

Examples for input files

In this section you will find some simple input examples. A much more comprehensive description of the program's capabilities is found in the user manual.

The first trivial calculation is a simple restricted Hartree-Fock SCF calculation on the CO molecule:

```
Orca1.inp
#
# My first ORCA calculation :-)
#
! HF SVP

* xyz 0 1
  C 0.0  0.0  0.0
  O 0.0  0.0  1.13
*
```

We can run a spin-unrestricted calculation on the cation and ask for tight SCF convergence:

```
Orca2.inp
#
# Unrestricted Hartree-Fock single point calculation
# with tight SCF convergence criteria
#
! UHF SVP TightSCF

* xyz 1 2
  C 0.0  0.0  0.0
  O 0.0  0.0  1.13
*
```

Now let's get a bit more serious and run a geometry optimization on some organic molecule at the B3LYP level. The program automatically generates internal coordinates and carries out the optimization in them.

```
Orca3.inp
#
# Test redundant internal optimization
#
! RKS B3LYP SVP Opt TightSCF SmallPrint
* xyz 0 1
C    -1.48746    -0.02867    -0.00006
O     0.37634     0.02867    -0.00006
H    -1.81891    -1.06706    -0.00006
H    -1.86647     0.47370     0.88993
H    -1.86647     0.47370    -0.89004
H     0.75672    -0.95001    -0.00006
*
```

It is a little bit more challenging to do calculations on transition metal complexes. Let us optimize the structure of $[\text{Fe}(\text{H}_2\text{O})_6]^{3+}$ ($S=5/2$) and use the very efficient RI approximation to reduce the computation time.

```
Orca4.inp
#
# Geometry optimization of [Fe(H2O)6]3+ employing DFT
# The RI approximation is used
# The SV(P) basis set was replaced by the TZVPP basis set for iron
#

! UKS BP SV(P) SV/J OPT Split-RI-J

%basis NewGTO 26 "TZVPP" end
      NewAuxGTO 26 "TZV/J" end
end

* xyz 3 6
Fe      0.000047      -0.000114      0.000013
O       -0.199873       1.108797       1.733279
H        0.380320       1.865880       2.020956
O       -1.236638       1.328040      -0.990513
H       -1.665421       2.138758      -0.601345
O       -1.643746      -1.133837       0.535682
H       -2.594241      -0.943118       0.306097
O        0.198381      -1.109845      -1.732630
H        0.891437      -0.986937      -2.437690
O        1.238604      -1.327482       0.989961
H        1.513573      -1.279077       1.946292
O        1.643403       1.134541      -0.535766
H        2.593848       0.945769      -0.304430
H       -1.516941       1.276571      -1.945157
H        1.632468       1.972748      -1.074090
H       -0.894758       0.986836       2.436707
H        1.671714      -2.135426       0.599824
H       -0.383130      -1.865932      -2.020344
H       -1.633554      -1.973176       1.072267
*
```

Let us predict properties – here we calculate the EPR parameters for an organic radical anion.

```
Orca5.inp
#
# g-tensor Calculation for an organic radical anion
#
#
! UKS BP SV(P) TightSCF Grid4 NoFinalGrid Direct

* xyz -1 2
c          1.672238      -1.264072      0.009796
c          0.335031      -0.940361     -0.075605
c         -0.121366       0.436182     -0.112778
c          0.914606       1.448908     -0.053979
c          2.251894       1.127195      0.031094
c          2.719187      -0.252390      0.069099
h          1.997766      -2.304445      0.036564
h         -0.429413      -1.716578     -0.118243
o         -1.362987       0.753407     -0.193423
h          0.584162       2.487790     -0.081799
```

```

h          3.017076    1.903066    0.073644
o          3.953182   -0.551604    0.148612
c         -4.499185    0.039361    0.381896
h         -5.467065   -0.483352    0.380119
h         -4.646728    1.027796   -0.090897
h         -4.211445    0.216196    1.434546
o         -3.563523   -0.755664   -0.309212
h         -2.692156   -0.268520   -0.298882

```

```

*

```

```

%epnrmr gtensor 1
end

```

A more complete set of properties for a transition metal complex. Use a specifically tailored uncontracted basis set

```

Orca6.inp
#
# [Fe(H2O)]3+
# Calculation of g-tensor, electric and 57Fe magnetic hyperfine data
# including second order spin-orbit coupling
#
! UKS B3LYP/G SV(P) SV/J TightSCF Direct Grid3 FinalGrid4
! Uncontract

%method SpecialGridAtoms 26
      SpecialGridIntAcc 7
end

%basis NewGTO 26 "CP(PPP)" end
      NewAuxGTO 26 "TZV/J" end
end

%rel    SOCType 3
      SOCFlags 1,3,3,1
end

* xyz 3 6
Fe      0.000047   -0.000114    0.000013
O       -0.199873    1.108797    1.733279
H        0.380320    1.865880    2.020956
H       -0.894758    0.986836    2.436707
*
#

%epnrmr nuclei = all 26 { aiso, adip, aorb, fgrad}
      gtensor 4
end

