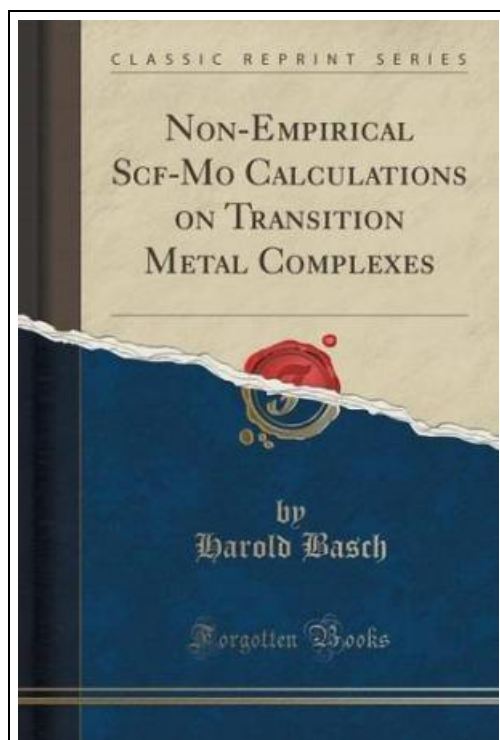# Non-Empirical Scf-Mo Calculations on Transition Metal Complexes (Classic Reprint)

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Forgotten Books, United States, 2015. Paperback. Book Condition: New. 229 x 152 mm. Language: English . Brand New Book ***** Print on Demand *****.Excerpt from Non-Empirical Scf-Mo Calculations on Transition Metal Complexes In this paper we shall demonstrate the feasibility of employing Gaussian functions as basis orbitals in molecular orbital computations on transition metal complexes. This calculation represents the first treatment of a transition metal complex ion involving all electrons and no approximations within the Roothaan SCF-MO formalism. The qualitative features of the calculation can be expected to have wide significance both for the understanding of the electronic structure of transition metal complexes and for the application of MO theory to large systems of this type. We will report the results of calculations on the (hypothetical) square planar N1F42- ion (the reasons for this particular choice will be explained later) and discuss those interesting ground and excited state molecular electronic properties which can be extracted from a computed wave function. It is well known that individual Gaussians are much poorer representations of atomic orbitals (AO s) than are single Slater type orbitals (STO s), especially in two very important areas: near the nucleus, and in the tail region of the AO. These deficiencies are very serious if one wants to use Gaussians as basis functions for molecular calculations. 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...

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