

## 1.28: Summary

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Hopefully this course has given you a reasonable introduction to the qualitative description of molecular symmetry, and also to the way in which it can be used quantitatively within the context of group theory to predict important molecular properties. These main things you should have learnt in this text are:

1. How to identify the symmetry elements possessed by a molecule and assign it to a point group.
2. The consequences of symmetry for chirality and polarity of molecules.
3. The effect of applying two or more symmetry operations consecutively (group multiplication)
4. How to construct a matrix representation of a group, starting from a suitable set of basis functions.
5. How to determine the irreducible representations spanned by a basis set, and construct symmetry adapted linear combinations (SALCs) of the original basis functions that transform as the irreducible representations of the group.
6. How to construct molecular orbitals by taking linear combinations of SALCs of the same symmetry species.
7. How to set up and solve the secular equations for the molecule in order to find the molecular energy levels and orbital coefficients – “Extra for experts”, though you will cover this in later courses
8. How to determine the symmetries of the various modes of motion (translational, rotational and vibrational) of a polyatomic molecule, and the symmetries of individual vibrational modes.
9. How to determine the atomic displacements in a given vibrational mode by constructing SALCs in the  $3N$  Cartesian basis.
10. How to determine atomic displacements in stretching and bending vibrations using internal coordinates.
11. The consequences of symmetry for the selection rules governing excitation to different electronic and vibrational states.

### Contributors and Attributions

[Claire Vallance](#) (University of Oxford)

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