

Welcome to Q-Chem  
A Quantum Leap Into The Future Of Chemistry

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Intel X86 Linux Version

Q-chem begins on Fri Dec 14 18:38:45 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:  
-----

\$molecule

0 1

H	0.774767	0.000000	0.458565
O	0.000000	0.000000	-0.114641
H	-0.774767	0.000000	0.458565

\$end

\$rem

jobtype sp  
exchange hf  
correlation ccsd  
basis 6-31+G\*  
cc\_nlowspin [1,0,1,1]  
cc\_ip\_proper true  
cc\_dconvergence 10  
cc\_exstates\_prop true  
cc\_trans\_prop true  
cc\_state\_deriv 1  
cc\_refsym 4

\$end

```
-----  
Writing REM_CC_EA          0  
-----  
          Standard Nuclear Orientation (Angstroms)  
          I      Atom      X      Y      Z  
-----  
          1      H      0.774767  0.000000  0.458565  
          2      O      0.000000  0.000000 -0.114641  
          3      H     -0.774767  0.000000  0.458565  
-----  
Molecular Point Group          C2v  NOp = 4  
Largest Abelian Subgroup      C2v  NOp = 4  
Nuclear Repulsion Energy =    9.1267391657 hartrees  
There are      5 alpha and      5 beta electrons  
Requested basis set is 6-31+G(d)  
There are 9 shells and 23 basis functions  
Total memory of 1361MB is distributed as follows:  
  QALLOC including MEM_STATIC uses 1301MB  
  MEM_STATIC is set to 301MB  
  CCMAN JOB total tmp buffer size is 1060MB  
  CC_TMPBUFFSIZE is set to 60MB  
  CC_BLK_TNSR_BUFFSIZE is set to 1000MB  
Warning: actual memory use might exceed 1361MB  
  
Total QAlloc Memory Limit  1301 MB  
Mega-Array Size           295 MB  
MEM_STATIC part           301 MB  
  
          Distance Matrix (Angstroms)  
          H ( 1)  O ( 2)  
O ( 2)  0.963758  
H ( 3)  1.549534  0.963758  
  
Standard Electronic Orientation quadrupole field applied  
Nucleus-field energy      =   -0.0000000001 hartrees  
A cutoff of 1.0D-14 yielded  45 shell pairs  
There are 309 function pairs  
Evaluating contribution to one-electron hamiltonian from nuclear  
Smallest overlap matrix eigenvalue = 1.81E-02  
Multipole matrices computed through 2nd order  
Guess from superposition of atomic densities  
Warning: Energy on first SCF cycle will be non-variational  
A restricted 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         -75.8955779457    1.43E-01  
2         -75.9837468790    2.43E-02  
3         -76.0087248191    1.36E-02  
4         -76.0170004486    1.47E-03  
5         -76.0171661520    3.32E-04  
6         -76.0171773389    4.93E-05  
7         -76.0171777289    1.04E-05  
-----
```

8	-76.0171777496	1.35E-06	
9	-76.0171777499	1.58E-07	
10	-76.0171777499	3.66E-08	
11	-76.0171777499	7.15E-09	Convergence criterion met

