CHEMICAL BONDING: LEARNING FROM SIMPLE MODELS

Presented by: Jerry Bell and Bonnie Bloom

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Chemical Bonding: Simple Models

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Lewis Structures

Jerry Bell, ACS (retired)
Bonnie Bloom, Hilliard Davidson HS, OH
Chemical Bonding: Simple Models

Examine the Lewis structure of water, $\text{H}_2\text{O}$, as a reminder of what makes up a Lewis structure.

$$\text{H} : \text{O} : \text{H}$$
Chemical Bonding: Simple Models

Examine the Lewis structure of water, H₂O, as a reminder of what makes up a Lewis structure.

\[
\begin{align*}
&\text{H : O : H} \\
\end{align*}
\]

What does the red-labeled part of this Lewis structure represent?

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&\text{H : O : H} \\
\end{align*}
\]

A: a proton  
B: an electron  
C: a neutron
Chemical Bonding: Simple Models

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This is, of course, why they are often called Lewis electron dot structures (or diagrams).
Chemical Bonding: Simple Models

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B: a pair of electrons  
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Chemical Bonding: Simple Models

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\text{O} \\
\text{H}
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Electron pairing has a special meaning. Paired electrons have opposite spins that we often represent by up- and down-pointing arrows.

The spins of the electrons are not shown in Lewis structures but have to be understood.
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Another way to represent a bonding pair of electrons is with a bond stroke.

\( \text{H—O—H} \)
Chemical Bonding: Simple Models

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\begin{array}{c}
\text{H} \quad \text{O} \quad \text{H} \\
\quad \bullet \\
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\]

Bond strokes remind us that bonding electron pairs hold the molecule together and, in the Lewis structure, readily show which atom centers are connected together.
Chemical Bonding: Simple Models

What is the total number of electrons in an H₂O molecule?

A: 6  
B: 8  
C: 10
Chemical Bonding: Simple Models

What is the total number of electrons in an H\textsubscript{2}O molecule?

A: 6  
B: 8  
C: 10

How many electrons are explicitly represented in the Lewis structure of H\textsubscript{2}O?

\[ \text{H} - \text{O} - \text{H} \]

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\text{H} \\
\text{O} \\
\text{H}
\end{array}
\]

A:  6  
B:  8  
C:  10

Where are the others? Do you have other questions before we consider this one?
Chemical Bonding: Simple Models

Questions?
Chemical Bonding: Simple Models

Electrons in Molecules
Chemical Bonding: Simple Models

What does the red-labeled part of this Lewis structure represent?

\[ \text{H} - \text{O} - \text{H} \]

A: an oxygen atom
B: an oxygen atom nucleus
C: an oxygen atom core
Chemical Bonding: Simple Models

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The oxygen atom core is the oxygen atom nucleus plus the non-valence electrons, that is, the electrons in inner shells.
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Chemical Bonding: Simple Models

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H—O—H

A: a hydrogen atom
B: a hydrogen atom nucleus
C: a hydrogen atom core
D: a proton

A hydrogen atom nucleus, a hydrogen atom core, and a proton are all the same thing. The hydrogen atom has a single valence electron (no core electrons), so the core is the nucleus, which is a proton.
Lewis structures are great for showing the connectivity of atomic cores in molecules. They also show which atomic cores have non-bonding electron pairs--sites of chemical reactivity and polarity in the molecule.
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Chemical Bonding: Simple Models

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To further understand reactivity and polarity, as well as the geometry of molecules, we need to have a model of the electrons in molecules. The model should also help us understand what holds molecules together.

