NATIONAL CENTER FOR CASE STUDY TEACHING IN SCIENCE

The Name's Bond, Chemical Bond: Agent Forever Chemical

by

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Preparation

Before beginning the case study, complete the five questions below, which review important topics you have previously learned about in class: (1) atomic structure, (2) electron configuration, and (3) valence, core, and outer electrons. If you are confused about any of these topics, refer to the supplementary tutorial videos and the OpenStax textbook listed below.

Atomic Structure

Resource

- Flowers, P., et al. (2022). Chapter 2.3 in *Chemistry 2e*. OpenStax. <https://openstax.org/details/books/chemistry-2e>

Videos

- *Nuclide Symbols: Atomic Number, Mass Number, Ions, and Isotopes*. Running time: 5:03 min. Produced by Professor Dave Explains. <https://youtu.be/5PyVoMnRTlQ>
- *How to Calculate the Number of Protons, Neutrons, and Electrons.* Running time: 13:11 min. Produced by The Organic Chemistry Tutor. <https://youtu.be/65dDZulPhtg>

Question

1. Give the number of protons, electrons, and neutrons for the following atoms:

	Protons	*Neutrons*	*Electrons*
^{10}B			
^{199}Hg			
$^{63}Cu^{+}$			
$^{77}Se^{-2}$			

Electron Configuration

Resource

- Flowers, P., et al. (2022). Chapter 6.4 in *Chemistry 2e*. OpenStax. <https://openstax.org/details/books/chemistry-2e>

Videos

- *Quantum Numbers, Atomic Orbitals, and Electron Configurations.* Running time: 8:41 min. Produced by Professor Dave Explains. <https://youtu.be/Aoi4j8es4gQ>
- *Pseudo Noble Gas Electroduced by ron Configurations.* Running time: 4:43 min. Produced by Professor Dave Explains. <https://youtu.be/zqxl3CdZDLM>

Questions

2. Predict the electron configuration of each of the following atoms.

   (a) ${}_{6}C$

   (b) ${}_{51}Sb$

   (c) ${}_{7}N^{-3}$

   (d) ${}_{16}S^{-}$

   (e) ${}_{20}Ca^{+2}$

   (f) ${}_{24}Cr^{+2}$

3. Identify the neutral element from the electron configurations given:

   (a) $[Ar]4s^2\ 3d^5$

   (b) $[Kr]\ 5s^2\ 4d^{10}$

Valence, Core and Outer Electrons

Resource

- Flowers, P., et al. (2022). Chapter 6.4 in *Chemistry 2e*. OpenStax. <https://openstax.org/details/books/chemistry-2e>

Videos

- *Electron Configurations (Part 9 of 12) – Inner, Outer, and Valence Electrons.* Running time: 4:16 min. Produced by Moof University. <https://youtu.be/l-eS6tKWT9Q>
- *Valence Electrons and the Periodic Table*. Running time: 16:52 min. Produced by Tyler DeWitt. <https://youtu.be/yADrWdNTWEc>

Questions

4. Define valence electrons.

5. Provide the number of valence, core, and outer electrons for the following atoms.

Atoms	*Number of Valence Electrons*	*Number of Core Electrons*	*Number of Outer Electrons*
${}_{6}C$			
${}_{51}Sb$			
${}_{23}V$			
${}_{27}Co$			

Introduction

Kayla Bond was just beginning her junior year of college as a biochemistry major. She loved science, especially the chemistry of biological systems. She thought of chemistry as a key for solving modern-day challenges and mysteries.

On a cool Monday morning, while walking across the empty quad on her way to class, Kayla got a call from her mom. She loved their weekly chats and enjoyed catching up on news regarding family and friends. This call, however, was different. She heard a shakiness in her mother's voice. Despite a lifetime of physical activity and a healthy diet, her mother had just been diagnosed with type II diabetes. Knowing the damaging health effects of the disease, Kayla was devastated. She just couldn't understand. *How could anyone without a family history or any risk factors suddenly develop diabetes?*

While considering possible reasons why her mother had developed diabetes, she thought about her home. Kayla had been born and raised in Parkersburg, a small town in West Virginia. Situated on the banks of the Ohio and Kanawha Rivers, for years it had played an important role in rail travel, oil, and gas production, and most recently, industrial chemical manufacturing.