```

A scalar relativistic single point calculation using the ZORA Hamiltonian. An uncontracted basis set is more accurate since segmented ZORA bases have not been developed.

```

Orca7.inp
#
# [Mn(II)(H2O)6]2+
# Scalar-relativistic single point calculation employing the ZORA method
#

```

```

! UKS BP SV(P) SV/J Direct TightSCF Grid3 NoFinalGrid
! Split-RI-J SlowConv Uncontract

# be careful with the numerical integration around manganese for
# relativistic potentials and uncontracted basis sets with steep
# s-functions.
%method SpecialGridAtoms =25
      SpecialGridIntAcc=7
    end
%basis NewGTO 25 "TZVPP" end
      NewAuxGTO 25 "TZV/J" end
    end

%rel method ZORA
      ModelPot 1,1,1,1
      ModelDens rhoZORA
      PictureChange true
    end

* xyz 2 6
mn -0.0012 -0.0002 0.0000
o -0.3280 1.5023 1.5581
h 0.3545 2.0232 2.0324
o -0.1563 1.5660 -1.5222
h -0.3178 2.5217 -1.3714
o -2.1595 -0.3443 -0.1250
h -2.8050 0.1230 -0.6969
o 0.3287 -1.5023 -1.5578
h 1.1868 -1.7790 -1.9443
o 0.1626 -1.5648 1.5229
h 0.0843 -1.4662 2.4956
o 2.1569 0.3439 0.1241
h 2.8011 -0.1169 0.7027
h -0.0921 1.4654 -2.4958
h 2.6863 0.9922 -0.3873
h -1.1837 1.7839 1.9462
h 0.3218 -2.5209 1.3722
h -0.3499 -2.0271 -2.0334
h -2.6880 -0.9991 0.3790
*
```

The COSMO model enables the simulation of solvent effects using a dielectric continuum approach.

```

Orca8.inp
#
# Geometry optimization of (H2O)2 using the COSMO continuum model
# and a dielectric constant of 80.4 (water)

! UKS B3LYP OPT TZVP TZV/J TightSCF

%cosmo epsilon 80.4
end

* xyz 0 1
O 22.002134 0.000000 -20.309542
H 21.914292 0.000000 -19.353569
H 22.873951 0.000000 -20.711455
H 21.255070 1.135019 -21.191600
```

```

O          20.812365    1.807624   -21.714301
H          21.001135    1.666089   -22.644857
*
```

Broken-symmetry calculations can be used to estimate singlet-triplet (generally high-spin low-spin) splittings in weakly interacting systems such as diradicals or magnetically interacting transition metal complexes. Here is a trivial example:

```

Orca9.inp
#
# Broken Symmetry Calculation on Li2 (singlet/triplet)
#
! B3LYP TZVPP

%scf BrokenSym 1,1
end

*int 0 3
Li  0  0  0  0  0  0
Li  1  0  0  4  0  0
*
```

MP2 calculations can be straightforwardly requested as well using RHF, ROHF or UHF reference wavefunctions. The RI approximation leads to large speedups (but note that no MP2 gradients are yet implemented).

```

Orca10.inp
#
# MP2 single point calculation for an organic radical
#
! UHF RI-MP2 SV(P) SV/C

* xyz 0 2
N      28.157954      -0.004768      -30.047552
O      27.124083      -0.112512      -30.810093
C      28.827154      -1.336941      -29.763613
C      28.747475       1.387942      -29.912897
C      30.016001       1.525763      -30.780098
H      30.376509       2.558810      -30.731210
H      30.828383       0.877656      -30.443657
H      29.794438       1.292768      -31.826310
C      29.041109       1.725750      -28.436344
H      28.172571       1.502625      -27.808513
H      29.906297       1.197349      -28.037064
H      29.248845       2.797600      -28.355708
C      27.688736       2.380459      -30.425568
H      28.082901       3.394215      -30.305800
H      27.457538       2.215998      -31.478855
H      26.759433       2.300258      -29.854951
C      27.719500      -2.276230      -29.245104
```

H	28.143299	-3.265342	-29.045764
H	27.292148	-1.891602	-28.312819
H	26.918821	-2.375064	-29.979214
C	29.938365	-1.274555	-28.706180
H	29.558236	-0.955053	-27.732751
H	30.339168	-2.286188	-28.587226
H	30.772041	-0.630613	-28.992920
C	29.389972	-1.879922	-31.094081
H	30.230458	-1.277863	-31.451349
H	29.743066	-2.907266	-30.957381
H	28.607181	-1.877518	-31.856971

*

Frequency calculations employ numerically differentiated analytical gradients and are available for all SCF methods (HF,DFT). From the output thermodynamical properties, vibrational spectra and stationary point characterizations are obtained.

```
Orca11.inp
#
# Frequency calculation for C2H2
#

! B3LYP TZVPP OPT NumFreq

%freq CentralDiff true
end

* int 0 1
C 0 0 0 0.000 0 0
C 1 0 0 1.22 0 0
H 1 2 0 1.08 180 0
H 2 1 3 1.08 180 0
*
```

