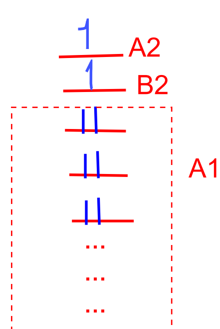
```
/home/qcsoftware/qchem070803/Linux64/exe/qcprog.exe .omx-uhf-ssq.in.12457.qcin.1
/scratch/krylov/qchem12457/
                  Welcome to Q-Chem
     A Quantum Leap Into The Future Of Chemistry

 Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld,
 S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko,S. V. Levchenko,
 D. P. O'Neill, R. A. DiStasio Jr., R. C. Lochan, T. Wang,
 G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin,
 T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele,
 V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson,
 B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen,
 A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani,
 S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora,
 R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang,
 I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek,
 Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill,
 A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III,
 W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman,
 F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III,
 J. Kong, A. I. Krylov, P. M. W. Gill, M. Head-Gordon,
 Q-Chem, Version 3.1, Q-Chem, Inc., Pittsburgh, PA (2007).

 Additional authors for Version 3.1:
 Z. Gan, Y. Zhao, N. E. Schultz, D. Truhlar, E. Epifanovsky and M. Oana.


 Intel X86 Linux Version

 Q-chem begins on Tue Aug 14 15:47:21 2007


theFileMan(): MAXOPENFILES=974 MAX_SUB_FILE_NUM=16
Maximum size of a physical file is 2.0 GB, maximum size of a tmp-file is 32.0 GB


--------------------------------------------------------------
User input:
--------------------------------------------------------------
$comment
Calculate <S^2> for the SF states. Do not use frozen core here, if
desired, use CC_RESTR_OCC instead.
$end

$molecule
-1 3
C    0.00000000   0.00000000   0.00000000
C   -0.05052600   0.00000000  -1.42736000
C   -1.25725500   0.00000000  -2.13235500
C   -2.46398400   0.00000000  -1.42736000
C   -2.51451000   0.00000000   0.00000000
C   -1.25725500   0.00000000   0.76755700
O   -1.25725500   0.00000000   2.03649900
C   -3.74642500   0.00000000   0.67053700
H   -3.77722100   0.00000000   1.75448300
H   -4.68434800   0.00000000   0.11772100
H   -3.40766600   0.00000000  -1.97606200
```

Use a high-spin (triplet) state as a reference

Reference state = $^3B_1$ (see page 6)



```
H   -1.25725500  0.00000000 -3.22174900
H    0.89315600  0.00000000 -1.97606200
C    1.23191500  0.00000000  0.67053700
H    1.26271100  0.00000000  1.75448300
H    2.16983800  0.00000000  0.11772100
$end

$rem
jobtype                 SP
CORRELATION             CCSD
BASIS                   6-31G*
CC_NLOWSPIN             [2,0,2,0]
CC_SPIN_FLIP            1
CC_EXSTATES_PROP        1
CC_EOM_TWOPART_PROP 1
CC_EOM_FULL_RESP        1
$end
```

In Q-Chem, C2v symmetry numbers translate as follows [A1, A2, B1, B2]. The numbers are the symmetries of the transitions and not the final states. Here 2 transitions of A1 symmetry and 2 transitions of B1 symmetry are requested, yielding two B1 states and two A1 states.

Perform Spin Flip (SF) calculation

Calculate one-electron properties for EOM states.

Calculate two-electron properties.

Calculate fully relaxed properties.

```
--------------------------------------------------------------
 Writing REM_CC_EA             0
 ----------------------------------------------------
       Standard Nuclear Orientation (Angstroms)
    I     Atom         X             Y            Z
 ----------------------------------------------------
    1      C       1.257255     0.000000     0.069970
    2      C       1.206729     0.000000    -1.357390
    3      C       0.000000     0.000000    -2.062385
    4      C      -1.206729     0.000000    -1.357390
    5      C      -1.257255     0.000000     0.069970
    6      C       0.000000     0.000000     0.837527
    7      O       0.000000     0.000000     2.106469
    8      C      -2.489170     0.000000     0.740507
    9      H      -2.519966     0.000000     1.824453
   10      H      -3.427093     0.000000     0.187691
   11      H      -2.150411     0.000000    -1.906092
   12      H       0.000000     0.000000    -3.151779
   13      H       2.150411     0.000000    -1.906092
   14      C       2.489170     0.000000     0.740507
   15      H       2.519966     0.000000     1.824453
   16      H       3.427093     0.000000     0.187691
 ----------------------------------------------------
 Molecular Point Group                 C2v   NOp =  4
 Largest Abelian Subgroup              C2v   NOp =  4
 Nuclear Repulsion Energy =   393.9616498128 hartrees
 There are         33 alpha and       31 beta electrons
 Requested basis set is 6-31G(d)
 There are 50 shells and 149 basis functions
Total memory of 2000MB is distributed as follows:
   QALLOC including MEM_STATIC uses 540MB
   MEM_STATIC is set to 241MB
   CCMAN JOB total tmp buffer size is  1060MB
   CC_TMPBUFFSIZE is set to 60MB
   CC_BLCK_TNSR_BUFFSIZE is set to 1000MB
Warning: actual memory use might exceed 2000MB

Total Memory Limit     540 MB
Mega-Array Size        236 MB
MEM_STATIC part        241 MB
```

```
 Standard Electronic Orientation quadrupole field applied
 Nucleus-field energy     =     -0.0000000705 hartrees
 A cutoff of  1.0D-14 yielded   1180 shell pairs
 There are  11139 function pairs
Evaluating contribution to one-electron hamiltonian from nuclear
 Smallest overlap matrix eigenvalue = 4.87E-04
 Multipole matrices computed through 2nd order
 Guess from superposition of atomic densities
 Warning:  Energy on first SCF cycle will be non-variational
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation
 SCF converges when DIIS error is below 1.0E-08
 ---------------------------------------
  Cycle       Energy         DIIS Error
 ---------------------------------------
    1    -384.7928514752      6.64E-02
    2    -381.6304149830      6.93E-03
    3    -381.7614109554      4.44E-03
    4    -381.8103132602      9.76E-04
    5    -381.8215355112      2.61E-04
    6    -381.8250925207      1.20E-04
    7    -381.8284617000      9.92E-05
    8    -381.8305249157      7.00E-05
    9    -381.8320600251      5.47E-05
   10    -381.8326697258      2.73E-05
   11    -381.8329397543      1.17E-05
   12    -381.8329636725      4.50E-06
   13    -381.8329682138      1.85E-06
   14    -381.8329684331      7.93E-07
   15    -381.8329685293      4.48E-07
   16    -381.8329685401      2.08E-07
   17    -381.8329685433      9.86E-08
   18    -381.8329685440      4.78E-08
   19    -381.8329685442      1.64E-08
   20    -381.8329685443      4.82E-09 Convergence criterion met
 ---------------------------------------
 <S^2> = 2.5063
 SCF time:  CPU 67.94 s  wall 68.27 s

******************************************************
*                    C C M A N                       *
*                                                    *
*                   Anna I. Krylov                   *
*                  C. David Sherrill                 *
*                  Steven R. Gwaltney                *
*                  Edward F. C. Byrd                 *
*                     June 2000                      *
*                                                    *
*                     AND                            *
*                                                    *
*                  Sergey V. Levchenko               *
*                  Lyudmila V. Slipchenko            *
*                  Tao Wang                          *
*                  Ana-Maria C. Cristian             *
*                                                    *
*                     November 2003                  *
******************************************************
```

