
 TD-DFT/TDA EXCITED STATES (SINGLETs)

the weight of the individual excitations are printed if larger than 1.0e-02

```

STATE 1:  E=   0.142238 au       3.870 eV    31217.5 cm**-1 <S**2> =   0.000000_
↪Mult 1
    7a ->   8a   :       0.999852 (c=  0.99992610)

STATE 2:  E=   0.279148 au       7.596 eV    61265.8 cm**-1 <S**2> =   0.000000_
↪Mult 1
    7a ->   9a   :       0.991058 (c=  0.99551880)

STATE 3:  E=   0.326547 au       8.886 eV    71668.9 cm**-1 <S**2> =   0.000000_
↪Mult 1
    5a ->   8a   :       0.992394 (c= -0.99618994)

STATE 4:  E=   0.339416 au       9.236 eV    74493.3 cm**-1 <S**2> =   0.000000_
↪Mult 1
    6a ->   8a   :       0.214928 (c=  0.46360308)
    7a ->  10a   :       0.760130 (c= -0.87185424)

STATE 5:  E=   0.357323 au       9.723 eV    78423.4 cm**-1 <S**2> =   0.000000_
↪Mult 1
    4a ->   8a   :       0.998607 (c=  0.99930350)

STATE 6:  E=   0.396031 au      10.777 eV    86918.7 cm**-1 <S**2> =   0.000000_
↪Mult 1
    7a ->  11a   :       0.995757 (c= -0.99787607)

STATE 7:  E=   0.412518 au      11.225 eV    90537.2 cm**-1 <S**2> =   0.000000_
↪Mult 1
    3a ->   8a   :       0.015703 (c=  0.12531336)
    6a ->   9a   :       0.982525 (c=  0.99122380)

STATE 8:  E=   0.420413 au      11.440 eV    92270.0 cm**-1 <S**2> =   0.000000_
↪Mult 1
    4a ->  10a   :       0.023644 (c= -0.15376603)
    5a ->   9a   :       0.184687 (c= -0.42975192)
    5a ->  11a   :       0.029413 (c= -0.17150093)
    6a ->   8a   :       0.535798 (c= -0.73198239)
    7a ->  10a   :       0.161330 (c= -0.40165919)
    7a ->  14a   :       0.031134 (c=  0.17644805)

STATE 9:  E=   0.454354 au      12.364 eV    99719.1 cm**-1 <S**2> =   0.000000_
↪Mult 1
    5a ->   9a   :       0.801630 (c=  0.89533782)
    5a ->  11a   :       0.012558 (c= -0.11206253)
    6a ->   8a   :       0.103311 (c= -0.32142015)
    7a ->  10a   :       0.051303 (c= -0.22650208)
    7a ->  14a   :       0.016544 (c=  0.12862428)

STATE 10: E=   0.474384 au      12.909 eV   104115.2 cm**-1 <S**2> =   0.000000_
↪Mult 1
    6a ->  10a   :       0.998860 (c= -0.99942977)
  
```

and the triplets:

 TD-DFT/TDA EXCITED STATES (TRIPLETS)

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```

the weight of the individual excitations are printed if larger than 1.0e-02

STATE 11:  E=   0.114291 au       3.110 eV   25084.1 cm**-1 <S**2> =   2.000000_
↳Mult 3
    7a ->   8a   :       0.999453 (c=  0.99972624)

STATE 12:  E=   0.213324 au       5.805 eV   46819.1 cm**-1 <S**2> =   2.000000_
↳Mult 3
    6a ->   8a   :       0.996522 (c=  0.99825941)

STATE 13:  E=   0.255583 au       6.955 eV   56094.1 cm**-1 <S**2> =   2.000000_
↳Mult 3
    7a ->   9a   :       0.992767 (c=  0.99637714)

STATE 14:  E=   0.276345 au       7.520 eV   60650.8 cm**-1 <S**2> =   2.000000_
↳Mult 3
    5a ->   8a   :       0.998251 (c= -0.99912505)

STATE 15:  E=   0.316749 au       8.619 eV   69518.3 cm**-1 <S**2> =   2.000000_
↳Mult 3
    7a ->  10a   :       0.991502 (c= -0.99574190)

STATE 16:  E=   0.327793 au       8.920 eV   71942.2 cm**-1 <S**2> =   2.000000_
↳Mult 3
    4a ->   8a   :       0.994029 (c=  0.99701018)

STATE 17:  E=   0.377551 au      10.274 eV   82862.9 cm**-1 <S**2> =   2.000000_
↳Mult 3
    7a ->  11a   :       0.998586 (c= -0.99929259)

STATE 18:  E=   0.400159 au      10.889 eV   87824.7 cm**-1 <S**2> =   2.000000_
↳Mult 3
    3a ->   8a   :       0.062364 (c=  0.24972706)
    6a ->   9a   :       0.934672 (c= -0.96678411)

STATE 19:  E=   0.433339 au      11.792 eV   95107.0 cm**-1 <S**2> =   2.000000_
↳Mult 3
    5a ->   9a   :       0.988277 (c=  0.99412115)

STATE 20:  E=   0.445213 au      12.115 eV   97713.0 cm**-1 <S**2> =   2.000000_
↳Mult 3
    3a ->   8a   :       0.934403 (c=  0.96664514)
    6a ->   9a   :       0.063400 (c=  0.25179341)

```

By default, it also prints the dipole absorption and circular dichroism spectra:

