



## Molecular Literacy for All

### making sense of the "monstrous and boundless thicket" of everyday chemistry

Every breath I take...the molecules in the air we breathe are used to teach a model for atomic bonding.

**ILLINOIS** Beckman Institute for Advanced Science & Technology

Jeff Moore (email: jsmoore@Illinois.edu)

## Today's Outline

### Connecting Atoms to Make Molecules

- The Octet Rule
- Covalency and electron pairs
- Exceeding the shell capacity is Not Allowed
- Valency of the Atoms (Carbon vs. Oxygen)
- Multiple Bonds Between Atom Pairs
- Electron Pair Domains

### Oxygen and the Energy that Fuels You

- Photosynthesis and respiration
- Tracking electrons in life's chemical symbiosis

#### **Bonding Patterns**

### Charge of the Whole Molecule

# Satisfying an atom's electron count

- The *electron count* is the total number electrons in the valence shell of an atom
- Atoms gain or lose electrons to achieve the valence electron count of its nearest noble gas
- Nearest noble gas for H, He, Li, Be  $\Rightarrow$  2 valence electrons
- Nearest noble gas for B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, Se, ⇒ 8 valence electrons
- Indicate the charge on each atom that gives it a filled shell
- Show the valence electrons as dots





Molecular dihydrogen: the most common molecule in the universe

Covalency: The prefix *co*- means *jointly, associated in action, partnered to a lesser degree,* etc.; thus a "co-valent bond", in essence, means that the atoms share "<u>valence</u>"



### The Universe's First Molecule

The molecule arose because hydrogen and helium were the two chief elements to emerge from the big bang. At the beginning, the universe was so hot that any electrons either element managed to capture would immediately be stripped away by high-energy radiation generated by the extreme heat. But as space expanded, it cooled, and about 100,000 years after the big bang, each helium nucleus grabbed two electrons and became neutral. Put H<sup>+</sup> and He together and you have the universe's first molecule, HeH<sup>+</sup>.



#### Space molecules

Methane teaches how heavier atoms acquire filled shells through covalent bonding

An electron count of eight fills the valence shell for B, C, N, O, F, and Ne (these are atoms of elements that reside in the second row of the periodic table).



By pooling valence electrons, then dividing the pool into pairs, then properly distributing them between the valence subshells, four hydrogen atoms and one carbon atom combine to make one  $CH_4$  (i.e., a methane molecule).

6

## Methane is a greenhouse gas in our everyday life

## Chicago: Snapshot of natural gas leaks under city streets

Leaked natural gas — mostly methane — is a powerful contributor to climate change.

### Explore Chicago map data



#### Findings

Our readings indicated an average of leak for every three miles we drove.

Readings are from September throug 2014 and may not reflect current leak repairs or other changes.

If you ever smell gas, or have any reason to suspect a say to immediately exit the building or area, then call the more see the Peoples Gas safety page.

### Hydrogen is a truncator atom

- A single covalent bond involves two electrons i.e., it's one electron pair.
- Hydrogen completes its valence shell with just two electrons.
- Therefore, hydrogen is bonded to, at most, one-and-only-one other atom.
- Because hydrogen is bonded to just one atom, it serves as a truncator to block the sites on carbon that could otherwise go on and bond to other carbon atoms.
- This will become important when we talk about implicit hydrogen atoms; i.e., it is implied that the "unsubstituted sites" in molecular drawings are capped by hydrogen atoms, even if they are not explicitly shown.

## Water (H<sub>2</sub>O)

(did you ever wonder why water is  $H_2O$  and not something else, like  $H_6O$ ?)







## Water – an essential nutrient – teaches the concept of the electron lone pair



# Electrons are usually paired

Valence-shell electron pairs come in two types: nonbonding and bonding. Nonbonding electrons, also called lone pairs or unshared pairs, are valence-shell electron pairs that are localized on only one atom. Bonding electrons are pairs of valence-shell electrons that are shared between two atoms.

# Exceeding valence shell capacity (Why water is $H_2O$ and not something else (e.g., $H_6O$ ))



# Molecular dioxygen teaches us about open shells, closed shells, and double bonds





### Every breath you take: dioxygen provides the chemical energy that fuels you

The chemical energy utilized by most complex multicellular organisms is not predominantly stored in glucose or fat, but rather in  $O_2$  with its relatively weak double bond. Methane (i.e., in combustion) or fatty acids (i.e., in cellular respiration) are "energyrich fuels" compared to, say, carbohydrates only because they unlock the energy of more  $O_2$  molecules than other "fuels". And so,  $O_2$ , rather than glucose, NAD(P)H, or ATP, is the molecule that provides the most energy to animals and plants.

