MENG 25510 Final Report: Hartree-Fock on HeH^+ with 6-311G

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(Dated: 30 May 2022)

Please see the corresponding code at `https://github.com/FitzSW/HF_HeH` for this project.

I. INTRODUCTION

This is a reference document to go with our submission for the MENG 25510 final coding project, for which we chose to implement the Hartree-Fock (HF) Self-Consistent Field (SCF) method on a HeH^+ molecular system using the 6-311G basis set on both atoms. The geometry at which we performed the calculation was optimized at the CCSD/aug-cc-pZTZ level of theory using Gaussian 16.