



Introduction to Gaussian 03 Package

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A variety of capabilities : (a)



By Andrew Weiser

1. Molecular structure :

- ✦ structural measurement
- ✦ optimization

2. Electronic structure :

- ✦ electronic energy
- ✦ molecular orbitals
- ✦ electron affinities
- ✦ ionization potentials
- ✦ atomic charges
- ✦ multipole moments
- ✦ electron densities
- ✦ electrostatic potentials
- ✦ polarizabilities and hyperpolarizabilities

3. Chemical reaction :

- ✦ bond energies
- ✦ reaction pathways
- ✦ transition states;
- ✦ reaction energetics
- ✦ potential surface

4. Thermochemistry analysis :

- ✦ thermal energies
- ✦ thermal enthalpies

A variety of capabilities : (b)



By Jack Haas

5. Vibrational frequencies

- ✦ normal frequency analysis
- ✦ IR intensities
- ✦ Raman intensities
- ✦ vibrational circular dichroism(VCD) intensities
- ✦ anharmonic vibrational analysis
- ✦ vibrational-rotational coupling

6. Chiroptics :

- ✦ Electronic circular dichroism(ECD) intensities
- ✦ Optical rotation

7. NMR :

- ✦ NMR shielding
- ✦ magnetic susceptibilities
- ✦ spin-spin coupling
- ✦ g-tensor; hyperfine NMR

8. More.

- ✦ molecular dynamics (ADMP, BOMD) ...

An arsenal of executables grouped into overlays (a)

Overlay 0 (initialization):

- ✦ **Link L0** : Initializes program and controls overlaying

Overlay 1 (initialization, optimization, miscellaneous):

- ✦ **Link L1** : Processes route section, builds list of links to execute, and initializes scratch files
- ✦ **L101** : Reads title and molecule specification
- ✦ **L102** : Nonderivative Fletcher-Powell (FP) optimization
- ✦ **L103** : Berny optimizations, Synchronous Transit-Guided Quasi-Newton (STQN) search of transition states
- ✦ **L105** : Murtaugh-Sargent optimization (obsolete)
- ✦ **L106** : Numerical differentiation of forces/dipoles to obtain polarizabilities / hyperpolarizabilities

An arsenal of executables grouped into overlays (b)

Overlay 1 (continued) :

- ✦ **L107** : Linear-synchronous-transit (LST) search of transition states
- ✦ **L108** : Potential energy surface scan
- ✦ **L109** : Newton-Raphson optimization
- ✦ **L110** : Double numerical differentiation of energies to produce frequencies
- ✦ **L111** : Double numerical differentiation of energies to compute polarizabilities & hyperpolarizabilities
- ✦ **L113** : Eigenvalue-following (EF) optimization using analytic gradients
- ✦ **L114** : Eigenvalue-following (EF) optimization using numeric gradients

An arsenal of executables grouped into overlays (c)

Overlay 1 (continued) :

- ✦ **L115** : Follows reaction path using the intrinsic reaction coordinate (IRC)
- ✦ **L116** : Numerical self-consistent reaction field (SCRFF)
- ✦ **L117** : Post-SCF SCRFF
- ✦ **L118** : Trajectory calculations (dynamics)
- ✦ **L120** : Controls ONIOM calculations
- ✦ **L121** : Atom Centered Density Matrix Propagation (ADMP) molecular dynamics calculations
- ✦ **L122** : Counterpoise calculations for Basis Set Superposition Error-correction (BSSE)

An arsenal of executables grouped into overlays (d)

Overlay 2 (molecular coordinates):

- ✦ **L202** : Reorients coordinates, calculates symmetry, and checks variables

Overlay 3 (integrals):

- ✦ **L301** : Generates basis set information
- ✦ **L302** : Calculates overlap, kinetic, and potential integrals
- ✦ **L303** : Calculates multipole integrals
- ✦ **L308** : Computes dipole velocity and Rx Del integrals
- ✦ **L310** : Computes spdf 2-electron integrals in a primitive fashion
- ✦ **L311** : Computes sp 2-electron integrals
- ✦ **L314** : Computes spdf 2-electron integrals

An arsenal of executables grouped into overlays (e)

Overlay 3 (continued) :

- ✦ **L316** : Prints 2-electron integrals
- ✦ **L319** : Computes 1-electron integrals for approximate spin orbital coupling

Overlay 4(initial guess):

- ✦ **L401** : Forms the initial MO guess
- ✦ **L402** : Performs semi-empirical and molecular mechanics calculations
- ✦ **L405** : Initializes an Complete Active Space Multiconfiguration SCF (MCSCF) calculation

An arsenal of executables grouped into overlays (f)

Overlay 5 (Self-consistent field -- SCF):

- ✦ **L502** : Iteratively solves the SCF equations
- ✦ **L503** : Iteratively solves the SCF equations using direct minimization
- ✦ **L506** : Performs a restricted open-shell HF (ROHF) or perfect-pairing General Valence Bond (GVB-PP) calculation
- ✦ **L508** : Quadratically convergent SCF program
- ✦ **L510** : MC-SCF

Overlay 6 (analysis of electronic properties):

- ✦ **L601** : Population and related analyses (including multipole moments)

An arsenal of executables grouped into overlays (g)

Overlay 6 (continued):

- ✦ **L602** : 1-electron properties (potential, field, and field gradient)
- ✦ **L604** : Evaluates MOs or density over a grid of points
- ✦ **L607** : Performs (Natural Bond Orbital) NBO analyses
- ✦ **L608** : Non-iterative DFT energies
- ✦ **L609** : Atoms in Molecules properties

Overlay 7 (derivatives):

- ✦ **L701** : 1-electron integral first or second derivatives
- ✦ **L702** : 2-electron integral first or second derivatives (sp)
- ✦ **L703** : 2-electron integral first or second derivatives (spdf)
- ✦ **L716** : Processes information for optimizations and frequencies

An arsenal of executables grouped into overlays (h)

Overlay 8 (transformation):

- ✦ **L801** : Initializes transformation of 2-electron integrals
- ✦ **L802** : Performs integral transformation
- ✦ **L804** : Integral transformation
- ✦ **L811** : Transforms integral derivatives & computes their contributions to MP2 2nd derivatives

Overlay 9 (post-HF):

- ✦ **L901** : Anti-symmetrizes 2-electron integrals
- ✦ **L902** : Determines the stability of the HF wavefunction
- ✦ **L903** : Old in-core MP2
- ✦ **L905** : Complex MP2
- ✦ **L906** : Semi-direct MP2

An arsenal of executables grouped into overlays (i)

Overlay 9 (continued) :

- ✦ **L908** : Outer Valence Green's Function (OVGF) closed shell
- ✦ **L909** : OVGF (open shell)
- ✦ **L913** : Calculates post-SCF energies and gradient terms
- ✦ **L914** : Excited states: CI-Singles; Random-phase approximation(RPA, a time-dependent HF) and Zindo; SCF stability
- ✦ **L915** : Computes fifth order quantities
(for MP5, QCISD(TQ) and BD(TQ))
- ✦ **L916** : Old MP4 and coupled cluster (CCSD)
- ✦ **L918** : Reoptimizes the wavefunction

An arsenal of executables grouped into overlays (j)

