Tutorial: Point groups

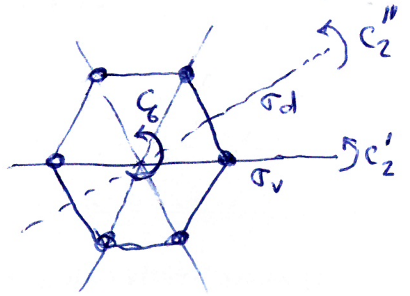
T1

- point groups in the 3D space are subgroups of $O(3)$ =
  = group of all proper and improper rotations (including reflections and inversion) in the space around all axes passing through a fixed point
  - these transformations preserve distances between points and they can be represented as 3x3 orthogonal matrices with determinant = +1 (proper) and −1 (improper rot.)
- we distinguish elements of symmetry (geometrical objects) and operations of symmetry (geometrical transformation) but they are often denoted in the same way
- elements of point groups can be (except identity E)

1) proper rotation C_n by angle $\varphi = \frac{2\pi}{n}$
   - symmetry element = rotation axis denoted also C_n
   - symmetry operations = rotation C_n, but also its multiples $C_n^2, C_n^3, \dots, C_n^{n-1}$ ($C_n^n = E$)
   - main rotation axis of a point group = C_n with the largest n

2) reflections σ_v, σ_d and σ_h
   - element = mirror plane, operation = reflection ($\sigma^2 = E$)
   - we use σ_h (horizontal) for the mirror plane $\perp$ to C_n and σ_v or σ_d for planes $\parallel$ with C_n
   - σ_v is more usual, used even when there is no axis $C_2 \perp C_n$
     if there is $C_2 \perp C_n$, then σ_v goes through C_n and C_2 and σ_d bisects the angle between C_2 axes
   - but sometimes not clear, then it depends on our choice

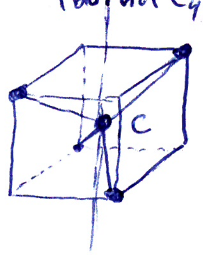
C_6H_6 (benzene)



3) improper rotations S_n by angle $\varphi = \frac{2\pi}{n}$

- at the same time as rotation, we reflect through $\sigma_h \perp S_n$

CH_4 $\circlearrowleft S_4$ (but not C_4)



- element = improper rotation axis S_n
- even though one can write $S_n = \sigma_h \cdot C_n$, that does not mean that if S_n is in a point group, there are also σ_h and C_n in this group (see CH_4)
- even multiples give proper rotations $S_n^{2k} = C_n^{2k}$
- $\sigma_h = S_1$ (no rotation)
- $S_n^n = \begin{cases} E & \text{for even } n \\ \sigma_h & \text{for odd } n \end{cases}$, as $S_n^n = \underbrace{C_n^n}_{=E} \sigma_h^n$ (note that C_n and σ_h commute)

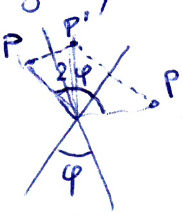
4) inversion i, element = point of inversion (usually origin)

- change of signs of all coordinates $x_i \Leftrightarrow -x_i$
- $i = S_2$ as rotation changes the sign of two axes and the reflection of the third axis

- thus i, σ_h, σ_v and σ_d are just special cases of S_n, but for simplicity these symbols are often used
- the presence of some symmetry elements forces the presence of others

for example: if there are C_n and $C_2 \perp C_n$ present then there are $n-1$ other C_2 axes $\perp C_n$

or if two mirror planes σ_v and σ_v' make an angle φ then a rotation by 2φ is forced: $\sigma_v \sigma_v' = C(2\varphi)$



Classification of point groups (for molecules)

- see the algorithm below in Czech (ano = yes, ne = no, jediná C_n = only one C_n)
- 7 infinite series - $\underbrace{C_n, S_{2n}, C_{nh}, C_{nv}}_{\text{only one rotational axis + possibly mirror planes}}$, $\underbrace{D_n, D_{nd}, D_{nh}}_{\text{dihedral groups with } C_2 \perp C_n}$
- notice $S_2 = C_i$, $C_s = C_{1h} = C_{1v}$
- 7 groups with more than one C_n: $T, \underset{\uparrow \text{ tetrahedron}}{T_d}, T_h, O, \underset{\uparrow \text{ cube}}{O_h}, I, \underset{\uparrow \text{ icosahedron}}{I_h}$
- linear molecules - limits as $n \to \infty$: $C_{\infty v}$ (heterogeneous mol.), $D_{\infty h}$ (homogeneous)

10.3. Schéma k určení bodové grupy symetrie