Entering Gaussian System, Link 0=g98
Initial command:
/ua1/usr/local/g98/l1.exe /ua1/arik/lab/Gau-11861.inp -scrdir=/ua1/arik/lab/
Entering Link 1 = /ua1/usr/local/g98/l1.exe PID= 11866.


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

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

Feb-2004

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

<table>
<thead>
<tr>
<th>CD</th>
<th>Cent</th>
<th>Atom</th>
<th>N1</th>
<th>Length/X</th>
<th>N2</th>
<th>Alpha/Y</th>
<th>N3</th>
<th>Beta/Z</th>
<th>J</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>H</td>
<td>1</td>
<td>0.712200</td>
<td>1</td>
<td>0.712200</td>
<td>1</td>
<td>1</td>
<td>1</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0</td>
</tr>
<tr>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0</td>
</tr>
</tbody>
</table>
Stoichiometry: H2
Framework group: D*H
Deg. of freedom: 1
Full point group: D*H
Largest Abelian subgroup: D2H
Largest concise Abelian subgroup: C2

Standard orientation:

Center | Atomic Number | Atomic Number | Type | Coordinates (Angstroms) |
-------|---------------|---------------|------|------------------------|
0.356100 | 0.000000 | 0.000000 | 0 | 1 | 1 |
0.356100- | 0.000000 | 0.000000 | 0 | 1 | 2 |

Rotational constants (GHZ): 0.000000 1977.2344452 1977.2344452
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 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 0.7430177605 Hartrees.

One-electron integrals computed using PRISM.

SCF Done: E(RHF) = -1.11750588424 A.U. after 1 cycles
Convg = 0.0000D+00 -V/T = 1.9248
S**2 = 0.0000

Range of M.O.s used for correlation: 1 2

NROrb = 2 NOA = 1 NOB = 1 NVA = 1

Differentiating once with respect to magnetic field using GIAOs.

Calculating GIAO nuclear magnetic shielding tensors.
GIAO Magnetic shielding tensor (ppm):

<table>
<thead>
<tr>
<th>1</th>
<th>H</th>
<th>Isotropic = 28.1938</th>
<th>Anisotropy = 0.6326</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>27.9830</td>
<td>YX = 0.0000</td>
<td>ZX = 0.0000</td>
</tr>
<tr>
<td>Y</td>
<td>0.0000</td>
<td>YY = 27.9830</td>
<td>ZY = 0.0000</td>
</tr>
<tr>
<td>Z</td>
<td>0.0000</td>
<td>YZ = 0.0000</td>
<td>ZZ = 28.6156</td>
</tr>
</tbody>
</table>

Eigenvalues: 27.9830 27.9830 28.6156

2 H Isotropic = 28.1938 Anisotropy = 0.6326

NMR results.
The two atoms magnetic shielding, these are two identical atoms, so the isotropic shielding is the same.
Population analysis using the SCF density.

Orbital Symmetries:

Occupied (SGG)
Virtual (SGU)

The electronic state is 1-SGG.
Alpha occ. eigenvalues -- -0.59023
Alpha virt. eigenvalues -- 0.70068

Condensed to atoms (all electrons):

<table>
<thead>
<tr>
<th>Atom</th>
<th>Mulliken Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>0.595917</td>
</tr>
<tr>
<td>H</td>
<td>0.404083</td>
</tr>
</tbody>
</table>

Total atomic charges:

1. 1 H 0.000000
2. 1 H 0.000000

Sum of Mulliken charges= 0.00000

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

Charge= 0.00000

Dipole moment (Debye): (x=0.000 y=0.000 z=0.000 tot=0.0000)

Quadrupole moment (Debye-Ang):

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>XX</td>
<td>YY</td>
<td>ZZ</td>
<td>-1.4475</td>
</tr>
</tbody>
</table>

Octapole moment (Debye-Ang**2):

<table>
<thead>
<tr>
<th>XXX</th>
<th>YYY</th>
<th>ZZZ</th>
<th>XYY</th>
<th>YZZ</th>
<th>ZXX</th>
<th>YXY</th>
<th>XXZ</th>
<th>YXZ</th>
<th>ZZX</th>
<th>ZYZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

Hexadecapole moment (Debye-Ang**3):

<table>
<thead>
<tr>
<th>XXXX</th>
<th>YYYY</th>
<th>ZZZZ</th>
<th>XXXY</th>
<th>YYYX</th>
<th>ZXXY</th>
<th>YXYX</th>
<th>XXXZ</th>
<th>ZYXZ</th>
<th>YXXZ</th>
<th>ZYYZ</th>
<th>ZZXY</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.5239</td>
<td>-1.5239</td>
<td>-2.3361</td>
<td>0.0000</td>
<td>0.0000</td>
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<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

N-N= 7.430177604605D-01 E-N=-3.74900565863D+00 KE= 1.208420152397D+00
Symmetry AG KE= 1.208420152397D+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

The second atom magnetic shielding tensor.
Note that: XX+YY+ZZ=Isotropic.
I (ERNEST RUTHERFORD) CAME INTO THE ROOM, WHICH WAS HALF DARK, AND PRESENTLY SPOTTED LORD KELVIN IN THE AUDIENCE AND REALIZED I WAS IN TROUBLE AT THE LAST PART OF MY SPEECH DEALING THE AGE OF THE EARTH, WHERE MY VIEWS CONFLICTED WITH HIS. TO MY RELIEF KELVIN FELL FAST ASLEEP, BUT AS I CAME TO THE IMPORTANT POINT, I SAW THE OLD BIRD SIT UP AND COCK A BALEFUL GLANCE AT ME! THEN A SUDDEN INSPIRATION CAME AND I SAID LORD KELVIN HAD LIMITED THE AGE OF THE EARTH PROVIDED NO NEW SOURCE WAS DISCOVERED. THAT PROPHETIC UTTERANCE REFERS TO WHAT WE ARE NOW CONSIDERING TONIGHT, RADIUM! BEHOLD! THE OLD BOY BEAMED UPON ME.

Job cpu time: 0 days 0 hours 0 minutes 4.5 seconds.
File lengths (MBytes): RWF= 11 Int= 0 D2E= 0 Chk= 8 Scr= 1
Normal termination of Gaussian 98.