The Covalent Bond Between Two Atoms

Learning Targets: At the end of this reading, I will be able to:

1. Define:
   a. covalent bond
   b. molecule
   c. Lewis structure
   d. bond dissociation energy
   f. endothermic
   g. exothermic

2. Relate the strength of covalent bonds to bond length and bond dissociation energy.

Open the http://phet.colorado.edu/

Click the "Play with Sims".

Click the "Chemistry" link on the left hand side of the page, then "General Chemistry".

Click the "Atomic Interactions" simulation. Press "Download" hard disk or "Run" for on-line interaction.

The Hydrogen Molecule, H_2

1. Toggle "Adjustable Interaction". Shift "Atom Diameter (σ)" to **Small**, and "Interaction Strength (ε)" three-quarters of the distance from the **Weak** setting to the **Strong** setting. Set the "Simulation Speed" to Fast. These settings models two interacting hydrogen atoms.

2. Separate the "moving atom" half way up the potential energy curve. Release and observe the behavior of the moving atom with respect to the "pinned atom". What do you see?

   _____

   _____

3. Move the "moving atom" closer to the "pinned atom". What happens to the potential energy of the H_2 molecule?

   _____

4. From a high potential energy position of the molecule, release the "moving atom". What happens?

   _____

5. Drag the "moving atom" to the right, increasing the distance between the atoms. What happens?

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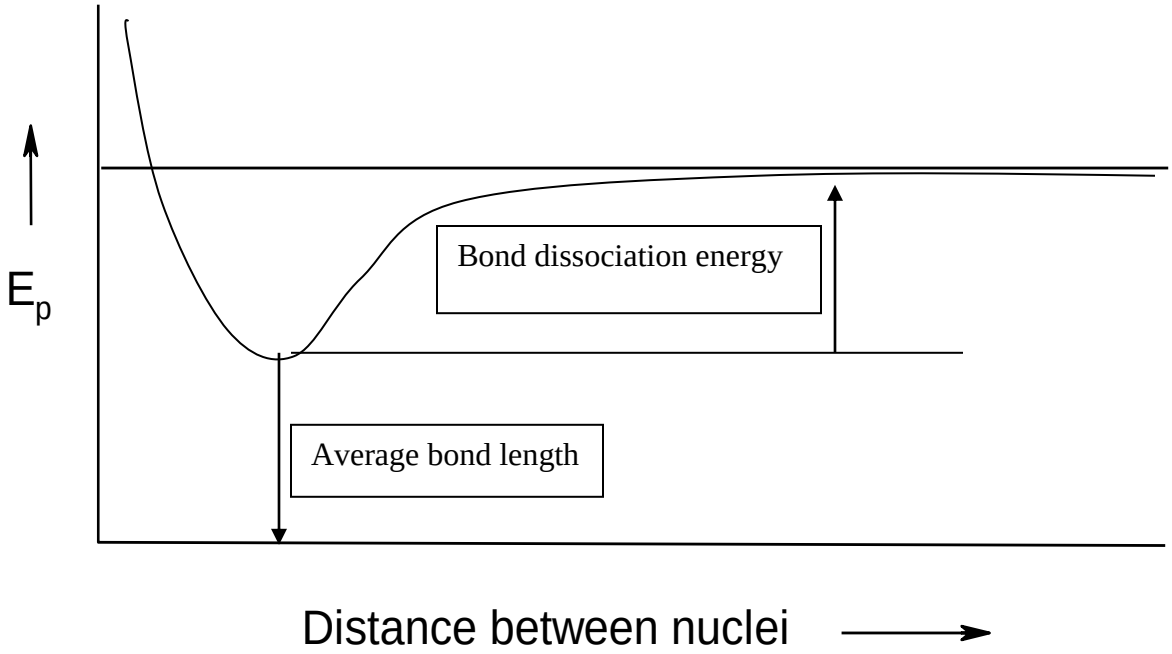
The potential energy profile of two interacting atoms with unpaired electrons is shown in Figure 1, below.

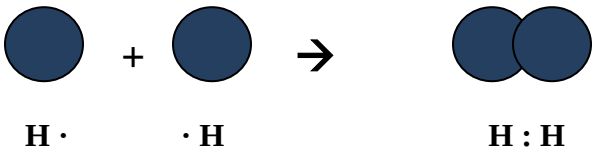
Figure 1. The potential energy profile of two interacting atoms and the formation of a covalent bond.



The potential energy of two hydrogen atoms, each with Lewis structures, **H ·**, lowers as the two atoms begin to approach. **By definition**, the potential energy between two atoms that are separated by an infinite distance**,** ∞**,** is **zero** Joules (0 J). At the close distances of atomic scale, the potential energy drops dramatically until it reaches a minimum. The energy difference between the bottom of the potential energy well and the potential energy when the atoms were separated is called the **bond dissociation energy**.

The minimum in the plot represents the average distance between the two nuclei, or **bond length**. Beyond that point, as the nuclei continue approaching, the coulombic repulsion of the positive nuclear charge become important and the potential energy rises asymptotically to the potential energy axis in the graph.

For the approach of two hydrogen atoms, the lowering of the potential energy is accompanied by the overlap of the outer shell electron clouds.



The sharing of two electrons in the H_2 single bond provides each hydrogen atom with an electronic configuration analogous to the He atom, **He:**.

