Electronic Supplementary Material (ESI) for Chemistry Education Research and Practice.

APPENDIX 3. Comparison of the standard and the enriched texts on chemical bonding

Electrostatic interactions

The standard text does not mention anywhere the term ‘electrostatic interactions’, but it does refer to “forces of an electrostatic nature (Coulomb forces) [that] are exerted between the positively charged nucleus and the negatively charged electrons” (p. 3), to “The ions formed are attracted to each other by electrostatic Coulomb forces” (p. 4), and to “the ions that are formed are held together in fixed positions in a NaCl crystal by means of electrostatic forces” (p. 5). The enriched text also did NOT refer to ‘electrostatic interactions’ but referred to “Central to any description of these electrical interactions is **Coulomb's law**” (p. 1), “forces of electrostatic nature (Coulomb forces)” (p. 3), to “ions with charges of the same sign will repel each other, through Coulombic interactions” (p. 7), and to “the attractive Coulomb forces between the cation and anion” (p. 11).

Octet rule

The standard textbook contained the following information about the octet rule:

Valence electrons

- It is known that the electronic structure, especially the outer (*valence*) electrons, is responsible for the chemical behavior of an atom. Elements that possess a completed outer shell of eight electrons (except the K shell, which is filled with two electrons) do not tend to form compounds. The noble gases belong to this category. Atoms of these elements exist in a very stable energy state, and this stability can be attributed to their filled outer shell.
  Atoms of the other elements are not “in the same boat”, that is, they do not have an octet of electrons in their outer shell (or a dyad of electrons in the case of the K shell) but try to acquire this structure, that is, to "look like" the noble gases. They can achieve this chemically by losing, gaining or sharing electrons to acquire the stable electronic structure of the noble gases (***octet rule***).
  Octet Rule: Atoms tend to fill their valence shell with eight electrons (unless it is the K shell which requires two electrons to be filled) to acquire a noble gas structure. (Appendix 1, p. 2)

The above text should be compared with the more detailed discussion provided by the entiched text, which includes the following information and comments about the octet rule.

- **The Octet Rule:** Atoms tend to fill their valence shell with eight electrons to obtain a noble gas structure - unless the outer shell is the K shell, where only two electrons are needed to obtain such a structure. (Appendix 2, covalent bonding, p. 5; and again in ionic bonding, p. 8.)
- The rule of eight electrons (**octet rule**) helps to predict: (a) the number of covalent bonds formed by any atom, and (b) the stoichiometry of a molecule of the resulting compound. (Appendix 2, covalent bonding, p. 5)
- It is evident from the above that the octet rule can help our understanding of: (a) the number of covalent bonds formed between two atoms, and (b) the stoichiometry of a molecule of the resulting compound [e.g. $(H)_1(Cl)_1$, $(H)_2(O)_1$, $(H)_3(N)_1$]. But note that

there are many covalent compounds for which this rule does not apply (e.g., BF_3). **EXERCISE:** *Confirm that in the case of the molecule* BF_3*, the octet rule does not apply.* (Appendix 2, covalent bonding, p. 7)

- To explain the charges on these ions, we use the MODEL of electron transfer from the atom of the more electropositive element to the atom of the more electronegative element, resulting in a cation and an anion, which obey the **octet rule.** (Appendix 2, ionic bonding, p. 8)
- We conclude that *it is NOT the octet rule that "imposes" the formation of an ionic bond*; however, *the octet rule is able to explain the charges on the ions and the stoichiometry of ionic compounds*. (Appendix 2, ionic bonding, p. 9)

Electronegativity

The enriched text gives a more detailed coverage, including the use of a quantitative scale (the Pauling scale), to this topic. Thus, in the standard text, the concept is discussed as follows:

- At this point it is appropriate to make brief reference to the notion of electronegativity. ***The electronegativity of an element refers to the tendency of an atom of the element to attract electrons, when it participates in the formation of polyatomic units*** (p. 7).
- The electronegativity of an atom indicates the force with which it attracts electrons in molecules of the compounds that it forms with other atoms. Note that as the atomic radius decreases and the number of valence electrons increases, the electronegativity value increases. (p. 7)
- Clearly the greater the electronegativity difference between the two atoms, the more polar the covalent bond will be (p. 8).