Kayla remembered that since the building of chemical manufacturing factories, her hometown had been struggling with unusually high rates of specific health problems. She and her mother had friends and family-members who had been diagnosed with ulcerative colitis, high-blood pressure, thyroid disease, and various cancers. Many people suspected these health problems were linked to the chemical factories located nearby. In 1948, the Dupont chemical company built a plant on the Ohio river just south of town to manufacture various products, including a popular chemical surfactant called Teflon. For years, Dupont had been dumping per- and polyfluoroalkyl substances (PFAS) into local landfills and rivers. Scientists had shown that there may be a link between these illnesses and the contaminated water supply (EPA, 2023). Was it possible that her mother's recent diabetes diagnosis was yet another consequence of PFAS contamination? If so, how? Could learning about the stability of PFAS compounds help her better understand the connection between the contaminated water resources and the increasing number of health problems in Parkersburg? Kayla decided to apply her passion for chemistry to researching PFAS and its negative health effects.

Chemistry of PFAS

Kayla decided to begin her investigation into the cause of her mother's illness by looking at the chemicals that were causing so many problems in Parkersburg: per- and polyfluoroalkyl substances (PFAS). She remembered that Dupont had phased out manufacturing PFAS containing substances like Teflon in 2011 because of the health problems connected with the compounds (Andrews & Walker, 2015). But if PFAS was a health issue, Kayla struggled to understand how her mother had developed type II diabetes several years *after* Dupont stopped the production of the compounds. She visited with her favorite chemistry professor, Dr. Johnson, to inquire about PFAS compounds and learn more about what makes them "forever compounds."

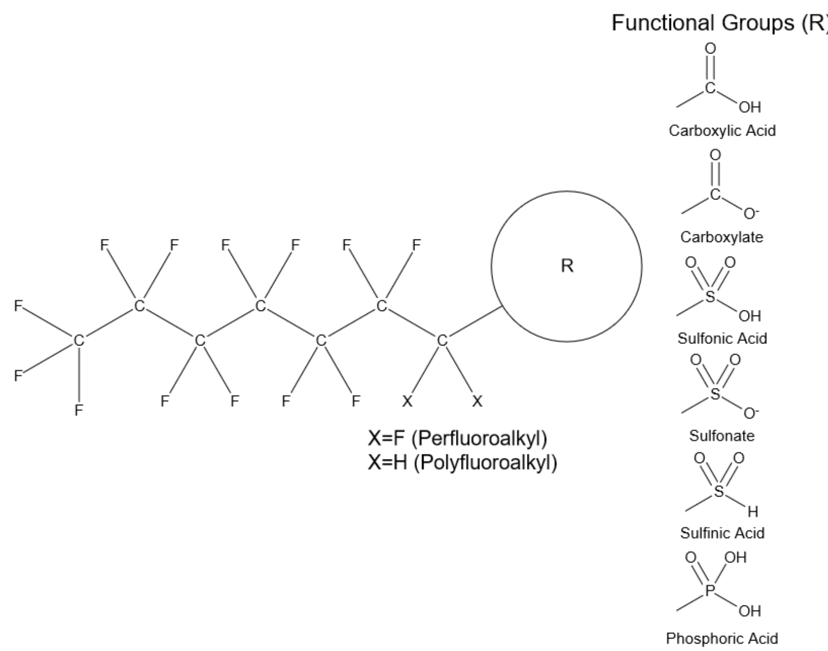

Figure 1. The structure of per- and polyfluoroalkyl (PFAS) compounds.

Dr. Johnson suggested that Kayla look at the chemical structure of PFAS compounds to understand how they could persist in the environment for a long time. Dr. Johnson showed her a diagram of a typical PFAS compound (Figure 1).

PFAS compounds are composed of a chain of carbon atoms, most of which are bonded to a fluorine atom, with the exception of the carbon attached to a functional group (R) at the end. To understand PFAS stability, Dr. Johnson told Kayla to focus on the carbon-fluorine (C–F) bonds that make up the majority of the chemical structure and compare the fluorine element to the other halogens (Figure 2).

