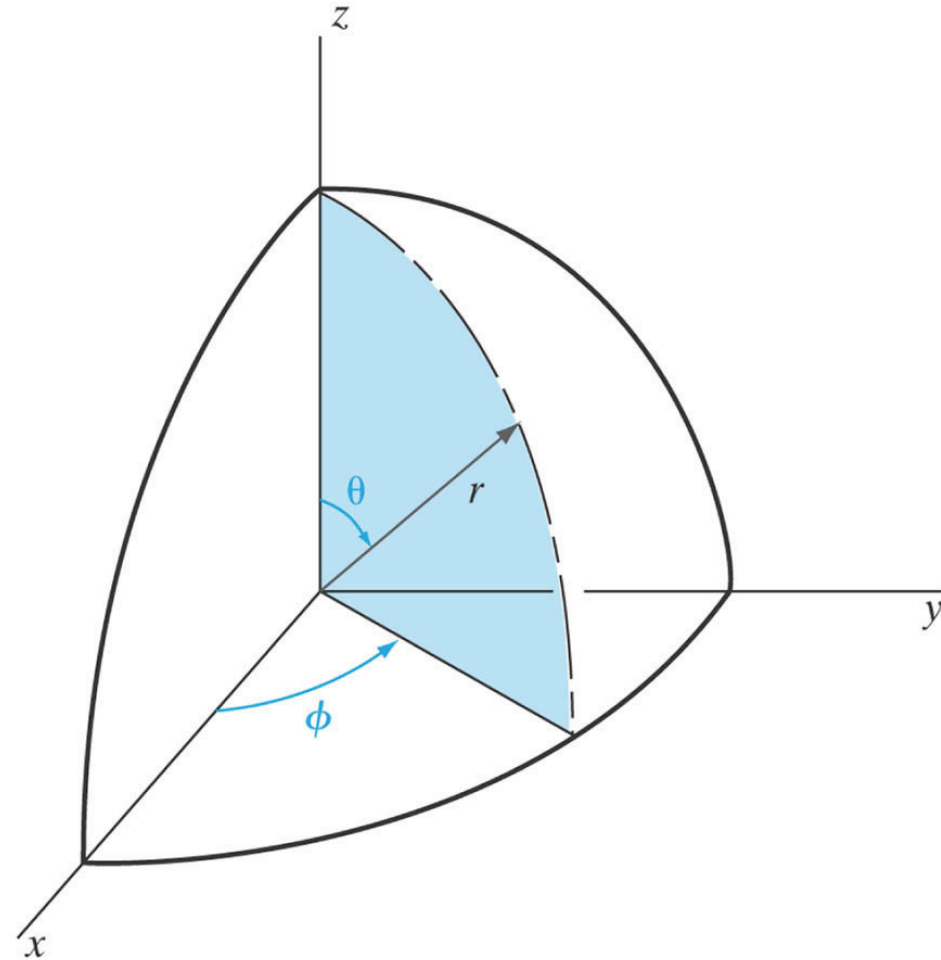


Atomic structure

The Hydrogen Atom

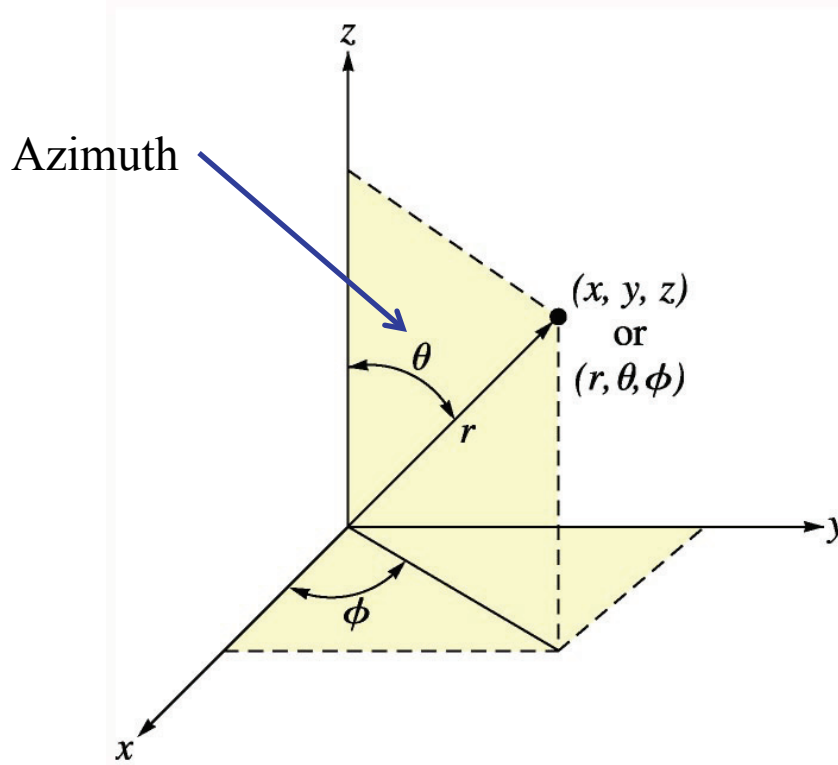
Finding the wave functions for the hydrogen atom requires a solution of the Schrödinger wave equation in *three dimensions* for a coulombic potential field.

