

Gaussian 98 Reference Card

Includes the most commonly-used keywords and options;
see the Gaussian 98 User's Reference for further information.

▼ Input Sections

*Starred sections are not terminated by a blank line.

- Link 0 commands (% commands)*
- Route section (# lines)
- Extra overlays (ExtraOverlays)
- Title section†
- Molecule specification†
- Red. internal coord. modifications (Opt=ModRedundant)†
- Connectivity specs. (Geom=Connect, ModConnect)†

Daggered sections repeated for Opt=QST2 and again for QST3.

- Cartesian initial force constants (Opt=FCCards)
- Accuracy of energy & forces (Opt=ReadError)*
- Trajectory input (Traj)
- Atomic masses (IRC=ReadIsotopes)
- Solvation model parameters (post-SCF SCRF)
- Basis set specification (Gen, ExtraBasis)
- Basis set alterations (Massage)
- ECP specification (ExtraBasis, Pseudo=Cards)
- Background charge distribution (Charge)
- Finite field coefficients (Field=Read)
- Symmetry types to combine (Guess=LowSymm)*
- Orbital specs. (UHF ⇒ separate α & β) (Guess=Cards)
- Orbital alterations (UHF ⇒ sep. α & β) (Guess=Alter)
- Solvation model parameters (HF or DFT SCRF)
- Weights for averaged states (CASSCF=StateAverage)*
- States of interest for spin coupling (CASSCF=Spin)*
- Number of orbitals per GVB pair (GVB)*
- Alternate atomic radii (Pop=ReadRadii or ReadAtRadii)
- Data for electrostatic properties (Prop=Read or Opt)
- Cube filename (& spec. for Cards option) (Cube)
- NBO input (Pop=NBORead)*
- Orbital freezing information (ReadWindow option)
- OVGf orbitals to refine (OVGF)
- Temp., pressure, atomic masses (Freq=ReadIsotopes)*
- PROAIMS wavefunction filename (Output=WFN)*

▼ Controlling Job Output

- Archive, Test Create/suppress archive entry
- Name=name Specify user for archive entry
- #T Produce less output
- #P Produce extra output
- Link1-- Begin new job step within input stream

▼ Link 0 Commands & MaxDisk Keyword

File/memory size units are: KW, MW, GW, KB, MB or GB (default=words).

- %Mem=size Set amount of dynamic memory to size
- %Chk=path Name and save the checkpoint file
- %RWF=list Name and save the read-write file(s)
- %Int=list Name and save the 2-electron int. file(s)
- %D2E=list Name and save the 2-elec. int. deriv. file(s)
- list A single pathname or a list of the form:
path1,size1,path2,size2,... (size = -1 ⇒ use all available space; 0 ⇒ retain current file size)
- %NProc=n Use n processors
- %[No]Save Discard/save named/unnamed scratch files
- %KJob Ln [m] Stop run after the mth occurrence of link n
- %Subst Ln dir Use .exe file in directory dir for link n
- MaxDisk=size Suggest disk use be limited to size

▼ Selecting the Job Type

- SP Single point energy (default job type)
- Opt Geometry optimization
- Opt=QST2 Generate guess for transition struct. & opt.
- Freq Frequency and thermochemical analysis
- Opt Freq Automated opt. followed by frequency
- m1//m2 Opt at model m2 followed by SP at model m1
- IRC Follow reaction path
- IRCMax(m1//m2) Find TS's max. E at model m1 on m2 rx. path
- ONIOM(high:med[:low]) Perform a layered ONIOM calculation
- Scan Potential energy surface scan
- Trajectory Direct dynamics trajectory calculation
- Stable Test wavefunction stability
- Polar Polarizabilities and hyperpolarizabilities
- Force Compute forces on nuclei
- Density=Check Redo population analysis only