```

↳-----
                                ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS
↳-----
↳-----
Transition      Energy      Energy      Wavelength      fosc(D2)      D2      DX      _
↳  DY          DZ          (eV)        (cm-1)        (nm)          (au**2)    (au)      _
↳ (au)        (au)
↳-----
0-1A -> 1-3A    3.110029    25084.1     398.7         0.0000000000  0.000000  0.000000  _
↳0.000000  0.000000
0-1A -> 1-1A    3.870479    31217.5     320.3         0.0000000000  0.000000 -0.000000  _

```

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↪0.00000	0.00000							
0-1A	→	2-3A	5.804830	46819.1	213.6	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	3-3A	6.954778	56094.1	178.3	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	4-3A	7.519743	60650.8	164.9	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	2-1A	7.595990	61265.8	163.2	0.139374365	0.74893	-0.000000 ↪
↪0.86541	-0.00000							
0-1A	→	5-3A	8.619170	69518.3	143.8	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	3-1A	8.885804	71668.9	139.5	0.002010847	0.00924	0.000000 -
↪0.00000	-0.09611							
0-1A	→	6-3A	8.919695	71942.2	139.0	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	4-1A	9.235990	74493.3	134.2	0.021695302	0.09588	-0.30964 -
↪0.00000	-0.00000							
0-1A	→	5-1A	9.723256	78423.4	127.5	0.0000000000	0.000000	-0.000000 ↪
↪0.00000	-0.00000							
0-1A	→	7-3A	10.273692	82862.9	120.7	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	6-1A	10.776542	86918.7	115.1	0.009793664	0.03709	0.000000 -
↪0.19260	-0.00000							
0-1A	→	8-3A	10.888868	87824.7	113.9	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	7-1A	11.225180	90537.2	110.5	0.002033718	0.00740	0.000000 -
↪0.00000	0.08599							
0-1A	→	8-1A	11.440020	92270.0	108.4	0.371220034	1.32448	-1.15086 -
↪0.00000	0.00000							
0-1A	→	9-3A	11.791761	95107.0	105.1	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	10-3A	12.114872	97713.0	102.3	0.0000000000	0.000000	0.000000 ↪
↪0.00000	0.00000							
0-1A	→	9-1A	12.363588	99719.1	100.3	0.259360077	0.85625	-0.92534 ↪
↪0.00000	0.00000							
0-1A	→	10-1A	12.908634	104115.2	96.0	0.0000000000	0.000000	-0.000000 -
↪0.00000	-0.00000							

↪-----	CD SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS						
↪-----							
↪-----	Transition	Energy	Energy	Wavelength	R	MX	MY
↪MZ		(eV)	(cm-1)	(nm)	(1e40*cgs)	(au)	(au)
↪(au)							
↪-----							
↪-----	0-1A → 1-3A	3.110029	25084.1	398.7	-0.00000	0.00000	0.00000 0.
↪00000	0-1A → 1-1A	3.870479	31217.5	320.3	0.00000	0.58235	0.00000 0.
↪00000	0-1A → 2-3A	5.804830	46819.1	213.6	-0.00000	0.00000	0.00000 0.
↪00000	0-1A → 3-3A	6.954778	56094.1	178.3	-0.00000	0.00000	0.00000 0.
↪00000	0-1A → 4-3A	7.519743	60650.8	164.9	-0.00000	0.00000	0.00000 0.
↪00000	0-1A → 2-1A	7.595990	61265.8	163.2	-0.00000	-0.00000	0.00000 0.
↪32961							

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0-1A -> 5-3A	8.619170	69518.3	143.8	-0.00000	0.00000	0.00000	0.
→00000							
0-1A -> 3-1A	8.885804	71668.9	139.5	-0.00000	-0.00000	-0.73058	0.
→00000							
0-1A -> 6-3A	8.919695	71942.2	139.0	-0.00000	0.00000	0.00000	0.
→00000							
0-1A -> 4-1A	9.235990	74493.3	134.2	-0.00000	-0.00000	-0.00000	-0.
→00000							
0-1A -> 5-1A	9.723256	78423.4	127.5	0.00000	0.31342	-0.00000	0.
→00000							
0-1A -> 7-3A	10.273692	82862.9	120.7	-0.00000	0.00000	0.00000	0.
→00000							
0-1A -> 6-1A	10.776542	86918.7	115.1	0.00000	0.00000	0.00000	0.
→58743							
0-1A -> 8-3A	10.888868	87824.7	113.9	-0.00000	0.00000	0.00000	0.
→00000							
0-1A -> 7-1A	11.225180	90537.2	110.5	-0.00000	0.00000	-0.06966	0.
→00000							
0-1A -> 8-1A	11.440020	92270.0	108.4	-0.00000	-0.00000	-0.00000	0.
→00000							
0-1A -> 9-3A	11.791761	95107.0	105.1	-0.00000	0.00000	0.00000	0.
→00000							
0-1A -> 10-3A	12.114872	97713.0	102.3	-0.00000	0.00000	0.00000	0.
→00000							
0-1A -> 9-1A	12.363588	99719.1	100.3	-0.00000	-0.00000	-0.00000	-0.
→00000							
0-1A -> 10-1A	12.908634	104115.2	96.0	0.00000	0.00260	0.00000	0.
→00000							

Which can be processed with *orca_mapspc* for plotting.

The triplets parameter is only valid for closed-shell references. If chosen as true the program will also determine the triplet excitation energies in addition to the singlets.

The collinear spin-flip version of CIS/TDA (always starting from an open-shell reference!) can be invoked in a similar manner, using:

```
%tddft
  Nroots 5
  sf      true
end
```

Please check the section *Collinear Spin-Flip TDA (SF-TD-DFT)* for more details on how to use it, and how to understand its results.

If one wants to compute transient spectra, or transition dipoles starting from a given excited state, the option DOTRANS must be set to TRUE and an IROOT should be given for the initial state (the default is 1). If DOTRANS ALL is requested instead, the transition dipoles between all states are computed. The transient transition dipoles will then be printed after the normal spectra.

This option is currently only available for CIS/TDA and is done using the expectation value formalism, as the other transition dipole moments in ORCA.

```
%tddft
  IROOT 2
  DOTRANS TRUE
        #or
  DOTRANS ALL
end
```

Capabilities

Currently, the TD-DFT/CIS module is able to calculate excitation energies, absorption spectra and circular dichroism spectra. Within the TD-DFT method, magnetic circular dichroism (see *Simulation of (Magnetic) Circular Dichroism and Absorption Spectra*) and transient spectra can also be calculated.

Analytical gradients are available for TD-DFT in both restricted and unrestricted formalisms and also for the collinear spin-flip variant, which allows for geometry optimizations of excited states as described in *Excited State Geometry Optimization*.

5.4.2 Excited States with Restricted Open-shell CIS - ROCIS

In addition to the CIS/TD-DFT description of excited states, ORCA features the ROCIS method[589], [590], which performs configuration interaction with single excitations calculations using a restricted open-shell Hartree-Fock (ROHF) reference.

Starting from ORCA 6.0, the general-spin ROCIS (GS-ROCIS) [591] implementation is available. This new implementation can handle CSFs with arbitrary spin couplings obtained via the CSF-ROHF method as references.

The main scope of ROCIS is to calculate L-edge and M-edge X-ray absorption spectra (XAS) as well as X-ray magnetic circular dichroism (XMCD) and resonant inelastic X-ray scattering (RIXS). The computational costs are usually larger than TD-DFT, but significantly smaller than coupled-cluster based methods. Together with the pair natural orbital approach (PNO-ROCIS), spectra of medium to large molecular sizes are feasible to be calculated.

For a detailed documentation check *Excited States via ROCIS and ROCIS/DFT*.

General Use

The method is invoked by providing the number of roots sought in the %rocis block of the input file:

```
!def2-SVP TightSCF

%scf
  HFTyp ROHF
  ROHF_CASE HIGHSPIN
  ROHF_NEL[1] 2
end

%rocis
  NRoots 10
end

* xyz 0 3
C 0 0 0.1058
H 0 0.9910 -0.3174
H 0 -0.9910 -0.3174
end
```

By default, the original ROCIS implementation is invoked, which is capable of dealing only with high-spin ROHF references, giving the following output:

```
Eigenvectors of ROCIS calculation:
the threshold for printing is: 1e-02

  i->a          single excitation from orbital i to a
  i->t->a        single excitation from orbital i to a with a spin flip in
->orbital t
  i->t ; w->a    double excitation from orbital i to t and orbital w to a

STATE   0   Exc. Energy:   0.000mEh   0.000eV   0.0cm**-1
```

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```

0                      : 0.9880 (0.993993)

STATE 1  Exc. Energy: 291.825mEh  7.941eV      64048.2cm**-1
2->3                      : 0.9602 (0.979900)

STATE 2  Exc. Energy: 307.258mEh  8.361eV      67435.4cm**-1
1->4                      : 0.0244 (-0.156226)
4->5                      : 0.9086 (-0.953183)
4->11                     : 0.0379 (-0.194741)
1->3 ; 4->5              : 0.0126 (-0.112387)

STATE 3  Exc. Energy: 311.967mEh  8.489eV      68468.7cm**-1
2->4                      : 0.9558 (-0.977660)
4->6                      : 0.0181 (0.134462)

STATE 4  Exc. Energy: 349.147mEh  9.501eV      76629.0cm**-1
3->5                      : 0.8588 (-0.926723)
3->11                     : 0.0299 (-0.173056)
1->3 ->5                 : 0.0561 (0.236925)

STATE 5  Exc. Energy: 374.241mEh  10.184eV     82136.4cm**-1
2->4                      : 0.0187 (0.136885)
4->6                      : 0.9224 (0.960395)
4->12                     : 0.0360 (0.189800)

STATE 6  Exc. Energy: 413.285mEh  11.246eV     90705.6cm**-1
3->6                      : 0.8368 (0.914777)
3->12                     : 0.0307 (0.175082)
1->6                      : 0.0148 (-0.121572)
1->3 ->6                 : 0.0376 (-0.193912)
2->3 ->5                 : 0.0456 (0.213492)

STATE 7  Exc. Energy: 474.514mEh  12.912eV     104143.8cm**-1
1->3                      : 0.8308 (-0.911467)
2->3 ->6                 : 0.0826 (0.287351)
2->3 ->12                : 0.0148 (0.121501)

STATE 8  Exc. Energy: 501.672mEh  13.651eV     110104.2cm**-1
1->4                      : 0.8364 (-0.914550)
4->5                      : 0.0249 (0.157804)
4->7                      : 0.0561 (0.236863)
2->4 ; 3->6              : 0.0324 (-0.180124)

STATE 9  Exc. Energy: 511.571mEh  13.921eV     112276.9cm**-1
3->6                      : 0.0580 (0.240898)
1->6                      : 0.0166 (-0.128707)
2->5                      : 0.1178 (0.343223)
2->3 ->5                 : 0.3041 (-0.551423)
2->4 ->5                 : 0.2625 (-0.512374)

```

The general-spin version GS-ROCIS can be requested via:

```

!def2-SVP TightSCF

%scf
  HFTyp ROHF
  ROHF_CASE HIGHSPIN
  ROHF_NEL[1] 2
end

%rocis

```

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```

DoGenROCIS true
ReferenceMult 3
NRoots 10
end

* xyz 0 3
C 0 0 0.1058
H 0 0.9910 -0.3174
H 0 -0.9910 -0.3174
end

```

The output gives the resulting spin coupling in addition to orbital information:

```

Eigenvectors of ROCIS calculation:
the threshold for printing is: 1e-02

i->a      single excitation from orbital i to a
i->t ; w->a double excitation from orbital i to t and orbital w to a

STATE 0  Exc. Energy: 0.000mEh 0.000eV 0.0cm**-1
      0      : 0.9880 (-0.993993) : spin coupling: 2+1+1 0

STATE 1  Exc. Energy: 291.825mEh 7.941eV 64048.2cm**-1
      2->3      : 0.9602 (0.979900) : spin coupling: +1 2+1 0

STATE 2  Exc. Energy: 307.258mEh 8.361eV 67435.4cm**-1
      1->4      : 0.0244 (-0.156226) : spin coupling: +1+1 2 0
      4->5      : 0.9086 (-0.953183) : spin coupling: 2+1 0+1
      4->11     : 0.0379 (-0.194741) : spin coupling: 2+1 0+1
      1->3 ; 4->5 : 0.0126 (0.112387) : spin coupling: +1 2 0+1

STATE 3  Exc. Energy: 311.967mEh 8.489eV 68468.7cm**-1
      2->4      : 0.9558 (0.977660) : spin coupling: +1+1 2 0
      4->6      : 0.0181 (-0.134462) : spin coupling: 2+1 0+1

STATE 4  Exc. Energy: 349.147mEh 9.501eV 76629.0cm**-1
      3->5      : 0.8588 (-0.926723) : spin coupling: 2 0+1+1
      3->11     : 0.0299 (-0.173056) : spin coupling: 2 0+1+1
      1->5      : 0.0695 (-0.263669) : spin coupling: +1-1+1+1

STATE 5  Exc. Energy: 374.241mEh 10.184eV 82136.4cm**-1
      2->4      : 0.0187 (-0.136885) : spin coupling: +1+1 2 0
      4->6      : 0.9224 (-0.960395) : spin coupling: 2+1 0+1
      4->12     : 0.0360 (-0.189800) : spin coupling: 2+1 0+1