Since the problem is *spherically symmetric*, the spherical coordinate system is used in the calculation:



Atomic structure – 2

The radial dependence of the potential suggests that we should go from Cartesian coordinates to spherical polar coordinates.



r = interparticle distance
($0 \leq r \leq \infty$)

θ = angle from z-axis to
“x-y plane”
($0 \leq \theta \leq \pi$)

ϕ = rotation in “x-y plane”
($0 \leq \phi \leq 2\pi$)

Atomic structure – 3

Potential term $U(x,y,z)$ in the Schrödinger equation written in *rectangular* coordinate system must be replaced by $U(r, \theta, \phi)$, representing the Coulomb potential the *spherical (polar)* coordinate system which the electron experiences in the vicinity of the proton.

The Coulomb potential varies only with r in spherical coordinates:

$$U(r) = -\frac{q^2}{4\pi\epsilon_0 r_n}$$

Then, the Schrödinger equation:

$$\nabla^2 \Psi(r, \theta, \phi) + \frac{2m}{\hbar^2} (E - U(r, \theta, \phi)) \Psi(r, \theta, \phi) = 0$$

(Note: the equation above is written in *rectangular* coordinate system. To work in *polar* coordinate system, it should be transformed.)

Atomic structure – 4

Coulomb potential which the electron experiences in the vicinity of the proton:

$$U(r, \theta, \phi) = U(r) = -\frac{1}{4\pi\epsilon_0} \frac{q^2}{r}$$

Now, variables in the Schrödinger equation can be separated:

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

This wave function of an electron in hydrogen atom $\psi(r, \theta, \phi)$ is a product of *three* parts. Three separate solutions must be obtained for:

- the *r*-dependent equation,
- the *θ*-dependent equation,
- the *φ*-dependent equation.

Atomic structure – 5

The wave functions for the ϕ -dependent equation are *quantized* with the following selection rule for the quantum numbers:

$$\mathbf{m} = \dots, -3, -2, -1, 0, +1, +2, +3, \dots$$

For the r -dependent equation, the *quantum number n* can be any positive integer (not zero).

For the θ -dependent equation the *quantum number l* can be zero or a positive integer.

Atomic structure – 6

These restrictions are summarized as follows:

Principal quantum number:

$$\mathbf{n} = 1, 2, 3, \dots$$

Azimuthal quantum number:

$$l = 0, 1, 2, \dots, (\mathbf{n} - 1)$$

Magnetic quantum number:

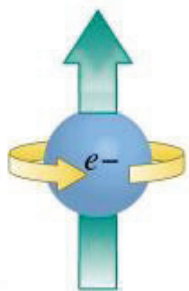
$$\mathbf{m} = -l, \dots, -2, -1, 0, +1, +2, \dots, +l$$

Atomic structure – 7

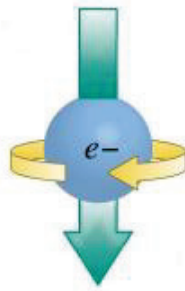
In addition to the three quantum numbers arising from the three parts of the wave equation, there is an important quantization condition on the "*spin*" of the electron.