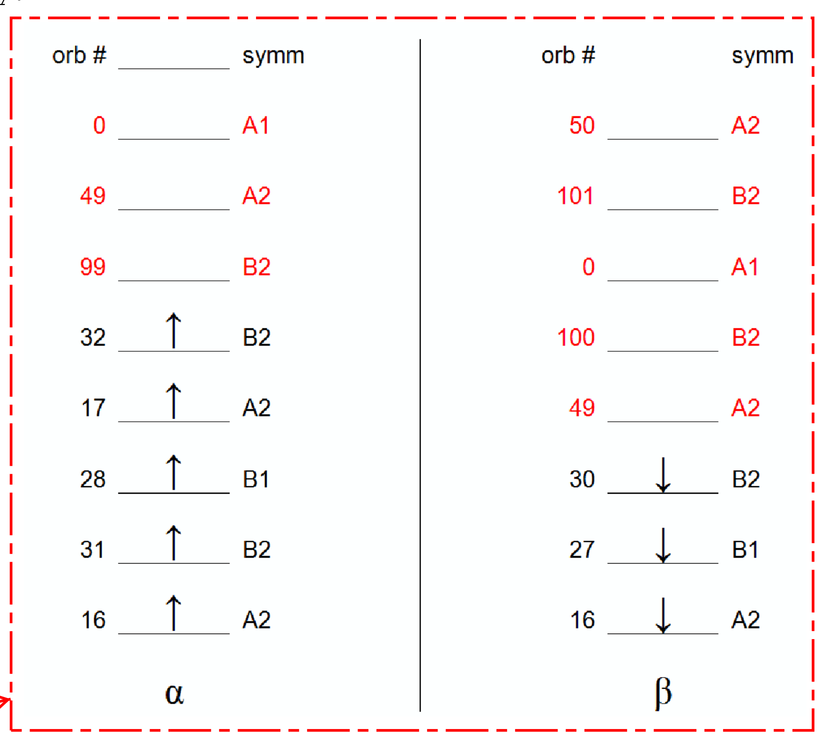
SCF energy and S^2 for the high-spin $^3B_1$ state.

```
USER PARAMETERS:
   PRINT                    1
   MAXITER                200    E CONVERG               8
   T CONVERG                8    Z CONVERG               8
   THETAGR CONV             6    THETA CONVERG           5
   THETA STEPSZ     1.0E+00    RESET THETA            15
   DIIS MODE                0    DIIS12 SWITCH           5
   DIIS SIZE                7    DIIS FREQ               1
   DIIS MIN OVLP           11    DIIS MAX OVLP     1.0E+00
   DIIS START               3
   SAVEAMLPL               no
   RESTART                 no    RESTART_NO_SCF         no
   REORTHOGONALIZE_MO      no
   PRECONV FROZEN           0    PRECONV TZ              0
   ITERATE OV               0    THETAGRAD TRESH         2
   PRECONV_TZ_EA            0
   HESS_THRESH      1.0E-02    DOV_THRESH        0.0E+00
   USE MP2-NO GUESS        no    OPDM FROM GRAD         no
   DO QCCD                 no    DO ED's CCD            no
   SCALE AMPL            1.00
   CALC_SSQ                no    ANALYZE_T2             no
   DO NUCLEAR GRAD         no
   CANONIZE               yes    CANONIZE_FREQ          50
   CANONIZE_FINAL         yes
   TMP_MAXBUFSZ            60    BLCK_TNSR_BUFFSZ     1000
   TOT_MEM (MB)          1060    NORBS_PER_BLOCK        16
   DO_DYNAMIC_CORR         no    DO_PARENTHESIS_T       no
   INCL_CORE_CORR         yes    INCL_VIRT_CORR        yes

PARAMETERS FOR EOM CALCULATIONS:
   NLOWSPIN             2 0 2 0 0 0 0 0 0 0 0 0
   NHIGHSPIN            0 0 0 0 0 0 0 0 0 0 0 0
   DO_DYSON                 0
   DO_CC_PROP               0    PLOT_CC_DENSITIES       0
   DO_EXS_PROP              1    DO_TRANS_PROP           0
   REF_SYM                  1    STATE_TO_OPT            0
   DO_SPIN_FLIP           yes
   DO PLAIN CIS            no    DO CIS(D)              no
   DO PLAIN CISD           no    DO PLAIN CISDT         no
   DO CC(2,3)              no    IF_RESTR_TRIPLES       no
   DO_SMALL_TRIPLES         0    IF_1ITER_FULL_TRIPLES    no
   PRECONV SD               0    SPIN_FLIP_MS            1
   DO_IP_FILTER            no
   DO DIP                  no
   DO_DISCNTD              no    IF_RESTR_AMPL          yes

PARAMETERS FOR DAVIDSON DIAGONALIZATION PROCEDURE:
   DMAXVECTORS             60    DMAXITER               30
   DCONVERGENCE             6    DTHRESHOLD        1.0E-06
   NGUESS_SINGLES           0    PRECONV_SINGLES        no
   NGUESS_DOUBLES           0    PRECONV_DOUBLES        no
   DO_APPR_DIAG           yes

Testing symmetry... Orbitals in the original order:
```

```
 Alpha MOs, Unrestricted
 -- Occupied --
-20.268 -11.078 -11.078 -11.070 -11.062 -11.057 -11.057 -11.038
  1 A1    2 A1    1 B1    3 A1    4 A1    5 A1    2 B1    3 B1
-11.038  -1.100  -0.959  -0.885  -0.836  -0.764  -0.722  -0.611
  6 A1    7 A1    8 A1    4 B1    9 A1    5 B1   10 A1   11 A1
 -0.590  -0.498  -0.482  -0.450  -0.413  -0.400  -0.377  -0.371
  6 B1   12 A1    7 B1   13 A1   14 A1    8 B1   15 A1    1 B2
 -0.364  -0.335  -0.310  -0.294  -0.271  -0.212  -0.173  -0.147
  9 B1   10 B1   16 A1    2 B2    1 A2    3 B2   11 B1    2 A2
 -0.037
  4 B2
 -- Virtual --
  0.351   0.373   0.382   0.418   0.425   0.472   0.473   0.483
  5 B2    3 A2   17 A1   12 B1   18 A1   13 B1   19 A1   20 A1
  0.491   0.565   0.593   0.614   0.659   0.664   0.686   0.734
 14 B1    6 B2   21 A1   15 B1   22 A1   16 B1   23 A1   24 A1
  0.740   0.873   0.888   0.891   0.897   0.912   0.948   0.954
 17 B1   25 A1    7 B2   18 B1   26 A1    4 A2   27 A1    8 B2
  0.954   0.993   0.995   1.006   1.016   1.042   1.044   1.050
 19 B1   28 A1   20 B1    5 A2   21 B1    9 B2   22 B1   29 A1
  1.094   1.157   1.182   1.218   1.246   1.248   1.262   1.280
 10 B2   30 A1    6 A2   31 A1   11 B2   23 B1   32 A1   33 A1
  1.292   1.299   1.348   1.359   1.368   1.388   1.401   1.413
 34 A1   24 B1   25 B1   35 A1   26 B1   36 A1   27 B1   37 A1
  1.470   1.473   1.545   1.545   1.584   1.646   1.675   1.688
 38 A1   28 B1   12 B2   39 A1   29 B1   40 A1    7 A2   30 B1
  1.704   1.781   1.781   1.805   1.866   1.882   1.898   1.901
 31 B1   41 A1   13 B2    8 A2   32 B1   42 A1   14 B2   33 B1
  1.914   1.926   2.107   2.108   2.178   2.224   2.227   2.318
 15 B2    9 A2   10 A2   16 B2   43 A1   44 A1   34 B1   11 A2
  2.321   2.345   2.361   2.396   2.407   2.435   2.439   2.480
 17 B2   45 A1   46 A1   35 B1   47 A1   36 B1   12 A2   48 A1
  2.523   2.557   2.607   2.639   2.685   2.689   2.777   2.788
 37 B1   49 A1   50 A1   18 B2   38 B1   51 A1   19 B2   13 A2
  2.788   2.826   2.866   2.884   2.889   2.951   3.029   3.130
 39 B1   52 A1   20 B2   40 B1   14 A2   53 A1   41 B1   15 A2
  3.131   3.154   3.201   3.280   3.344   3.425   3.427   3.438
 54 A1   42 B1   21 B2   55 A1   43 B1   56 A1   44 B1   57 A1
  3.616   3.802   3.918   4.614   4.683   4.691   4.735   4.754
 58 A1   45 B1   59 A1   60 A1   61 A1   46 B1   62 A1   47 B1
  4.930   5.033   5.123   5.430
 63 A1   48 B1   64 A1   65 A1

 Beta MOs, Unrestricted
 -- Occupied --
-20.257 -11.075 -11.062 -11.062 -11.061 -11.051 -11.051 -11.037
  1 A1    2 A1    1 B1    3 A1    4 A1    2 B1    5 A1    3 B1
-11.037  -1.075  -0.947  -0.867  -0.826  -0.703  -0.677  -0.597
  6 A1    7 A1    8 A1    4 B1    9 A1    5 B1   10 A1   11 A1
 -0.577  -0.493  -0.476  -0.442  -0.402  -0.392  -0.371  -0.357
  6 B1   12 A1    7 B1   13 A1   14 A1    8 B1   15 A1    9 B1
 -0.328  -0.326  -0.302  -0.235  -0.202  -0.165  -0.124
 10 B1    1 B2   16 A1    2 B2    1 A2   11 B1    3 B2
 -- Virtual --
  0.275   0.321   0.386   0.406   0.423   0.430   0.433   0.482
```

```
 2 A2     4 B2    17 A1     5 B2     3 A2    12 B1    18 A1    19 A1
 0.487    0.492    0.500    0.590    0.593    0.619    0.663    0.667
13 B1    20 A1    14 B1     6 B2    21 A1    15 B1    22 A1    16 B1
 0.695    0.740    0.742    0.880    0.893    0.901    0.927    0.958
23 A1    17 B1    24 A1    25 A1    18 B1    26 A1     7 B2    19 B1
 0.960    0.987    0.999    1.000    1.003    1.025    1.073    1.074
27 A1    28 A1     8 B2    20 B1     4 A2    21 B1    22 B1    29 A1
 1.083    1.088    1.105    1.156    1.168    1.226    1.244    1.263
 9 B2     5 A2    10 B2     6 A2    30 A1    31 A1    11 B2    23 B1
 1.270    1.284    1.300    1.310    1.359    1.365    1.383    1.388
32 A1    33 A1    34 A1    24 B1    25 B1    35 A1    26 B1    36 A1
 1.412    1.428    1.474    1.481    1.551    1.592    1.595    1.647
27 B1    37 A1    28 B1    38 A1    39 A1    12 B2    29 B1    40 A1
 1.685    1.696    1.708    1.784    1.809    1.829    1.867    1.885
 7 A2    30 B1    31 B1    41 A1    13 B2     8 A2    32 B1    42 A1
 1.899    1.904    1.930    1.951    2.180    2.181    2.189    2.223
14 B2    33 B1    15 B2     9 A2    10 A2    16 B2    43 A1    44 A1
 2.228    2.344    2.354    2.354    2.382    2.398    2.417    2.445
34 B1    11 A2    17 B2    45 A1    46 A1    35 B1    47 A1    36 B1
 2.470    2.483    2.543    2.578    2.609    2.648    2.704    2.714
12 A2    48 A1    37 B1    49 A1    50 A1    18 B2    51 A1    38 B1
 2.788    2.793    2.814    2.840    2.881    2.893    2.902    2.973
19 B2    13 A2    39 B1    52 A1    20 B2    40 B1    14 A2    53 A1
 3.034    3.134    3.137    3.159    3.221    3.283    3.345    3.426
41 B1    15 A2    54 A1    42 B1    21 B2    55 A1    43 B1    56 A1
 3.429    3.442    3.623    3.803    3.919    4.620    4.686    4.702
44 B1    57 A1    58 A1    45 B1    59 A1    60 A1    61 A1    46 B1
 4.757    4.774    4.927    5.033    5.129    5.434
62 A1    47 B1    63 A1    48 B1    64 A1    65 A1
Setting symmetry... Orbitals will be reordered.
No MO reordering is requested

The orbitals are ordered and numbered as follows:
Alpha orbitals:
Number     Energy      Type     Symmetry:
  0     -20.268      AOCC      A1
  1     -11.078      AOCC      A1
  2     -11.070      AOCC      A1
  3     -11.062      AOCC      A1
  4     -11.057      AOCC      A1
  5     -11.038      AOCC      A1
  6      -1.100      AOCC      A1
  7      -0.959      AOCC      A1
  8      -0.836      AOCC      A1
  9      -0.722      AOCC      A1
 10      -0.611      AOCC      A1
 11      -0.498      AOCC      A1
 12      -0.450      AOCC      A1
 13      -0.413      AOCC      A1
 14      -0.377      AOCC      A1
 15      -0.310      AOCC      A1
 16      -0.271      AOCC      A2
 17      -0.147      AOCC      A2
 18     -11.078      AOCC      B1
 19     -11.057      AOCC      B1
 20     -11.038      AOCC      B1
 21      -0.885      AOCC      B1
```