-----  
SCF time: CPU 0.24 s wall 0.37 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      *
*                               *
*           AND                 *
*                               *
*           Piotr A. Pieniazek  *
*           C. Melania Oana     *
*           E. Epifanovsky      *
*                               *
*           October 2007       *
*                               *
*****

```

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_BUFSZ	1000
TOT_MEM (MB)	1060	NORBS_PER_BLOCK	16
DO_DYNAMIC_CORR	no	DO_PARENTHESES_T	no
INCL_CORE_CORR	yes	INCL_VIRT_CORR	yes

PARAMETERS FOR EOM CALCULATIONS:

NLOWSPIN	1 0 1 1 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	1
REF_SYM	4	STATE_TO_OPT	1
DO_SPIN_FLIP	no		
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
PRECONV SD	0	EOM2MS	1
DO IP	no	DO EA	no
DO_IP_FILTER	no		
DO DIP	no	DO IP_PROPER	yes
IF_RESTR_AMPL	yes		

PARAMETERS FOR DAVIDSON DIAGONALIZATION PROCEDURE:

DMAXVECTORS	60	DMAXITER	30
DCONVERGENCE	10	DTHRESHOLD	1.0E-10
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, Restricted

-- Occupied --

-20.581	-1.352	-0.724	-0.579	-0.508			
1 A1	2 A1	1 B1	3 A1	1			

B2

-- Virtual --

0.147	0.220	0.251	0.253	0.353	0.381	1.238	1.322
4 A1	2 B1	5 A1	2 B2	3 B1	6 A1	4 B1	7

A1

1.394	1.405	1.414	1.474	2.015	2.018	2.057	2.618
5 B1	3 B2	8 A1	9 A1	10 A1	1 A2	4 B2	11

A1

3.007	4.098						
6 B1	12						

A1

Beta MOs, Restricted

-- Occupied --

-20.581	-1.352	-0.724	-0.579	-0.508
1 A1	2 A1	1 B1	3 A1	1

B2

