From Phenyl Chlorides to α,n-Didehydrotoluenes (α,n-DHTs) via Phenyl Cations. A CPCM-CASMP2 Investigation.

Davide Ravelli, Stefano Protti, Maurizio Fagnoni* and Angelo Albini

PhotoGreen Lab, Department of Chemistry,

University of Pavia, Viale Taramelli 12, 27100 Pavia, Italy

*Email of corresponding author: fagnoni@unipv.it

webpage: www.unipv.it/photochem

Supporting Information

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1. Computational details

All of the calculations were carried out using the Gaussian 03 program package.[S1] The CASMP2/6-31G(d) Gibbs free energies reported in the text (see also Tables S1, S3 and S5) have thus been calculated by means of Eq. 1 reported below:

$$G_{CASMP2} = E_{0(CASSCF,CPCM)} + \Delta E_{CORR(MP2,vacuo)} + \Delta G_{CORR(CASSCF,vacuo)} \quad (1)$$

Where:

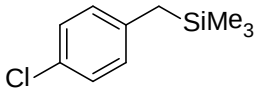
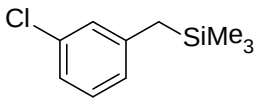
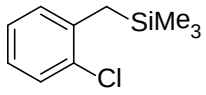
- $E_{0(CASSCF,CPCM)}$ is the total electronic energy calculated at the CPCM-CASSCF level (MeOH bulk);
- $\Delta E_{CORR(MP2,vacuo)}$ is the MP2 correction calculated in vacuo on the geometry optimized at the CASSCF level;
- $\Delta G_{CORR(CASSCF,vacuo)}$ is the unscaled thermal correction to Gibbs Free Energy as from the output of the frequency calculation at the CASSCF level (in vacuo), also including the zero-point vibrational energy (ZPVE).

Further notice that the three terms from Eq. 1 have been reported in blue color for all of the stationary points reported below.

Optimized geometry listed in cartesian format (coordinates are given in Å), minimum energies and thermochemical data (in Hartree; the default options were adopted in the latter case, *viz.* temperature: 298.150 K and pressure: 1.00000 atm) are reported below.

The conversion factor between Hartree and kcal mol^{-1} has been: 1 Hartree = 627.509 kcal mol^{-1}.

Table S1. Gibbs free energies of the stationary points described in the text for the three isomeric (chlorobenzyl)trimethylsilanes (**1a-c**) calculated at the CPCM-CASMP2(10,10)/6-31G(d) level of theory in MeOH bulk. The values reported below have been determined according to Eq. 1.

Species	**G_{CASMP2} [Hartree]**			
	1a-c	**^{1}1a-c**[a]	**^{3}1a-c(α)**	**^{3}1a-c(β)**
 **1a**	-1137.134751	-1136.962855	-1137.026393	-1137.026061
	$\Delta G(\alpha$ *vs* $\beta) = -0.55$ kcal mol^{-1} $\Delta G(^1$**1a-1a**$) = 107.66$ kcal mol^{-1} $\Delta G(^3$**1a(α)-1a**$) = 67.42$ kcal mol^{-1}			
 **1b**	-1137.134471	-1136.974705	-1137.025325	-1137.025861
	$\Delta G(\alpha$ *vs* $\beta) = 0.10$ kcal mol^{-1} $\Delta G(^1$**1b-1b**$) = 100.04$ kcal mol^{-1} $\Delta G(^3$**1b(β)-1b**$) = 67.98$ kcal mol^{-1}			
 **1c**	-1137.132767	-1136.972970	-1137.022436	-1137.025995
	$\Delta G(\alpha$ *vs* $\beta) = 2.87$ kcal mol^{-1} $\Delta G(^1$**1c-1c**$) = 99.95$ kcal mol^{-1} $\Delta G(^3$**1c(β)-1c**$) = 66.13$ kcal mol^{-1}			

[a] The role of higher excited states has been safely ruled out by calculation of the vertical excitation energy starting from the equilibrium geometry of **1a**. Thus, only the excitation energy to the first excited singlet (^{1}**1a**) was compatible with the actual wavelength used in the experiment (254 nm; data not reported).

Table S2. Total electronic energy (E_0(CASSCF,CPCM)) calculated at the CPCM-CASSCF(10,10)/6-31G(d) level of theory (MeOH bulk).

C-Cl length	E_0(CASSCF,CPCM) [Hartree]*		
	1a	**^{1}1a**	**^{3}1a(α)**
1.4	-1135.851726	-1135.686185	-1135.727865
1.5	-1135.917390	-1135.747576	-1135.790153
1.6	-1135.952328	-1135.779738	-1135.823872
1.7	-1135.967794	-1135.793409	-1135.839923
1.8	-1135.971078	-1135.795529	-1135.845369
1.9	-1135.966940	-1135.790660	-1135.844964
2.0	-1135.958545	-1135.781825	-1135.841832
2.1	-1135.947924	-1135.770991	-1135.837920
2.2	-1135.936398	-1135.759400	-1135.834164
2.3	-1135.925151	-1135.748191	-1135.831274
2.4	-1135.913822	-1135.737045	-1135.828072
2.5	-1135.903099		-1135.825441
2.6	-1135.893164		-1135.823899
2.7	-1135.884144		
2.8	-1135.876148		
2.9	-1135.869243		
3.0	-1135.863450		

* The energies reported refer to single point calculations carried out starting from the equilibrium geometries.

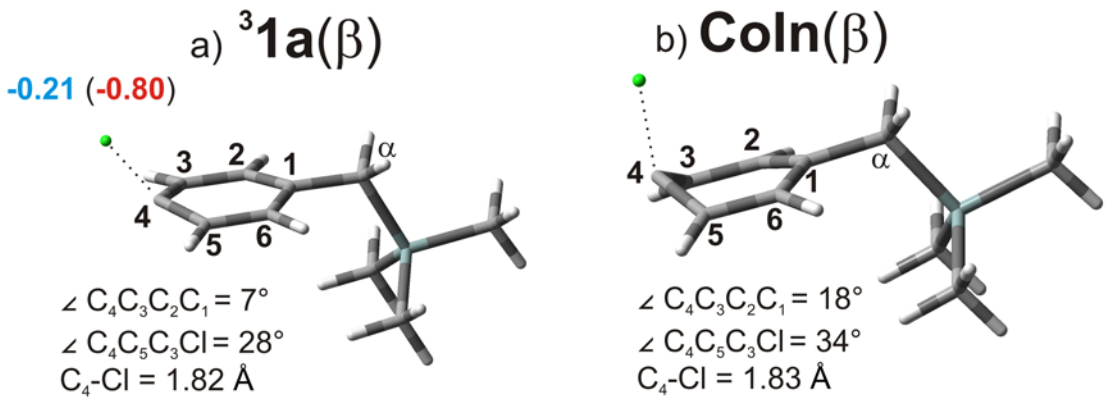


Fig. S1. a) Optimized geometries at the CASSCF/6-31G(d) of the triplet state ^{3}**1a(β)** (relative minimum) for compound **1a**. ESP charges for the Cl atom at the equilibrium geometry and upon stretching of the C-Cl bond up to 2.6 Å are reported in blue and red colours, respectively, as from the results of calculations at the CPCM-CASSCF/6-31G(d) level of theory in MeOH bulk. b) Optimized geometry at the CASSCF/6-31G(d) of the Conical Intersection (CoIn) connecting the ^{1}**1a** and ^{3}**1a** (β structure) PESs, along with some of the most relevant parameters of this structure.

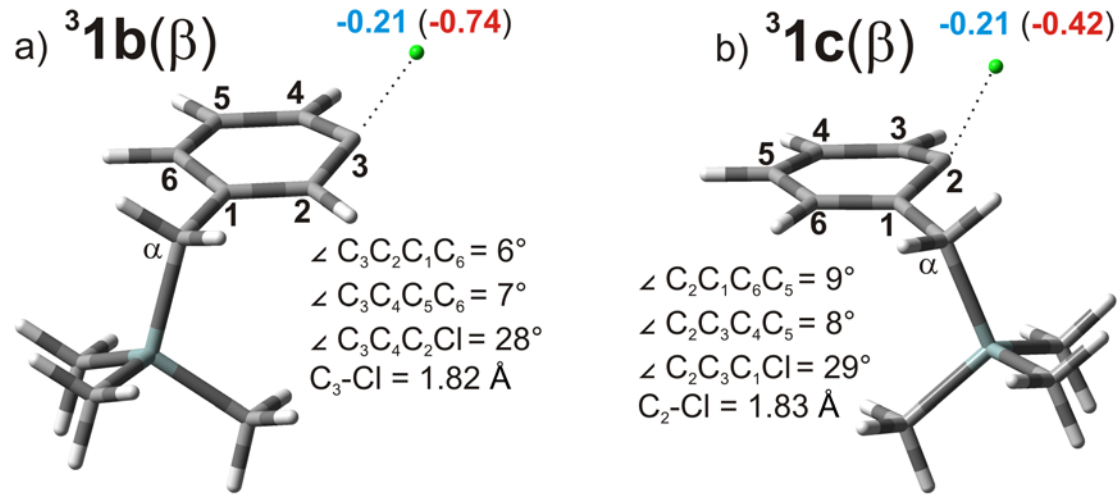
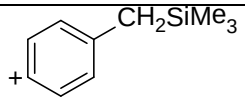
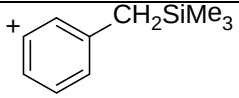
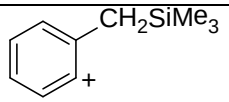
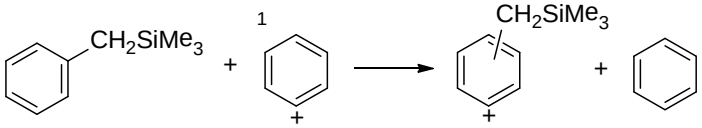


Fig. S2. Optimized geometries at the CASSCF/6-31G(d) of the triplet states: a) ^{3}**1b(β)** (absolute minimum) and b) ^{3}**1c(β)** (absolute minimum). ESP charges for the Cl atom at the equilibrium geometry and upon stretching of the C-Cl bond up to 2.6 Å are reported in blue and red colours, respectively, as from the results of calculations at the CPCM-CASSCF/6-31G(d) level of theory in MeOH bulk.

Table S3. Gibbs free energies of the stationary points described in the text for the three isomeric phenyl cations (**2$^+$a-c**) calculated at the CPCM-CASMP2(8,9)/6-31G(d) level of theory in MeOH bulk. The values reported below have been determined according to Eq. 1.

Species	G_{CASMP2} [Hartree]	
	SINGLET	**TRIPLET**
 **2$^+$a**	-677.222380	-677.225776
 **2$^+$b**	-677.222187	-677.220374
 **2$^+$c**	-677.228804	-677.222516

The isodesmic reaction reported in Eq. 2 (see main text and below) was used to quantify the stabilization of the isomeric phenyl cations **2$^+$a-c**. The results are reported in Table S4 and in Fig. 5 (see main text).



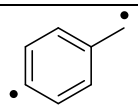
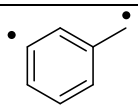
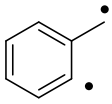
(2)

Table S4. Relative stability of phenyl cations **2$^+$a-c** according to the isodesmic reaction in Eq. 2.

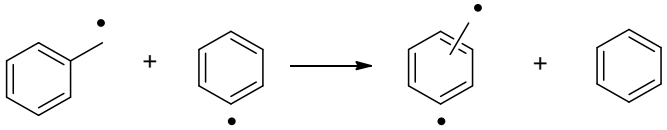
Species	ΔG_{CASMP2} [kcal mol^{-1}]*	
	SINGLET	**TRIPLET**
2$^+$a	8.28	6.14
2$^+$b	8.40	9.53
2$^+$c	4.24	8.19

* These values have been calculated by taking the difference between the G_{CASMP2} (as from Eq. 1) values among the required species (see Eq. 2).

Table S5. Gibbs free energies of the stationary points described in the text for the three isomeric DHTs (**3a-c**) calculated at the CPCM-CASMP2(8,8)/6-31G(d) level of theory in MeOH bulk. The values reported below have been determined according to Eq. 1.

Species	**G_{CASMP2} [Hartree]**	
	SINGLET	**TRIPLET**
 **3a**	-269.196588	-269.206038
 **3b**	-269.207215	-269.204886
 **3c**	-269.197005	-269.205973

The isodesmic reaction reported in Eq. S1 was used to quantify the stabilization of the isomeric DHTs **3a-c**. The results are reported in Table S6 and in Fig. S3.



Eq. S1

Table S6. Relative stability of DHTs **3a-c** according to the isodesmic reaction in Eq. S1.