▼ Computing Molecular Properties

- Pop Atomic charges
- AIM Atoms in Molecules atomic charges & props.
- Pop Dipole & higher multipole moments
- CIS, RPA, ZINDO Excited states
- OVGF Electron affinities
- Cube=Density Electron density
- Cube=Potential Electrostatic potential
- Pop Electrostatic-potential derived charges
- Prop Electrostatic properties
- G2; CBS-4,-QB3 High accuracy energies
- OVGF Ionization potentials
- Freq IR and Raman Spectra
- Pop=Regular Molecular orbitals
- NMR NMR properties
- Freq, Polar Polarizabilities & hyperpolarizabilities
- Freq Thermochemical analysis
- CIS, RPA, ZINDO UV/visible spectra
- Freq=VCD Vibrational circular dichroism intensities

▼ Basis Set Specifications

◆ Available Basis Sets and Associated Keywords

STO-3G	3-21G	6-21G	4-31G	6-31G†
6-311G‡	CEP-4G	CEP-31G	CEP-121G	D95
D95V	SEC	LANL2MB	LANL2DZ	SDD
SV	SVP	TZV	MidiX (Midi!)	

[aug-]cc-pVxZ where x = D, T, Q, 5 or 6

[aug-]Dcc-pVxZ where x = D or T (Davidson-modified cc-pV*Z)

†For 6-31G† & †† (CBS methods), specify 6-31G(d') & (d',p').

‡6-311G yields 6-311G for 1st row, McLean-Chandler for 2nd row, Wachters-Hay for 1st transition row & 6-311G of McGrath, Curtiss, and coworkers for rest of third row.

- +, ++ Add diffuse functions (as available)
- *, ** Add polarization functions (as available)
- (x,y) Place x polarization functions on heavy atoms and y functions on hydrogens (e.g. 3df,2p)

◆ Basis-Set Related Keywords

- ChkBasis Read basis set from the checkpoint file
- ExtraBasis Add functions to built-in basis set
- Gen Read basis set specification from input stream
- GFInput Print current basis set in G98 input format
- GFPrint Print current basis set in tabular format
- nD, mF Use pure (n=5, m=7) or Cartesian (n=6, m=10) functions (F applies to f & all higher functions)
- Pseudo Substitute ECP's for core electrons;
Read option ⇒ read from input

▼ Molecule Specifications

◆ Cartesian coordinates:

elem. x y z

◆ Z-Matrix format:

elem., atom1, bond-len, atom2, bond-∠, atom3, tors-∠ [,0]

◆ Z-Matrix variable definitions:

var = value [H diag | D | S steps incr]
H = diagonal Hessian element; D = numer. differentiate;
S = relaxed potential energy surface scan

◆ Modifying redundant internal coordinates:

{kind} n₁ {n₂ {n₃ {n₄}} [+ = [val]] [C [args]] [[min] max]
C=B (add & build related), R (remove), K (remove/kill related),
A (activate), F (freeze), D (diff.), H hval (Hessian diag. elem),
S n step (scan). The default is to add the coordinate.
+ = val increments current value; min & max set wildcard limits;
type forces coordinate type: X (Cart.), B (bond len.), A (angle),
D (dihedral), L (linear bend), O (out-of-plane bend)

◆ Specifying atom types and partial charges:

elem--atom_type[-partial_charge] (e.g. C-CT-0.32)

▼ Quantum Mech. Procedure Keywords

As available, keywords may be prefaced with R, U or RO.

◆ SCF Methods

HF Hartree-Fock
 CASSCF Complete Active Space SCF (MC-SCF)
 GVB Generalized Valence Bond

◆ Electron Correlation Methods

MP n HF calc. followed by Møller-Plesset electron corr. energy corrections through order n
 $n=2,3,4,5$
 QCISD Quadratic Configuration Interaction; (T) adds triples, (TQ) add triples & quadruples, (...E4T) includes triples in the MP4
 CCD, CCSD Coupled Cluster calc. with doubles or singles & doubles; accepts (T) and (T,E4T)
 BD Brueckner Doubles; accepts (T)
 ROVGF, UOVGF Outer Valence Green's Function calc. for electron affinities and ionization potentials