```

-- Virtual --
  0.147  0.220  0.251  0.253  0.353  0.381  1.238  1.322
  4 A1   2 B1   5 A1   2 B2   3 B1   6 A1   4 B1   7
A1
  1.394  1.405  1.414  1.474  2.015  2.018  2.057  2.618
  5 B1   3 B2   8 A1   9 A1  10 A1   1 A2   4 B2  11
A1
  3.007  4.098
  6 B1  12

```

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	-20.581	AOCC	A1
1	-1.352	AOCC	A1
2	-0.579	AOCC	A1
3	-0.724	AOCC	B1
4	-0.508	AOCC	B2
0	0.147	AVIRT	A1
1	0.251	AVIRT	A1
2	0.381	AVIRT	A1
3	1.322	AVIRT	A1
4	1.414	AVIRT	A1
5	1.474	AVIRT	A1
6	2.015	AVIRT	A1
7	2.618	AVIRT	A1
8	4.098	AVIRT	A1
9	2.018	AVIRT	A2
10	0.220	AVIRT	B1
11	0.353	AVIRT	B1
12	1.238	AVIRT	B1
13	1.394	AVIRT	B1
14	3.007	AVIRT	B1
15	0.253	AVIRT	B2
16	1.405	AVIRT	B2
17	2.057	AVIRT	B2

MOLECULAR PARAMETERS:

ORB SYMM INFO:

POINT GROUP=C2v  
MOL ORB= 23

NIRREPS = 4

IRREPS =	A1	A2	B1	B2
ORBSP1 =	12	1	6	4
DOCC =	3	0	1	1
SOCC =	0	0	0	0
FDOCC =	0	0	0	0
RDOCC =	0	0	0	0
AAOCC =	3	0	1	1
BAOCC =	3	0	1	1
AAVIRT =	9	1	5	3

BAVIRT = 9 1 5 3  
 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 B1 B2 A1 A1 A1 A1 A1  
 A1 A1 A1 A1 A2 B1 B1 B1 B1 B1  
 B2 B2 B2  
 ORBSYM BETA = A1 A1 A1 B1 B2 A1 A1 A1 A1 A1  
 A1 A1 A1 A1 A2 B1 B1 B1 B1 B1  
 B2 B2 B2

BASIS ORBS	=	23	MOL ORBS	=	23
FROZEN OCC	=	0	FROZEN VIR	=	0
CORR ORBS	=	23	CORR SP ORBS	=	46
NUM ALP ELEC	=	5	NUM BET ELEC	=	5
NUM ALP EXPL	=	5	NUM BET EXPL	=	5
NUM SO OCC	=	10	NUM SO VIR	=	36
NUM RESTR DOCC	=	0	NUM RESTR DVIRT	=	0
ORBS PER BLCK	=	16	RESTRICTED_REF	=	1

BLOCKING PARAMETERS:

NUM ROCC BLOCKS = 0 NUM AOCC BLOCKS= 3  
 NUM AVIRT BLOCKS= 4 NUM RVIRT BLOCKS= 0

ORBITALS/BLOCK = 3 1 1 3 1 1 9 1 5 3 9 1 5 3

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

Integral transformation job: CPU 0.16 s wall 0.22 s  
 EHF = -76.017177750 EMP2 = -76.212163259

Beginning CC iterations

Itr	Var	D	Energy	Delta_E	Delta_t	Comments
1	CC	-	-76.214719135	2.6E-03	7.1E-02	
2	CC	-	-76.218658901	3.9E-03	2.5E-02	
3	CC	-	-76.219323577	6.6E-04	9.6E-03	
4	CC	+	-76.219819255	5.0E-04	3.7E-03	
5	CC	+	-76.219963278	1.4E-04	5.8E-04	
6	CC	+	-76.219964350	1.1E-06	1.1E-04	
7	CC	+	-76.219963989	3.6E-07	3.3E-05	
8	CC	+	-76.219964075	8.6E-08	7.8E-06	
9	CC	+	-76.219964101	2.6E-08	2.2E-06	
10	CC	+	-76.219964091	1.0E-08	6.2E-07	
11	CC	+	-76.219964089	1.5E-09	2.2E-07	
12	CC	+	-76.219964088	9.7E-10	5.6E-08	
13	CC	+	-76.219964089	3.0E-10	1.6E-08	
14	CC	+	-76.219964089	2.4E-10	4.7E-09	

Calculation converged, 14 iterations

Largest T amplitudes

Largest singles amplitudes:

Value	i	->	a
0.0245	4( B2 ) B	->	15( B2 ) B
0.0245	4( B2 ) A	->	15( B2 ) A
0.0126	2( A1 ) B	->	1( A1 ) B
0.0126	2( A1 ) A	->	1( A1 ) A
-0.0068	2( A1 ) B	->	2( A1 ) B

Largest doubles amplitudes:

Value	i	j	->	a	b
-0.0389	4( B2 ) A,	4( B2 ) B	->	16( B2 ) A,	16( B2 ) B
-0.0317	3( B1 ) A,	3( B1 ) B	->	11( B1 ) A,	11( B1 ) B
-0.0270	3( B1 ) A,	3( B1 ) B	->	12( B1 ) A,	12( B1 ) B
-0.0264	4( B2 ) A,	4( B2 ) B	->	15( B2 ) A,	15( B2 ) B
-0.0255	2( A1 ) A,	2( A1 ) B	->	4( A1 ) A,	4( A1 ) B

EHF = -76.017177750  
EMP2 = -76.212163259  
Correlation Energy = -0.202786339  
CCSD Total Energy = -76.219964089

CCSD or (V)OO-CCD job: CPU 0.78 s wall 0.84 s  
Removing integral transformation files: 151 153 152  
SIZE OF R2 LEQ 0.0 MB BLCK\_TNSR\_BUFFSZ=1000 INCORE=127007  
SOLVE EOM EQUATIONS FOR THE 1 LOWEST IONIZED STATES, TRANSITION OF A1 IRREP

State 1: 7 -> inf ( 0.6415)

1 guess vectors generated

0		0		1.9E-01		1	
1		0		6.1E-01		2	
2		0		2.7E-03		3	
3		0		3.3E-04		4	
4		0		8.8E-06		5	
5		0		3.8E-07		6	
6		0		2.3E-08		7	
7		0		3.5E-10		8	

NSDavidsonRight<T>::CalcCorrectionVec(): Warning!  
Scaled norm for root 0 is too small: 2.72E-11; ||Res||=3.47E-10

8| 1 |1.4E-11 | 9 |Collapse current subspace  
DAVIDSON ITERATIONS CONVERGED, 8 ITERATIONS  
Excitation energies, hartree

0  
0 0.526818

1 lowest roots of symmetry A1 :  
Root 1 Conv-d yes Tot Ene= -75.693146569 hartree (Ex Ene 14.3354 eV),  
U1^2=0.942837, U2^2=0.057163, ||Res||=1.4E-11  
Right U1:

Value	i	->	a
-0.9703	2( A1 ) B	->	inf

