CHEM110 – Chapter 5
Chemical Bonding and Molecular Structure

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Introduction / Learning OBJECTIVES

- Atoms bond together to form molecules using their electrons
- How are electrons shared between atoms ?
- Can we predict geometry of molecules or their reactivity ?

- Different theories will be explored to answer these questions

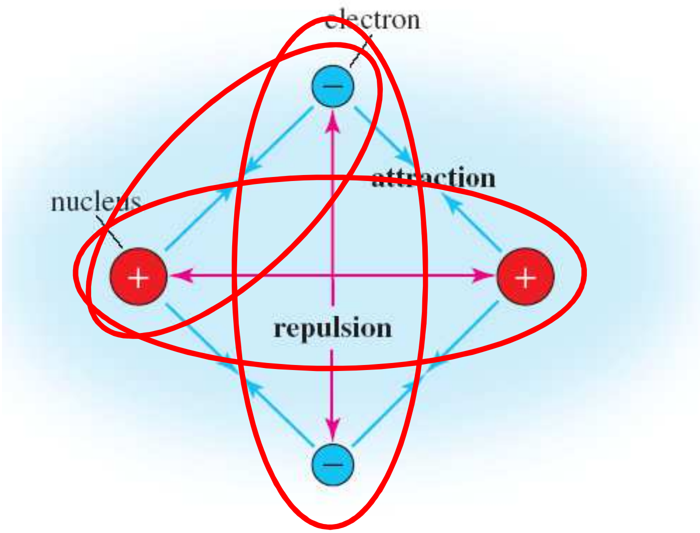
5.1 Fundamentals of Bonding

There are three types of interactions within a molecule:

– Electrons and nuclei attract one another

– Electrons repel each other

– Nuclei repel each other



The hydrogen molecule H_2

5.1 Fundamentals of Bonding

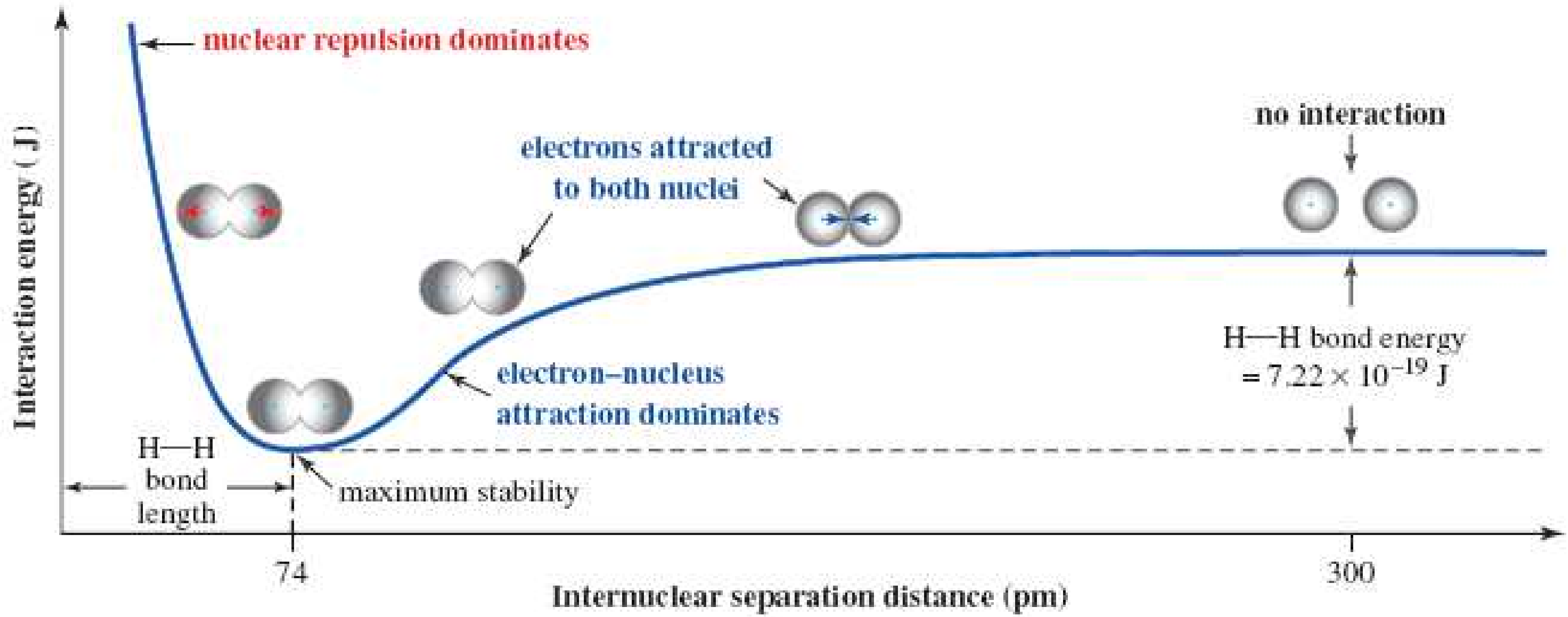
- The molecule is most stable when the attractive and repulsive forces are balanced
- This occurs when the electron density is situated between the nuclei of bonded atoms
- This shared electron density is called a **covalent bond**

