Schrödinger Equation

Schrödinger combined the idea that an electron has wave properties with classical equations of wave motion to give a wave equation for the energy of an electron in an atom.

Wave equation (Schrödinger equation) gives a series of solutions called wave functions (ψ).

Wave Functions

Only certain values of ψ are allowed.

Each ψ corresponds to a certain energy.

The probability of finding an electron at a particular point with respect to the nucleus is given by ψ^2.

Each energy state corresponds to an orbital.

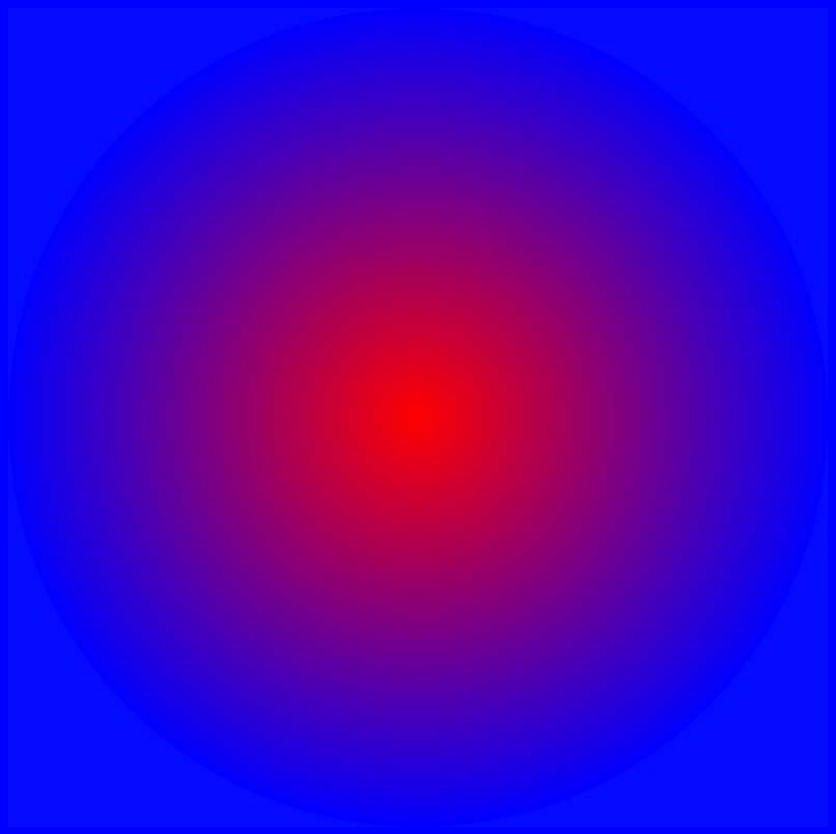


Figure 1.1 Probability distribution (ψ^2) for an electron in a 1*s* orbital.

A boundary surface encloses the region where the probability of finding an electron is high—on the order of 90-95%

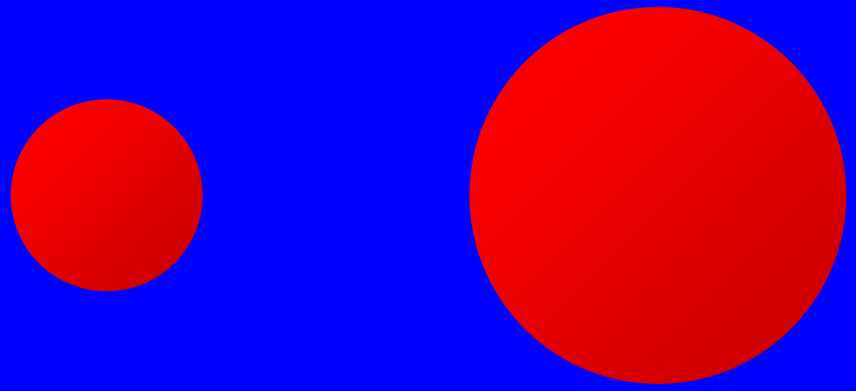


Figure 1.2 Boundary surfaces of a 1*s* orbital and a 2*s* orbital.

Quantum Numbers

Each orbital is characterized by a unique set of quantum numbers.

The principal quantum number *n* is a whole number (integer) that specifies the shell and is related to the energy of the orbital.

The angular momentum quantum number is usually designated by a letter (*s*, *p*, *d*, *f*, etc) and describes the shape of the orbital.

The Pauli Exclusion Principle

No two electrons in the same atom can have the same set of four quantum numbers.

