



List of New Course(s) Introduced

Department : **Chemistry**

Programme Name : **M.Sc.**

Academic Year : **2018-19**

List of New Course(s) Introduced

Sr. No.	Course Code	Name of the Course
01.	CMT-405	Advanced Quantum and Computational Chemistry



Minutes of Meetings (MoM) of Board of Studies (BoS)

Academic Year : 2018-19

School : School of Studies of Physical Science

Department : Chemistry

Date and Time : Nov. 03, 2017 - 11:30 AM

Venue : Meeting room

The scheduled meeting of member of Board of Studies (BoS) of Department of Chemistry, School of Studies of Physical Science, Guru Ghasidas Vishwavidyalaya, Bilaspur was held to design and discuss the structure and scheme of examination of Integrated UG/PG, M. Sc. Chemistry syllabi.

The following members were present in the meeting:

1. Prof. Bali Ram (External Expert Member BoS, Dept. of Chemistry, BHU, Varanasi)
2. Prof. G. K. Patra (Member BoS, Dept. of Chemistry)
3. Dr. Charu Arora (HOD, Associate Prof., Dept. of Chemistry-cum Chairman, BOS)
4. Dr. Arti Srivastava (Member BoS, Assistant Professor, Dept. of Chemistry)

Following points were discussed during the meeting

1. Draft prepared to revise course structure and scheme of examination in the light of UGC directives (as per CBCS Scheme) to be implemented from 2018-19.
2. Elective paper Advanced Quantum and Computational Chemistry (CMT-405) has been incorporated in M.Sc. IV sem.
3. The core paper Organic Chemistry-IV (CBT-503) of B.Sc.-Vth sem has been interchanged with core paper Physical Chemistry-IV (CBT-601) to justify semester wise teaching load.

The following new courses were introduced in the B. Sc. and M. Sc.:

- ❖ B. Sc. CBCS scheme
- ❖ Advanced Quantum and Computational Chemistry (CMT-405)

अध्यक्ष/Head
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Scheme and Syllabus

CMT-407: Advanced Quantum and Computational Chemistry

Credits:3

Note: Prerequisite for this course: B Sc with Mathematics

1. Approximation Methods in Quantum Chemistry: Angular momentum: commutative relations and ladder operators. Addition of angular momenta—Clabsch-Gordan series, Term symbols for two equivalent electrons, Total angular momentum and spin-orbit interaction. Condon Slater Rules. Variation method, Stationary perturbation theory for non-degenerate and degenerate. Ground state of He atom. Time-dependent perturbation theory. Radiative transition, Einstein coefficients.
2. Many Electron atoms: Hartree-Fock SCF method, Roothaan-Hartree-Fock method. Selection of basis sets. Electronic structure calculations, Population analysis, Response properties, Electron correlation. Valence bond and molecular orbital theory
3. Correlated methods in quantum chemistry: Configuration interaction, Coupled cluster theory, Density functional Theory. Open shell systems; introduction to multi-reference methods of Hartree-Fock and correlated methods.
4. Applications of Quantum Chemistry: Computational Chemistry: Brief introduction. Application of quantum chemistry: Potential energy surface, Chemical reactivity, HSAB principle, Study of reaction mechanism (Finding Transition state), Rotational, vibrational and electronic Spectroscopy.

Books Recommended

1. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 3rd edition (1997), Oxford University Press. Oxford.
2. H. Eyring, J. Walter and G.E. Kimball, *Quantum Chemistry*, John Wiley, New York (1944)
3. I.N. Levine, *Quantum Chemistry*, 5th edition (2000), Pearson Educ., Inc., New Delhi.
4. G. M. Barrow, *Physical Chemistry*, Fifth edition, Tata MacGraw Hill, New delhi (1994).
5. J. N. Gurtu and A. Gurtu, *Advanced Physical Chemistry*, Pragati Edition, Meerut (2009).

Dr. H. H. S.

Dr. S.S.
23.06.18

Cham Akash
23-6-18
27.06.18

Dr. P. P.
23.06.18