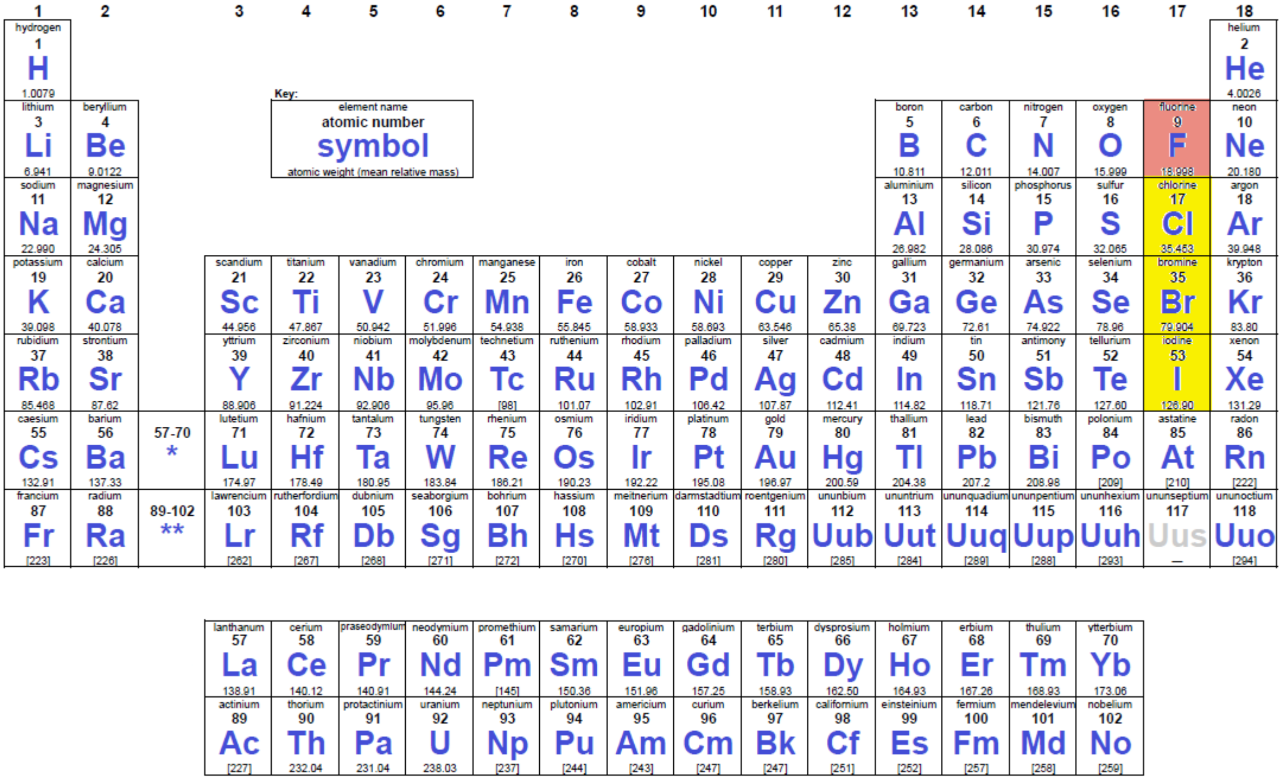

Figure 2. The location of the fluorine element and other halogens in the periodic table.

Types of Bonds

"Let's start by exploring chemical bonds," said Dr. Johnson "Chemical bonds are formed between atoms trying to reach the most stable energy state by obtaining a noble gas configuration. Consider three major categories of chemical bonds: ionic, pure covalent, and polar covalent."

Ionic Bonds

"Ionic bonds are formed through the exchange of one or more valence electrons between a metal and a nonmetal. Ionic bonds are defined as electrostatic forces of attraction between oppositely charged cations and anions (Flowers et al., 2019b). Let's look at how a sodium atom (Na) and a chlorine (Cl) atom react to form sodium chloride (NaCl)." Dr. Johnson grabbed a piece of paper and drew Figure 3. "Sodium loses an electron and chlorine accepts an electron and the resulting ions join together to form an ionically bonded NaCl."

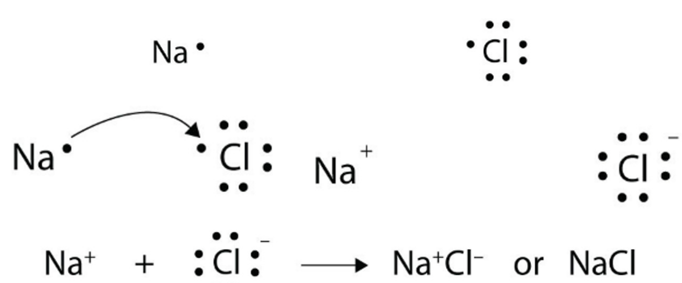

Figure 3. The formation of an ionic bond (Anon, 2012b). The NaCl is a simplification of ionic bonding and the actual structure of NaCl is a lattice (Flowers et al., 2019b).

Questions

1. Does a cation gain protons to form a positive charge or does it lose electrons?

2. Which of the following atoms would be expected to form negative ions in binary ionic compounds and which would be expected to form positive ions: Br, Ca, Na, and F?

