Example of the Population analysis Single Point Hartree-Fock SCF Calculation output of the Nitrogen Molecule.

```
Entering Gaussian System, Link 0=g98
Initial command:
/ua1/usr/local/g98/l1.exe /ua1/arik/lab/Gau-25108.inp -scrdir=/ua1/arik/lab/
Entering Link 1 = /ua1/usr/local/g98/l1.exe PID=     25105.
```

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,
Gaussian, Inc., Pittsburgh PA, 1998.

START HERE

The route section of a Gaussian job is initiated by a pound sign (#). #p=Additional output, to the defult print level, is generated.

POP:This properties keyword controls printing of molecular orbitals and several types of population analysis and atomic charge assignments. Regular=The five highest occupied and five lowest virtual orbitals are printed, along with the density matrices and a full ,Mulliken population analysis.

```
 ******************************************
 Gaussian 98:  DEC-AXP-OSF/1-G98RevA.4 11-Sep-1998
                      6-Mar-2003
 ******************************************
 ----------------------------------
 #p RHF/6-31G(D) SCF=Tight pop=regular
 ----------------------------------
 1/38=1/1;
 2/17=6,18=5/2;
 3/5=1,6=6,7=1,11=1,25=1,30=1/1,2,3;
 4/7=1/1;
 5/5=2,32=2,38=4/2;
 6/28=1/1;
 99/5=1,9=1/99;
 Leave Link    1 at Thu Mar  6 17:04:44 2003, MaxMem=           0 cpu:        0.2
 (Enter /ua1/usr/local/g98/l101.exe)
 --
 N2
 --
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 N                     0.         0.         0.
 N                     1.0784     0.         0.
 Leave Link  101 at Thu Mar  6 17:04:45 2003, MaxMem=     6291456 cpu:        0.2
 (Enter /ua1/usr/local/g98/l202.exe)
```

This method keyword requests a Restricted Hartree-Fock calculation.

This keyword controls the functioning of the SCF procedure. Defult single point direct SCF calculations are run with modest convergence criteria automatically in the interest of speed. Tight keyword request tight SCF convergence criteria, calculations involving basis sets which include diffuse functions should always use the SCF=Tight.

This keyword specifies the basis set used in this process, in this case it is the same as using the 6-31G* basis set.

INPUT

```
                         Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 --------------------------------------------------------------------------------
   1    1  N     0    0.000000          0.000000          0.000000
   2    2  N     0    1.078400          0.000000          0.000000
 --------------------------------------------------------------------------------
                         Z-Matrix orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          7           0        0.000000    0.000000    0.000000
    2          7           0        1.078400    0.000000    0.000000
 ---------------------------------------------------------------------
```

Cartesian coordinates of atoms in the molecule

```
Stoichiometry    N2
Framework group  D*H[C*(N.N)]
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
---------------------------------------------------------------------
   1          7             0        0.000000    0.000000    0.539200
   2          7             0        0.000000    0.000000   -0.539200
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000     62.0674791     62.0674791
Isotopes: N-14,N-14
Leave Link  202 at Thu Mar  6 17:04:45 2003, MaxMem=    6291456 cpu:       0.1
(Enter /ua1/usr/local/g98/l301.exe)
Standard basis: 6-31G(d) (6D, 7F)
There are     8 symmetry adapted basis functions of AG  symmetry.
There are     1 symmetry adapted basis functions of B1G symmetry.
There are     3 symmetry adapted basis functions of B2G symmetry.
There are     3 symmetry adapted basis functions of B3G symmetry.
There are     1 symmetry adapted basis functions of AU  symmetry.
There are     8 symmetry adapted basis functions of B1U symmetry.
There are     3 symmetry adapted basis functions of B2U symmetry.
There are     3 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.
   30 basis functions       56 primitive gaussians
    7 alpha electrons        7 beta electrons
      nuclear repulsion energy        24.0445893926 Hartrees.
Leave Link  301 at Thu Mar  6 17:04:45 2003, MaxMem=    6291456 cpu:       0.2
(Enter /ua1/usr/local/g98/l302.exe)
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
NBasis=    30 RedAO= T  NBF=     8     1     3     3     1     8     3     3
NBsUse=    30 1.00D-04 NBFU=     8     1     3     3     1     8     3     3
Leave Link  302 at Thu Mar  6 17:04:46 2003, MaxMem=    6291456 cpu:       0.5
```

N2 group symetry.

set the origin to be the molecular center and the interatomic axis to be the z axis.

