Molecular Structures of Acids and Bases

In our introduction to acids and bases, we asserted that different molecules react based on the role they play with protons and what they are reacting with. For example, we know that if a molecule has a proton that they really want to get rid of, they're a strong acid. On the other hand, if we have another molecule that only somewhat readily accepts a proton, they're a weak base.

Understanding these trends and how acids and bases react with each other is critical to succeeding in AP Chemistry. However, being able to discern why these rules are true is just as important.

Overview

- In this lesson, we'll discover the general structure of acids and bases.
- Then, we'll learn how this structure influences the functionality and strength of acids and bases.
- Afterwards, we'll learn about molecular structure equilibria in acids and bases.
- Finally, for each of these concepts, we will step through different practice problems to ensure you conceptually grasp how acids and bases are influenced by structure.

Structure of Acids and Bases

Before we continue, let's have a quick refresher on what acids and bases do. Acids are hydrogen atom (proton) donors, and bases are proton acceptors. As mentioned in the Introductory Lesson and the start of this lesson, how readily acids and bases do these jobs determine their strength. Also recall that molecules can be assigned a number on the pH scale that corresponds with how acidic or basic it is, with 0 being the former and 14 being the latter. Again, if you need a reminder, be sure to read our Introduction to Acids and Bases.

Now that we understand the roles of acids and bases, let's try to understand their general structure. Starting with acids, there are three general types of acids: binary acids, oxyacids, and carboxylic acids. If you recall the strong acids that you need to be familiar with, most of them are binary and oxyacids.

Definition

Binary acids are acids with the formula **H-X**, where a hydrogen atom is bonded to an electronegative nonmetal atom, X. X is typically a halogen.

The strong acids hydrochloric acid (HCl), hydrobromic acid (HBr), and hydroiodic acid (HI) are all binary acids. Next, we have oxyacids.

Definition

Oxyacids are acids that have **one (or multiple) H-O bonds**, where a hydrogen atom is bonded to an oxygen atom.

Note: This hydrogen atom directly bonded to the oxygen atom is what makes it acidic.

Recalling our strong acids, nitric acid (HNO_3) and sulfuric acid (H_2SO_4) are oxyacids. Lastly, we have carboxylic acids. These typically appear more in organic chemistry and higher-level chemistry courses, but for the sake of being thorough, we will briefly cover them as well.

Definition

Carboxylic acids have the general structure of **COOH**, where a carbon atom is 1. double bonded to a single oxygen atom, and 2. bonded separately to an alcohol group (OH).

But why do acids typically appear in these three general structures? As it turns out, there's a common denominator: these structures promote hydrogen atom donation, (which defines what an acid is), through bond strength and conjugate base stability. But before we get into that, let's quickly cover the general structure of bases.

Definition

Bases almost always have the structure of **MOH**, where metal M+ and hydroxide OH- are in an ionic compound that will dissociate to free OH- to accept a donated hydrogen atom (proton) H+. Hydroxide doesn't always have to be the proton acceptor, however.

Common strong bases include sodium hydroxide (NaOH), potassium hydroxide (KOH), and other group 1 and 2 metals bonded to one or more hydroxides (based on the charge of the metal.) An example of a non-hydroxide base is ammonia (NH_3).

As we mentioned briefly. acids and bases generally appear this way to perfectly complement each other's functions. Let's discover how the structure of each does this.

Acid and Base Structure Influences Functionality

If we were to generalize the three types of acid structures that we just covered, how would we do so? Let's imagine that for each kind of acid we covered, we have a hydrogen attached to some group Z. This means that in the case of binary acids, Z = a halogen (typically denoted as an X), while in oxyacids, it would be some group with an oxygen atom. To solidify this concept, let's try an example.

If we have the acid HBr, what group would Z be? Z would be Br. What about H_2SO_4? Z would be HSO_4. There's a reason we do this separation exercise. If we want to discern why acids appear in this form, we have to ask: what qualities does Z have that make the proton so ready to leave?

Why do Binary Acids Appear? (Z is a halogen, typically denoted as an X)
There are three primary reasons that binary structures in the form of H-X tend to be acidic.

1. H-X becomes more acidic the more electronegative the X group is (usually a halogen).
   This is because the more electronegative the halogen is, the more it likes retaining its electrons. This means that the conjugate base that it forms is far more stable than other negative ions.

2. The more stable the conjugate base X^- is, the more acidic H-X is.
   If we imagine a conjugate base as extremely stable, it would make intuitive sense that the molecule would want to become that base. If you recall from the Introduction to Acids and Bases lesson, conjugate bases are formed once acids go through an acid-base reaction. A stable conjugate base prefers that form. We know that a strong acid forms a weak conjugate base, which will stay in that form due to its weakness. From this, we can infer that the more stable a conjugate base is, the stronger an acid is.