Species	ΔG_{CASMP2} [kcal mol^{-1}]*	
	SINGLET	TRIPLET
3a	5.00	-0.93
3b	-1.66	-0.20
3c	4.74	-0.89

* These values have been calculated by taking the difference between the G_{CASMP2} (as from Eq. 1) values among the required species (see Eq. S1).

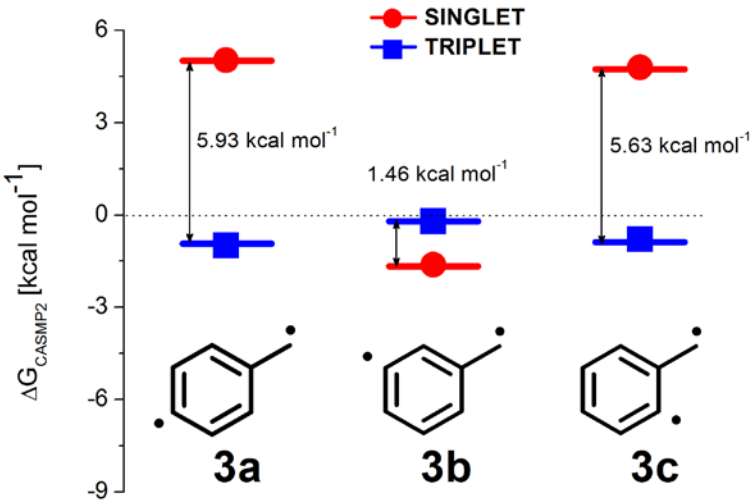


Fig. S3. Relative energies of DHTs **3a-c** according to the isodesmic reaction reported in Eq. S1.

2. Cartesian coordinates and CASSCF output data for structures 1a-c

The level of theory chosen for optimizing these structures was the CASSCF(10,10)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π^* orbitals of the aromatic ring and the σ/σ^* couple of the C-Cl and C-Si bonds (see Fig. S4 for a graphical representation of the orbitals included in the active space in the case of **1a**, taken as a model). For all of the structures reported in this section, numerical frequency calculations (FREQ=NUMER) have been adopted.

As mentioned in the text, two different minima were located for the lowest-energy triplet states of compounds **1a-c**, *viz.* a geometry with the chlorine atom and the TMS group on the same side (hereafter tagged as geometry "α") or opposite (hereafter tagged as geometry "β") with respect to the plane of the aromatic ring, in accordance with the results previously obtained having recourse to Density Functional Theory (DFT, UB3LYP/6-311+G(2d,p) level of theory).[S2]

The entries named " E_0(CASSCF,CPCM,STRETCH,#)" refer to the total electronic energy as from single point calculations carried out at the CPCM-CASSCF(10,10)/6-31G(d) (MeOH bulk) level of theory, when imposing an elongation to the C-Cl bond up to # Å. Thus, the energies reported in the test only consider the total electronic energy variation.

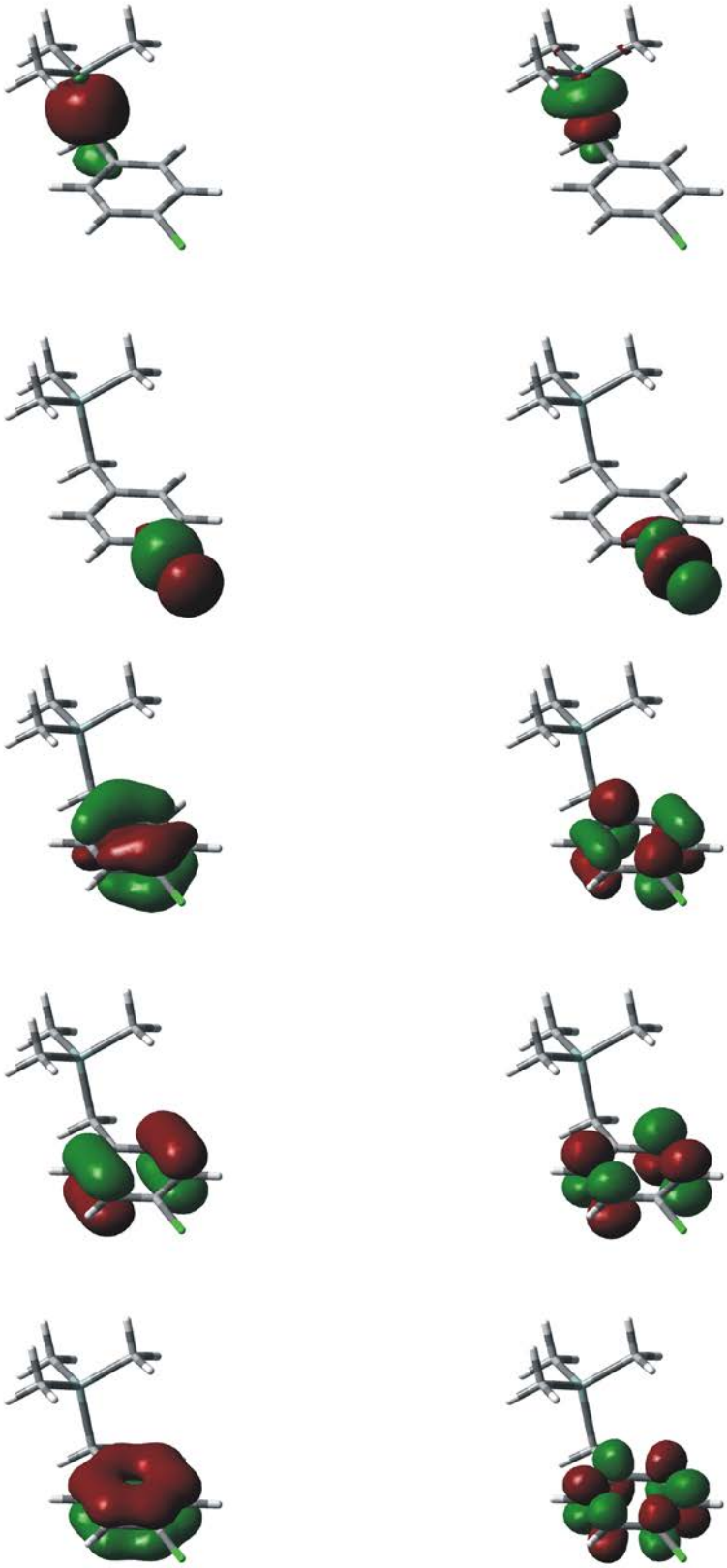
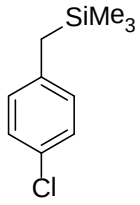


Fig. S4. Orbitals included in the active space for the CASSCF calculations in the case of **1a**, taken as a model.



1a

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39040000
C	1.21902100	0.00000000	2.06861000
C	2.43962000	0.00021500	1.37989800
C	2.40098100	0.00234800	-0.02106100
C	1.19164100	0.00236700	-0.71638200
H	-0.92734800	0.00400900	1.93117800
H	1.21513900	0.00605900	3.14438600
H	3.32096800	0.01024100	-0.57865400
H	1.17730700	0.00819000	-1.78978400
C	3.75571000	-0.02358300	2.12427800
H	3.65663200	0.51024700	3.06719900
H	4.51227400	0.51195100	1.55444900
C	4.77142600	-2.74173700	0.91841400
H	5.19292700	-3.72198700	1.12820100
H	3.85408300	-2.89501700	0.35694000
H	5.47139900	-2.22089500	0.26923000
C	3.24816700	-2.74479200	3.61141400
H	3.64609900	-3.72507600	3.86292300
H	3.05188300	-2.22573100	4.54668300
H	2.29448100	-2.89817300	3.11419900
C	6.09670400	-1.55043400	3.44669700
H	5.95602300	-1.00178900	4.37488600
H	6.54703700	-2.50711100	3.70029500
H	6.81917900	-0.99999800	2.84887900
Si	4.46112200	-1.78502100	2.52128600
Cl	-1.55024400	0.00355800	-0.87684700

E_0(CASSCF,vacuo) -1135.965437

Zero-point correction=	0.233630
Thermal correction to Energy=	0.247665
Thermal correction to Enthalpy=	0.248609
Thermal correction to Gibbs Free Energy=	**0.192357**

E_0(CASMP2,vacuo) -1137.325164

ΔE_{CORR}(MP2) **-1.359727**

E_0(CASSCF,CPCM) **-1135.971145**

E_0(CASSCF,CPCM,STRETCH,2.3) -1135.925150

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.9654365869
Full Convergence on CI vector     -0.11359654E+04
          ( 1)        EIGENVALUE
(     1) 0.9300895 ( 1711)-0.1457611 (   21)-0.1418912 ( 1833)-0.1319749 ( 2279)-0.1080916 ( 8128)-0.1035699 ( 1719) 0.0886927
(    59) 0.0871899 (  325)-0.0842320 ( 1662) 0.0640057 (   42) 0.0617320 (   36)-0.0420267 (   66)-0.0389694 ( 8007)-0.0388083
(    45)-0.0372260 (    6)-0.0364283 (   10)-0.0331000 ( 1770)-0.0318473 ( 2346) 0.0313815 ( 1891)-0.0304803 (  191) 0.0254579
( 2851) 0.0246870 ( 1659)-0.0238833 ( 8005)-0.0210032 ( 3069)-0.0209618 ( 8517)-0.0208661 ( 2433)-0.0207941 ( 8012) 0.0203098
( 9046) 0.0179423 ( 9180) 0.0174290 (19503) 0.0164216 (  305)-0.0153924 (20032) 0.0150298 ( 2926) 0.0133450 ( 4753) 0.0132396
( 2298)-0.0132289 (  666) 0.0130884 ( 2918)-0.0130693 (  210) 0.0129726 ( 8010) 0.0126452 (21863) 0.0126049 ( 5082) 0.0120045
( 3176) 0.0117288 (  310)-0.0110747 ( 8258)-0.0108971 ( 3061)-0.0107724 ( 2418)-0.0107247 (10573)-0.0105524 ( 2151) 0.0104433
( 8522) 0.0103790 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197074D+01
     2  0.396844D-08  0.190243D+01
     3 -0.448865D-07  0.234844D-05  0.198266D+01
     4 -0.152620D-06 -0.425169D-05  0.331490D-05  0.196015D+01
     5 -0.196060D-06  0.568260D-05 -0.171954D-05 -0.789583D-07  0.190055D+01
     6  0.174057D-05 -0.252688D-08  0.146458D-06 -0.151844D-05 -0.326702D-05
     7  0.257897D-07  0.212255D-04 -0.295813D-05  0.283905D-05  0.114796D-05
     8  0.354975D-06  0.429310D-05 -0.161977D-06 -0.202267D-05 -0.903442D-05
     9 -0.100237D-06 -0.183192D-05 -0.374389D-06  0.225712D-05  0.101406D-05
    10  0.107220D-06  0.403240D-05 -0.334270D-05  0.250627D-05 -0.222331D-04
                6             7             8             9            10
     6  0.292503D-01
     7 -0.297343D-07  0.100054D+00
     8  0.236053D-05 -0.419545D-05  0.375100D-01
     9  0.107371D-06 -0.945478D-06 -0.296877D-06  0.174427D-01
    10 -0.628309D-06  0.134592D-05  0.141315D-06 -0.188393D-06  0.992087D-01
MCSCF converged.
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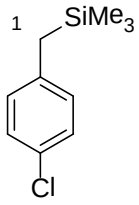

[1]1a

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.42707100
C	1.25744300	0.00000000	2.11555000
C	2.50040500	0.00188800	1.38980900
C	2.46055200	0.00281900	-0.04894000
C	1.21196200	0.00284100	-0.75339600
H	-0.92636200	0.00371800	1.96527400
H	1.26796500	0.00946700	3.18881300
H	3.37760100	0.01441000	-0.60659700
H	1.17997000	0.00865300	-1.82426800
C	3.81256700	-0.04301200	2.11909800
H	3.72886800	0.48148100	3.06948200
H	4.57494300	0.48346300	1.54731700
C	4.79278200	-2.76996300	0.89054000
H	5.20722900	-3.75509200	1.09156500
H	3.86976700	-2.91139600	0.33531100
H	5.49210300	-2.25151900	0.23882100
C	3.28964100	-2.77352500	3.59466500
H	3.68027500	-3.75870000	3.83858100
H	3.10469700	-2.25716200	4.53367200
H	2.33099400	-2.91507000	3.10354400
C	6.14814600	-1.60577300	3.41531700
H	6.01968600	-1.06108200	4.34759200
H	6.59093900	-2.56827900	3.66014500
H	6.87149000	-1.05900400	2.81519600
Si	4.50332500	-1.81903600	2.50073200
Cl	-1.54577800	-0.00199400	-0.85919500