Covalent Bonds

Dr. Johnson continued, "Next, there are covalent bonds. While ionic bonds are formed when one atom gives up an electron completely to another atom, covalent bonds are formed when one or more electron pairs are *shared* by two atoms (1 bond = 2 electrons; multiple bonds are possible). When there are not enough electrons for each atom to fill their octet, they share electrons in a covalent bond, allowing each to complete their octet. This type of bond is usually formed between two nonmetals. Let's look at the covalent bond in fluorine, F_2 (Figure 4). Each fluorine has seven valence electrons, so how can two fluorine atoms create a covalent bond?"

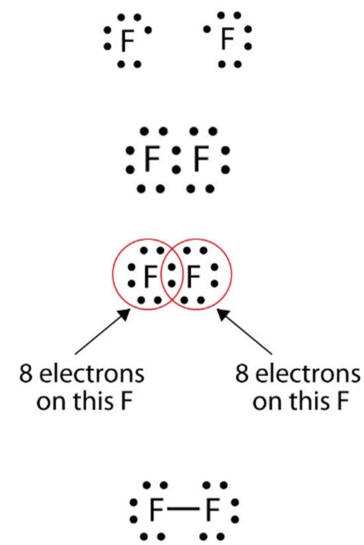

Figure 4. The formation of a covalent bond (Anon, 2012c).

"Well, since each fluorine is one electron short of completing its octet, the two atoms would share a pair of electrons. This would give each fluorine atom eight valence electrons and complete the octets," Kayla replied.

"Great job, Kayla!" Dr. Johnson smiled. "You're catching on very quickly!"

Electronegativity

"Now let's look at two different types of covalent bonds: polar and pure. To differentiate between these two bond types, you need to know an important concept in chemistry called electronegativity."

"I remember electronegativity," Kayla exclaimed. "That's a measure of how well an atom attracts electrons in a bond."

"Very good. Electronegativity is very important when trying to distinguish the type of bond between two atoms." Dr Johnson pulled out a periodic table and began drawing two arrows (Figure 5).

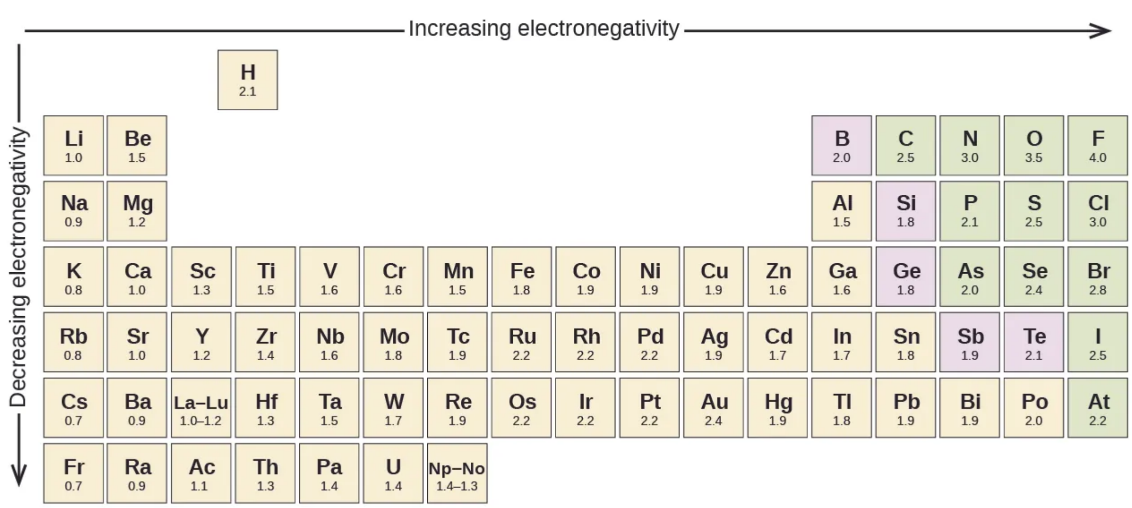

Figure 5. Periodic table electronegativity distribution (Flowers et al., 2019a).

Dr. Johnson pointed to the arrow at the top of the periodic table. "As you can see, electronegativity increases from left to right across the periodic table and decreases from top to bottom. Electronegativity is measured using the Pauling scale and higher number values indicate more electronegative elements. Therefore, many of the most electronegative elements are found in the upper right-hand corner of the periodic table."

"I see, so fluorine is the most electronegative atom at 4, while cesium and francium are the least electronegative at 0.7."

"Yes, and now to determine the type of bond between two atoms you must look at the difference in electronegativity of the two bonded atoms. Generally, the rule of thumb is if the difference between the bonding atoms is less than 0.4 the type of bond is pure covalent. If the difference in electronegativity is between 0.4 and 1.8 the bond is polar covalent. If the difference is greater than 1.8 the bond is ionic. While there are some exceptions to this rule, you can generally figure out the type of bond with this rule (Figure 6)."