Investigations of electron spin employ the theory of relativity as well as quantum mechanics; therefore, we shall simply state that the intrinsic angular momentum s of an electron with ψ_{nlm} specified is

$$s = \pm \frac{\hbar}{2}$$



"spin up"



"spin down"

That is, in units of \hbar , the electron has a spin of $\frac{1}{2}$, and the angular momentum produced by this spin is positive or negative depending on whether the electron is "*spin up*" or "*spin down*".

Atomic structure – 8

Summary:

Each allowed energy state of the electron in the hydrogen atom is uniquely described by the set of four quantum numbers: ***n***, ***l***, ***m***, and ***s***.

Using these *four quantum numbers*, we can identify the various states which the electron can occupy in a hydrogen atom.

The number ***n***, called the *principal quantum number*, specifies the “orbit” of the electron in Bohr terminology.

There is considerable fine structure in the energy levels about the Bohr orbits, for example:

- an electron with ***n*** = 1 can have only ***l*** = 0 and ***m*** = 0, but there are two spin states allowed.
- for ***n*** = 2, ***l*** can be 0 or 1, and ***m*** can be -1, 0, or +1 with two spins for each state.

Atomic structure – 9

These four quantum numbers with the selection rules precisely describe the structure of *energy states* in hydrogen atom.

Electron in a hydrogen atom can occupy *only* one of a large number of excited states including the lowest (*ground*) state.

Energy differences between the various states properly account for the observed lines in the hydrogen spectrum.

The Periodic Table – 1

The structure of energy states and quantum numbers arise from solutions to the hydrogen atom problem.

Question: How can we extend the knowledge of hydrogen atom energy structure on description of more complex atoms?

Answer: The *quantum number selection rules* are valid for more complicated structures. They can be used to describe the arrangement of atoms in the *periodic table* of chemical elements.

The Periodic Table – 2

Pauli exclusion principle.



Wolfgang Pauli

In multi-electron system *only one electron* may occupy a specific discrete energy level.

or in other words:

No two electrons can have the same set of quantum numbers n , l , m , s .

or in other words:

Only two electrons can have the same three quantum numbers n , l , m , and those two must have opposite spin.

The Periodic Table – 3

Pauli exclusion principle is basic to the electronic structure of all atoms in the periodic table

n	l	m	s/ħ	Allowable states in subshell	Allowable states in complete shell
1	0	0	½	2	2
2	0	0	½	2	8
	1	-1	½	6	
		0	½		
3	1	1	½	6	18
		0	½		
	2	-2	½	10	
2	-1	½			
	0	½			
	1	½			
2	1	½	10		
	0	½			

Quantum numbers to $n = 3$ and allowable states for the electron in a hydrogen atom.

The first four columns show the various combinations of quantum numbers allowed by the selection rules.

The last two columns indicate the number of allowed states (combinations of **n**, **l**, **m**, and **s**) for each **l** (subshell) and **n** (shell, or Bohr orbit).

The Periodic Table – 4

Atomic number (Z)	Element	n = 1 l = 0		2		3		4		
		1s	2s	2p	3s	3p	3d	4s	4p	
		Number of electrons						Shorthand notation		
1	H	1						1s ¹		
2	He	2						1s ²		
3	Li		1					1s ² 2s ¹		
4	Be		2					1s ² 2s ²		
5	B		2	1				1s ² 2s ² 2p ¹		
6	C	helium core, 2 electrons	2	2				1s ² 2s ² 2p ²		
7	N		2	3				1s ² 2s ² 2p ³		
8	O		2	4				1s ² 2s ² 2p ⁴		
9	F		2	5				1s ² 2s ² 2p ⁵		
10	Ne		2	6				1s ² 2s ² 2p ⁶		
11	Na				1				[Ne] 3s ¹	
12	Mg				2				3s ²	
13	Al				2	1			3s ² 3p ¹	
14	Si	neon core, 10 electrons	2	2				3s ² 3p ²		
15	P		2	3				3s ² 3p ³		
16	S		2	4				3s ² 3p ⁴		
17	Cl		2	5				3s ² 3p ⁵		
18	Ar		2	6				3s ² 3p ⁶		
19	K						1		[Ar] 4s ¹	
20	Ca					2		4s ²		
21	Sc			1		2		3d ¹ 4s ²		
22	Ti			2		2		3d ² 4s ²		
23	V			3		2		3d ³ 4s ²		
24	Cr			5	1	1		3d ⁵ 4s ¹		
25	Mn			5	2	2		3d ⁵ 4s ²		
26	Fe			6	2	2		3d ⁶ 4s ²		
27	Co			7	2	2		3d ⁷ 4s ²		
28	Ni			8	2	2		3d ⁸ 4s ²		
29	Cu			10	1	1		3d ¹⁰ 4s ¹		
30	Zn			10	2	2		3d ¹⁰ 4s ²		
31	Ga			10	2	1		3d ¹⁰ 4s ² 4p ¹		
32	Ge			10	2	2		3d ¹⁰ 4s ² 4p ²		
33	As			10	2	3		3d ¹⁰ 4s ² 4p ³		
34	Se			10	2	4		3d ¹⁰ 4s ² 4p ⁴		
35	Br			10	2	5		3d ¹⁰ 4s ² 4p ⁵		
36	Kr			10	2	6		3d ¹⁰ 4s ² 4p ⁶		