For almost a century (since de Broglie’s work), we have known that electrons have wave properties that have to be accounted for in models of matter at the atomic and molecular level.
Chemical Bonding: Simple Models

The simplest possible three dimensional wave is a spherical wave. Think of a spherical gong that is struck and vibrates with a sort of in-and-out “breathing” motion. The wave motion of the sphere (gong) can be described in terms of the radius of the sphere and the location of its center.
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For our simple model of chemical bonding, we will assume that any pair of electrons (spin-paired) can be represented as a spherical wave that excludes all other electron waves. The exclusion is due to the Pauli exclusion principle that does not permit electrons of the same spin to occupy the same space.
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As a physical representation of these electron waves we will use balloons (assumed to be spherical) that we can manipulate to see how electron wave pairs would interact when attracted to positive atomic core centers. Let’s see what questions you might have.
Chemical Bonding: Simple Models

Questions?
Chemical Bonding: Simple Models

Spherical Packing
Chemical Bonding: Simple Models

Consider two spherical objects pulled together at a point, like two balloons whose stems are twisted together.
Chemical Bonding: Simple Models

Consider two spherical objects pulled together at a point, like two balloons whose stems are twisted together. What is the geometry of the three points defined by the center of each balloon and their mutual contact?

A: linear
B: bent
C: other
Chemical Bonding: Simple Models

Consider two spherical objects pulled together at a point, like two balloons whose stems are twisted together. What is the geometry of the three points defined by the center of each balloon and their mutual contact?

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The three points lie on a line. Is it mathematically required that the three points must lie on a line?
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A: linear  
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C: other

The three points lie on a line. Is it mathematically required that the three points must lie on a line?

NO. Two points define a line, but a third point can be anywhere else in space. The linearity in this model is required by the physics.
Chemical Bonding: Simple Models

Consider three spherical objects pulled together at a point, like three balloons whose stems are twisted together.
Chemical Bonding: Simple Models

Consider three spherical objects pulled together at a point, like three balloons whose stems are twisted together. What is the geometry of the four points defined by the center of each balloon and their mutual contact?

A: planar
B: triangular planar
C: pyramidal
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A: planar
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The four points lie on a plane. Planarity must be part of the description. Geometry on the plane is necessary as well. Trigonal planar is also OK. Is it mathematically required that the four points must lie on a plane?
Consider three spherical objects pulled together at a point, like three balloons whose stems are twisted together. What is the geometry of the four points defined by the center of each balloon and their mutual contact?

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The four points lie on a plane. **Planarity** must be part of the description. Geometry on the plane is necessary as well. Trigonal planar is also OK. Is it mathematically required that the four points must lie on a plane?

**NO.** Three points define a plane, but a fourth point can be anywhere else in space. The **planarity in this model is required by the physics.**
Chemical Bonding: Simple Models

Consider four spherical objects pulled together at a point, like four balloons whose stems are twisted together. What is the geometry of the five points defined by the center of each balloon and their mutual contact?

A: triangular pyramidal  
B: tetrahedral  
C: square planar
Chemical Bonding: Simple Models

Consider four spherical objects pulled together at a point, like four balloons whose stems are twisted together. What is the geometry of the five points defined by the center of each balloon and their mutual contact?

A: triangular pyramidal
B: tetrahedral
C: square planar

The four balloon points define a triangular pyramid. The geometry of these points about the central point is usually called tetrahedral. Is it mathematically required that the five points must take up a tetrahedral arrangement?
Chemical Bonding: Simple Models

Is it mathematically required that the five points must take up a tetrahedral arrangement?

NO. A square planar arrangement of the five points is also possible. Physics determines the more stable tetrahedral arrangement.
Chemical Bonding: Simple Models

Questions?
Chemical Bonding: Simple Models

Spherical Electron Waves in Molecules
Chemical Bonding: Simple Models

The Lewis structure for water has two non-bonding electron pairs and two bonding electron pairs surrounding the oxygen atomic core, $\text{O}^{6+}$.
The Lewis structure for water has two non-bonding electron pairs and two bonding electron pairs surrounding the oxygen atomic core, O\(^{6+}\).