E_0(CASSCF,vacuo) -1135.790557

Zero-point correction= 0.228834
Thermal correction to Energy= 0.243969
Thermal correction to Enthalpy= 0.244913
Thermal correction to Gibbs Free Energy= **0.186568**

E_0(CASMP2,vacuo) -1137.147722
ΔE_{CORR}(MP2) **-1.357719**

E_0(CASSCF,CPCM) **-1135.795794**

E_0(CASSCF,CPCM,STRETCH,2.3) -1135.748191

DATA from the CASSCF calculation in vacuo:

```
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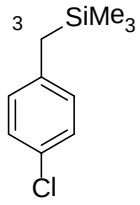
 Full Convergence on CI vector
 Energy state  2 =    -1135.7905566058
 Full Convergence on CI vector
                 ( 1)      EIGENVALUE     -0.1135952 7E+04
 (     1) 0.9175989 ( 1711)-0.1589353 (    21)-0.1549273 ( 1833)-0.1477982 ( 2279)-0.1170564 ( 8128)-0.1013350 ( 1719) 0.0972907
 (    59) 0.0944858 (  325)-0.0819923 ( 1662) 0.0700325 (   42) 0.0661390 (   36)-0.0432395 (   45)-0.0410716 (   66)-0.0392784
 ( 2346) 0.0373183 (    6)-0.0371082 ( 1770)-0.0356210 (   10)-0.0349279 ( 8007)-0.0339004 ( 1891)-0.0314900 ( 1659)-0.0307417
 (  191) 0.0283467 ( 2851) 0.0272581 ( 2433)-0.0251448 ( 3069)-0.0250903 (  305)-0.0224804 (   56) 0.0214917 ( 8517)-0.0208382
 ( 8005)-0.0195059 ( 8012) 0.0188425 ( 9180) 0.0185038 (19503) 0.0178059 (    7)-0.0166975 (20032) 0.0166840 (  331) 0.0165907
 ( 1654)-0.0164956 ( 2298)-0.0161229 ( 2926) 0.0160534 ( 2918)-0.0156181 (  210) 0.0153576 ( 2203)-0.0147464 (  666) 0.0144530
 ( 3176) 0.0142700 ( 4753) 0.0142471 ( 1848)-0.0138566 (21863) 0.0134869 ( 5082) 0.0133822 ( 9046) 0.0130634 (  156)-0.0129470
 ( 8010) 0.0125852 (
                 ( 2)      EIGENVALUE     -0.1135790 6E+04
 (     4) 0.6513549 ( 1831)-0.5713020 ( 1661) 0.1652253 (   34)-0.1626359 ( 1841)-0.1570621 (   58)-0.1514115 ( 1834) 0.1498174
 (     9) 0.1460472 ( 1769)-0.1421115 ( 1717) 0.1388726 (  164)-0.0865206 ( 3011) 0.0808870 ( 2204)-0.0753879 ( 8773) 0.0733797
 ( 2419) 0.0682462 (20027)-0.0626902 (  521)-0.0580443 ( 5075) 0.0511887 ( 1669) 0.0404667 ( 3166)-0.0354051 (  126) 0.0333842
 ( 3218)-0.0310836 ( 3019) 0.0273603 ( 1850) 0.0270217 ( 2868) 0.0259693 ( 3238) 0.0254998 (  208)-0.0245941 ( 2911) 0.0245163
 ( 2161)-0.0239500 ( 2435) 0.0234165 ( 2920)-0.0231712 ( 2853)-0.0226715 ( 3226)-0.0222132 (  193)-0.0193963 (10146) 0.0188996
 (19448)-0.0186967 ( 2281)-0.0182197 (20045) 0.0181751 ( 2153) 0.0177953 (20033)-0.0177582 (10572) 0.0166599 ( 8910)-0.0160298
 (19638)-0.0159318 (19700) 0.0158128 ( 8652) 0.0156537 ( 8572) 0.0154606 (  129)-0.0151191 ( 4698) 0.0147672 (  897)-0.0147367
 ( 8130) 0.0146466 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.197133D+01
      2 -0.329893D-07  0.148839D+01
      3 -0.292955D-07 -0.181122D-05  0.198231D+01
      4  0.207241D-06  0.203611D-05 -0.118021D-05  0.184831D+01
      5  0.122577D-05 -0.681481D-05  0.198372D-04 -0.319021D-04  0.138638D+01
      6  0.219291D-05 -0.125486D-06  0.203798D-05 -0.253226D-05 -0.314294D-05
      7  0.841914D-08  0.229031D-04 -0.527771D-05  0.321803D-05  0.387367D-04
      8  0.644856D-06 -0.393809D-05  0.386443D-05 -0.109794D-05  0.881702D-05
      9 -0.118418D-05 -0.191707D-06 -0.303912D-05  0.287147D-05 -0.518188D-06
     10  0.129486D-05  0.427969D-04 -0.580519D-05  0.211159D-05  0.910073D-05
                   6             7             8             9            10
      6  0.286354D-01
      7 -0.488773D-07  0.628903D+00
      8 -0.973894D-06 -0.333119D-05  0.125125D+00
      9 -0.141778D-05  0.546849D-07 -0.171489D-05  0.175928D-01
     10 -0.347583D-05  0.795874D-05 -0.132823D-04 -0.150568D-05  0.523026D+00
 MCSCF converged..
```



^{3}1a(α)

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48025600
C	1.18845400	0.00000000	2.14383100
C	2.44662400	-0.15647200	1.45502800
C	2.41180900	-0.43593300	0.03990200
C	1.24651500	-0.44397100	-0.66355500
H	-0.93857700	0.06512700	1.99766700
H	1.19751300	0.06348700	3.21829300
H	3.33238000	-0.69694100	-0.45309800
H	1.21450700	-0.70164800	-1.70541700
C	3.74996000	-0.06963500	2.19492500
H	4.48626400	-0.72695100	1.73514600
H	3.62354200	-0.41908800	3.21838900
C	3.35630300	2.88960000	3.17198200
H	3.79206700	3.88257700	3.25328000
H	2.41255900	2.99083900	2.64329200
H	3.13350500	2.55057800	4.18098500
C	4.88710200	2.34325400	0.53645900
H	5.35156000	3.32598800	0.56839400
H	5.56319800	1.68336500	-0.00215800
H	3.97741200	2.43234400	-0.05085200
C	6.15502800	1.56855300	3.25247600
H	6.85401100	0.89046500	2.76881400
H	6.64674600	2.53455900	3.33821600
H	5.98707500	1.19929800	4.26131500
Si	4.53457200	1.70691300	2.28257600
Cl	-0.72031400	1.50377400	-0.73009200

E_0(CASSCF,vacuo) -1135.839478

Zero-point correction= 0.229811
Thermal correction to Energy= 0.244502
Thermal correction to Enthalpy= 0.245446
Thermal correction to Gibbs Free Energy= **0.186611**

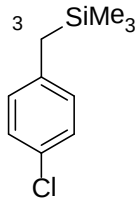
E_0(CASMP2,vacuo) -1137.211522
ΔE_{CORR}(MP2) **-1.372043**

E_0(CASSCF,CPCM) **-1135.845640**

E_0(CASSCF,CPCM,STRETCH,2.6) -1135.823899

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.8394784465
Full Convergence on CI vector
         ( 1)        EIGENVALUE     -0.1135839E+04
(     1) 0.9245075 (14731)-0.1254331 (  239)-0.1131088 (  505) 0.0978408 ( 7782)-0.0959627 ( 3787)-0.0829284 (26492) 0.0754624
(14997) 0.0723524 (26547)-0.0667853 ( 1080) 0.0661644 (14788) 0.0655264 (14785) 0.0638566 (26701) 0.0624543 ( 1079) 0.0601273
(14942)-0.0596949 (26758)-0.0569283 (14701) 0.0553840 (   31)-0.0550878 ( 1345)-0.0543324 ( 1346)-0.0535425 (  240)-0.0504585
(14939)-0.0486009 (26671)-0.0465021 (   88) 0.0459681 (  451)-0.0455609 (26489) 0.0445160 (  297) 0.0398583 (  506) 0.0381692
(  638)-0.0317746 ( 7779)-0.0273674 ( 7781)-0.0272247 (15682)-0.0266841 ( 7572)-0.0265549 (  242)-0.0263026 (38370) 0.0229194
(15541) 0.0223220 (  142)-0.0221612 (14786) 0.0206652 (16801)-0.0197687 (  642)-0.0176153 ( 1479) 0.0172705 ( 1291) 0.0172469
(26755)-0.0167149 (   86)-0.0159326 ( 1137)-0.0154058 ( 1261) 0.0149368 ( 1687) 0.0144299 (14940)-0.0140130 (16942) 0.0137027
(15149) 0.0135007 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192518D+01
     2  0.114150D-05  0.188513D+01
     3 -0.304723D-05  0.159154D-06  0.196915D+01
     4  0.114997D-05  0.237037D-06 -0.107391D-06  0.198252D+01
     5  0.165260D-04  0.306750D-04 -0.352791D-05 -0.451452D-05  0.102541D+01
     6  0.100217D-05  0.380680D-05  0.200742D-05 -0.614649D-06 -0.364715D-06
     7  0.138543D-05  0.745886D-05  0.665359D-06 -0.983876D-07 -0.678607D-05
     8 -0.215045D-05  0.218056D-05 -0.130804D-05  0.358680D-06  0.744756D-05
     9  0.123402D-04  0.125087D-05 -0.104142D-05  0.196192D-05  0.585755D-05
    10 -0.184974D-06  0.414044D-06 -0.540128D-06 -0.237218D-05  0.170252D-05
                6             7             8             9            10
     6  0.979207D+00
     7 -0.922855D-05  0.114442D+00
     8 -0.213410D-04 -0.112632D-05  0.718439D-01
     9 -0.259674D-04  0.691118D-06 -0.517166D-05  0.296236D-01
    10  0.205251D-05 -0.133318D-06 -0.384865D-06  0.212948D-05  0.174949D-01
MCSCF converged.
```



^{3}1a(β)

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48086200
C	1.18626600	0.00000000	2.14810400
C	2.44872600	-0.14626900	1.46368300
C	2.42017800	-0.40301800	0.04350500
C	1.25791600	-0.41086000	-0.66467600
H	-0.93904900	0.07249100	1.99637100
H	1.18987300	0.06781200	3.22220700
H	3.34541400	-0.63622300	-0.45435100
H	1.23622600	-0.63799900	-1.71384600
C	3.74327000	-0.16516300	2.22628200
H	3.68029600	0.50275300	3.08338100
H	4.54833200	0.21941100	1.60284200
C	4.56000100	-3.10449100	1.45099200
H	4.90738600	-4.07037300	1.81006000
H	3.63773700	-3.27440300	0.90226500
H	5.30055400	-2.73701800	0.74453500
C	3.01663600	-2.60087500	4.08290300
H	3.33896100	-3.55861500	4.48461300
H	2.84784900	-1.93668700	4.92723900
H	2.06001900	-2.75952500	3.59274200
C	5.94938000	-1.65380600	3.80478900
H	5.84137500	-0.96576700	4.63974800
H	6.32444700	-2.59292200	4.20441200
H	6.71637000	-1.25127200	3.14758900
Si	4.30996100	-1.90240200	2.89100500
Cl	-0.76073000	1.48099100	-0.72962200

E_0(CASSCF,vacuo) -1135.838787

Zero-point correction= 0.229806
Thermal correction to Energy= 0.244509
Thermal correction to Enthalpy= 0.245453
Thermal correction to Gibbs Free Energy= **0.186677**

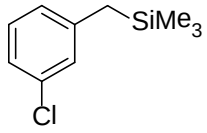
E_0(CASMP2,vacuo) -1137.210602
ΔE_{CORR}(MP2) **-1.371815**

E_0(CASSCF,CPCM) **-1135.845050**

E_0(CASSCF,CPCM,STRETCH,2.6) -1135.824125

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.8387872118
Full Convergence on CI vector
         ( 1)        EIGENVALUE     -0.11358388E+04
(     1) 0.9241336 (14731)-0.1251878 (  239)-0.1161687 (  505)-0.0999758 ( 3787)-0.0961139 ( 7782)-0.0831617 (26492)-0.0756304
(14997)-0.0725601 (26547)-0.0670823 ( 1080) 0.0662869 (14788)-0.0657256 (14785) 0.0640817 (26701)-0.0627502 (14942)-0.0599662
( 1079) 0.0584678 (26758)-0.0567820 (14701) 0.0542158 (   31)-0.0539500 ( 1346) 0.0537200 ( 1345) 0.0530565 (  240)-0.0498168
(14939) 0.0490647 (  451) 0.0464042 (26671) 0.0456642 (26489) 0.0452131 (   88)-0.0451438 (  297) 0.0406361 (  506)-0.0377845
(  842)-0.0312918 (  242) 0.0274430 (15682) 0.0273240 ( 3785) 0.0270258 ( 3783)-0.0268994 ( 3367) 0.0263722 (38370) 0.0229810
(15541)-0.0223295 (  142)-0.0220397 (14786) 0.0201512 (16801) 0.0192263 (  847)-0.0175907 (26755) 0.0175773 ( 1683) 0.0168297
( 1291)-0.0167659 (   86)-0.0165313 ( 1261)-0.0155317 ( 1137)-0.0149999 ( 1482)-0.0144151 (14940) 0.0137775 (38362) 0.0135810
(16942)-0.0133753 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192471D+01
     2  0.754230D-07  0.188466D+01
     3  0.115551D-05  0.128107D-07  0.198241D+01
     4  0.333460D-05 -0.219203D-07  0.100832D-06  0.196927D+01
     5  0.123316D-04 -0.750924D-06 -0.346222D-05 -0.419897D-05  0.102674D+01
     6 -0.391042D-06 -0.481486D-07 -0.277856D-06  0.250872D-05 -0.317803D-06
     7  0.113431D-07  0.614452D-05  0.527866D-08 -0.509105D-07  0.113582D-06
     8  0.300121D-05  0.601366D-07 -0.562596D-06 -0.659934D-06 -0.207873D-05
     9  0.476435D-06  0.137353D-07  0.239149D-05 -0.806140D-06 -0.222144D-05
    10  0.144906D-04 -0.514642D-07  0.144964D-05 -0.652721D-07 -0.599528D-05
                6             7             8             9            10
     6  0.977789D+00
     7  0.933638D-07  0.114971D+00
     8  0.121866D-04  0.660355D-07  0.723298D-01
     9 -0.122173D-05  0.909603D-08 -0.347946D-06  0.175972D-01
    10 -0.704263D-05  0.373001D-07  0.505811D-05 -0.206604D-05  0.295059D-01
 MCSCF converged.
```