5.1 Fundamentals of Bonding

- **Bond length** - distance at which the molecule has the maximum energetic advantage over individual atoms

5.1 Fundamentals of Bonding

H_2 : Bond length and bond energy



5.1 Fundamentals of Bonding

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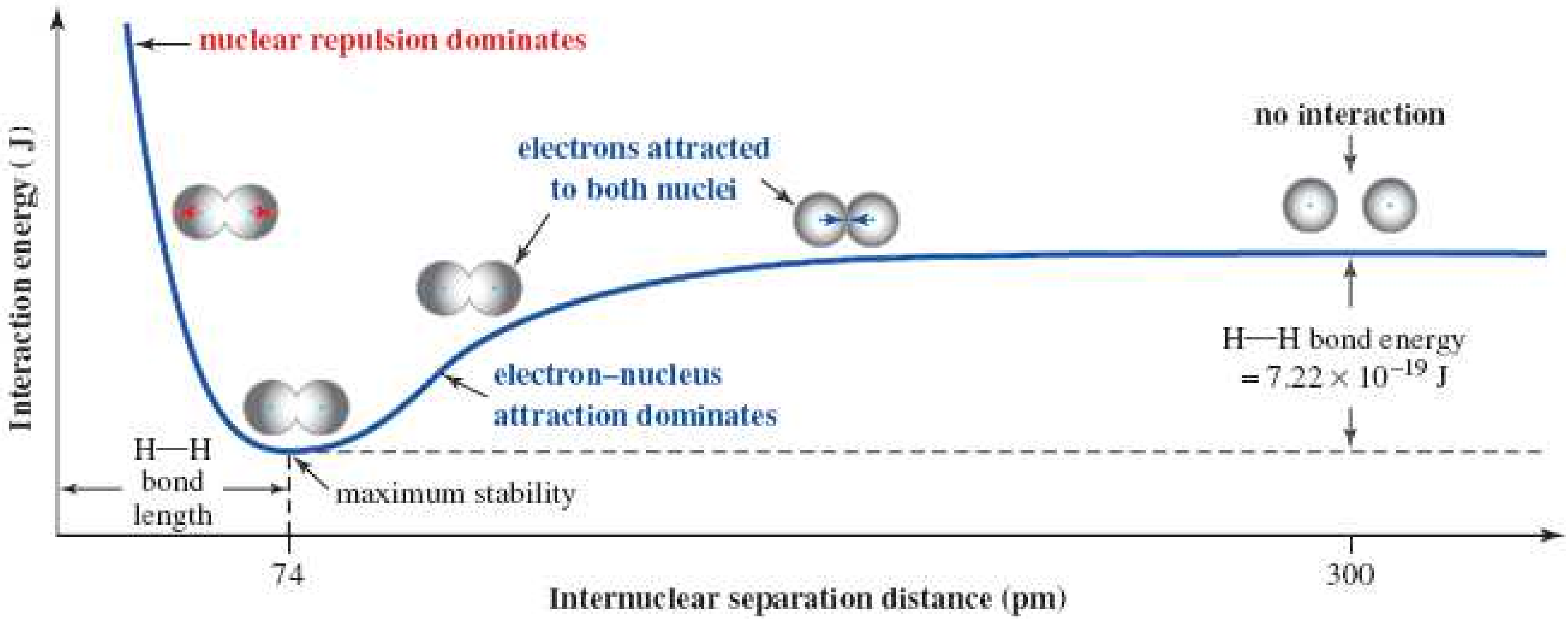
- **Bond length** - distance at which the molecule has the maximum energetic advantage over individual atoms

- **Bond energy** - energy required to break the bond, it is always positive (kJ mol^{-1})

5.1 Fundamentals of Bonding

H_2 : Bond length and bond energy



5.1 Fundamentals of Bonding

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- **Bond length** - distance at which the molecule has the maximum energetic advantage over individual atoms