Oxygen (not proteins, carbohydrates, or fats) is the high-energy molecule that powers life.

### Oxygen—A Critical, but Overlooke Nutrient

Paul Trayhurn 1,2\*

14

## The Jekyll and Hyde of dioxygen

*Science* 07 May 1954: Vol. 119, Issue 3097, pp. 623-626 DOI: 10.1126/science.119.3097.623

#### Oxygen Poisoning and X-irradiation: A Mechanism in Common<sup>1</sup>

Rebeca Gerschman, Daniel L. Gilbert, Sylvanus W. Nye, Peter Dwyer, and Wallace O. Fenn<sup>2</sup>

Department of Physiology and Vital Economics, The University of Rochester School of Medicine and Dentistry, Rochester, New York

CONSIDERATION of various isolated reports in the literature has led us to the hypothesis that oxygen poisoning and radiation injury have at least one common basis of action, possibly through the formation of oxidizing free radicals. This article reviews the pertinent material that led to this hypothesis and also presents the supporting evidence obtained from (i) experiments on the protective action against oxygen poisoning by substances of varied chemical nature known to increase resistance to irradiation, and (ii) experiments on the survival in oxygen of mice irradiated and exposed to high oxygen tensions simultaneously or at different intervals.

Concerning free-radical formation, it is generally believed that the chemical actions of ionizing radiation on aqueous solutions are mainly indirect (1), involving the primary formation of the free radicals  $H^{\bullet}$  and  $OH^{\bullet}$ with subsequent formation of  $H_2O_2$ , atomic oxygen, and  $HO_4^{\bullet}$  (2). In the presence of oxygen, increased amounts of the powerful and quantitatively important  $OH^{\bullet}$ , as well as the less reactive but more persistent  $HO_2^{\bullet}$ , would be expected.

as such or bound with enzymes in normal metab reactions. As one of the reactants, it might be expethat increased concentrations of oxygen would incrthe formation of oxidizing free radicals.

Indication of certain similarities between oxy poisoning and x-irradiation results from the study the many reports in the literature dealing with t effects. On the basis that increased metabolism mi result in an increased production of free radicals, vice versa, it is not surprising that variations in c gen toxicity with metabolic activity have been no Thus, in oxygen poisoning, it has been observed i a decreased metabolism has a protective effect and increased metabolism has a detrimental effect (11, Several reports indicate that the same may be i for x-irradiation, but this matter has not been o clusively clarified (13-15).

The *in vitro* inactivation of some thiol enzymes been demonstrated in oxygen poisoning (16, 17), in irradiation (6, 18). On the other hand, a measur*in vivo* decrease of SH groups right after irradia: (14) has not been observed. However, one must necessarily rule out the possibility that the inactiva





### Life's chemical symbiosis



## Dinitrogen and the triple bond



The dinitrogen molecule

## Nitrogen fixation



## Molecular difluorine



### Pattern seekers

Given our results, deduce the patterns for bonding across the periodic table. Use this observation to write a hypothesis about dicarbon. Write your hypothesis as a factual statement. Name your hypothesis. Now test your hypothesis.



### Diatomic carbon breaks the pattern

(quadruple bonding is not possible with 2<sup>nd</sup> row elements)



# Room-temperature chemical synthesis of C<sub>2</sub> and role in nanocarbon formation

Nature Communications volume 11, Article number: 2134 (2020)





Electron Pair Domain	Number of Bonding Pairs	Representation	Total Electron Count
nonbonding domain	0	Ä	2
single bond domain	1	A-A	2
double bond domain	2	A=A	4
triple bond domain	3	A≡A	6

### Electron pair domains (EPDs)

Regions around an atom having a high density of valence-shell electrons are called electron pair domains. An **electron-pair domain** consists of either a nonbonding pair of electrons, a single pair of bonding electrons, two pairs of bonding electrons, or three pairs of bonding electrons. A single pair of bonding electrons is known as a single bond; two or more pairs of bonding electrons are called multiple bonds.

# Charge of the whole molecule

Molecules are neutral, cationic, or anionic according to their overall state of charge. Here's a look at how molecular charge is calculated for ammonia.

