This book is intended as a guide to the ab initio calculation of molecular structure and properties. It provides the necessary working information to enable the non-specialist to use and understand electronic structure methods and related computing technology, despite the high level of sophistication of quantum chemical methods.The initial chapters define and outline theoretical concepts, methods and computational approaches. Descriptive information and definitions of the terminology are given first; more detailed and mathematical explanations follow. These first chapters thus provide the background information needed to use the extensive literature of ab initio electronic structure theory. The next chapter first provides an overview of the technical issues relating to molecular properties, and then gives a rather detailed but general development. The latter part of this chapter is mainly intended for those first encountering the methodologies of properties determination and intending to pursue further developments. The other chapters provide reviews of calculations in the literature and assessments of factors influencing accuracy.The book is particularly useful to those who need a working understanding of ab initio calculations and well-suited to graduate students and researchers in computational and theoretical chemistry, researchers in electronic structure, spectroscopists and organic chemists.

DMZ #55, Graphis New Media 1: A Compilation of New Media Design (v. 1), D. H. Lawrence (Modern masters ; M20), El Diablo de la Botella (Spanish Edition), Babbling Corpse: Vaporwave And The Commodification Of Ghosts,