We are applying Symmetry and Group Theory to molecules for the purpose of explaining/predicting spectroscopic features. You already know the relevant symmetry operations: identity (E), rotations (Cn), reflections (σv/h/d), inversion (i), and improper rotations (Sn). “Groups” are the point groups.

Point groups follow the mathematical rules of Group Theory, listed below. **We will use dichloromethane, the C2v point group, and its operations for this exercise.** **For each rule, provide an example that follows the rule. Use an algebraic representation of the rule and show the symmetry operation(s) associated with the algebraic representation.** Use my answer for the first rule as a model for providing answers for the rest of the rules.

**C2v point group has symmetry operations: E, C2, σv(xz), σv(yz). The major rotational axis is defined as z.**

1. *A group has an identity operation such that it commutes with all symmetry operations in the group and leaves them unchanged.*
2. *Each operation can operate as an inverse such that when an operation is combined with its inverse, the result is the identity.*
3. *The product of any two operations in the group must produce an operation that is also a member of the group.* (Products of operations act like performing a sequence of operations, one after another.)
4. *Symmetry operations in a group have the associative property of combination such that (AB)C = A(BC).* [Meaning that if you perform 3 operations one after the other, you can do them in any order, like multiplying numbers together: (2 x 3) x 5 = 2 x (3 x 5).]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **C2v** | E | C2 (z) | σv(xz) | σv(yz) |
| x |  | -1 |  |  |
| y |  | -1 |  |  |
| z |  | 1 |  |  |
| Rx |  |  |  |  |
| Ry |  |  |  |  |
| Rz |  |  |  |  |

Consider an x, y, z coordinate system like the one sketched nearby with a positive and negative direction associated with each axis. A table of the C2v with its operations is also shown.

+z

+x

+y

For each linear function, x, y, z, consider what happens to the “sense of direction” when performing each symmetry operation.

*If I perform the C2 operation around the z axis, the sense of direction changes for x and y, but stays the same for z.* The notation shown in the table indicates these results.

+z

+x

+y

+z

+x

+y

*C2 around z-axis*

Perform the rest of the operations for x, y, z and the sense of rotation around each axis. Fill in the rest of the table: if the sense of direction stays the same (1) or changes to the opposite sense of direction under the operation (-1).

**Show each of your operations; attach scrap if needed.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **C2v** | E | C2 (z) | σv(xz) | σv(yz) | *Linear functions (x,y,z) and/or rotations (Rx, Ry, Rz)* |
| A1 | 1 | 1 | 1 | 1 |  |
| A2 | 1 | 1 | -1 | -1 |  |
| B1 | 1 | -1 | 1 | -1 |  |
| B2 | 1 | -1 | -1 | 1 |  |

In character tables, the most “symmetric” mode is often labeled A1. *Which linear &/or rotational function matches the pattern for A1? What about the others?*

*Did you just build a character table??? I think you did!*