Semiempirical Hartree-Fock in NWChem (semiemp module)

Below is a sample input for a single point calculation:

```
start h2o_scf

charge 0
geometry noautosym noautoz
O      -0.249678801     0.000000000    -1.056890908
H      -0.249678801     0.759337000    -0.460847908
H      -0.249678801    -0.759337000    -0.460847908
end

semiemp
mult 1
apx INDO/1
scftype rhf
maxiter 50
end


task semiemp energy
```

No basis set is needed.

MULT- MULTIPLICITY

Multiplicity of the system can be defined here.

APX-Approximate Hamiltonian

Currently available methods are CNDO/1, CNDO/2, INDO/1 and INDO/2. (1 and 2 indicates two different parametrization for one centre core integrals).

SCFTYPE-Wave function type

Currently only RHF and UHF is available.

MAXITER-Iteration limit.

This keyword indicate maximum allowed iterations. Default is 50.

SCFTOL-Convergence criteria for density.

Default value is 10^{-7}.

INTTYP- Integral type

0 (default) for ground state calculations

1 for spectroscopic calculations (INDO/S etc)

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RT-INDO/S

Input for Ag_{20}

start Ag20_y

memory total 84 stack 24 heap 24 global 36 mb

charge 0
geometry noautosym noautoz
 Ag -4.18425 -2.41578 -1.70821
 Ag -1.38662 -2.52547 -1.78578
 Ag   1.38662 -2.52547 -1.78578
 Ag   4.18425 -2.41578 -1.70821
 Ag -2.88043   0.06189 -1.78578
 Ag   0.00000   0.00000 -1.89153
 Ag   2.88043   0.06189 -1.78578
 Ag -1.49381   2.46358 -1.78578
 Ag   1.49381   2.46358 -1.78578
 Ag   0.00000   4.83155 -1.70821
 Ag -2.88043 -1.66302   0.65361
 Ag   0.00000 -1.78335   0.63051
 Ag   2.88043 -1.66302   0.65361
 Ag -1.54443   0.89167   0.63051
 Ag   1.54443   0.89167   0.63051
 Ag   0.00000   3.32604   0.65361
 Ag -1.49381 -0.86245   2.91795
 Ag   1.49381 -0.86245   2.91795
 Ag   0.00000   1.72491   2.91795
 Ag   0.00000   0.00000   5.12463
end

semiemp
mult 1.0
apx INDO/1
scftype rhf
maxiter 100
inttyp 1
end

rt_semiemp
nrestarts 100
tmax 1000
dt 0.1
tag "kick_y"
field_type delta
field_max 0.0001
polarization y

print dipole
end

task semiemp rt_semiemp

RT-INDO/S is currently available only for RHF wave functions.

NRESTARTS

This sets the number of run-time check points where the time-dependent complex density matrix is saved to file, allowing the simulation to be restarted from that point.

TMAX

This option specifies the maximum time (in au) to run the simulation before stopping, which must be a positive real number.

DT

This specifies the electronic time step for time integration.

TAG -- Output label

This option sets a label for the output for convenient parsing (e.g., with "grep").

Tag “kick_y”

It appears in the output as:

Kick_ytotal 0.1 2.20000 -7.589146713114E+001 -7.589146713114E+001 -7.589146713114E+001 #Dipole moment [system]

FIELD_TYPE

This option sets type of external electric field. Only option available currently is “delta”.

FIELD_MAX

This option sets the maximum value of the electric field

Polarization

This option sets the polarization direction. It can be x, y or z.

PRINT

This option sets the different time-dependent properties to be computed and printed at each time step.

Dipole: Dipole moment