By LYH

Gaussian (NOT case sensitive)	**ORCA** (NOT case sensitive)	Note
%nprocshared=8	pal8	supports only pal2 ~ pal8, default pal1
%nprocshared=16	%pal nprocs 16 end	for >8 threads
%mem=32GB	%maxcore 1500	MEM **per core**/MB, with (large) redundancy
%rwf=/gaussian/name.rwf		name.hess <==> name.rwf
%oldchk=/gaussian/name_old.chk	%base=name (Without extension!)	name.gbw <==> name.chk. And it's always %oldchk:
%chk=/gaussian/name.chk		restart.gbw can't have the same name with old.gbw.
%nosave	*NOT SUPPORTED*	ORCA suggests writing a script to do this.
#	!	
#p	! LargePrint	
	! PrintBasis	Specific print Basis Set)
	%geom ReducePrint false end	Suppress reduced printing in opt
	%scf print[p_mos] 1 end	Print MO
	! RKS	Restricted 需要明确声明
B3LYP/6-31+G(d,p)	! B3LYP**/G** 6-31+g(d,p)	B3LYP ma-def2-SVP
BLYP/def2TZVP/W06 DensityFit	! BLYP def2-TZVP def2-TZVP/J RI	def2-TZVP def2-TZVP/JK RIJK def2-TZVP def2-TZVP/C RIJCOSX GridX4
M062X/def2TZVP	! M062X def2-TZVP	
opt freq	! Opt Freq	• Freq available for HF & GGA/hybrid-GGA DFT & MP2 • ORCA suggest use *TightSCF*, *Grid4* and occasionally *TightOPT*. Give as much *%maxcore* as possible. • Anal. freq. not avail. for meta-GGA (e.g. m06-2X) & COSMO solvation. • *NumFreq* is much more expensive (time), but universally available. • *NumGrad* is required when Anal. Grad. is not avail. *(like M06-2X + RIJK)*.
	! Opt NumFreq	
	! Opt NumFreq NumGrad	
empiricaldispersion=gd3bj	! D3	D3 means D3-BJ by default.
empiricaldispersion=gd3	! D3Zero	The Gaussian "GD3" (like in B3LYP-D3) with 0 damping.

SCF=tight (default)	! NormalSCF (default for SP) or SCFConv6 ! TightSCF (default for opt) or SCFConv8	△E<1D-6 △E<1D-8 *At least TolE<1D-7, TolRMSP<1D-6 for Freq.*
int=fine int=ultrafine	! Grid4 NoFinalGrid ! Grid6 NoFinalGrid default is Grid2 FinalGrid4	302 angular grid points 590 angular grid points *Grid**X**4 or Grid**X**5 for RIJCOSX* *At least Grid4 for Freq.*
scrf=(smd, solvent=water)	%cosmo smd true solvent “water” end	不确定是否需要再重新算真空下 SCF
[Blank Line]	*NOT REQUIRED*	
[Title] [Blank Line]	*NOT SUPPORTED* Use “#” to comment everywhere	
0 1	* xyz 0 1	
C 0.56115 -0.80370 -0.25733 C -1.71781 -2.65758 -0.68753 [Geometry Continue] [Blank Line]	C 0.56115 -0.80370 -0.25733 C -1.71781 -2.65758 -0.68753 [Geometry Continue] *	Also accept xyz file path directly.
--link1--	$new_job	

“!” before keywords will be omitted below

Program issue

Run a job: Windows: via G09W Linux : g09 input output	 FullOrcaPath\orca input > output full_orca_path/orca input >& output	 Windows [Note: never “*orca input output*”] Linux
Monitor calculation: G09W tail –f output	 GabEdit tail –f output	
UI Interface: G09W GaussView	 GabEdit (Generate and run input file) ChemCraft (Visualization) Multiwfn (Visualization)	 (Be prepared for its one-of-the-ugliest GUI) Use orca_2mkl.exe to convert .gbw → .molden