◆ Density Functional Methods

◆ Functional Component Keyword Units

S Local Spin Density (LSD) exchange
 XA X α exchange
 B Becke 1988 exchange
 PW91 Perdew-Wang 1991 exchange
 MPW Barone's Modified PW91
 G96 Gill 1996 exchange
 B96 Becke 1996 gradient-corrected correlation
 VWN Vosko, Wilk, & Nusair local correlation
 VWN5 Vosko, Wilk, & Nusair functional V
 LYP Lee, Yang, & Parr grad.-corrected correlation
 PL Perdew 1981 local correlation
 P86 Perdew 1986 gradient-corrected correlation
 PW91 Perdew/Wang 1991 grad.-corr. correlation

◆ DFT Method Keyword

LSDA Equivalent to SVWN

◆ Hybrid Functionals

B3LYP, B3PW91 Becke-style 3-parameter hybrids
 B1B96 Becke 1-parameter hybrid
 B1LYP, MPW1PW91, G961LYP Becke-style 1-parameter hybrids

◆ High Accuracy Energies:

G1 Gaussian-1 Theory
 G2, G2MP2 Gaussian-2 Theory & G2(MP2) variation
 CBS- x Complete Basis Set (CBS) methods, where $x = 4, Lq, Q, Q3$ or APNO

◆ Excited State Calculations

CIS CI-Singles method
 TD Time-dependent HF and DFT
 ZINDO ZINDO semi-empirical method

◆ Ground State Semi-Empirical Methods

AM1, CNDO, INDO, MNDO, MINDO3, PM3 and PM3MM

◆ Molecular Mechanics Methods

AMBER, DREIDING and UFF force fields

Method Availabilities in *Gaussian 98*

	SP ^a	Opt ^b	Freq ^c	IRC	Traj	ONIOM	Polar	Stable
HF	*	*	*	*	*	*	*	*
CASSCF	*	*	*	*	*		*	
GVB	*	*		*				
MP2	*	*	*	*		*	*	
MP3, MP4(SDQ)	*	*		*		*		
MP4(SDTQ)	*					*		
MP5	*					*		
CI	*	*		*				
QCISD, CCD	*	*		*		*		
QCISD(T), CCSD	*					*		
BD	*					*		
OVGF	*							
<i>DFT Methods</i>	*	*	*	*	*	*	*	*
G1, G2, G2MP2	*							
<i>CBS Methods</i>	*							
CIS	*	*	*	*			*	
ZINDO, RPA	*							
<i>Semi-Empirical</i>	*	*	^d	*	*	*		
<i>Mol. Mechanics</i>	*	*	^d			*		

^a Note that the availability for Scan is the same as that for SP.

^b Refers to the availability of analytic gradients. Note that the availability for Force and the IRC portion of IRCmax is the same as that for Opt.

^c Refers to the availability of analytic second derivatives.

^d Frequencies are computed numerically but options like Opt=CalcFC are still valid.

▼ SCF Options

◆ SCF-Related Keyword

Complex Allow MOs to become complex

◆ Options to the SCF Keyword

FON Start SCF with a superposition of states
 Conventional Perform a conventional SCF calculation
 NoDIIS Disable DIIS extrapolation method
 FullLinear Perform full linear searches at each iteration
 InCore Use the in-core SCF algorithm
 IntRep Replicate integrals to account for symmetry
 MaxCycle= n Set max. # of SCF iterations [64; 512 for QC]
 NoSymm Lift all orbital symmetry constraints
 Symm Retain symmetry constraints in final wavefn.
 IDSymm Symmetrize density matrix at first iteration

◆ Options to the SCF Keyword Continued

DSymm Symmetrize density matrix every iteration
 QC Use quadratically-convergent SCF procedure
 Restart Restart SCF calculation from the checkpt. file
 Tight Use normal, tight convergence even for single point energy calculations
 TightLinEq Use tight convergence in the linear equation solution (SCF=QC)
 VShift= $[n]$ Shift orbital energies .001 n millihartrees [100]
 NoVarAcc Use full accuracy from the start of the SCF

