

Elevia Manual

Haoyu Lin (1801110300)

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1 Input File Format

Listing 1: **test.vie**

```
1 RHF STO-3G 3 0 1
2
3 O    0.01984457   -0.19931037   0.00000000
4 H    0.97984454   -0.19906927   0.00000000
5 H   -0.30038273    0.70570591   0.00000000
```

2 Basis Set

Currently supported basis sets:

- STO-3G
- 3-21G
- 6-31G
- 6-31G(d)
- 6-31G(d,p)
- 6-311G(d,p)

3 SCF Procedure

The SCF procedure is carried out as follows:

1. Specify a system (a set of nuclear coordinates $\{\mathbf{R}_a\}$, atomic numbers $\{Z_a\}$, and the total number of electrons N) and a basis set $\{\chi_s\}$.
2. Calculate all required molecular integrals S_{rs} , h_{rs} , and $(rp|sq)$, $(rp|qs)$.
3. Diagonalize the overlap matrix \mathbf{S} and obtain a transformation matrix $\mathbf{X} = \mathbf{U}\mathbf{S}^{-1/2}$.
4. Assume an initial bond-order matrix \mathbf{P} (often in the first iteration, we put $\mathbf{P} = \mathbf{0}$, as if there were no electron repulsion).
5. Find the \mathcal{F} matrix using matrix \mathbf{P} .
6. Calculate the transformed Fock matrix $\mathcal{F}' = \mathbf{X}^\dagger \mathcal{F} \mathbf{X}$.

7. Diagonalize \mathcal{F}' to obtain \mathbf{C}' and ϵ .
8. Calculate $\mathbf{C} = \mathbf{X}\mathbf{C}'$.
9. Form a new \mathbf{P} from \mathbf{C} .
10. Calculate the total energy E .
11. Determine whether the procedure has converged, i.e., determine whether the difference between two successive total energy is less than a threshold (10^{-8}). If the procedure has not converged, return to step (5) with the new bond-order matrix. If the procedure has converged, then calculate and output the quantities of interest.

References