3. The weaker the bond between H and X, the more acidic H-X is.
   This makes intuitive sense. If the bond between the hydrogen atom and X can be broken easily, the proton will be given up much more readily. This makes the compound more acidic. Recall that the higher a bond's enthalpy is, the more energy is required to break it. This would mean the bond is stronger and therefore less acidic.

Why do Oxyacids Appear?
For oxyacids, the same trends as binary acids are true. However, there is an additional trend:

1. The acidity of an oxyacid increases with the number of oxygen atoms.
   This happens due to their collective electronegativity forming a much more stable conjugate base. In reality, this is just an extension of the "electronegativity" rule.

On the AP Chemistry exam, you'll most likely be dealing with binary acids, and possibly oxyacids. The characteristics of carboxylic acids, however, will not be tested until organic chemistry.

How do Bases Structurally Appear?
If you understand the rules behind how acids structurally appear, understanding bases will be easy to comprehend. Remember, acids and bases perform complementary roles. This means that the rules that dictate how acids structurally appear are just reversed for bases.

1. The less electronegative a molecule is, the more basic it is.
2. The weaker a conjugate acid, the more strong a base is.
3. The stronger the bonds within a molecule, the more likely it is to be basic.

What we can gather from this is a simple rule: acids and bases are opposites in strength. This means that a strong acid would be a weak base, and a strong base would be a weak acid. As long as you can grasp one set of structural rules, the other is intuitive.

Check Your Comprehension

Let's walk through a few example problems to see if you understand how structure influences acid-base functionality. As always, try to answer these on your own before referring to the answers below each question.

> **Example**
>
> You want to find out if hydrochloric acid or hydrobromic acid is more acidic. The bond enthalpy between H-Cl is ~432 kJ/mol, while for H-Br it is ~366 kJ/mol. Which acid is stronger? Which structural rules are you applying to determine this?

This is an application of the structural rule that states that acid strength increases as bond strength between the hydrogen atom and the Z/X group decrease. Bond enthalpy tells us how much energy is required to break a bond. This means that a higher bond enthalpy implies a stronger bond. Hydrobromic acid's lower bond enthalpy implies a weaker bond, meaning an easier release of the proton, making it a stronger acid.

> **Example**
>
> What does it mean for a conjugate base to be stable? Are stable conjugate bases weak or strong?

A stable conjugate base has no alternative preferential form. In other words, any molecule in its stable form *wants* to stay that way. Therefore, a stable conjugate base wants to stay a base. A molecule that wants to stay a base certainly won't want to fulfill the base's role by accepting a proton. This means that stable conjugate bases are weak bases.

> **Example**
>
> You are asked to explain to your peer why H_2SO_4 is a stronger acid than H_2SO_3. How would you go about explaining this?

This can be answered through the oxyacid extension of the electronegativity rule. The additional oxygen atom in H_2SO_4 provides additional electronegativity, and therefore, a greater electron density, and a more stable conjugate base. The more electronegative the group attached to the hydrogen atom is, the more acidic the molecule is overall. Or, in other words, the more stable the conjugate base is, the stronger the acid will be. H_2SO_4's conjugate base being stable is consistent with it being a stronger acid.

Using Acid-Base Structure to Understand Equilibria

We'll have a separate lesson diving into acid-base equilibria more in-depth releasing soon. However, we can apply the rules we just learned to determine what side of a reaction will be preferred in an acid-base equilibrium problem.

You'll learn in this lesson that acid-base equilibrium reactions prefer the side of a reaction that has weaker acids and bases. In short, this is because stronger acids and bases can perform their roles of donating and accepting protons more readily, making them much more likely to react than weaker acids and bases. If these weaker acids and bases aren't reacting, this means they are staying in their weak forms, making them the preferred product of our equilibrium problem.

This means that we can apply the structural rules that we just learned about acids and bases to determine which side of an equilibrium reaction will be preferred. Let's try a simple example.

> Example
>
> Which side of this acid-base equilibrium reaction will be preferred?
>
> $$HF + NH3 \rightleftharpoons NH4+ + F-$$

Recall that we want to find out which side of our reaction has the weaker acid. We can identify HF as the acid and NH_3 as the base, meaning that NH_4^+ is our conjugate acid and F^- is our conjugate base. Now, it's simply a matter of comparing acid strengths. Using our structural rules, we know that hydrofluoric acid is going to be much more strong than the conjugate acid, NH_4^+. This means that equilibrium will favor the **right** side of this reaction.

As you learn more about how acid-base equilibria works in the remainder of AP Chemistry and higher-level chemistry courses, these trends will reappear again and again. Therefore, if you understand how acid and base structure influences their functionality, you'll be able to comprehend not just the *how*, but the *why* behind acid-base equilibria.

Molecular Structures of Acids and Bases - Key takeaways

- In this lesson, we discovered the general structure of acids and bases.
- Then, we learned how this structure influences the functionality and strength of acids and bases.
- Afterwards, we learned about molecular structure equilibria in acids and bases.
- Lastly, we reviewed different practice problems for each concept to ensure comprehension.