MRCI- and MRPT calculations can be used to calculate the ground and excited states of molecules. There are a few reasonably efficient approximate methods available which are described in detail in the manual. Let us only look at a simple example. The first few states of formaldehyde.

```
Orca12.inp
#
#
#
! SV(P)+ SV/C SmallPrint Conv

%mrcki EWin -3,5
CITYPE MRCI
EUnselOpt FullMP2
DavidsonOpt Davidson1
IntMode RITrafo
Solver DIIS
```

```

CIMode          Direct2
UseIVOs          true
tsel            1e-6
tpre            1e-6
tstore          1e-7
NewBlock 1 *
  NRoots 2
  Excitations cisd
  Refs CAS(2,2) end
end
NewBlock 3 *
  NRoots 1
  Excitations cisd
  Refs CAS(2,2) end
end
end

* int 0 1
C      0  0  0  0.000000  0.000  0.000
O      1  0  0  1.200371  0.000  0.000
H      1  2  0  1.107372 121.941  0.000
H      1  2  3  1.107372 121.941 180.000
*
```

How to run ORCA

ORCA can be run in serial and parallel versions. For the serial version the program usage is trivial. Simply make sure that the binaries are somewhere located in your PATH and type

```
orca myinput.inp > myinput.out
```

Some additional hints can be found in the manual.

The parallel ORCA is based on the MPI protocol (Message Passing Interface). Therefore, if you want to do parallel ORCA calculations you have to install an MPI implementation on your computer system (see www-unix.mcs.anl.gov/mpi/mpich/download.html). Here is how you can make it happen:

1. INSTALL MPI

1. Download MPI
2. Install MPI (follow instructions given by MPI distribution)
3. Make sure that the directory of mpirun is available in your \$PATH

2. INSTALL ORCA

1. Download ORCA (see ???)
2. Unpack ORCA to a directory where you'll want to find it

```
bzip2 -d orca.tbz
tar -xvf orca.tar
```
3. Make sure that the directory /where/to/find/ORCA is available in your \$PATH

If you want to run ORCA in a PBS batch environment, please contact the developers team in order to obtain a reasonable example for a submit script.

3. Start ORCA

- a. edit your ORCA input file (some examples are provided below; more can be found in the manual.

For parallel calculations:

add PALx to the simple input line; 1<=x<=8 (syntax is ! PALx)

or include a block %pal which looks like

```
%PAL NPROCS x END
```

Note that more of eight processors usually make not much sense since you will ultimately run into the diagonalization penalty and obtain poor scaling with large number of processes. Up to

eight processors, the speedups are usually reasonable (note – they are necessarily worse for RI-DFT compared to hybrid DFT or Hartree-Fock).

b. start your job with:

```
/where/to/find/ORCA/orca myinput.inp
```

NOTE: the full path name is mandatory if you want to start a parallel ORCA calculation with MPI

or (for PBS) submit your job with:

```
suborca myinput
```

Frequently asked questions

- How to get ORCA?
ORCA can be downloaded for free from our ORCA website. After signing the license agreement and sending it back to the MPI for Bioinorganic Chemistry you will get the access code for downloading the ORCA binaries for your platform.
- Why can't I read my old .gbw files into the new ORCA version?
The .gbw files are thoroughly version dependent. ORCA tries to recover your orbitals and basis functions when reading your .gbw file via MOREAD. Unfortunately, this is not always possible (yet).
- Why is my orca_plot not working correctly?
Same problem as with .gbw files. The created .gbw files should only be read by the same program version as used when creating the files.
- Why can the program not read orbitals from a .gbw file?
The program always rewrites the gbw file at the beginning of the calculation. Thus you cannot read orbitals from `test.gbw` if your input file is named `test.inp`. In the case that you want identical filenames please FIRST rename the old .gbw file (e.g. `test.ges`) and then read the orbitals from there.
- My SCF calculations refuse to converge. What can I do?
At the end of the ORCA manual there are a few hints as to how to proceed in those cases. A rough rule of thumb would be setting the SCF to SlowConv mode (Keyword ! SlowConv) . If it still does not converge setting the SCF convergence limits to less strict values might be the only option.
- Why is my platform, cpu, and/or MPI library not supported?
Our access to different computer platforms and operating systems is limited, of course. But we hope that the ORCA versions we provide should be adequate for most people's wishes. The same holds true for the MPI versions. If you have questions with regards to platforms and libraries, please contact the ORCA development team.
- What are the benefits of running ORCA in parallel?
Our aim at parallelizing ORCA are distributed memory architectures of up to 8 CPUs. Up to this number the speed increase should be reasonable. The parts of ORCA that have been parallelized so far are the SCF, SCFGRAD, CIS/TDDFT, SOC, EPRNMR parts.
- How to cite ORCA?
A publication dedicated to the features of ORCA is in preparation. Until this one is published, please refer to the citations in the ORCA manual on page 10.

To be continued.....