

Example of geometry optimization calculation of the H₂ molecule. Similar features will appear also in transition state and reaction path calculations.

```
Entering Gaussian System, Link 0=g98
Initial command:
/ ual/usr/local/g98/l1.exe /ual/arik/lab/Gau-11867.inp -screedir=/ual/arik/lab/
Entering Link 1 = /ual/usr/local/g98/l1.exe PID= 11872.
```

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Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

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Cite this work as:

Gaussian 98, Revision A.4,
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C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen ,
M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon ,
E. S. Replogle, and J. A. Pople ,
Gaussian, Inc., Pittsburgh PA, 1998.

```
*****  
Gaussian 98: DEC-AXP-OSF/1-G98RevA.4 11-Sep-1998  
-17 Feb-2004  
*****
```

```
-----  
# n RHF/STO-3G SCF=Tight opt  
-----
```

Route section line from the input file.

```
;1/1,3=20,38=1/18  
;5/2=6,18=110,17=2/9  
;1/1,2,3=1,30=1,25=3/11  
;1/1=4/7  
;4/2=2,38=2,32=5/5  
;1/1=2,28=2,10=2,9=2,8=6/7  
;1,2,3,16//7  
;(1)20/3=1/18  
;99//99  
;110/2=2/9  
;1/1,2,3=1,30=1,25=3/11  
;2/1=1,16=5,7=4/5  
;4/2=2,38=2,32=5/5  
;1,2,3,16//7  
;(5-)20/3=1/18  
;110/2=2/9  
;1/1=2,28=2,19=2,10=2,9=2,8=6/7  
;1/99=99/9  
--
```

This keyword requests that a geometry optimization be performed. The geometry will be adjusted until a stationary point on the potential surface is found.

Title from input.

```
--  
H2  
--
```

```
Symbolic Z-matrix:  
Charge = 0 Multiplicity = 1  
H  
H          1      R  
Variables:  
R          0.71
```

atoms Z-matrix from input.

```
-----  
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad  
Berny optimization.  
Initialization pass.  
-----
```

Beginning of the optimization process.

! Initial Parameters!
) ! Angstroms and Degrees! (

! Name	Definition	Value	Derivative	Info!
! R1	R(1,2)	0.71		estimate D2E/DX2!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.000000	0.000000	0.000000	0	1	1
0.710000	0.000000	0.000000	0	1	2

Stoichiometry H2
Framework group D*H[C*(H.H[(

Deg. of freedom 1
Full point group D*H NOp 8
Largest Abelian subgroup D2H NOp 8
Largest concise Abelian subgroup C2 NOp 2

symmetry information.

Standard orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.355000	0.000000	0.000000	0	1	1
0.355000-	0.000000	0.000000	0	1	2

Rotational constants (GHZ): 0.0000000 1989.5067130 1989.5067130

Isotopes: H-1,H-1

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

There are 1 symmetry adapted basis functions of AG symmetry.
There are 0 symmetry adapted basis functions of B1G symmetry.
There are 0 symmetry adapted basis functions of B2G symmetry.
There are 0 symmetry adapted basis functions of B3G symmetry.
There are 0 symmetry adapted basis functions of AU symmetry.
There are 1 symmetry adapted basis functions of B1U symmetry.
There are 0 symmetry adapted basis functions of B2U symmetry.
There are 0 symmetry adapted basis functions of B3U symmetry.

Crude estimate of integral set expansion from redundant integrals=1.000.

Integral buffers will be 131072 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

2 basis functions 6 primitive gaussians

1 alpha electrons 1 beta electrons

nuclear repulsion energy 0.7453200690 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 2 RedAO= T NBF= 1 0 0 0 0 1 0 0

NBsUse= 2 1.00D-04 NBFU= 1 0 0 0 0 1 0 0

Projected INDO Guess.

Initial guess orbital symmetries:

Occupied (SGG(

Virtual (SGU(

Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Keep R1 integrals in memory in canonical form, NReq= 806066.

SCF calculations and Population analysis of the first step in the optimization process.

SCF Done: E(RHF) = -1.11750077541 A.U. after 1 cycles
 Convg = 0.0000D+00 -V/T = 1.9243
 S**2 = 0.0000

Population analysis using the SCF density.

Orbital Symmetries:

Occupied (SGG(
 Virtual (SGU(

The electronic state is 1-SGG.