- **Bond energy** - energy required to break the bond, it is always positive (kJ mol^{-1})

- Each different chemical bond has a characteristic bond length and energy

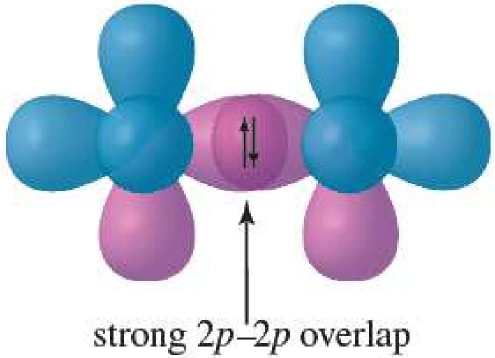
5.1 Fundamentals of Bonding

- The most probable position of the electrons is between the nuclei

- This symmetrical bond is called a **sigma** (**σ**) **bond**

5.1 Fundamentals of Bonding

Other diatomic molecules : e.g. F_2



- Even when the atoms within a molecule contain many electrons, bond formation is still considered as the sharing of only two electrons
- The resulting bond is also a **sigma bond**

5.1 Fundamentals of Bonding

Unequal electron sharing

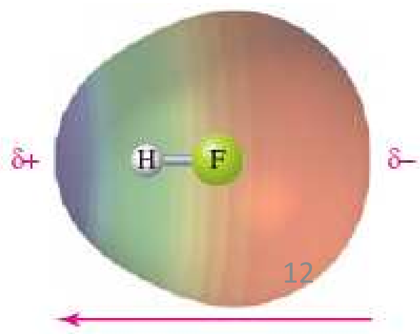
- Two identical atoms: e.g. H_2, F_2

  the nuclei share the bonding electrons equally

- Two different atoms: e.g. HF

  unequal attractive forces lead to an unsymmetrical distribution of the bonding electrons

