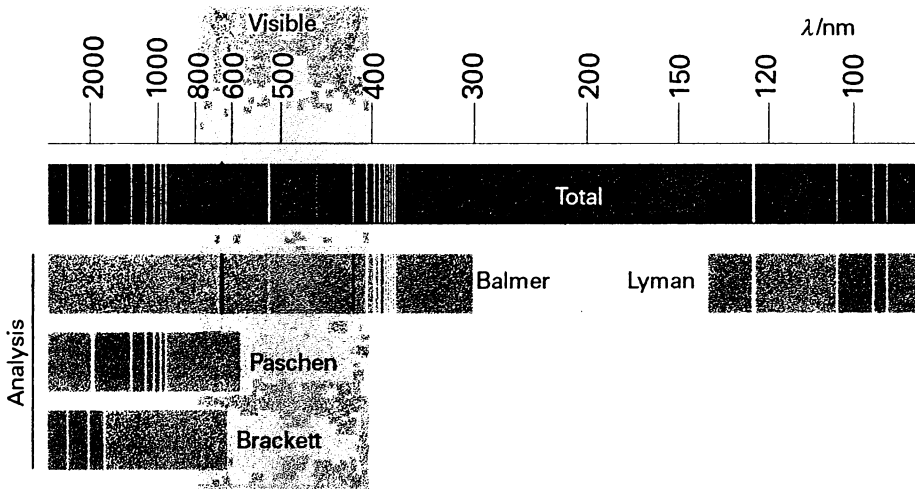


# 2013 化学結合論配布資料 01

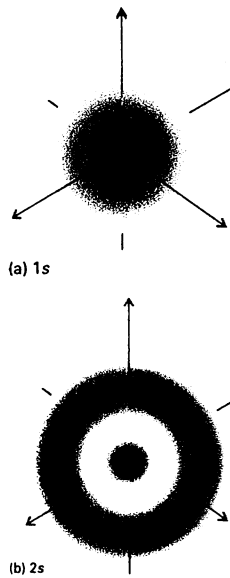
## ・水素原子のスペクトル



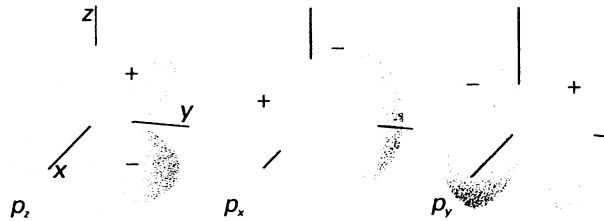
**Fig. 10.1** The spectrum of atomic hydrogen. Both the observed spectrum and its resolution into overlapping series are shown. Note that the Balmer series lies in the visible region.

Peter Atkins, Julio de Paula, Physical Chemistry 8<sup>th</sup> edition (2006).

## ・水素様原子の原子オービタル

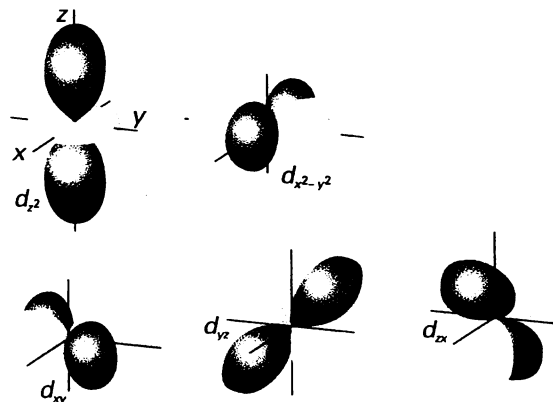


**Fig. 10.10** Representations of the 1s and 2s hydrogenic atomic orbitals in terms of their electron densities (as represented by the density of shading)



**Fig. 10.15** The boundary surfaces of *p* orbitals. A nodal plane passes through the nucleus and separates the two lobes of each orbital. The dark and light areas denote regions of opposite sign of the wavefunction.

