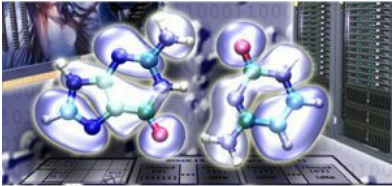




TeraChem 1.93P Linux x64

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Scratch directory: ./scr
Random number seed: 1521474850

XYZ coordinates C6H6.pdb
Molden File Output: ./scr/C6H6.molden
Using basis set: 6-31gss
Spin multiplicity: 1
DIIS will use up to 10 vectors.
WF convergence threshold: 3.00e-05
Using DIIS algorithm to converge WF
Maximum number of SCF iterations: 100
Incremental fock with rebuild ever 8 iterations
Will switch to conventional Fock if diffuse functions are detected
X-matrix tolerance: 1.00e-04
PRECISION: DYNAMIC
DFT Functional requested: b3lyp
Method: B3LYP
  Hartree-Fock exact exchange:      0.20
  Slater exchange functional:      0.80
  Becke 1988 exchange functional:  0.72
  Lee-Yang-Parr correlation functional: 0.81
  VWN(I) correlation functional:    0.19
Wavefunction: RESTRICTED
DFT grid type: 1
Using dynamic DFT grids.
Initial guess generated by maximum overlap

*****
*****  RUNNING GEOMETRY OPTIMIZATION  *****
*****

Geometry optimization parameters:
Max number of optimization cycles: 1000
Convergence threshold (Max grad component): 4.50e-04
Convergence threshold (energy change): 1.00e-06
using L-BFGS method
Optimization checkpoint file will be dumped every 10 cycles
Atomic displacement in finite-difference Hessian (Bohr) 0.003000
Each step will be scaled by 1.00
Maximum step size in internal coordinates 0.50
Minimization SCF guess will be regenerated every 10 steps
Job started from scratch
SCF:  Initial guess is taken from previous step
CIS:  Initial guess is taken from previous step
Z-vec: Initial guess is taken from previous step
```



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