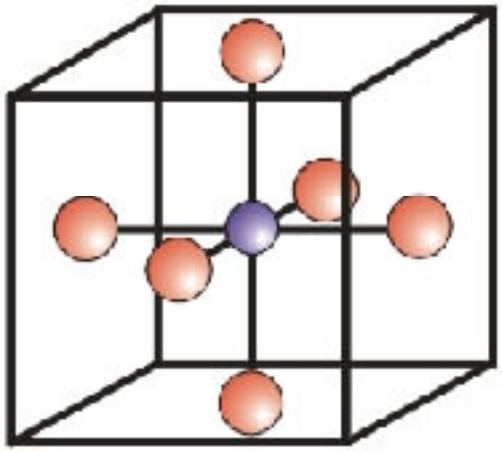


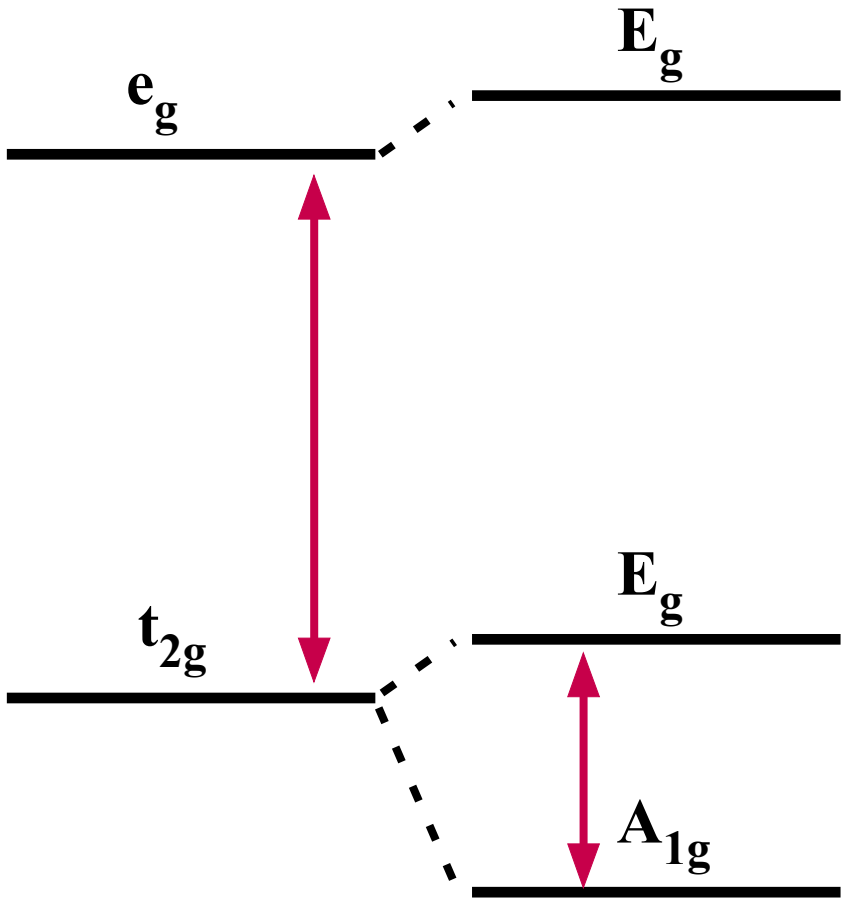
d-Orbitale