```
0.0373          1( A1 ) B  ->  inf
-0.0002         0( A1 ) B  ->  inf
```

CALCULATING LEFT VECTORS:

Re-orthogonalize vecs

Itr	ConvR	ResNormR	NVecs	Comments
0	0	8.2E-03	1	
1	0	4.6E-03	2	
2	0	9.2E-05	3	
3	0	5.7E-06	4	
4	0	3.5E-07	5	
5	0	1.9E-08	6	
6	0	1.5E-09	7	
7	1	5.8E-11	8	Collapse current subspace

DAVIDSON ITERATIONS CONVERGED, 7 ITERATIONS

Excitation energies, hartree

```
0
0 0.526818
```

Re-orthogonalize vecs

Biorthogonalize left and right vectors

CALCULATE LEFT AND RIGHT VECTORS:

Itr	ConvR	ConvL	ResNormR	ResNormL	NVecs	Lock	Comments
0	1	1	1.4E-11	5.8E-11	1	1	Collapse current subspace

DAVIDSON ITERATIONS CONVERGED, 0 ITERATIONS

Excitation energies, hartree

```
0
0 0.526818
```

SIZE OF R2 LEQ 0.0 MB BLCK\_TNSR\_BUFFSZ=1000 INCORE=127007

SOLVE EOM EQUATIONS FOR THE 1 LOWEST IONIZED STATES, TRANSITION OF B1 IRREP

State 1: 8 -> inf ( 0.7884)

1 guess vectors generated

0	0	1.6E-01	1	
1	0	4.1E-01	2	
2	0	1.3E-03	3	
3	0	9.4E-05	4	
4	0	4.9E-06	5	
5	0	1.9E-07	6	
6	0	1.9E-08	7	
7	0	6.8E-10	8	NSDavidsonRight<T>::CalcCorrectionVec(): Warning!

Scaled norm for root 0 is too small: 4.57E-11; ||Res||=6.77E-10

8| 1 |1.3E-11 | 9 |Collapse current subspace

DAVIDSON ITERATIONS CONVERGED, 8 ITERATIONS

Excitation energies, hartree

