APPENDIX A: Selection of Oxidation State Definitions

1. 'Chemistry: A Structural View' first published in 1965 as a secondary school senior chemistry text book for use in Australia. I used the Second Edition version as a school student in South Australia 1976.

   "Oxidation Number: A formally similar reaction to $2\mathrm{Mg} + \mathrm{O}_2 \rightarrow 2\mathrm{MgO}$ is the burning of sulphur in oxygen $S + \mathrm{O}_2 \rightarrow S\mathrm{O}_2$. Remembering that sulphur dioxide consists of discrete covalently-bonded molecules, we cannot readily regard this as oxidation-reduction in the sense of complete electron transfer from one species to another. Nevertheless, it is desirable that this reaction should be viewed as a redox reaction, and this is achieved through framing an alternative definition in terms of directed numbers assigned to the atoms, called *oxidation numbers*. The use of such numbers provides a means of deciding whether oxidation-reduction is involved in a particular reaction under consideration."
   (Stranks, 1970, p. 301)

2. 'Chemistry: Principles and Applications' published 1974 as an undergraduate text book for first year Chemistry students in U.S.A. I used the First Edition version as an undergraduate at Flinders University, South Australia 1977.

   "In assigning oxidation states to the various elements in a species or compound, we use the following conventions (or rules) that are to be applied in the order given:

   1. All elements in the elementary state are assigned an oxidation state of zero.
   2. The alkali metals (Li, Na, K, Rb, and Cs) in any compound are assigned an oxidation state of +1; the alkaline earth metals (Be, Mg, Ca, Sr, Ba, and Ra) and also Zn and Cd in any compound are assigned an oxidation state of +2.
   3. Oxygen is assigned an oxidation state of –2 in all of its compounds except the peroxides and superoxides (e.g., Na_2O_2 and K_2O_2).
   4. Hydrogen is assigned an oxidation state of +1 in all of its compounds except the hydrides (e.g., NaH).
   5. Oxidation states of all the other elements in a species usually can be determined by the requirement that the algebraic sum of the oxidation state values for all of the elements in the species must equal the net charge of the species.

   If a conflict arises, then the rule with the lower number takes precedence. In other words, apply the rules in the order given until there is only one element left, which is then assigned an oxidation state consistent with the net-charge condition (rule 5).

   These rules have their origin in the atomic structures and electronegativities of the various elements. However, it is important to realise that the oxidation state does not, in general, correspond to the actual charge on an element in a chemical species. Oxidation states are primarily a convenient bookkeeping device that is useful in balancing reactions." (Rock & Gerhold, 1974, p. 204)

3. 'Chemical Experience' first published 1981 as a secondary school senior chemistry practical activity text book for use in Australia. I used the first and second Edition versions as a teacher of chemistry in South Australia from 1985 onwards. It remains a valued resource of clear and concise practical activities.

   "This extension uses the concept of oxidation number. Numbers are given to atoms according to a set of rules. When these numbers increase atoms are oxidized; when they decrease, atoms are reduced. This concept has the major advantage of bringing all previous definitions together. It Is therefore, widely used." (Cross & Stanley, 1981, pp. 80, 89)

4. 'Dictionary.com'

   "oxidation state (noun, Chemistry): the state of an element or ion in a compound with regard to the electrons gained or lost by the element or ion in the reaction that formed the compound, expressed as a positive or negative number indicating the ionic charge of the element or ion." (American Heritage, 2011)

5. 'Chemistry Workbook: Essentials Education' first published in 1996 specifically as a study guide for the South Australian Certificate of Education (SACE). All eight editions have been well valued resources to teachers and students of chemistry in South Australia.

   "Oxidation Number: This is the charge an atom would have if any electron pairs being shared in a compound were imagined to be transferred completely to the atoms with the greater ability to attract electrons (the higher electronegativity). An oxidation number can be assigned to an atom or ion in any compound and this is done by applying a set of rules." (Evans & McCann, 2014, p. 417)

6. The UK based website' Chemguide' has been providing excellent pragmatic support to secondary school students for many years.

   "Oxidation state shows the total number of electrons which have been removed from an element (a positive oxidation state) or added to an element (a negative oxidation state) to get to its present state.

   Oxidation involves an increase in oxidation state
   Reduction involves a decrease in oxidation state

   … If you know how the oxidation state of an element changes during a reaction, you can instantly tell whether it is being oxidised or reduced without having to work in terms of electron half-equations and electron transfers” (Clark, 2002) last modified July 2018

7. Recommendations to IUPAC from the “Toward a comprehensive definition of oxidation state” project team.

   “Oxidation state (OS) gives the degree of oxidation of an atom in terms of counting electrons. It scales trends in redox and acid-base properties, as well as physical properties such as magnetism, and is a key component when tracking the course of chemical reactions.” (Karen, McArdle, & Takats, 2016, p. 832)

8. IUPAC 2016

   “Oxidation state (OS) is a simple numerical attribute of an atom in a compound, which aids the systematic descriptive chemistry of the elements, scales trends in properties, and tracks key chemistry changes in reactions. Lacking a comprehensive definition, OS has so far been defined via algorithms for its calculation or with postulated values. This document provides a definition of OS based on ionic approximation of chemical bonds. Associated with the definition’s underlying principle of bond-electron allegiance, two general algorithms are outlined for OS determination in a molecule, ion, or a solid, described by a Lewis formula or a bond graph. Typical origins of ambiguous OS values are pointed out, and the relationship between OS and the d-electron configuration of transition metals is commented on.” (IUPAC, 2016)

9. Wikipedia Oxidation State

   “The oxidation state, sometimes referred to as oxidation number, describes the degree of oxidation of an atom in a chemical compound. Conceptually, the oxidation state, which may be positive, negative or zero, is the hypothetical charge that an atom would have if all bonds to atoms of different elements were 100% ionic, with no covalent component. This is never exactly true for real bonds.” (Wikipedia, 2018)

10. ‘Khan Academy’ website

   “What are oxidation numbers? Chemists use oxidation numbers (or oxidation states) to keep track of how many electrons an atom has. Oxidation numbers don’t always correspond to real charges on molecules, and we can calculate oxidation numbers for atoms that are involved in covalent (as well as ionic) bonding.

   Guidelines for determining the oxidation number: Oxidation numbers are usually written with the sign $(+ \text{ or } -)$ first, then the magnitude, which is the opposite of charges on ions. Chemists use the following guidelines to determine oxidation numbers:

Step 1. Atoms in their elemental state have an oxidation number of 0.

Step 2. Atoms in monatomic (i.e. single atom) ions have an oxidation number equal to their charge.

Step 3. In compounds: fluorine is assigned a −1 oxidation number; oxygen is usually assigned a −2 oxidation number (except in peroxide compounds where it is −1, and in binary compounds with fluorine where it is positive); and hydrogen is usually assigned a +1 oxidation number except when it exists as the hydride ion, H^-, in which case rule 2 wins.

Step 4. In compounds, all other atoms are assigned an oxidation number so that the sum of the oxidation numbers on all the atoms in the species equals the charge on the species." (Khan Academy, 2019)