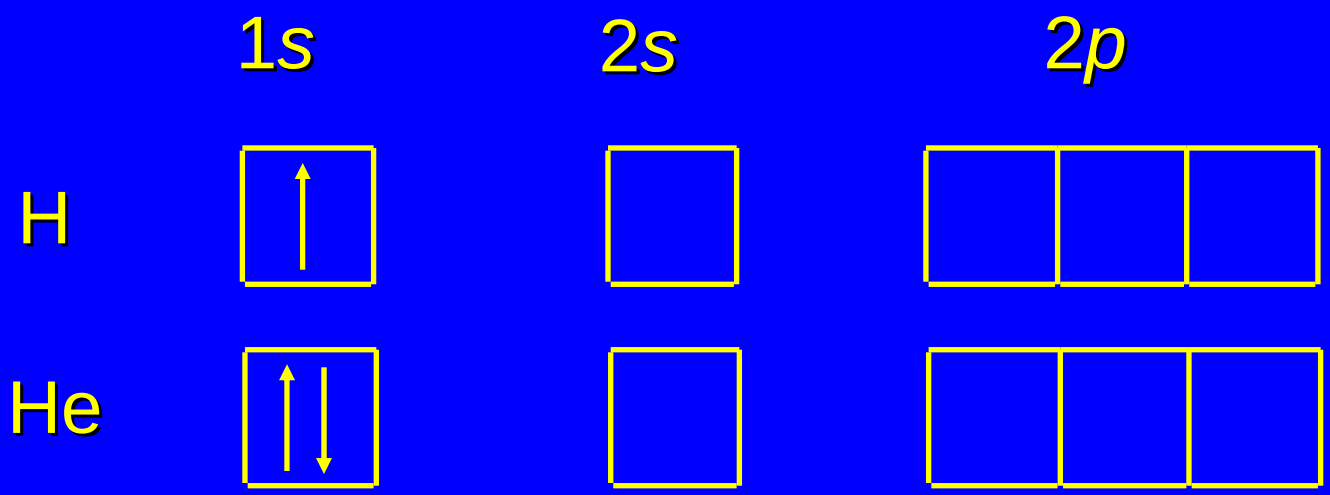
Two electrons can occupy the same orbital only when they have opposite spins.

There is a maximum of two electrons per orbital.

First Period

Principal quantum number (n) = 1

Hydrogen	Helium
$Z = 1$	$Z = 2$
$1s^1$	$1s^2$

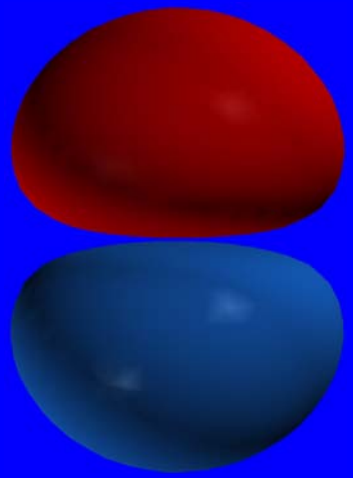


p *Orbitals*

p Orbitals are shaped like dumbells.

Are not possible for $n = 1$.

Are possible for $n = 2$ and higher.



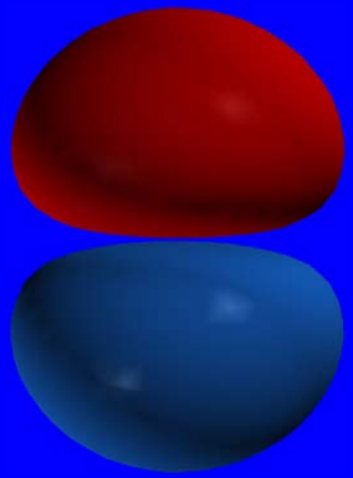
p *Orbitals*

p Orbitals are shaped like dumbells.

Are not possible for $n = 1$.

Are possible for $n = 2$ and higher.

There are three p orbitals for each value of n (when n is greater than 1).