Alpha occ. eigenvalues -- -0.59117
 Alpha virt. eigenvalues -- 0.70309

Condensed to atoms (all electrons:(

2 1
 1 H 0.595405 0.404595
 2 H 0.404595 0.595405

Total atomic charges:

1
 1 H 0.000000
 2 H 0.000000

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

1
 1 H 0.000000
 2 H 0.000000

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): <R**2>= 4.7173

Charge= 0.0000 electrons

Dipole moment (Debye:(

X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

Quadrupole moment (Debye-Ang:(

XX= -1.8427 YY= -1.8427 ZZ= -1.4490
 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (Debye-Ang**2:(

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

Hexadecapole moment (Debye-Ang**3:(

XXXX= -1.5235 YYYY= -1.5235 ZZZZ= -2.3303 XXXY= 0.0000
 XXXZ= 0.0000 YYYZ= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000
 ZZZY= 0.0000 XXYX= -0.5078 XXZZ= -0.6517 YYZZ= -0.6517
 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 7.453200690141D-01 E-N=-3.752314390080D+00 KE= 1.209011849970D+00

Symmetry AG KE= 1.209011849970D+00
 Symmetry B1G KE= 0.000000000000D+00
 Symmetry B2G KE= 0.000000000000D+00
 Symmetry B3G KE= 0.000000000000D+00
 Symmetry AU KE= 0.000000000000D+00
 Symmetry B1U KE= 0.000000000000D+00
 Symmetry B2U KE= 0.000000000000D+00
 Symmetry B3U KE= 0.000000000000D+00

forces calculation

**** Axes restored to original set****

Center Number	Atomic Number	Forces (Hartrees/Bohr(
		X	Y	Z
0.002430640-	0.000000000	0.000000000	1	1

0.002430640 0.000000000 0.000000000 1 2

Cartesian Forces: Max 0.002430640 RMS 0.001403331

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Bery optimization.

Internal Forces: Max 0.002430640 RMS 0.002430640

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:

R1
R1 0.43489
Eigenvalues --- 0.43489
RFO step: Lambda=-1.35845809D-05.
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.00395194 RMS(Int)= 0.00000000
Iteration 2 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000000
Variable Old X -DE/DX Delta X Delta X Delta X New X
)
R1 1.34171 0.00243 0.00000 0.00559 0.00559 1.34729

Item	Value	Threshold	Converged?
Maximum Force	0.002431	0.000450	NO
RMS Force	0.002431	0.000300	NO
Maximum Displacement	0.002794	0.001800	NO
RMS Displacement	0.003952	0.001200	NO

Checking for convergence of the optimization: Not converged!

Predicted change in Energy=-6.792078D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.356479-	0.000000	0.000000	0	1	1
0.356479	0.000000	0.000000	0	1	2

Starting the second step, changing the position of the atoms.

Stoichiometry H2
Framework group D*H[C*(H.H[(
Deg. of freedom 1
Full point group D*H NOp 8
Largest Abelian subgroup D2H NOp 8
Largest concise Abelian subgroup C2 NOp 2

Standard orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.356479	0.000000	0.000000	0	1	1
0.356479-	0.000000	0.000000	0	1	2

Rotational constants (GHZ): 0.0000000 1973.0350754 1973.0350754

Isotopes: H-1,H-1

Standard basis: STO-3G5) D, 7F(

There are 1 symmetry adapted basis functions of AG symmetry.
There are 0 symmetry adapted basis functions of B1G symmetry.
There are 0 symmetry adapted basis functions of B2G symmetry.
There are 0 symmetry adapted basis functions of B3G symmetry.
There are 0 symmetry adapted basis functions of AU symmetry.
There are 1 symmetry adapted basis functions of B1U symmetry.

New atoms coordinates .
(Note the minus sign has moved dew to the convert to WORD.)

There are 0 symmetry adapted basis functions of B2U symmetry.
 There are 0 symmetry adapted basis functions of B3U symmetry.
 Crude estimate of integral set expansion from redundant integrals=1.000.
 Integral buffers will be 131072 words long.
 Raffanetti 1 integral format.
 Two-electron integral symmetry is turned on.
 2 basis functions 6 primitive gaussians
 1 alpha electrons 1 beta electrons
 nuclear repulsion energy 0.7422283081 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis= 2 RedAO= T NBF= 1 0 0 00 0 1 0
 NBSUse= 2 1.00D-04 NBFU= 1 0 0 0 0 1 0 0
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:

Occupied (SGG(
 Virtual (SGU(
 Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Keep R1 integrals in memory in canonical form, NReq= 806066.
 SCF Done: E(RHF) = -1.11750534437 A.U. after 1 cycles
 Convq = 0.0000D+00 -V/T = 1.9249
 S**2 = 0.0000
 ***** Axes restored to original set*****

SCF of the second step.