Basis set information

30 basis function contracted from 56 primitive gaussians. 14 occupied electrons of N2 are devided to 7 alpha and 7 beta spin functions.

```
(Enter /ua1/usr/local/g98/l303.exe)
DipDrv:  MaxL=1.
Leave Link  303 at Thu Mar  6 17:04:46 2003, MaxMem=    6291456 cpu:       0.3
(Enter /ua1/usr/local/g98/l401.exe)
Projected INDO Guess.
Initial guess orbital symmetries:
      Occupied  (SGG) (SGU) (SGG) (SGU) (PIU) (PIU) (SGG)
      Virtual   (PIG) (PIG) (SGU) (SGG) (SGG) (SGG) (?A) (?A)
                (?A) (PIG) (PIG) (PIG) (PIG) (DLTU) (SGU) (SGU)
                (SGU) (SGU) (DLTU) (PIU) (PIU) (PIU) (PIU)
Leave Link  401 at Thu Mar  6 17:04:47 2003, MaxMem=    6291456 cpu:       0.4
(Enter /ua1/usr/local/g98/l502.exe)
IExCor=   0 DFT=F Ex=HF Corr=None ScaHFX= 1.0000
ScaDFX=  0.0000  0.0000  0.0000  0.0000
IRadAn=      0 IRanWt=     -1 IRanGd=            0 ICorTp=0
Using DIIS extrapolation.
Closed shell SCF:
Requested convergence on RMS density matrix=1.00D-08 within  64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Integral symmetry usage will be decided dynamically.
Keep R1 integrals in memory in canonical form, NReq=      936192.
IEnd=      7833 IEndB=      7833 NGot=   6291456 MDV=   6180419
LenX=   6180419
Symmetry not used in FoFDir.
MinBra= 0 MaxBra= 2 Meth= 1.
IRaf=       0 NMat=   1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.
```

begining of the iterative SCF process.

```
Cycle   1  Pass 1  IDiag 1:
E=-0.132701884733295D+03
DIIS: error= 2.74D-01 at cycle   1.
T=  950. NK=0  NO(<0.9)=   0  NV(>0.1)=   0   7.00e < EF 0.00e >EF  Err=0.0D+00
RMSDP=1.68D-02 MaxDP=9.82D-02

Cycle   2  Pass 1  IDiag 1:
E=-0.132980009095215D+03 Delta-E=       -0.278124361921
DIIS: error= 2.82D-02 at cycle   2.
T=  883. NK=0  NO(<0.9)=   0  NV(>0.1)=   0   7.00e < EF 0.00e >EF  Err=0.0D+00
RMSDP=4.79D-03 MaxDP=5.57D-02

Cycle   3  Pass 1  IDiag 1:
E=-0.132988056734500D+03 Delta-E=       -0.008047639285
```

```
DIIS: error= 6.50D-03 at cycle   3.
Coeff: 0.246D+00-0.125D+01
T=  766. NK=0  NO(<0.9)=   0  NV(>0.1)=   0   7.00e < EF 0.00e >EF  Err=0.0D+00
RMSDP=1.53D-03 MaxDP=1.78D-02

Cycle   4  Pass 1  IDiag 1:
E=-0.132988534737858D+03 Delta-E=       -0.000478003358
DIIS: error= 5.20D-04 at cycle   4.
Coeff:-0.957D-02 0.883D-01-0.108D+01
RMSDP=1.06D-04 MaxDP=1.02D-03

Cycle   5  Pass 1  IDiag 1:
E=-0.132988538705782D+03 Delta-E=       -0.000003967924
DIIS: error= 1.22D-04 at cycle   5.
Coeff:-0.601D-02 0.342D-01-0.970D-02-0.102D+01
RMSDP=1.46D-05 MaxDP=1.31D-04

Cycle   6  Pass 1  IDiag 1:
E=-0.132988538856445D+03 Delta-E=       -0.000000150663
DIIS: error= 1.25D-05 at cycle   6.
Coeff: 0.382D-03-0.361D-02 0.311D-01 0.488D-01-0.108D+01
RMSDP=4.81D-06 MaxDP=5.48D-05

Cycle   7  Pass 1  IDiag 1:
E=-0.132988538860877D+03 Delta-E=       -0.000000004432
DIIS: error= 2.14D-06 at cycle   7.
Coeff: 0.995D-04-0.376D-03-0.436D-02 0.248D-01 0.851D-01-0.111D+01
RMSDP=1.08D-06 MaxDP=1.27D-05

Cycle   8  Pass 1  IDiag 1:
E=-0.132988538860977D+03 Delta-E=       -0.000000000099
DIIS: error= 3.06D-07 at cycle   8.
Coeff:-0.227D-04 0.111D-03 0.475D-03-0.483D-02-0.848D-02 0.266D+00
Coeff:-0.125D+01
RMSDP=1.11D-07 MaxDP=1.18D-06

Cycle   9  Pass 1  IDiag 1:
E=-0.132988538860979D+03 Delta-E=       -0.000000000002
DIIS: error= 1.02D-08 at cycle   9.
Coeff: 0.182D-05-0.925D-05-0.289D-04 0.379D-03 0.556D-03-0.237D-01
Coeff: 0.146D+00-0.112D+01
```

```
 RMSDP=3.08D-09 MaxDP=3.74D-08
```