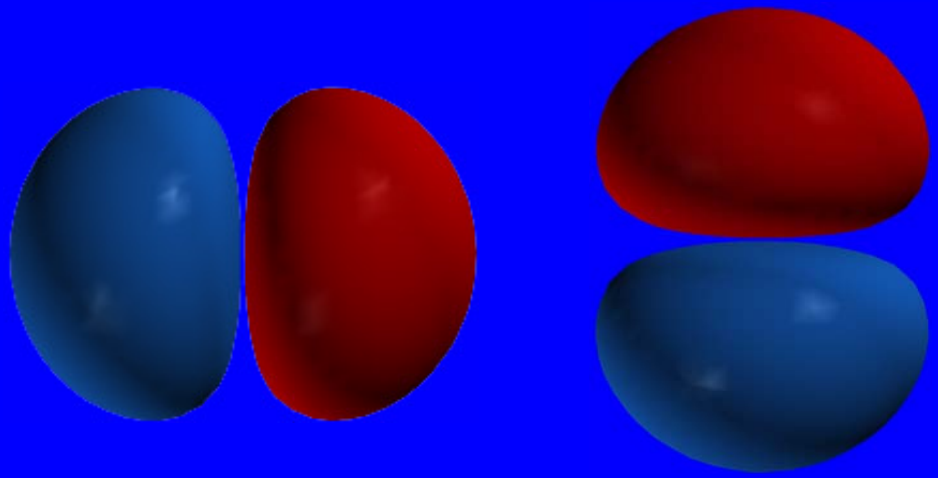
p *Orbitals*

p Orbitals are shaped like dumbells.

Are not possible for $n = 1$.

Are possible for $n = 2$ and higher.

There are three p orbitals for each value of n (when n is greater than 1).



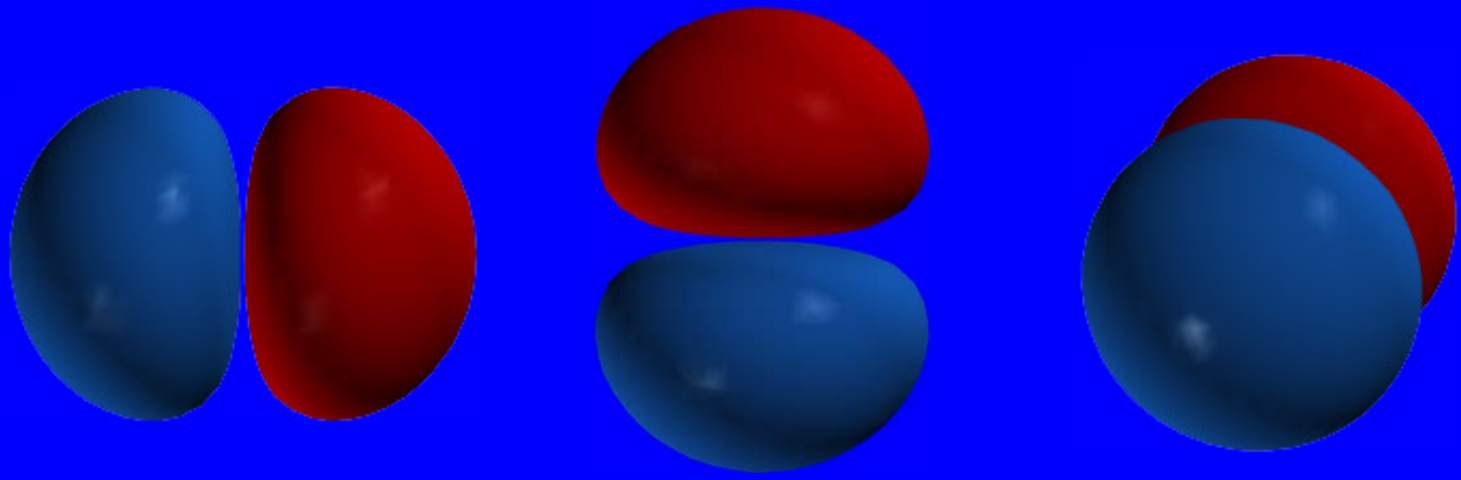
p *Orbitals*

p Orbitals are shaped like dumbells.

Are not possible for $n = 1$.