Overlay 10 (Coupled Perturbed Hartree-Fock --CPHF):

- ✦ **L1002** : Iteratively solves CPHF equations; properties (e.g.NMR)
- ✦ **L1003** : Iteratively solves the CP-MCSCF equations
- ✦ **L1014** : Computes analytic CI-Singles second derivatives

Overlay 11 (Fock matrix derivatives):

- ✦ **L1101** : Computes 1-electron integral derivatives
- ✦ **L1102** : Computes dipole derivative integrals
- ✦ **L1110** : 2-electron integral derivative contribution to Fx
- ✦ **L1111** : 2 particle density matrix (PDM) & post-SCF derivatives
- ✦ **L1112** : MP2 second derivatives

Overlay 99 (Termination):

- ✦ **Link L9999** : Finalizes calculation and output

Gaussian job → Route: a sequence of links (a)

A simple example: Compute the **electronic energy of formaldehyde (CH₂O)** using **Hartree-Fock** method with a minimum basis set **STO-3G**

→ **Standard route**: in input file, we specify in a line

HF/STO-3G

→ **Non-standard route** : **Link 1** reads **HF/STO-3G** and generates the following route in output file

```
# HF/STO-3G
```

```
-----
```

```
1/38=1/1;
```

```
To call Link 101
```

```
2/17=6,18=5,40=1/2;
```

```
To call Link 202
```

```
3/6=3,11=9,16=1,25=1,30=1/1,2,3;
```

```
To call Links 301, 302, 303
```

```
4//1;
```

```
To call Link 401
```

```
5/5=2,32=1,38=5/2;
```

```
To call Link 502
```

```
6/7=2,8=2,9=2,10=2,28=1/1;
```

```
To call Link 601
```

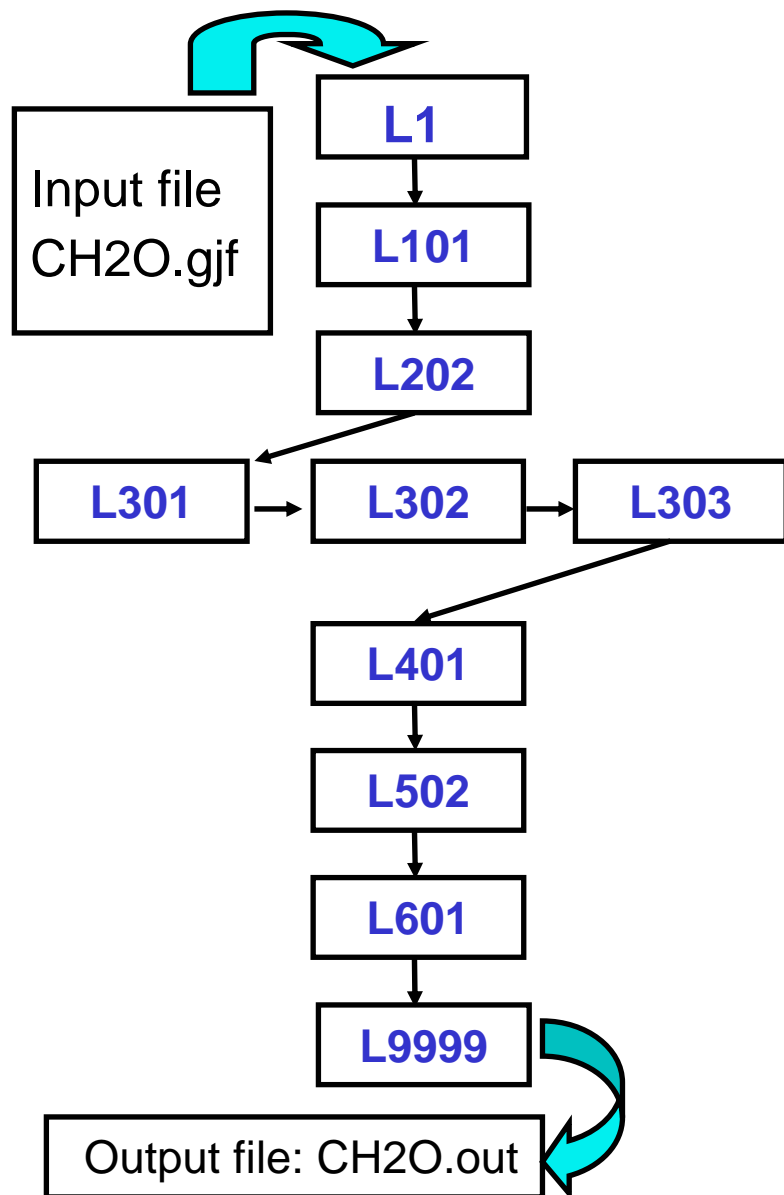
```
99/5=1,9=1/99;
```

```
To call Link 9999
```

```
-----
```

→ **Non-standard route**: **Overlay / Opt=val, Opt=Val, ... / Link, Link₁₄**.

Gaussian job → Route: a sequence of links (b)



HF/STO-3G

Link 1 : Reads and parses route section. Builds links.

Link 101 : Reads in title and molecule specification

Link 202 : calculates molecular symmetry

Link 301 : Generates basis set information

Link 302 : Overlap, kinetic, and potential integrals

Link 303 : Calculates multipole integrals

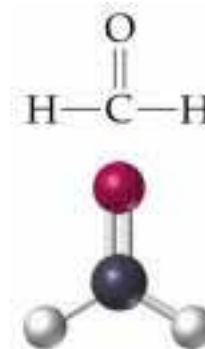
Link 401 : Forms the initial MO guess

Link 502 : Iteratively solves the SCF equations

Link 601 : Assigns orbital and wavefunction symmetries; Performs Mulliken population analysis

Link 9999 : Finalizes calculation and output

Example of CH₂O with HF/STO-3G: Input file



Input file 1 : molecule in Z-matrix

HF/STO-3G

Example: aldehyde

0 1

C1

O2 1 A

H3 1 B 2 C

H4 1 B 2 C 3 D

A = 1.28

B = 1.10

C = 121.0

D = 180.0

Input file 2 : molecule in Z-matrix

HF/STO-3G

Example: aldehyde

0 1

C1

O2 1 1.28

H3 1 1.10 2 121.0

H4 1 1.10 2 121.0 3 180.0

Input file 3 : molecule in Cartesian

HF/STO-3G

Example: aldehyde

0 1

C1 0.00 0.00 0.00

O2 0.00 0.00 1.28

H3 0.94 0.00 -0.57

H4 -0.94 0.00 -0.57

More about Gaussian Input file: Section layout

Input file 1 : molecule in Z-matrix

HF/STO-3G

Example: aldehyde

0 1

C1

O2 1 A

H3 1 B 2 C

H4 1 B 2 C 3 D

A = 1.28

B = 1.10

C = 121.0

D = 180.0

% Resources management
(link 0 commands)

Route card

[*blank line*]

Title section

[*blank line*]

Molecular coordinates

[*blank line*]

Internal coordinates variables

[*blank line*]

Other specification

[*blank line*]

More About Gaussian Input file: Link 0 Commands

%Mem=N Sets the amount of dynamic memory used to N words (8N bytes).
The default is 6MW. N may be followed by a units designation:
KB, MB, GB, KW, MW or GW