Electronic configuration of atoms in the ground state

The Periodic Table – 5

In **1869** Mendeleev and Lothar Meyer (Germany) published nearly identical classification schemes for elements known to date.

The periodic table is based on the similarity of properties and reactivities exhibited by certain elements.

Later, Henri Moseley (England, 1887-1915) established that each element has a unique atomic number (Z), which is how the current periodic table is organized.



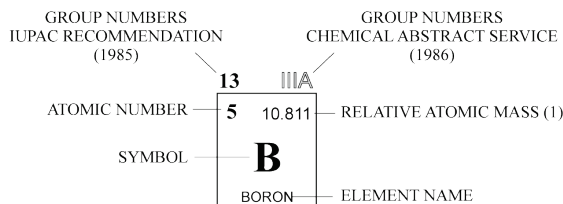
Dmitri Mendeleev.

Row	Group I — R ₂ O	Group II — RO	Group III — R ₂ O ₃	Group IV RH ₄ RO ₂	Group V RH ₃ R ₂ O ₅	Group VI RH ₂ RO ₃	Group VII RH R ₂ O ₇	Group VIII — RO ₄
1	H = 1							
2	Li = 7	Be = 9.4	B = 11	C = 12	N = 14	O = 16	F = 19	
3	Na = 23	Mg = 24	Al = 27.3	Si = 28	P = 31	S = 32	Cl = 35.5	
4	K = 39	Ca = 40	— = 44	Ti = 48	V = 51	Cr = 52	Mn = 55	Fe = 56, Co = 59, Ni = 59, Cu = 63
5	(Cu = 63)	Zn = 65	— = 68	— = 72	As = 75	Se = 78	Br = 80	
6	Rb = 85	Sr = 87	?Yt = 88	Zr = 90	Nb = 94	Mo = 96	— = 100	Ru = 104, Rh = 104, Pd = 106, Ag = 108
7	(Ag = 108)	Cd = 112	In = 113	Sn = 118	Sb = 122	Te = 125	I = 127	
8	Cs = 133	Ba = 137	?Di = 138	?Ce = 140				
9								
10			?Er = 178	?La = 180	Ta = 182	W = 184		Os = 195, Ir = 197, Pt = 198, Au = 199
11	(Au = 199)	Hg = 200	Tl = 204	Pb = 207	Bi = 208			
12				Th = 231		U = 240		