STATE 6  Exc. Energy: 413.285mEh 11.246eV 90705.6cm**-1
      3->6      : 0.8368 (-0.914777) : spin coupling: 2 0+1+1
      3->12     : 0.0307 (-0.175082) : spin coupling: 2 0+1+1
      1->6      : 0.0609 (-0.246700) : spin coupling: +1-1+1+1
      2->5      : 0.0242 (-0.155666) : spin coupling: +1+1+1-1
      2->5      : 0.0345 (0.185684) : spin coupling: +1-1+1+1

STATE 7  Exc. Energy: 474.514mEh 12.912eV 104143.8cm**-1
      1->3      : 0.8308 (-0.911467) : spin coupling: +1 2+1 0
      2->6      : 0.0374 (0.193474) : spin coupling: +1+1+1-1
      2->6      : 0.0631 (-0.251226) : spin coupling: +1-1+1+1
      2->12     : 0.0134 (-0.115919) : spin coupling: +1-1+1+1

STATE 8  Exc. Energy: 501.672mEh 13.651eV 110104.2cm**-1
      1->4      : 0.8364 (0.914550) : spin coupling: +1+1 2 0
      4->5      : 0.0249 (-0.157804) : spin coupling: 2+1 0+1

```

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```

4->7      : 0.0561 (-0.236863) : spin coupling: 2+1 0+1
2->4      ; 3->6      : 0.0324 (0.180124) : spin coupling: +1 0 2+1

STATE 9   Exc. Energy: 511.571mEh 13.921eV      112276.9cm**-1
3->6      : 0.0580 (0.240898) : spin coupling: 2 0+1+1
1->6      : 0.0311 (0.176432) : spin coupling: +1+1+1-1
2->5      : 0.6111 (-0.781719) : spin coupling: +1+1+1-1
2->5      : 0.0557 (0.235994) : spin coupling: +1+1-1+1
2->5      : 0.2060 (0.453844) : spin coupling: +1-1+1+1
2->11     : 0.0115 (0.107060) : spin coupling: +1-1+1+1

```

GS-ROCIS requires a valid ROHF solution as reference (either high-spin or a specific CSF). For this, one would use the CSF-ROHF method to obtain the reference wavefunction for which GS-ROCIS will be performed:

```

%scf
  HFTyp ROHF
  ROHF_CASE HIGHSPIN, USER_CSF or AF_CSF
end

```

For more details on the CSF-ROHF method, check [ROHF Options](#).

The parametrized ROCIS/DFT formulation can be requested by:

```

%rocis
  DoGenROCIS      false # ROCIS/DFT is available only for the high-spin_
  ↳implementation of ROCIS.
  DoDFTCIS        true  # Switches on the ROCIS/DFT method.
  DFTCIS_c = 0.18, 0.20, 0.40 # Array input of the three parameters.
end

```

Important

- Currently, ROCIS/DFT is not implemented for the general-spin (GS-ROCIS) procedure.

Capabilities

At the present, ROCIS can be used to calculate excitation energies, absorption, circular dichroism and magnetic circular dichroism spectra. It is also capable of calculating resonant inelastic X-ray scattering (RIXS) spectra. Magnetic properties such as g-tensors, zero-field splittings, hyperfine couplings and electric field gradients are also available.

5.4.3 Excited States for Open-Shell Molecules with CASSCF Linear Response (MC-RPA)

ORCA has the possibility to calculate excitation energies, oscillator and rotatory strengths for CASSCF wave functions within the response theory (MC-RPA) formalism.[592, 593, 594] The main scope of MC-RPA is to simulate UV/Vis and ECD absorption spectra of open-shell molecules like transition metal complexes and organic radicals. MC-RPA absorption spectra are usually more accurate than those obtained from the state-averaged CASSCF ansatz as orbital relaxation effects for excited states are taken into account. The computational costs are usually larger than those of SA-CASSCF and should be comparable to a TD-DFT calculation for feasible active space sizes.

General Use

MC-RPA needs a converged state-specific CASSCF calculation of the electronic ground state. The only necessary information that the user has to provide is the desired number of excited states (roots). All other keywords are just needed to control the Davidson algorithm or post process the results. A minimal input for calculating the four lowest singlet excited states of ethylene could like the following:

```
#
# CASSCF + MCRPA for C2H4
#
! DEF2-SVP DEF2-TZVP/C VeryTightSCF

%casscf
  nel          2
  norb          2
  mult          1
  nroots        1
  gtol 1e-6
  etol 1e-10
end

%mcrrpa
  nroots        8
end

* int 0 1
C 0 0 0 0      0 0
C 1 0 0 1.3385 0 0
H 1 2 0 1.07   120 0
H 1 2 3 1.07   120 180
H 2 1 3 1.07   120 0
H 2 1 3 1.07   120 180
*
```

After the residual norm is below a user-given threshold TolR we get the following information

```
-----
->-----
      All 8 RPA Roots CONVERGED Below 1.000e-05
-----
->-----
      3 (root 0)      3.352976e-01      3.489323e-07      Yes
        (root 1)      3.485288e-01      1.656998e-08      Yes
        (root 2)      3.514846e-01      2.178527e-08      Yes
        (root 3)      3.741213e-01      2.577113e-07      Yes
        (root 4)      3.743973e-01      2.416887e-08      Yes
        (root 5)      4.040700e-01      4.609207e-08      Yes
        (root 6)      4.479248e-01      1.240222e-08      Yes
        (root 7)      4.609744e-01      6.311327e-09      Yes
```

and the absorption and ECD spectrum

```
-----
->-----
      ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS
-----
->-----
      Transition      Energy      Energy      Wavelength      fosc(D2)      D2      DX      <
      DY      DZ      (eV)      (cm-1)      (nm)      (au**2)      (au)      <
      (continues on next page)
```

