



Implementation of the Gaussian 78 Programs on the Nyu VAX/11-780: A Probe Into Basis Set and Correlation Effects on the Structure of Molecular Complexes (Classic Reprint) (Paperback)

By Sid Topiol

Fb C Ltd, 2016. Paperback. Condition: New. Language: English. Brand New Book ***** Print on Demand *****. Excerpt from Implementation of the Gaussian 78 Programs on the Nyu Vax/11-780: A Probe Into Basis Set and Correlation Effects on the Structure of Molecular Complexes We report the implementation of the gaussian 78 system of programs for ab-initio quantum mechanical calculations of molecular electronic structure of the New York University vax/ll-780 minicomputer. We illustrate the use of the program package in a theoretical investigation of a model for drug receptor complexes. About the Publisher Forgotten Books publishes hundreds of thousands of rare and classic books. Find more at This book is a reproduction of an important historical work. Forgotten Books uses state-of-the-art technology to digitally reconstruct the work, preserving the original format whilst repairing imperfections present in the aged copy. In rare cases, an imperfection in the original, such as a blemish or missing page, may be replicated in our edition. We do, however, repair the vast majority of imperfections successfully; any imperfections that remain are intentionally left to preserve the state of such historical works.



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