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<tr><td>Course Code</td><td colspan="3">CHE302M3</td></tr>
<tr><td>Course Title</td><td colspan="3">Molecular Symmetry, Group Theory and Diffraction methods</td></tr>
<tr><td>Credit Value</td><td colspan="3">03</td></tr>
<tr><td rowspan="2">Hourly Breakdown</td><td>Theory</td><td>Practical</td><td>Independent Learning</td></tr>
<tr><td>45</td><td>-</td><td>105</td></tr>
<tr><td>Objective/s</td><td colspan="3">• Recognize symmetry elements in molecules
• Reduce a reducible representation to its component as irreducible representation
• Define the character of matrix representing a symmetry operation
• Identify the Symmetry Adapted Linear Combinations of molecular orbitals
• Develop the concepts of unit cells and lattices to describe diffraction patterns</td></tr>
<tr><td>Intended Learning Outcomes</td><td colspan="3">• Determine symmetry elements and point group of molecules
• Deduce irreducible and reducible representations of point group
• Predict the number of vibrational bands and their symmetries in IR and Raman spectra of molecules
• Predict the formation of molecular orbital
• Explain crystal systems and diffraction methods
• Apply diffraction techniques for three dimensional structural elucidation</td></tr>
<tr><td>Course Content</td><td colspan="3">• Point groups: Symmetry operations and elements, classification of molecules based on symmetry, group multiplication, creating higher groups from simpler groups and identifying the point groups for specific molecules.
• Group representations: Characters of representations, reduction of representations, non-degenerate and degenerate representations, irreducible and reducible representations, matrix, characters and character tables.
• Symmetry adapted linear combinations: General concepts of orthogonality and its relationships in group theory, determination of irreducible representations</td></tr>
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<tr><td></td><td colspan="2">MolecularOrbitals and Group Theory: Bonding in diatomics, bonding in polyatomics, projection and transfer Operators, calculating the orbital energies and expansion coefficients, constructing molecular orbitals
Application to molecular vibration: Brief review of molecular degrees of freedom, determining the symmetries of molecular motions, molecular vibrations using internal coordinates. Infrared and Raman active modes of vibrations.
Diffraction Methods: Brief review of crystal systems and diffraction method, space groups, reciprocal lattices and Fourier transforms, determination of crystal structure, Fourier synthesis, ionic crystals and cohesive energy</td></tr>
<tr><td>Teaching learning Methods/Activities</td><td colspan="2">Lectures, tutorial discussions, small group assignment and home-work assignments</td></tr>
<tr><td rowspan="2">Evaluation/Assessment Strategy</td><td>In-course Assessment</td><td>End-of-course Examination</td></tr>
<tr><td>30 %</td><td>70 %</td></tr>
<tr><td>Recommended References</td><td colspan="2">Atkins, P. and Paula, J. D., Physical Chemistry, 11th Edition Oxford University Press, 2017.
Vincent, A., Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edition, John Wiley & Sons, 2013.
Atkins, P. W., and Friedman, R. S., Molecular Quantum Mechanics, 5th Edition, Oxford University Press, 2010
Atkins, P. W., Overton, T., Rourke, J. Weller, M. and Armstrong, F., Shriver & Atkins' Inorganic Chemistry, 5th Edition, Oxford University Press, 2010
Kettle, S. F. A., Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edition, John Wiley & Sons, 2007
Ogden, J. S., Introduction to Molecular Symmetry, Oxford University Press, 2001
Davidson, G., Group Theory for Chemists, Macmillan Physical Science book series, 1991
Cotton, F. A., Chemical Applications of Group Theory, 3rd Edition, John Wiley & Sons, 1990</td></tr>
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