Example of the NMR calculation output of H_2 in Gaussian.

```
 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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 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 ,
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 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 nmr
----------------------------
;1/1=1/38
;5/2=6,18=2/17
;1/1,2,8,3=1,30=1,25=3/11
;1/1=4/7
;4/2=2,38=2,32=5/5
;11/1=1,11=8/6
;100/2=10/13
;1/1=2,28=2,10=2,9=2,8=6/7
;1/99=1,9=99/5
--
 H2
--
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 H
 H    1                    R
      Variables:
  R                     0.7122
-------------------------------------------------------------------------
                         Z-MATRIX (ANGSTROMS AND DEGREES(
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
-------------------------------------------------------------------------
  1   1   H
  2   2   H     1   0.712200(  1(
-------------------------------------------------------------------------
                         Z-Matrix orientation                          :
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms(
 Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
0.000000    0.000000    0.000000        0           1           1
0.712200    0.000000    0.000000        0           1           2
```

This properties keyword predicts NMR shielding tensors

```
 ---------------------------------------------------------------------
 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     Atomic     Atomic              Coordinates (Angstroms(
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
0.356100    0.000000    0.000000        0              1           1
0.356100-   0.000000    0.000000        0              1           2
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.0000000   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     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         0.7430177605 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 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
 NBasis=     2 NAE 1     =NBE=     1 NFC=     0 NFV=     0
 NROrb=      2 NOA=     1 NOB=     1 NVA=     1 NVB=     1
          Differentiating once with respect to magnetic field using GIAOs.
          Store integrals in memory, NReq=      820092.
          There are   3 degrees of freedom in the 1st order CPHF.
 0   vectors were produced by pass  0.
 Calculating GIAO nuclear magnetic shielding tensors.
 GIAO Magnetic shielding tensor (ppm:(
  1  H    Isotropic =    28.1938   Anisotropy =     0.6326
   XX=    27.9830   YX=    0.0000     =ZX=     0.0000
   XY=     0.0000   YY=   27.9830   ZY=     0.0000
   XZ=     0.0000   YZ=    0.0000   ZZ=    28.6156
   Eigenvalues:    27.9830    27.9830    28.6156
  2  H    Isotropic =    28.1938   Anisotropy =     0.6326
```

Convergence of the SCF calculations.

Compute NMR properties using the Gauge-Independent Atomic Orbital (GIAO) method only. This is the default.

NMR results.

The two atoms magnetic shielding, these are two identical atoms, so the isotropic shielding is the same.

```
  XX=    27.9830   YX=     0.0000   ZX=     0.0000
  XY=     0.0000   YY=    27.9830   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=    28.6156
   Eigenvalues:    27.9830    27.9830    28.6156

*******************************************************************

           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:(
2          1
  1  H    0.595917   0.404083
  2  H    0.404083   0.595917
 Total atomic charges:
1
  1  H    0.000000
  2  H0.000000
 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=    -1.4475
   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=    -1.5239 YYYY=    -1.5239 ZZZZ=    -2.3361 XXXY=     0.0000
 XXXZ=     0.0000 YYYX=     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= 7.430177604605D-01 E-N=-3.749005665863D+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
\1\1 GINC-ATTO\SP\RHF\STO-3G\H2\ARIK\17-Feb-2004\0\\#N RHF/STO-3G SCF=T
 IGHT NMR\\H2\\0,1\H\H,1,0.7122\\Version=DEC-AXP-OSF/1-G98RevA.4\State=
-1 SGG\HF\1.1175059-=RMSD=0.000e+00\Dipole=0.,0.,0.\PG=D*H [C*(H1.H1\[(
@\
```

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.