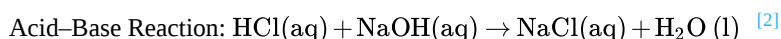
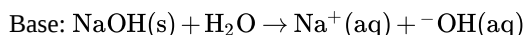
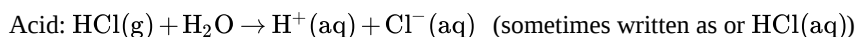


1.1: A Quick Review of the Models of Acid-Base Reactions.

There are a number of ways to discuss acid–base reactions, depending on what aspects of the reaction we want to highlight. They range from the extremely simplified (and not useful) Arrhenius model, to the Brønsted–Lowry model that we use only for reactions in which protons are transferred, and finally to the Lewis model, which can encompass any type of acid–base reaction.

Arrhenius:

The Arrhenius acid–base model is probably the first acid–base model that you were introduced to in the course of your education. In this model, when an acid dissolves in water it dissociates to release a hydrogen ion (H^+); when a base dissolves it releases a hydroxide ion (OH^-).

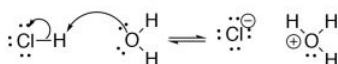


Although simple, the Arrhenius model is not particularly useful when it comes to understanding the reactions considered in organic chemistry. This of course raises the obvious question: so why are we mentioning it? The answer is two fold: i) because you might well vaguely remember it as a description of acid–base behaviors and ii) so that we can consider why it is not useful and why you should not use it. The Arrhenius acid–base model applies only when water is the solvent—as we will see many organic reactions do not occur in water. The Arrhenius model also, falsely implies that there are free protons (H^+) roaming around in water and it restricts bases to those substances that release a hydroxide ion. Finally, it implies that an acid can exist independent of a base—and vice versa, which doesn't make a great deal of sense.

Brønsted–Lowry:

The Brønsted–Lowry model is a much more useful and flexible model for considering acid base reactions. In this model an acid is a proton (H^+) donor and a base is a proton acceptor. In the Brønsted–Lowry model you cannot have an acid without a base, and vice versa; the acid has to donate its H^+ to something (the base), and similarly the base has to accept it. The H^+ doesn't just “drop off”—it is **transferred**.^[3] In the case of reactions that occur within aqueous solution, the H^+ is transferred to a water molecule to form H_3O^+ . Consider, as an example, HCl; in aqueous solution HCl transfer a H^+ group to a water molecule. The products are H_3O^+ (the conjugate acid of water) and Cl^- , the conjugate base of HCl.

$\text{HCl(g)} +$	$\text{H}_2\text{O(l)}$	\rightleftharpoons	$\text{H}_3\text{O}^+(\text{aq})$	+	$\text{Cl}^-(\text{aq})$
acid	base		conjugate acid		conjugate base



The key point here is that the H^+ is transferred from one molecule to the other—it doesn't drop off and then reattach.

The flexibility of the Brønsted–Lowry model lies in the fact that the base does not necessarily have to be water. For example, if we look at the reaction of hydrogen chloride and ammonia (NH_3), we see that the proton transfer from acid to base is analogous to the reaction in water.

HCl	+	NH_3	\rightleftharpoons	NH_4^+	+	Cl^-
acid		base		conjugate acid		conjugate base

In the Brønsted–Lowry model, as for all chemical reactions considered at the molecular level, there is the possibility for the reaction to reverse, which is denoted by the use of equilibrium arrows (\rightleftharpoons).

At the macroscopic level the extent to which the reaction proceeds (from reactants on the left to products on the right) is determined by a number of factors. That is, we need more information to predict (or calculate) the concentrations of reactants and

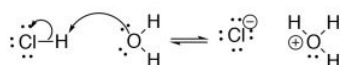
projects at equilibrium. This is information that also enables us to predict whether the reaction will proceed in the forward direction (to the right) or not and how the reaction might change if we add or remove reactants (or products).