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→ (au)	(au)							
→-----								
0-1A → 1-1A	9.123912	73589.3	135.9	0.430768702	1.92710	1.38820	-	
→0.00000 -0.00000								
0-1A → 2-1A	9.483952	76493.2	130.7	0.009915132	0.04267	0.00000	-	
→0.00000 -0.20657								
0-1A → 3-1A	9.564384	77142.0	129.6	0.000000000	0.00000	0.00000	-	
→0.00000 -0.00000								
0-1A → 4-1A	10.180358	82110.1	121.8	0.000000000	0.00000	-0.00000	-	
→0.00000 -0.00000								
0-1A → 5-1A	10.187869	82170.7	121.7	0.000000000	0.00000	-0.00000	-	
→0.00000 0.00000								
0-1A → 6-1A	10.995304	88683.1	112.8	0.000000000	0.00000	0.00000	-	
→0.00000 -0.00000								
0-1A → 7-1A	12.188654	98308.1	101.7	0.000000000	0.00000	-0.00000	-	
→0.00000 -0.00000								
0-1A → 8-1A	12.543751	101172.2	98.8	0.000000000	0.00000	-0.00000	-	
→0.00000 -0.00000								
...								
→-----								
CD SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS								
→-----								
Transition	Energy	Energy	Wavelength	R	MX	MY		
→MZ	(eV)	(cm-1)	(nm)	(1e40*cgs)	(au)	(au)		
→(au)								
→-----								
0-1A → 1-1A	9.123912	73589.3	135.9	-0.00000	0.00000	0.00000	0.	
→00000								
0-1A → 2-1A	9.483952	76493.2	130.7	-0.00000	-0.00000	0.00000	-0.	
→00000								
0-1A → 3-1A	9.564384	77142.0	129.6	-0.00000	0.69943	0.00000	0.	
→00000								
0-1A → 4-1A	10.180358	82110.1	121.8	-0.00000	-0.15776	0.00000	0.	
→00000								
0-1A → 5-1A	10.187869	82170.7	121.7	-0.00000	0.00000	0.73302	-0.	
→00000								
0-1A → 6-1A	10.995304	88683.1	112.8	0.00000	-0.00000	0.54037	0.	
→00000								
0-1A → 7-1A	12.188654	98308.1	101.7	0.00000	-0.00000	0.00000	0.	
→00000								
0-1A → 8-1A	12.543751	101172.2	98.8	-0.00000	-0.00000	0.00000	-0.	
→90854								

Capabilities

At the moment, we can simulate UV/Vis and ECD absorption spectra by computing excitation energies, oscillator and rotatory strengths (check section *One Photon Spectroscopy* for more information). The code is parallelized and the computational bottleneck is the integral direct AO-Fock matrix construction. All intermediates that depend on the number of states are stored on disk, which makes the MC-RPA implementation suitable for computing many low-lying electronic states of larger molecules. Abelian point-group symmetry can be exploited in the calculation (up to D_{2h}). But there are no calculations of spin-flip excitations possible at the moment. That means all excited states will have the same spin as the reference state, which is specified in the %casscf input block.

It is also possible to analyze and visualize the ground-to-excited-state transitions by means of natural transition orbitals[595] (NTO), which is explained in more detail in section *Excited States for Open-Shell Molecules with CASSCF*

Linear Response (MC-RPA).

For further details, please study our recent publications[594, 596].

5.4.4 Excited States with ADC2

Among the various approximate correlation methods available for excited states, one of the most popular one is algebraic diagrammatic construction(ADC) method. The ADC has its origin in the Green's function theory. It expands the energy and wave-function in perturbation order and can directly calculate the excitation energy, ionization potential and electron affinity, similar to that in the EOM-CCSD method. Because of the symmetric eigenvalue problem in ADC, the calculation of properties are more straight forward to calculate than EOM-CCSD. In ORCA, only the second-order approximation to ADC(ADC2) is implemented. It scales as $O(N^5)$ power of the basis set.

General Use

The simplest way to perform an ADC2 calculation is via the usage of the ADC2 keyword, together with the specification of the desired number of roots:

```
! ADC2 cc-pVDZ cc-pVDZ/C TightSCF

%mdci
  nroots 9
end

*xyz 0 1
  C      0.016227   -0.000000    0.000000
  O      1.236847    0.000000   -0.000000
  H     -0.576537    0.951580   -0.000000
  H     -0.576537   -0.951580   -0.000000
*
```

The above input will call the ADC2 routine with default settings. The main output is a list of excitation energies, augmented with some further state specific data. The integral transformation in the ADC2 implementation of ORCA is done using the density-fitting approximation. Therefore, one needs to specify an auxiliary basis. For the above input, the following output is obtained:

```
-----
ADC (2) RESULTS (RHS)
-----

IROOT=  1:  0.146914 au      3.998 eV   32243.8 cm**-1
  Amplitude   Excitation
  -0.116970    4 ->   8
    0.672069    7 ->   8
IROOT=  2:  0.286012 au      7.783 eV   62772.3 cm**-1
  Amplitude   Excitation
  -0.659777    7 ->   9
IROOT=  3:  0.341919 au      9.304 eV   75042.5 cm**-1
  Amplitude   Excitation
  -0.676913    5 ->   8
IROOT=  4:  0.352206 au      9.584 eV   77300.2 cm**-1
  Amplitude   Excitation
    0.126824    4 ->  10
    0.360690    6 ->   8
   -0.547670    7 ->  10
IROOT=  5:  0.393965 au     10.720 eV   86465.3 cm**-1
  Amplitude   Excitation
    0.551345    6 ->   8
    0.363450    7 ->  10
```

