

Modern Quantum Chemistry, Szabo & Ostlund

HW

WSF

May 14, 2020

Contents

A	Integral Evaluation with 1s Primitive Gaussians	2
B	2-Electron Self-consistent-field Program	2
C	Analytic Derivative Methods and Geometry Optimization	2
C.1	Introduction	2

A	Integral Evaluation with 1s Primitive Gaussians
B	2-Electron Self-consistent-field Program
C	Analytic Derivative Methods and Geometry Optimization
C.1	Introduction
C.2	General Considerations
C.3	Analytic Derivatives
C.4	Optimization Techniques
C.5	Some Optimization Algorithms
Ex C.1	
Ex C.2	
Ex C.3	
Ex C.4	
C.6	Transition States
C.7	Constrained Variation
D	Molecular Integrals for H₂ as a Function of Bond Length