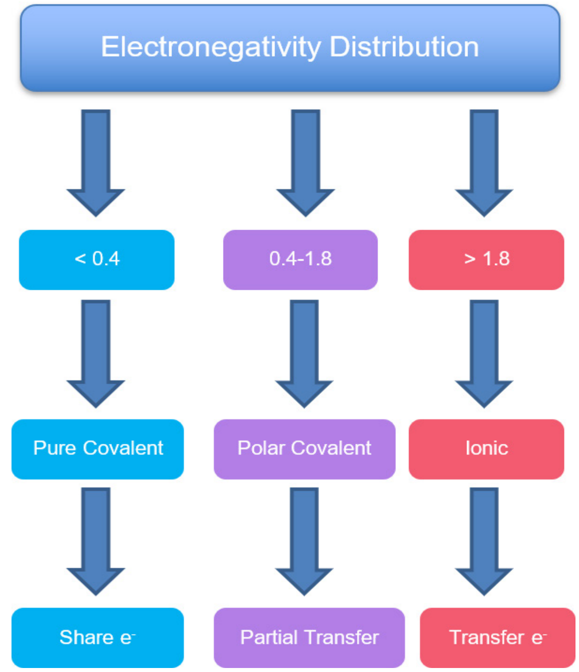

Figure 6. Type of bond from electronegativity difference (Flowers et al., 2019a).

"Okay," Kayla nodded her head. "So, when the difference in electronegativity is zero then the electrons are shared equally between the two atoms. However, when the difference is between 0.4 and 1.8, the electrons are shifted towards the more electronegative atom in the bond."

"Yes! This creates a partial transfer of electron density since the electrons spend more time near the more electronegative atom. This will give the more electronegative atom a partial negative charge (δ–) and the less electronegative atom a partial positive charge (δ+). So, now knowing this information can you tell me what type of bond the C–F bond is in the PFAS compounds?"

"Well," Kayla began, "fluorine has an electronegativity of 4 and carbon has an electronegativity of 2.5. Therefore, the difference in electronegativity of the two bonded atoms is 1.5, so the bond is a polar covalent bond."

"Okay," replied Dr. Johnson, "now let's compare the fluorine carbon bond to the other halogen carbon bonds, starting with chlorine."

"Well," reasoned Kayla, "the electronegativity difference between chlorine and carbon is 0.5 so the bond is polar covalent. The electronegativity difference between bromine and carbon is 0.3 so the bond is pure covalent. However, iodine also has an electronegativity of 2.5 so the bond is pure covalent."

Table 1. Bond Classification for Different Carbon-Halogen Bonds

Bond	*Electronegativity of First Atom*	*Electronegativity of Second Atom*	*Electronegativity Difference*	*Bond Type*
Na–Cl	0.9	3.0	2.1	Ionic
C–F	2.5	4.0	1.5	Polar Covalent
C–Cl	2.5	3.0	0.5	Polar Covalent
C–Br	2.5	2.8	0.3	Pure Covalent
C–I	2.5	2.5	0.0	Pure Covalent

Questions

3. From their positions in the periodic table, arrange the atoms in each of the following series in order of increasing electronegativity:
   a. C, F, H, N, O ____________________
   b. Br, Cl, F, H, I ____________________
   c. F, O, P, S ____________________

4. What information can you use to predict whether a bond between two atoms is pure covalent, polar covalent or ionic?

5. Classify the following bonds as ionic, pure covalent, or polar covalent using electronegativity.

Bond	*Electronegativity of First Atom*	*Electronegativity of Second Atom*	*Electronegativity Difference*	*Bond Type*
HCl				
KF				
C–C bond in H_3CCH_3				

Bond Dipole Moment

Kayla now understood how to classify the different carbon-halogen bonds, but there was still one major question on her mind. "Dr. Johnson, how does the type of bond relate to the bond strength and if two of the carbon halogen bonds are polar covalent does that mean their bonds are similar in strength?"

"Another good question. To answer that, let's look at something called bond dipole moment. Bond dipole moment is a measure of the separation of charges between two atoms. Can you tell me from the different bonds we just learned which of them would have a dipole moment?"

"Well, it would be ionic bonds and polar covalent bonds because the atoms in those bonds have different electronegativities," replied Kayla.

