Chapter 1
Carbon as the Basis of Organic Chemistry

Clayden, Greeves, Warren, Wothers, *Organic Chemistry*, Oxford University Press, **2001**, Chapter 4, pp. 81–110.
Arnaud, *Chimie Organique*, Paul Arnaud, Dunod Editeur, **2009**, Chapitre 4, pp 73-103.

Definition of Organic Chemistry

- organic chemistry is the chemistry of carbon-containing molecules (compounds)
- organic molecules contain carbon "covalently" bonded to other (non-metallic) elements

group 4

	Ia	IIa	IIIa	IVa	Va	VIa	VIIa	VIII			Ib	IIb	IIIb	IVb	Vb	VIb	VIIb	0
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H 1.008 Wasserstoff																	2 He 4.0003 Helium
2	3 Li 6.94 Lithium	4 Be 9.01 Beryllium				2nd period							5 B 10.81 Bor	6 C 12.011 Kohlenstoff	7 N 14.01 Stickstoff	8 O 16.00 Sauerstoff	9 F 19.00 Fluor	10 Ne 20.18 Neon
3	11 Na 22.99 Natrium	12 Mg 24.31 Magnesium											13 Al 26.98 Aluminium	14 Si 28.09 Silicium	15 P 30.97 Phosphor	16 S 32.06 Schwefel	17 Cl 35.45 Chlor	18 Ar 39.95 Argon
4	19 K 39.10 Kalium	20 Ca 40.08 Calcium	21 Sc 44.96 Scandium	22 Ti 47.90 Titan	23 V 50.94 Vanadium	24 Cr 52.00 Chrom	25 Mn 54.94 Mangan	26 Fe 55.85 Eisen	27 Co 58.93 Cobalt	28 Ni 58.71 Nickel	29 Cu 63.55 Kupfer	30 Zn 65.37 Zink	31 Ga 69.72 Gallium	32 Ge 72.59 Germanium	33 As 74.92 Arsen	34 Se 78.96 Selen	35 Br 79.90 Brom	36 Kr 83.80 Krypton
5	37 Rb 85.47 Rubidium	38 Sr 87.62 Strontium	39 Y 88.91 Yttrium	40 Zr 91.22 Zirconium	41 Nb 92.91 Niob	42 Mo 95.94 Molybdän	43 Tc 98.91 Technecium	44 Ru 101.07 Ruthenium	45 Rh 102.91 Rhodium	46 Pd 106.4 Palladium	47 Ag 107.87 Silber	48 Cd 112.40 Cadmium	49 In 114.82 Indium	50 Sn 118.69 Zinn	51 Sb 121.75 Antimon	52 Te 127.60 Tellur	53 I 126.90 Iod	54 Xe 131.30 Xenon
6	55 Cs 132.91 Cäsium	56 Ba 137.34 Barium	57 La 138.91 Lanthan	72 Hf 178.49 Hafnium	73 Ta 180.95 Tantal	74 W 183.85 Wolfram	75 Re 186.2 Rhenium	76 Os 190.2 Osmium	77 Ir 192.22 Iridium	78 Pt 195.09 Platin	79 Au 196.97 Gold	80 Hg 200.59 Quecksilber	81 Tl 204.37 Thallium	82 Pb 207.2 Blei	83 Bi 209.98 Bismut	84 Po 208.98 Polonium	85 At 209.99 Astat	86 Rn 222.02 Radon
7	87 Fr 223.02 Francium	88 Ra 226.03 Radium	89 Ac 227.03 Actinium	104 Rf 261.11 Rutherfordium	105 Db 262.11	106 Sg 263.12	107 Bh 262.12	108 Hs	109 Mt									

- carbon is in 4th group of the 2nd period of the PSE; 4 valence electrons on 2nd shell for bonding
- carbon is tetravalent, can connect with a maximum of four bonds (electron pairs) to other atoms

The Time-Independent Schrödinger Equation

- **electrons (waves) around a nucleus, have to fulfill the time-independent Schrödinger equation**

$$\hat{H}\psi = E\psi$$

- Schrödinger equation is a differential equation that describes the allowed states (stationary state wave functions ψ) of an electron in the field of an atomic nucleus
- if the Hamilton operator $\hat{H}$ *(Hamiltonian)* acts on a wave function ψ and the result is proportional to ψ, then ψ is an allowed stationary state and the proportionality constant (Eigen value) is its energy E

