# Introduction to Q-Chem and QCMagic

*A brief tutorial*



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## Contents

# 1 Single-Point Calculations

We begin with a simple Hartree–Fock calculation for the simplest closed-shell system, a He atom, to familiarise ourselves with the syntax of Q-Chem.

```
$ qchem -nt 6 test.inp test.out
```

Shown in Listing 1

**Listing 1:** singlepoint/codesnippets/He.inp

```
$molecule
  0 1
  He  0 0 0
$end
$rem
  BASIS STO-3G
  EXCHANGE hf
  CORRELATION none
  UNRESTRICTED false
  SCF_GUESS CORE
  SCF_ALGORITHM DIIS
  SCF_CONVERGENCE 13
  SCF_MAX_CYCLES 1000
  MOM_START 1
  SCF_PRINT 1
  PRINT_ORBITALS true
$end
```