%NProcShared=N Requests that the job use up to N processors

%Chk=file Locates and names the checkpoint file

%RWF=file Locates and names a single, unified Read-Write file

%RWF=loc1,size1,loc2,size2,... Locates and names split Read-Write file

%Int=spec Locates and names two-electron integral file(s)

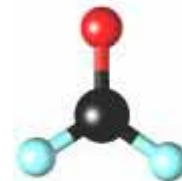
%D2E=spec Locates and names two-electron integral derivative file(s)

%KJob LN [M] Tells the program to stop the run after the Mth occurrence of link N

%save (%nosave) Causes Link 0 (not) to save scratch files at the end of the run

%subst LN dir Tells Link 0 to the executable for a link from alternate directory

Example of CH₂O: Output file (a) : Link 1



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Cite this work as:

Gaussian 03, Revision B.03,

M. J. Frisch, G. W. Trucks, H. B. Schlegel,

(many many other), and J. A. Pople,

Gaussian, Inc., Pittsburgh PA, 2003.

Gaussian 03: x86-Win32-G03RevB.03 4-May-2003

16-Jan-2006

%chk=Nosave

HF/STO-3G

1/38=1/1;

2/17=6,18=5,40=1/2;

3/6=3,11=9,16=1,25=1,30=1/1,2,3;

4//1;

5/5=2,32=1,38=5/2;

6/7=2,8=2,9=2,10=2,28=1/1;

99/5=1,9=1/99;

Input file 2 : molecule in Z-matrix

HF/STO-3G

Example: aldehyde

0 1

C1

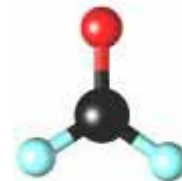
O2 1 1.28

H3 1 1.10 2 121.0

H4 1 1.10 2 121.0 3 180.0

Link 1 : Reads and parses
route section. Builds links.

Example of CH₂O: Output file (b) : Link 101



test aldehyde

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C1							
O2	1	1.28					
H3	1	1.1	2	121.			
H4	1	1.1	2	121.	3	180.	0

Link 101 : Reads in title and molecule specification.

----- The following is not printed unless requested -----

Isotopes and Nuclear Properties:

Atom	1	2	3	4		
IAtWgt=	12	16	1	1		
AtmWgt=	12.0000000	15.9949146	1.0078250	1.0078250		
IAtSpn=	0	0	1	1		
AtZEff=	0.0000000	0.0000000	0.0000000	0.0000000		
AtQMom=	0.0000000	0.0000000	0.0000000	0.0000000		
AtGFac=	0.0000000	0.0000000	2.7928460	2.7928460		

Example of CH₂O: Output file (c) : Link 202



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.280000
3	1	0	0.942884	0.000000	-0.566542
4	1	0	-0.942884	0.000000	-0.566542

Distance matrix (angstroms):

	1	2	3	4
1 C	0.000000			
2 O	1.280000	0.000000		
3 H	1.100000	2.073342	0.000000	
4 H	1.100000	2.073342	1.885768	0.000000

Stoichiometry CH₂O

Framework group C₂V[C₂(CO),SGV(H₂)]

Deg. of freedom 3

Full point group C₂V NOp 4

Largest Abelian subgroup C₂ NOp 4

Largest concise Abelian subgroup C₂ NOp 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	-0.569182
2	8	0	0.000000	0.000000	0.710818
3	1	0	0.000000	0.942884	-1.135724
4	1	0	0.000000	-0.942884	-1.135724

Rotational constants (GHZ): 282.0236292 35.0946253 31.2107974

Link 202 : calculates molecular symmetry

Terminology reminder

rotational constants

Coefficients of quantum numbers in the rotational *term* expression and inversely proportional to the *principal moments of inertia*. Symbols: A , B , C . $\tilde{A} = h/8\pi^2 c I_A$ (dimension wavenumber), $A = h/8\pi^2 I_A$ (dimension frequency) where h is the Planck constant and c the speed of light in vacuum.

G.B. 23

Example of CH₂O: Output file (d)



Link 301 : Generates basis set information.

Link 302 : Overlap, kinetic, and potential integrals

Link 303 : Calculates multipole integrals

Standard basis: STO-3G (5D, 7F)

There are 7 symmetry adapted basis functions of A1 symmetry.

There are 0 symmetry adapted basis functions of A2 symmetry.

There are 2 symmetry adapted basis functions of B1 symmetry.

There are 3 symmetry adapted basis functions of B2 symmetry.

Integral buffers will be 262144 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

12 basis functions, 36 primitive gaussians, 12 cartesian basis functions

8 alpha electrons 8 beta electrons

nuclear repulsion energy 29.9812693439 Hartrees.

NAtoms= 4 NActive= 4 NUniq= 3 SFac= 2.05D+00 NAtFMM= 60 Big=F

One-electron integrals computed using PRISM.

NBasis= 12 RedAO= T NBF= 7 0 2 3

NBsUse= 12 1.00D-06 NBFU= 7 0 2 3

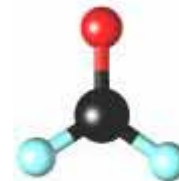
Example of CH₂O: Output file (e) : [Link 401](#)



Link 401 : Forms the initial MO guess.

```
Harris functional with IExCor= 205 diagonalized for initial guess.  
ExpMin= 1.69D-01 ExpMax= 1.31D+02 ExpMxC= 1.31D+02  
          IAcc=1 IRadAn=      1 AccDes= 1.00D-06  
HarFok: IExCor= 205 AccDes= 1.00D-06 IRadAn=      1 IDoV=1  
ScaDFX= 1.000000 1.000000 1.000000 1.000000  
Initial guess orbital symmetries:  
  Occupied (A1) (A1) (A1) (A1) (B2) (A1) (B1) (B2)  
  Virtual  (B1) (A1) (B2) (A1)  
The electronic state of the initial guess is 1-A1.
```

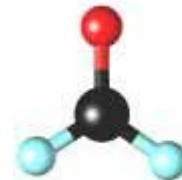

Example of CH₂O: Output file (f) : [Link 502](#)



Link 502 : Iteratively solves the SCF equations.

```
Warning! Cutoffs for single-point calculations used.  
Requested convergence on RMS density matrix=1.00D-04 within 128 cycles.  
Requested convergence on MAX density matrix=1.00D-02.  
Requested convergence on          energy=5.00D-05.  
No special actions if energy rises.  
Keep R1 integrals in memory in canonical form, NReq=  422883.  
SCF Done: E(RHF) = -112.347061089  A.U. after  6 cycles  
          Convg =  0.4290D-04          -V/T =  2.0095  
          S**2  =  0.0000
```

Example of CH₂O: Output file (g) : Link 601



Link 601 : Assigns orbital and wavefunction symmetries;
Performs Mulliken population analysis.

Population analysis using the SCF density.

Orbital symmetries:

Occupied (A1) (A1) (A1) (A1) (B2) (A1) (B1) (B2)

Virtual (B1) (A1) (B2) (A1)

The electronic state is 1-A1.