On the other hand, the enriched text discusses electronegativity extensively (pp. 3-4), and subsequently with reference to nonpolar covalent bonding (p. 6), nonpolar and polar covalent bonds (pp. 12-13), the ionic bond (p. 14), the continuum percentage between ionic and covalent bonding (p. 14), the percentage ionic and covalent character of a bond (p. 14), e.g.:

- the difference in electronegativity between the two atoms involved in forming a chemical bond can vary significantly, giving rise to a variety of polarity of bonds. The difference in electronegativity between the two atoms participating in the bond and the resulting polarity of the bond allows us to assign a percentage ionic character and a percentage covalent character to the bond. (p. 14)
- The continuum between ionic and covalent bonding is illustrated by the variety of values observed for the melting points of different halogen compounds (see table below). (p. 14)
- According to Pauling, a difference of 1.7 in electronegativity between the bonded atoms (on the Pauling scale) corresponds to 50% ionic character, so a difference of more than 1.7 corresponds to a bond that is primarily ionic. (p. 14)
- the electronegativity difference is not the only criterion for the prediction of the type of bond formed. (p. 15)

Bond polarity

It is noteworthy that the standard text does not use the term ‘bond polarity’ or ‘polarity’, while the enriched text refers explicitly to this concept:

- The nature of the chemical bond in this case is also covalent and is indeed similar to that for the case of homonuclear molecules. The basic difference is that the two atoms now have different, but not very different, electronegativities. This results in *bond polarization*, which we will study later. (p. 7)
- The *ionic bond* can be regarded as an *extreme case* of a *polar covalent bond*, with bond polarity even larger for an ionic bond. (p. 13)
- **IMPORTANT NOTE:** It is evident that bond polarity also occurs in an ionic bond. The difference from a polar covalent bond is that while in the ionic bond we have separation of integer electric charges (multiples of the elementary electric charge) (1+, 2+, 3+, 1−, 2−, 3−), in a polar covalent bond we have a fraction of the elementary charge δ+ and δ - where δ is a positive number <1. (p. 13)
- The difference in electronegativity between the two atoms involved in forming a chemical bond can vary significantly, giving rise to a variety of polarity of bonds. The difference in electronegativity between the two atoms participating in the bond and the resulting polarity of the bond allows us to assign a percentage ionic character and a percentage covalent character to the bond. (p. 14)

Both texts, however, refer extensively to nonpolar and polar bonds, e.g. in the standard text:

- Where the atoms forming a covalent bond are identical as e.g. in the H2 molecule, the common pair of electrons of the covalent bond is attracted equally by both nuclei, in which case we have a uniform distribution of the shared electron pair between the two atoms and *a nonpolar covalent bond is produced.* (pp. 7-8)
- However, this will not be the case when the atoms forming a covalent bond are different, e.g. in the HCl molecule. In this case, the shared pair of electrons will be attracted more strongly by the more electronegative atom. Thus, there will be an uneven distribution of the shared electron pair with a greater proportion toward the more electronegative atom (in this case, Cl). Such a bond is called ***a polar covalent bond***. Clearly the greater the electronegativity difference between the two atoms, the more polar the covalent bond will be. (p. 8)
- Purely covalent or purely ionic bonds represent extreme cases. Most bonds are intermediate in nature. A polar covalent bond indicates the existence of ionic character in the covalent bond.
- **FIGURE 2.9.** The polar covalent bond (*in the middle*) is an intermediate state between the nonpolar bond (*left*) and the ionic bond (*right*).
- Electronic formulas for the polyatomic molecules water (H_2O) and ammonia (NH_3), and molecules with multiple covalent bonds: carbon dioxide (CO_2) and nitrogen (N_2) are given below. Note that in all cases, except for N_2, the covalent bonds are polar. (p. 8)

Of particular relevance is the following statement in the enriched text in relation to polar covalent and ionic bonds:

- Chemical bonds between atoms of different elements are polar, with a partially ionic and a partially covalent character. If the covalent character is dominant, we have a *polar covalent bond,* if the ionic character dominates, we have *ionic bonding*. (p. 15)