1.7: Mathematical Definition of a Group

Now that we have explored some of the properties of symmetry operations and elements and their behavior within point groups, we are ready to introduce the formal mathematical definition of a group.

A mathematical group is defined as a set of elements (g_1, g_2, g_3...) together with a rule for forming combinations $g_i g_j$. The number of elements h is called the *order* of the group. For our purposes, the elements are the symmetry operations of a molecule and the rule for combining them is the sequential application of symmetry operations investigated in the previous section. The elements of the group and the rule for combining them must satisfy the following criteria.

1. The group must include the identity E, for which
$$Eg_i = g_i \tag{7.1}$$
for all the elements of the group.
2. The elements must satisfy the *group property* that the combination of any pair of elements is also an element of the group.
3. Each element g_i must have an inverse g_i^{-1}, which is also an element of the group, such that
$$g_i g_i^{-1} = g_i^{-1} g_i = E \tag{7.2}$$
(e.g. in C_{3v} the inverse of C_3^+ is C_3^-, the inverse of (σ_v is σ_v', the inverse g_i^{-1} effectively 'undoes' the effect of the symmetry operation g_i).
4. The rule of combination must be associative i.e.
$$(g_i g_j)(g_k) = g_i(g_j g_k) \tag{7.3}$$

The above definition **does not** require the elements to commute, which would require

$$g_i g_k = g_k g_i \tag{7.4}$$

As we discovered in the C_{3v} example above, in many groups the outcome of consecutive application of two symmetry operations depends on the order in which the operations are applied. Groups for which the elements do not commute are called *non-Abelian* groups; those for which they elements do commute are *Abelian*.

Group theory is an important area in mathematics, and luckily for chemists the mathematicians have already done most of the work for us. Along with the formal definition of a group comes a comprehensive mathematical framework that allows us to carry out a rigorous treatment of symmetry in molecular systems and learn about its consequences.

Many problems involving operators or operations (such as those found in quantum mechanics or group theory) may be reformulated in terms of matrices. Any of you who have come across transformation matrices before will know that symmetry operations such as rotations and reflections may be represented by matrices. It turns out that the set of matrices representing the symmetry operations in a group obey all the conditions laid out above in the mathematical definition of a group, and using matrix representations of symmetry operations simplifies carrying out calculations in group theory. Before we learn how to use matrices in group theory, it will probably be helpful to review some basic definitions and properties of matrices.