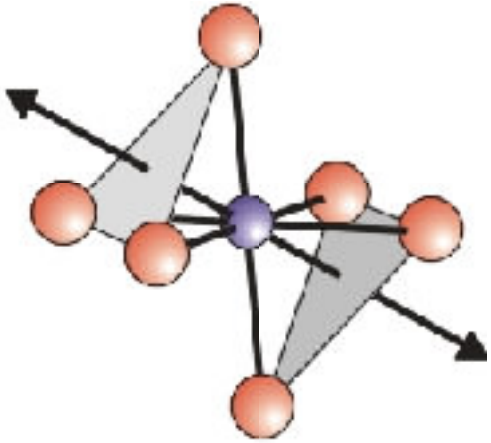
Energien

oktaedrische Symmetrie

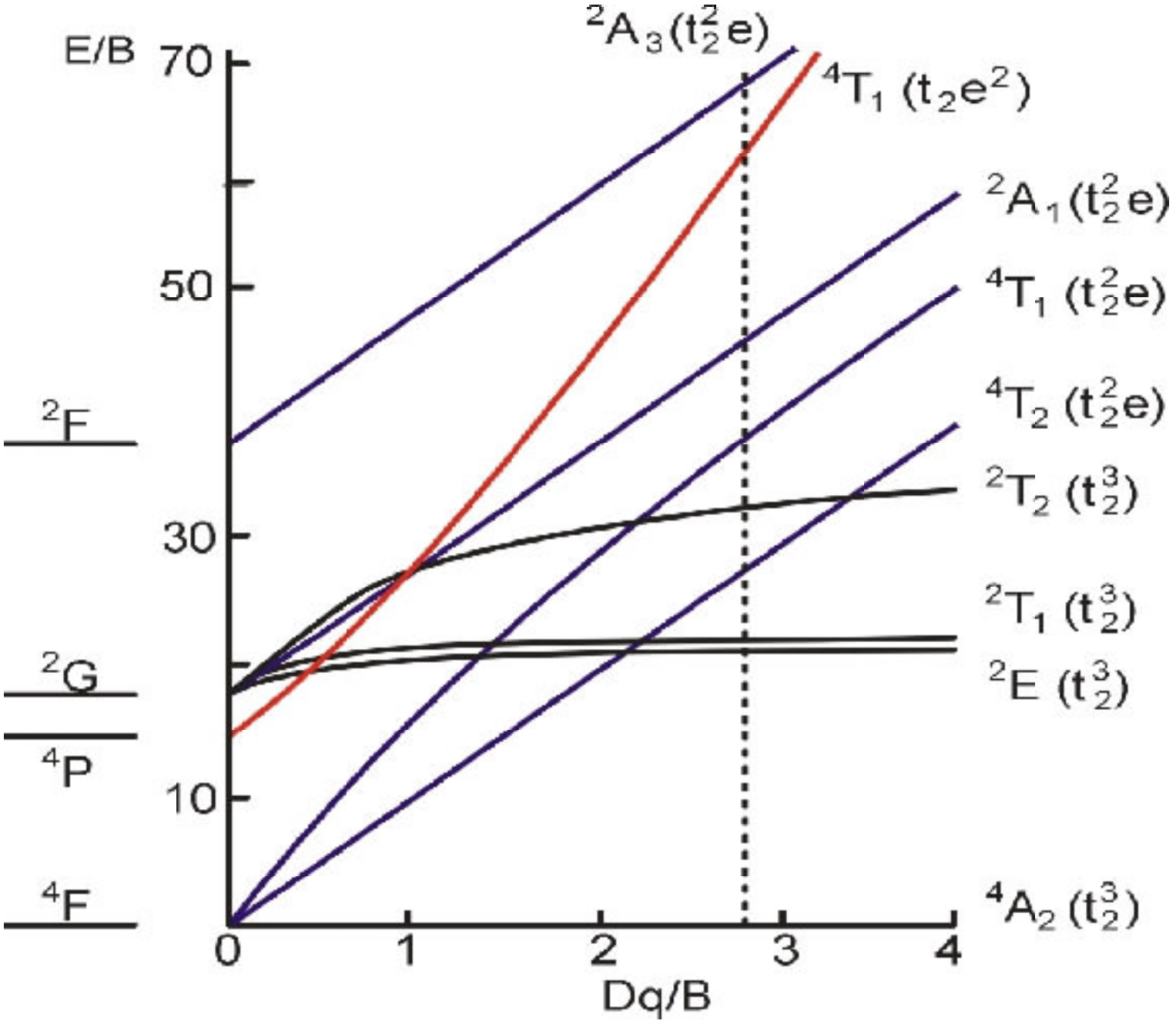