```
0
```

0 0.695595

1 lowest roots of symmetry B1 :  
Root 1 Conv-d yes Tot Ene= -75.524368802 hartree (Ex Ene 18.9281 eV),  
U1^2=0.952964, U2^2=0.047036, ||Res||=1.3E-11

Right U1:

Value	i	->	a
0.9762	3( B1 ) B	->	inf

CALCULATING LEFT VECTORS:

Re-orthogonalize vecs

Itr	ConvR	ResNormR	NVecs	Comments
0	0	6.0E-03	1	
1	0	2.1E-03	2	
2	0	5.3E-05	3	
3	0	4.0E-06	4	
4	0	2.2E-07	5	
5	0	8.0E-09	6	
6	0	5.9E-10	7	
7	1	5.2E-11	8	Collapse current subspace

DAVIDSON ITERATIONS CONVERGED, 7 ITERATIONS

Excitation energies, hartree

0  
0 0.695595

Re-orthogonalize vecs

Biorthogonalize left and right vectors

Negative norm is detected for vector 0: NORM=-0.999158

CALCULATE LEFT AND RIGHT VECTORS:

Itr	ConvR	ConvL	ResNormR	ResNormL	NVecs	Lock	Comments
0	1	1	1.3E-11	5.2E-11	1	1	Collapse current subspace

DAVIDSON ITERATIONS CONVERGED, 0 ITERATIONS

Excitation energies, hartree

0  
0 0.695595

SIZE OF R2 LEQ 0.0 MB BLCK\_TNSR\_BUFFSZ=1000 INCORE=127007

SOLVE EOM EQUATIONS FOR THE 1LOWEST IONIZED STATES, TRANSITION OF B2 IRREP

State 1: 9 -> inf ( 0.5677)

1 guess vectors generated

0	0	2.0E-01	1	
1	0	5.3E-01	2	
2	0	2.3E-03	3	
3	0	2.0E-04	4	
4	0	6.0E-06	5	
5	0	2.3E-07	6	
6	0	1.2E-08	7	

7| 0 |3.4E-10 | 8 |NSDavidsonRight<T>::CalcCorrectionVec(): Warning!  
Scaled norm for root 0 is too small: 1.05E-11; ||Res||=3.44E-10

8| 1 |7.2E-12 | 9 |Collapse current subspace  
DAVIDSON ITERATIONS CONVERGED, 8 ITERATIONS  
Excitation energies, hartree  
0  
0 0.445666

1 lowest roots of symmetry B2 :  
Root 1 Conv-d yes Tot Ene= -75.774297979 hartree (Ex Ene 12.1272 eV),  
U1^2=0.940265, U2^2=0.059735, ||Res||=7.2E-12  
WARNING: Total energy for excited state 1 has been written in energy location  
Right U1:

Value	i	->	a
0.9697	4( B2 ) B	->	inf

CALCULATING LEFT VECTORS:

Re-orthogonalize vecs

Itr	ConvR	ResNormR	NVecs	Comments
0	0	8.6E-03	1	
1	0	4.0E-03	2	
2	0	1.3E-04	3	
3	0	5.7E-06	4	
4	0	3.2E-07	5	
5	0	1.1E-08	6	
6	0	5.6E-10	7	NSDavidsonRight<T>::CalcCorrectionVec(): Warning!

Scaled norm for root 0 is too small: 4.71E-11; ||Res||=5.60E-10

7| 1 |3.0E-11 | 8 |Collapse current subspace  
DAVIDSON ITERATIONS CONVERGED, 7 ITERATIONS  
Excitation energies, hartree  
0  
0 0.445666

Re-orthogonalize vecs

Biorthogonalize left and right vectors

CALCULATE LEFT AND RIGHT VECTORS:

Itr	ConvR	ConvL	ResNormR	ResNormL	NVecs	Lock	Comments
0	1	1	7.2E-12	3.0E-11	1	1	Collapse current subspace

DAVIDSON ITERATIONS CONVERGED, 0 ITERATIONS  
Excitation energies, hartree  
0  
0 0.445666

<STATE 1/B2 |Mu|STATE 1/A1 >  
Energies= -75.774297983 -75.693146584 hartree (Delta Ene 2.2082 eV)

Transition dipole	x	y	z	
<Gr.St. mu Exc.St.>	0.000000000	-0.137607865	-0.000000000	a.u.
<Exc.St. mu Gr.St.>	0.000000000	-0.141510587	-0.000000000	a.u.

mu^2 = 0.019472970 a.u.  
f\_L = 0.001053506 a.u.

<STATE 1/B2 |Mu|STATE 1/B1 >  
Energies= -75.774297983 -75.524368806 hartree (Delta Ene 6.8009 eV)