◆ Options to CASSCF(n,m)

n,m Uses n electrons and m orbitals in active space
 FullDiag Use full (Jacobi) diag. meth. (vs. Lanczos)
 DavidsonDiag Use Davidson diagonalization
 NoOrbRot Exclude orbital rotation deriv. contributions
 NRoot= n Compute the n th root of the CI (excited state)
 OrbLocal= $[=n]$ Localize 1st n strongly-occupied orbitals [all]
 QC Use a quadratically convergent algorithm
 SlaterDet Use Slater determs. (HW uses Hartree-Waller)
 Spin Compute approx. spin orbit coupling between two states (specified in input)
 StateAverage State-averaged CAS (all states up to NRoot)
 StateGuess= k Starting vector to config. k (k =Read to input)
 UNO Read UHF orbs. to produce NO initial guess
 MP2States= m Compute MP2 corr. for states in mask m
 NFC, NFV Specify frozen orbitals for CAS MP2

◆ Related Keywords

Opt=Conical Search for conical intersect./avoided crossing
 CASSCF MP2 Add MP2 electron correlation to CAS calc.

◆ Options to GVB(n)

n Specifies the number of perfect-pairing pairs
 Freeze Allow only 2nd and higher orbitals to vary
 InHam= n Read in n Hamiltonians
 OSS Perform a two-electron, two orthogonal orbital open shell singlet calculation

◆ Options to Scan

Restart Restart scan calculation

◆ Options to FMM (Fast Multipole Method)

LMax= n Set maximum order multipole to n
 Levels= n Set number of FMM levels to n
 Tolerance= n Set accuracy level to 10^{-n}
 BoxLen= n Set minimum box length size to $n/10$ Bohrs

◆ Options to Sparse

n Sets cutoff for 10^{-n} . Loose= $5 * 10^{-5}$, Medium= $5 * 10^{-7}$, Tight= 10^{-10}

▼ Options for Post-SCF Methods

◆ General Options for Post-SCF Method Keywords

Conver=*n* Set convergence in CI, CC, and QCISD to 10^{-n} on energies, 10^{-n+2} on wavefunc.
[7 for single pts.; 8 for grads.; 4 & 6 for CIS]

FC Frozen core: exclude inner and outer shell

Full Include all electrons

RW Read window: input orbitals to retain

Window=(*n*,*m*) Set orbitals to retain in route section

◆ MP2 and Transformation Keyword Options

Direct Select a direct alg. based on avail. resources

FullDirect Force fully direct algorithm

InCore Force in-core algorithm

SemiDirect Force semi-direct algorithm

▼ Geometry Optimizations & Related Calcs.

◆ Geometry Optimization Keywords

Opt Opt. geometry in redundant internal coords.

Opt Freq Automated opt. followed by frequency calc.

m1/m2 Optimize at *m2* & then compute *m1* energy

◆ Options to the Opt Keyword

ModRedundant Modify redundant internal coordinates

AllHBond Generate hydrogen bonds and all related angles (NoHBond stops H bond generation)

QST2, QST3 Generate initial TS from reactants & products (& TS guess for QST3) and then optimize

Path=*n* Simultaneous opt. of TS & *n*-point rx. Path

OptReactant Optimize the reactant prior to a simul. opt

OptProduct Optimize the product prior to a simul. opt

CalcAll Compute force constants at every point

CalcFC Compute force constants at 1st point

CalcHFFC Compute HF force constants at 1st point

Big Use fast equation solving methods

GDIIS Use the modified GDIIS algorithm

Cartesian Perform opt. in Cartesian coordinates

Conical Locate conical intersection/avoided crossing

EF Use eigenvalue-following algorithm

Expert Relax limits on force constants and step size

FCCards Read force constants from input stream

MaxCyc=*n* Set maximum optimization cycles to *n*

NoEigenTest Suppress curvature testing

NoFreeze Activate (unfreeze) all variables

NoRaman Suppress Raman intensities for CalcAll

RCFC Read Cart. force constants from checkpt. file

ReadFC Read internal coord. force constants

Restart Restart optimization from checkpoint file

Saddle=*n* Proceed to an *n*th-order saddle point

Tight Tighten forces and step size cutoffs

TS Proceed to a transition structure

Z-matrix Optimize in internal coords.