1b

GEOMETRY

C	-2.78779900	1.17691500	0.33978800
C	-1.82464100	2.17709100	0.20582200
C	-0.56190700	1.88106500	-0.30683400
C	-0.22688300	0.57789500	-0.69983700
C	-1.19726700	-0.42401400	-0.56506900
C	-2.45265500	-0.11413000	-0.05199700
H	-2.06183300	3.18436400	0.49724300
H	0.16472400	2.66787600	-0.40791700
H	-0.98113100	-1.43347500	-0.86174600
C	1.14973400	0.25103800	-1.23374300
H	1.54705600	1.10698000	-1.77521400
H	1.08333500	-0.55818700	-1.95788500
C	1.89921900	-1.81919800	1.00860400
H	2.64259700	-2.13115400	1.73846000
H	0.96656100	-1.65874600	1.54209600
H	1.74766900	-2.65160700	0.32547100
C	2.72164300	1.14605700	1.33537100
H	3.47714200	0.88049600	2.07108200
H	3.05459400	2.05741900	0.84420500
H	1.80827700	1.37858700	1.87569700
C	4.08808300	-0.61029500	-0.81311000
H	4.44185900	0.26589900	-1.35113300
H	4.87274600	-0.90435300	-0.12015600
H	3.97621200	-1.41422100	-1.53662200
Si	2.46419100	-0.26105900	0.09645200
H	-3.76397400	1.39198600	0.73023000
Cl	-3.66586300	-1.41068200	0.10128700

E_0(CASSCF,vacuo) -1135.965551

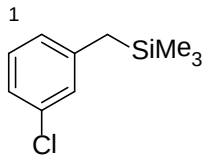
Zero-point correction= 0.233698
Thermal correction to Energy= 0.247704
Thermal correction to Enthalpy= 0.248648
Thermal correction to Gibbs Free Energy= **0.192440**

E_0(CASMP2,vacuo) -1137.325413
ΔE_{CORR}(MP2) **-1.359862**

E_0(CASSCF,CPCM) **-1135.971169**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.9655509023
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.11359656E+04
(     1) 0.9300882 (     6)-0.1340639 (   351)-0.1324367 (   259) 0.1167047 (   529)-0.1081798 (    28)-0.1038363 ( 1830)-0.0841654
( 8539) 0.0841539 ( 8132)-0.0829535 ( 8282) 0.0610358 ( 8259)-0.0584146 (   348)-0.0479625 (   256) 0.0468415 (    21)-0.0453728
(  331)-0.0451951 (    18) 0.0448405 (   276)-0.0424682 ( 8646)-0.0417365 ( 8256)-0.0392085 ( 8385)-0.0372365 (   300)-0.0327782
(   10)-0.0321451 (   561) 0.0313926 (   332) 0.0280674 ( 8152) 0.0275263 ( 8519) 0.0272905 ( 9181) 0.0245390 (14366) 0.0231181
(   27) 0.0227506 ( 8522)-0.0201333 ( 9484)-0.0198902 (14063)-0.0198116 ( 8279) 0.0196410 ( 8262) 0.0195613 (   283) 0.0166274
(  242) 0.0163654 (   820) 0.0155320 (    78) 0.0151251 ( 1775) 0.0150422 (   681) 0.0137524 (   260)-0.0133177 ( 9213)-0.0127511
( 8263)-0.0127179 ( 1183)-0.0126427 ( 2278) 0.0123484 (14398)-0.0122534 (    25) 0.0122313 (   106)-0.0122302 (14535) 0.0122009
( 5151) 0.0120164 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.196006D+01
     2 -0.337716D-05  0.198267D+01
     3 -0.592609D-05 -0.850177D-05  0.190151D+01
     4  0.168496D-06 -0.835152D-07 -0.340787D-06  0.197068D+01
     5  0.734354D-06 -0.233562D-05 -0.152196D-02 -0.178092D-06  0.190161D+01
     6  0.137665D-05 -0.996767D-08 -0.221041D-05 -0.209744D-05 -0.146033D-05
     7  0.440187D-05  0.510670D-07  0.835993D-05  0.490894D-07 -0.153085D-04
     8 -0.392139D-05 -0.195837D-06 -0.340615D-05  0.651006D-06  0.501711D-05
     9 -0.204188D-05  0.486393D-07 -0.270367D-05 -0.390402D-07 -0.473048D-06
    10  0.523077D-05  0.111725D-04  0.185773D-04 -0.165871D-06  0.143244D-04
                6             7             8             9            10
     6  0.293008D-01
     7  0.573117D-07  0.985363D-01
     8  0.289506D-05 -0.322313D-05  0.374840D-01
     9 -0.849925D-07  0.101170D-06  0.999982D-07  0.174347D-01
    10 -0.523624D-06 -0.549457D-05 -0.454951D-05  0.649027D-07  0.100722D+00
MCSCF converged.
```



^{1}1b

GEOMETRY

C	-2.81861700	1.18965100	0.35286400
C	-1.83796100	2.22252900	0.21364300
C	-0.54290700	1.91778300	-0.32058000
C	-0.20286400	0.58004200	-0.72844900
C	-1.19254000	-0.45642600	-0.58900600
C	-2.47872000	-0.13565200	-0.05349200
H	-2.07734100	3.22610800	0.50737100
H	0.18240200	2.70188900	-0.42881900
H	-0.97929900	-1.46169700	-0.89387100
C	1.17035800	0.25549300	-1.24323600
H	1.57963500	1.11298700	-1.77470500
H	1.11481900	-0.55374700	-1.96947500
C	1.90166700	-1.82678900	1.00164400
H	2.63889700	-2.14250700	1.73615300
H	0.96438100	-1.66867500	1.52767800
H	1.75547700	-2.65570900	0.31316900
C	2.71981700	1.13700800	1.34915400
H	3.46924200	0.86911700	2.09025600
H	3.05567300	2.05093100	0.86485800
H	1.80131900	1.36635000	1.88214400
C	4.10703800	-0.60961900	-0.79405300
H	4.46580200	0.26901300	-1.32476100
H	4.88514200	-0.90681600	-0.09502200
H	4.00201900	-1.41023800	-1.52226000
Si	2.47408800	-0.26436600	0.10128900
H	-3.79143900	1.39706000	0.75139300
Cl	-3.68562300	-1.41982700	0.10511300

E_0(CASSCF,vacuo) -1135.790482

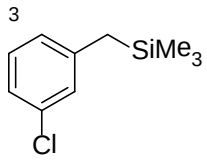
Zero-point correction= 0.228948
Thermal correction to Energy= 0.244063
Thermal correction to Enthalpy= 0.245007
Thermal correction to Gibbs Free Energy= **0.186697**

E_0(CASMP2,vacuo) -1137.199795
ΔE_{CORR}(MP2) **-1.370139**

E_0(CASSCF,CPCM) **-1135.795729**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.9528642081
Full Convergence on CI vector
Energy state  2 =    -1135.7904821532
Full Convergence on CI vector
                ( 1)      EIGENVALUE     -0.1135952 9E+04
(     1) 0.9177856 (     3)-0.1592346 (   276)-0.1573722 (   234) 0.1456467 (   352)-0.1171375 (    66)-0.1017036 ( 8005)-0.0967317
( 8152) 0.0951158 ( 1830)-0.0820086 ( 8258)-0.0692965 ( 8279) 0.0668775 ( 8128)-0.0426739 ( 8385)-0.0410933 ( 8256)-0.0398951
(  378) 0.0372552 (   10)-0.0355261 (   300)-0.0352791 (   253)-0.0350093 (     6)-0.0304429 (  255) 0.0285091 (13696)-0.0282381
( 8779) 0.0274350 (13072) 0.0251541 ( 8674)-0.0250995 ( 1795)-0.0216948 (   242) 0.0200746 (   58)-0.0199638 (  120) 0.0180453
(  946) 0.0176963 (  798) 0.0171316 (13722) 0.0160526 ( 8911) 0.0159877 ( 8805)-0.0157049 (13861) 0.0155689 ( 1676) 0.0153781
(   57)-0.0151624 ( 4753) 0.0146028 (     2)-0.0145235 ( 8012) 0.0143430 ( 2080) 0.0142776 (13339)-0.0141814 (   59) 0.0140096
( 1187)-0.0135173 ( 8139) 0.0134586 ( 4438)-0.0132267 (   287)-0.0131397 (    27)-0.0129067 ( 8129) 0.0123713 ( 8267)-0.0123082
(  264) 0.0121522 (
                ( 2)      EIGENVALUE     -0.1135790 5E+04
(  232) 0.6370892 (     4) 0.5862173 ( 8003)-0.1233579 ( 8024)-0.1221997 ( 8131) 0.1189863 ( 8150)-0.1161169 (  279)-0.1094866
( 8004)-0.1081215 (  298) 0.1079607 (     8)-0.1062808 ( 8023) 0.1051716 (  257)-0.1046745 ( 8130)-0.1034572 ( 8151)-0.1027187
(  278) 0.0993975 (  299) 0.0979308 (     9)-0.0957236 (  235) 0.0947479 (13169)-0.0859199 ( 8773) 0.0819424 (  382) 0.0740848
(  791) 0.0708436 (  489)-0.0698205 (  164)-0.0655052 ( 4431)-0.0567812 ( 2271)-0.0525231 (13205)-0.0374251 (13226) 0.0350089
( 9203) 0.0346014 ( 9182)-0.0334363 ( 8781)-0.0256152 (13698) 0.0244165 (13717) 0.0223558 ( 8800)-0.0215148 (13335) 0.0199639
(13174) 0.0193958 ( 9312)-0.0190006 (13857) 0.0186026 (13231)-0.0179131 ( 8910) 0.0177833 (13726) 0.0176391 ( 8809) 0.0175366
(13365)-0.0175019 (13827) 0.0174324 ( 9208) 0.0170674 (13177) 0.0168973 ( 8029) 0.0159103 (13234)-0.0157747 (   27) 0.0154805
(  373)-0.0154693 (
Final one electron symbolic density matrix:
                  1             2             3             4             5
     1  0.184774D+01
     2 -0.844136D-06  0.198229D+01
     3 -0.302806D-04 -0.809427D-05  0.140505D+01
     4  0.241580D-07 -0.300098D-07  0.364185D-07  0.197118D+01
     5 -0.145484D-04 -0.126820D-04 -0.103093D-04 -0.122535D-06  0.146945D+01
     6  0.525451D-06 -0.174622D-07  0.424344D-04  0.297120D-07 -0.428753D-04
     7  0.889761D-06 -0.436668D-05  0.826322D-05  0.296404D-07  0.314050D-04
     8 -0.223020D-05 -0.349007D-05  0.115333D-04  0.360836D-07 -0.318543D-06
     9 -0.255112D-05 -0.255927D-05  0.905702D-06 -0.801977D-06 -0.304887D-05
    10  0.103539D-06 -0.468166D-06  0.465026D-06 -0.544349D-06  0.600142D-06
                  6             7             8             9            10
     6  0.609990D+00
     7  0.188766D-05  0.542372D+00
     8 -0.975079D-05  0.694214D-05  0.125513D+00
     9  0.182216D-05 -0.925380D-06  0.134709D-05  0.176135D-01
    10  0.149407D-05 -0.166239D-05  0.511869D-07  0.394569D-06  0.288010D-01
MCSCF converged.
```



