Entering Gaussian System, Link 0=g98
Initial command:
/ ual/usr/local/g98/l1.exe /ua1/arik/lab/Gau-11867.inp -scrdir=/ua1/arik/lab/
Entering Link 1 = /ual/usr/local/g98/l1.exe PID= 11872.

All Rights Reserved.

This is part of the Gaussian(R) 98 program. It is based on
the Gaussian 94(TM) system (copyright 1995 Gaussian, Inc,).
the Gaussian 92(TM) system (copyright 1992 Gaussian, Inc,).
the Gaussian 90(TM) system (copyright 1990 Gaussian, Inc,).
the Gaussian 88(TM) system (copyright 1988 Gaussian, Inc,).
the Gaussian 86(TM) system (copyright 1986 Carnegie Mellon
University), and the Gaussian 82(TM) system (copyright 1983
Carnegie Mellon University). Gaussian is a federally registered
trademark of Gaussian, Inc.

This software contains proprietary and confidential information,
including trade secrets, belonging to Gaussian, Inc.

This software is provided under written license and may be
used, copied, transmitted, or stored only in accord with that
written license.

The following legend is applicable only to US Government
contracts under DFARS:

RESTRICTED RIGHTS LEGEND

Use, duplication or disclosure by the US Government is subject
to restrictions as set forth in subparagraph (c)(1)(ii) of the
Rights in Technical Data and Computer Software clause at DFARS
.7013-252.227

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

The following legend is applicable only to US Government
contracts under FAR:

RESTRICTED RIGHTS LEGEND

Use, reproduction and disclosure by the US Government is subject
to restrictions as set forth in subparagraph (c) of the
Commercial Computer Software - Restricted Rights clause at FAR
.19-52.227

Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

------------------------------------------------------------------------

Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc. The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the

Example of geometry optimization calculation of the
H2 molecule. Similar features will appear also in
transition state and reaction path calculations.
licensee that it is not a competitor of Gaussian, Inc. and that it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 98, Revision A.4,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr,
R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam,
A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,
V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo,
S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui,
K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov, G. Liu,
A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin,
D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara,
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,

-17 Feb-2004

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

H
H
Variables: 1 R
R 0.71

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

H2

Initialization pass.

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

Angstroms and Degrees!

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Value</th>
<th>Derivative Info</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R(1,2)</td>
<td>0.71</td>
<td>Estimate D2E/DX2</td>
</tr>
</tbody>
</table>

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.

Input orientation:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0</td>
<td>X</td>
</tr>
<tr>
<td>0.710000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0</td>
<td>X</td>
</tr>
</tbody>
</table>

Stoichiometry: H2
Framework group: D*H|C*(H.H){
Deg. of freedom: 1
Full point group: D*H
Largest Abelian subgroup: D2H
Largest concise Abelian subgroup: C2

Standard orientation:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.355000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0</td>
<td>X</td>
</tr>
<tr>
<td>0.355000-</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0</td>
<td>X</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ): 0.000000 1989.5067130 1989.5067130
Isotopes: H-1, H-1

Crude estimate of integral set expansion from redundant integrals=1.000.
Integral buffers will be 131072 words long.

Two-electron integral symmetry is turned on.
2 basis functions 6 primitive gaussians
1 alpha electrons 1 beta electrons

One-electron integrals computed using PRISM.

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.
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=  0.00000 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 XZZ=   0.0000 XYZ=  -0.0000
YYZ=    0.0000 YYY=  -0.5078 XXZ=  -0.6517 YZZ=   -0.6517
XYZ=    0.0000 YYZ=  -0.5078 XXY=  -0.6517 ZZZ=   -2.3303
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
**** Axes restored to original set****

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Forces (Hartrees/Bohr)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>0.002430640</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
</tbody>
</table>
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
GradGradGradGrad
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:
R
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
                 Linear) (Quad) (Total)
R1  1.34171  0.00243  0.00000  0.00559  0.00559  1.34729

Checking for convergence of the optimization: Not converged!
Starting the second step, changing the position of the atoms.

New atoms coordinates.
(Note the minus sign has moved down 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.
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 = 0.742283081 Hartrees.
One-electron integrals computed using PRISM.
NBasis= 2 RedAO= T NBF= 1 0 0 0 0 1 0
NBsUse= 2 1.00D-04 NBFU= 1 0 0 0 0 1 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
Convg = 0.00000000D+00 -V/T = 1.9249
S**2 = 0.0000
Axes restored to original set

Center Atomic Forces (Hartrees/Bohr)
Number Number 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
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny 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
R1 0.57555
Eigenvalues --- 0.57555
RFO step: Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.24602.
Iteration 1 RMS(Cart)= 0.00097226 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
 ) Linear) (Quad) (Total( Linear)
R1 1.34729 -0.00079 -0.00137 0.00000 -0.00137 1.34592
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
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Input orientation

SCF of the second step.
Checking for convergence, not yet.
starting third step of the optimization.
### Calculated Properties

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.356115</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.00000000</td>
</tr>
<tr>
<td>0.356115</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.00000000</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.356115</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.00000000</td>
</tr>
<tr>
<td>0.356115</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.00000000</td>
</tr>
</tbody>
</table>

- **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 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
  - Convg = 0.000000D+00 -V/T = 1.9248
  - S**2 = 0.0000

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

### Cartesian Forces

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Forces (Hartrees/Bohr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000000004</td>
<td>0.0000000000</td>
<td>0.0000000000 1 1</td>
</tr>
<tr>
<td>0.0000000004</td>
<td>0.0000000000</td>
<td>0.0000000000 1 2</td>
</tr>
</tbody>
</table>

**Cartesian Forces:** Max 0.0000000004 RMS 0.0000000002

---

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

Eigenvalues --- 0.57168

RFO step: Lambda= 0.00000000D+00.

Quartic linear search produced a step of -0.00001.

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

Variable Old X -DE/DX Delta X Delta X Delta X New X

R1 1.34592 0.00000 0.00000 0.00000 0.00000 1.34592

Optimized Parameters!

Angstroms and Degrees!

Name Definition Value Derivative Info!

R1 R(1,2) 0.7122 -DE/DX = 0!

Optimized geometry:

The optimized geometry energy can be found above.

Input orientation:

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:

Rotational constants (GHZ): 0.0000000 1977.0682421 1977.0682421

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):

<table>
<thead>
<tr>
<th>Atom</th>
<th>Occupancy</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>0.595924</td>
<td>0.404076</td>
</tr>
<tr>
<td>H</td>
<td>0.404076</td>
<td>0.595924</td>
</tr>
</tbody>
</table>

Total atomic charges:

<table>
<thead>
<tr>
<th>Atom</th>
<th>Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>H</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.000000

Atomic charges with hydrogens summed into heavy atoms:

<table>
<thead>
<tr>
<th>Atom</th>
<th>Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>H</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.000000

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
XYX= 0.0000  ZXZ= 0.0000  YYZ= 0.0000
XYZ= 0.0000  XZZ= 0.0000  ZZY= 0.0000

Hexadecapole moment (Debye-Ang**3):

XXXX= -1.5240  YYYY= -1.5240  ZZZZ= -2.3362  XXXY= 0.0000
XXZ= 0.0000  YYXX= 0.0000  ZZYY= 0.0000  ZZZX= 0.0000
XXXZ= 0.0000  YYZZ= 0.0000  XZZY= 0.0000  XXYZ= 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
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*