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```

-0.109270      6 -> 8      6 -> 8
IROOT= 6: 0.404946 au      11.019 eV      88875.4 cm**-1
  Amplitude      Excitation
    0.669682      4 -> 8
    0.126557      7 -> 8
IROOT= 7: 0.412800 au      11.233 eV      90599.2 cm**-1
  Amplitude      Excitation
   -0.100274      4 -> 11
    0.671884      7 -> 11
IROOT= 8: 0.439251 au      11.953 eV      96404.5 cm**-1
  Amplitude      Excitation
   -0.674114      6 -> 9
    0.104541      6 -> 9      6 -> 8
IROOT= 9: 0.486582 au      13.241 eV      106792.5 cm**-1
  Amplitude      Excitation
   -0.654624      5 -> 9

```

The transition moment for ADC2 in ORCA is calculated using an EOM-like expectation value approach, unlike the traditionally used intermediate state representation. However, the two approaches gives almost identical result.

SPECTRUM FOR LEFT-RIGHT TRANSITION MOMENTS								

↪-----								
ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS								

↪-----								
Transition	Energy	Energy	Wavelength	fosc(D2)	D2	DX		
↪ DY DZ	(eV)	(cm-1)	(nm)		(au**2)	(au)		
↪ (au) (au)								

↪ 0-1A -> 1-1A	3.997726	32243.8	310.1	0.000000000	0.00000	0.00000	↪	
↪ 0.00000 0.00000								
↪ 0-1A -> 2-1A	7.782776	62772.3	159.3	0.096710371	0.50720	-0.00000	-	
↪ 0.70536 0.00000								
↪ 0-1A -> 3-1A	9.304078	75042.5	133.3	0.002261744	0.00992	-0.00000	↪	
↪ 0.00000 -0.09835								
↪ 0-1A -> 4-1A	9.584003	77300.2	129.4	0.007937829	0.03381	-0.18502	-	
↪ 0.00000 -0.00000								
↪ 0-1A -> 5-1A	10.720332	86465.3	115.7	0.465055079	1.77067	1.32377	↪	
↪ 0.00000 -0.00000								
↪ 0-1A -> 6-1A	11.019150	88875.4	112.5	0.000000000	0.00000	-0.00000	↪	
↪ 0.00000 -0.00000								
↪ 0-1A -> 7-1A	11.232869	90599.2	110.4	0.022236623	0.08080	0.00000	-	
↪ 0.28105 -0.00000								
↪ 0-1A -> 8-1A	11.952640	96404.5	103.7	0.009103120	0.03109	0.00000	-	
↪ 0.00000 0.17328								
↪ 0-1A -> 9-1A	13.240575	106792.5	93.6	0.071433742	0.22021	-0.46692	-	
↪ 0.00000 0.00000								

The IP and EA versions can be called using the keywords IP-ADC2 and EA-ADC2, respectively.

Capabilities

At present, the ADC2 module is able to perform excited, ionized and electron attached state calculations, only for closed-shell systems. No open-shell version of the ADC2 is currently available. Below are all the parameters that influence the ADC2 module.

```
%mdci
#ADC2 parameters - defaults displayed
NDav 20          # maximum size of reduced space (i.e. 20*NRoots)
CheckEachRoot true # check convergence for each root separately
RootHoming true  # apply root homing
DoLanczos false  # use the Lanczos procedure rather than Davidson
UseCISUpdate true # use diagonal CIS for updating
NInitS 0         # number of roots in the initial guess, if 0, use preset
↪value
DoRootwise false # solves for each root separately,
                  # more stable for large number of roots
FOLLOWCIS false  # follows the initial singles guess
end
```

One can notice that features available in the ADC2 module is quite limited as compared to the EOM module and the option to specifically target the core-orbitals are yet not available. A word of caution, **The ‘second order black magic’ of ADC2 can fail in many of the cases.** The readers are encouraged to try the DLPNO based EOM-CCSD methods(*Excited States with DLPNO based coupled cluster methods*) which are much more accurate and computationally efficient.

5.4.5 Excited States with STEOM-CCSD

The STEOM-CCSD method provides an efficient way to calculate excitation energies, with an accuracy comparable to the EOM-CCSD approach, at a nominal cost. A detailed description will be given in Section *Excited States via STEOM-CCSD*.

General Use

The simplest way to perform a STEOM calculation is using the STEOM-CCSD keyword, together with the specification of the desired number of roots (NRoots):

```
! STEOM-CCSD cc-pVDZ TightSCF

%mdci
  NRoots 9          # Number of excited states
  DoDbfilter true   # Remove doubly excited states
end

*xyz 0 1
C      0.016227    -0.000000     0.000000
O      1.236847     0.000000    -0.000000
H     -0.576537     0.951580    -0.000000
H     -0.576537    -0.951580    -0.000000
*
```

The above input calls the STEOM routine with default settings, where, for instance, the doubly excited states are eliminated (DoDbFilter true). The main output is a list of excitation energies, augmented with some further state specific data. The STEOMCC approach in ORCA uses state-averaged CIS natural transition orbitals (NTO) for the selection of the active space. For the above input, the following output is obtained:

```
-----
STEOM-CCSD RESULTS (SINGLETs)
-----
```

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```

IROOT= 1: 0.145378 au      3.956 eV   31906.7 cm**-1
  Amplitude   Excitation
-0.168322    4 -> 8
-0.984801    7 -> 8
  Ground state amplitude: -0.000000

```

```

Percentage Active Character      99.91

```

```

  Amplitude   Excitation in Canonical Basis
-0.166144    4 -> 8
-0.975626    7 -> 8
  0.123172    7 -> 13

```

```

IROOT= 2: 0.309944 au      8.434 eV   68024.9 cm**-1
  Amplitude   Excitation
-0.993139    7 -> 9
  Ground state amplitude: 0.000000

```

```

Percentage Active Character      99.94

```

```

  Amplitude   Excitation in Canonical Basis
-0.989653    7 -> 9

```

```

IROOT= 3: 0.337588 au      9.186 eV   74092.0 cm**-1
  Amplitude   Excitation
-0.993709    5 -> 8
  Ground state amplitude: -0.000002

```

```

Percentage Active Character      99.23

```

```

  Amplitude   Excitation in Canonical Basis
-0.984171    5 -> 8
  0.136295    5 -> 13

```

```

IROOT= 4: 0.357393 au      9.725 eV   78438.7 cm**-1
  Amplitude   Excitation
-0.186839    4 -> 10
-0.755864    6 -> 8
-0.601549    7 -> 10
-0.112921    7 -> 12
  Ground state amplitude: 0.026385

```

```

Percentage Active Character      99.71

```

```

  Amplitude   Excitation in Canonical Basis
-0.182608    4 -> 10
-0.752095    6 -> 8
-0.598472    7 -> 10

```

```

IROOT= 5: 0.386751 au      10.524 eV   84882.0 cm**-1
  Amplitude   Excitation
-0.980511    4 -> 8
  0.178900    7 -> 8
  Ground state amplitude: 0.000000

```

```

Percentage Active Character      99.90

```

```

  Amplitude   Excitation in Canonical Basis
-0.971593    4 -> 8
  0.121664    4 -> 13

```

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```

0.179278      7 ->  8

IROOT=  6:  0.406225 au      11.054 eV      89156.2 cm**-1
  Amplitude      Excitation
    0.532674      6 ->  8
   -0.825021      7 -> 10
  Ground state amplitude: -0.065794