- This results in a **polar covalent bond**



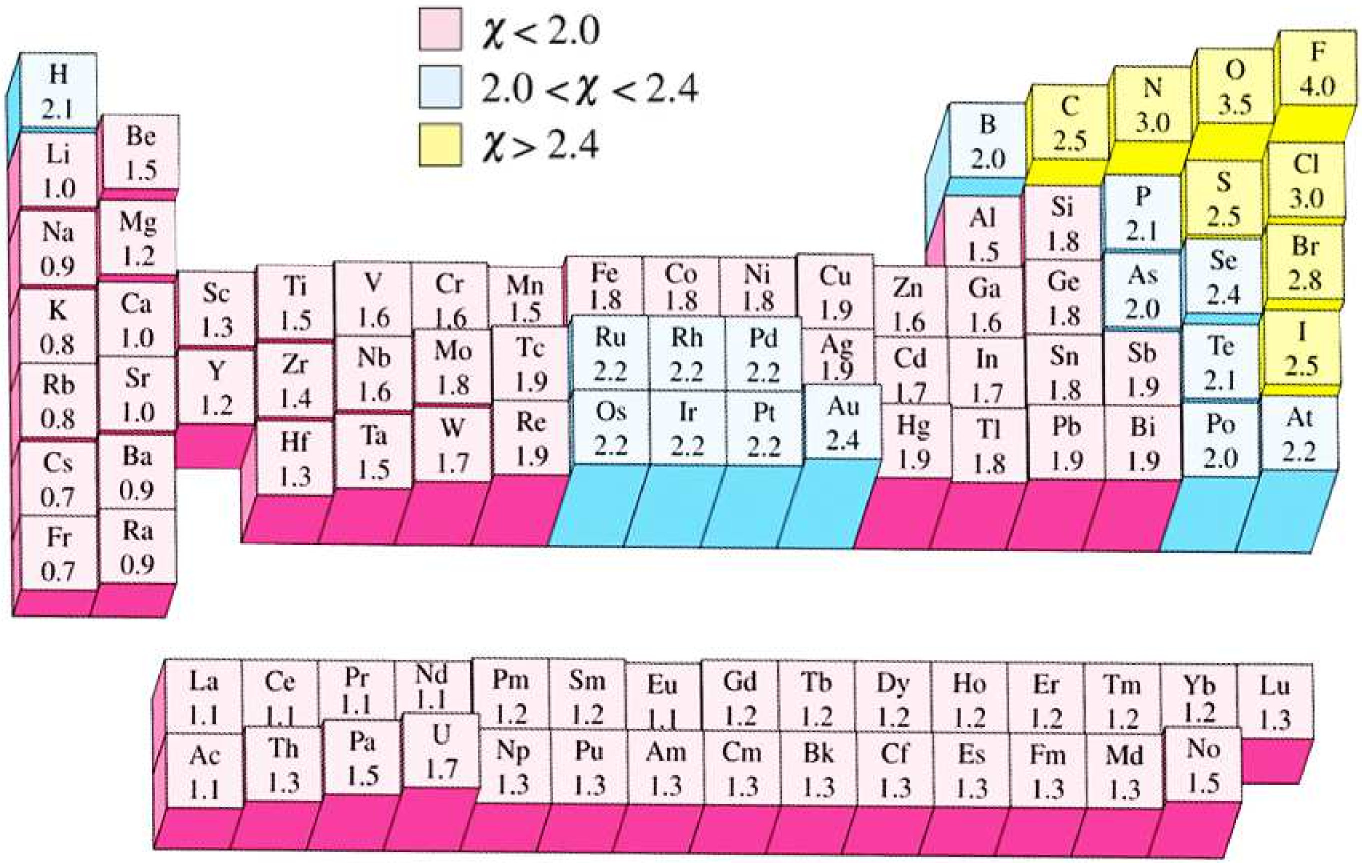
5.1 Fundamentals of Bonding

Unequal electron sharing

Electronegativity gives a numerical value of how strongly an atom attracts the electrons in a chemical bond

5.1 Fundamentals of Bonding

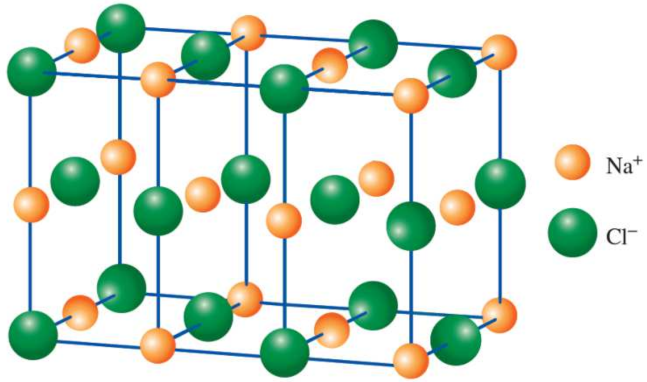
- Electronegativity (χ)is the ability of an element to attract electrons to itself



χ = 'chi'

5.2 Ionic Bonding

- Compounds formed between elements of very different electronegativities are ionic. e.g. NaCl



- Most ionic compounds are solids with high melting points
- They are held together by the attractive forces between oppositely charged ions

5.3 Lewis Structures

The conventions

- An atom is represented by its elemental symbol
- Only the valence electrons are shown
- A line represents one pair of electrons that is shared between two atoms (double bond : 2 lines, triple bond : 3 lines…)
- Dots represent the non-bonding electrons on that atom (non-bonding pairs are called lone pairs)

5.3 Lewis Structures

Building Lewis structures

1. Count the valence electrons
2. Assemble the bonding framework using single bonds
3. Place three nonbonding pairs of electrons on each outer atom except H
4. Assign the remaining valence electrons to inner atoms
5. Minimise formal charges on all atoms

5.3 Lewis Structures

Example from textbook: SO_2

1. Count the valence electrons =

atomic number — 1

chemical symbol — H

atomic mass — 1.008

metals | nonmetals | metalloids

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (97.91)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	57–71 *	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209.0)	85 At (210.0)	86 Rn (222.0)
7	87 Fr (223)	88 Ra (226)	89–103 **	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (271)	111 Rg (272)	112 Uub (285)	113 Uut (284)	114 Uuq (289)	115 Uup (288)	116 Uuh (292)		118 Uuo (294)

*lanthanide series	57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
**actinide series	89 Ac (227)	90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

5.3 Lewis Structures

Example from textbook: SO_2

1. Count the valence electrons

   $O = 2s^2 2p^4 = 6 \times 2 = 12$

   $S = 3s^2 3p^4 = 6$

   Total = 18 e^-

5.3 Lewis Structures

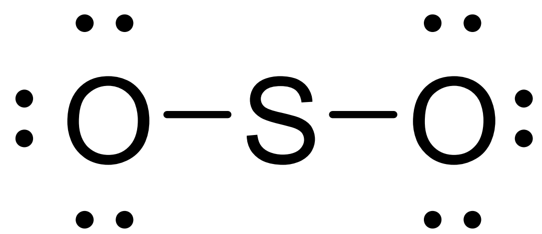
2. Assemble the bonding framework using single bonds