This is how orbitals will be ordered and numbered in the CC and EOM-CC calculations.



Some of the relevant orbitals.

22	-0.764	AOCC	B1
23	-0.590	AOCC	B1
24	-0.482	AOCC	B1
25	-0.400	AOCC	B1
26	-0.364	AOCC	B1
27	-0.335	AOCC	B1
28	-0.173	AOCC	B1
29	-0.371	AOCC	B2
30	-0.294	AOCC	B2
31	-0.212	AOCC	B2
32	-0.037	AOCC	B2

0	0.382	AVIRT	A1
1	0.425	AVIRT	A1
2	0.473	AVIRT	A1
3	0.483	AVIRT	A1
4	0.593	AVIRT	A1
5	0.659	AVIRT	A1
6	0.686	AVIRT	A1
7	0.734	AVIRT	A1
8	0.873	AVIRT	A1
9	0.897	AVIRT	A1
10	0.948	AVIRT	A1
11	0.993	AVIRT	A1
12	1.050	AVIRT	A1
13	1.157	AVIRT	A1
14	1.218	AVIRT	A1
15	1.262	AVIRT	A1
16	1.280	AVIRT	A1
17	1.292	AVIRT	A1
18	1.359	AVIRT	A1
19	1.388	AVIRT	A1
20	1.413	AVIRT	A1
21	1.470	AVIRT	A1
22	1.545	AVIRT	A1
23	1.646	AVIRT	A1
24	1.781	AVIRT	A1
25	1.882	AVIRT	A1
26	2.178	AVIRT	A1
27	2.224	AVIRT	A1
28	2.345	AVIRT	A1
29	2.361	AVIRT	A1
30	2.407	AVIRT	A1
31	2.480	AVIRT	A1
32	2.557	AVIRT	A1
33	2.607	AVIRT	A1
34	2.689	AVIRT	A1
35	2.826	AVIRT	A1
36	2.951	AVIRT	A1
37	3.131	AVIRT	A1
38	3.280	AVIRT	A1
39	3.425	AVIRT	A1
40	3.438	AVIRT	A1
41	3.616	AVIRT	A1
42	3.918	AVIRT	A1
43	4.614	AVIRT	A1
44	4.683	AVIRT	A1

45	4.735	AVIRT	A1
46	4.930	AVIRT	A1
47	5.123	AVIRT	A1
48	5.430	AVIRT	A1
49	0.373	AVIRT	A2
50	0.912	AVIRT	A2
51	1.006	AVIRT	A2
52	1.182	AVIRT	A2
53	1.675	AVIRT	A2
54	1.805	AVIRT	A2
55	1.926	AVIRT	A2
56	2.107	AVIRT	A2
57	2.318	AVIRT	A2
58	2.439	AVIRT	A2
59	2.788	AVIRT	A2
60	2.889	AVIRT	A2
61	3.130	AVIRT	A2
62	0.418	AVIRT	B1
63	0.472	AVIRT	B1
64	0.491	AVIRT	B1
65	0.614	AVIRT	B1
66	0.664	AVIRT	B1
67	0.740	AVIRT	B1
68	0.891	AVIRT	B1
69	0.954	AVIRT	B1
70	0.995	AVIRT	B1
71	1.016	AVIRT	B1
72	1.044	AVIRT	B1
73	1.248	AVIRT	B1
74	1.299	AVIRT	B1
75	1.348	AVIRT	B1
76	1.368	AVIRT	B1
77	1.401	AVIRT	B1
78	1.473	AVIRT	B1
79	1.584	AVIRT	B1
80	1.688	AVIRT	B1
81	1.704	AVIRT	B1
82	1.866	AVIRT	B1
83	1.901	AVIRT	B1
84	2.227	AVIRT	B1
85	2.396	AVIRT	B1
86	2.435	AVIRT	B1
87	2.523	AVIRT	B1
88	2.685	AVIRT	B1
89	2.788	AVIRT	B1
90	2.884	AVIRT	B1
91	3.029	AVIRT	B1
92	3.154	AVIRT	B1
93	3.344	AVIRT	B1
94	3.427	AVIRT	B1
95	3.802	AVIRT	B1
96	4.691	AVIRT	B1
97	4.754	AVIRT	B1
98	5.033	AVIRT	B1
99	0.351	AVIRT	B2
100	0.565	AVIRT	B2
101	0.888	AVIRT	B2

102	0.954	AVIRT	B2
103	1.042	AVIRT	B2
104	1.094	AVIRT	B2
105	1.246	AVIRT	B2
106	1.545	AVIRT	B2
107	1.781	AVIRT	B2
108	1.898	AVIRT	B2
109	1.914	AVIRT	B2
110	2.108	AVIRT	B2
111	2.321	AVIRT	B2
112	2.639	AVIRT	B2
113	2.777	AVIRT	B2
114	2.866	AVIRT	B2
115	3.201	AVIRT	B2

Beta orbitals:

Number	Energy	Type	Symmetry:
0	-20.257	AOCC	A1
1	-11.075	AOCC	A1
2	-11.062	AOCC	A1
3	-11.061	AOCC	A1
4	-11.051	AOCC	A1
5	-11.037	AOCC	A1
6	-1.075	AOCC	A1
7	-0.947	AOCC	A1
8	-0.826	AOCC	A1
9	-0.677	AOCC	A1
10	-0.597	AOCC	A1
11	-0.493	AOCC	A1
12	-0.442	AOCC	A1
13	-0.402	AOCC	A1
14	-0.371	AOCC	A1
15	-0.302	AOCC	A1
16	-0.202	AOCC	A2
17	-11.062	AOCC	B1
18	-11.051	AOCC	B1
19	-11.037	AOCC	B1
20	-0.867	AOCC	B1
21	-0.703	AOCC	B1
22	-0.577	AOCC	B1
23	-0.476	AOCC	B1
24	-0.392	AOCC	B1
25	-0.357	AOCC	B1
26	-0.328	AOCC	B1
27	-0.165	AOCC	B1
28	-0.326	AOCC	B2
29	-0.235	AOCC	B2
30	-0.124	AOCC	B2