Percentage Active Character      99.70

  Amplitude      Excitation in Canonical Basis
    0.526200      6 ->  8
   -0.817279      7 -> 10

IROOT=  7:  0.421236 au      11.462 eV      92450.6 cm**-1
  Amplitude      Excitation
   -0.125749      4 -> 11
   -0.985406      7 -> 11
  Ground state amplitude:  0.000000

Percentage Active Character      99.85

  Amplitude      Excitation in Canonical Basis
    0.124222      4 -> 11
    0.983485      7 -> 11

IROOT=  8:  0.443588 au      12.071 eV      97356.3 cm**-1
  Amplitude      Excitation
    0.106457      3 ->  8
    0.992884      6 ->  9
  Ground state amplitude:  0.000092

Percentage Active Character      99.78

  Amplitude      Excitation in Canonical Basis
    0.106009      3 ->  8
    0.987228      6 ->  9

IROOT=  9:  0.512311 au      13.941 eV     112439.3 cm**-1
  Amplitude      Excitation
   -0.995561      6 -> 10
  Ground state amplitude: -0.000001

Percentage Active Character      99.94

  Amplitude      Excitation in Canonical Basis
   -0.985669      6 -> 10
    0.157781      6 -> 15

```

The first set of excitation amplitudes, printed for each root, have been calculated in the CIS NTO (Natural Transition Orbitals) basis. The second set of amplitudes have been evaluated in the RHF canonical basis.

Capabilities

At present, the STEOM routine is able to calculate excitation energies, for both closed- or open-shell systems, using an RHF or UHF reference function, respectively. It can be used for both serial and parallel calculations. The method is available in the back-transformed PNO and DLPNO framework allowing the calculation of large molecules (Section *Capabilities* and *Excited States with DLPNO based coupled cluster methods*). In the closed-shell case (RHF), a lower scaling version can be invoked by setting the CCSD2 keyword to true in the %mdci section, which sets a second order approximation to the exact parent approach. The transition moments can also be obtained for closed- and open-shell systems. For more details see Section *Excited States via STEOM-CCSD*.

5.4.6 Excited States with IH-FSMR-CCSD

The intermediate Hamiltonian Fock-space coupled cluster method (IH-FSMR-CCSD) provides an alternate way to calculate excitation energies, with an accuracy comparable to the STEOM-CCSD approach. A detailed description is given in Section *Excited States via IH-FSMR-CCSD*.

General Use

The IH-FSMR-CCSD calculation is called using the simple input keyword IH-FSMR-CCSD and specifying the desired number of excited states (NRoots) in the %mdci block.:

```
! IH-FSMR-CCSD cc-pVDZ TightSCF

%mdci
  nroots 6
end

*xyz 0 1
  C      0.016227   -0.000000    0.000000
  O      1.236847    0.000000   -0.000000
  H     -0.576537    0.951580   -0.000000
  H     -0.576537   -0.951580   -0.000000
*
```

The above input will call the IH-FSMR-CCSD routine with default settings. The main output is a list of excitation energies, augmented with some further state specific data. The IH-FSMR-CCSD approach in ORCA uses state-averaged CIS natural transition orbitals(NTO) for the selection of the active space - similar to STEOM-CCSD. For the above input, the following output is obtained:

```
-----
IH-FSMR-CCSD RESULTS (SINGLETs)
-----

IROOT=  1:  0.144808 au      3.940 eV   31781.8 cm**-1
  Amplitude      Excitation
  -0.171178      4 ->    8
  -0.984024      7 ->    8
  Ground state amplitude:  0.000000

Percentage Active Character      99.96

  Amplitude      Excitation in Canonical Basis
  -0.169804      4 ->    8
  -0.976596      7 ->    8
   0.111105      7 ->   13

IROOT=  2:  0.309569 au      8.424 eV   67942.6 cm**-1
  Amplitude      Excitation
  -0.994029      7 ->    9
```

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```

Ground state amplitude: 0.000000

Percentage Active Character      99.79

Amplitude      Excitation in Canonical Basis
-0.991036      7 -> 9

IROOT= 3: 0.337609 au      9.187 eV      74096.7 cm**-1
Amplitude      Excitation
0.992246      5 -> 8
Ground state amplitude: 0.000000

Percentage Active Character      99.29

Amplitude      Excitation in Canonical Basis
0.985970      5 -> 8
-0.120519      5 -> 13

IROOT= 4: 0.354726 au      9.653 eV      77853.3 cm**-1
Amplitude      Excitation
-0.167422      4 -> 10
0.125754      5 -> 11
-0.748485      6 -> 8
-0.575997      7 -> 10
-0.204999      7 -> 14
Ground state amplitude: 0.000000

Percentage Active Character      94.11

Warning:: the state may have not converged with respect to active space
----- Handle with Care -----

Amplitude      Excitation in Canonical Basis
-0.175024      4 -> 10
0.110821      5 -> 11
-0.745514      6 -> 8
-0.609903      7 -> 10

IROOT= 5: 0.386134 au      10.507 eV      84746.6 cm**-1
Amplitude      Excitation
-0.980436      4 -> 8
0.180972      7 -> 8
Ground state amplitude: 0.000000

Percentage Active Character      99.91

Amplitude      Excitation in Canonical Basis
-0.972869      4 -> 8
0.111877      4 -> 13
0.180279      7 -> 8

IROOT= 6: 0.443256 au      12.062 eV      97283.4 cm**-1
Amplitude      Excitation
-0.110780      3 -> 8
-0.991903      6 -> 9
Ground state amplitude: 0.000000

Percentage Active Character      99.71

Amplitude      Excitation in Canonical Basis
-0.109728      3 -> 8

```

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```
-0.988030      6 -> 9
```

The first set of excitation amplitudes, printed for each root, have been calculated in the CIS NTO (Natural Transition Orbitals) basis. The second set of amplitudes have been evaluated in the RHF canonical basis.

Capabilities

At present, the IH-FSMR-CCSD routine is able to calculate excitation energies, for only closed shell systems using an RHF reference. It can be used for both serial and parallel calculations. In the closed-shell case (RHF), a lower scaling version can be invoked by using bt-PNO approximation. The transition moments and solvation correction can be obtained using the CIS approximation.

5.4.7 Excited States with PNO based coupled cluster methods

The methods described in the previous section are performed over a canonical CCSD or MP2 ground state. The use of canonical CCSD amplitudes restricts the use of EOM-CC and STEOM-CC methods to small molecules. The use of MP2 amplitudes is possible (e.g. the EOM-CCSD(2) or STEOM-CCSD(2) approaches), but it seriously compromises the accuracy of the method.

The bt-PNO-EOM-CCSD methods gives an economical compromise between accuracy and computational cost by replacing the most expensive ground state CCSD calculation with a DLPNO based CCSD calculation. The typical deviation of the results from the canonical EOM-CCSD results is around 0.01 eV. A detailed description will be given in *Excited States via PNO-based coupled cluster*.

General Use

The simplest way to perform a PNO based EOM calculation is via the usage of the bt-PNO-EOM-CCSD keyword, together with the specification of the desired number of roots. The specification of an auxiliary basis set is also required, just as for ground state DLPNO-CCSD calculations.

