

Electronic Structure of Tetracyanonickelate(II)

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Example TD-DFT Calculation Input Parameters:

```
! PBE0  
! ma-def2-TZVPP TIGHTSCF Opt Grid3 FinalGrid5 xyzfile
```

```
! CPCM  
%cpcm  
epsilon 37.5  
end
```

```
* xyzfile -2 1 guess.xyz
```

```
$new_job
```

```
! ma-def2-TZVPP Grid5 FinalGrid6 TightSCF  
! PBE0
```

```
! CPCM  
%cpcm  
epsilon 37.5  
end
```

```
%tddft  
nroots 25  
maxdim 5  
tda true  
triplets true  
end
```

```
*xyzfile -2 1
```

```
Example of EOM-CCSD calculation  
! RHF EOM-CCSD def2-SVP TightSCF
```

```
%maxcore 8000
```

```
!moread  
%moinp "16eeeom.gbw"
```

```
%mdci  
NInitS 30  
nroots 9  
DoCOSXEOM true  
DoAOX3e true  
KCOpt KC_AOBLAS  
end
```

```
* xyz -2 1
Ni 0 0 0
C 1.87 0 0
C -1.87 0 0
C 0 1.87 0
C 0 -1.87 0
N 3.03 0 0
N -3.03 0 0
N 0 3.03 0
N 0 -3.03 0
*
```

Example of CASSCF calculation

```
! CASSCF ma-def2-TZVPP NoIter
```

```
%maxcore 600000
```

```
!moread
%moinp "11.gbw"
```

```
! CPCM
%cpcm
epsilon 37.5
end
```

```
%casscf
nel 10
norb 10
mult 3,1
nroots 4,5
NEVPT2 SC
nevpt
d4tpre 1e-8
end
end
```

```
* xyz -2 1
Ni 0 0 0
C 1.87 0 0
C -1.87 0 0
C 0 1.87 0
C 0 -1.87 0
N 3.03 0 0
N -3.03 0 0
```

N 0 3.03 0
N 0 -3.03 0
*