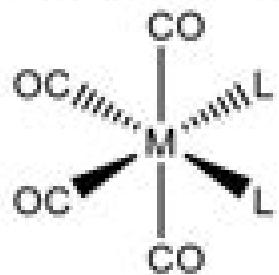
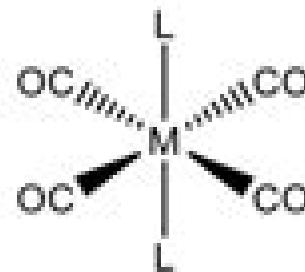


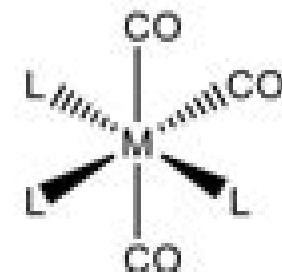
- Completed online (Molecular symmetry (Group theory) Quiz) [4]
- Completed online (Molecular symmetry (Group theory) Quiz) [6]
- M(CO)₆ (where M = transition metal) has been utilised in a reaction. The product was analysed by infra-red and Raman spectroscopy. The CO ligands of the product produced three frequencies in the infra-red spectrum and three frequencies in the Raman spectrum. The infra-red and Raman frequencies were co-incident.
The possible structures (A-C) and their point groups (in parentheses) are shown below.
Deduce, using a group theory approach, which of the compounds has been synthesised.



A (C_{2v})



B (D_{4h})



C (C_{2v})

N.B. The identity of the ligand, L, can be taken to be a single atom to simplify analysis.

You must include the following in your answer:

- The reducible representation of Γ_{M-CO} for each complex [9]
- The irreducible representation of Γ_{M-CO} for each complex, stating clearly which labels are infra-red and / or Raman active. The reduction formula must be used (and calculations shown) to deduce the labels present for each complex [12]
- Which complex has been synthesised and brief reasoning for your answer [2]

Molecular Symmetry Group Theory Answers To

R. Mirman

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Molecular Symmetry and Group Theory Alan Vincent,2013-06-05 This substantially revised and expanded new edition of the bestselling textbook addresses the difficulties that can arise with the mathematics that underpins the study of symmetry and acknowledges that group theory can be a complex concept for students to grasp Written in a clear concise manner the author introduces a series of programmes that help students learn at their own pace and enable to them understand the subject fully Readers are taken through a series of carefully constructed exercises designed to simplify the mathematics and give them a full understanding of how this relates to the chemistry This second edition contains a new chapter on the projection operator method This is used to calculate the form of the normal modes of vibration of a molecule and the normalised wave functions of hybrid orbitals or molecular orbitals The features of this book include A concise gentle introduction to symmetry and group theory Takes a programmed learning approach New material on projection operators and the calcultaion of normal modes of vibration and normalised wave functions of orbitals This book is suitable for all students of chemistry taking a first course in symmetry and group theory

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Molecular

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GROUP THEORY AND ITS

APPLICATIONS IN CHEMISTRY, SECOND EDITION KUNJU, A. SALAHUDDIN, KRISHNAN, G., 2015-08-31 This book divided into two parts now in its second edition presents the basic principles of group theory and their applications in chemical theories While retaining the thorough coverage of the previous edition the book in Part I discusses the symmetry elements point groups and construction of character tables for different point groups In Part II it describes the concept of hybridization to explain the shapes of molecules and analyzes the character tables to predict infrared and Raman active vibrational modes of molecules It also brings into fore the molecular orbital theory and the techniques of group theory to interpret bonding in transition metal complexes and their electronic spectra Finally the book describes the crystal symmetry in detail as well as the Woodward Hoffmann rules to determine the pathways of electrocyclic and cycloaddition reactions

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Molecular Dynamics and Spectroscopy by Stimulated Emission Pumping
Hai-Lung Dai, 1995 Since the first stimulated emission pumping SEP experiments more than a decade ago this technique has proven powerful for studying vibrationally excited molecules SEP is now widely used by increasing numbers of research groups to investigate fundamental problems in spectroscopy intramolecular dynamics intermolecular interactions and even reactions SEP provides rotationally pre selected spectra of vibrationally highly excited molecules undergoing large amplitude motions A unique feature of SEP is the ability to access systematically a wide variety of extreme excitations localized in various parts of a molecule and to prepare populations in specific high vibrational levels SEP has made it possible to ask and answer specific questions about intramolecular vibrational redistribution and the role of vibrational excitation in chemical reactions

Mathematical Crystallography and the Theory of Groups of Movements Harold Hilton, 1908

The Union of Chemistry and Physics Hinne Hettema, 2017-08-01 This monograph deals with the interrelationship between chemistry and physics and especially the role played by quantum chemistry as a theory in between these two disciplines The author uses structuralist approach to explore the overlap between the two sciences looking at their theoretical and ontological borrowings as well as their continuity The starting point of this book is that there is at least a form of unity between chemistry and physics where the reduction relation is conceived as a special case of this unity However matters are never concluded so simply within philosophy of chemistry as significant problems exist around a number of core chemical ideas

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