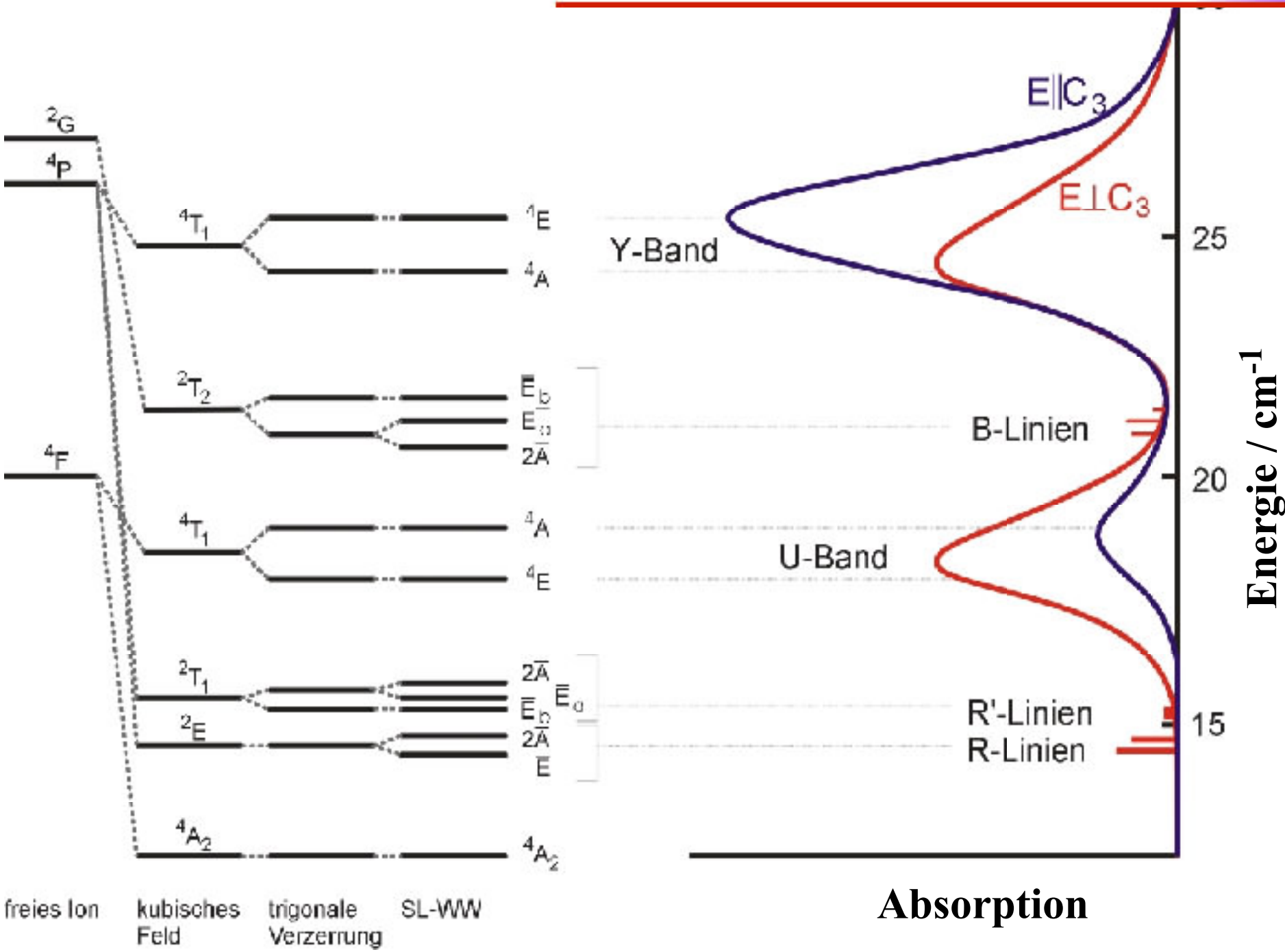
trigonale Symmetrie



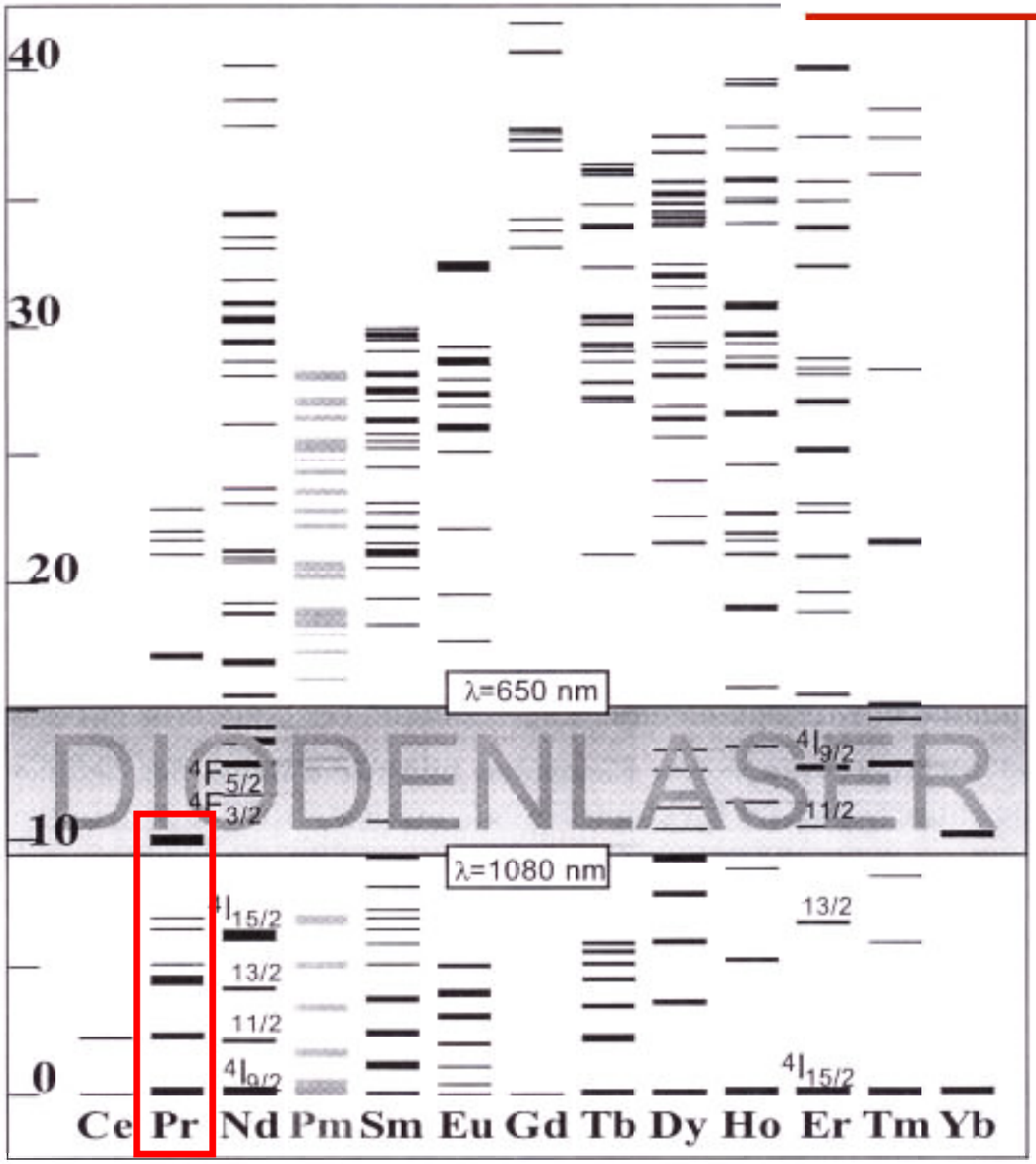
d^3 Zustände im Kristallfeld