Center Number	Atomic Number	Forces (Hartrees/Bohr(
		X	Y	Z
0.000786042	0.000000000	0.000000000	1	1
0.000786042-	0.000000000	0.000000000	1	2

Cartesian Forces: Max 0.000786042 RMS 0.000453822

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 Bery optimization.
 Internal Forces: Max 0.000786042 RMS 0.000786042
 Search for a local minimum.
 Step number 2 out of a maximum of 20
 All quantities printed in internal units (Hartrees-Bohrs-Radians(
 Update second derivatives using information from points 12
 Trust test= 6.73D-01 RLast= 5.59D-03 DXMaxT set to 3.00D-01
 The second derivative matrix:

R1	Eigenvalues	Value	Threshold	Converged?		
R1	---	0.57555	0.000450	NO		
RFO step: Lambda=		0.00000000D+00.				
Quartic linear search produced a step of		-0.24602.				
Iteration 1 RMS(Cart)=		0.00097226				
Iteration 2 RMS(Cart)=		0.00000000				
Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	1.34729	-0.00079	-0.00137	0.00000	-0.00137	1.34592

Checking for convergence, not yet.

Item	Value	Threshold	Converged?
Maximum Force	0.000786	0.000450	NO
RMS Force	0.000786	0.000300	NO
Maximum Displacement	0.000687	0.001800	YES
RMS Displacement	0.000972	0.001200	YES

Predicted change in Energy= 5.440623D-07
 Grad

Input orientation :

starting third step of the optimization.

new atomic
coordination

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.356115-	0.000000	0.000000	0	1	1
0.356115	0.000000	0.000000	0	1	2

Stoichiometry H2
 Framework group D*H[C*(H.H[(
 Deg. of freedom 1
 Full point group D*H NOp 8
 Largest Abelian subgroup D2H NOp 8
 Largest concise Abelian subgroup C2 NOp 2
 Standard orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.356115	0.000000	0.000000	0	1	1
0.356115-	0.000000	0.000000	0	1	2

Rotational constants (GHZ): 0.0000000 1977.0684221 1977.0684221

Isotopes: H-1,H-1

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

There are 1 symmetry adapted basis functions of AG symmetry.

There are 0 symmetry adapted basis functions of B1G symmetry.

There are 0 symmetry adapted basis functions of B2G symmetry.

There are 0 symmetry adapted basis functions of B3G symmetry.

There are 0 symmetry adapted basis functions of AU symmetry.

There are 1 symmetry adapted basis functions of B1U symmetry.

There are 0 symmetry adapted basis functions of B2U symmetry.

There are 0 symmetry adapted basis functions of B3U symmetry.

Crude estimate of integral set expansion from redundant integrals=1.000.

Integral buffers will be 131072 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

2 basis functions 6 primitive gaussians

1 alpha electrons 1 beta electrons

nuclear repulsion energy 0.7429865652 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 2 RedAO= T NBF= 1 0 0 0 0 1 0 0

NBsUse= 2 1.00D-04 NBFU= 1 0 0 0 0 1 0 0

Initial guess read from the read-write file:

Initial guess orbital symmetries:

Occupied (SGG(

Virtual (SGU(

Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Keep R1 integrals in memory in canonical form, NReq= 806066.

SCF Done: E(RHF) = -1.11750588516 A.U. after 1 cycles

Conv = 0.0000D+00 -V/T = 1.9248

S**2 = 0.0000

***** Axes restored to original set*****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
0.000000004-	0.000000000	0.000000000	1	1
0.000000004	0.000000000	0.000000000	1	2

Cartesian Forces: Max 0.000000004 RMS 0.000000002

SCF calculation of the third step, if convergence is achieved this is the optimized geometry ground state energy.

Grad
Berny optimization.

Internal Forces: Max 0.000000004 RMS 0.000000004

Search for a local minimum.

