

1.13: Irreducible representations and symmetry species

The two one-dimensional irreducible representations spanned by s_N and s'_1 are seen to be identical. This means that s_N and s'_1 have the 'same symmetry', transforming in the same way under all of the symmetry operations of the point group and forming bases for the same matrix representation. As such, they are said to belong to the same *symmetry species*. There are a limited number of ways in which an arbitrary function can transform under the symmetry operations of a group, giving rise to a limited number of symmetry species. Any function that forms a basis for a matrix representation of a group must transform as one of the symmetry species of the group. The irreducible representations of a point group are labeled according to their symmetry species as follows:

- i. 1D representations are labeled A or B , depending on whether they are symmetric (character +1) or antisymmetric (character -1) under rotation about the principal axis.
- ii. 2D representations are labeled E , 3D representations are labeled T .
- iii. In groups containing a center of inversion, g and u labels (from the German *gerade* and *ungerade*, meaning symmetric and antisymmetric) denote the character of the irreducible representation under inversion (+1 for g , -1 for u)
- iv. In groups with a horizontal mirror plane but no center of inversion, the irreducible representations are given prime and double prime labels to denote whether they are symmetric (character +1) or antisymmetric (character -1) under reflection in the plane.
- v. If further distinction between irreducible representations is required, subscripts 1 and 2 are used to denote the character with respect to a C_2 rotation perpendicular to the principal axis, or with respect to a vertical reflection if there are no C_2 rotations.

The 1D irreducible representation in the C_{3v} point group is symmetric (has character +1) under all the symmetry operations of the group. It therefore belongs to the irreducible representation A_1 . The 2D irreducible representation has character 2 under the identity operation, -1 under rotation, and 0 under reflection, and belongs to the irreducible representation E .

Sometimes there is confusion over the relationship between a function f and its irreducible representation, but it is quite important that you understand the connection. There are several different ways of stating the relationship. For example, the following statements all mean the same thing:

- " f has A_2 symmetry"
- " f transforms as A_2 "
- " f has the same symmetry"

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