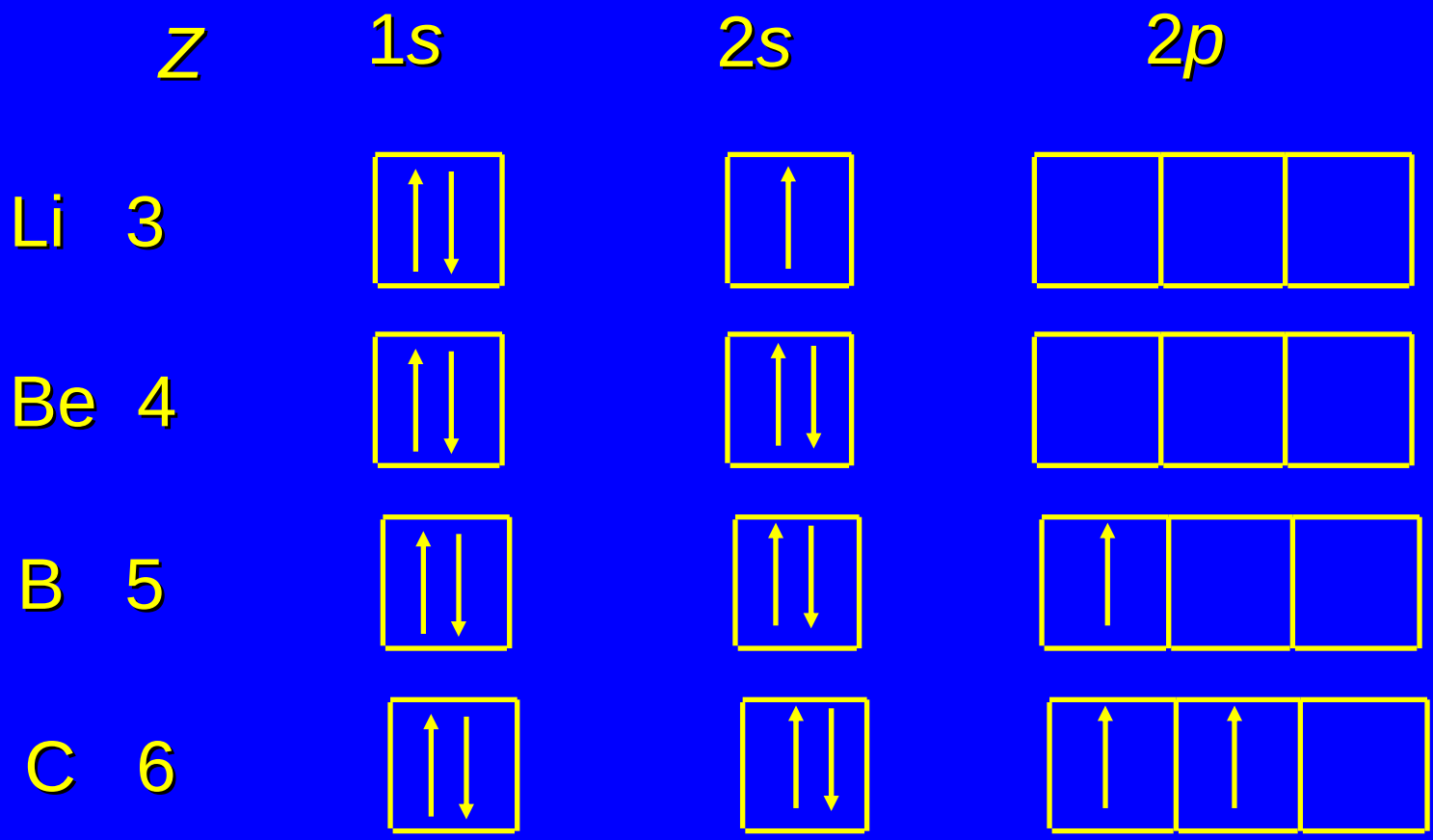
Are possible for $n = 2$ and higher.

There are three p orbitals for each value of n (when n is greater than 1).