^{3}1b(α)

GEOMETRY

C	-3.04534900	-1.10334600	0.04279000
C	-2.11195600	-2.01346400	0.44025200
C	-0.72585000	-1.82971900	0.12612000
C	-0.29005000	-0.73831100	-0.72209400
C	-1.20978200	0.18298600	-1.12973500
C	-2.58439900	0.15826400	-0.58346600
H	-2.41404600	-2.90936100	0.95288100
H	-0.01162400	-2.56550600	0.44398300
H	-0.94406000	0.98622200	-1.79237400
C	1.15625200	-0.67466900	-1.15380500
H	1.23355700	-0.13291600	-2.09396500
H	1.52945500	-1.67811500	-1.35093600
C	2.35494500	-0.69725000	1.76600600
H	3.06282600	-0.23424000	2.44949000
H	1.37709200	-0.66012800	2.23795500
H	2.63615600	-1.74342900	1.67011000
C	1.85743700	1.99552600	0.32384900
H	2.53115500	2.50457900	1.00911100
H	1.88043800	2.54003100	-0.61717100
H	0.85274600	2.08310400	0.72755800
C	4.10296900	0.10068500	-0.65408600
H	4.14833100	0.59626500	-1.62083700
H	4.83424900	0.58133000	-0.00869200
H	4.42453800	-0.92787600	-0.79925000
Si	2.36507900	0.18904000	0.09321400
H	-4.09426000	-1.24060100	0.22500000
Cl	-3.01076300	1.63940400	0.38395100

E_0(CASSCF,vacuo) -1135.838299

Zero-point correction=	0.229549
Thermal correction to Energy=	0.244220
Thermal correction to Enthalpy=	0.245164
Thermal correction to Gibbs Free Energy=	**0.186512**

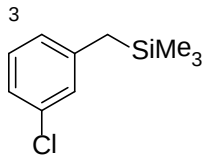
E_0(CASMP2,vacuo) -1137.210211

ΔE_{CORR}(MP2) **-1.371912**

E_0(CASSCF,CPCM) **-1135.844703**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.8382989292
Full Convergence on CI vector
          ( 1)        EIGENVALUE     -0.11358383E+04
(     1) 0.9231456 (14731)-0.1249460 (  239) 0.1172888 (  505) 0.1009669 ( 7993)-0.0961301 ( 3576)-0.0835050 (26492)-0.0748634
(14997)-0.0717434 ( 1080)-0.0676303 (26547)-0.0641778 (14788)-0.0640033 ( 1079)-0.0628925 (14785) 0.0614850 (26701)-0.0614737
(14942)-0.0596712 (26758)-0.0582600 (14701)-0.0575642 (   31) 0.0573662 ( 1345)-0.0560651 ( 1346)-0.0551845 (  240) 0.0521550
(26671)-0.0484342 (   88) 0.0478704 (14939) 0.0474550 (  451)-0.0455203 (26489) 0.0409966 (  506) 0.0402798 (  297)-0.0389954
(  848)-0.0317826 (  242)-0.0284026 ( 7991)-0.0270552 (15682)-0.0269592 ( 7989) 0.0268099 ( 7573)-0.0262802 (  142)-0.0234155
(38370) 0.0227935 (15541) 0.0207771 (14786) 0.0202944 (16801)-0.0180776 (  853) 0.0177711 ( 1291) 0.0172759 ( 1689) 0.0171596
( 1261)-0.0153062 (   86) 0.0152611 ( 1137) 0.0146657 (14940) 0.0142196 (26755) 0.0141525 (15359)-0.0139526 (16942) 0.0139202
(27443)-0.0137762 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192457D+01
     2 -0.993994D-06  0.188362D+01
     3  0.842759D-06  0.519173D-07  0.196914D+01
     4  0.278635D-06  0.516360D-06 -0.254563D-07  0.198279D+01
     5  0.304862D-04 -0.203291D-04  0.101145D-04  0.322649D-05  0.102632D+01
     6  0.147114D-04 -0.230416D-04 -0.510796D-05  0.221925D-06 -0.151388D-06
     7  0.556032D-06 -0.327914D-05 -0.345896D-05  0.277859D-06 -0.154210D-04
     8 -0.943737D-06 -0.149201D-05 -0.107374D-05 -0.997344D-06 -0.153855D-04
     9 -0.126114D-05 -0.195961D-05  0.120326D-06  0.395341D-06 -0.236558D-06
    10 -0.396620D-05  0.127171D-05  0.581934D-06 -0.233617D-06 -0.549987D-05
                6             7             8             9            10
     6  0.977999D+00
     7 -0.349965D-04  0.115159D+00
     8 -0.198476D-04 -0.117943D-05  0.734232D-01
     9 -0.193679D-06 -0.960981D-07  0.282275D-06  0.173674D-01
    10 -0.197218D-05 -0.799797D-06  0.119204D-05 -0.135217D-06  0.296194D-01
MCSCF converged.
```



^{3}1b(β)

GEOMETRY

C	-0.00015700	0.00046400	0.00003100
C	-0.00011800	0.00033400	1.36309800
C	1.23016400	0.00000300	2.09727200
C	2.50820300	-0.11206700	1.41697900
C	2.52939700	-0.09668900	0.05455000
C	1.29085900	0.16278600	-0.71158400
H	-0.92840200	-0.04790400	1.90416600
H	1.20526000	0.01143000	3.17046100
H	3.44883500	-0.19413300	-0.49321000
C	3.76016300	-0.31184200	2.23970500
H	3.70544900	0.29585900	3.14117800
H	4.62421300	0.04894000	1.68642700
C	4.41762200	-3.20311100	1.22867200
H	4.65966800	-4.22738900	1.50212600
H	3.53124600	-3.23329100	0.60121900
H	5.23698500	-2.82768100	0.62030100
C	2.73683500	-2.85919000	3.80202300
H	2.98026800	-3.86617500	4.13280600
H	2.54424500	-2.26484600	4.69211900
H	1.81000900	-2.91792400	3.23821600
C	5.73227400	-2.10000600	3.80468200
H	5.61011100	-1.49495500	4.69986500
H	6.01746800	-3.09928700	4.12472500
H	6.56788400	-1.68793900	3.24418800
Si	4.14841200	-2.13672500	2.76762300
H	-0.90636800	-0.04771900	-0.57329000
Cl	1.36559000	1.65714700	-1.74031500

E_0(CASSCF,vacuo) -1135.837905

Zero-point correction= 0.229404
Thermal correction to Energy= 0.244144
Thermal correction to Enthalpy= 0.245088
Thermal correction to Gibbs Free Energy= **0.186205**

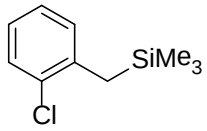
E_0(CASMP2,vacuo) -1137.209835
ΔE_{CORR}(MP2) **-1.371930**

E_0(CASSCF,CPCM) **-1135.844531**

E_0(CASSCF,CPCM,STRETCH,2.6) -1135.818517

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.8379052494
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.11358379E+04
(     8) 0.9231930 ( 3165) 0.1243481 (  212) 0.1200830 (  925)-0.1030671 ( 1271) 0.0964020 (15173)-0.0835976 (26478)-0.0748143
( 3887) 0.0719260 ( 7364) 0.0678557 (26567)-0.0646161 ( 3260) 0.0641831 (27105)-0.0617664 ( 3235) 0.0616302 ( 7352)-0.0604075
( 3798) 0.0600354 (27200)-0.0581235 ( 3158)-0.0555683 (   15)-0.0554016 ( 8086) 0.0552208 ( 8065) 0.0530748 (  224)-0.0506222
( 3782)-0.0477753 (  855)-0.0462930 (27098) 0.0460561 (  110)-0.0455179 (26462) 0.0418719 (  317)-0.0393921 (  946)-0.0385198
(  421)-0.0311151 (  228)-0.0295585 ( 4502) 0.0275508 ( 1273) 0.0266156 ( 1269) 0.0260462 ( 1691) 0.0258875 (   92)-0.0229327
(31207)-0.0228379 ( 4418)-0.0206189 ( 3256) 0.0192521 (  431) 0.0176945 (11978)-0.0172737 ( 7569)-0.0167624 ( 7995) 0.0162816
(27175)-0.0162199 ( 7988) 0.0161355 (  106) 0.0160223 (  950)-0.0142100 (27815)-0.0140058 ( 7457) 0.0137687 ( 3794) 0.0135017
( 3362) 0.0133934 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192428D+01
     2  0.241637D-06  0.198273D+01
     3 -0.122208D-04 -0.203048D-05  0.102771D+01
     4 -0.282379D-06 -0.311993D-06  0.203490D-04  0.188376D+01
     5  0.203934D-05 -0.259087D-06 -0.351138D-04  0.869219D-06  0.196934D+01
     6 -0.141987D-06 -0.272266D-05  0.848160D-07 -0.356330D-05  0.214762D-04
     7 -0.212276D-05  0.221366D-05  0.745559D-05 -0.695405D-05 -0.350453D-05
     8  0.716040D-06 -0.122987D-06  0.243004D-04 -0.107886D-04 -0.769592D-05
     9  0.668484D-05 -0.521033D-05 -0.578242D-07 -0.448644D-05  0.400799D-06
    10 -0.147317D-05 -0.449886D-05  0.737007D-05  0.155457D-05 -0.648360D-06
                6             7             8             9            10
     6  0.976533D+00
     7  0.489786D-06  0.115123D+00
     8 -0.484749D-04  0.854671D-06  0.294586D-01
     9  0.191650D-05 -0.228652D-07 -0.287845D-06  0.174026D-01
    10 -0.215298D-04  0.472336D-07 -0.179269D-05 -0.140538D-06  0.736572D-01
MCSCF converged.
```



1c

GEOMETRY

C	-0.00272500	-0.00096100	-0.00534300
C	-0.00505300	0.00463400	1.39041600
C	1.19932600	0.01128400	2.08735500
C	2.44380600	0.00981700	1.43191300
C	2.40584900	0.00829500	0.03314100
C	1.21038600	0.00400700	-0.68630200
H	-0.93467300	0.00845000	1.93038000
H	1.18558100	0.02427300	3.16280100
C	3.71944500	-0.00348800	2.24149400
H	3.57024400	0.59191100	3.13993200
H	4.52582100	0.47155500	1.69467800
C	4.54185400	-2.94505200	1.38506900
H	4.87401000	-3.91812400	1.74008900
H	3.60691800	-3.09419500	0.85195900
H	5.27356300	-2.58955800	0.66584000
C	3.10678500	-2.47205300	4.07478000
H	3.46420100	-3.42434800	4.45962800
H	2.95884900	-1.81372700	4.92775700
H	2.13467700	-2.64978400	3.62303900
C	6.00716200	-1.48002100	3.68686600
H	5.92218500	-0.79451600	4.52672500
H	6.40766500	-2.41536000	4.07044900
H	6.74387000	-1.06756900	3.00188800
Si	4.33858900	-1.74644300	2.83200200
H	-0.92617000	-0.00390100	-0.55512100
H	1.23891200	0.00756100	-1.75919900
Cl	3.91699000	0.03397500	-0.92318000

E_0(CASSCF,vacuo) -1135.963588

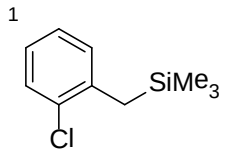
Zero-point correction= 0.233899
Thermal correction to Energy= 0.247832
Thermal correction to Enthalpy= 0.248776
Thermal correction to Gibbs Free Energy= **0.192948**

