

Week 1

A Rigorous Definition of Symmetry

1.1 Symmetry: Symmetry Elements and Operations

- 9/28:
- Dr. Anna Wuttig (AH-nuh WUH-tig).
 - Teaches exclusively on the blackboard.
 - Will record lectures, however; if there is a technical error, she will upload last year's lecture.
 - Syllabus.
 - PSets graded on completion, not accuracy.
 - Two exams: One on the first half of the course; one on the second half of the course.
 - Cumulativeness: You'll need to understand the first half to do the second half, but there won't be questions specifically targeted to first-half material.
 - No final.
 - Participation. Showing up to class and working in groups.
 - Chris, Dan, Amy, Matt, Jintong, Yibin, Ben, Sara, Ryan, Joe, Owen, Isabella, Pierce are the people.
 - People come from a diversity of chemistry subfields (physical, inorganic, organic, materials, biological).
 - Every day will have a handout that we will write on (in pencil).
 - Study the learning objectives!
 - (Local) symmetry of a molecule helps us predict and describe bonding, spectroscopic properties, and reactivity.
 - We describe symmetry with group theory.
 - **Symmetry operation:** An operation which moves a molecule into a new orientation equivalent to its original one (geometrically indistinguishable).
 - Symmetry operations that can be applied to an object always form a **group**.
 - **Symmetry element:** A point, line, or plane about which a symmetry operation is applied.
 - Symmetry operations.
 1. Identity operation (E): Do nothing; null operation.
 2. Reflection through a plane (σ): Subdivided into...

- σ_d : dihedral mirror planes, which contain the principle C_n axis and bisect the angles formed between adjacent C_2 axes;
 - σ_h : horizontal mirror planes, in which the mirror plane is perpendicular to the principal C_n axis;
 - σ_v : vertical mirror planes, which contain the C_n axis and are not dihedral mirror planes.
3. Rotation about an axis (C_n): A clockwise^[1] rotation about the C_n axis.
 4. Improper rotation (S_n): A two-step symmetry operation consisting of a C_n followed by a σ that is perpendicular to C_n (i.e., σ_h).
 5. Inversion (i): Take any point with coordinates (x, y, z) to $(-x, -y, -z)$.
- To describe the operations, we'll introduce **stereographic projections**.



Table 1.1: Symbols for stereographic projections.

- We have a working area (the plane of the page is the xy -plane). It is useful to draw quadrants.
- We describe a general point which experiences our symmetry operation.
- We need a gear symbol in the middle for rotations and improper rotations (see Table 1.1).
 - Must stereographic projections be drawn one at a time because it seems that the squares should not be in a reflection?
 - No — the symbols are to help us and should be included somewhere, but there are no hard-and-fast rules.
- Stereographic projections for each of the five elementary symmetry operations.

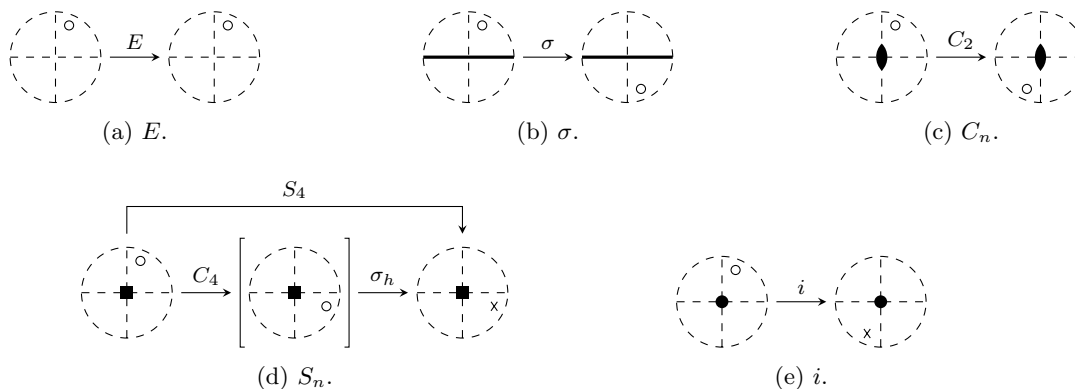


Figure 1.1: Stereographic projections of the elementary symmetry operations.

- Principal C_n axis: The C_n axis for which n is the highest.
 - In a stereographic projection, the C_n axis is the one that is perpendicular to the working area (goes in/out of the page).
- Example: Give the symmetry elements of NH_3 .

¹Really?

- C_3 axis, 3 σ_v mirror planes (denoted σ_v , σ'_v , and σ''_v).
 - The symmetry operations are E , C_3 , C_3^2 , σ_v , σ'_v , and σ''_v . These operations form the C_{3v} point group.
- Direct products of symmetry operations: $YX = Z$ means “operation X is carried out first and then operation Y ,” giving the same net effect as would the carrying out of the single operation Z .
 - If $YX = XY = Z$, then the two operations Y and X commute.
- What is the direct product of C_2 and σ_h ?
 - $\sigma_h C_2 = S_2 = i$. They do commute.
- Do C_4 and $\sigma_{x,z}$ commute? Take the plane of this page as xy .
 - They do not (determine by drawing out both sets of stereographic projections).
- Don't get careless, Steven. This is easy, but it's also easy to make easy mistakes.
- New symmetry operations *of your group* are generated by taking the direct product of two.