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Fachgruppe Chemie & Biologie

BERGISCHE UNIVERSITÄT WUPPERTAL

Fundamentals of Molecular Symmetry

An internet lecture course

Welcome to Fundamentals of Molecular Symmetry – The Lecture Course!

The lectures introduce group theory with special emphasis on representations and their use in describing the symmetry of molecules in theoretical chemistry and in molecular physics generally. The theory is accompanied by a series of "prototypical" examples, mostly concerned with applications of symmetry principles in high-resolution molecular spectroscopy.

Format

This course is planned in the classical, so-called 2+1 format of German universities: a 90-minute lecture session and a 45-minute exercise session per week for 11 weeks.

The exercise session should be taught by a 'local' 'lab instructor', for whom solutions to the exercise problems will be provided. For each of the 11 weeks of the course, the following internet resources should be made available to the students:

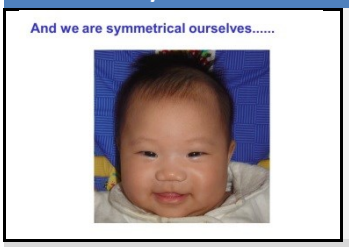
- A video file with the lecture of the week.
- A pdf file with powerpoint slides shown during the week's lecture.
- A sheet with the problems suggested for the exercise session of the week.

All files can be freely downloaded from the internet; the corresponding links are given below together with keywords for the individual lectures.

When the video files are being watched on the screen of an ordinary computer, the picture of the powerpoint slides is relatively small. It is conceivable that there will be occasional difficulties reading the smaller print directly from the video file. To circumvent this problem, we supply the pdf files generated from the powerpoint files. In my experience, these files are readable also on small screens. A few typographical problems were discovered as the lectures were recorded. I have generally tried to correct these in the pdf files generated from the powerpoint files. That is, for a few slides distributed over the 11 lectures, the layout in the pdf file is

nicer and clearer than in the file used for the video recording. However, these changes are purely cosmetic, there has been no change of the informational content. In the same vein, I discovered two mistakes, one in Lecture 10 and one in Lecture 11, while giving these lectures and I pointed out the mistakes and corrected them with the red pen. These mistakes have been corrected in the pdf files.

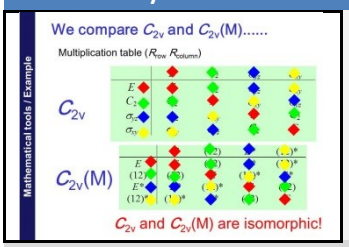
Week 1/11



The concept of symmetry in everyday life, geometrical symmetry, symmetry in quantum mechanics, permutation-inversion symmetry, groups and symmetry groups.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung1.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture1.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week1.pdf

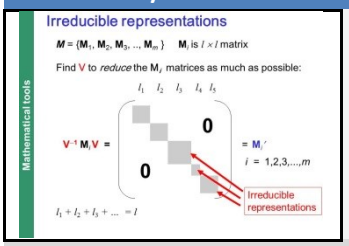
Week 2/11



Permutation-inversion symmetry and groups continued, subgroups, isomorphism, homomorphism, classes, point groups, matrix groups, representations.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung2.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture2.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week2.pdf

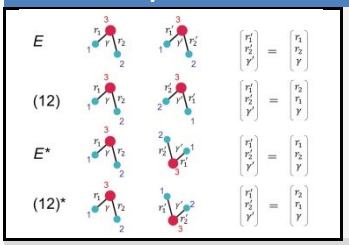
Week 3/11



Equivalent representations, characters, characters and classes, irreducible representations, determination of irreducible representations.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung3.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture3.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week3.pdf

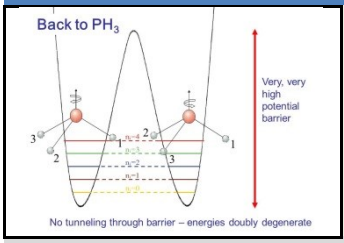
Week 4/11



Irreducible representations continued, generation of representations, reduction of representations, effect of a symmetry operation on a wavefunction.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung4.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture4.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week4.pdf

