Simple Theorems, Proofs, and Derivations in Quantum Chemistry (Mathematical and Computational Chemistry)

By Istvan Mayer

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Since 1983 I have been delivering lectures at Budapest University that are mainly attended by chemistry students who have already studied quantum chem istry in the amount required by the (undergraduate) chemistry curriculum of the University, and wish to acquire deeper insight in the field, possibly in prepara tion of a master's or Ph.D. thesis in theoretical chemistry. In such a situation, I have the freedom to discuss, in detail, a limited number of topics which I feel are important for one reason or another. The exact coverage may vary from year to year, but I usually concentrate on the general principles and theorems and other basic theoretical results which I foresee will retain their importance despite the rapid development of quantum chemistry. I commonly organize my lectures by treating the subject from the begin ning, without referring explicitly to any actual previous knowledge in quantum chemistry-only some familiarity with its goals, approaches and, to a lesser ex tent, techniques is supposed. I concentrate on the formulae and their derivation, assuming the audience essentially understands the reasons for deriving these results. This book is basically derived from the material of my lectures. The spe cial feature, distinguishing it from most other textbooks, is that all results are explicitly proved or derived, and the derivations are presented completely, step by step. True understanding of a theoretical result can be achieved only if one has gone through its derivation.

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