"Yes, bonds with different electronegativities create a shift in electron density surrounding the atoms; the electrons are more attracted to one of the atoms in the bond. Remember that we said that this gives the less electronegative atom a partial positive charge (δ+) and the more electronegative atoms a partial negative charge (δ–). Now, the greater the difference in electronegativity between two atoms, the greater the dipole moment and thus the stronger a bond is (Figure 7).

"Ok so with that concept, the carbon-fluorine bond is the strongest because it has the greatest electronegativity difference and therefore the greatest dipole moment."

"Correct, if you look at this table (Table 2) you can see the differences in dipole moment for the carbon-halogen bonds."

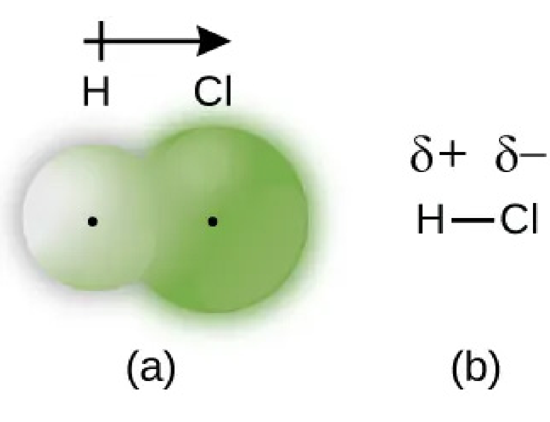

Figure 7. Electronegativity distribution of H–Cl (Flowers et al., 2019c).

Table 2. Carbon-Halogen Dipole Moments	
Bond	*Dipole Moment (D)*
C–F	1.6
C–Cl	1.5
C–Br	1.4
C–I	1.2

Question

6. Using the electronegativity values in Figure 5 (p. 5 above), arrange the following covalent bonds in order of increasing polarity. Then designate the dipole moment using arrows similar to Figure 7:

   O–H, C–O, C–H

Bond	*Electronegativity Difference*	*Dipole Moment*

Atomic Radius

Dr. Johnson told Kayla that another important component regarding the strength of the carbon-fluorine bond is the atomic radius of each atom.

She explained, “The atomic radius is defined as one-half the distance between the two nuclei of two adjacent metal atoms or in a diatomic molecule. On the periodic table, the atomic radius of elements decreases from left to right and increases from top to bottom (Figure 8). This means that helium would be expected to have the smallest atomic radius and Fr (francium) would have the largest. Looking at the periodic table, where is carbon and fluorine and what does their position indicate about their size?”

“Let’s see...they are both in the upper right-hand corner. That means their atomic radii should both be small.”

“That’s correct!” Excited at Kayla’s quick grasp of chemistry concepts, Dr. Johnson asked, “Now, let’s look at why atomic radius would be important for bond strength by looking at bond length.”

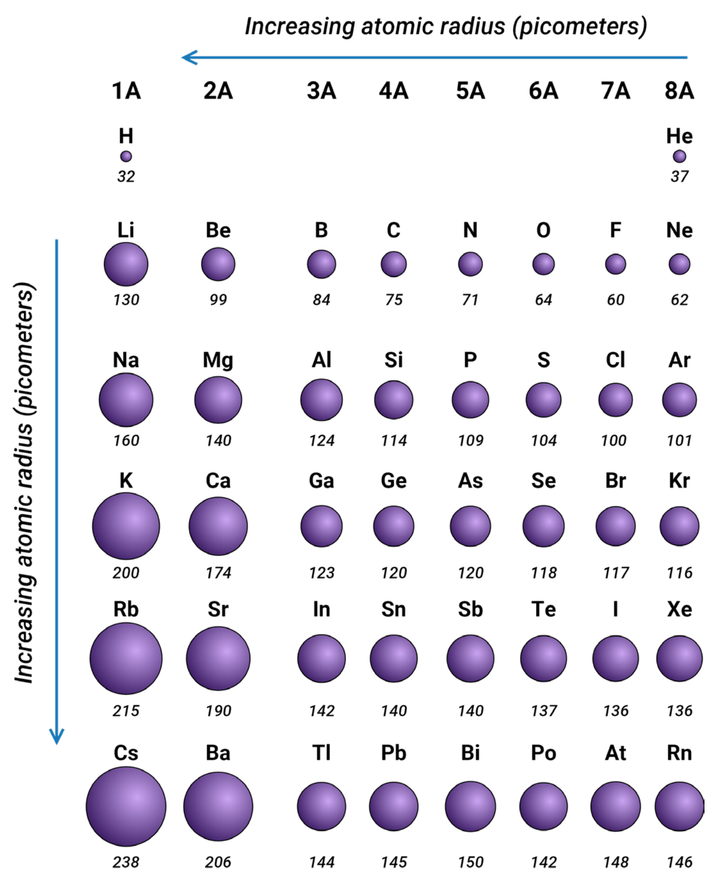

Figure 8. Periodic table atomic radius distribution. (CK-12, 2023)