- in one dimension: $$\hat{H}\psi(x) = -\frac{h^2}{8\pi^2 m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

- in three dimensions: $$\hat{H}\psi(r) = -\frac{h^2}{8\pi^2 m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r)$$

$$\hat{H}\psi(r) = -\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(r) + V(r)\psi(r) = E\psi(r)$$

- ∇^2 is the Laplace operator, $V(r)$ is potential energy, m is electron mass, h is the Planck constant

Quantum Numbers and Exclusion Principle

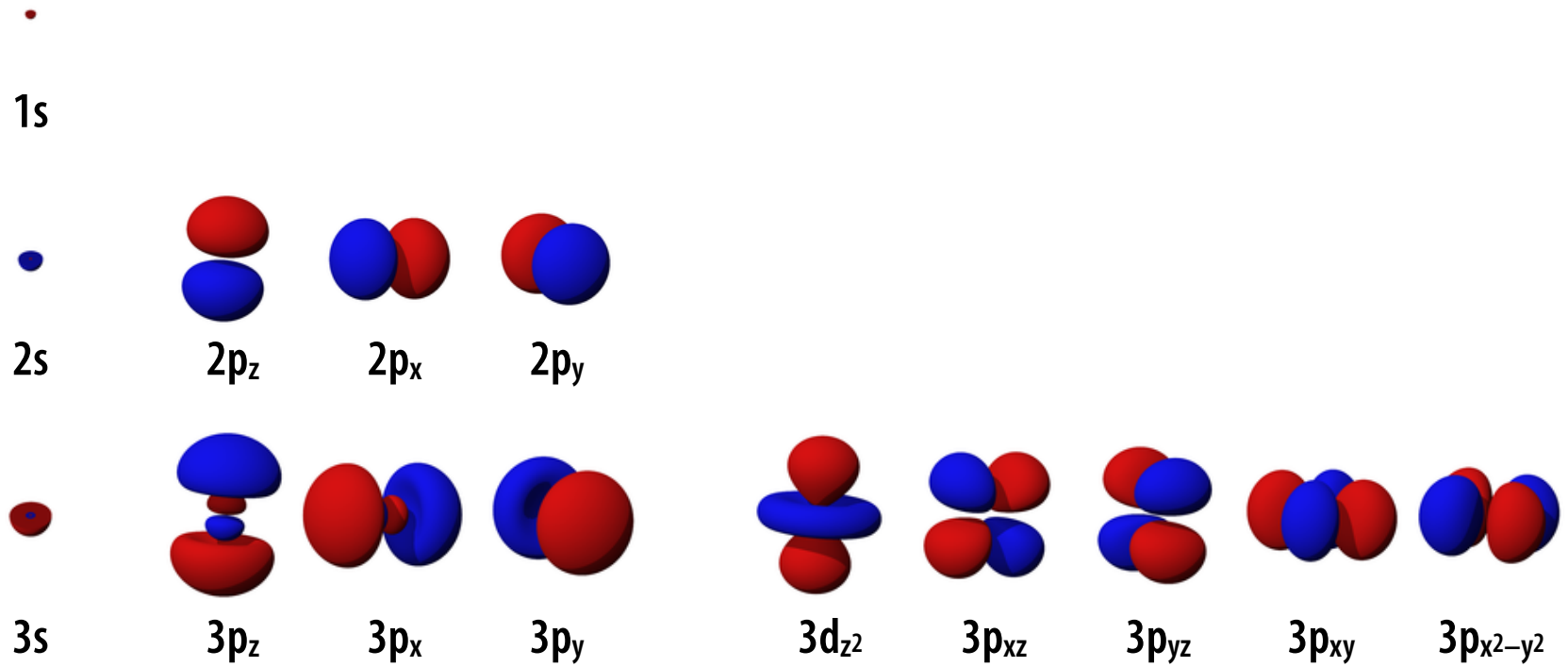
- the different allowed stationary states ψ are described by unique combinations of quantum numbers