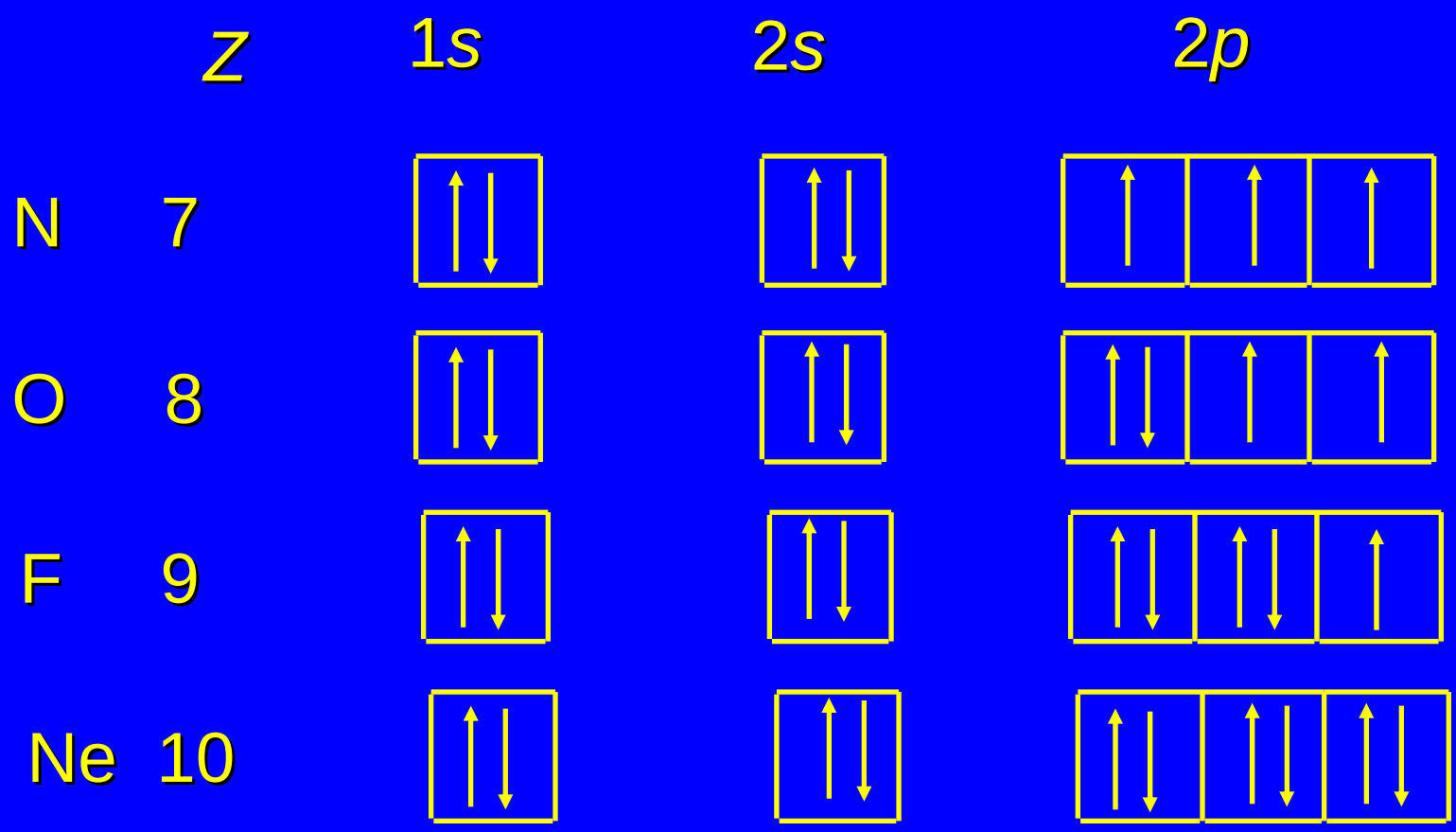


Second Period

Principal quantum number (*n*) = 2



Second Period



Covalent Bonding in H_2

Two hydrogen atoms, each with 1 electron,

H· ·H

can share those electrons in a covalent bond.

H:H

Sharing the electron pair gives each hydrogen an electron configuration analogous to helium.

1.6
Structural Formulas of Organic Molecules

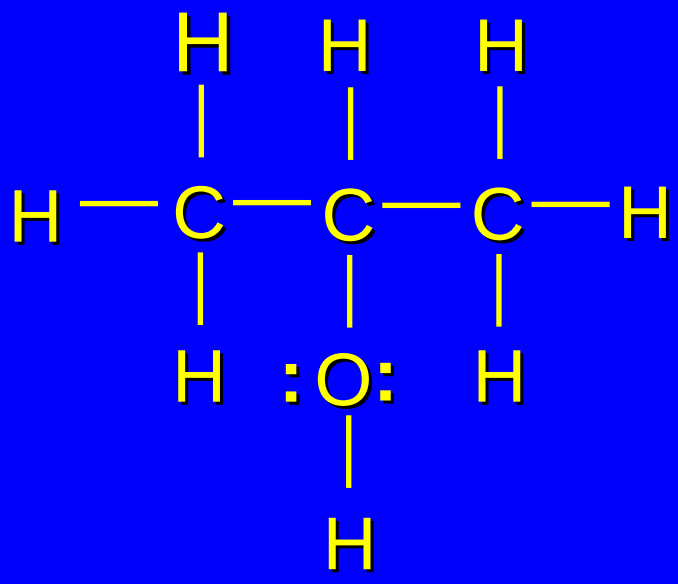
Constitution

The order in which the atoms of a molecule are connected is called its *constitution* or *connectivity*.

The constitution of a molecule must be determined in order to write a Lewis structure.

Condensed structural formulas

Lewis structures in which many (or all) covalent bonds and electron pairs are omitted.