O–S–O

4 e^- Used

5.3 Lewis Structures

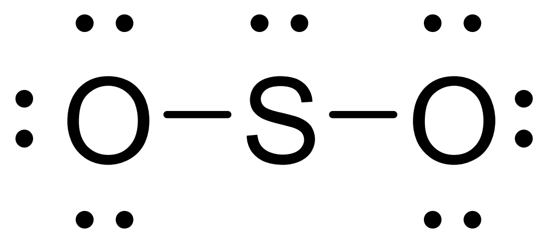
3. Place three nonbonding pairs of electrons on each outer atom except H



16 e^- Used

5.3 Lewis Structures

4. Assign the remaining valence electrons to inner atoms



18 e^- Used

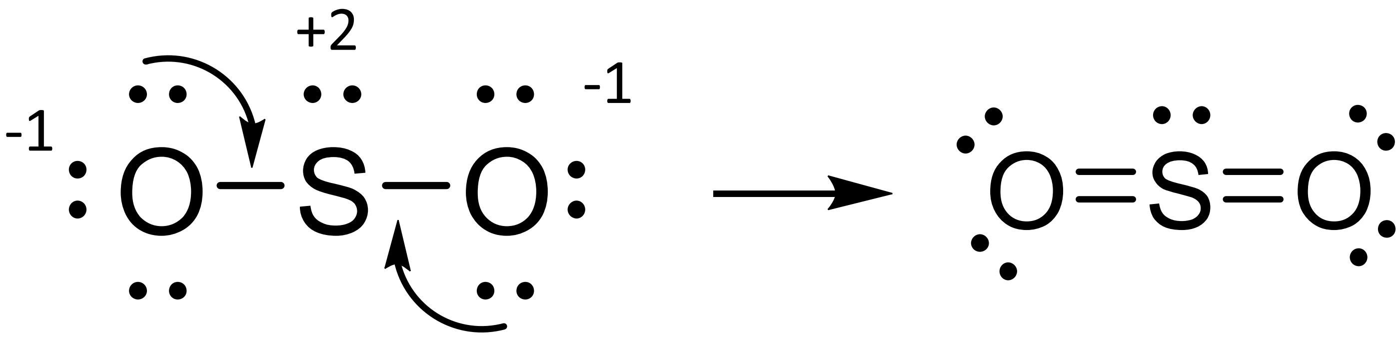
5.3 Lewis Structures

5. Minimise formal charges on all atoms

Formal charge = (valence e^- of free atom) - (lone pair e^-) - $\frac{1}{2}$ (shared e^-)

$$O = 6 - 6 - \frac{1}{2}(2) = -1$$

$$S = 6 - 2 - \frac{1}{2}(4) = +2$$



5.3 Lewis Structures

Worked Example 5.1:

Chlorine Trifluoride, ClF_3, is used to recover uranium from nuclear fuel rods in a high-temperature reaction that produces gaseous uranium hexafluoride

$$2ClF_3\,(g) + U\,(s) \longrightarrow UF_6\,(g) + Cl_2\,(g)$$

Determine the Lewis structure of ClF_3

atomic number — 1
chemical symbol — H
atomic mass — 1.008

metals | nonmetals | metalloids

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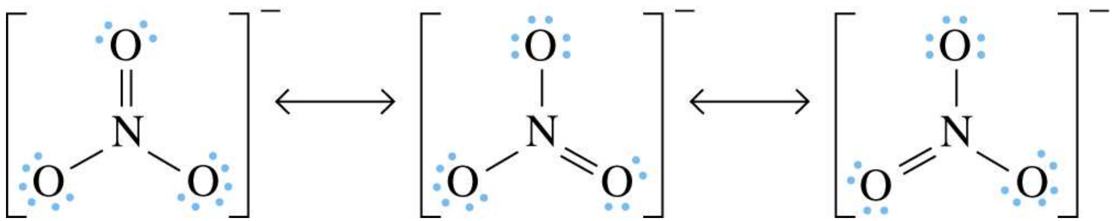
5.3 Lewis Structures

Resonance structures

- Composites of **equivalent** Lewis structures
- Resonance structures differ only in the position of the electrons, not atoms



5.3 Lewis Structures

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Worked Example 5.2:

Determine the possible resonance structures of the phosphate anion, PO_4^{3-}.

5.3 Lewis Structures

Worked Example 5.3:

Determine the possible resonance structures of dinitrogen oxide, N_2O, a gas used as an anesthetic, a foaming agent and a propellant.