Convergence now achieved

computed ground state energy

```
 SCF Done:  E(RHF) =  -108.943949468     A.U. after    9 cycles
            Convg  =    0.3082D-08             -V/T =  2.0034
            S**2   =    0.0000
 KE= 1.085745380364D+02 PE=-3.035367944144D+02 EE= 6.197371751696D+01
 Leave Link  502 at Thu Mar  6 17:04:47 2003, MaxMem=    6291456 cpu:       0.3
 (Enter /ua1/usr/local/g98/l601.exe)
 Copying SCF densities to generalized density rwf, ISCF=0 IROHF=0.

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

        Population analysis using the SCF density.

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

 Orbital Symmetries:
      Occupied  (SGG) (SGU) (SGG) (SGU) (SGG) (PIU) (PIU)
      Virtual   (PIG) (PIG) (SGU) (SGG) (PIU) (PIU) (SGG) (PIG)
                (PIG) (SGU) (SGU) (DLTG) (DLTG) (PIU) (PIU) (DLTU)
                (DLTU) (SGG) (PIG) (PIG) (SGU) (SGG) (SGU)
  The electronic state is 1-SGG.
 Alpha  occ. eigenvalues --  -15.69065 -15.68682  -1.48817  -0.76996  -0.63159
 Alpha  occ. eigenvalues --   -0.62011  -0.62011
 Alpha virt. eigenvalues --    0.18075   0.18075   0.59134   0.76911   0.83104
 Alpha virt. eigenvalues --    0.83104   0.83858   1.01938   1.01938   1.09369
 Alpha virt. eigenvalues --    1.51666   1.71185   1.71185   1.87357   1.87357
 Alpha virt. eigenvalues --    2.27244   2.27244   2.74818   2.96488   2.96488
 Alpha virt. eigenvalues --    3.28013   3.68355   4.00876
      Molecular Orbital Coefficients
                            3         4         5         6         7
                         (SGG)--O  (SGU)--O  (SGG)--O  (PIU)--O  (PIU)--O
      EIGENVALUES --    -1.48817  -0.76996  -0.63159  -0.62011  -0.62011
    1  1   N  1S         -0.16104  -0.14579  -0.05459   0.00000   0.00000
    2        2S          0.33667   0.32941   0.10699   0.00000   0.00000
    3        2PX         0.00000   0.00000   0.00000   0.43500   0.00000
    4        2PY         0.00000   0.00000   0.00000   0.00000   0.43500
    5        2PZ        -0.22458   0.22494   0.45811   0.00000   0.00000
    6        3S          0.18075   0.49011   0.33525   0.00000   0.00000
    7        3PX         0.00000   0.00000   0.00000   0.24460   0.00000
    8        3PY         0.00000   0.00000   0.00000   0.00000   0.24460
```

converged! - difference between energies in the two last successive iterations

sigma-g, sigma-u, pi-g, pi-u

occupied

symmetry of the ground molecular state

Eigenvalues of the single electron states

virtual orbital

3-orbital no. SGG=Sigma-g symetry. O = occupied orbital.

Nitrogen atom no. 1

From here on: Expansion coefficients of the molecular orbitals (5 upper occupied and 5 lower unoccupied is the default) in the atomic orbitals (each atomic orbital is a contraction of several Gaussians defined by the chosen basis)

This column (continued below) shows expansion coefficients of molecular "orbital 3" (occupied) in terms of the atomic orbitals shown on the left.