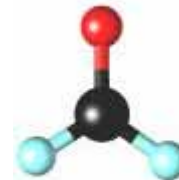
Alpha occ. eigenvalues -- -20.29858 -11.11185 -1.29494 -0.80966 -0.61970

Alpha occ. eigenvalues -- -0.52527 -0.40809 -0.35764

Alpha virt. eigenvalues -- 0.26125 0.61732 0.73989 0.82421

Condensed to atoms (all electrons):

	1	2	3	4
1 C	4.789993	0.415588	0.373985	0.373985
2 O	0.415588	7.798242	-0.020016	-0.020016
3 H	0.373985	-0.020016	0.614031	-0.031677
4 H	0.373985	-0.020016	-0.031677	0.614031



Mulliken atomic charges:

1

1 C 0.046448
2 O -0.173799
3 H 0.063675
4 H 0.063675

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

1

1 C 0.173799
2 O -0.173799
3 H 0.000000
4 H 0.000000

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): $\langle R^2 \rangle = 60.8056$

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= -1.6140 Tot= 1.6140

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -10.4576 YY= -10.4527 ZZ= -11.1925
XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 0.2433 YY= 0.2482 ZZ= -0.4916
XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang²):

XXX= 0.0000 YYY= 0.0000 ZZZ= 2.7749 XYY= 0.0000
XXY= 0.0000 XXZ= 1.6848 XZZ= 0.0000 YZZ= 0.0000
YYZ= 0.3381 XYZ= 0.0000

Hexadecapole moment (field-independent basis, Debye-Ang³):

XXXX= -6.9188 YYYY= -14.5631 ZZZZ= -42.0114 XXXY= 0.0000
XXXZ= 0.0000 YYYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000
ZZZY= 0.0000 XYYX= -3.8439 XXZZ= -8.0695 YYZZ= -8.5413
XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 2.998126934395D+01 E-N=-3.250968571591D+02 KE= 1.112917498530D+02

Symmetry A1 KE= 1.008213329811D+02

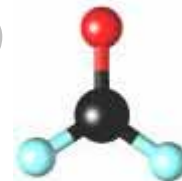
Symmetry A2 KE= 0.000000000000D+00

Symmetry B1 KE= 3.600811981759D+00

Symmetry B2 KE= 6.869604890141D+00

Link 601 : Assigns orbital and wavefunction symmetries; Performs Mulliken population analysis.

Example of CH₂O: Output file (h) : Link 9999



Link 9999 : Finalizes calculation and output.

```
1|1|UNPC-UNK|SP|RHF|STO-3G|C1H2O1|PCUSER|16-Jan-2006|0||# HF/STO-3G||t
est aldehyde||0,1|C|O,1,1.28|H,1,1.1,2,121.|H,1,1.1,2,121.,3,180.,0||V
ersion=x86-Win32-G03RevB.03|State=1-A1|HF=-112.3470611|RMSD=4.290e-005
|Dipole=0.,0.,-0.6350015|PG=C02V [C2(C1O1),SGV(H2)]||@
```

You don't have to suffer to be a poet.
Adolescence is enough suffering for anyone.

-- John Ciardi

Job cpu time: 0 days 0 hours 1 minutes 17.0 seconds.

File lengths (MBytes): RWF= 11 Int= 0 D2E= 0 Chk= 8 Scr= 1

Normal termination of Gaussian 03 at Mon Jan 16 16:13:09 2006.

Back to check route : Internal Options (IOP)

→ Non-standard route: *Overlay / Opt=val, Opt=Val, ... / Link, Link,...*

```
# HF/STO-3G
```

```
-----
```

```
1/38=1/1;
```

```
2/17=6,18=5,40=1/2;
```

```
3/6=3,11=9,16=1,25=1,30=1/1,2,3;
```

```
4//1;
```

```
5/5=2,32=1,38=5/2;
```

```
6/7=2,8=2,9=2,10=2,28=1/1;
```

```
99/5=1,9=1/99;
```

```
-----
```

Example:

3/6=3,11=9,16=1,25=1,30=1/1,2,3;

Means:

run through links 301, 302, and 303,
with options 6 set equal to 3, option
11 set to 9, etc. in each of the links (in
overlay 3).

Check the options and their values at <http://www.gaussian.com/iops.htm>

Consider options that control methods, basis set and integrals

- IOP(3/6) Number of Gaussian Functions. Here IOP(3/6=3) for STO-3G
- IOP(3/11) Control of 2-electron integral storage format
- IOP(3/16) Pseudopotential option (=1: Yes, read if general basis.)
- IOP(3/25) Number of last 2-electron integral link (=1 : Direct SCF.)
- IOP(3/30) Control of 2-electron integral symmetry (=1: symmetry turned on)

Option and values for basis sets (in overlay 3)

For example, compare:

HF/**STO-3G**

→ 3/6=3,11=9,16=1,25=1,30=1/1,2,3;

HF/**6-31+G(d,p)**

→ 3/5=1,**6=6**,7=111,11=9,16=1,25=1,30=1/1,2,3;

Explanation:

STO-3G

I_{Op}(3/6) Number of Gaussian Functions. Here I_{Op}(3/6=3) for STO-3G

6-31+G**

I_{Op}(3/5) Number of Gaussian Functions. Here I_{Op}(3/6=6) for 6-31+G(d,p)

I_{Op}(3/6) Type of basis set. Here I_{Op}(3/5=1) for Extended 4-31G,5-31G,6-31G

I_{Op}(3/7=111) Diffuse and polarization functions. Here I_{Op}(3/7=111) for
d-functions on heavy atoms (1) **PLUS**
a set of sp functions on heavy atoms (10) **PLUS**
p-functions on H atoms (100)

An array of Basis sets are available

Basis Set	Applies To	Polarization Functions	Diffuse Functions
STO-3G	H--Xe	*	
3-21G	H--Xe	* or **	+
6-21G	H--Cl	(d)	
4-31G	H--Ne	(d) or (d,p)	
6-31G	H--Kr	(3df,3pd)	++
6-311G	H--Kr	(3df,3pd)	++
D95	H--Cl except Na, Mg	(3df,3pd)	++
D95V	H--Ne	(d) or (d,p)	++
SHC	H--Cl	*	
CEP-4G	H--Rn	*	
CEP-31G	H--Rn	*	
CEP-121G	H--Rn	*	
LanL2MB	H--Ba, La--Bi		
LanL2DZ	H, Li--Ba, La--Bi		
SDD	all but Fr and Ra		
cc-pV[DTQ5]Z			
Dcc-pV[DT]Z	H-He, B-Ne, Al-Ar	included indefiniton	added via AUG-prefix
cc-pV6Z	H, B-Ne	included indefiniton	added via AUG-prefix
SV	H--Kr		
SVP	H--Kr	included indefiniton	
TZV	H--Kr	(3df,3pd)	
MidiX	H, C, N, O, F, P, S, Cl	included indefiniton	
EPR-II,III	H, B, C, N, O, F	included indefiniton	

You can also specify particular basis functions, using keyword "Gen".

Option and values for DFT methods (in overlay 3)

For example, compare:

HF/6-31+G(d,p)

→ 3/5=1,6=6,7=111,11=9,16=1,25=1,30=1/1,2,3;

B3LYP/6-31+G(d,p)

→ 3/5=1,6=6,7=111,11=2,16=1,25=1,30=1,**74=-5**/1,2,3;

Explanation:

IOP(3/74) Type of exchange and correlation potentials.

