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Semiempirical Hartree-Fock in NWChem (semiemp module)

Below is a sample input for a single point calculation for INDO Hamiltonian:

```
start benzene_scf

charge 0
geometry noautosym noautoz
C      -0.804616000    0.000000000   -2.637508000
C      -1.968653000   -0.357135000   -1.934532000
C       0.359421000    0.357135000   -1.934532000
H      -2.876005000   -0.635517000   -2.482493000
H       1.266773000    0.635517000   -2.482493000
C      -1.968653000   -0.357135000   -0.528579000
C       0.359421000    0.357135000   -0.528579000
H      -2.876005000   -0.635517000    0.019382000
H       1.266773000    0.635517000    0.019382000
C      -0.804616000    0.000000000    0.174397000
H      -0.804616000    0.000000000    1.270320000
H      -0.804616000    0.000000000   -3.733431000
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.

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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)

RT-INDO/S

Input for RT-INDO/S

start benzene_y

charge 0

geometry noautosym noautoz

C	-0.804616000	0.000000000	-2.637508000
C	-1.968653000	-0.357135000	-1.934532000
C	0.359421000	0.357135000	-1.934532000
H	-2.876005000	-0.635517000	-2.482493000
H	1.266773000	0.635517000	-2.482493000
C	-1.968653000	-0.357135000	-0.528579000
C	0.359421000	0.357135000	-0.528579000
H	-2.876005000	-0.635517000	0.019382000
H	1.266773000	0.635517000	0.019382000
C	-0.804616000	0.000000000	0.174397000
H	-0.804616000	0.000000000	1.270320000
H	-0.804616000	0.000000000	-3.733431000

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

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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