Frequently used combination

opt B3LYP/6-31G(d)	Medium-opt (BP86/DefBasis_2 RI)	DefBasis_2 ~ SV(P) ~ 6-31G(d)

opt=(TS,calcfc) freq	OptTS <==> %geom TS_search EF end Freq %geom Calc_Hess True Num_Hess True *ReCalc_Hess True* end	ORCA suggests *SCAN* relaxed PES before *optTS* *Re-calculate Hessian every 5 steps*
	Opt Freq %geom TS_Mode {M *x*} end %geom TS_Mode {B atom1 atom2} end %geom TS_Mode {A atom1 atom2 atom3} end %geom TS_Mode {D atom1 ...} end	Choose the x^{th} lowest Hessian eigen, start from 0. (choose neg. vibration) May prevent this in Gaussian: *Wrong number of Negative eigenvalues:*
	ScanTS	先进行 Relaxed PES Scan，取最高点和前后两点进行 TS 计算。尚未尝试如何使用
opt=modredundant B *1 2* F	opt %geom Constraints {B *1 2 length* C} end	Constrained optimization “C” for “Constrain”
opt=modredundant B *1 2* S *NSteps StepSize*	opt %geom Scan B *1 2 = START End NStep* end %geom Scan B *1 2 [value1 value2 ...]* end	Relaxed PES
Scan R1 1.4(A) 3(steps) 0.1(A)	*NOT REQUIRED* %paras R1=1.4,1.7,4 end %paras R1 [1.4,1.5,1.6,1.7] end	*Scan* can be omitted, chosen automatically R1 is a bond length defined in Z-Matrix
Gen C H 0 6-31G(d) **** F 0 6-31G(d,p) **** 1 0 # add to atom No.1	%basis newgto C “6-31G(d)” end newgto H “6-31G(d)” end [No blank line here, just match left cell] newgto F “6-31G(d,p)” end C 0 0 0 0.0 0.0 0.0 # a line in coord. section addgto	Self-define basis set # use GAMESS file format from EMSL

SP 1 1.00 0.4380D-01 0.1000D+01 0.1000D+01 ****	SP 1 1.00 0.4380D-01 0.1000D+01 0.1000D+01	
genecp C O Cl H 6-31+g(d) **** Rh lanl2dz **** Rh lanl2dz	ECP{LanL=[Rh]} ECP{LanL=[Rb-Ag]} ECP{LanL=[Rh],def2-TZVP/J} ECP{LanL=[Rh],LanLDZ,def2-TZVP/J} ORCA suggests: First TM row : No ECP Many 2~3 TM row atoms : Use ECP Only one 2/3 TM row atoms : Use relativistic: ! *method* ZORA def2-SVP def2-SVP/J TIGHTSCF ! *method* DKH2 def2-SVP def2-SVP/J TIGHTSCF	Add ECP only for certain element (in this case: Rh) Choose Aux Basis. *LanL* and *SDD* will choose valence basis automatically; can be override. Relativistic ZORA/DKH recontracted basis sets will be automatically chosen. Use *PrintBasis* to confirm. For 3rd TM row: use *Grid7* & *IntAcc 10~20* (says ORCA). 不确定如何选择 ZORA vs DKH2
Debug		
opt=restart	Run new job copying LAST OUTPUT STRUCTURE. (Use with guess=read)	WHAT AN EXCELLENT SOLUTION!
guess=read	MORead Rescue %moinp “old.gbw”	New %base and input filename cannot be same as “old”
Restart (Frequency)	%freq restart true end	Same base name .hess file should be present
opt=GDIIS	GDIIS-Opt	Replace *opt*
opt=ReadFC	%geom InHess Read InHessName “filename.hess”	Read Hessian matrix from “filename.hess”
opt=CalcFC	%geom Calc_Hess True	Combine with *NumHess* if Anal. Hess. is not avail.
opt=CalcAll	%geom Recalc_Hess 1 %geom Recalc_Hess 5	Combine with *NumHess* if Anal. Hess. is not avail. Re-calculate Hess. every 5 steps besides the first.
opt=(maxstep=3)	%geom MaxStep 0.03	Both default: 0.3 au For 0.03 au.: Gaussian maxstep=3 ~ ORCA MaxStep 0.03
opt=NoTrustUpdate	%geom Trust 0.3	Default is Trust -0.3, means fixed 0.3 au. Trust 0.3, means start at 0.3 au and update after each step.
opt=Cartesian	copt	

opt (MaxD=1.8E-3, MaxF=4.5E-4) opt=tight (RMSD=4.0E-5, MaxD=6.0E-5, RMSF=1.0E-5, MaxF=1.5E-5)	NormalOPT (MaxD=4E-3, MaxG=3E-3) TightOPT (MaxD=1E-3, MaxF=?) %geom TolRMSD 4.0E-5 TolMaxD 6.0E-5 TolRMSG 1.0E-5 TolMaxG 1.5E-5	Seems ORCA opt is much more loose: Gaussian NormalOpt ≈ Orca TightOpt Use with *int=ultrafine* Use Gaussian Version opt=tight criteria