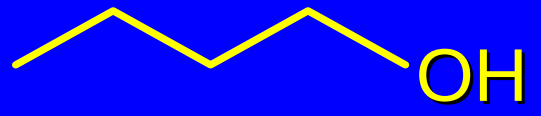
can be condensed to:

CH_3CHCH_3 or $(CH_3)_2CHOH$

OH

Bond-line formulas

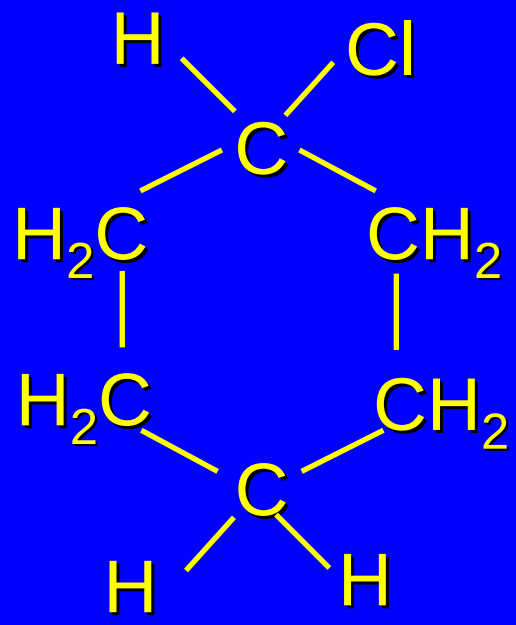
$CH_3CH_2CH_2CH_3$ is shown as 

$CH_3CH_2CH_2CH_2OH$ is shown as 

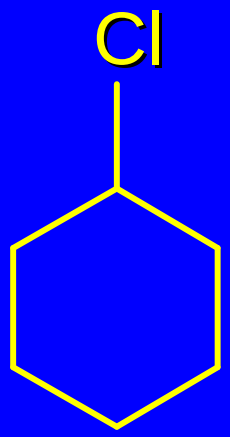
Omit atom symbols. Represent structure by showing bonds between carbons and atoms other than hydrogen.

Atoms other than carbon and hydrogen are called *heteroatoms*.

Bond-line formulas



is shown as



Omit atom symbols. Represent structure by showing bonds between carbons and atoms other than hydrogen.

Atoms other than carbon and hydrogen are called *heteroatoms*.

1.8
Resonance

Resonance

two or more Lewis structures may be written for certain compounds (or ions)

Recall from Table 1.6

Table 1.6 Introduction to the Rules of Resonance

Step 1:

The connectivity must be the same in all resonance structures

Example:

The Lewis formulas below are **not** resonance forms of the same compound.

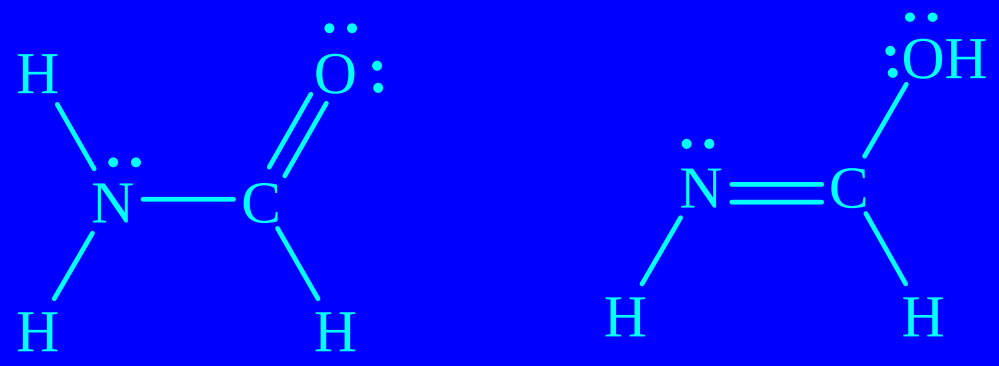


Table 1.6 Introduction to the Rules of Resonance

Step 2:

Each contributing structure must have the same number of electrons and same net charge.

Example:

All structures have 18 electrons and a net charge of 0.