E_0(CASMP2,vacuo) -1137.325189
ΔE_{CORR}(MP2) **-1.361601**

E_0(CASSCF,CPCM) **-1135.968419**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.9635876483
Full Convergence on CI vector
         ( 1)        EIGENVALUE      -0.11359636E+04
(     1) 0.9299121 (  276)-0.1149038 (    3)-0.1109706 (  352)-0.1080605 ( 8515)-0.1039309 (  234) 0.0880955 (   66)-0.0841212
( 1677)-0.0752160 ( 1600) 0.0738637 (  233) 0.0722343 (  275)-0.0717236 (  256)-0.0685950 (    5) 0.0682886 (    6)-0.0648296
(  253)-0.0637862 ( 1734)-0.0541996 ( 1713) 0.0524016 ( 1657)-0.0469334 ( 1620)-0.0462564 ( 1711)-0.0418508 ( 1653)-0.0390331
( 1770)-0.0372039 ( 1714)-0.0343913 (   10)-0.0330544 ( 1733)-0.0322243 (  300)-0.0318569 (  378) 0.0314030 ( 8388) 0.0309267
( 1954)-0.0214621 ( 4561) 0.0210164 ( 8389)-0.0206170 (  255)-0.0199650 ( 8387)-0.0190881 ( 4217)-0.0178061 ( 1919) 0.0176257
( 8443)-0.0169688 ( 9317) 0.0158741 ( 8133) 0.0150527 ( 4279) 0.0140321 ( 8444) 0.0134520 ( 9045) 0.0129551 (14028) 0.0126853
(15008) 0.0126194 ( 1841)-0.0126046 ( 2146) 0.0125421 ( 8442) 0.0125273 ( 8006)-0.0123850 (   61) 0.0119040 ( 8407)-0.0118428
( 1980) 0.0112033 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197045D+01
     2  0.163137D-06  0.195999D+01
     3  0.211213D-06 -0.278826D-05  0.190134D+01
     4 -0.407932D-06 -0.167467D-05 -0.371534D-05  0.198257D+01
     5  0.171951D-06 -0.383324D-05 -0.627811D-03 -0.556975D-05  0.190145D+01
     6 -0.612662D-06 -0.618225D-05 -0.277946D-04  0.666036D-05  0.317832D-04
     7  0.124280D-06  0.824396D-05 -0.121237D-04 -0.696225D-05 -0.135405D-04
     8  0.162997D-06  0.180973D-05  0.619034D-05  0.175393D-06  0.448225D-05
     9 -0.129564D-05  0.352013D-06 -0.309954D-06 -0.410636D-06  0.590508D-06
    10  0.780980D-06  0.796256D-06  0.708976D-06  0.103309D-05  0.227698D-05
                6             7             8             9            10
     6  0.984224D-01
     7 -0.249464D-05  0.101086D+00
     8  0.297817D-05 -0.252932D-05  0.376176D-01
     9  0.389591D-07  0.123234D-06 -0.959004D-06  0.295570D-01
    10 -0.452465D-06  0.306614D-06  0.407708D-06  0.657733D-07  0.175247D-01
MCSCF converged.
```



^{1}1c

GEOMETRY

C	-0.02816900	-0.02660100	-0.03813400
C	-0.04365600	-0.00844700	1.39053800
C	1.18963400	0.02154400	2.11976900
C	2.46702600	0.03376500	1.45121800
C	2.44124200	0.02082500	0.00952400
C	1.21996100	-0.00538500	-0.73647600
H	-0.97694400	-0.01431700	1.91986700
H	1.16981100	0.04570300	3.19261100
C	3.73131300	0.00799400	2.26024000
H	3.58586800	0.59869700	3.16338000
H	4.54669700	0.47500900	1.71869100
C	4.51586200	-2.93609200	1.38514000
H	4.85523500	-3.91159100	1.72630000
H	3.57057500	-3.08198400	0.86946600
H	5.23324800	-2.57533900	0.65399000
C	3.11733000	-2.46831100	4.09637400
H	3.47306800	-3.42374600	4.47507500
H	2.98250200	-1.81116900	4.95240900
H	2.13939800	-2.63812200	3.65442700
C	6.02131400	-1.50031300	3.68007900
H	5.95263500	-0.81720800	4.52338800
H	6.41636300	-2.44119900	4.05574000
H	6.75456800	-1.09268500	2.98854700
Si	4.34029900	-1.74611100	2.84313300
H	-0.94680100	-0.05168400	-0.59186100
H	1.25335800	-0.00472700	-1.80722100
Cl	3.94633300	0.10815400	-0.92715500

E_0(CASSCF,vacuo) -1135.788403

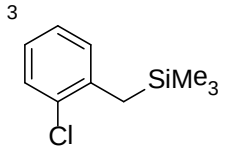
Zero-point correction= 0.229126
Thermal correction to Energy= 0.244201
Thermal correction to Enthalpy= 0.245145
Thermal correction to Gibbs Free Energy= **0.187051**

E_0(CASMP2,vacuo) -1137.199672
ΔE_{CORR}(MP2) **-1.371968**

E_0(CASSCF,CPCM) **-1135.792873**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.9508147195
Full Convergence on CI vector
Energy state  2 =    -1135.7884032748
Full Convergence on CI vector
                ( 1)      EIGENVALUE     -0.1135950 8E+04
(     1) 0.9175035 (  276)-0.1600952 (     3)-0.1570005 (  234) 0.1462308 (  352)-0.1172632 ( 8515)-0.1018100 ( 1677)-0.0971382
( 1600) 0.0951798 (   66)-0.0821661 ( 1734)-0.0694080 ( 1713) 0.0669485 ( 1711)-0.0427052 ( 1770)-0.0412389 ( 1653)-0.0399659
(  378) 0.0373879 (  300)-0.0354769 (   10)-0.0351918 (    6)-0.0350947 (  253)-0.0303557 (  255) 0.0289675 ( 1954)-0.0282311
( 4561) 0.0277300 ( 4217)-0.0252657 ( 1919) 0.0251762 (   61) 0.0218914 ( 8388) 0.0213796 ( 8407)-0.0187927 (14028) 0.0181878
( 9045) 0.0178102 ( 8408) 0.0172804 (13503)-0.0172037 ( 4656) 0.0161099 ( 1980) 0.0160376 (   23)-0.0158771 ( 4587)-0.0158224
( 2016) 0.0155826 (  120) 0.0146406 (  946) 0.0143860 ( 4344)-0.0142361 ( 8409)-0.0140625 ( 8443)-0.0140333 ( 8389)-0.0138433
( 8153) 0.0137484 (15008) 0.0135239 (  798) 0.0132897 ( 8387)-0.0123038 ( 8442) 0.0121421 ( 1597) 0.0119110 ( 8444) 0.0118212
( 9317) 0.0116997 (
                ( 2)      EIGENVALUE     -0.1135788 4E+04
(     4) 0.6331205 (  232) 0.5897426 ( 1676)-0.1396871 ( 1655)-0.1383173 ( 1618) 0.1353237 ( 1599)-0.1324409 (  235)-0.1258756
(     9) 0.1245640 (  299)-0.1226368 (  278)-0.1211589 ( 1948) 0.0855792 ( 1675) 0.0853782 ( 1656)-0.0831400 ( 4244)-0.0825980
( 1619) 0.0823406 ( 1598) 0.0803220 (  257)-0.0770103 (    8)-0.0749432 (  298) 0.0742922 (  489)-0.0739529 (  279)-0.0738786
( 9446)-0.0704514 (  382) 0.0700562 (13496)-0.0661303 (  164)-0.0565454 (  791) 0.0529611 ( 2168)-0.0377480 ( 4280) 0.0351169
( 2147) 0.0344167 ( 4301)-0.0333875 ( 4582)-0.0251488 ( 1975) 0.0246986 ( 4252)-0.0229728 ( 4622)-0.0223847 ( 1956) 0.0222179
( 4563)-0.0221005 ( 4370) 0.0219907 ( 2015)-0.0215631 ( 2176) 0.0203141 ( 1981)-0.0200198 ( 4588)-0.0199105 ( 4309)-0.0194493
(20468) 0.0160494 ( 8153)-0.0159241 ( 8006)-0.0157212 ( 1684)-0.0156476 (20435) 0.0155671 (19838) 0.0155442 ( 8387)-0.0154301
( 8408)-0.0154239 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197090D+01
     2 -0.157799D-06  0.184735D+01
     3  0.702434D-06 -0.658513D-05  0.146418D+01
     4 -0.223708D-06 -0.214858D-05 -0.350557D-05  0.198214D+01
     5 -0.420438D-06  0.193328D-04  0.942313D-06  0.940158D-05  0.140989D+01
     6 -0.116449D-05  0.214933D-05 -0.531870D-04  0.668020D-05 -0.196030D-05
     7  0.370687D-06  0.609787D-05 -0.137983D-04 -0.316957D-05 -0.574210D-04
     8 -0.501199D-06  0.660679D-06  0.322234D-06  0.122410D-05  0.133963D-04
     9  0.174930D-05  0.129349D-05  0.203798D-05 -0.243198D-05  0.113135D-05
    10  0.458160D-06 -0.155370D-05 -0.231795D-05 -0.141069D-05  0.104264D-05
                6             7             8             9            10
     6  0.547063D+00
     7  0.169469D-05  0.605789D+00
     8  0.190319D-05  0.307609D-05  0.125849D+00
     9 -0.420938D-06  0.491298D-06  0.508541D-06  0.291000D-01
    10 -0.856524D-07 -0.326519D-06 -0.116396D-05 -0.432790D-07  0.177370D-01
MCSCF converged.
```



^{3}1c(α)

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.43773700
C	1.23150800	0.00000000	2.15328100
C	2.44210000	0.12936000	1.51513800
C	2.39570400	0.47353600	0.06725700
C	1.16780700	0.13319200	-0.68528700
H	-0.92549200	-0.10990600	1.97013500
H	1.20815900	-0.18772000	3.21323900
H	1.21145900	0.10079600	-1.75766300
H	4.51047900	-0.38637300	1.49285600
C	3.76738000	-0.04687600	2.21094600
H	3.66544400	-0.84760300	2.94003900
H	3.66772600	3.50929800	4.29379200
C	3.22212000	2.70771700	3.70900400
H	2.73673200	3.15800300	2.84875900
H	2.44860100	2.25159200	4.32164200
H	6.38267100	3.08180800	2.78251000
C	5.90438400	2.30175700	2.19424300
H	6.67831400	1.59363600	1.90684100
H	5.52340600	2.75833900	1.28725800
H	6.07340700	-0.04223400	4.50291800
C	5.32915500	0.71066900	4.75269400
H	5.82759800	1.47393200	5.34549000
H	4.58738000	0.23613400	5.39103700
H	-0.92440200	-0.16099500	-0.52526700
Si	4.54214900	1.45523300	3.19612700
Cl	2.97725600	2.16791700	-0.31981900

E_0(CASSCF,vacuo) -1135.835332

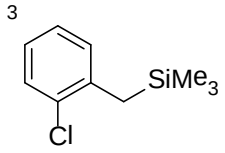
Zero-point correction= 0.229799
Thermal correction to Energy= 0.244447
Thermal correction to Enthalpy= 0.245391
Thermal correction to Gibbs Free Energy= **0.187167**