0	0.386	AVIRT	A1
1	0.433	AVIRT	A1
2	0.482	AVIRT	A1
3	0.492	AVIRT	A1
4	0.593	AVIRT	A1
5	0.663	AVIRT	A1
6	0.695	AVIRT	A1
7	0.742	AVIRT	A1

8	0.880	AVIRT	A1
9	0.901	AVIRT	A1
10	0.960	AVIRT	A1
11	0.987	AVIRT	A1
12	1.074	AVIRT	A1
13	1.168	AVIRT	A1
14	1.226	AVIRT	A1
15	1.270	AVIRT	A1
16	1.284	AVIRT	A1
17	1.300	AVIRT	A1
18	1.365	AVIRT	A1
19	1.388	AVIRT	A1
20	1.428	AVIRT	A1
21	1.481	AVIRT	A1
22	1.551	AVIRT	A1
23	1.647	AVIRT	A1
24	1.784	AVIRT	A1
25	1.885	AVIRT	A1
26	2.189	AVIRT	A1
27	2.223	AVIRT	A1
28	2.354	AVIRT	A1
29	2.382	AVIRT	A1
30	2.417	AVIRT	A1
31	2.483	AVIRT	A1
32	2.578	AVIRT	A1
33	2.609	AVIRT	A1
34	2.704	AVIRT	A1
35	2.840	AVIRT	A1
36	2.973	AVIRT	A1
37	3.137	AVIRT	A1
38	3.283	AVIRT	A1
39	3.426	AVIRT	A1
40	3.442	AVIRT	A1
41	3.623	AVIRT	A1
42	3.919	AVIRT	A1
43	4.620	AVIRT	A1
44	4.686	AVIRT	A1
45	4.757	AVIRT	A1
46	4.927	AVIRT	A1
47	5.129	AVIRT	A1
48	5.434	AVIRT	A1
49	0.275	AVIRT	A2
50	0.423	AVIRT	A2
51	1.003	AVIRT	A2
52	1.088	AVIRT	A2
53	1.156	AVIRT	A2
54	1.685	AVIRT	A2
55	1.829	AVIRT	A2
56	1.951	AVIRT	A2
57	2.180	AVIRT	A2
58	2.344	AVIRT	A2
59	2.470	AVIRT	A2
60	2.793	AVIRT	A2
61	2.902	AVIRT	A2
62	3.134	AVIRT	A2
63	0.430	AVIRT	B1
64	0.487	AVIRT	B1

65	0.500	AVIRT	B1
66	0.619	AVIRT	B1
67	0.667	AVIRT	B1
68	0.740	AVIRT	B1
69	0.893	AVIRT	B1
70	0.958	AVIRT	B1
71	1.000	AVIRT	B1
72	1.025	AVIRT	B1
73	1.073	AVIRT	B1
74	1.263	AVIRT	B1
75	1.310	AVIRT	B1
76	1.359	AVIRT	B1
77	1.383	AVIRT	B1
78	1.412	AVIRT	B1
79	1.474	AVIRT	B1
80	1.595	AVIRT	B1
81	1.696	AVIRT	B1
82	1.708	AVIRT	B1
83	1.867	AVIRT	B1
84	1.904	AVIRT	B1
85	2.228	AVIRT	B1
86	2.398	AVIRT	B1
87	2.445	AVIRT	B1
88	2.543	AVIRT	B1
89	2.714	AVIRT	B1
90	2.814	AVIRT	B1
91	2.893	AVIRT	B1
92	3.034	AVIRT	B1
93	3.159	AVIRT	B1
94	3.345	AVIRT	B1
95	3.429	AVIRT	B1
96	3.803	AVIRT	B1
97	4.702	AVIRT	B1
98	4.774	AVIRT	B1
99	5.033	AVIRT	B1
100	0.321	AVIRT	B2
101	0.406	AVIRT	B2
102	0.590	AVIRT	B2
103	0.927	AVIRT	B2
104	0.999	AVIRT	B2
105	1.083	AVIRT	B2
106	1.105	AVIRT	B2
107	1.244	AVIRT	B2
108	1.592	AVIRT	B2
109	1.809	AVIRT	B2
110	1.899	AVIRT	B2
111	1.930	AVIRT	B2
112	2.181	AVIRT	B2
113	2.354	AVIRT	B2
114	2.648	AVIRT	B2
115	2.788	AVIRT	B2
116	2.881	AVIRT	B2
117	3.221	AVIRT	B2

MOLECULAR PARAMETERS:
ORB SYMM INFO:
POINT GROUP=C2v NIRREPS = 4

```
MOL ORB=149

IRREPS =   A1   A2   B1   B2
ORBSPI =   65   15   48   21
DOCC   =   16    1   11    3
SOCC   =    0    1    0    1

FDOCC  =    0    0    0    0
RDOCC  =    0    0    0    0
AAOCC  =   16    2   11    4
BAOCC  =   16    1   11    3
AAVIRT =   49   13   37   17
BAVIRT =   49   14   37   18
RUOCC  =    0    0    0    0
FUOCC  =    0    0    0    0

IRREP MULT TABLE:
  0   1   2   3
  1   0   3   2
  2   3   0   1
  3   2   1   0

ORBSYM ALPHA= A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A2   A2   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B2
              B2   B2   B2   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A2   A2   A2   A2   A2   A2   A2   A2
              A2   A2   A2   A2   A2   B1   B1   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B1
              B1   B1   B2   B2   B2   B2   B2   B2   B2   B2
              B2   B2   B2   B2   B2   B2   B2   B2   B2
ORBSYM BETA = A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A2   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B2   B2
              B2   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A1   A1   A1   A1   A1   A1   A1   A1   A1   A1
              A2   A2   A2   A2   A2   A2   A2   A2   A2   A2
              A2   A2   A2   A2   B1   B1   B1   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B1
              B1   B1   B1   B1   B1   B1   B1   B1   B1   B1
              B1   B2   B2   B2   B2   B2   B2   B2   B2   B2
              B2   B2   B2   B2   B2   B2   B2   B2   B2


BASIS ORBS    =      149      MOL ORBS      =      149
FROZEN OCC    =        0      FROZEN VIR    =        0
CORR ORBS     =      149      CORR SP ORBS  =      298
```

```
   NUM ALP ELEC =      33      NUM BET ELEC =      31
   NUM ALP EXPL =      33      NUM BET EXPL =      31
   NUM SO OCC   =      64      NUM SO VIR   =     234
   NUM RESTR DOCC=      0      NUM RESTR DVIRT=     0
   ORBS PER BLCK =     16      RESTRICTED_REF =    0

BLOCKING PARAMETERS:
   NUM ROCC BLOCKS =     0      NUM AOCC  BLOCKS=     4
   NUM AVIRT BLOCKS=    10      NUM RVIRT BLOCKS=     0

   ORBITALS/BLOCK =  16   2  11   4  16   1  11   3  13  12  12  12  13  13  12
12   9   8  13  12  12  12  14  13  12  12   9   9

BIRREP = A1   A2   B1   B2   A1   A2   B1   B2   A1   A1   A1   A1   A2   B1
B1   B1   B2   B2   A1   A1   A1   A1   A2   B1   B1   B1   B2   B2



 Integral transformation job:   CPU 583.47 s  wall 586.57 s
EHF =  -381.832968544 EMP2 =  -382.998563150

Beginning CC iterations
Itr|Var|D|Energy         |Delta_E|Delta_t|Comments
  1| CC|-| -383.020537977|2.2E-02|2.4E-01|
  2| CC|-| -383.059200988|3.9E-02|1.1E-01|
  3| CC|-| -383.063289781|4.1E-03|6.8E-02|
  4| CC|+| -383.069279860|6.0E-03|4.6E-02|
  5| CC|+| -383.075730124|6.5E-03|2.0E-02|
  6| CC|+| -383.077387138|1.7E-03|9.9E-03|
  7| CC|+| -383.077922397|5.4E-04|4.0E-03|
  8| CC|+| -383.078009107|8.7E-05|2.1E-03|
  9| CC|+| -383.078061360|5.2E-05|9.3E-04|
 10| CC|+| -383.078057523|3.8E-06|4.9E-04|
 11| CC|+| -383.078058638|1.1E-06|2.7E-04|
 12| CC|+| -383.078061670|3.0E-06|1.2E-04|
 13| CC|+| -383.078061395|2.8E-07|6.3E-05|
 14| CC|+| -383.078061287|1.1E-07|3.6E-05|
 15| CC|+| -383.078059932|1.4E-06|2.0E-05|
 16| CC|+| -383.078058772|1.2E-06|1.2E-05|
 17| CC|+| -383.078058017|7.5E-07|6.8E-06|
 18| CC|+| -383.078057574|4.4E-07|3.8E-06|
 19| CC|+| -383.078057423|1.5E-07|2.1E-06|
 20| CC|+| -383.078057394|3.0E-08|1.2E-06|
 21| CC|+| -383.078057377|1.7E-08|6.8E-07|
 22| CC|+| -383.078057367|9.5E-09|3.7E-07|
 23| CC|+| -383.078057359|7.9E-09|2.3E-07|
 24| CC|+| -383.078057355|4.2E-09|1.4E-07|
 25| CC|+| -383.078057354|1.6E-09|7.8E-08|
 26| CC|+| -383.078057355|1.1E-09|4.6E-08|
 27| CC|+| -383.078057356|1.1E-09|2.9E-08|
 28| CC|+| -383.078057357|1.3E-09|1.6E-08|
 29| CC|+| -383.078057358|7.1E-10|9.2E-09|
Calculation converged,    29 iterations

Largest T amplitudes
Largest singles amplitudes:
       Value                  i            ->    a
```

```
       0.1606                  32( B2  ) A   ->   99( B2  ) A
      -0.1241                  30( B2  ) B   ->  100( B2  ) B
      -0.1034                  16( A2  ) A   ->   49( A2  ) A
       0.0990                  16( A2  ) B   ->   50( A2  ) B
      -0.0972                  29( B2  ) B   ->  101( B2  ) B

Largest doubles amplitudes:
       Value      i             j            ->   a             b
      0.0579     17( A2  ) A,  16( A2  ) B  ->  49( A2  ) A,  49( A2  ) B
     -0.0456     16( A2  ) A,  16( A2  ) B  ->  49( A2  ) A,  50( A2  ) B
     -0.0454     17( A2  ) A,  29( B2  ) B  ->  99( B2  ) A,  49( A2  ) B
      0.0421     30( B2  ) A,  29( B2  ) B  ->  99( B2  ) A, 101( B2  ) B
     -0.0413     32( B2  ) A,  30( B2  ) B  ->  99( B2  ) A, 101( B2  ) B

EHF                        =  -381.832968544
EMP2                       =  -382.998563150
Correlation Energy         =    -1.245088813
CCSD Total Energy          =  -383.078057358
```