Transition dipole  
<Gr.St.|mu|Exc.St.> x y z a.u.  
<Exc.St.|mu|Gr.St.> x y z a.u.  
mu^2 = -0.000000000 a.u.  
f\_L = -0.000000000 a.u.

EOM-IP-CCSD PROPERTIES FOR 1/A1 TRANSITION:

Dipole moment  
Total x y z a.u.  
|mu| = 0.729991543 a.u.  
XX

<R^2> x^2 y^2 z^2 a.u.  
Total <R^2> = 14.663105795 a.u.  
XX

EOM-IP-CCSD PROPERTIES FOR 1/B1 TRANSITION:

Dipole moment  
Total x y z a.u.  
|mu| = 1.116674999 a.u.  
XX

<R^2> x^2 y^2 z^2 a.u.  
Total <R^2> = 14.737060634 a.u.  
XX

EOM-IP-CCSD PROPERTIES FOR 1/B2 TRANSITION:  
WARNING: density has been written in density file  
Write\_OPDM(): position=0, offset=0 FILE=54  
Write\_OPDM(): offset=0 FILE=54

Dipole moment  
Total x y z a.u.  
|mu| = 0.899644878 a.u.  
XX

<R^2> x^2 y^2 z^2 a.u.  
Total <R^2> = 14.784767501 a.u.  
XX

EOM-IP-CCSD job: CPU 0.36 s wall 0.36 s

CCMAN JOB: ALL CPU 1.14 s wall 1.20 s  
 Cleaning up statics....  
 Analysis of SCF Wavefunction

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

Alpha MOs, Restricted  
 -- Occupied --  
 -20.581 -1.352 -0.579 -0.724 -0.508  
 1 A1 2 A1 3 A1 1 B1 1  
 B2  
 -- Virtual --  
 0.147 0.251 0.381 1.322 1.414 1.474 2.015 2.618  
 4 A1 5 A1 6 A1 7 A1 8 A1 9 A1 10 A1 11  
 A1  
 4.098 2.018 0.220 0.353 1.238 1.394 3.007 0.253  
 12 A1 1 A2 2 B1 3 B1 4 B1 5 B1 6 B1 2  
 B2  
 1.405 2.057  
 3 B2 4  
 B2

Beta MOs, Restricted  
 -- Occupied --  
 -20.581 -1.352 -0.579 -0.724 -0.508  
 1 A1 2 A1 3 A1 1 B1 1  
 B2  
 -- Virtual --  
 0.147 0.251 0.381 1.322 1.414 1.474 2.015 2.618  
 4 A1 5 A1 6 A1 7 A1 8 A1 9 A1 10 A1 11  
 A1  
 4.098 2.018 0.220 0.353 1.238 1.394 3.007 0.253  
 12 A1 1 A2 2 B1 3 B1 4 B1 5 B1 6 B1 2  
 B2  
 1.405 2.057  
 3 B2 4  
 B2

-----  
 Mulliken Net Atomic Charges  
 -----

Atom	Charge (a.u.)
1 H	0.599248
2 O	-0.197537
3 H	0.599248
-----	
Sum of atomic charges =	1.000960

-----  
 Cartesian Multipole Moments  
 -----

Charge (ESU x 10<sup>10</sup>)

```

          4.8078
Dipole Moment (Debye)
  X      0.0000      Y      0.0000      Z      2.2867
  Tot    2.2867
Quadrupole Moments (Debye-Ang)
  XX     -2.1212     XY      0.0000     YY     -4.9026
  XZ      0.0000     YZ      0.0000     ZZ     -4.5708
Octapole Moments (Debye-Ang^2)
  XXX      0.0000   XXY      0.0000   XYY      0.0000
  YYY      0.0000   XXZ      1.8226   XYZ      0.0000
  YYZ      0.2699   XZZ      0.0000   YZZ      0.0000
  ZZZ      1.5782
Hexadecapole Moments (Debye-Ang^3)
  XXXX     -2.9354   XXXY      0.0000   XXYY     -1.3621
  XYYY      0.0000   YYYY     -3.0402   XXXZ      0.0000
  XXYZ      0.0000   XYYZ      0.0000   YYYZ      0.0000
  XXZZ     -0.8957   XYZZ      0.0000   YYZZ     -1.3382
  XZZZ      0.0000   YZZZ      0.0000   ZZZZ     -4.7393

```

---

Total job time: 1.95s(wall), 1.75s(cpu)  
 Fri Dec 14 18:38:47 2007

```

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

```