9			3PZ	-0.03337	0.08178	0.20031	0.00000	0.00000
10			4XX	-0.01197	0.00171	0.00709	0.00000	0.00000
11			4YY	-0.01197	0.00171	0.00709	0.00000	0.00000
12			4ZZ	0.03096	-0.01726	-0.02990	0.00000	0.00000
13			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
14			4XZ	0.00000	0.00000	0.00000	-0.04819	0.00000
15			4YZ	0.00000	0.00000	0.00000	0.00000	-0.04819
16	2	N	1S	-0.16104	0.14579	-0.05459	0.00000	0.00000
17			2S	0.33667	-0.32941	0.10699	0.00000	0.00000
18			2PX	0.00000	0.00000	0.00000	0.43500	0.00000
19			2PY	0.00000	0.00000	0.00000	0.00000	0.43500
20			2PZ	0.22458	0.22494	-0.45811	0.00000	0.00000
21			3S	0.18075	-0.49011	0.33525	0.00000	0.00000
22			3PX	0.00000	0.00000	0.00000	0.24460	0.00000
23			3PY	0.00000	0.00000	0.00000	0.00000	0.24460
24			3PZ	0.03337	0.08178	-0.20031	0.00000	0.00000
25			4XX	-0.01197	-0.00171	0.00709	0.00000	0.00000
26			4YY	-0.01197	-0.00171	0.00709	0.00000	0.00000
27			4ZZ	0.03096	0.01726	-0.02990	0.00000	0.00000
28			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29			4XZ	0.00000	0.00000	0.00000	0.04819	0.00000
30			4YZ	0.00000	0.00000	0.00000	0.00000	0.04819
				8	9	10	11	12
				(PIG)--V	(PIG)--V	(SGU)--V	(SGG)--V	(PIU)--V
EIGENVALUES --				0.18075	0.18075	0.59134	0.76911	0.83104
1	1	N	1S	0.00000	0.00000	-0.09051	0.02964	0.00000
2			2S	0.00000	0.00000	0.20474	0.51782	0.00000
3			2PX	0.00000	0.43109	0.00000	0.00000	0.62738
4			2PY	0.43109	0.00000	0.00000	0.00000	0.00000
5			2PZ	0.00000	0.00000	-0.04357	-0.32182	0.00000
6			3S	0.00000	0.00000	4.42045	-0.40357	0.00000
7			3PX	0.00000	0.69787	0.00000	0.00000	-0.61909
8			3PY	0.69787	0.00000	0.00000	0.00000	0.00000
9			3PZ	0.00000	0.00000	-2.84978	0.87816	0.00000
10			4XX	0.00000	0.00000	-0.00429	0.07138	0.00000
11			4YY	0.00000	0.00000	-0.00429	0.07138	0.00000
12			4ZZ	0.00000	0.00000	0.08752	0.16309	0.00000
13			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
14			4XZ	0.00000	0.01331	0.00000	0.00000	-0.10130
15			4YZ	0.01331	0.00000	0.00000	0.00000	0.00000
16	2	N	1S	0.00000	0.00000	0.09051	0.02964	0.00000

Atomic orbitals or basis set contracted function. here the 2s and 2px orbitals of the second Nitrogen atom.

altogether 30 basis functions in this calculation.

from here - unoccupied (virtual) molecular orbitals

17		2S	0.00000	0.00000	-0.20474	0.51782	0.00000
18		2PX	0.00000	-0.43109	0.00000	0.00000	0.62738
19		2PY	-0.43109	0.00000	0.00000	0.00000	0.00000
20		2PZ	0.00000	0.00000	-0.04357	0.32182	0.00000
21		3S	0.00000	0.00000	-4.42045	-0.40357	0.00000
22		3PX	0.00000	-0.69787	0.00000	0.00000	-0.61909
23		3PY	-0.69787	0.00000	0.00000	0.00000	0.00000
24		3PZ	0.00000	0.00000	-2.84978	-0.87816	0.00000
25		4XX	0.00000	0.00000	0.00429	0.07138	0.00000
26		4YY	0.00000	0.00000	0.00429	0.07138	0.00000
27		4ZZ	0.00000	0.00000	-0.08752	0.16309	0.00000
28		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29		4XZ	0.00000	0.01331	0.00000	0.00000	0.10130
30		4YZ	0.01331	0.00000	0.00000	0.00000	0.00000

DENSITY MATRIX.

