Point symmetry groups of SF_6

Deadline: Monday, **November 4, 2024**

1. (5 points) For the molecule of sulfur hexafluoride SF_6 (it is used as electrical insulation) in its equilibrium geometry, determine

   (a) its point group of symmetry (for further reference, let us denote it as G_1),

   (b) the conjugacy classes of this group,

   (c) and whether this group is a direct or semidirect product of its two subgroups.

   Explain briefly your answers for (b) and (c), based on general considerations discussed during lectures.

2. (10 points) Three fluorine atoms of SF6 with the same distance from each other form an equilateral triangle. We can deform the molecule by rotating this triangle by an angle φ around the axis that goes through its center of mass and the sulfur atom.

   (a) Determine the symmetry group of this new non-equilibrium configuration for $\varphi = 60°$ (let us denote it as G_2) and also for $0° < \varphi < 60°$ (a group G_3).

   (b) Are these groups a direct or semidirect product of its two subgroups?

   (c) Are these groups isomorphic to some subgroups of G_1?

   (d) For the group G_2, find its conjugacy classes and for two chosen classes with more than one element determine their corresponding isotropy groups (when the inner automorphism on G_2 is considered) and also class constants of their product.

   (e) Find a subgroup of order 4 of the group G_2 and determine all its left cosets. Is it a normal subgroup?

3. (5 points) When using some particular codes in quantum chemistry calculations, we can often choose only commutative point groups of symmetry, even for molecules with higher symmetry.

   (a) What are the largest commutative subgroups of G_1, G_2, and G_3? To what point groups are they isomorphic? What relations are among them?

   (b) Find examples of non-equilibrium configurations of SF_6 which have as their symmetry groups these commutative subgroups.