Installation (Linux)

Assume Route: $HOME = /home/gauuser $HOME/g09	Assume Route: $HOME = /home/gauuser $HOME/orca $HOME/orca/mpi	 for OpenMPI
“unzip” g09 mkdir $HOME/g09/scratch chmod -R 0770 $HOME/g09/ “append” *.bashrc* ---------- g09root=$HOME export g09root GAUSS_SCRDIR GAUSS_SCRDIR=$HOME/g09/scratch . $g09root/g09/bsd/g09.profile ----------	“unzip” ORCA “unzip” OpenMPI chmod -R 0777 $HOME/orca/ “append” *.bashrc* ---------- export ORCA=$HOME/orca export PATH=$PATH:$ORCA export PATH=$HOME/orca/mpi/bin:$PATH export LD_LIBRARY_PATH= $HOME/orca/mpi/lib:$LD_LIBRARY_PATH ---------- cd $HOME/orca/mpi ./confgiure --prefix=$HOME/orca/mpi sudo make -j4 all sudo make install	words in “” is not actual command For OpenMPI <-- In ONE LINE # Compile OpenMPI

	`./bin/mpirun`	`# Check whether OpenMPI work`

`su -`
`source /home/gauuser/.bashrc`
`echo 0 > /proc/sys/kernel/randomize_va_space`
`logout`
`# now ready to use`
	`su -`
	`source /home/gauuser/.bashrc`
	`echo 0 > /proc/sys/kernel/randomize_va_space`
	`logout`
	`# now ready to use`
		`<-- In ONE LINE. And... no idea why I have to do this.`

Links vs components		***(Not sure at all, use with caution)***
`L0, L1, L101`	`orca.exe`	Input & driver
	`orca_anoint.exe`	Integral generation over ANOs
	`orca_ciprep.exe`	Preparation of data for MRCI calculations
	`orca_cis.exe`	Excited states via CIS and TD-DFT.
	`orca_cpscf.exe`	Solution of the coupled-perturbed SCF equations.
	`orca_casscf.exe`	Main program for CASSCF driver
`L1002`	`orca_eprnmr.exe`	SCF approximation to EPR and NMR parameters.
	`orca_fci.exe`	Full-CI
	`orca_gtoint.exe`	Gaussian integrals.
`L102, L103, L105, L107` `L109, L113, L114, L115`	`orca_gstep.exe`	Relaxation of the geometry based on energies and gradients.
	`orca_loc.exe`	Localized MO
`L118, L121`	`orca_md.exe`	MD
	`orca_mdci.exe`	Matrix driven CI,CEPA,CPF,QCISD,CCSD(T)
`L903, L905, L906`	`orca_mp2.exe`	MP2
	`orca_mrci.exe`	MRCI, MRPT
	`orca_ndoint.exe`	Semiempirical integrals and gradients.
`L1101, L1102, L1110 (numeric)`	`orca_numfreq.exe`	Numerical hessian
	`orca_pc.exe`	Addition of point charge terms to the one-electron matrix.
	`orca_plot.exe`	Generation of orbital and density plots.
	`orca_pop.exe`	External program for population analysis on a given density.
	`orca_rel.exe`	(Quasi) Relativistic corrections.
	`orca_rocis.exe`	Excited states via the ROCIS method
`L502`	`orca_scf.exe`	SCF

L701, L702, L703	orca_scfgrad.exe	Analytic derivatives of SCF energies (HF and DFT).
L1101, L1102, L1110 (analytic)	orca_scfhess.exe	Analytical hessian of SCF
	orca_soc.exe	Spin-orbit coupling matrices.
	orca_vpot.exe	Electrostatic potential on a given molecular surface.
	orca_asa.exe	Absorption, fluorescence and resonance Raman spectra.
	orca_vib.exe	Vibrational frequencies, isotope shift.
	orca_pltvib.exe	Produces files for the animation of vibrations.
	orca_2mkl.exe	ASCII for molekel, molden…
	orca_2aim.exe	WFN files for AIM analysis.
	orca_fitpes.exe	Fit PES of diatomics.
	orca_mapspc.exe	Produces files for transfer into plotting programs.
	orca_euler.exe	Calculate Euler angles from .prop file
	orca_chelpg.exe	Electrostatic potential derived charges.
	otool_gcp.exe	Geometrical Counterpose Correction

UPDATE

NumGrad issue.

ECP.

Options during failed optimization process in *sobereva.com/164.*

User Gaussian version opt=tight optimization convergence criteria.

Installation procedure comparison.