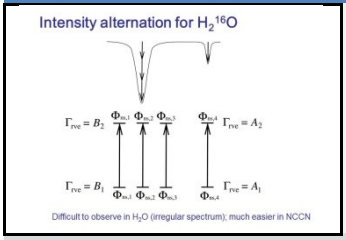
Week 5/11



The molecular Hamiltonian and its symmetry, symmetry classification for non-degenerate and degenerate molecular states, the Complete Nuclear Permutation-Inversion Group, feasibility, the Molecular Symmetry (MS) Group, isomorphism of MS group and point group at equilibrium for rigid molecules.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung5.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture5.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week5.pdf

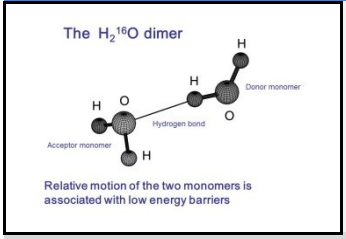
Week 6/11



Nonrigid molecules, nuclear spin statistical weight factors.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung6.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture6.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week6.pdf

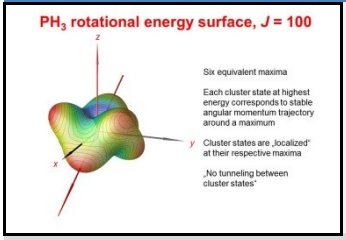
Week 7/11



Hyperfine structure, forward and reverse correlation.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung7.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture7.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week7.pdf

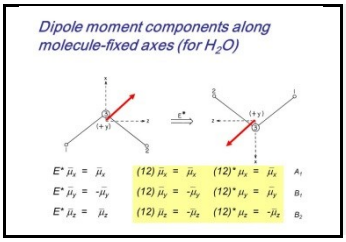
Week 8/11



Energy level cluster formation, vanishing integral rule, symmetry of a product, optical selection rules.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung8.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture8.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week8.pdf

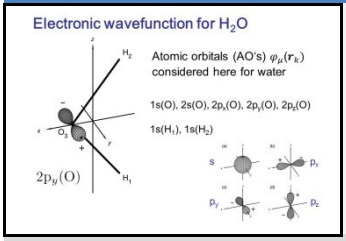
Week 9/11



Optical selection rules continued, the molecular wavefunction.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung9.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture9.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week9.pdf

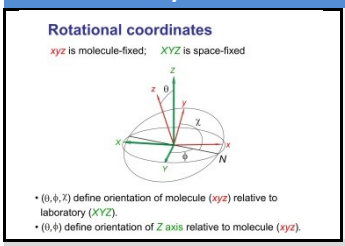
Week 10/11



Electronic wavefunctions and their symmetries, vibrational wavefunctions and their symmetries.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung10.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture10.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week10.pdf

Week 11/11



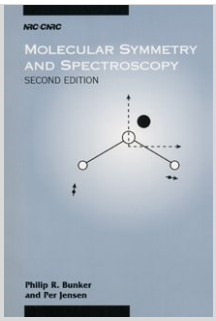
Rigid (static) rotor wavefunctions and their symmetries, rotational selection rules.

- Video file: http://podcast.uni-wuppertal.de/wp-content/uploads/2014/01/Vorlesung11.mp4
- Slides: http://www.chem.uni-wuppertal.de/theochem/FMS-lecture11.pdf
- Problems: http://www.chem.uni-wuppertal.de/theochem/FMS_exercise_week11.pdf

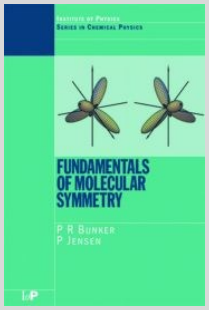
Literature

The recommended literature for this lecture course are the two monographs on the subject by Bunker and Jensen together with the review article in “Encyclopedia of Chemical Physics and Physical Chemistry”:

- P. R. Bunker and P. Jensen: “Molecular Symmetry and Spectroscopy, 2nd Edition,” NRC Research Press, Ottawa, 1998 (ISBN 0-660-17519-3).
- 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 P. Jensen: “Fundamentals of Molecular Symmetry,” IOP Publishing, Bristol, 2004 (ISBN 0-7503-0941-5).