**Fig. 10.16** The boundary surfaces of *d* orbitals. Two nodal planes in each orbital intersect at the nucleus and separate the lobes of each orbital. The dark and light areas denote regions of opposite sign of the wavefunction.



## ・水素様原子の原子オービタル(動径部分)

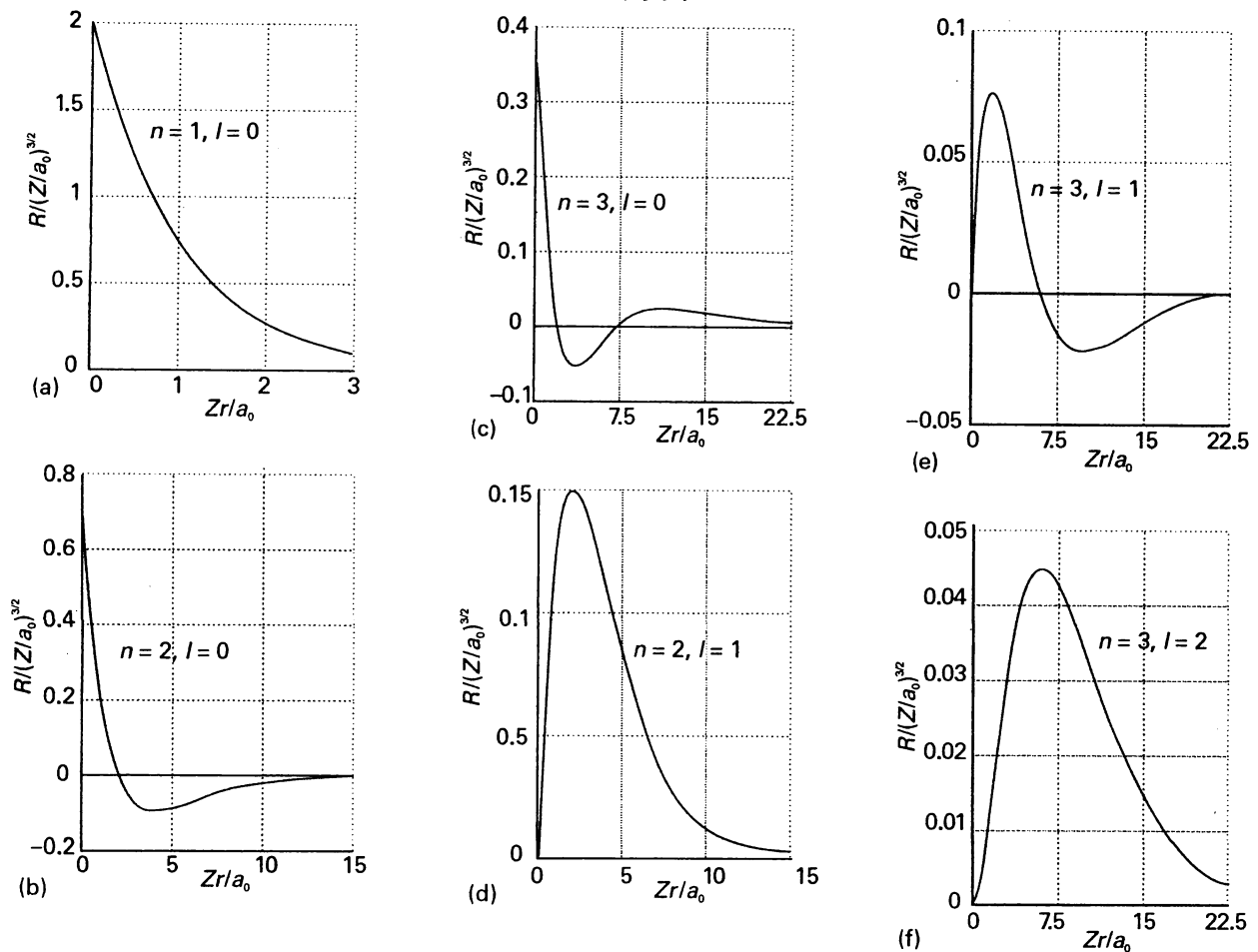


Fig. 10.4 The radial wavefunctions of the first few states of hydrogenic atoms of atomic number  $Z$ . Note that the orbitals with  $l=0$  have a nonzero and finite value at the nucleus. The horizontal scales are different in each case: orbitals with high principal quantum numbers are relatively distant from the nucleus.