Questions

7. Arrange the following atoms in order of atomic radius:
   a. P, Si, N ______________________
   b. Na, Al, P, Cl, Mg ______________________
   c. Mg, Sr, Si, Cl ______________________

Bond Length

"Bond length, also called bond distance, is the distance between the nuclei of two covalently bonded atoms. The bond length is proportional to atomic radius and therefore follows the same periodic trends as atomic radius." Dr. Johnson added, "However this is only true for diatomic molecules where one atom remains the same such as C–Cl and C–Br."

"I get it, so if atomic radius decreases across a period and increases down a group, then the same goes for bond length."

"Very good!" Dr. Johnson smiled. "In general, the stronger the bond between the two atoms, the shorter the bond length."

"Therefore," Kayla began, "the smaller the atomic radius, the shorter the bond length will be. Since bond length is inversely related to bond strength, the shorter the bond length, the stronger the bond strength."

"Great. Now think about carbon and fluorine. We saw that their atomic radii are quite small. With that information, do you think their bond would be considered strong or weak?"

"Their small atomic radius must mean that they have a strong bond," answered Kayla.

"That's right!" said Dr. Johnson "You're beginning to put together the pieces of this chemistry puzzle. Now look at this table (Table 3) that shows the bond lengths of several single bonds to carbon."

Table 3. Single Bond Lengths

Bond	*Length (Å)*
C–F	1.35
C–Cl	1.77
C–Br	1.94
C–I	1.73

Note: As the number of electron pairs in the bond increases, the bond length decreases. Therefore, triple bonds are shorter than double bonds between the same two atoms; likewise, double bonds are shorter than single bonds between the same two atoms.

Bond Enthalpy

Kayla was beginning to understand the different properties that made the C–F bond so strong, however there was one more concept that she wanted to learn. "Thanks to your help I know how to predict which chemical bonds will be stronger, but how do you quantify a bond's strength?"

Dr Johnson nodded her head, "So basically you're asking how to tell the difference between the strength of different bonds?"

"Yes, so if I were to compare the bond between C–F or C–Cl, how would I know which one is stronger?"

"Well to answer that, you'll have to look at bond enthalpy, which is an important measure of stability of a molecule. Bond enthalpy is the measure of the amount of energy needed to break a mole of the stated bond (Flowers et al., 2019a). For example, the bond energy of a H–Cl bond is 431.9 kJ/mol. This means that it takes 431.9 kJ of energy to break one mole of H–Cl bonds.

"I get it! It takes energy to break a chemical bond, right?"

"Correct, and on the other hand, when a bond is formed energy is released. Table 4 shows the bond energies of several single bonds to carbon. Can you tell me what's important about the C–F bond?"

Table 4. Single Bond Energies

Bond	*Energy (kJ/mol)*
C–F	485
C–C	346
C–Cl	339
C–Br	285
C–I	213

"Let me see," Kayla examined the table. "Wow, the C–F bond has one of the highest bond energies at 485 kJ/mol and the highest bond energy of all the single carbon-halogen bonds."

"Correct! As you can see because of the different concepts we talked about before, the C–F bond is extremely strong. Therefore, that allows compounds such as PFAS compounds, which are composed of many C–F bonds to be extremely stable."

"Thank you, Dr. Johnson! This all makes much more sense."

Question

8. The bond energy for N–N is 167 kJ/mol, while the bond energy for N–F 283 kJ/mol. Explain why N–F has a higher bond energy than N–N.

Conclusion

Table 5 below summarizes the chemical properties of different carbon-halogen bonds mentioned in this case study.

Table 5. Properties of Different Carbon-Halogen Bonds

Bond	*Electronegativity Difference*	*Type of Bond*	*Dipole Moment (D)*	*Bond Length (Å)*	*Bond Energies (kJ/mol)*
C–F	1.5	Polar Covalent	1.6	1.35	485
C–Cl	0.5	Polar Covalent	1.5	1.77	339
C–Br	0.3	Pure Covalent	1.4	1.94	285
C–I	0	Pure Covalent	1.2	1.73	213