The spherical electron wave model for this molecule is shown in this balloon model. Each balloon represents a pair of electrons, -2 charge. The two yellow balloons each contain a proton, H\(^+\); their net charge is -1.
The Lewis structure for water has two non-bonding electron pairs and two bonding electron pairs surrounding the oxygen atomic core, \( \text{O}^{6+} \).

The spherical electron wave model for this molecule is shown in this balloon model. Each balloon represents a pair of electrons, -2 charge. The two yellow balloons each contain a proton, \( \text{H}^+ \); their net charge is -1.

All four spherical electron pairs are attracted to the +6 oxygen atomic core, which is what holds the molecule together in this tetrahedral geometry.

The net charge on the four electron pairs is \((-2) + (-2) + (-1) + (-1) = -6\), balancing the \( \text{O}^{6+} \) charge to give an overall neutral molecule.
Although the molecule is overall electrically neutral, the charge is not distributed uniformly around the oxygen atomic core.
Chemical Bonding: Simple Models

Although the molecule is overall electrically neutral, the charge is not distributed uniformly around the oxygen atomic core. The geometry of the atomic cores shown here is the familiar bent structure of water due to the tetrahedral packing of the spherical electron waves.
Chemical Bonding: Simple Models

Although the molecule is overall electrically neutral, the charge is not distributed uniformly around the oxygen atomic core.

The geometry of the atomic cores shown here is the familiar bent structure of water due to the tetrahedral packing of the spherical electron waves.

One side of the molecule (the top here) has more net negative charge than the other side, so the molecule is polar.

The polarity and geometry of water molecules have profound effects on the properties of water that we will explore in the next NSTA-ACS web seminar.
Chemical Bonding: Simple Models

A Lewis structure for ammonia is $\text{H} - \text{N} - \text{H}$.
A Lewis structure for ammonia is \( \text{H} \text{N} \text{H} \).

The Lewis structure shows that there are four electron pairs surrounding the nitrogen atom core. A representation of the spherical electron wave model of ammonia is shown here. What is the geometric arrangement of the electron wave pairs?

A: trigonal planar
B: trigonal pyramidal
C: tetrahedral
D: square planar
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The inclusion of the atomic cores may be confusing. We have to distinguish between the geometry of the spherical electron wave pairs and the geometry of the atomic cores.
Chemical Bonding: Simple Models

What is the geometric arrangement of the atomic cores?

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The water and ammonia examples demonstrate that the geometries of the spherical electron waves and the atomic cores are related, but, in general not the same.
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The water and ammonia examples demonstrate that the geometries of the spherical electron waves and the atomic cores are related, but, in general not the same.
The experimentally observable geometry of the cores is usually referred to as the shape or structure of the molecule.
The geometry of the electron wave distribution is not readily observable, but is responsible for the geometry of the cores.
Chemical Bonding: Simple Models

A Lewis structure for methane is

\[
\begin{array}{c}
  \text{H} \\
  \text{H} \\
  \text{H} \\
  \text{H} \\
  \text{C} \\
\end{array}
\]
Chemical Bonding: Simple Models

A Lewis structure for methane is \( \text{H--C--H} \).

The Lewis structure shows that there are four identical bonding electron pairs surrounding the carbon atom core. A representation of the spherical electron wave model of methane is shown here.

This is a relatively rare example where the geometry of the spherical electron wave pairs and the geometry of the atomic cores are the same.
Those of you fortunate enough to be familiar with the Chemical Bond Approach curriculum developed about 50 years ago might recognize the spherical electron wave model presented here as the Kimball “charge cloud” model: J. Chem. Educ., 1959, 36, 233. For an expanded discussion by Kimball, send me an e-mail request with the subject line “Kimball model”.


A similar approach, focusing more quantitatively on the energetics of assemblies of -2 non-bonding electron spheres and -1 hydride spheres (2 electrons and a proton), was developed by Larry Sacks: J. Chem. Educ., 1986, 63, 288, 373, 487; 2000, 77, 445.
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Save the date:
16 November, “Chemical Bonding: Why is Water Different?”
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