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Eugen Merzbacher

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Computer Generated Physical Properties Stan Bumble, 1999-06-01 Computer Generated Physical Properties offers the environmental scientist a basis to predict the properties of molecules and reengineer them to remove those properties that are harmful to the environment This technology is currently used in other fields and is now becoming popular in the environmental engineering field because of its pollution prevention and waste reduction capabilities This book interdisciplinary in scope treats the physical properties of matter as generated by computers It covers a wide variety of topics pointing towards synthesizing new molecules to substitute for reactants intermediaries and products in industrial processes with better physical and environmental properties than the original The author achieves this with a spreadsheet program called SYNPROPS that operates on a PC computer with optimization features A radar type graph one for each property visually sorts the various groups in order of their contribution to the property creating the necessity for a computer to obtain answers for the structure of the optimum molecules for substitution or synthesis The author discusses applications to biologically active molecules without side effects including antineoplatic drugs Additionally he demonstrates model compounds and the applications of SYNPROPS optimization and substitution This book has everything you need to know Statistical Thermodynamics Lukong about deriving properties and combinational chemistry from molecular structure Cornelius Fai, Gary Matthew Wysin, 2012-10-19 Statistical thermodynamics and the related domains of statistical physics and quantum mechanics are very important in many fields of research including plasmas rarefied gas dynamics nuclear systems lasers semiconductors superconductivity ortho and para hydrogen liquid helium and so on Statistical Thermodynamics Understanding the Properties of Macroscopic Systems provides a detailed overview of how to apply statistical principles to obtain the physical and thermodynamic properties of macroscopic systems Intended for physics chemistry and other science students at the graduate level the book starts with fundamental principles of statistical physics before diving into thermodynamics Going further than many advanced textbooks it includes Bose Einstein Fermi Dirac statistics and Lattice dynamics as well as applications in polaron theory electronic gas in a magnetic field thermodynamics of dielectrics and magnetic materials in a magnetic field The book concludes with an examination of statistical thermodynamics using

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