Step number 3 out of a maximum of 20

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

Update second derivatives using information from points 2 3

Trust test= 9.94D-01 RLast= 1.37D-03 DXMaxT set to 3.00D-01

The second derivative matrix:

R1
R1 0.57168
Eigenvalues --- 0.57168
RFO step: Lambda= 0.00000000D+00.

Quartic linear search produced a step of -0.00001.

Iteration 1 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000000

Variable	Old X	-DE/DX	Delta X Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	1.34592	0.00000	0.00000	0.00000	0.00000	1.34592

Item	Value	Threshold	Converged?
Maximum Force	0.000000	0.000450	YES
RMS Force	0.000000	0.000300	YES
Maximum Displacement	0.000000	0.001800	YES
RMS Displacement	0.000000	0.001200	YES

Checking for convergence of the optimization process. SUCCESS!!!!

~~Predicted change in Energy= -1.468146D-17~~

Optimization completed.

-- Stationary point found.

the optimized geometry energy can be found above.

! Optimized Parameters!
) ! Angstroms and Degrees! (

Name	Definition	Value	Derivative Info!
R1	R(1,2)	0.7122	-DE/DX = 0!

Grad

Input orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.356115-	0.000000	0.000000	0	1	1
0.356115	0.000000	0.000000	0	1	2

Stoichiometry H2
Framework group D*H[C*(H.H[(
Deg. of freedom 1
Full point group D*H NOp 8
Largest Abelian subgroup D2H NOp 8
Largest concise Abelian subgroup C2 NOp 2

Standard orientation :

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
0.356115	0.000000	0.000000	0	1	1
0.356115-	0.000000	0.000000	0	1	2

Rotational constants (GHZ): 0.000000 1977.0684221 1977.0684221
Isotopes: H-1,H-1

Population analysis using the SCF density.

Orbital Symmetries:

Occupied (SGG(

Virtual (SGU(

The electronic state is 1-SGG.

Alpha occ. eigenvalues -- -0.59022

Alpha virt. eigenvalues -- 0.70065

Condensed to atoms (all electrons:(

2 1
1 H 0.595924 0.404076
2 H 0.404076 0.595924

Total atomic charges:

1
1 H 0.000000
2 H 0.000000

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

1
1 H 0.000000
2 H 0.000000

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): <R**2>= 4.7223

Charge= 0.0000 electrons

Dipole moment (Debye:(

X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

Quadrupole moment (Debye-Ang:(

XX= -1.8430 YY= -1.8430 ZZ= -1.4474
XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (Debye-Ang**2:(

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

Hexadecapole moment (Debye-Ang**3:(

XXXX= -1.5240 YYYY= -1.5240 ZZZZ= -2.3362 XXXY= 0.0000
XXXZ= 0.0000 YYYY= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000
ZZZY= 0.0000 XXYY= -0.5080 XXZZ= -0.6529 YYZZ= -0.6529
XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 7.429865652147D-01 E-N=-3.748960750344D+00 KE= 1.208412137734D+00

Symmetry AG KE= 1.208412137734D+00

Symmetry B1G KE= 0.000000000000D+00

Symmetry B2G KE= 0.000000000000D+00

Symmetry B3G KE= 0.000000000000D+00

Symmetry AU KE= 0.000000000000D+00

Symmetry B1U KE= 0.000000000000D+00

Symmetry B2U KE= 0.000000000000D+00

Symmetry B3U KE= 0.000000000000D+00

Final structure in terms of initial Z-matrix:

H
H,1,R

Variables:

R=0.7122299

\1\1 GINC-ATTO\FOpt\RHF\STO-3G\H2\ARIK\17-Feb-2004\0\#\N RHF/STO-3G SCF
= TIGHT OPT\H2\0,1\H,0.,0.,-0.3561149513\H,0.,0.,0.3561149513\Versio
n=DEC-AXP-OSF/1-G98RevA.4\State=1-SGG\HF=-1.1175059\RMSD=0.000e+00\RMS
F=2.371e-09\Dipole=0.,0.,0.\PG=D*H [C*(H1.H1@\\((

ANYONE WHO IS NOT SHOCKED BY QUANTUM THEORY HAS
NOT UNDERSTOOD IT. -- NIELS BOHR(1885-1962(

Job cpu time: 0 days 0 hours 0 minutes 10.4 seconds.

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

(Normal) termination of Gaussian 98.