E_0(CASMP2,vacuo) -1137.208934
ΔE_{CORR}(MP2) **-1.373602**

E_0(CASSCF,CPCM) **-1135.840673**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.8353316122
Full Convergence on CI vector     -0.1135853E+04
          ( 1)        EIGENVALUE
(     1) 0.9209708 (14731)-0.1282643 (  239)-0.1135201 ( 7993)-0.0944007 (  505)-0.0941338 ( 3576)-0.0850572 (26492)-0.0753889
(14997)-0.0716804 ( 1079)-0.0712888 ( 1080) 0.0695965 (14701)-0.0661992 (   31) 0.0656728 (14788)-0.0618725 (26758)-0.0608943
(  240) 0.0607373 (26547)-0.0606394 ( 1345)-0.0605087 (26701)-0.0592930 (14942)-0.0586394 (14785)-0.0556522 ( 1346) 0.0549536
(26671)-0.0535909 (    88) 0.0529771 (  506) 0.0460944 (14939)-0.0429629 (  451)-0.0420866 (  297)-0.0367043 (26489)-0.0342877
(  848) 0.0337347 ( 7989)-0.0294691 ( 7991) 0.0287158 ( 7573) 0.0279376 (15682) 0.0249832 (  142) 0.0237731 (15541) 0.0233276
(38370) 0.0229160 (16801) 0.0219887 (  242)-0.0219183 (14786) 0.0213598 ( 1291)-0.0194689 ( 1689)-0.0185577 (  853)-0.0172081
( 1137)-0.0171517 (  146)-0.0155496 (16942) 0.0151827 (15359)-0.0148464 ( 1348) 0.0146411 (14850)-0.0140490 (27443) 0.0139645
(14940) 0.0137915 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192554D+01
     2  0.113551D-05  0.188015D+01
     3 -0.144365D-05  0.125813D-06  0.196859D+01
     4  0.604920D-06  0.140776D-05 -0.177851D-06  0.198186D+01
     5  0.345110D-04 -0.436121D-04  0.487189D-05  0.104013D-06  0.102175D+01
     6 -0.113099D-04 -0.189773D-05  0.192177D-05  0.187662D-06 -0.187093D-06
     7 -0.555596D-05  0.330956D-05 -0.213617D-05 -0.347711D-05 -0.100822D-04
     8  0.119595D-05  0.791400D-05  0.248021D-06  0.164595D-05 -0.130736D-04
     9 -0.153372D-05 -0.332937D-05  0.608094D-05  0.235000D-05 -0.149057D-05
    10  0.970948D-05  0.170554D-05 -0.392066D-05  0.199944D-05 -0.873475D-05
                6             7             8             9            10
     6  0.981607D+00
     7  0.122880D-04  0.118563D+00
     8  0.238568D-04  0.299666D-06  0.737844D-01
     9 -0.716080D-07 -0.105289D-05  0.550144D-07  0.181985D-01
    10 -0.891117D-05  0.114964D-05 -0.331012D-05 -0.729171D-06  0.299576D-01
 MCSCF converged.
```



^{3}1c(β)

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.43718800
C	1.23391400	0.00000000	2.15526300
C	2.44241700	0.11674700	1.51619500
C	2.40179100	0.45068400	0.06427400
C	1.16790200	0.12782800	-0.68731200
H	-0.92656300	-0.09535900	1.97038900
H	1.21020200	-0.15980000	3.21955400
C	3.77300600	-0.04047100	2.19807400
H	3.65201100	0.10222100	3.27004900
H	4.45843100	0.73309400	1.86027800
C	4.86888800	-2.14809300	0.11270700
H	5.41822500	-3.07779500	-0.01714200
H	3.91840700	-2.25828000	-0.40219800
H	5.42683100	-1.36547400	-0.39475300
C	3.57865600	-3.11083300	2.75340900
H	4.04266000	-4.08816700	2.64385100
H	3.44457700	-2.93281400	3.81782100
H	2.59082800	-3.16651600	2.30388200
C	6.32292600	-1.67830600	2.80219400
H	6.22647200	-1.44961600	3.86084000
H	6.85262600	-2.62447200	2.72119400
H	6.95513900	-0.91268800	2.35921700
Si	4.63441300	-1.76086800	1.94981300
H	-0.92604900	-0.15274700	-0.52492100
H	1.20886000	0.09610800	-1.75982800
Cl	3.03152500	2.12291100	-0.31641700

E_0(CASSCF,vacuo) -1135.839318

Zero-point correction= 0.229676
Thermal correction to Energy= 0.244374
Thermal correction to Enthalpy= 0.245318
Thermal correction to Gibbs Free Energy= **0.186533**

E_0(CASMP2,vacuo) -1137.212512
ΔE_{CORR}(MP2) **-1.373194**

E_0(CASSCF,CPCM) **-1135.845025**

E_0(CASSCF,CPCM,STRETCH,2.6) -1135.819217

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =    -1135.8393181921
Full Convergence on CI vector      -0.11358393E+04
          ( 1)        EIGENVALUE
(     1) 0.9220136 ( 7360)-0.1272714 (  218)-0.1136363 (  505)-0.0957740 (15153)-0.0950427 ( 3787)-0.0833405 (26471)-0.0753316
( 7647)-0.0716325 ( 1059) 0.0688011 ( 1058) 0.0686727 ( 7351) 0.0641120 (   10)-0.0636032 ( 7438)-0.0623259 (26547)-0.0613620
( 1345) 0.0599134 (26758)-0.0598828 (26680)-0.0598238 (  219)-0.0591793 ( 7571)-0.0589985 ( 7435)-0.0570357 ( 1346) 0.0552914
(26671) 0.0532141 (    88)-0.0526253 (  506)-0.0459575 ( 7568)-0.0442023 (  430)-0.0434468 (  297)-0.0376191 (26468)-0.0357779
(  659)-0.0330705 (15152)-0.0285086 (15150)-0.0283648 (14943)-0.0277017 ( 8297) 0.0254274 (  107) 0.0237645 (  221)-0.0234657
( 8191) 0.0231900 (33925) 0.0227906 ( 7436)-0.0213266 ( 9451)-0.0212854 ( 1270) 0.0194588 ( 1500) 0.0182771 (  663)-0.0172788
( 1137) 0.0170385 (  111) 0.0152560 ( 9557)-0.0149401 ( 7778) 0.0143594 ( 7569)-0.0139183 ( 7465) 0.0138734 ( 1348)-0.0138407
(27408) 0.0138013 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192581D+01
     2 -0.615681D-07  0.196877D+01
     3 -0.158696D-06 -0.185664D-07  0.188171D+01
     4 -0.930624D-07  0.139061D-06 -0.886762D-07  0.198270D+01
     5 -0.354486D-04  0.329525D-05  0.360407D-05  0.257730D-05  0.102244D+01
     6 -0.102263D-04  0.439986D-06 -0.670769D-05  0.124683D-05 -0.150455D-07
     7 -0.391842D-06 -0.140935D-05  0.332491D-05 -0.827886D-07 -0.533449D-05
     8 -0.367626D-06 -0.160856D-06  0.137677D-05  0.345544D-06 -0.110928D-04
     9  0.129691D-05  0.680175D-06  0.217458D-05  0.135156D-07  0.154451D-05
    10  0.245511D-06 -0.109940D-05  0.894357D-07 -0.279674D-07  0.595714D-07
                6             7             8             9            10
     6  0.980913D+00
     7 -0.707822D-05  0.117025D+00
     8 -0.270827D-04  0.193141D-06  0.734222D-01
     9 -0.101030D-04  0.341455D-07 -0.246567D-07  0.298228D-01
    10 -0.117535D-05 -0.881929D-07 -0.350636D-06 -0.824055D-06  0.173841D-01
MCSCF converged.
```

3. Conical Intersections (CoIns) geometries

The level of theory chosen for optimizing these structures was the CASSCF(6,6)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring. Unfortunately, it was not possible to adopt the same (10,10) active space adopted for the optimization of **1a-c**, due to the huge memory requirements of this kind of jobs. Further notice that the optimizations of the structures reported below were carried out using the %MEM=11600MB keyword. Nevertheless, the change in the active space is not expected to introduce a severe approximation, since the two σ/σ* couples showed little electron displacements, with values close to 2 and 0 for the σ and σ* orbitals, respectively (see above). Of course, due to the change in the active space, it is not possible to make a direct comparison among the energies of these CoIns and those of the stationary points reported above.

As mentioned in the text, the keyword CASSCF=SLATERDET has been used, since this is required when looking for CoIns between states of different spin. The actual involvement of a triplet root in the CoIns reported below can be demonstrated having recourse to arguments based on spin algebra, as previously reported in the literature.[S3]

CoIn(α) for 1a

GEOMETRY

C	0.04166556	-0.01315645	0.01247177
C	0.00990132	0.00892723	1.49875608
C	1.24916064	0.02632900	2.07242152
C	2.39969105	0.41234780	1.28855212
C	2.18733727	1.03516977	0.00240252
C	0.94586307	1.01538620	-0.56637588
H	-0.91159016	-0.05596303	2.04438714
H	1.37762201	-0.12223242	3.13067571
H	2.98949918	1.61105252	-0.42581482
H	0.64936179	1.62256070	-1.39974054
C	3.78145405	0.32263082	1.87107217
H	3.73602929	0.43630450	2.95320400
H	4.39395204	1.14378260	1.50154495
C	4.93459780	-1.51790244	-0.36518138
H	5.50156534	-2.41836771	-0.58975248
H	3.97798793	-1.59956324	-0.87302161
H	5.47200343	-0.67993002	-0.80327116
C	3.76496849	-2.77562932	2.21552152
H	4.30512226	-3.70492795	2.05011288
H	3.61761064	-2.67399747	3.28831314
H	2.78669443	-2.88058602	1.75548174
C	6.41465163	-1.18050971	2.33192522
H	6.32515511	-1.05088297	3.40785255
H	7.00402576	-2.07827423	2.16150917
H	6.98684390	-0.33935533	1.94788394
Si	4.71794473	-1.30860471	1.50051348
Cl	0.44065705	-1.68536667	-0.62166215

E_0(CASSCF,vacuo) -1135.791827

DATA from the CASSCF calculation in vacuo:

```
 EIGENVALUES AND  EIGENVECTORS OF CI MATRIX

 ( 1)     EIGENVALUE    -1135.7918472081
(    3)-0.6597071 (    2) 0.6597071 (   27) 0.1073044 (   25)-0.1073044 (  110)-0.0958647 (  116) 0.0958647 (   80)-0.0875464
(   67) 0.0875464 (   10) 0.0572144 (   17)-0.0572144 (  191) 0.0553936 (  210)-0.0553936 (  197)-0.0549642 (  204) 0.0549642
(   41)-0.0512689 (   54) 0.0512689 (  208) 0.0487996 (  193)-0.0487996 (   57) 0.0475760 (   36)-0.0475760 (  214)-0.0470477
(  187) 0.0470477 (  291) 0.0461027 (  285)-0.0461027 (  195) 0.0459293 (  189)-0.0459293 (  212) 0.0451444 (  206)-0.0451444
(  128)-0.0421037 (   95) 0.0421037 (   74)-0.0365091 (   66) 0.0365091 (  109) 0.0290875 (  104)-0.0290875 (   72) 0.0289540
(   79)-0.0289540 (   81) 0.0240412 (   76)-0.0240412 (  334) 0.0236478 (  321)-0.0236478 (   83)-0.0227379 (   64) 0.0227379
(   63)-0.0225308 (   77) 0.0225308 (  107)-0.0219917 (  120) 0.0219917 (  399)-0.0184636 (  398) 0.0184636 (  122) 0.0171957
(  111)-0.0171957 (

 ( 2)     EIGENVALUE    -1135.7918270700
(    1) 0.7252065 (    6)-0.5874939 (   25)-0.1069266 (   27)-0.1069266 (   75)-0.1052635 (   67) 0.0882524 (   80) 0.0882524
(  157) 0.0859513 (   33) 0.0606551 (   21) 0.0606551 (  159) 0.0603314 (  147) 0.0603314 (  143) 0.0518795 (  163) 0.0518795
(  244)-0.0503616 (  145)-0.0498418 (  254)-0.0496939 (  242)-0.0496939 (  161)-0.0480462 (   23)-0.0462715 (   30)-0.0462715
(   60)-0.0442161 (   90)-0.0442161 (   87) 0.0440363 (   62) 0.0440363 (  238)-0.0432490 (  258)-0.0432490 (  326) 0.0414942
(  256) 0.0412716 (  240) 0.0412122 (   66) 0.0337118 (   74) 0.0337118 (  104)-0.0308768 (  109)-0.0308768 (  120) 0.0251285
(  107) 0.0251285 (   79)-0.0248802 (   72)-0.0248802 (  321)-0.0237433 (  334)-0.0237433 (  111)-0.0221444 (  122)-0.0221444
(   97) 0.0208500 (  124) 0.0208500 (  395) 0.0199692 (   77) 0.0195177 (   63) 0.0195177 (    2) 0.0186887 (    3) 0.0186887
(   76)-0.0180547 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192441D+01
     2  0.210568D-09  0.187774D+01
     3 -0.905637D-02  0.593520D-09  0.119311D+01
     4 -0.777442D-02  0.115280D-07  0.537402D-02  0.811598D+00
     5  0.100077D-08  0.555238D-03  0.175530D-08 -0.636124D-08  0.120144D+00
     6 -0.314330D-03 -0.170322D-08 -0.202839D-01 -0.222092D-01 -0.370563D-09
                6
     6  0.729913D-01
 Density Matrix for State     1
                1             2             3             4             5
     1  0.192367D+01
     2 -0.210426D-09  0.187657D+01
     3  0.905650D-02 -0.592292D-09  0.100645D+01
     4  0.777455D-02 -0.115282D-07 -0.537399D-02  0.998404D+00
     5 -0.100078D-08 -0.555214D-03 -0.175458D-08  0.636215D-08  0.121297D+00
     6  0.314338D-03  0.170357D-08  0.202842D-01  0.222096D-01  0.370431D-09
                6
     6  0.736073D-01
 Final State Averaged  Density Matrix
                1             2             3             4             5
     1  0.192404D+01
     2  0.708975D-13  0.187716D+01
     3  0.651602D-07  0.614037D-12  0.109978D+01
     4  0.652038D-07 -0.867282D-13  0.109242D-07  0.905001D+00
     5 -0.632352D-14  0.118569D-07  0.358683D-12  0.456676D-12  0.120720D+00
     6  0.397187D-08  0.175771D-12  0.144586D-06  0.161882D-06 -0.663355D-13
                6
     6  0.732993D-01
```