Problem Set:

1. Many molecular model systems use perforated styrofoam, wooden, or plastic balls to represent atoms and wooden sticks to connect the atom models. The ball and stick model gives the impression of a rigid chemical bond. Based on your observation on the simulation, rather than describing a chemical bond as rigid as a wooden stick, how would you describe the interaction of two atoms in a covalent bond?

2. Based on the behavior of the interacting atoms, how would you define "bond length"?

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3. How would you define "bond dissociation energy"?

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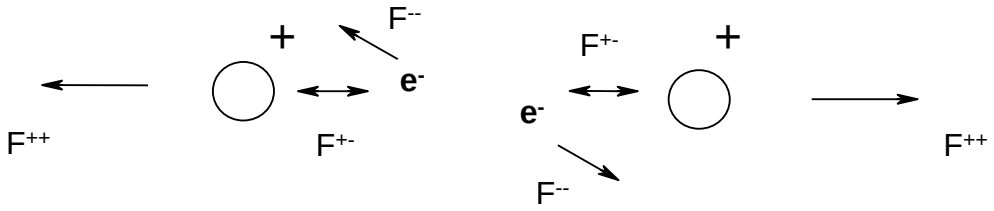
4. The coulombic repulsion between the two nuclei, F^{++}, and the two electrons, F^{--}, is offset by the attractive forces between the protons and the electrons, F+-. This coulombic balancing act is the chemical covalent bond.



Based on your knowledge of Coulomb's Law, why should nature prefer the probability of finding the electrons in the hydrogen molecule in the axis between the two nuclei? Support your answer with the sketch, above.

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Your answers to Problem 1 - 4, above, should have been:

1. Based on your observation on the simulation, rather than describing a chemical bond as rigid as a wooden stick, interacting atoms behave as if attached by a spring, *a harmonic oscillator*.

2. Bond length is the average distance between the interacting atoms when oscillating close to the bottom of the potential energy curve.

3. Bond dissociation energy is the difference in energy of two atoms separated by an infinite distance and the energy of the lowest vibration energy level in the lower portion of the potential energy curve.

4. In the sigma bond, the electrons shield the nuclear positive charges and reduce the repulsion between them.

<u>The He-He interaction: A He_2 molecule?</u>

1. Change the "Interaction Strength (ε)" to **Weak**.

2. Pull the "moving atom" of helium to the right.

3. Record what happens: _____

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4. Push the "moving atom" of helium close to the "pinned atom". Then, release the "moving atom". What do you observe?

5. What do you infer from the shape of the potential energy curve and the behavior of the two interacting helium atoms?

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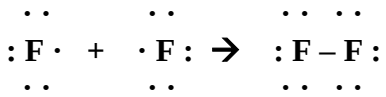
The fluorine molecule, F_2

Elemental fluorine, F_2, forms a single covalent bond. The unpaired electron in atomic fluorine is available to form a chemical bond**.**



- The seven valence electrons each fluorine atom are represented in the Lewis structure of the F_2 molecule. They are arranged so that each fluorine atom has a complete octet.

- Elemental fluorine, F_2, has **one** covalent bond.

1. Set the "Atom Diameter (σ)" halfway between the settings of **Small** and **Large**, and the "Interaction Strength (ε) a quarter of the distance from **Small** to **Large.**

2. How does the depth of the potential energy curve compare with that observed for H_2?

_____

3. Which molecule, H_2 or F_2, has a larger bond energy:

_____

4. Move the "moving atom" of fluorine. What can you infer about the strength of the F_2 covalent bond?

_____

The neon-neon interaction.

1. Toggle the neon-neon "pinned atom/moving atom" combination.

2. What can you infer about the strength of a neon-neon interaction? Do you expect this interaction to be in the order of a strong covalent bond?

_____

3. What happens when you attempt to move the "moving atom" of neon toward the "pinned atom" of neon?

The argon-argon interaction.

1. Toggle the argon-argon "pinned atom/moving atom" combination.

2. What happens when you attempt to move the "moving atom" of argon toward the "pinned atom" of argon?

3. What can you infer about the strength of the argon-argon interaction?

The oxygen molecule, O_2

1. Toggle the oxygen-oxygen "pinned atom/moving atom" combination.

2. Based on the observed potential energy curve, rank the strength of the oxygen-oxygen bond relative to the fluorine-fluorine bond and the hydrogen-hydrogen bond?

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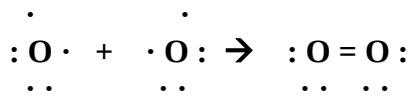
← greatest bond strength

3. The number of covalent bonds in O_2 is two, with a Lewis structure as shown:



The carbon monoxide molecule, CO:

1. Toggle the "Adjustable Attraction" setting.

2. Set the "Atom Diameter (σ)"at **Small** and the "Interaction Strength (ε)" at **Strong. This setting models the carbon-oxygen triple bond in carbon monoxide: one σ bond and two π bonds.**

3. Note the bond length between the atoms. Observe the change in position if you toggle the oxygen-oxygen pair. You might have to reset the CO molecule and repeat this one more time.

4. Based on your observation, which bond is longer: a triple bond or a double bond? _____

5. By employing the "Adjustable Attraction" settings used for F_2, above, to generate the potential energy curve and comparing it to the oxygen molecule, O_2, which of the two molecules has a shorter bond length?

6. What is the order of relative bond length for F_2, O_2, and CO? > >

← greater bond length

7. What rule would you establish for the relative bond strengths of a single, double, and triple covalent bond between the same pair of atoms?