> This is NOT the Spin Flip energy. It is the CCSD energy for the reference state.

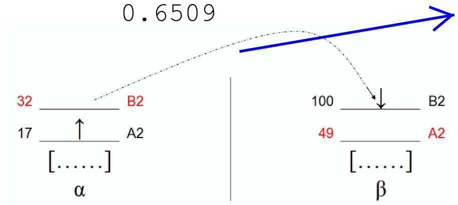
```
 CCSD or (V)OO-CCD job:  CPU 5333.28 s  wall 5856.76 s
Removing integral transformation files: 151 153 152
SOLVE EOM EQUATIONS FOR THE 2 LOWEST LOWSPIN STATES, TRANSITION OF A1   IRREP

State   1:  32 ->216    (  0.4533)
State   2:  17 ->165    (  0.4868)
```

> This is the symmetry of the transition, and NOT the symmetry of the resulting state. The target states are:
>
> B_1 (ref) x A_1 = B_1

```
2 guess vectors generated

Itr|ConvR|ResNormR|NVecs|Comments
  0|  0  |2.8E-01 |  2  |
  1|  0  |2.6E-02 |  4  |
  2|  0  |5.0E-03 |  6  |
  3|  0  |1.7E-03 |  8  |
  4|  0  |5.9E-04 | 10  |
  5|  0  |1.9E-04 | 12  |
  6|  0  |7.0E-05 | 14  |
  7|  0  |2.2E-05 | 16  |
  8|  0  |4.3E-06 | 18  |NSDavidsonRight&lt;T&gt;::CalcCorrectionVec(): Warning!
Scaled norm for root   0 is too small: 2.76E-07; ||Res||=1.34E-06

  9|  1  |8.2E-07 | 20  |NSDavidsonRight&lt;T&gt;::CalcCorrectionVec(): Warning!
Scaled norm for root   1 is too small: 4.31E-07; ||Res||=1.43E-06

 10|  2  |2.9E-07 | 21  |Collapse current subspace
DAVIDSON ITERATIONS CONVERGED,    10 ITERATIONS
Excitation energies, hartree
                                0
    0    0.009144
    1    0.057738

  2 lowest roots of symmetry A1  :
Root 1 Conv-d yes Tot Ene= -383.068913021 hartree (Ex Ene 0.2488 eV),
U1^2=0.945064, U2^2=0.054936, ||Res||=2.0E-07
Right U1:
       Value                        i            ->    a
       0.6509                  32( B2  ) A   ->  100( B2  ) B
```

> Energy of the lowest state with B_1 symmetry.

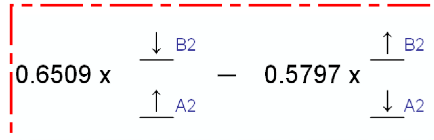
> Ignore this.



> orbital #

> alpha spin

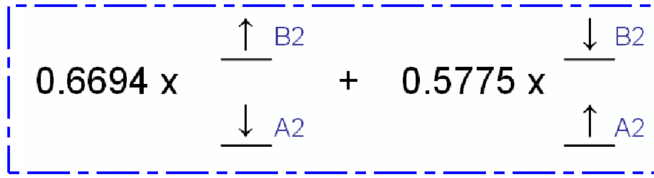
> beta spin




```
      -0.5797                17( A2  ) A   ->   49( A2  ) B
       0.3060                31( B2  ) A   ->  100( B2  ) B
       0.1315                16( A2  ) A   ->   50( A2  ) B
```

Root 1 looks like this, so it is a $^1B_1$ state.

```
 Root 2 Conv-d yes Tot Ene= -383.020319257 hartree (Ex Ene 1.5711 eV),
 U1^2=0.913903, U2^2=0.086097, ||Res||=3.8E-07
 Right U1:
        Value                 i              ->     a
      -0.6694                17( A2  ) A   ->   49( A2  ) B
      -0.5775                32( B2  ) A   ->  100( B2  ) B
       0.2365                32( B2  ) A   ->  101( B2  ) B
       0.1178                17( A2  ) A   ->   50( A2  ) B
```



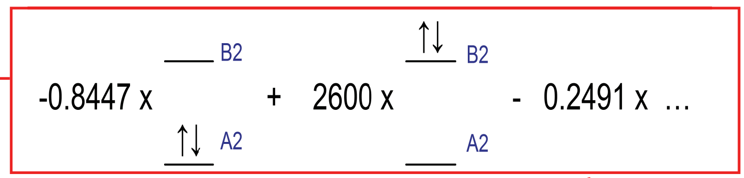
Root 2 is the M_s = 0 triplet state. ($^3B_1$)

```
 CALCULATING LEFT VECTORS:

 Re-orthogonalize vecs
 Itr|ConvR|ResNormR|NVecs|Comments
   0|  0  |1.2E-02 |  2  |
   1|  0  |1.9E-03 |  4  |
   2|  0  |3.8E-04 |  6  |
   3|  0  |7.8E-05 |  8  |
   4|  0  |1.6E-05 | 10  |
   5|  0  |5.3E-06 | 12  |
   6|  0  |2.4E-06 | 14  |NSDavidsonRight<T>::CalcCorrectionVec(): Warning!
 Scaled norm for root   0 is too small: 3.35E-07; ||Res||=1.32E-06

   7|  1  |8.4E-07 | 16  |NSDavidsonRight<T>::CalcCorrectionVec(): Warning!
 Scaled norm for root   1 is too small: 4.20E-07; ||Res||=1.34E-06

   8|  2  |4.4E-07 | 17  |Collapse current subspace
 DAVIDSON ITERATIONS CONVERGED,      8 ITERATIONS
 Excitation energies, hartree
                 0
     0     0.009147
     1     0.057741

 Re-orthogonalize vecs
 Biorthogonalize left and right vectors


 CALCULATE LEFT AND RIGHT VECTORS:

 Itr|ConvR|ConvL|ResNormR|ResNormL|NVecs|Lock|Comments
   0|  2  |  2  |3.0E-07 |4.4E-07 |  2  |  2 |Collapse current subspace
 DAVIDSON ITERATIONS CONVERGED,      0 ITERATIONS
 Excitation energies, hartree
                 0
     0     0.009147
     1     0.057741

 SOLVE EOM EQUATIONS FOR THE 2 LOWEST LOWSPIN STATES, TRANSITION OF B1   IRREP

 State   1:  32 ->165     (  0.4054)
 State   2:  17 ->216     (  0.5347)
```