				1	2	3	4	5
1	1	N	1S	2.08088				
2			2S	-0.16779	0.46780			
3			2PX	0.00000	0.00000	0.37846		
4			2PY	0.00000	0.00000	0.00000	0.37846	
5			2PZ	-0.04880	0.09487	0.00000	0.00000	0.62181
6			3S	-0.23871	0.51631	0.00000	0.00000	0.44647
7			3PX	0.00000	0.00000	0.21280	0.00000	0.00000
8			3PY	0.00000	0.00000	0.00000	0.21280	0.00000
9			3PZ	-0.03384	0.07430	0.00000	0.00000	0.23530
10			4XX	-0.00496	-0.00560	0.00000	0.00000	0.01266
11			4YY	-0.00496	-0.00560	0.00000	0.00000	0.01266
12			4ZZ	-0.00546	0.00299	0.00000	0.00000	-0.04905
13			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
14			4XZ	0.00000	0.00000	-0.04193	0.00000	0.00000
15			4YZ	0.00000	0.00000	0.00000	-0.04193	0.00000
16	2	N	1S	0.01342	-0.02474	0.00000	0.00000	0.08926
17			2S	-0.02474	0.03253	0.00000	0.00000	-0.20135
18			2PX	0.00000	0.00000	0.37846	0.00000	0.00000
19			2PY	0.00000	0.00000	0.00000	0.37846	0.00000
20			2PZ	-0.08926	0.20135	0.00000	0.00000	-0.41940
21			3S	0.04998	-0.12940	0.00000	0.00000	0.00548
22			3PX	0.00000	0.00000	0.21280	0.00000	0.00000
23			3PY	0.00000	0.00000	0.00000	0.21280	0.00000
24			3PZ	-0.01281	0.03348	0.00000	0.00000	-0.16172
25			4XX	0.00344	-0.00767	0.00000	0.00000	0.01110

Note that number 3 refer to atomic orbital 3 (2Px orbital on Nitrogen atom number 1) in both places

Here we see large mixing between the 2pz orbital of N no.2 and the 2s orbital of N no.1 (0.2) and the 2pz of N no.1 (-0.42). These matrix elements coresponds to a singele chemical bond.

26			4YY	0.00344	-0.00767	0.00000	0.00000	0.01110
27			4ZZ	-0.01369	0.02577	0.00000	0.00000	-0.03353
28			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29			4XZ	0.00000	0.00000	0.04193	0.00000	0.00000
30			4YZ	0.00000	0.00000	0.00000	0.04193	0.00000
				6	7	8	9	10
6			3S	0.77054				
7			3PX	0.00000	0.11966			
8			3PY	0.00000	0.00000	0.11966		
9			3PZ	0.20240	0.00000	0.00000	0.09585	
10			4XX	0.00211	0.00000	0.00000	0.00391	0.00042
11			4YY	0.00211	0.00000	0.00000	0.00391	0.00042
12			4ZZ	-0.02577	0.00000	0.00000	-0.01687	-0.00121
13			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
14			4XZ	0.00000	-0.02358	0.00000	0.00000	0.00000
15			4YZ	0.00000	0.00000	-0.02358	0.00000	0.00000
16	2	N	1S	0.04998	0.00000	0.00000	0.01281	0.00344
17			2S	-0.12940	0.00000	0.00000	-0.03348	-0.00767
18			2PX	0.00000	0.21280	0.00000	0.00000	0.00000
19			2PY	0.00000	0.00000	0.21280	0.00000	0.00000
20			2PZ	-0.00548	0.00000	0.00000	-0.16172	-0.01110
21			3S	-0.19029	0.00000	0.00000	0.04208	-0.00126
22			3PX	0.00000	0.11966	0.00000	0.00000	0.00000
23			3PY	0.00000	0.00000	0.11966	0.00000	0.00000
24			3PZ	-0.04208	0.00000	0.00000	-0.06910	-0.00336
25			4XX	-0.00126	0.00000	0.00000	0.00336	0.00038
26			4YY	-0.00126	0.00000	0.00000	0.00336	0.00038
27			4ZZ	0.00806	0.00000	0.00000	-0.01122	-0.00110
28			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29			4XZ	0.00000	0.02358	0.00000	0.00000	0.00000
30			4YZ	0.00000	0.00000	0.02358	0.00000	0.00000
				11	12	13	14	15
11			4YY	0.00042				
12			4ZZ	-0.00121	0.00431			
13			4XY	0.00000	0.00000	0.00000		
14			4XZ	0.00000	0.00000	0.00000	0.00465	
15			4YZ	0.00000	0.00000	0.00000	0.00000	0.00465
16	2	N	1S	0.00344	-0.01369	0.00000	0.00000	0.00000
17			2S	-0.00767	0.02577	0.00000	0.00000	0.00000
18			2PX	0.00000	0.00000	0.00000	-0.04193	0.00000
19			2PY	0.00000	0.00000	0.00000	0.00000	-0.04193