We can identify a potentially acidic H^+ because it will be bonded to a more electronegative atom; the result is that the electron density in the bond will lie mainly with the more electronegative atom (e.g. O, N, or Cl). The outcome is that, for example, an $\text{H}-\text{O}$ bond will be weakened (require less energy to break); the H will have a large partial positive charge on it, and will be strongly attracted to basic centers (as described in the next section). Similarly, simple **bases** can be identified by the presence of an atom (within the molecule) that has a partial negative charge; this partial negative charge arises because the atom (the basic center) is bonded to less electronegative atoms. Now we add one further consideration, this base center atom also needs to be able to accept the incoming H^+ . In practice, this means that a **basic molecule will contain an atom that has a lone (non-bonding) pair of electrons that can form a bond to the H^+** .

The Brønsted–Lowry model is useful for acid–base reactions that involve proton transfer, but even so, it is limited to proton transfer reactions. We also note here that the solvent in which the proton transfer takes place will have an effect on the reaction, and we will return to this idea later in the course. If we extend the Brønsted model to other reactions where a base uses its lone electron pair to form a new bond with an electropositive center, we can expand the class of acid–base reactions even further. Which brings us to the next model of acid base chemistry: the Lewis model.

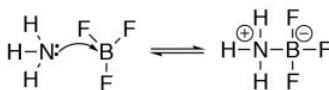
Lewis:

The Lewis model allows us to describe exactly the same set of reactions as does the Brønsted–Lowry model, but from a different perspective, and it also allows us to expand on the model. In the Lewis model **a base has the ability to donate an electron pair to form a new bond** with the **acid that accepts this new bond**, often but not always with the concomitant breaking of a bond within the acid molecule. We use same rationale for why the reaction occurs between two oppositely charged centers, but from the perspective of the electrons, rather than the H^+ . A base must therefore have a lone pair of electrons that can take part in a bond while an acid must have an atom that can accept that lone pair of electrons. Using the reaction of HCl and water as an example, we use the curved arrow notation to denote how the electrons move between base and acid. Recall^[4] that we use this curved arrow notation to indicate the movement of electron pair



from a source of electrons to a sink. Here the source is the lone pair on the oxygen, and the sink is the hydrogen (which has a δ^+ due to its bonding to a Cl). The second arrow moves from the source (the bond between H and Cl, to the sink—the electronegative Cl which ends up with the negative charge, while the O that donated the original electron pair ends up with a positive charge).

The Lewis model encompasses the Brønsted–Lowry model, that is, all Brønsted–Lowry acid–base reactions that can be described using the Lewis model. However, the Lewis model extends the range of reaction types that can be considered as acid–base reactions. Take for example the reaction of ammonia (NH_3) and boron trifluoride (BF_3). This reaction is classified as a Lewis acid–base reaction, but it is not a Brønsted acid–base reaction.



Why use different models of acid–base chemistry? While at first the idea of using different models to explain acid–base chemistry may be a little confusing. Why not use the all-encompassing Lewis model for everything? It turns out that both the Brønsted–Lowry and Lewis models are particularly useful depending on the system under consideration. The trick is to recognize which is the most useful when describing, predicting, and explaining a particular type of chemical reaction.^[5]

In our explorations in organic chemistry we will be using both Brønsted–Lowry (proton transfer) and Lewis (electron pair donation) models to describe acid–base chemistry, depending on the type of reaction. In practice, the Brønsted–Lowry model is simple and useful; it tells you what is happening (proton transferred from acid to base) but nothing about the mechanism by which the H^+ moves. For that we must turn to the Lewis model, which tells us how the electrons rearrange during the reaction. It is also important to keep in mind **why** these reactions happen—they are caused by an electrostatic interaction between two oppositely charged parts of molecules: δ^- is attracted to δ^+ .

One further note, all reactions are initiated by random collisions of molecules, but only collisions that allow the electrostatic interaction of the acid and base to occur are productive (that is, collisions that involve two similarly charged parts of molecules will not give rise to a reaction. Again we will have more to say about this later.

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