The Periodic Table – 6

<http://www.ktf-split.hr/periodni/en/>

PERIOD	GROUP																18				
	1	IIA												IIIA		14	15	16	17	VIIIA	
1	1 1.0079 H HYDROGEN																				2 4.0026 He HELIUM
2	3 6.941 Li LITHIUM	4 9.0122 Be BERYLLIUM												5 10.811 B BORON		6 12.011 C CARBON	7 14.007 N NITROGEN	8 15.999 O OXYGEN	9 18.998 F FLUORINE	10 20.180 Ne NEON	
3	11 22.990 Na SODIUM	12 24.305 Mg MAGNESIUM												13 26.982 Al ALUMINIUM		14 28.086 Si SILICON	15 30.974 P PHOSPHORUS	16 32.065 S SULPHUR	17 35.453 Cl CHLORINE	18 39.948 Ar ARGON	
4	19 39.098 K POTASSIUM	20 40.078 Ca CALCIUM	21 44.956 Sc SCANDIUM	22 47.867 Ti TITANIUM	23 50.942 V VANADIUM	24 51.996 Cr CHROMIUM	25 54.938 Mn MANGANESE	26 55.845 Fe IRON	27 58.933 Co COBALT	28 58.693 Ni NICKEL	29 63.546 Cu COPPER	30 65.39 Zn ZINC	31 69.723 Ga GALLIUM	32 72.64 Ge GERMANIUM	33 74.922 As ARSENIC	34 78.96 Se SELENIUM	35 79.904 Br BROMINE	36 83.80 Kr KRYPTON			
5	37 85.468 Rb RUBIDIUM	38 87.62 Sr STRONTIUM	39 88.906 Y YTTRIUM	40 91.224 Zr ZIRCONIUM	41 92.906 Nb NIOBIUM	42 95.94 Mo MOLYBDENUM	43 (98) Tc TECHNETIUM	44 101.07 Ru RUTHENIUM	45 102.91 Rh RHODIUM	46 106.42 Pd PALLADIUM	47 107.87 Ag SILVER	48 112.41 Cd CADMIUM	49 114.82 In INDIUM	50 118.71 Sn TIN	51 121.76 Sb ANTIMONY	52 127.60 Te TELLURIUM	53 126.90 I IODINE	54 131.29 Xe XENON			
6	55 132.91 Cs CAESIUM	56 137.33 Ba BARIUM	57-71 La-Lu Lanthanide	72 178.49 Hf HAFNIUM	73 180.95 Ta TANTALUM	74 183.84 W TUNGSTEN	75 186.21 Re RHENIUM	76 190.23 Os OSMIUM	77 192.22 Ir IRIDIUM	78 195.08 Pt PLATINUM	79 196.97 Au GOLD	80 200.59 Hg MERCURY	81 204.38 Tl THALLIUM	82 207.2 Pb LEAD	83 208.98 Bi BISMUTH	84 (209) Po POLONIUM	85 (210) At ASTATINE	86 (222) Rn RADON			
7	87 (223) Fr FRANCIUM	88 (226) Ra RADIUM	89-103 Ac-Lr Actinide	104 (261) Rf RUTHERFORDIUM	105 (262) Db DUBNIUM	106 (266) Sg SEABORGIUM	107 (264) Bh BOHRIUM	108 (277) Hs HASSIUM	109 (268) Mt MEITNERIUM	110 (281) Uun UNUNNILIUM	111 (272) Uuu UNUNUNIUM	112 (285) Uub UNUNBIUM		114 (289) Uuq UNUNQUADIUM							



LANTHANIDE

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57 138.91 La LANTHANUM	58 140.12 Ce CERIUM	59 140.91 Pr PRASEODYMIUM	60 144.24 Nd NEODYMIUM	61 (145) Pm PROMETHIUM	62 150.36 Sm SAMARIUM	63 151.96 Eu EUROPIUM	64 157.25 Gd GADOLINIUM	65 158.93 Tb TERBIUM	66 162.50 Dy DYSPROSIUM	67 164.93 Ho HOLMIUM	68 167.26 Er ERBIUM	69 168.93 Tm THULIUM	70 173.04 Yb YTTTERBIUM	71 174.97 Lu LUTETIUM
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ACTINIDE

89 (227) Ac ACTINIUM	90 232.04 Th THORIUM	91 231.04 Pa PROTACTINIUM	92 238.03 U URANIUM	93 (237) Np NEPTUNIUM	94 (244) Pu PLUTONIUM	95 (243) Am AMERICIUM	96 (247) Cm CURIUM	97 (247) Bk BERKELIUM	98 (251) Cf CALIFORNIUM	99 (252) Es EINSTEINIUM	100 (257) Fm FERMIUM	101 (258) Md MENDELEVIUM	102 (259) No NOBELIUM	103 (262) Lr LAWRENCIUM
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(1) Pure Appl. Chem., 73, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements having no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@netlinx.com)