20		2PZ	-0.01110	0.03353	0.00000	0.00000	0.00000
21		3S	-0.00126	0.00806	0.00000	0.00000	0.00000
22		3PX	0.00000	0.00000	0.00000	-0.02358	0.00000
23		3PY	0.00000	0.00000	0.00000	0.00000	-0.02358
24		3PZ	-0.00336	0.01122	0.00000	0.00000	0.00000
25		4XX	0.00038	-0.00110	0.00000	0.00000	0.00000
26		4YY	0.00038	-0.00110	0.00000	0.00000	0.00000
27		4ZZ	-0.00110	0.00312	0.00000	0.00000	0.00000
28		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29		4XZ	0.00000	0.00000	0.00000	-0.00465	0.00000
30		4YZ	0.00000	0.00000	0.00000	0.00000	-0.00465
			16	17	18	19	20
16	2 N	1S	2.08088				
17		2S	-0.16779	0.46780			
18		2PX	0.00000	0.00000	0.37846		
19		2PY	0.00000	0.00000	0.00000	0.37846	
20		2PZ	0.04880	-0.09487	0.00000	0.00000	0.62181
21		3S	-0.23871	0.51631	0.00000	0.00000	-0.44647
22		3PX	0.00000	0.00000	0.21280	0.00000	0.00000
23		3PY	0.00000	0.00000	0.00000	0.21280	0.00000
24		3PZ	0.03384	-0.07430	0.00000	0.00000	0.23530
25		4XX	-0.00496	-0.00560	0.00000	0.00000	-0.01266
26		4YY	-0.00496	-0.00560	0.00000	0.00000	-0.01266
27		4ZZ	-0.00546	0.00299	0.00000	0.00000	0.04905
28		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29		4XZ	0.00000	0.00000	0.04193	0.00000	0.00000
30		4YZ	0.00000	0.00000	0.00000	0.04193	0.00000
			21	22	23	24	25
21		3S	0.77054				
22		3PX	0.00000	0.11966			
23		3PY	0.00000	0.00000	0.11966		
24		3PZ	-0.20240	0.00000	0.00000	0.09585	
25		4XX	0.00211	0.00000	0.00000	-0.00391	0.00042
26		4YY	0.00211	0.00000	0.00000	-0.00391	0.00042
27		4ZZ	-0.02577	0.00000	0.00000	0.01687	-0.00121
28		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29		4XZ	0.00000	0.02358	0.00000	0.00000	0.00000
30		4YZ	0.00000	0.00000	0.02358	0.00000	0.00000
			26	27	28	29	30
26		4YY	0.00042				
27		4ZZ	-0.00121	0.00431			

28		4XY	0.00000	0.00000	0.00000		
29		4XZ	0.00000	0.00000	0.00000	0.00465	
30		4YZ	0.00000	0.00000	0.00000	0.00000	0.00465

Full Mulliken population analysis:

				1	2	3	4	5
1	1	N	1S	2.08088				
2			2S	-0.03729	0.46780			
3			2PX	0.00000	0.00000	0.37846		
4			2PY	0.00000	0.00000	0.00000	0.37846	
5			2PZ	0.00000	0.00000	0.00000	0.00000	0.62181
6			3S	-0.04103	0.40040	0.00000	0.00000	0.00000
7			3PX	0.00000	0.00000	0.11051	0.00000	0.00000
8			3PY	0.00000	0.00000	0.00000	0.11051	0.00000
9			3PZ	0.00000	0.00000	0.00000	0.00000	0.12219
10			4XX	-0.00025	-0.00356	0.00000	0.00000	0.00000
11			4YY	-0.00025	-0.00356	0.00000	0.00000	0.00000
12			4ZZ	-0.00028	0.00190	0.00000	0.00000	0.00000
13			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
14			4XZ	0.00000	0.00000	0.00000	0.00000	0.00000
15			4YZ	0.00000	0.00000	0.00000	0.00000	0.00000
16	2	N	1S	0.00000	-0.00065	0.00000	0.00000	-0.00488
17			2S	-0.00065	0.00767	0.00000	0.00000	0.06326
18			2PX	0.00000	0.00000	0.05164	0.00000	0.00000
19			2PY	0.00000	0.00000	0.00000	0.05164	0.00000
20			2PZ	-0.00488	0.06326	0.00000	0.00000	0.14712
21			3S	0.00366	-0.05094	0.00000	0.00000	-0.00132
22			3PX	0.00000	0.00000	0.05455	0.00000	0.00000
23			3PY	0.00000	0.00000	0.00000	0.05455	0.00000
24			3PZ	-0.00171	0.01907	0.00000	0.00000	0.01701
25			4XX	0.00001	-0.00099	0.00000	0.00000	-0.00181
26			4YY	0.00001	-0.00099	0.00000	0.00000	-0.00181
27			4ZZ	-0.00180	0.01253	0.00000	0.00000	0.01468
28			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29			4XZ	0.00000	0.00000	0.01284	0.00000	0.00000
30			4YZ	0.00000	0.00000	0.00000	0.01284	0.00000