The target states are:

B_1 (ref) x B_1 = A_1

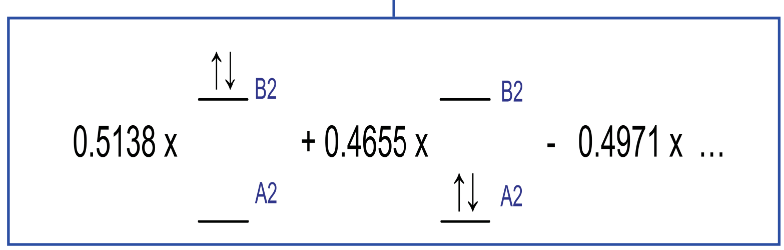
```
2 guess vectors generated

Itr|ConvR|ResNormR|NVecs|Comments
  0|  0  |3.0E-01 |  2  |
  1|  0  |3.3E-02 |  4  |
  2|  0  |8.3E-03 |  6  |
  3|  0  |3.8E-03 |  8  |
  4|  0  |1.2E-03 | 10  |
  5|  0  |3.1E-04 | 12  |
  6|  0  |7.4E-05 | 14  |
  7|  0  |2.0E-05 | 16  |NSDavidsonRight<T>::CalcCorrectionVec(): Warning!
Scaled norm for root   0 is too small: 4.98E-07; ||Res||=2.40E-06

  8|  1  |4.2E-06 | 18  |
  9|  1  |1.1E-06 | 19  |
 10|  2  |3.0E-07 | 20  |Collapse current subspace
DAVIDSON ITERATIONS CONVERGED,    10 ITERATIONS
Excitation energies, hartree
                0
    0    0.002742
    1    0.081832
```



$^1A_1$ state

```
  2 lowest roots of symmetry B1  :
Root 1 Conv-d yes Tot Ene= -383.075315180 hartree (Ex Ene 0.0746 eV),
U1^2=0.921512, U2^2=0.078488, ||Res||=1.1E-07
Right U1:
       Value                   i            ->    a
      -0.8447                 32( B2   ) A   ->   49( A2   ) B
       0.2600                 17( A2   ) A   ->  100( B2   ) B
      -0.2491                 31( B2   ) A   ->   49( A2   ) B
      -0.1582                 16( A2   ) A   ->  100( B2   ) B

Root 2 Conv-d yes Tot Ene= -382.996225190 hartree (Ex Ene 2.2268 eV),
U1^2=0.928647, U2^2=0.071353, ||Res||=4.9E-07
Right U1:
       Value                   i            ->    a
       0.5138                 17( A2   ) A   ->  100( B2   ) B
      -0.4971                 31( B2   ) A   ->   49( A2   ) B
       0.4655                 32( B2   ) A   ->   49( A2   ) B
      -0.2807                 32( B2   ) A   ->   50( A2   ) B
```

Higher energy $^1A_1$ state




```
CALCULATING LEFT VECTORS:

Re-orthogonalize vecs
Itr|ConvR|ResNormR|NVecs|Comments
  0|  0  |1.2E-02 |  2  |
  1|  0  |1.9E-03 |  4  |
  2|  0  |3.7E-04 |  6  |
  3|  0  |7.0E-05 |  8  |
  4|  0  |1.2E-05 | 10  |
  5|  0  |3.1E-06 | 12  |
  6|  1  |8.7E-07 | 14  |NSDavidsonRight<T>::CalcCorrectionVec(): Warning!
Scaled norm for root   1 is too small: 4.89E-07; ||Res||=1.15E-06

  7|  2  |5.7E-07 | 15  |Collapse current subspace
```

```
DAVIDSON ITERATIONS CONVERGED,     7 ITERATIONS
Excitation energies, hartree
                0
    0    0.002741
    1    0.081831

Re-orthogonalize vecs
Biorthogonalize left and right vectors
Negative norm is detected for vector 1: NORM=-0.993990


CALCULATE LEFT AND RIGHT VECTORS:

Itr|ConvR|ConvL|ResNormR|ResNormL|NVecs|Lock|Comments
  0|  2  |  2  |3.1E-07 |5.7E-07 |  2  |  2 |Collapse current subspace
DAVIDSON ITERATIONS CONVERGED,     0 ITERATIONS
Excitation energies, hartree
                0
    0    0.002741
    1    0.081831

EOM-CCSD PROPERTIES FOR LOWSPIN    1/A1    STATE:
Solve amplitude response equations
```

Again, this is the symmetry of the transition, and NOT the symmetry of the resulting state. The target state is the lower energy:

B_1 (ref) x A_1 = B_1 ($^1B_1$ state)

```
  0|  Z|-|1.2E-01|
  1|  Z|-|6.3E-02|
  2|  Z|+|3.8E-02|
  3|  Z|-|2.7E-02|
  4|  Z|+|7.7E-03|
  5|  Z|-|5.4E-03|
  6|  Z|+|1.7E-03|
  7|  Z|-|1.2E-03|
  8|  Z|+|4.2E-04|
  9|  Z|-|3.1E-04|
 10|  Z|+|1.0E-04|
 11|  Z|-|7.4E-05|
 12|  Z|+|2.4E-05|
 13|  Z|-|1.7E-05|
 14|  Z|+|5.9E-06|
 15|  Z|-|4.4E-06|
 16|  Z|+|1.6E-06|
 17|  Z|-|1.2E-06|
 18|  Z|+|5.3E-07|
 19|  Z|-|4.2E-07|
 20|  Z|+|1.4E-07|
 21|  Z|-|1.1E-07|
 22|  Z|+|3.9E-08|
 23|  Z|-|2.9E-08|
 24|  Z|+|1.0E-08|
 25|  Z|-|8.4E-09|
Z-vector converged in 26 iterations

Solve orbital response equations

  0| Lambda|-|1.1E-01|
  1| Lambda|-|1.1E-01|
  2| Lambda|-|1.2E-01|
```

```
  3| Lambda|-|1.5E-01|
  4| Lambda|+|1.2E-02|
  5| Lambda|-|8.4E-03|
  6| Lambda|+|1.9E-03|
  7| Lambda|-|1.5E-03|
  8| Lambda|+|2.9E-04|
  9| Lambda|-|2.3E-04|
 10| Lambda|+|4.8E-05|
 11| Lambda|-|3.5E-05|
 12| Lambda|+|1.6E-05|
 13| Lambda|-|1.6E-05|
 14| Lambda|+|2.7E-06|
 15| Lambda|-|1.8E-06|
 16| Lambda|+|9.2E-07|
 17| Lambda|-|5.9E-07|
 18| Lambda|+|2.3E-07|
 19| Lambda|-|1.5E-07|
 20| Lambda|+|3.1E-08|
 21| Lambda|-|2.2E-08|
 22| Lambda|+|1.1E-08|
 23| Lambda|-|7.9E-09|
Lambda-equations converged in 24 iterations
```

Dipole moment for the $^1B_1$ state.

```
Dipole moment                  x               y               z
Total                    0.000000000     0.000000000     1.620082775    a.u.
|mu| = 1.620082775 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

<R^2>                   x^2              y^2              z^2
                    605.901954262    44.156890432   472.514557551    a.u.
Total <R^2> = 1122.573402244 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

NAlpha=   32 ; NBeta=   32
<S^2> = 1.966516397


EOM-CCSD PROPERTIES FOR LOWSPIN   2/A1   STATE:
Solve amplitude response equations

  0|  Z|-|1.2E-01|
  1|  Z|-|6.2E-02|
  2|  Z|+|3.8E-02|
  3|  Z|-|2.8E-02|
  4|  Z|+|9.8E-03|
  5|  Z|-|7.4E-03|
  6|  Z|+|2.6E-03|
  7|  Z|-|2.0E-03|
  8|  Z|+|6.7E-04|
  9|  Z|-|5.3E-04|
 10|  Z|+|1.7E-04|
 11|  Z|-|1.3E-04|
 12|  Z|+|4.4E-05|
 13|  Z|-|3.3E-05|
 14|  Z|+|1.1E-05|
```

```
 15|  Z|-|8.1E-06|
 16|  Z|+|2.8E-06|
 17|  Z|-|2.1E-06|
 18|  Z|+|7.7E-07|
 19|  Z|-|5.9E-07|
 20|  Z|+|2.4E-07|
 21|  Z|-|1.9E-07|
 22|  Z|+|6.8E-08|
 23|  Z|-|5.2E-08|
 24|  Z|+|1.8E-08|
 25|  Z|-|1.3E-08|
 26|  Z|+|5.0E-09|
Z-vector converged in 27 iterations

Solve orbital response equations

  0| Lambda|-|1.4E-01|
  1| Lambda|-|1.2E-01|
  2| Lambda|-|1.3E-01|
  3| Lambda|-|1.5E-01|
  4| Lambda|+|1.1E-02|
  5| Lambda|-|6.2E-03|
  6| Lambda|+|2.5E-03|
  7| Lambda|-|1.7E-03|
  8| Lambda|+|3.0E-04|
  9| Lambda|-|2.5E-04|
 10| Lambda|+|1.0E-04|
 11| Lambda|-|7.5E-05|
 12| Lambda|+|2.0E-05|
 13| Lambda|-|2.1E-05|
 14| Lambda|+|3.9E-06|
 15| Lambda|-|3.0E-06|
 16| Lambda|+|1.4E-06|
 17| Lambda|-|1.3E-06|
 18| Lambda|+|3.2E-07|
 19| Lambda|-|2.4E-07|
 20| Lambda|+|1.5E-07|
 21| Lambda|-|1.0E-07|
 22| Lambda|+|4.9E-08|
 23| Lambda|-|3.7E-08|
 24| Lambda|+|1.1E-08|
 25| Lambda|-|9.1E-09|
Lambda-equations converged in 26 iterations
```