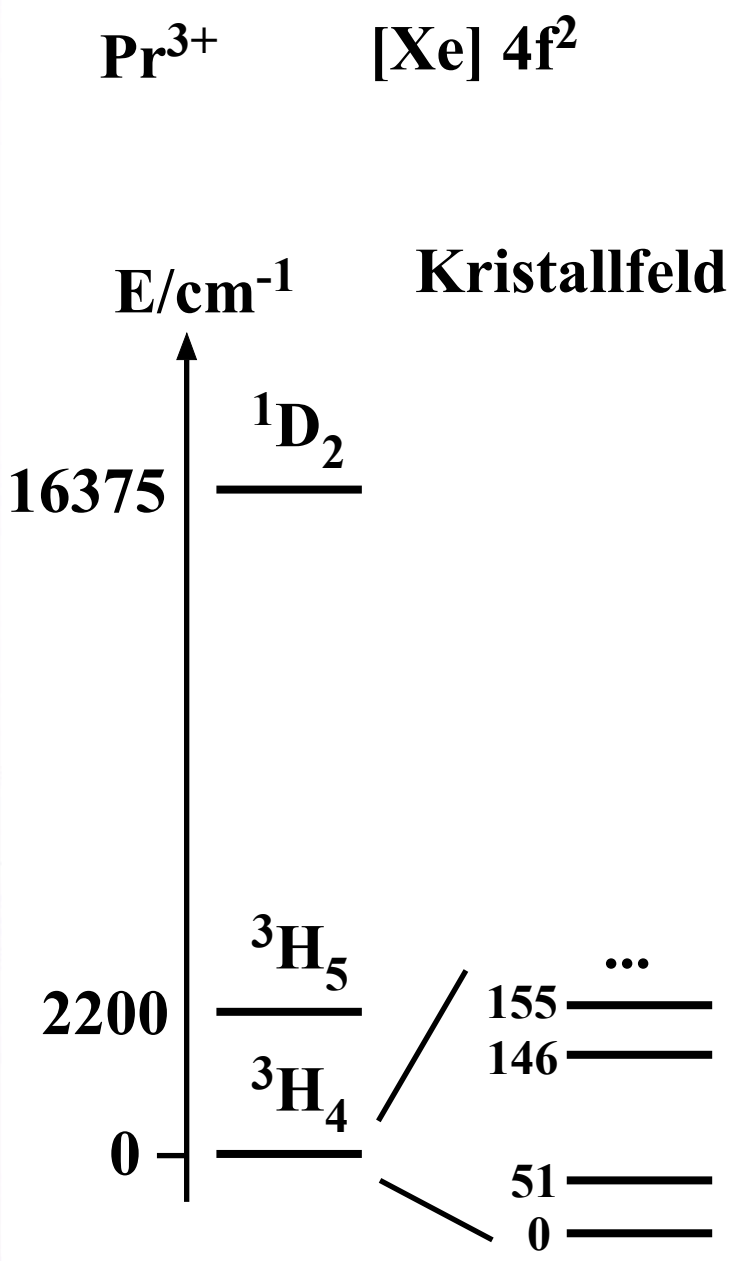


Rubin Spektrum

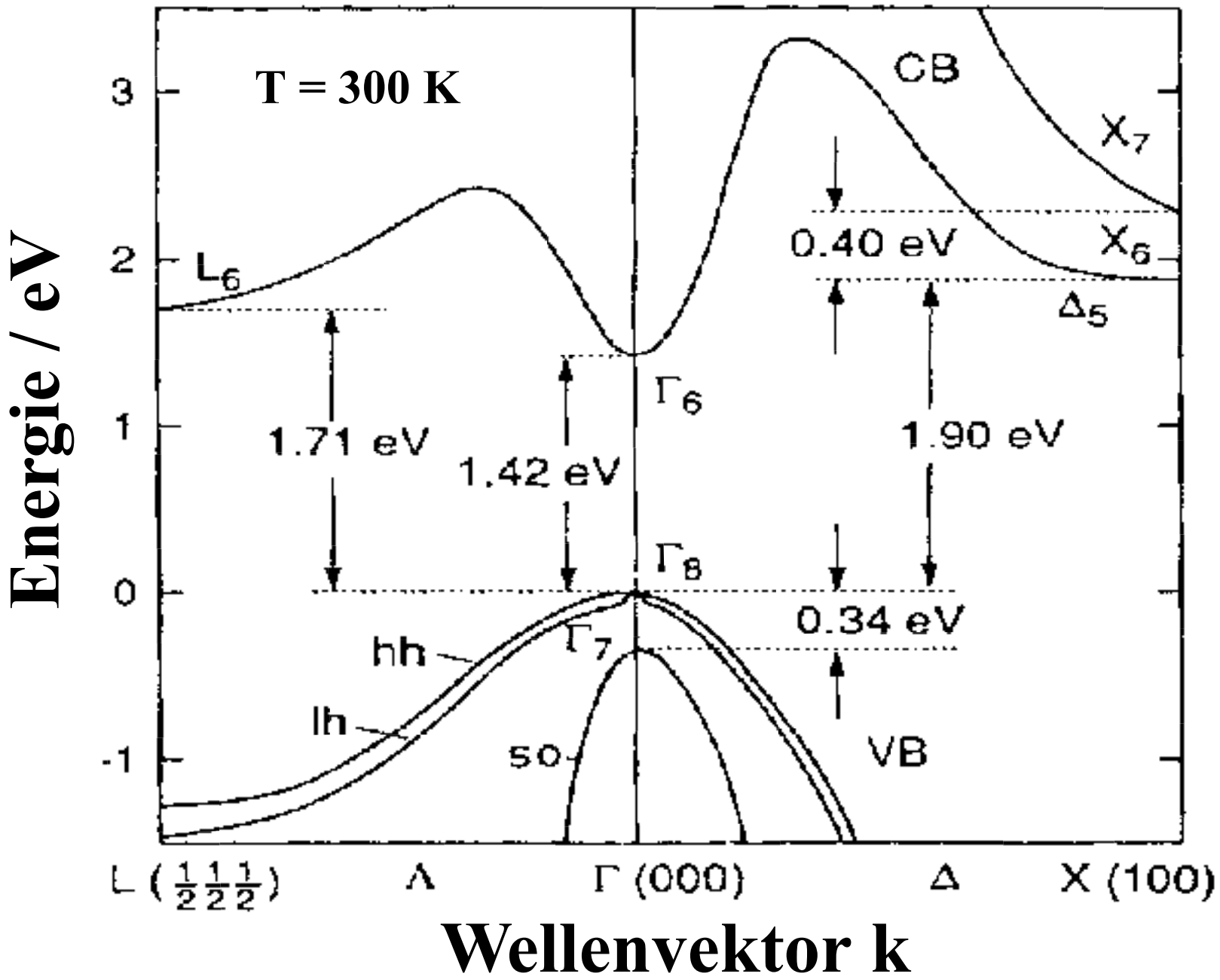


Seltene Erden





GaAs


T = 300 K
CB
X_7
X_6
L_6
Δ_5
0.40 eV
Γ_6
1.71 eV
1.42 eV
1.90 eV
Γ_8
0.34 eV
hh
Γ_7
lh
so
VB
3
2
1
0
-1
Energie / eV
L ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$)
Λ
Γ (000)
Δ
X (100)
Wellenvektor k

GaAs Übergänge