Schema KZ4012 Kemisk bindning, 5 hp

HT2018-VT2019 (17.12.2017 – 18.01.2018)

dag vecka	måndag	tisdag	onsdag	torsdag	fredag
51 17/12-22/12	F1 Math/RÖ1	F2 RÖ2	F3 RÖ3	F4 Labb1	F5 RÖ4
2018					
01 31/12- 04/01				Labb2 Labb2	Utvärdering Rapportskr. Labb 2
02 07/01- 11/01	F6 RÖ5	F7 RÖ6	F8 RÖ7	Labb3 Labb3	Utvärdering Rapportskr. Labb3
03 14/01- 18/01	Reservlabb 1 och Reservlabb 2		F9 (Q&A)		Tenta

Tider: fm 9:15 – 12; em: 13 – 17
F (1-8) föreläsningar, RÖ (1-7) räkneövningar, L (1-3) labbar
F1-3, F5-9: Ulrich Häussermann (ulrich.haussermann@mmk.su.se)
F4: Lorenzo Agosta (lorenzo.agosta@mmk.su.se)
Math: Lorenzo Agosta (lorenzo.agosta@mmk.su.se
RÖ1-3: Lorenzo Agosta (lorenzo.agosta@mmk.su.se),
RÖ4-6 Ulrich Häussermann (ulrich.haussermann@mmk.su.se
Labb 1,2: Lorenzo Agosta (lorenzo.agosta@mmk.su.se),
Labb3: Lorenzo Agosta , Zoltan Bacsik (zoltan.bacsik@mmk.su.se)

Plats: Sal **K447** för föreläsningar och övninar. Datasalen för labbarna 1 och 2.

Kurslitteratur:

1) P. Atkins, J. de Paula, R. Friedman, “Quanta, Matter and Change”, Second edition, Oxford, 2014; (används tidigare i fysikalisk kemi)
2) “Inorganic Chemistry” 7th edition , 2018 (by Mark Weller, Tina Overton, Jonathan Rourke, Fraser Armstrong) ISBN: 9780198768128 (används senare i oorganisk kemi), Kapitel 1, 2, 3.

Notera att vi har inte möjlighet att erbjuda reservlab till labb3

Föreläsningar (focus & topic info refer to the Atkins book)

F1 – F4: Molecular structure (Focus 6)

F1: Repetition H-atom and many-electron atoms (topics 18, 19), periodicity (topic 20), atomic spectroscopy (brief) (topic 21). Outlook molecules.

F2: Molecular orbital theory, effective Hamiltonians, variation principle (topic 23), homonuclear and heteronuclear diatomic molecules, the polar bond (topics 24, 25),

F3: Polyatomic molecules, π-systems and Hückel approach (topic 26), valence bond theory (topic 22)

F4: Introduction into Gaussian program package (used in the computer lab), self consistent fields (topic 27), ab-inito methods and DFT (excerpts topics 29, 30), examples of computational chemistry

F5 – F7: Molecular symmetry (Focus 7)

F5: Symmetry in chemistry, analysis of molecular shape, symmetry elements and operations, symmetry classification of molecules (topic 31)

F6: Group theory and its tools (topic 32), applications of symmetry (topic 33)

F7: Application of symmetry to orbitals: revisit ring systems (organic molecules), MOs for basic shapes of inorganic molecules, symmetry adaption of ligand basis functions, valence bond theory vs MO theory

F8: Vibrational and electronic spectroscopy (Focus 9)

F8: Vibrational spectroscopy of polyatomic molecules: IR and Raman spectrometers (topic 40, excerpts), normal modes, selection rules, interpretation of spectra (topic 44), utilizing spectroscopy for the characterization of molecules. Application of symmetry to vibrational and electronic spectroscopy: irreducible representation of modes, establishing modes for basic shapes of inorganic molecules, principles of UV-VIS (absorption)spectrometers (topic 40, excerpts), electronic spectroscopy, electronic transitions (topic 45).

F9: Q&A, Exam preparation (frågestund…).

Räkneövningar:

Math: introduction/repetition of some linear algebra (linear equation systems, matrices, determinants)

RÖ1: Properties of atomic orbitals, construction of diatomic MOs

RÖ2 and 3: Exercising the Hückel method (setting up hamiltonian matrices and diagonalization): allyl system, butadien system, general ring systems. By hand and with Matlab. Introduction of take-home exercise (e.g. benzene and cyclopentadiene).

RÖ4: Finding symmetry elements, handling symmetry operations, symmetry classification of molecules.

RÖ5: Application of symmetry to orbitals, part1

RÖ6: Application of symmetry to orbitals, part 2

RÖ7: Application of symmetry to vibrations

Laboratory:

1. Computer-lab 1: Atoms and diatomic molecules (homo- and heteronuclear) O_2, LiF. MO diagrams, potential energy curves, dissociation energy.

2. Computer-lab2: Polyatomic molecules. AH_2 (BeH_2, OH_2). Walsh diagram, number of valence electrons governs molecular structure. Organic molecules (isomers of butadiene). Geometry optimization, determination of most stable isomers from Gaussian calculations. Calculation of vibrational frequencies.

3. Spectroscopy-lab: Collecting Raman, IR, UV-VIS spectra of various compounds. Evaluation and interpretation of spectroscopic data.