Dipole moment for the $^3B_1$ state.

```
Dipole moment                x              y              z
Total                  0.000000000    0.000000000    2.038804975    a.u.
|mu| = 2.038804975 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx


<R^2>                x^2              y^2              z^2
                 608.341096468    44.277817228   471.277643366    a.u.
Total <R^2> = 1123.896557062 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

NAlpha=   32 ; NBeta=   32
```

```
<S^2> = 0.143364295


EOM-CCSD PROPERTIES FOR LOWSPIN   1/B1   STATE:
Solve amplitude response equations

  0|  Z|-|1.2E-01|
  1|  Z|-|6.2E-02|
  2|  Z|+|3.7E-02|
  3|  Z|-|2.7E-02|
  4|  Z|+|8.4E-03|
  5|  Z|-|5.9E-03|
  6|  Z|+|1.8E-03|
  7|  Z|-|1.3E-03|
  8|  Z|+|4.2E-04|
  9|  Z|-|3.2E-04|
 10|  Z|+|1.1E-04|
 11|  Z|-|8.0E-05|
 12|  Z|+|2.4E-05|
 13|  Z|-|1.8E-05|
 14|  Z|+|6.3E-06|
 15|  Z|-|5.0E-06|
 16|  Z|+|1.8E-06|
 17|  Z|-|1.5E-06|
 18|  Z|+|5.7E-07|
 19|  Z|-|4.6E-07|
 20|  Z|+|1.8E-07|
 21|  Z|-|1.4E-07|
 22|  Z|+|5.6E-08|
 23|  Z|-|4.3E-08|
 24|  Z|+|1.6E-08|
 25|  Z|-|1.3E-08|
 26|  Z|+|5.6E-09|
Z-vector converged in 27 iterations

Solve orbital response equations

  0| Lambda|-|1.7E-01|
  1| Lambda|-|1.8E-01|
  2| Lambda|-|2.0E-01|
  3| Lambda|-|2.4E-01|
  4| Lambda|+|2.0E-02|
  5| Lambda|-|1.2E-02|
  6| Lambda|+|4.1E-03|
  7| Lambda|-|3.1E-03|
  8| Lambda|+|5.7E-04|
  9| Lambda|-|4.3E-04|
 10| Lambda|+|8.0E-05|
 11| Lambda|-|5.1E-05|
 12| Lambda|+|1.6E-05|
 13| Lambda|-|1.4E-05|
 14| Lambda|+|3.4E-06|
 15| Lambda|-|2.2E-06|
 16| Lambda|+|1.2E-06|
 17| Lambda|-|8.5E-07|
 18| Lambda|+|3.1E-07|
 19| Lambda|-|2.1E-07|
```

Properties for the lower energy: B_1 (ref) x B_1 = A_1 target state ($^1A_1$).

```
 20| Lambda|+|5.1E-08|
 21| Lambda|-|2.9E-08|
 22| Lambda|+|1.4E-08|
 23| Lambda|-|1.2E-08|
 24| Lambda|+|3.2E-09|
Lambda-equations converged in 25 iterations

Dipole moment                  x              y               z
Total                   -0.000000000     0.000000000     0.612371735    a.u.
|mu| = 0.612371735 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx


<R^2>                x^2              y^2              z^2
                   606.910671681    44.339481555   472.430432169    a.u.
Total <R^2> = 1123.680585405 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

NAlpha=   32 ; NBeta=   32
<S^2> = -0.079489928


EOM-CCSD PROPERTIES FOR LOWSPIN   2/B1   STATE:
Solve amplitude response equations
```