IOP(3/74=-5) means “Becke’s three-parameter hybrid exchange functional with Lee-Yang-Parr correlation functional”.

IOP(3/74=100) or by default is Hartree-Fock

DFT methods: IOP(3/74)

-34	BMK.	-9	LG1LYP.
-33	X3LYP	-8	B1LYP.
-32	t-HCTH hybrid	-7	mPW91PW91.
-31	t-HCTH	-6	Becke3 with Perdew 91 correlation.
-30	OmPW3PBE.	-5	Becke3 using VWN/LYP for correlation.
-29	OmPW1PBE.	-4	Becke 3 with Perdew 86 correlation.
-28	OmPW1LYP.	-3	Becke "Half and Half" with LYP/VWN correlation.
-27	OmPW1PW91.	-2	Becke "Half and Half": 0.5 HF + 0.5 LSD
-24	O3LYP.	-1	Do only coulomb part; skip exchange-correlation.
-23	HCTH407.	00	Default, same as 100.
-22	HCTH147.	00	No correlation.
-21	B97-2.	01	Vosko-Wilk-Nusair method 5 correlation.
-20	B97-1.	02	Lee-Yang-Parr correlation.
-19	HCTH93.	03	Perdew 81 correlation.
-18	B98.	04	Perdew 81 + Perdew 86 correlation.
-17	B1B95.	05	VWN 80 (LSD) correlation
-16	BA3PBE.	06	VWN 80 (LSD) + Perdew 86 correlation
-15	BA1PBE.	07	OS1 correlation
-14	PBE3PBE.	08	PW91
-13	PBE1PBE	09	PBE
-12	mPW3PBE.	10	VSXC
-11	mPW1PBE.	11	Bc96
-10	mPW1LYP.		

DFT methods: IOP(3/74) more

18	VWN5+P86	1400 B98 (JCP 108,9624(1998) eq.2c) exchange
19	LYP+VWN5 for scaling	1500 HCTH (JCP 109,6264 (1998) exchange
20	KCIS	1600 B97-1 (CPL 316,160(2000)) exchange
100	Hartree-Fock exchange.	1700 B97-2 (JCP 115,9233(2001)) exchange
200	Hartree-Fock-Slater exchange (Alpha = 2/3).	1800 HCTH147 exchange
300	X-alpha exchange (alpha= 0.7)	1900 HCTH407 exchange
400	Becke 1988 exchange.	2000 OPTX exchange
500	LG exchange.	2100 OPTX exchange as in O3LYP
600	PW91 exchange	2800 Old mPW exchange (local scaling in non-local ter
700	Gill 96 exchange	
800	PW86 exchange	
900	mPW exchange	
1000	PBE exchange	
1100	BA exchange	
1200	VSXC exchange	

3/74= Ex+Corr

3/74=100 is Hartree-Fock
3/74=200 is Hartree-Fock-Slater,
3/74=205 is Local Spin Density,
3/74=402 is BLYP.
3/74=-5 is B3LYP
etc.

Option & values for post-HF methods

For example, compare:

HF/6-31+G(d,p)

→ 1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=1,6=6,7=111,11=9,16=1,25=1,30=1/1,2,3;
4//1;
5/5=2,32=1,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/5=1,9=1/99;

MP2/6-31+G(d,p)

→ 1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=1,6=6,7=111,11=9,16=1,25=1,30=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/10=2/1;
9/16=-3/6;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99

Link 801 : Performs integral transformation.

Link 906 : Semi-direct MP2.

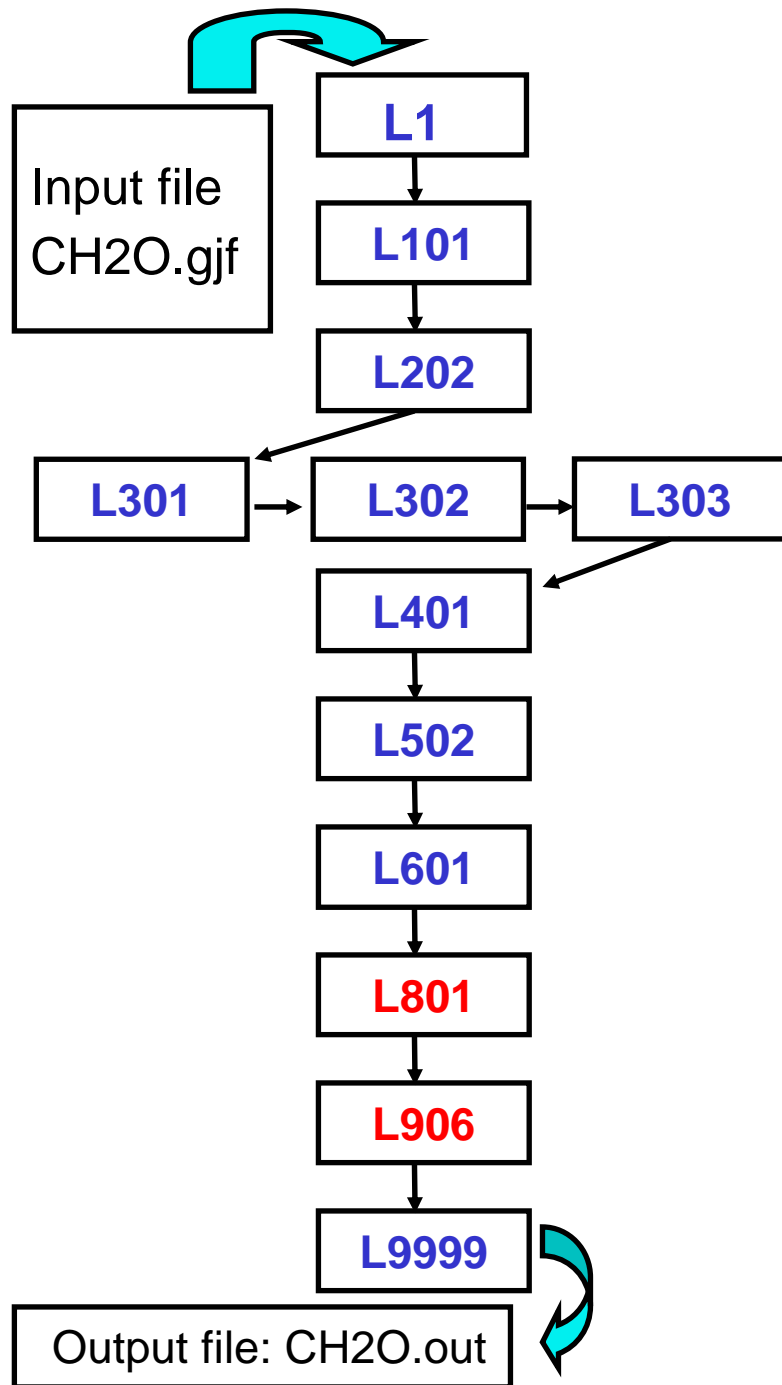
IOP(9/16) : Control of Semi-/ Direct MP2

IOP(9/16=3) : Try to minimize integral evaluations, using fully direct methods if possible, otherwise spilling to disk.

