Module: Elective Advanced Lectures: BCGS Courses

Module No.: physics70d

Course: Fundamentals of Molecular Symmetry (E/A/T)

Course No.:

Category	Type	Language	Teaching hours	CP	Semester
Elective	Lecture	English	2	4	ST

Requirements for Participation:

Preparation:
Basic knowledge of quantum mechanics

Form of Testing and Examination:
Oral Examination

Length of Course:
1 semester

Aims of the Course:
Understanding the fundamental concepts of representation theory and its application to describe the symmetry of molecules

Contents of the Course:
The lecture introduces to group theory with special emphasis on representations and their use to describe the symmetry of molecules in high-resolution spectroscopy and in molecular physics generally. The theory is accompanied by a series of "prototypical" examples Topics covered are
- symmetry in general and symmetry of a molecule.
- groups and point groups.
- irreducible representations, characters.
- vanishing integral rule
- the Complete Nuclear Permutation-Inversion (CNPI) group.
- the Molecular Symmetry (MS) group).
- the molecular point group.
- classification of molecular states: electronic, vibrational, rotational, and nuclear spin states
- nuclear spin statistical weights
- hyperfine structure
- non-rigid molecules (inversion, internal rotation)

Recommended Literature:
Jensen: Script (text of powerpoint presentation files; available during the course)
P. Jensen and P. R. Bunker: The Symmetry of Molecules, in: "Encyclopedia of Chemical Physics and Physical Chemistry" (J. H. Moore and N. D. Spencer, Eds.), IOP Publishing, Bristol, 2001.
P. R. Bunker and Per Jensen: "Molecular Symmetry and Spectroscopy, 2nd Edition," NRC Research Press, Ottawa, 1998 (ISBN 0-660-17519-3).
P. R. Bunker and P. Jensen: "Fundamentals of Molecular Symmetry", IOP Publishing, Bristol, 2004 (ISBN 0-7503-0941-5).