◆ Options to IRC

CalcFC, RCFC and ReadFC as for Opt above

Phase=(*atoms*) Define the phase for the transition vector

Cartesian Follow path in Cartesian coordinates

Forward Follow reaction in forward direction only

Reverse Follow reaction in reverse direction only

Downhill Follow the path downhill (start is not a TS)

Internal Follow path in internal coordinates

MassWeight Follow path in mass-weighted int. coords.

MaxPoint=*n* Examine up to *n* points in each direction

ReadIso Read in masses for each atom

ReadVector Read in vector to follow

Restart Restart/resume IRC from checkpoint file

StepSize=*n* Set step size to $0.01n$ au.

VeryTight Tighten convergence criteria for opts.

▼ Options to Trajectory

NTraj=*N* *N* trajectories will be propagated

Steps=*N* Specifies the maximum number of steps

Phase=(*N1 N2* [*N3* [*N4*]]) Defines the phase for the transition vector

ReadIsotopes Read in a list of atomic isotopic masses

ReadVelocity Read in an initial Cartesian velocity

RTemp=*N* Specifies the rotational temperature

[Non]Adiabatic Perform only the non/adiabatic hop test (CASSCF method only)

▼ Options to Frequency

VCD Compute vibr. circular dichroism intensities

[No]Raman Compute/suppresses Raman intensities

HPModes Include 5-figure normal mode output

Projected Compute projected freqs. perp. to IRC path

Numer Computer frequencies numerically

ReadFC Read force constants from a previous frequency calculation from the checkpoint file

ReadIso Input temp., pressure & atomic masses

Restart Restart frequency calculation from chkpt. file

Step=*n* Set numer. differentiation step-size to $n \times 10^{-4}$

▼ Options to Polar (Polarizabilities)

EnergyOnly Numer. differentiate energy twice to produce polarizabilities (& poss. hyperpolarizabilities)

Numer Force a numerical calculation

Restart Restart numerical polar. calculation

Step=*n* Set electric field step size to $n \times 10^{-4}$ au.

▼ Options to CIS, RPA and ZINDO (Excited States)

NStates=*n* Determine *n* states [3]

Singlets Solve only for singlet states

Triplets Solve only for triplet states

50-50 Solve for singlet and triplet states

Root=*n* Designates state *n* as state of interest

◆ Options to CIS, RPA and ZINDO (Excited States) Continued

AllTransitionDen Calc. trans. dens. btwn. every pair of states

Add=*n* Solve for *n* addl. states for a prev. calculation

Direct Perform direct SCF and CIS calculations

Densities Compute 1-particle densities for each state

Read Read initial guesses from checkpoint file

Restart Restart CIS calculation from checkpoint file

RWFRestart Restart CIS iterations from RW file

IOP(9/40=*n*) Display coefficients $\geq 10^{-n}$

▼ Options to SCRF (Solvent Effects)

Dipole Onsager (dipole & sphere) model

PCM, CPCM, IEFCM Tomasi's Polarized Continuum Models (use Read option to specify further input)

IPCM Isodensity Polarized Continuum Model

SCIPCM Self-Consistent Isodensity PCM model

Solvent=*s* Specify solvent by name or ID number

▼ Options to Geom (Molecule Spec. Source)

AllCheck Read title, charge & spin, and molecule spec.

Checkpoint Read molecular spec. from the checkpoint file

ModRedundant Modify retrieved or specified geometry

Modify Modify retrieved geometry from checkpt. File

Connect Input explicit atom bonding data

ModConnect Modify current atom bonding

NoCrowd Allow atoms to be closer than 0.5 Å

NoKeep Discard information about frozen variables

▼ Options to Guess (SCF Initial Guess)

Alter Swap orbitals as specified in input

Always Generate new guess at each point of an opt.

