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Methods of Electronic Structure Theory

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Preface

These two volumes deal with the quantum theory of the electronic structure of molecules. Implicit in the term *ab initio* is the notion that approximate solutions of Schrödinger's equation are sought "from the beginning," i.e., without recourse to experimental data. From a more pragmatic viewpoint, the distinguishing feature of *ab initio* theory is usually the fact that no approximations are involved in the evaluation of the required molecular integrals. Consistent with current activity in the field, the first of these two volumes contains chapters dealing with methods *per se*, while the second concerns the application of these methods to problems of chemical interest. In a sense, the motivation for these volumes has been the spectacular recent success of *ab initio* theory in resolving important chemical questions. However, these applications have only become possible through the less visible but equally important efforts of those developing new theoretical and computational methods and models.

Henry F. Schaefer

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