Name	principal QN n	azimuthal QN ℓ	magnetic QN m	spin QN s	electrons
1s	1	0	0	+½, –½	2
2s	2	0	0	+½, –½	2
2p	2	1	+1, 0, –1	+½, –½	6
3s	3	0	0	+½, –½	2
3p	3	1	+1, 0, –1	+½, –½	6
3d	3	2	+2, +1, 0, –1, –2	+½, –½	10

- each orbital described by unique set of quantum numbers n, ℓ, and m
- n, ℓ, m correspond to electron energy, angular momentum, angular momentum vector component
- each orbital then filled with up to two electrons with different spin QN s (Pauli exclusion principle)

Representations of Atomic Orbitals

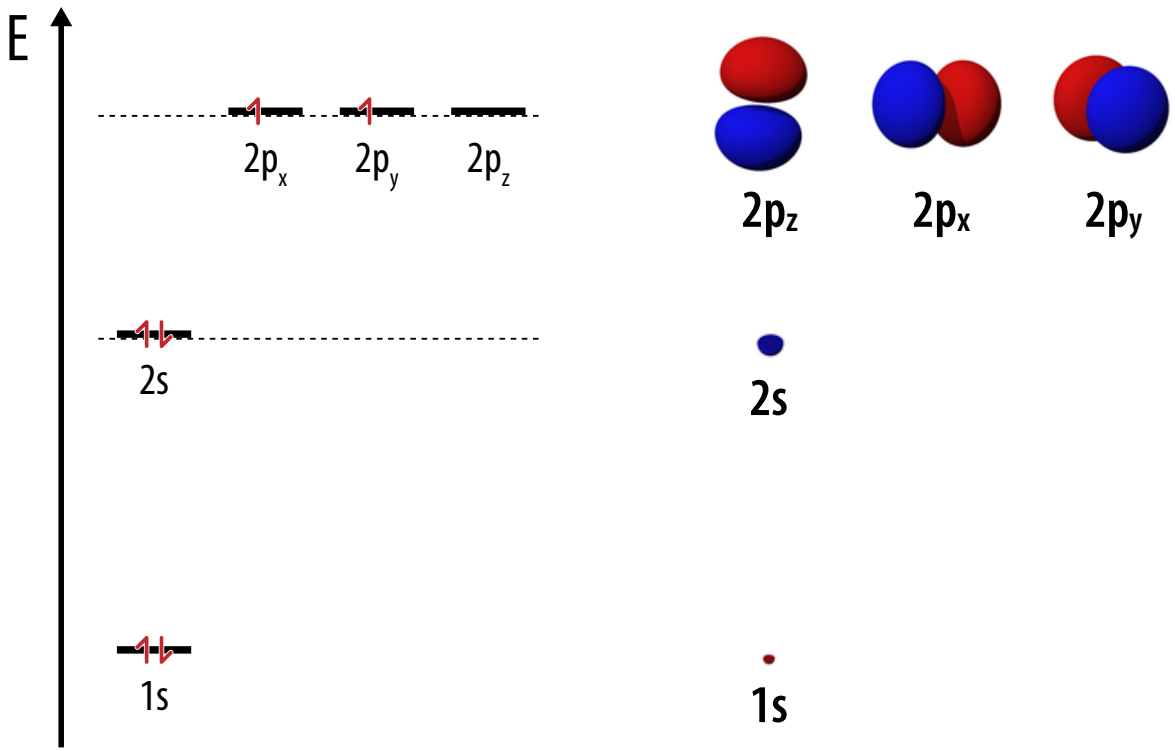
- atomic orbitals are space where the electron has a certain non-zero probability to be observed



- pictorial representations of atomic orbitals use $|\psi|^2$ representing the probability density to find electron
- approximate representations of contour surfaces with given probability density $|\psi|^2 = const.$
- representations often use color coding to show phase (sign) of ψ itself (important for bonding)

Valence Electrons and the Electronic Configuration of Carbon

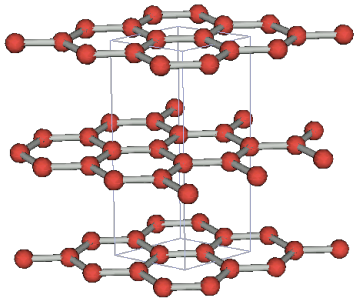
- atomic orbitals filled with electrons starting from low to high energy states (Aufbau principle)