Cards Read occupied orbitals from input stream

Check Read initial guess from checkpoint file

Core Diagonalize core Hamiltonian for initial guess

Huckel Generate pseudo-extended Huckel guess

Local Localize orbitals using the Boys method

LowSymm Lower symmetry of guess by combining irreducible representations

Mix Mix HOMO and LUMO to destroy α - β and spatial symmetries

NoSymm Lift all symmetry constraints

NoTranslate Don't translate guess to curr. atomic coords.

Only End job after printing initial guess

Print Adds printing of initial guess to output

Read Retrieve initial guess from checkpoint file

▼ Options to Density (Select Density Matrix)

All Use all available densities (for pop. analysis)

Check Recover density matrix from checkpoint file

Current Use density matrix of current method

▼ Options to Pop (Population Analysis)

Charge	Fit charges to electrostatic potential at each atomic center (add AtomDipole to also fit dipoles)
CHelp	Fit charges to electrostatic potential via CHelp
CHelpG	Fit charges using CHelpG scheme
Dipole	Constrain fitted charge to reproduce μ
Full	Same as Reg except all orbitals are printed
MK	Fit charges via Merz-Kollman/Singh scheme
NaturalOrb	Do natural orbital analysis of the total density
NaturalSpin	Do sep. nat. orb. analysis for α & β densities
NBO	Perform Natural Bond Orbital analysis
NBODel	Analyze effects of deleting some interactions
NBORead	Natural Bond Orbital analysis with user input
None	Suppress orbital printing and pop. analysis
NPA	Perform only NBO natural pop. analysis
ReadAtRadii	Read alternate radii for each atom
ReadRadii	Read alternate radii for elements
Reg	Print highest 5 occupied and lowest 5 virtual orbitals, density matrices & Mulliken pop.

▼ Options to Cube

n	Use n^3 points (evenly distributed) Coarse, Medium, Fine mean $n = 40, 80, 100$
Alpha	Use only alpha spin density
Beta	Use only beta spin density
Cards	Input cube parameters (as required in G92)
Density	Compute density over the cube (default)
Full	Evaluate density including all electrons
Orbitals	Compute MO(s) at each point
Potential	Compute electrostatic potential at each point
Spin	Use difference of alpha and beta densities

▼ Options to Field

One of the first two sets of parameters is required.

$m \pm n$	Apply specified field where m is a multipole, and the field magnitude is $.0001n$ (e.g. $x+10$)
$F(m)n$	Apply Fermi contact perturbation for atom m of magnitude $0.0001n$
Read	Read coefficients of all 35 electric multipole components from the input stream
Check	Read coefficients from the checkpoint file

▼ Options to Charge

Check	Read background charge dist. from chkpt. file
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▼ Options to Integral

Grid=grid	Use specified numerical integration grid
IntBufferSize= n	Set integral buffer size to $8n$ MB
SSWeights	Use Stratman and Scuseria's weights
NoSymm	Disable use of symmetry
ReUse	Use an existing integral file
Rys1E, Rys2E	Evaluate 1- or 2-electron integrals with Rys method (for systems with limited memory)

▼ Options to Units (Changing Input Units)

Bohr	Distances are in bohrs (atomic units)
Radian	Angles are in radians

▼ Creating Additional Output Files

Output=WFN	Write a PROAIMS .wfn file
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◆ Options to Punch

All	Punch everything except natural orbitals
Archive	Punch archive entry
Coord	Punch atomic numbers and Cartesian coords.
Deriv	Punch energy, nuclear coord. and 2nd derivs.
Games	Punch Games input file
MO	Punch molecular orbitals
NaturalOrb	Punch natural orbitals for selected density

▼ General Internal Option

IOP($ov/p=n$)	Set option p in overlay ov to n
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▼ Modifications to Standard Routes

ExtraLinks	Execute extra links listed as options
ExtraOverlays	Execute extra overlays listed in input
Skip=Ovn	Skip all overlays preceding overlay n
Skip= n	Skip first n overlays
Use=link	Use specified alternate link

See also the %KJob Link 0 command.

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