



COURSE DATASHEET

Semester:	2016/17/1
Course:	Theoretical Inorganic Chemistry
Code:	VEMKAKM112E
Responsible department:	Department of General and Inorganic Chemistry
Department code:	MKAK
Responsible instructor:	dr. Zsolt Valicsek

Course objectives:

Better understanding the relationship between the structure and physico-chemical properties of inorganic compounds

Course content:

1. Introduction. Foundation of quantum mechanics. Wave-particle duality. Uncertainty relationships, physical meaning of Schrödinger equation. Tunnel effect. 2. Electronic structure and spectra of hydrogen atom and many electron atoms 3. Spin-orbit coupling, heavy atom effect, Russell-Saunders and j-j coupling scheme, microstates, atomic terms. symmetry and/or spin forbidden transitions, Zeeman effect 4. Symmetry of molecules: symmetry operation, symmetry elements, pointgroup 5. Basic concepts of group theory, reducible and irreducible representation, character table, formula for reduction 6. Application of character tables for simple molecules. Determination of the symmetry of normal vibrations. Assignment of IR and Raman band. 7. Middle semester test. Basic concept of LCAO method: secular determinant, solution for homonuclear case. 8. Electronic structure of homonuclear diatomic molecule for the second row elements of periodic table. Molecular terms. Spin or/and symmetry forbidden transitions 9. Electronic structure of heteronuclear diatomic triatomic molecules: LIH, HF, CO, NO CN-, H₂O, CO₂ 10. Many atom molecules. Walsh diagram. Hückel method for conjugate system. 11. Interpretation of the electronic structure of many atom molecules by VSEPR model 12. Interpretation of the electronic structure of many atom molecules by VB method 13. Interpretation of the electronic structure of transition metal complexes by VB method 14. Interpretation of the electronic structure of transition metal complexes by LCAO-MO method 15. Final semester test

Requirements, evaluation and grading:

The weighted average of middle and final semester test has to reach 2,00. The final mark is calculated from average of the tests and results of exam (weight ratio is 1:2, respectively)

Required and recommended readings:

1. Papp Sándor; Szervetlen Kémia II, Tankönyvkiadó Budapest 1983 2. F. A. Cotton and G. Wilkinson; Advanced Inorganic Chemistry John Wiley and Sons, New York, 1980