In HF, **IOP(5/32=1)** means sleazy (low-quality) SCF, using loose integral cutoffs, convergence on either energy or density.

In MP2 **IOP(5/32) by default** is not to use sleazy SCF.

MP2 Route



Link 1 : Reads and parses route section. Builds links.

Link 101 : Reads in title and molecule specification

Link 202 : calculates molecular symmetry

Link 301 : Generates basis set information

Link 302 : Overlap, kinetic, and potential integrals

Link 303 : Calculates multipole integrals

Link 401 : Forms the initial MO guess

Link 502 : Iteratively solves the SCF equations

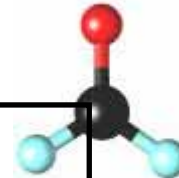
Link 601 : Assigns orbital and wavefunction symmetries; Performs Mulliken population analysis

Link 801 : Performs integral transformation.

Link 906 : Semi-direct MP2.

Link 9999 : Finalizes calculation and output

Output electronic energy : a comparison



HF/6-31+G(d,p)

After Link **502** (Iteratively solves the SCF equations.)

SCF Done: E(RHF) = -113.860654385 A.U. after 5 cycles
Conv γ = 0.8268D-04 -V/T = 2.0057
S**2 = 0.0000

B3LYP/6-31+G(d,p)

After Link **502**

SCF Done: E(RB+HF-LYP) = -114.505038857 A.U. after 5 cycles
Conv γ = 0.3438D-04 -V/T = 2.0113
S**2 = 0.0000

MP2/6-31+G(d,p)

After Link **502**

SCF Done: E(RHF) = -113.860667838 A.U. after 11 cycles
Conv γ = 0.6467D-08 -V/T = 2.0057
S**2 = 0.0000

After Link **906** (semi-direct MP2)

E2 = -0.3280486809D+00 EUMP2 = -0.11418871651932D+03

An array of methods are available

Method Availabilities in *Gaussian 03*

	SP, Scan	Opt, Force, BOMD	Freq	IRC	ADMP	Polar	Stable	ONIOM	SCRF	PBC
Molecular Mechanics	*	*	*					*		
AM1, PM3 (etc.)	*	*	<i>num.</i>	*				*		
HF	*	*	*	*	*	*	*	*	*	*
DFT methods	*	*	*	*	*	*	*	*	*	*
CASSCF	*	*	*	*		*		*	*	
MP2	*	*	*	*		*		*		
MP3, MP4(SDQ)	*	*		*				*		
MP4(SDTQ), MP5	*							*		
QCISD, CCD, CCSD	*	*		*				*		
QCISD(T) or (TQ)	*							*		
BD	*							*		
OVGF	*									
CBS, G _n , W1 methods	*									
CIS	*	*	*	*		*		*	*	
TD	*							*	*	
ZINDO	*							*		
CI	*	*		*				*		
GVB	*	*		*				*		

Some New, for example,

1. Periodic Boundary Conditions (**PBC**) calculations for periodic systems
2. Atom-Centered Density Matrix Propagation (**ADMP**) molecular dynamics.

Methods / basis set

FCI	FCI/ STO-3G	FCI/ 3-21G	FCI/ 6-31G*	FCI/ 6-311G(2df)		exact

CCSD(T)	CCSD(T)/ STO-3G	CCSD(T)/ 3-21G	CCSD(T)/ 6-31G*	CCSD(T)/ 6-311G(2df)		CCSD(T) limit
CCSD	CCSD/ STO-3G	CCSD/ 3-21G	CCSD/ 6-31G*	CCSD/ 6-311G(2df)		CCSD limit
MP2	MP2/ STO-3G	MP2/ 3-21G	MP2/ 6-31G*	MP2/ 6-311G(2df)		MP2 limit
HF	HF/ STO-3G	HF/ 3-21G	HF/ 6-31G*	HF/ 6-311G(2df)		HF limit
	STO-3G	3-21G	6-31G*	6-311G(2df)	***	complete

↑
Correlation

→
AO Basis Set

A theoretical model chemistry is defined by the two main approximations that are made in order to make solution of the time-independent Schrödinger equation tractable. These are the level of correlation treatment and the extent of completeness of the set of basis functions which are used to represent the molecular orbitals.

(Martin Head-Gordon, *J. Phys. Chem.* **1996**, *100*, 13213-13225)

Scaling features of computational methods

Method	Formal CPU	Formal Memory	Formal Disk	Actual CPU	Actual Disk
Conv. SCF	N^4	N^2	N^4	$N^{3.5}$	$N^{3.5}$
Incore SCF	N^4	N^4	-	N^4	N^2
Direct SCF	N^4	N^2	-	$N^{2.3}$	N^2
Conv. MP2	ON^4	N^2	N^4	ON^4	N^4
Dir MP2 SP	ON^4	OVN	-	O^2N^3	N^2
SD MP2 SP	ON^4	N^2	VN^2	O^2N^3	VN^2
Conv. MP2 Force	ON^4	N^2	N^4	ON^4	N^4
Dir MP2 Force	ON^4	N^3	-	O^2N^3	N^2
SD MP2 Force	ON^4	N^2	N^3	O^2N^3	N^3
MP3, CISD, QCISD	O^2N^4	N^2	N^4	O^2N^4	N^4
MP4, QCISD(T)	O^3V^4	N^2	N^4	O^3V^4	N^4

O: Number of occupied orbitals; V: Number of virtual orbitals; N: Number of basis functions

Tell G 03 what to do: keywords in # route card

Input file 1 : single-point

```
# B3LYP/6-31G
```

Example: aldehyde

```
0 1
C1
O2 1 A
H3 1 B 2 C
H4 1 B 2 C 3 D
```

```
A = 1.28
B = 1.10
C = 121.0
D = 180.0
```

Input file 2 : optimization

```
# B3LYP/6-31G OPT
```

Example: aldehyde

```
0 1
C1
O2 1 A
H3 1 B 2 C
H4 1 B 2 C 3 D
```

```
A = 1.28
B = 1.10
C = 121.0
D = 180.0
```

Options of OPT, for example:

```
# B3LYP/6-31G OPT(Tight, Z-matrix)
```

Opt=tight: tightens the cutoffs on forces and step size that are used to determine convergence