Later, Kayla called her mother to tell her all the new information she learned about PFAS compounds and how they are extremely persistent in the environment. Kayla told her mother that she believed that the PFAS compounds dumped into local water may be harmful and that her family should be careful with local water. She explained that chemical companies were beginning to take responsibility for the dangers posed by PFAS compounds. Dupont settled a class action lawsuit in 2004 for the dumping of PFAS chemicals around Parkersburg, agreeing to pay plaintiffs a total of $670.7 million (Lammi, 2020). Additionally, DuPont and other major chemical companies have had numerous individual lawsuits over health issues regarding PFAS contaminated water. In June 2023, Dupont along with Chemours and Corteva agreed to fund a $1.19 billion clean-up of PFAS contaminated drinking water, while 3M has settled for a $10 billion clean-up of PFAS (Casselman et al., 2023). Kayla had recently learned the DuPont chemical company had begun manufacturing two new chemicals: PFBS and GenX (Figure 9). These compounds were intended as replacements for PFOA and PFOS and reported safer by DuPont (Draft Toxicity, 2018). Litigation is currently pending concerning pollution of the Cape Fear River in North Carolina by the new, "safer" GenX.

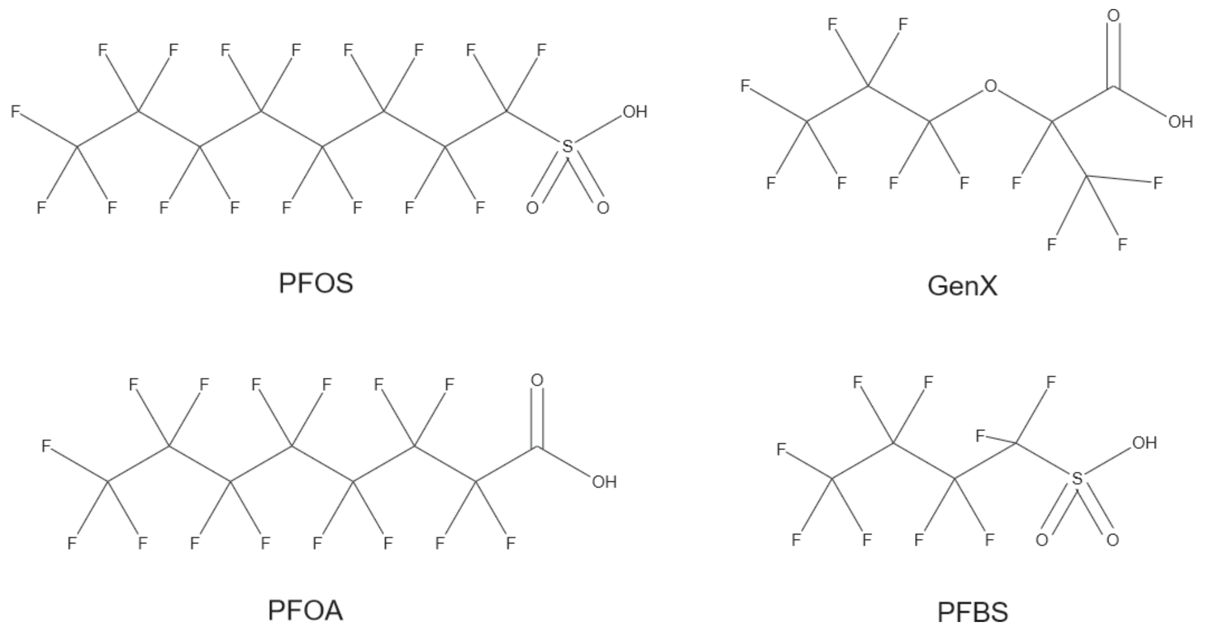

Figure 9. The chemical compositions of PFBS, GenX, PFOS and PFOA.

Kayla looked at the chemical compositions of the new compounds (PFBS and GenX) and found many similarities to the chemical compositions of both PFOA and PFOS. What are the similarities between PFBS and GenX and PFOA and PFOS? What are the differences? Why would both GenX and PFBS also be difficult to break down?

Additional Resources

For further information about PFAS compounds, the following movie, book, and documentary film are recommended.

- *Dark Waters:* This movie is based on the true story of a corporate defense attorney and his environmental lawsuit against a major chemical company. Directed by Todd Haynes and starring Mark Ruffalo, Anne Hathaway, and Tim Robbins. <https://www.imdb.com/title/tt9071322/>
- *Exposure: Poisoned Water, Corporate Greed, and One Lawyer's Twenty-Year Battle against DuPont:* This is the book on which *Dark Waters* is based; by Robert Bilott (2019, Atria Books).
- *The Devil We Know:* This 2018 documentary film by Stephanie Soechtig investigates the health hazards posed by perfluorooctanoic acid and DuPont's responsibility. <https://www.imdb.com/title/tt7689910/>

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