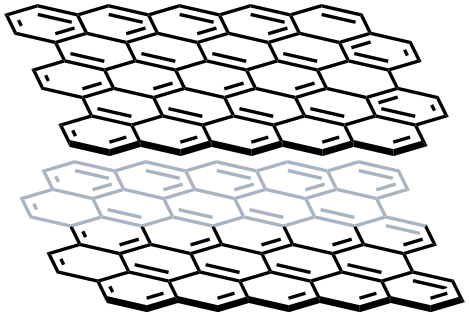
- valence shell is outer-most, highest-energy shell (highest principal QN *n*) filled with electrons
- only valence shell and valence electrons relevant for chemical bonding and reactions
- electronic configuration of carbon in the ground state $1s^2\ 2s^2\ 2p^2$

Modifications (Allotropes) of Carbon

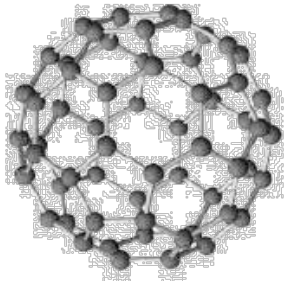
Graphite



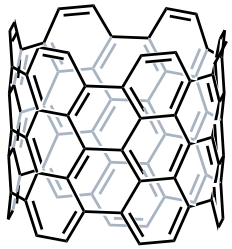
every carbon has 3 neighbors
every carbon has 4 bonds



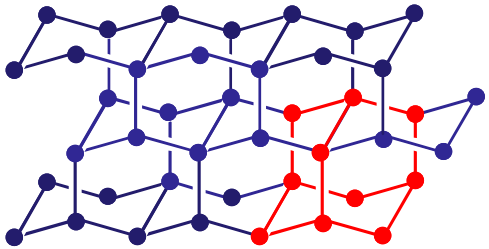
Fullerenes, Nanotubes



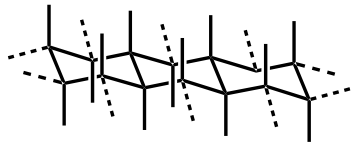
every carbon has 3 neighbors
every carbon has 4 bonds



Diamond

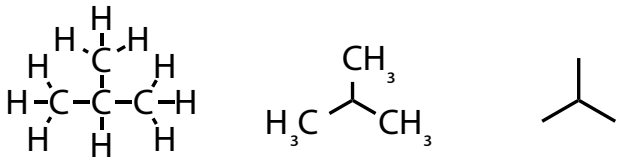
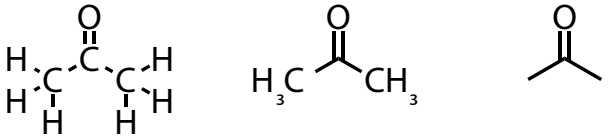
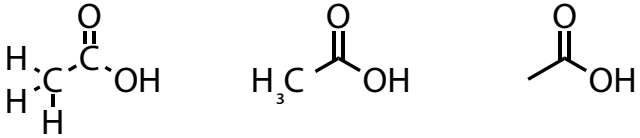
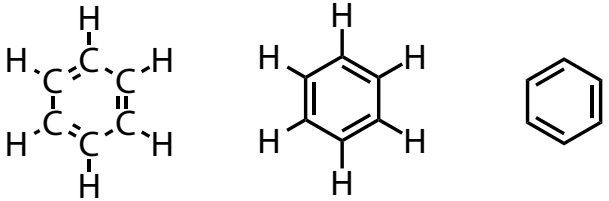


every carbon has 4 neighbors
every carbon has 4 bonds



- carbon is always tetravalent (connected with four bonds to other atoms)
- variable coordination geometry: tetrahedral (4 neighbors), trigonal (3 neighbors), linear (2 neighbors)

Different Types of Chemical Formulae

trivial name	IUPAC name	molecular formula	condensed formula	structure formulae
isobutane	2-methylpropane	C_4H_{10}	CH_3 -CH(CH_3)-CH_3	
acetone	propan-2-one	C_3H6O	CH_3 -C(O)-CH_3	
acetic acid	ethanoic acid	$C_2H_4O_2$	CH_3-C(O)-OH CH_3COOH	
benzene	benzene	C_6H_6	C_6H_6	
styrene	1-phenylethene	C_8H_8	C_6H_5-CH=CH_2