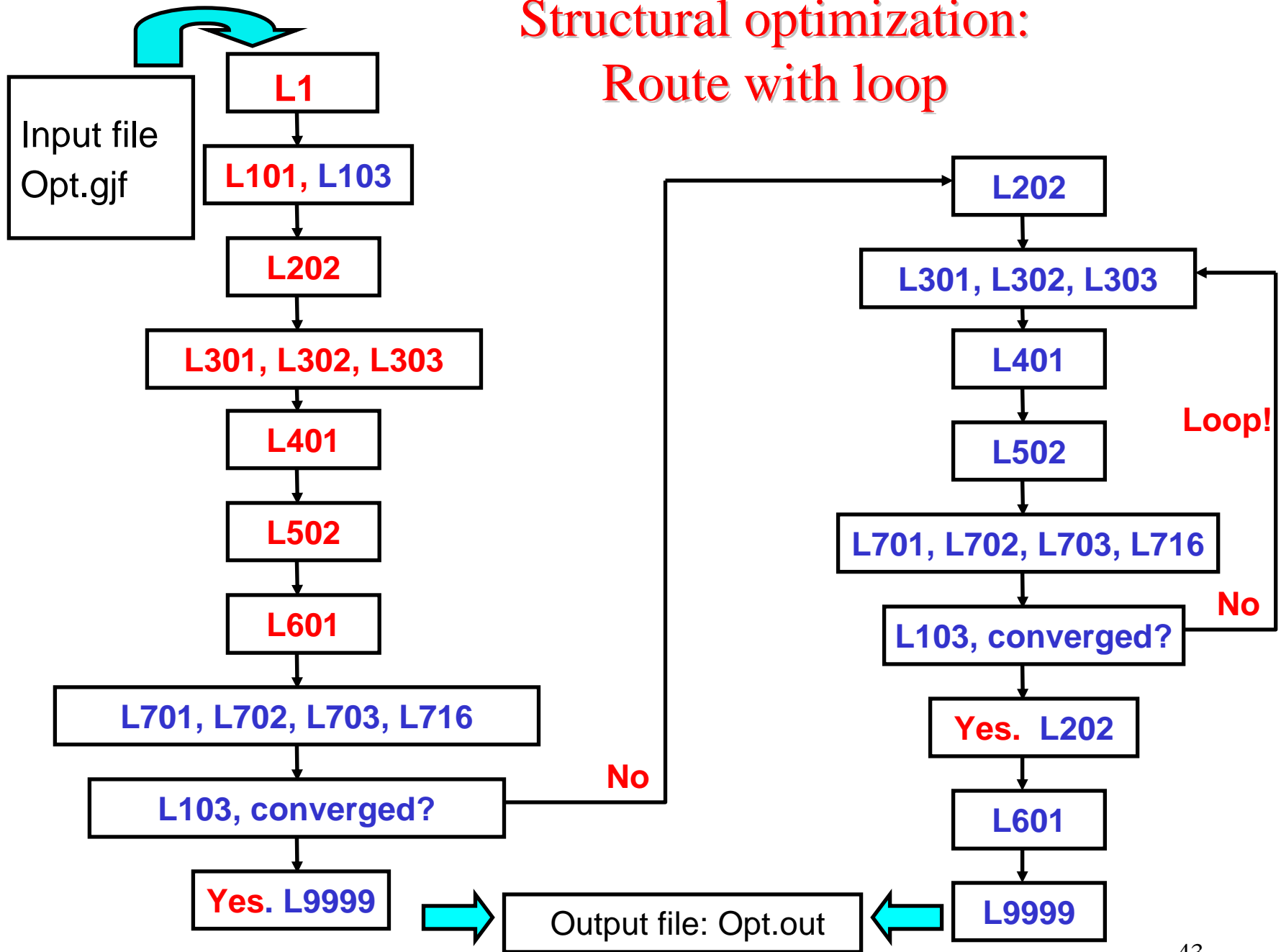
Structural optimization: Option & values

For example :

B3LYP/6-31G **OPT(Tight, Z-matrix)**

→ 1/7=10,10=7,14=-1,18=40,26=3,38=1/1,3;
2/17=6,18=5,29=3,40=1/2;
3/5=1,6=6,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2; (missing 5/32=1)
6/7=2,8=2,9=2,10=2,28=1/1;
7/29=1/1,2,3,16;
1/10=7,14=-1,18=40/3(1);
99//99;
2/29=3/2;
3/5=1,6=6,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=40/3(-5);
2/29=3/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Structural optimization: Route with loop



Structural optimization: links and options

Link 103 : Performs optimization using Berny algorithm

Link 701 : 1-electron integral first or second derivatives

Link 702 : 2-electron integral first or second derivatives (sp)

Link 703 : 2-electron integral first or second derivatives (spdf)

Link 716 : Processes information for optimizations and frequencies

Example of option values for # B3LYP/6-31G OPT(Tight, Z-matrix)

IOP(1/7) : Convergence of the 1st derivative (forces).

IOP(1/7=10) : 10^{-10} , that is, **Tight**

IOP(1/26) : Accuracy of function being optimized .

IOP(1/26=3) : Fine grid accuracy for DFT
(Energy 1.d-7, gradient 1.d-6)

IOP(1/10) : Input of initial Hessian.

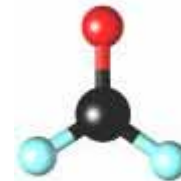
IOP(1/10=7) : Use semiempirical force constants.

IOP(2/29) : Update of coordinates from current **Z-matrix**. IOP(2/29=3): YES.

IOP(7/29) : Mode of Use of L 716.

IOP(7/29=1) Normal + Generate estimated initial force constants.

CH₂O optimization: Output (a) : Link 103, 1st



Link 103 : Performs optimization using Bery algorithm.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Bery optimization.

Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name Value Derivative information (Atomic Units) !

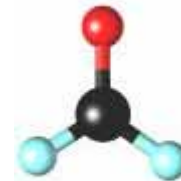
! A 1.28 estimate D2E/DX2 !
! B 1.1 estimate D2E/DX2 !
! C 121.0 estimate D2E/DX2 !
! D 180.0 estimate D2E/DX2 !

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 20 maximum allowed number of steps= 100.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

CH₂O optimization: Output (b) : Link 103, 2nd



Link 103 : Performs optimization using Bery algorithm.

Grad

Bery optimization.

Search for a local minimum.

Step number 1 out of a maximum of 20

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Second derivative matrix not updated -- first step.

The second derivative matrix:

	A	B	C	D
A	0.73068			
B	0.00000	0.67364		
C	0.00000	0.00000	0.96000	
D	0.00000	0.00000	0.00000	0.03306

Eigenvalues --- 0.03306 0.67364 0.73068 0.96000

RFO step: Lambda=-4.87629959D-03.

Linear search not attempted -- first point.

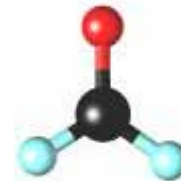
Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
A	2.41885	-0.05962	0.00000	-0.08105	-0.08105	2.33780
B	2.07870	-0.00285	0.00000	-0.00419	-0.00419	2.07451
C	2.11185	0.00558	0.00000	0.00579	0.00579	2.11763
D	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159

Item	Value	Threshold	Converged?
Maximum Force	0.059618	0.000015	NO
RMS Force	0.029973	0.000010	NO
Maximum Displacement	0.081051	0.000060	NO
RMS Displacement	0.040683	0.000040	NO

Predicted change in Energy=-2.454290D-03

Grad

CH₂O optimization: Output (c) : Link 103, last



Link 103 : Performs optimization using Bery algorithm.

Grad

Bery optimization.

Search for a local minimum.

Step number 5 out of a maximum of 20

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Update second derivatives using D2CorN and points 1 2 3 5

Trust test= 9.73D-01 RLast= 7.12D-05 DXMaxT set to 3.00D-01

The second derivative matrix:

	A	B	C	D
A	0.70717			
B	0.03146	0.64966		
C	0.09438	-0.06550	0.80879	
D	0.00000	0.00000	0.00000	0.03306

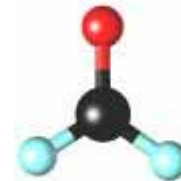
Eigenvalues --- 0.03306 0.58664 0.70603 0.87295

RFO step: Lambda= 0.00000000D+00.