				6	7	8	9	10
6			3S	0.77054				
7			3PX	0.00000	0.11966			
8			3PY	0.00000	0.00000	0.11966		
9			3PZ	0.00000	0.00000	0.00000	0.09585	
10			4XX	0.00141	0.00000	0.00000	0.00000	0.00042

11		4YY	0.00141	0.00000	0.00000	0.00000	0.00014
12		4ZZ	-0.01727	0.00000	0.00000	0.00000	-0.00040
13		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
14		4XZ	0.00000	0.00000	0.00000	0.00000	0.00000
15		4YZ	0.00000	0.00000	0.00000	0.00000	0.00000
16	2 N	1S	0.00366	0.00000	0.00000	-0.00171	0.00001
17		2S	-0.05094	0.00000	0.00000	0.01907	-0.00099
18		2PX	0.00000	0.05455	0.00000	0.00000	0.00000
19		2PY	0.00000	0.00000	0.05455	0.00000	0.00000
20		2PZ	-0.00132	0.00000	0.00000	0.01701	-0.00181
21		3S	-0.12252	0.00000	0.00000	-0.02543	-0.00042
22		3PX	0.00000	0.07704	0.00000	0.00000	0.00000
23		3PY	0.00000	0.00000	0.07704	0.00000	0.00000
24		3PZ	-0.02543	0.00000	0.00000	-0.00531	-0.00166
25		4XX	-0.00042	0.00000	0.00000	-0.00166	0.00007
26		4YY	-0.00042	0.00000	0.00000	-0.00166	0.00002
27		4ZZ	0.00369	0.00000	0.00000	0.00467	-0.00030
28		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29		4XZ	0.00000	0.00537	0.00000	0.00000	0.00000
30		4YZ	0.00000	0.00000	0.00537	0.00000	0.00000

			11	12	13	14	15
11		4YY	0.00042				
12		4ZZ	-0.00040	0.00431			
13		4XY	0.00000	0.00000	0.00000		
14		4XZ	0.00000	0.00000	0.00000	0.00465	
15		4YZ	0.00000	0.00000	0.00000	0.00000	0.00465
16	2 N	1S	0.00001	-0.00180	0.00000	0.00000	0.00000
17		2S	-0.00099	0.01253	0.00000	0.00000	0.00000
18		2PX	0.00000	0.00000	0.00000	0.01284	0.00000
19		2PY	0.00000	0.00000	0.00000	0.00000	0.01284
20		2PZ	-0.00181	0.01468	0.00000	0.00000	0.00000
21		3S	-0.00042	0.00369	0.00000	0.00000	0.00000
22		3PX	0.00000	0.00000	0.00000	0.00537	0.00000
23		3PY	0.00000	0.00000	0.00000	0.00000	0.00537
24		3PZ	-0.00166	0.00467	0.00000	0.00000	0.00000
25		4XX	0.00002	-0.00030	0.00000	0.00000	0.00000
26		4YY	0.00007	-0.00030	0.00000	0.00000	0.00000
27		4ZZ	-0.00030	0.00146	0.00000	0.00000	0.00000
28		4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29		4XZ	0.00000	0.00000	0.00000	0.00205	0.00000
30		4YZ	0.00000	0.00000	0.00000	0.00000	0.00205

				16	17	18	19	20
16	2	N	1S	2.08088				
17			2S	-0.03729	0.46780			
18			2PX	0.00000	0.00000	0.37846		
19			2PY	0.00000	0.00000	0.00000	0.37846	
20			2PZ	0.00000	0.00000	0.00000	0.00000	0.62181
21			3S	-0.04103	0.40040	0.00000	0.00000	0.00000
22			3PX	0.00000	0.00000	0.11051	0.00000	0.00000
23			3PY	0.00000	0.00000	0.00000	0.11051	0.00000
24			3PZ	0.00000	0.00000	0.00000	0.00000	0.12219
25			4XX	-0.00025	-0.00356	0.00000	0.00000	0.00000
26			4YY	-0.00025	-0.00356	0.00000	0.00000	0.00000
27			4ZZ	-0.00028	0.00190	0.00000	0.00000	0.00000
28			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29			4XZ	0.00000	0.00000	0.00000	0.00000	0.00000
30			4YZ	0.00000	0.00000	0.00000	0.00000	0.00000