Peter Atkins, Julio de Paula, Physical Chemistry 8<sup>th</sup> edition (2006).

## ・水素様原子の原子オービタルの式

K 殻

$$n=1, l=0, m=0:$$

$$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\sigma}$$

L 殻

$$n=2, l=0, m=0:$$

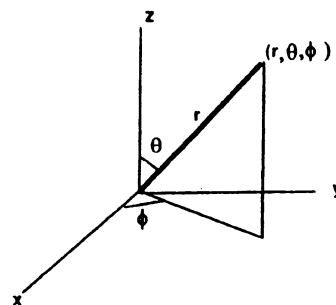
$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (2-\sigma) e^{-\frac{\sigma}{2}}$$

$$n=2, l=1, m=0:$$

$$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma e^{-\frac{\sigma}{2}} \cos \vartheta$$

極座標

$$\begin{cases} x = r \sin \theta \cos \phi \\ y = r \sin \theta \sin \phi \\ z = r \cos \theta \end{cases} \Leftrightarrow \begin{cases} r = x^2 + y^2 + z^2 \\ \theta = \cos^{-1} z / r \\ \phi = \tan^{-1} y / x \end{cases}$$



$n = 2, l = 1, m = \pm 1:$

$$\psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma e^{-\frac{\sigma}{2}} \sin \vartheta \cos \varphi$$

$$\psi_{2p_y} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma e^{-\frac{\sigma}{2}} \sin \vartheta \sin \varphi$$

M殻

$n = 3, l = 0, m = 0:$

$$\psi_{3s} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (27 - 18\sigma + 2\sigma^2) e^{-\frac{\sigma}{3}}$$

$n = 3, l = 1, m = 0:$

$$\psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (6 - \sigma) \sigma e^{-\frac{\sigma}{3}} \cos \vartheta$$

$n = 3, l = 1, m = \pm 1:$

$$\psi_{3p_x} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (6 - \sigma) \sigma e^{-\frac{\sigma}{3}} \sin \vartheta \cos \varphi$$

$$\psi_{3p_y} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} (6 - \sigma) \sigma e^{-\frac{\sigma}{3}} \sin \vartheta \sin \varphi$$

$n = 3, l = 2, m = 0:$

$$\psi_{3d_z} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} (3 \cos^2 \vartheta - 1)$$

$n = 3, l = 2, m = \pm 1:$

$$\psi_{3d_{xy}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} \sin \vartheta \cos \vartheta \cos \varphi$$

$$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} \sin \vartheta \cos \vartheta \sin \varphi$$

$n = 3, l = 2, m = \pm 2:$

$$\psi_{3d_{x^2-y^2}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} \sin^2 \vartheta \cos 2\varphi$$

$$\psi_{3d_{xy}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} \sin^2 \vartheta \sin 2\varphi$$

ここに  $\sigma = \frac{Z}{a_0} r$ .

ポーリング・ウィルソン「量子力学序論」(1965) 白水社の160ページより。

### ・ギリシャ文字一覧表

A, α	アルファ	N, ν	ニュー
B, β	ベータ	Ξ, ξ	グザイ (クシー、クサイ)
Γ, γ	ガンマ	O, o	オミクロン
Δ, δ	デルタ	Π, π	パイ
E, ε	イプシロン	P, ρ	ロー
Z, ζ	ゼータ	Σ, σ	シグマ
H, η	イータ (エータ)	T, τ	タウ
Θ, θ	シート (テータ)	Υ, υ	ウプシロン (ユプシロン)
I, i	イオタ	Φ, φ	ファイ
K, κ	カッパ	X, χ	カイ
Λ, λ	ラムダ	Ψ, ψ	プサイ
M, μ	ミュー	Ω, ω	オメガ