Quartic linear search produced a step of -0.01838.

Variable	Old X	-DE/DX (Linear)	Delta X (Quad)	Delta X (Total)	Delta X	New X
A	2.32732	0.00000	0.00000	0.00000	0.00000	2.32732
B	2.08364	0.00000	0.00000	0.00000	0.00000	2.08364
C	2.13198	0.00000	0.00000	0.00000	0.00000	2.13198
D	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159

CH₂O optimization: Output (d) : Link 103, last



Link 103 : Performs optimization using Bery algorithm.

```
Item      Value  Threshold Converged?
Maximum Force  0.000002  0.000015  YES
RMS Force     0.000001  0.000010  YES
Maximum Displacement  0.000002  0.000060  YES
RMS Displacement  0.000001  0.000040  YES
Predicted change in Energy=-2.811879D-12
Optimization completed.
-- Stationary point found.
```

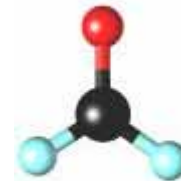
! Optimized Parameters !
! (Angstroms and Degrees) !

!	Name	Value	Derivative information (Atomic Units)	!
!	A	1.2316	-DE/DX = 0.0	!
!	B	1.1026	-DE/DX = 0.0	!
!	C	122.1532	-DE/DX = 0.0	!
!	D	180.0	-DE/DX = 0.0	!

Grad

Largest change from initial coordinates is atom 1 0.011 Angstroms.

CH₂O optimization: Output (e) : Link 202, first



Link 202 : Reorients coordinates, calculates symmetry

Z-MATRIX (ANGSTROMS AND DEGREES)

CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J

```
-----  
1 1 C  
2 2 O 1 1.280000( 1)  
3 3 H 1 1.100000( 2) 2 121.000( 4)  
4 4 H 1 1.100000( 3) 2 121.000( 5) 3 180.000( 6) 0  
-----
```

Z-Matrix orientation:

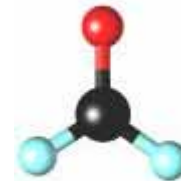
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

```
-----  
1 6 0 0.000000 0.000000 0.000000  
2 8 0 0.000000 0.000000 1.280000  
3 1 0 0.942884 0.000000 -0.566542  
4 1 0 -0.942884 0.000000 -0.566542  
-----
```

Distance matrix (angstroms):

```
-----  
1 C 0.000000  
2 O 1.280000 0.000000  
3 H 1.100000 2.073342 0.000000  
4 H 1.100000 2.073342 1.885768 0.000000  
-----
```

CH₂O optimization: Output (f) : Link 202, first



Link 202 : Reorients coordinates, calculates symmetry

Interatomic angles:

O2-C1-H3=121. O2-C1-H4=121. H3-C1-H4=118.

Stoichiometry CH2O

Framework group C2V[C2(CO),SGV(H2)]

Deg. of freedom 3

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2 NOp 2

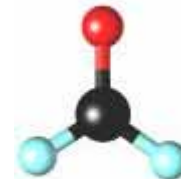
Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1	6	0	0.000000	0.000000	-0.569182
2	8	0	0.000000	0.000000	0.710818
3	1	0	0.000000	0.942884	-1.135724
4	1	0	0.000000	-0.942884	-1.135724

Rotational constants (GHZ): 282.0236292 35.0946253 31.2107974

CH₂O optimization: Output (g) : Link 202, last



Link 202 : Reorients coordinates, calculates symmetry

Z-MATRIX (ANGSTROMS AND DEGREES)

CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z J

```
-----  
1 1 C  
2 2 O 1 1.231562( 1)  
3 3 H 1 1.102613( 2) 2 122.153( 4)  
4 4 H 1 1.102613( 3) 2 122.153( 5) 3 180.000( 6) 0  
-----
```

Z-Matrix orientation:

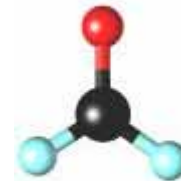
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

```
-----  
1 6 0 0.000000 0.000000 0.000000  
2 8 0 0.000000 0.000000 1.231562  
3 1 0 0.933503 0.000000 -0.586794  
4 1 0 -0.933503 0.000000 -0.586794  
-----
```

Distance matrix (angstroms):

```
1 2 3 4  
1 C 0.000000  
2 O 1.231562 0.000000  
3 H 1.102613 2.043978 0.000000  
4 H 1.102613 2.043978 1.867006 0.000000
```

CH₂O optimization: Output (h) : Link 202, last



Link 202 : Reorients coordinates, calculates symmetry

Interatomic angles:

O2-C1-H3=122.1532 O2-C1-H4=122.1532 H3-C1-H4=115.6936

Stoichiometry CH2O

Framework group C2V[C2(CO),SGV(H2)]

Deg. of freedom 3

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1 6 0 0.000000 0.000000 -0.542432

2 8 0 0.000000 0.000000 0.689130

3 1 0 0.000000 0.933503 -1.129226

4 1 0 0.000000 -0.933503 -1.129226

Rotational constants (GHZ): 287.7203705 37.3517737 33.0599418

Tell G 03 what to do: keywords in # route card

Input file 1 : single-point

B3LYP/6-31G

Example: aldehyde

```
0 1
C1
O2 1 A
H3 1 B 2 C
H4 1 B 2 C 3 D
```

A = 1.28
B = 1.10
C = 121.0
D = 180.0

Input file 2 : frequency

B3LYP/6-31G Freq

Example: aldehyde

```
0 1
C1
O2 1 A
H3 1 B 2 C
H4 1 B 2 C 3 D
```

A = 1.28
B = 1.10
C = 121.0
D = 180.0

Example of options of Freq:

B3LYP/6-31G Freq(Anharmonic, VibRot, Raman)

Gaussian 03 keywords

ADMP	Density Functional Methods	IRC
AM1	Dreiding	IRCMax
Amber	ExtendedHuckel	LSDA
Archive	External	MaxDisk
B3LYP	ExtraBasis	MINDO3
BD	Frozen Core Options	MM
BOMD	Field	MNDO
CASSCF	FMM	MP* Keywords
CBS Keywords	Force	Name
CBSExtrapolate	Frequency	NMR
CCD	G* Keywords	ONIOM
Charge	Gen	Opt
ChkBasis	Geom	Output
CID	GfInput	OVGF
CIS	GfPrint	PBC
CNDO	Guess	PM3
Complex	GVB	Polar
Constants	Hartree-Fock	Population
Counterpoise	Huckel	Pressure
CPHF	INDO	Prop
Density	Integral	Pseudo
DensityFit	IOp	Punch

Gaussian 03 keywords (continued)

QCISD

ReArchive

SAC-CI

Scale

Scan

SCF

SCRF

SP

Sparse

Stable

Symmetry

TD

Temperature

Test

TestMO

TrackIO

Transformation

UFF

Units

Volume

W1U

Zindo

Link 0 Commands

Non-Standard Routes

Obsolete Keywords

Program Development Keywords