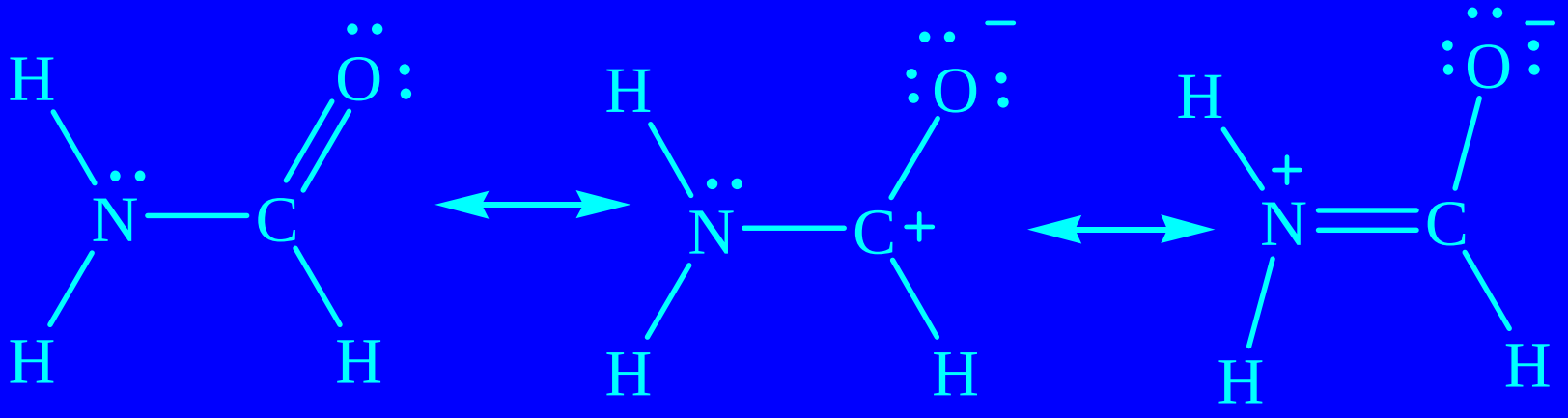


Table 1.6 Introduction to the Rules of Resonance

Step 3:

Calculate formal charges on the first structure.

Example:

None of the atoms possess a formal charge in this Lewis structure.

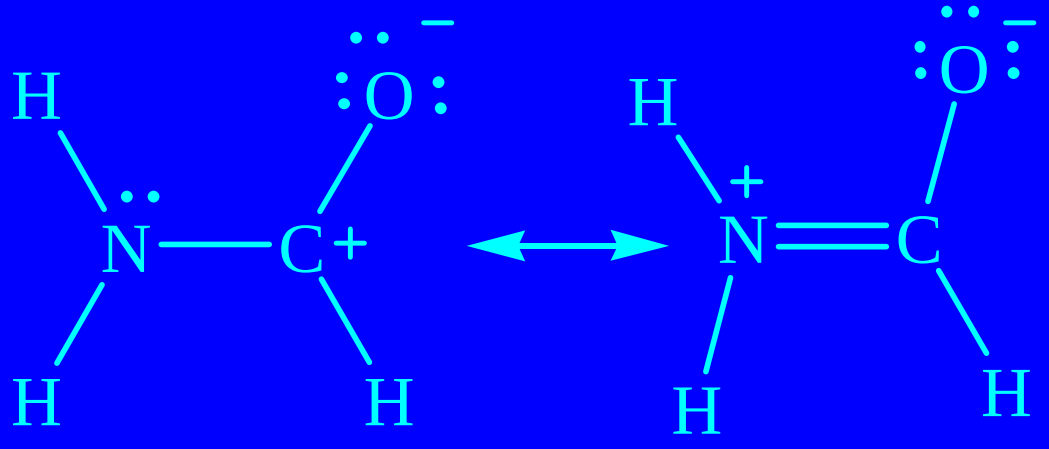
Table 1.6 Introduction to the Rules of Resonance

Step 4:

Calculate formal charges on the second and third structures.

Example:

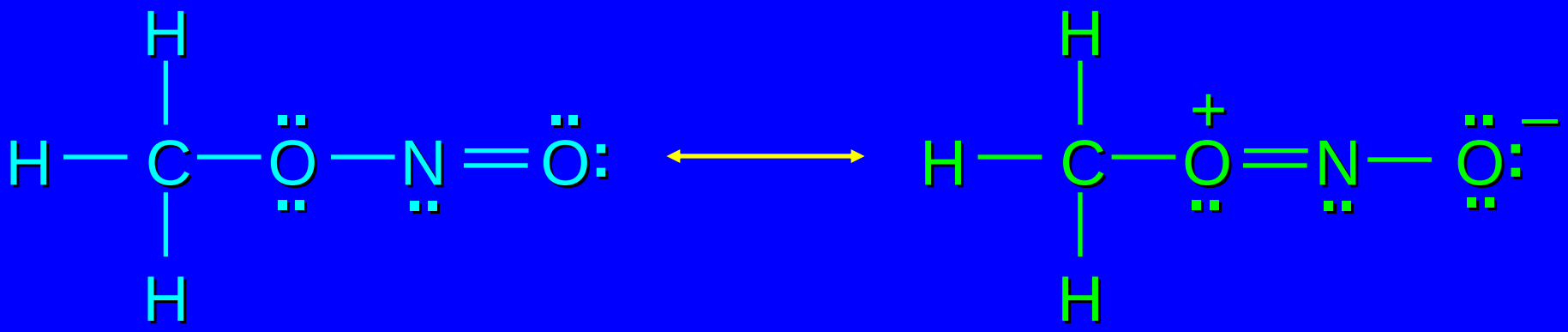
These structures have formal charges; these are less stable Lewis structures.