"Molecular Symmetry and Spectroscopy, 2nd Edition" is at a level appropriate for graduate students and researchers in molecular sciences. It is now out of regular print but an e-book version is available from NRC Research Press, see http://www.nrcresearchpress.com/doi/book/10.1139/9780660196282, and print-on-demand paper books are available from the company *Volumes* (in Kitchener, Ontario, Canada), see http://www.volumesdirect.com/detail.aspx?ID=5126.



"Fundamentals of Molecular Symmetry" is an introductory text, suitable for students starting out in the field. It is in regular print, see http://www.crcpress.com/product/isbn/9780750309417.

The review article in "Encyclopedia of Chemical Physics and Physical Chemistry" is a highly condensed presentation of the theory covered in the lecture; it may also be useful for readers starting out in the field.

Acknowledgments

The lectures in this series have reached their present form through writing and teaching activities taking place over a period of many years. Many of these activities involved collaboration with my erstwhile Ph.D. supervisor, Dr. Phil(ip R.) Bunker (National Research Council of Canada, Ottawa), and I thank him for introducing me to the subject of molecular symmetry now more than 30 years ago and inviting me to join him in extending the first edition of "Molecular Symmetry and Spectroscopy."

The first time I gave a complete lecture course on this subject was in the Winter Term 2002/2003 at the University of Cologne. This course took place at the initiative of the late Professor Gisbert Winnewisser, for whose enthusiastic support I am grateful. The exercises accompanying these first lectures were led by (present-day) Drs. Petra Neubauer-Guenther and Guido Fuchs, whose assistance with the preparation of the exercise problems was very helpful. (Present-day) Drs. Oliver Baum and Monika Körber gave similar help at later times.

Since the start of the present millennium, I have had the pleasure of being invited to teach this lecture course, or parts of it, at several locations away from Wuppertal. I thank the various colleagues who invited me for this and have endeavoured to remember them all: Professor Štěpán Urban (Vysoká Škola Chemicko-Technologická v Praze, Prague), Professors Stephan Schlemmer and Thomas Giesen (Universität zu Köln), Professor Pedro Gómez Calzada (Universidad Complutense, Madrid), Professors Keiko Takano and Keiko Miyamoto (Ochanomizu University, Tokyo), Professors Miguel Carvajal Zaera and Francisco Pérez-Bernal (Universidad de Huelva), Professors Rafael Escribano and Victor Herrero (Consejo Superior de Investigaciones Científicas, Madrid), and Professor Takayoshi Amano (then at Ibaraki University in Mito).

Some slides in the powerpoint presentations were originally prepared by (present-day) Drs. Sergei N. Yurchenko, Miguel Carvajal Zaera, and Vladlen V. Melnikov – I thank them for this. I also thank Professor Hai Lin (University of Colorado at Denver) for permission to use the picture of his baby daughter to illustrate the point of human beings having geometrical near-symmetry.

The present electronic version of the lecture has been prepared through the efforts of Messrs. Marc Stania, Hubertus Knopff, and Uli Christmann of the Zentrum für Informations- und Medienverarbeitung (ZIM) at the University of Wuppertal. I am very grateful to these three gentlemen, to the director of ZIM Mr. Dieter Huth, and to M.Sc. Saskia Springmann for being a highly active member of the audience, whose constructive suggestions for improvements of the lecture were very valuable.

I thank in advance Professors Thomas Giesen (now at the University of Kassel) and Stephan Schlemmer (Universität zu Köln) for them kindly giving me the opportunity to try out the electronic version of the lecture at their respective institutions in the Summer Term of 2014.

Wuppertal, January 2014
Per Jensen