Properties for the higher energy: B_1 (ref) x B_1 = A_1 target state ($^1A_1$).

```
  0|  Z|-|1.1E-01|
  1|  Z|-|4.8E-02|
  2|  Z|+|2.6E-02|
  3|  Z|-|1.8E-02|
  4|  Z|+|6.2E-03|
  5|  Z|-|4.4E-03|
  6|  Z|+|1.3E-03|
  7|  Z|-|9.5E-04|
  8|  Z|+|3.1E-04|
  9|  Z|-|2.2E-04|
 10|  Z|+|7.5E-05|
 11|  Z|-|5.5E-05|
 12|  Z|+|1.8E-05|
 13|  Z|-|1.3E-05|
 14|  Z|+|4.3E-06|
 15|  Z|-|3.1E-06|
 16|  Z|+|1.0E-06|
 17|  Z|-|7.8E-07|
 18|  Z|+|3.4E-07|
 19|  Z|-|2.6E-07|
 20|  Z|+|1.0E-07|
 21|  Z|-|8.1E-08|
 22|  Z|+|3.0E-08|
 23|  Z|-|2.3E-08|
 24|  Z|+|8.4E-09|
Z-vector converged in 25 iterations

Solve orbital response equations

  0| Lambda|-|1.4E-01|
  1| Lambda|-|1.5E-01|
```

```
  2| Lambda|-|1.7E-01|
  3| Lambda|-|2.1E-01|
  4| Lambda|+|8.7E-03|
  5| Lambda|-|6.5E-03|
  6| Lambda|+|2.8E-03|
  7| Lambda|-|2.1E-03|
  8| Lambda|+|3.5E-04|
  9| Lambda|-|3.1E-04|
 10| Lambda|+|5.4E-05|
 11| Lambda|-|3.6E-05|
 12| Lambda|+|2.2E-05|
 13| Lambda|-|1.8E-05|
 14| Lambda|+|3.7E-06|
 15| Lambda|-|2.6E-06|
 16| Lambda|+|1.2E-06|
 17| Lambda|-|1.2E-06|
 18| Lambda|+|3.8E-07|
 19| Lambda|-|2.7E-07|
 20| Lambda|+|8.2E-08|
 21| Lambda|-|5.1E-08|
 22| Lambda|+|2.7E-08|
 23| Lambda|-|2.4E-08|
 24| Lambda|+|5.5E-09|
Lambda-equations converged in 25 iterations

Dipole moment                x              y              z
Total                   0.000000000    0.000000000    1.477000563    a.u.
|mu| = 1.477000563 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx


<R^2>                x^2             y^2             z^2
                  607.134891157    44.147993947   471.918489033    a.u.
Total <R^2> = 1123.201374137 a.u.
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

NAlpha=   32 ; NBeta=   32
<S^2> = 0.650755401



 EOM job:  CPU 27647.72 s  wall 35579.20 s


 CCMAN JOB: ALL  CPU 32981.08 s  wall 41436.06 s
Cleaning up statics....
 Analysis of SCF Wavefunction

 --------------------------------------------------------------
             Orbital Energies (a.u.) and Symmetries
 --------------------------------------------------------------

 Alpha MOs, Unrestricted
 -- Occupied --
-20.268 -11.078 -11.070 -11.062 -11.057 -11.038  -1.100  -0.959
```

```
  1 A1    2 A1    3 A1    4 A1    5 A1    6 A1    7 A1    8 A1
 -0.836  -0.722  -0.611  -0.498  -0.450  -0.413  -0.377  -0.310
  9 A1   10 A1   11 A1   12 A1   13 A1   14 A1   15 A1   16 A1
 -0.271  -0.147 -11.078 -11.057 -11.038  -0.885  -0.764  -0.590
  1 A2    2 A2    1 B1    2 B1    3 B1    4 B1    5 B1    6 B1
 -0.482  -0.400  -0.364  -0.335  -0.173  -0.371  -0.294  -0.212
  7 B1    8 B1    9 B1   10 B1   11 B1    1 B2    2 B2    3 B2
 -0.037
  4 B2
 -- Virtual --
  0.382   0.425   0.473   0.483   0.593   0.659   0.686   0.734
 17 A1   18 A1   19 A1   20 A1   21 A1   22 A1   23 A1   24 A1
  0.873   0.897   0.948   0.993   1.050   1.157   1.218   1.262
 25 A1   26 A1   27 A1   28 A1   29 A1   30 A1   31 A1   32 A1
  1.280   1.292   1.359   1.388   1.413   1.470   1.545   1.646
 33 A1   34 A1   35 A1   36 A1   37 A1   38 A1   39 A1   40 A1
  1.781   1.882   2.178   2.224   2.345   2.361   2.407   2.480
 41 A1   42 A1   43 A1   44 A1   45 A1   46 A1   47 A1   48 A1
  2.557   2.607   2.689   2.826   2.951   3.131   3.280   3.425
 49 A1   50 A1   51 A1   52 A1   53 A1   54 A1   55 A1   56 A1
  3.438   3.616   3.918   4.614   4.683   4.735   4.930   5.123
 57 A1   58 A1   59 A1   60 A1   61 A1   62 A1   63 A1   64 A1
  5.430   0.373   0.912   1.006   1.182   1.675   1.805   1.926
 65 A1    3 A2    4 A2    5 A2    6 A2    7 A2    8 A2    9 A2
  2.107   2.318   2.439   2.788   2.889   3.130   0.418   0.472
 10 A2   11 A2   12 A2   13 A2   14 A2   15 A2   12 B1   13 B1
  0.491   0.614   0.664   0.740   0.891   0.954   0.995   1.016
 14 B1   15 B1   16 B1   17 B1   18 B1   19 B1   20 B1   21 B1
  1.044   1.248   1.299   1.348   1.368   1.401   1.473   1.584
 22 B1   23 B1   24 B1   25 B1   26 B1   27 B1   28 B1   29 B1
  1.688   1.704   1.866   1.901   2.227   2.396   2.435   2.523
 30 B1   31 B1   32 B1   33 B1   34 B1   35 B1   36 B1   37 B1
  2.685   2.788   2.884   3.029   3.154   3.344   3.427   3.802
 38 B1   39 B1   40 B1   41 B1   42 B1   43 B1   44 B1   45 B1
  4.691   4.754   5.033   0.351   0.565   0.888   0.954   1.042
 46 B1   47 B1   48 B1    5 B2    6 B2    7 B2    8 B2    9 B2
  1.094   1.246   1.545   1.781   1.898   1.914   2.108   2.321
 10 B2   11 B2   12 B2   13 B2   14 B2   15 B2   16 B2   17 B2
  2.639   2.777   2.866   3.201
 18 B2   19 B2   20 B2   21 B2

 Beta MOs, Unrestricted
 -- Occupied --
-20.257 -11.075 -11.062 -11.061 -11.051 -11.037  -1.075  -0.947
  1 A1    2 A1    3 A1    4 A1    5 A1    6 A1    7 A1    8 A1
 -0.826  -0.677  -0.597  -0.493  -0.442  -0.402  -0.371  -0.302
  9 A1   10 A1   11 A1   12 A1   13 A1   14 A1   15 A1   16 A1
 -0.202 -11.062 -11.051 -11.037  -0.867  -0.703  -0.577  -0.476
  1 A2    1 B1    2 B1    3 B1    4 B1    5 B1    6 B1    7 B1
 -0.392  -0.357  -0.328  -0.165  -0.326  -0.235  -0.124
  8 B1    9 B1   10 B1   11 B1    1 B2    2 B2    3 B2
 -- Virtual --
  0.386   0.433   0.482   0.492   0.593   0.663   0.695   0.742
 17 A1   18 A1   19 A1   20 A1   21 A1   22 A1   23 A1   24 A1
  0.880   0.901   0.960   0.987   1.074   1.168   1.226   1.270
 25 A1   26 A1   27 A1   28 A1   29 A1   30 A1   31 A1   32 A1
  1.284   1.300   1.365   1.388   1.428   1.481   1.551   1.647
```

```
33 A1   34 A1   35 A1   36 A1   37 A1   38 A1   39 A1   40 A1
 1.784   1.885   2.189   2.223   2.354   2.382   2.417   2.483
41 A1   42 A1   43 A1   44 A1   45 A1   46 A1   47 A1   48 A1
 2.578   2.609   2.704   2.840   2.973   3.137   3.283   3.426
49 A1   50 A1   51 A1   52 A1   53 A1   54 A1   55 A1   56 A1
 3.442   3.623   3.919   4.620   4.686   4.757   4.927   5.129
57 A1   58 A1   59 A1   60 A1   61 A1   62 A1   63 A1   64 A1
 5.434   0.275   0.423   1.003   1.088   1.156   1.685   1.829
65 A1    2 A2    3 A2    4 A2    5 A2    6 A2    7 A2    8 A2
 1.951   2.180   2.344   2.470   2.793   2.902   3.134   0.430
 9 A2   10 A2   11 A2   12 A2   13 A2   14 A2   15 A2   12 B1
 0.487   0.500   0.619   0.667   0.740   0.893   0.958   1.000
13 B1   14 B1   15 B1   16 B1   17 B1   18 B1   19 B1   20 B1
 1.025   1.073   1.263   1.310   1.359   1.383   1.412   1.474
21 B1   22 B1   23 B1   24 B1   25 B1   26 B1   27 B1   28 B1
 1.595   1.696   1.708   1.867   1.904   2.228   2.398   2.445
29 B1   30 B1   31 B1   32 B1   33 B1   34 B1   35 B1   36 B1
 2.543   2.714   2.814   2.893   3.034   3.159   3.345   3.429
37 B1   38 B1   39 B1   40 B1   41 B1   42 B1   43 B1   44 B1
 3.803   4.702   4.774   5.033   0.321   0.406   0.590   0.927
45 B1   46 B1   47 B1   48 B1    4 B2    5 B2    6 B2    7 B2
 0.999   1.083   1.105   1.244   1.592   1.809   1.899   1.930
 8 B2    9 B2   10 B2   11 B2   12 B2   13 B2   14 B2   15 B2
 2.181   2.354   2.648   2.788   2.881   3.221
16 B2   17 B2   18 B2   19 B2   20 B2   21 B2
--------------------------------------------------------------

        Mulliken Net Atomic Charges

    Atom                 Charge (a.u.)    Spin (a.u.)
  --------------------------------------------------------
      1 C                  -0.021858      -0.684822
      2 C                  -0.212508       0.855419
      3 C                  -0.220700      -0.737897
      4 C                  -0.212508       0.855419
      5 C                  -0.021858      -0.684822
      6 C                   0.390094       0.486195
      7 O                  -0.811627       0.202881
      8 C                  -0.430421       1.057954
      9 H                   0.181474      -0.082573
     10 H                   0.104394      -0.085105
     11 H                   0.133848      -0.060342
     12 H                   0.132374       0.047757
     13 H                   0.133848      -0.060342
     14 C                  -0.430421       1.057954
     15 H                   0.181474      -0.082573
     16 H                   0.104394      -0.085105
  --------------------------------------------------------
  Sum of atomic charges =    -1.000000
  Sum of spin   charges =     2.000000

-----------------------------------------------------------------
                   Cartesian Multipole Moments
-----------------------------------------------------------------
   Charge (ESU x 10^10)
             -4.8032
   Dipole Moment (Debye)
```

```
        X       0.0000      Y       0.0000      Z      -5.1884
      Tot       5.1884
   Quadrupole Moments (Debye-Ang)
       XX     -61.4734     XY       0.0000     YY     -59.5424
       XZ       0.0000     YZ       0.0000     ZZ     -70.3537
   Octapole Moments (Debye-Ang^2)
      XXX       0.0000    XXY       0.0000    XYY       0.0000
      YYY       0.0000    XXZ      -2.4707    XYZ       0.0000
      YYZ       4.1850    XZZ       0.0000    YZZ       0.0000
      ZZZ     -21.3044
   Hexadecapole Moments (Debye-Ang^3)
     XXXX    -918.5617   XXXY       0.0000   XXYY    -174.0161
     XYYY       0.0000   YYYY     -62.6785   XXXZ       0.0000
     XXYZ       0.0000   XYYZ       0.0000   YYYZ       0.0000
     XXZZ    -245.6738   XYZZ       0.0000   YYZZ    -125.8554
     XZZZ       0.0000   YZZZ       0.0000   ZZZZ    -701.3491
-----------------------------------------------------------------
Total job time:  41527.15s(wall), 33052.41s(cpu)
Wed Aug 15 03:19:28 2007

       *************************************************************
       *                                                           *
       *  Thank you very much for using Q-Chem.  Have a nice day.  *
       *                                                           *
       *************************************************************
```