Resonance Structures of Methyl Nitrite

same atomic positions

differ in electron positions



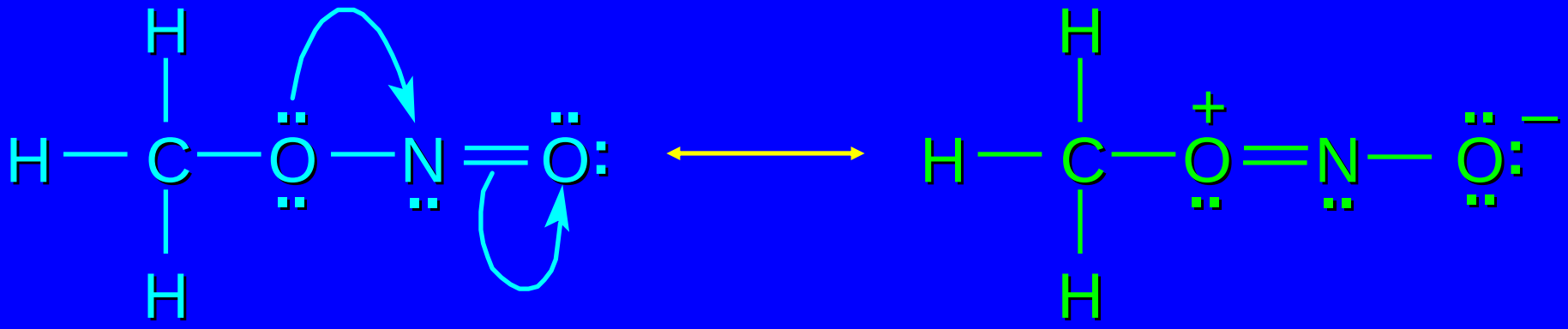
more stable Lewis structure

less stable Lewis structure

Resonance Structures of Methyl Nitrite

same atomic positions

differ in electron positions



more stable Lewis structure

less stable Lewis structure

Why Write Resonance Structures?

Electrons in molecules are often delocalized between two or more atoms.

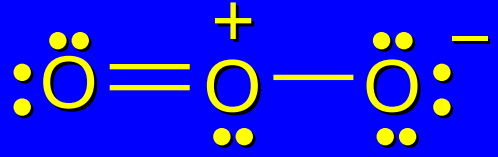
Electrons in a single Lewis structure are assigned to specific atoms-a single Lewis structure is insufficient to show electron delocalization.

Composite of resonance forms more accurately depicts electron distribution.

Example

Ozone (O_3)

Lewis structure of ozone shows one double bond and one single bond



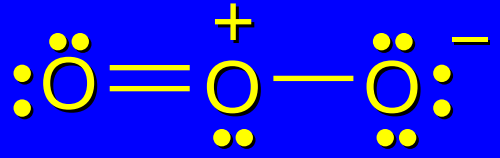
Expect: one short bond and one long bond

Reality: bonds are of equal length (128 pm)

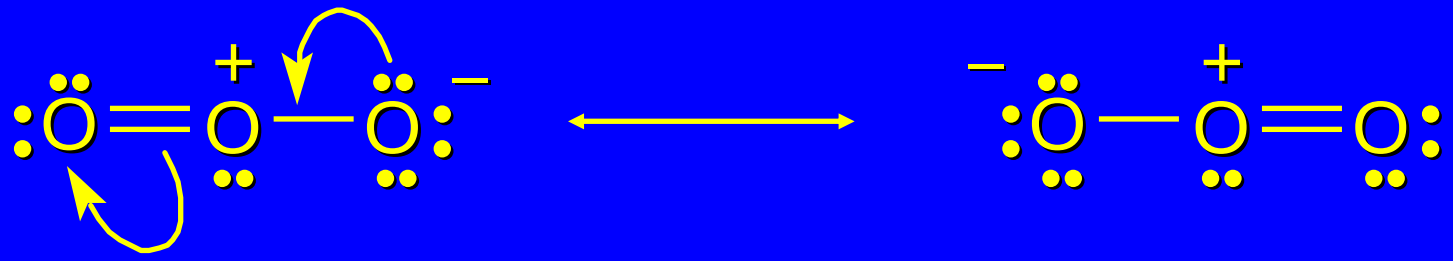
Example

Ozone (O_3)

Lewis structure of ozone shows one double bond and one single bond



Resonance:



Example

Ozone (O_3)

Electrostatic potential map shows both end carbons are equivalent with respect to negative charge. Middle carbon is positive.