				21	22	23	24	25
21			3S	0.77054				
22			3PX	0.00000	0.11966			
23			3PY	0.00000	0.00000	0.11966		
24			3PZ	0.00000	0.00000	0.00000	0.09585	
25			4XX	0.00141	0.00000	0.00000	0.00000	0.00042
26			4YY	0.00141	0.00000	0.00000	0.00000	0.00014
27			4ZZ	-0.01727	0.00000	0.00000	0.00000	-0.00040
28			4XY	0.00000	0.00000	0.00000	0.00000	0.00000
29			4XZ	0.00000	0.00000	0.00000	0.00000	0.00000
30			4YZ	0.00000	0.00000	0.00000	0.00000	0.00000

				26	27	28	29	30
26			4YY	0.00042				
27			4ZZ	-0.00040	0.00431			
28			4XY	0.00000	0.00000	0.00000		
29			4XZ	0.00000	0.00000	0.00000	0.00465	
30			4YZ	0.00000	0.00000	0.00000	0.00000	0.00465

Gross orbital populations:

				1
1	1	N	1S	1.99644
2			2S	0.87466
3			2PX	0.60799
4			2PY	0.60799
5			2PZ	0.97626
6			3S	0.92178

```
  7        3PX          0.36712
  8        3PY          0.36712
  9        3PZ          0.22301
 10        4XX         -0.00731
 11        4YY         -0.00731
 12        4ZZ          0.02247
 13        4XY          0.00000
 14        4XZ          0.02490
 15        4YZ          0.02490
 16 2   N  1S           1.99644
 17        2S           0.87466
 18        2PX          0.60799
 19        2PY          0.60799
 20        2PZ          0.97626
 21        3S           0.92178
 22        3PX          0.36712
 23        3PY          0.36712
 24        3PZ          0.22301
 25        4XX         -0.00731
 26        4YY         -0.00731
 27        4ZZ          0.02247
 28        4XY          0.00000
 29        4XZ          0.02490
 30        4YZ          0.02490
         Condensed to atoms (all electrons):
              1          2
 1  N    6.335915   0.664085
 2  N    0.664085   6.335915
Total atomic charges:
              1
 1  N    0.000000
 2  N    0.000000
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
 1  N    0.000000
 2  N    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=     38.3530
Charge=     0.0000 electrons
Dipole moment (Debye):
```

information on charge distribution in the molecule

```
   X=     0.0000   Y=     0.0000   Z=     0.0000  Tot=     0.0000
Quadrupole moment (Debye-Ang):
  XX=   -10.1825   YY=   -10.1825   ZZ=   -11.6708
  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=    -8.2506 YYYY=    -8.2506 ZZZZ=   -30.0130 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.7502 XXZZ=    -5.9785 YYZZ=    -5.9785
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.404458939262D+01 E-N=-3.035367943962D+02  KE= 1.085745380364D+02
Symmetry AG   KE= 5.328351969243D+01
Symmetry B1G  KE= 1.454130887039D-34
Symmetry B2G  KE= 1.654370109182D-32
Symmetry B3G  KE= 1.463530463780D-32
Symmetry AU   KE= 7.683458813815D-34
Symmetry B1U  KE= 4.877353380758D+01
Symmetry B2U  KE= 3.258742268217D+00
Symmetry B3U  KE= 3.258742268217D+00
Leave Link  601 at Thu Mar  6 17:04:48 2003, MaxMem=    6291456 cpu:       0.4
(Enter /ua1/usr/local/g98/l9999.exe)
1\1\GINC-ATTO\SP\RHF\6-31G(d)\N2\ARIK\06-Mar-2003\0\\#P RHF/6-31G(D) S
CF=TIGHT POP=REGULAR\\N2\\0,1\N,0,0.,0.,0.\N,0,1.0784,0.,0.\\Version=D
EC-AXP-OSF/1-G98RevA.4\State=1-SGG\HF=-108.9439495\RMSD=3.082e-09\Dipo
le=0.,0.,0.\PG=D*H [C*(N1.N1)]\\@


HO!  SUCH BUGS AND GOBLINS IN MY LIFE!

                          -- HAMLET, ACT 5, SCENE 2
Job cpu time:  0 days  0 hours  0 minutes  3.6 seconds.
File lengths (MBytes):  RWF=   11 Int=    0 D2E=    0 Chk=    8 Scr=    1
Normal termination of Gaussian 98.
```

No permanent dipole on the nitrogen molecule