Elevia Manual

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1 Input File Format

Elevia assumes a new input format:

```
[method] [basis] [the number of atoms] [charge] [spin multiplicity]

[atom symbol]   [ Rx ]   [ Ry ]   [ Rz ]
[atom symbol]   [ Rx ]   [ Ry ]   [ Rz ]
[atom symbol]   [ Rx ]   [ Ry ]   [ Rz ]
... ...
```

For instance, an input file for test is

2 Method

Only support RHF.

3 Basis Set

Currently supported basis sets:

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

Basis must strictly be typed in these displayed forms, only for that could Elevia recognize. The source code about reading basis data (dat/basis/*.g94) into the program is included in ”intro_basis.cpp”.

4 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 $\boldsymbol{\mathcal{F}}$ matrix using matrix $\mathbf{P}$.
6. Calculate the transformed Fock matrix $\boldsymbol{\mathcal{F}}' = \mathbf{X}^{\dagger}\boldsymbol{\mathcal{F}}\mathbf{X}$.
7. Diagonalize $\boldsymbol{\mathcal{F}}'$ to obtain $\mathbf{C}'$ and $\boldsymbol{\epsilon}$.
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.

[1] [2] [3]

References

[1] L. Piela. *Ideas of Quantum Chemistry*. Elsevier, USA, second edition, 2014.

[2] A. Szabo and N. S. Ostlund. *Modern Quantum Chemistry*. Dover Publications, USA, 1996.

[3] S. Obara and A. Saika. Efficient recursive computation of molecular integrals over cartesian gaussian functions. *J. Chem. Phys.*, 84(7):3963–3974, 1986.