Point group theory

Introduction

During the laboratory, you will familiarize yourselves with the Point group theory. We will analyze the vibrational properties of different molecules.
The Point Group describes all the symmetry operations that can be performed on a molecule that result in a conformation indistinguishable from the original. Point groups are used in the Points Group Theory, the mathematical analysis of groups, to determine properties such as types of vibrations.

1. Familiarize yourself with basic information about group theory.
a. Characterize the basic elements of symmetry: proper axis, symmetry plane, center of symmetry, improper axis.
b. Describe the symmetry operations associated with the symmetry elements listed in point 1a.
c. Define the concepts of irreducible and reducible representations.
2. Based on the Points group theory, perform the analysis of water molecule vibrations.
3. Based on the Points group theory, perform the analysis of ammonia molecule vibrations.
4. Based on the Points group theory, perform the analysis of one, other molecule than those mentioned in points 3 and 4.
5. Prepare your report.
The report should contain the following parts: 1. Theoretical introduction. 2. Analysis of 3 molecules based on the Point group theory. 4. The conclusions of the performed exercise. 5. References.

The report should be returned in two weeks from the laboratory. Please deliver the report to secretary of MITR (room 101 at the ground floor of the building). The 0.5 will be deducted from the final grade after each week of the delay in delivery of the report.

Literature:

1. Z. Kęcki, Podstawy spektroskopii molekularnej, PWN, Warszawa 1992
2. Peter Atkins, Atkins' Physical Chemistry