

Problem #7, 10 points, McQuarrie and Simon: Chapter 12, Problem 28 + Extra.

Given the four symmetry orbitals of butadiene:

$$\phi_1 = \frac{1}{\sqrt{2}}(\psi_1 - \psi_4)$$

$$\phi_2 = \frac{1}{\sqrt{2}}(\psi_2 - \psi_3)$$

$$\phi_3 = \frac{1}{\sqrt{2}}(\psi_1 + \psi_4)$$

$$\phi_4 = \frac{1}{\sqrt{2}}(\psi_2 + \psi_3)$$

Derive the Hückel theory secular determinant

$$\begin{vmatrix} \alpha - E & \beta & 0 & 0 \\ \beta & \alpha - \beta - E & 0 & 0 \\ 0 & 0 & \alpha - E & \beta \\ 0 & 0 & \beta & \alpha + \beta - E \end{vmatrix} = 0$$

Which, given the substitution $x = \frac{\alpha - E}{\beta}$, reduces to

$$(x^2 - x - 1)(x^2 + x - 1) = 0.$$

Use this expression to solve for the four values of x , which yield four values of E . Specify these values, and plot them on an energy diagram.

Mcquarrie Problem 7

Paul J. Reier



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Introduction to Computational Physical Chemistry Joshua Schrier, 2017-06-16 This book will revolutionize the way physical chemistry is taught by bridging the gap between the traditional solve a bunch of equations for a very simple model approach and the computational methods that are used to solve research problems This book will revolutionize the way physical chemistry is taught by bridging the gap between the traditional solve a bunch of equations for a very simple model approach and the computational methods that are used to solve research problems While some recent textbooks include exercises using pre packaged Hartree Fock DFT calculations this is largely limited to giving students a proverbial black box The DIY do it yourself approach taken in this book helps student gain understanding by building their own simulations from scratch The reader of this book should come away with the ability to apply and adapt these techniques in computational chemistry to his or her own research problems and have an enhanced ability to critically evaluate other computational results This book is mainly intended to be used in conjunction with an existing physical chemistry text such as McQuarrie Simon s Physical Chemistry A Molecular Approach but it is also well suited as a stand alone text for upper level undergraduate or intro graduate computational chemistry courses Assumes no computational background Enables students to build simulations from scratch to reproduce famous literature calculations Teaches a variety of computational numerical simulation methods applicable to solving chemical problems Designed to play well with McQuarrie Simon s landmark P CHEM text but can be used with others as well *Official Gazette of the United States Patent and Trademark Office*, 1982 Introduction to Cell Mechanics and Mechanobiology Hayden Huang, Ronald Kwon, 2012-11-16 Introduction to Cell Mechanics and Mechanobiology is designed for a one semester course in the mechanics of the cell offered to advanced undergraduate and graduate students in biomedical engineering bioengineering and mechanical engineering It teaches a quantitative understanding of the way cells detect modify and respond to the physical prope Post-Lesion Neural Plasticity Hans Flohr, 2012-12-06 Neural networks are not rigidly wired but rather highly plastic structures the functional architecture of which can be actively reorganized in response to external or internal events Lesions of such networks induce plastic processes which in time may lead to a recovery of the initially disrupted function This type of neural plasticity is the main focus of the book which presents a broad spectrum of experimental paradigms for lesion induced plasticity as in the spinal cord the vestibular oculomotor visual and olfactory system the cerebellum and the cerebral cortex including recent methodological developments Concepts and perspectives in understanding neural plasticity are reported in reviews and original research reports and are thoroughly discussed *Bulletin* University of Minnesota, 1954 **School Health Problems** Laurence Benjamin Chenoweth, Theodore King Selkirk, 1953 **Problems in Quantum Physics, Gdańsk '87** Ludwik Kostro, 1988 **Cumulated Index Medicus**, 1968 **Journal of Applied Probability**, 1971 **Many-body Problems** William Edward Parry, 1969 Principles of Accounting: Advanced Harry Anson Finney, Herbert E. Miller, 1958

Current Issues in Neural Regeneration Research Paul J. Reier, 1988 *Management of Peripheral Nerve Problems* George E. Omer, Morton Spinner, 1998 Here s a completely expanded and restructured edition of the classic work on nerve problems outside the brain and spine Coverage ranges from surgical anatomy and diagnostic and basic techniques through trauma compression syndromes and limb reconstruction Current and comprehensive this text is the result of contributions from experts in hand surgery orthopedics plastic surgery neurosurgery and rehabilitation **IBM Systems Journal** ,1972

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