



PROGRAMS AND BIBLIOGRAPHY

| Subject | |
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| Code | Name |
| QI145 | Chemical Interactions |

Vector

OF:S-5 T:002 P:000 L:000 O:002 D:000 HS:004 SL:002 C:004 AV:N EX:S FM:75%

Pre requirement

QG108

Summary

Molecular orbital theory for polyatomic molecules. Introduction to group theory. Acids and bases.

Program

Molecular Orbitals

Introduction to group theory: symmetry, point groups and the use of the character table in the classification of molecules and orbitals. Molecular orbitals adapted by symmetry. Molecular orbital theory for polyatomic molecules (single species: H_3 and H_3^+ , H_2O , NH_3 and Walsh diagrams for molecules EH_2); Molecular orbitals for chains of atoms, hypervalent molecules, molecules with π bond and electron deficient molecules (examples: SF_6 fragment B-H-B of boranes, NO_2^-)

Acids and Bases

Bronsted acidity: H^+ in H_2O ; conjugate acids and bases; acidity and basicity of solvents. Periodic trends in Bronsted acidity: aqua-acids; oxo-acids (Pauling Rule); anhydrous oxides; amphoterism. Lewis acids and bases: periodic trends; examples of reactions: adduct formation (correlating with the molecular orbital); displacement reactions; metathesis. Structural and steric considerations on the strength of acids and bases in several theories. Hard and soft acids and bases including f elements. The interpretation of hardness/softness and usefulness of this concept. Surface acidity, for example, silica, alumina, aluminosilicates. Generalized concept of acids and bases. Hydrides - periodic trends.

Bibliography

Textbooks

C. E. Housecroft, A. G. Sharpe. Inorganic Chemistry. 4th ed. Upper Saddle River. NJ : Prentice-Hall, 2012. 754p.

G. L. Miessler, D. A. Tarr. Inorganic Chemistry. 4th ed., Harlow : Pearson, 2011. 1213p.

D. F. Shriver, P. W. Atkins, C.H. Langford. Inorganic Chemistry. 2nd. ed. Oxford : Oxford University Press, 1994. 819p.

Supplemental Readings

J. E. Huheey, E. A. Keiter, R. L. Keiter. Inorganic Chemistry: Principles of Structure and Reactivity. 4th ed. New York : Harper Collins, 1993. 964p.

S. F. A. Kettle. Symmetry and Structure: (Readable Group Theory for Chemists). 2nd ed. Chichester : John Wiley, 1995. 416p.

F. A. Cotton. Chemical Applications of Group Theory. 3th ed. New York: John Wiley, 1990. 461p.

G. M. Oliveira. Simetria de Moléculas e Cristais: Fundamentos da Espectroscopia Vibracional. Porto Alegre : Bookman, 2009. 269p.

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures.

For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.