```
! bt-PNO-EOM-CCSD def2-TZVP def2-TZVP/C def2/J TightSCF

%mdci
  nroots 9
end

*xyz 0 1
  C      0.016227   -0.000000    0.000000
  O      1.236847    0.000000   -0.000000
  H     -0.576537    0.951580   -0.000000
  H     -0.576537   -0.951580   -0.000000
*
```

The output is similar to that from a canonical EOM-CCSD calculation:

```
-----
EOM-CCSD RESULTS (RHS)
-----
```

```
IROOT=  1:  0.145420 au      3.957 eV   31915.9 cm** -1
  Amplitude   Excitation
    0.650351    7 ->  8
   -0.162540    7 -> 13
  Ground state amplitude: 0.000000
Percentage singles character=      92.33

IROOT=  2:  0.311168 au      8.467 eV   68293.4 cm** -1
```

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```

Amplitude   Excitation
  0.650800   7 ->  9
 -0.155532   7 -> 11
Ground state amplitude: -0.000000
Percentage singles character=      90.95

IROOT=  3:  0.337404 au      9.181 eV   74051.7 cm**-1
Amplitude   Excitation
  0.652018   5 ->  8
 -0.169980   5 -> 13
Ground state amplitude:  0.000000
Percentage singles character=      91.87

IROOT=  4:  0.348225 au      9.476 eV   76426.6 cm**-1
Amplitude   Excitation
  0.152132   7 ->  9
  0.652819   7 -> 11
Ground state amplitude:  0.000000
Percentage singles character=      92.35

IROOT=  5:  0.354668 au      9.651 eV   77840.6 cm**-1
Amplitude   Excitation
  0.545649   6 ->  8
 -0.339835   7 -> 10
  0.170720   6 ->  8      6 ->  8
Ground state amplitude:  0.032711
Percentage singles character=      87.10

IROOT=  6:  0.379606 au     10.330 eV   83313.9 cm**-1
Amplitude   Excitation
  0.636153   4 ->  8
 -0.160301   4 -> 13
 -0.109552   7 ->  8
  0.143497   7 ->  8      6 ->  8
Ground state amplitude:  0.000000
Percentage singles character=      88.55

IROOT=  7:  0.386807 au     10.526 eV   84894.3 cm**-1
Amplitude   Excitation
  0.257812   6 ->  8
  0.584151   7 -> 10
  0.181783   7 -> 14
Ground state amplitude:  0.038804
Percentage singles character=      90.30

IROOT=  8:  0.440552 au     11.988 eV   96690.1 cm**-1
Amplitude   Excitation
 -0.655574   6 ->  9
 -0.104097   6 -> 16
 -0.112700   6 ->  9      6 ->  8
Ground state amplitude:  0.000000
Percentage singles character=      87.92

IROOT=  9:  0.447219 au     12.169 eV   98153.2 cm**-1
Amplitude   Excitation
  0.162756   7 ->  8
  0.651078   7 -> 13
Ground state amplitude:  0.000000
Percentage singles character=      90.36

```

The IP and EA versions can be called by using the keywords bt-PNO-IP-EOM-CCSD and bt-PNO-EA-EOM-CCSD, respectively. Furthermore, the STEOM version can be invoked by using the keywords bt-PNO-STEOM-CCSD.

Capabilities

All of the features of canonical EOM-CC and STEOM-CC are available in the PNO based approaches for both closed- and open-shell systems.

5.4.8 Excited States with DLPNO based coupled cluster methods

The DLPNO-STEOM-CCSD method uses the full potential of DLPNO to reduce the computational scaling while keeping the accuracy of STEOM-CCSD.

Important

- DLPNO-STEOM-CCSD is currently only available for closed-shell systems!

General Use

The simplest way to perform a DLPNO based STEOM calculation is via the usage of the STEOM-DLPNO-CCSD keyword, together with the specification of the desired number of roots. The specification of an auxiliary basis set is also required, just as for ground state DLPNO-CCSD calculations.

As any CCSD methods, it is important to allow ORCA to access a significant amount of memory. In terms of scaling the limiting factor of the method is the size of temporary files and thus the disk space. For molecules above 1500 basis functions it starts to increase exponentially up to several teraoctets.

Here is the standard input we would recommend for STEOM-DLPNO-CCSD calculations. More information on the different keywords and other capabilities are available in the detailed part of the manual [Excited States via STEOM-CCSD](#), [Excited States via DLPNO-STEOM-CCSD](#). The following publications referenced some applications for this method either in organic molecules [597], [598] or for Semiconductors [599].

```
! STEOM-DLPNO-CCSD def2-TZVP def2-TZVP/C def2/J TightSCF

%mdci
  NRoots 6
  DoRootWise true
  OThresh 0.005
  VThresh 0.005
  TCutPNOSingles 1e-11
  NDAV 400
  DoStoreSTEOM true
  DoSimpleDens false
  AddL2Term True
  DTol 1e-5
end

* xyz 0 1
  C    0.016227   -0.000000    0.000000
  O    1.236847    0.000000   -0.000000
  H   -0.576537    0.951580   -0.000000
  H   -0.576537   -0.951580   -0.000000
*
```

The output is similar to that from a canonical DLPNO-STEOM-CCSD calculation:

```
-----
STEOM-CCSD RESULTS (SINGLETs)
-----
```

```
IROOT=  1:  0.144275 au      3.926 eV   31664.7 cm**-1
```

(continues on next page)