CoIn(β) for 1a

GEOMETRY

C	0.04792139	-0.06214744	-0.00884484
C	0.00635789	-0.03209769	1.47739367
C	1.24406507	-0.00072666	2.05590496
C	2.39165356	0.40000393	1.27590794
C	2.17830459	1.01449990	-0.01359391
C	0.93785882	0.98015420	-0.58603955
H	-0.91605291	-0.11357164	2.01925435
H	1.37064248	-0.15946423	3.11263371
H	2.97835797	1.58762025	-0.44872929
H	0.63940386	1.57672763	-1.42634751
C	3.76833542	0.37893306	1.88705064
H	4.51163177	0.22864068	1.10686930
H	3.86032097	-0.47913696	2.54963252
C	3.11742035	2.20584423	4.34480296
H	3.43965068	3.05822814	4.93826842
H	2.10021543	2.40399386	4.01850632
H	3.08991494	1.34359339	5.00676909
C	4.27711368	3.46610347	1.77585078
H	4.61797965	4.33876400	2.32799746
H	4.93554161	3.34925955	0.91838217
H	3.28222018	3.68848375	1.40012151
C	6.04069239	1.62417419	3.52373525
H	6.74217536	1.46434587	2.70854557
H	6.40253676	2.47067013	4.10234849
H	6.08371487	0.74878728	4.16716703
Si	4.28672636	1.93128740	2.88260945
Cl	0.48638320	-1.72781358	-0.62802929

E_0(CASSCF,vacuo) -1135.789721

DATA from the CASSCF calculation in vacuo:

```
                EIGENVALUES AND  EIGENVECTORS OF CI MATRIX

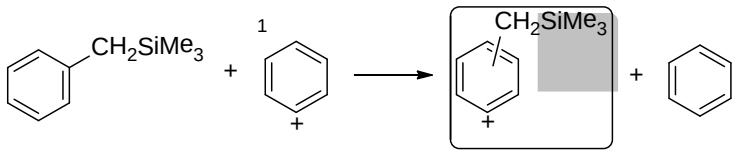
 ( 1)     EIGENVALUE    -1135.7897216850
(    65) 0.7254640 (     1)-0.5860839 (    77) 0.1079705 (    63) 0.1079705 (   319)-0.1059419 (    87)-0.0886676 (    62)-0.0886676
(    75) 0.0863326 (    66) 0.0610224 (    74) 0.0610224 (   316) 0.0605397 (   328) 0.0605397 (   325) 0.0519306 (   320) 0.0519306
(   326)-0.0506357 (   240)-0.0498066 (    73)-0.0497846 (    85)-0.0497846 (   373)-0.0480728 (    59) 0.0469480 (    89) 0.0469480
(    80)-0.0444280 (    67)-0.0444280 (    90)-0.0442396 (    60)-0.0442396 (    81)-0.0432038 (    76)-0.0432038 (    82) 0.0416947
(   161) 0.0412487 (    28) 0.0409902 (   127) 0.0338651 (    93) 0.0338651 (    30) 0.0305611 (    23) 0.0305611 (   216)-0.0250875
(   179)-0.0250875 (    79)-0.0249483 (    72)-0.0249483 (   339) 0.0239487 (   314) 0.0239487 (   163)-0.0221060 (   143)-0.0221060
(    83) 0.0209817 (    64) 0.0209817 (   400) 0.0200923 (   118) 0.0195352 (    96) 0.0195352 (   279) 0.0182422 (   290) 0.0182422
(    16) 0.0181913 (

 ( 2)     EIGENVALUE    -1135.7897206684
(     9) 0.6591379 (    16)-0.6591379 (    63) 0.1087121 (    77)-0.1087121 (   182) 0.0964621 (   213)-0.0964621 (    62)-0.0882611
(    87) 0.0882611 (   181) 0.0579054 (   198)-0.0579054 (   221) 0.0555709 (   180)-0.0555709 (   191)-0.0551407 (   210) 0.0551407
(    17)-0.0516986 (    10) 0.0516986 (   214) 0.0487455 (   187)-0.0487455 (   199) 0.0477159 (   186)-0.0477159 (   183)-0.0470487
(   218) 0.0470487 (   188) 0.0463697 (   219)-0.0463697 (    97) 0.0457660 (   124)-0.0457660 (   277) 0.0451086 (   304)-0.0451086
(    12)-0.0422929 (    18) 0.0422929 (    93) 0.0361851 (   127)-0.0361851 (    23) 0.0291787 (    30)-0.0291787 (   179)-0.0287347
(   216) 0.0287347 (   290) 0.0239899 (   279)-0.0239899 (   314) 0.0239269 (   339)-0.0239269 (   195)-0.0228896 (   189) 0.0228896
(    72)-0.0221432 (    79) 0.0221432 (    96) 0.0220518 (   118)-0.0220518 (   385) 0.0185786 (   392)-0.0185786 (   143)-0.0173337
(   163) 0.0173337 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.998345D+00
     2 -0.170716D-06  0.187514D+01
     3  0.642185D-02 -0.273609D-08  0.192319D+01
     4 -0.528809D-02 -0.145743D-07  0.826076D-02  0.100637D+01
     5  0.776433D-07 -0.634006D-03 -0.140933D-07 -0.389941D-07  0.122761D+00
     6  0.225021D-01  0.240275D-07  0.315403D-03  0.200350D-01  0.490936D-08
                6
     6  0.741863D-01
Density Matrix for State     1             2             3             4             5
     1  0.809268D+00
     2  0.170731D-06  0.187646D+01
     3 -0.642183D-02  0.273505D-08  0.192397D+01
     4  0.528811D-02  0.145534D-07 -0.826062D-02  0.119534D+01
     5 -0.776800D-07  0.633992D-03  0.141282D-07  0.389729D-07  0.121428D+00
     6 -0.225018D-01 -0.240737D-07 -0.315440D-03 -0.200348D-01 -0.490798D-08
                6
     6  0.735370D-01
 Final State Averaged  Density Matrix
                1             2             3             4             5
     1  0.903806D+00
     2  0.713841D-11  0.187580D+01
     3  0.858380D-08 -0.520460D-12  0.192358D+01
     4  0.130707D-07 -0.104128D-10  0.677476D-07  0.110086D+01
     5 -0.183840D-10 -0.701567D-08  0.174437D-10 -0.106178D-10  0.122095D+00
     6  0.157634D-06 -0.230895D-10 -0.182023D-07  0.922721D-07  0.688298D-12
                6
     6  0.738617D-01
```

4. Cartesian coordinates and CASSCF output data for structures 2^+a-c

The level of theory chosen for optimizing these structures was the CASSCF(8,9)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring, the σ/σ* couple of the C-Si bond and the orbital at the dicoordinated carbon (see Fig. S5 for a graphical representation of the orbitals included in the active space in the case of ^{3}**2$^+$a**, taken as a model). For all of the structures reported in this section, numerical frequency calculations (FREQ=NUMER) have been adopted.

As stated in the text, the energies reported in Fig. 5 have been calculated according to the isodesmic reaction reported below.



The level of theory of theory chosen for describing the compounds involved is as in the following:

- Benzytrimethylsilane: CASSCF(8,8)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring and the σ/σ* couple of the C-Si bond; numerical frequency calculations (FREQ=NUMER) have been adopted.
- Parent singlet phenyl cation: CASSCF(6,7)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring and the orbital at the dicoordinated carbon; analytical frequency calculations have been adopted.
- Benzene: CASSCF(6,6)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring; analytical frequency calculations have been adopted.

The optimization of parent singlet phenyl cation was quite troublesome, due to the inclusion of the orbital at the dicoordinated carbon in the active space. This is probably related to the low occupancy of this orbital (less than 0.01, both in vacuo and in MeOH bulk), as hinted from the output of the CASSCF calculation (see below). Thus, the geometry was optimized applying a symmetry constraint (C_{2v}) and all of the calculations were carried out applying a loose convergence criterion (SCF=CONVER=4). Despite the above mentioned approximations, the geometry was successfully optimized and checked to be a minimum, and indeed the data are in accordance with the literature.[S4]

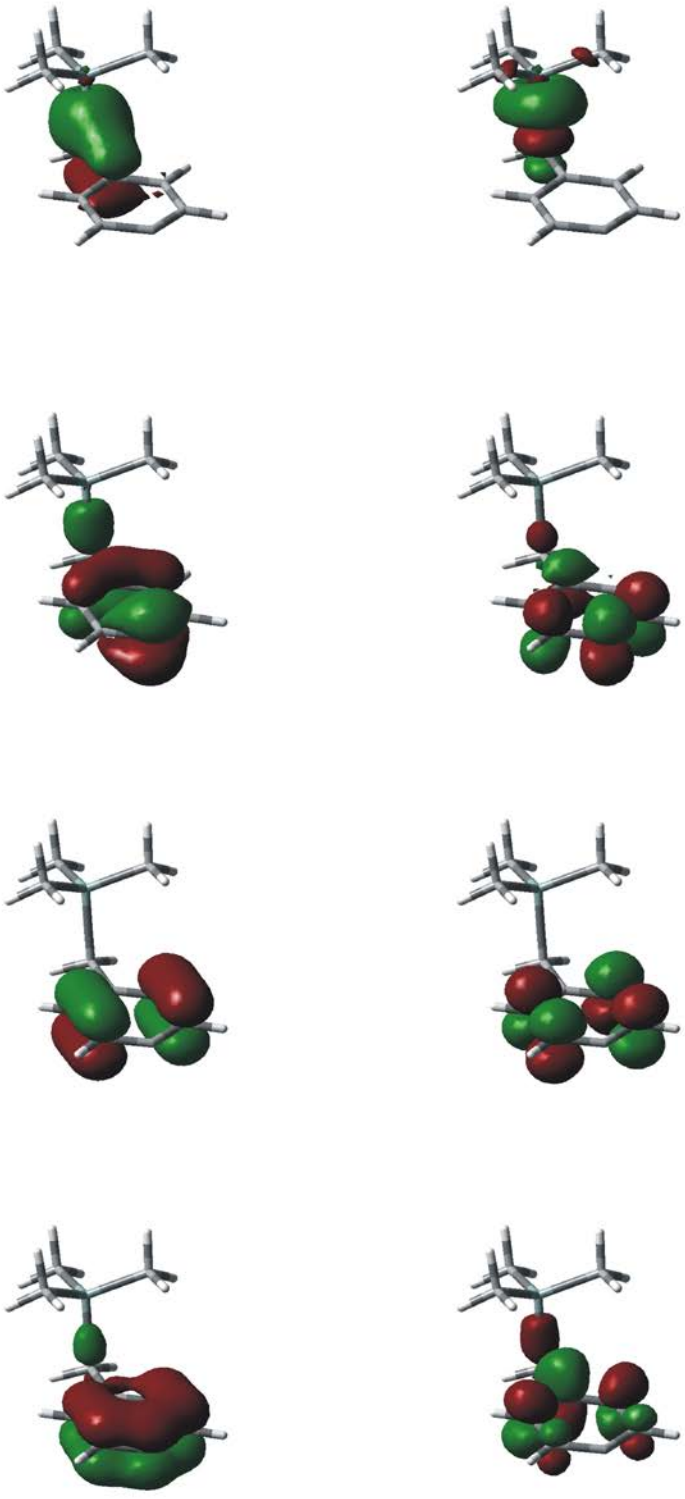
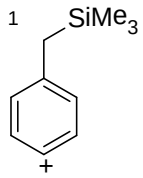


Fig. S5. Orbitals included in the active space for the CASSCF calculations in the case of $^{3}\mathbf{2}^{+}\mathbf{a}$, taken as a model. Further notice that the above orbitals have been employed for all of the cations and that they differ slightly for singlet cations, due to the orbitals mixing mentioned in the main text.



$^{1}2^{+}$a

GEOMETRY

C	3.32556200	0.05367300	0.53328000
C	2.97907300	-1.21487800	0.17075700
C	1.65761400	-1.27851900	-0.30108100
C	1.00924500	-0.08057500	-0.63589200
C	1.68439700	1.16062700	-0.40178000
C	3.00783000	1.28292700	0.07245200
H	3.65248400	-2.05036300	0.20622700
H	1.21799600	-2.23130100	-0.52633700
H	1.11135100	2.06928500	-0.44810400
H	3.44427500	2.22044800	0.35163300
C	-0.36624000	-0.06821800	-1.21154900
H	-0.52685100	-0.96660100	-1.79962000
H	-0.48753900	0.77909200	-1.87967400
C	-1.65329600	1.57612500	1.13523100
H	-2.49159600	1.67370900	1.81985800
H	-0.75225600	1.56999000	1.74404300
H	-1.64145600	2.47445000	0.52274000
C	-1.75474600	-1.52726400	1.18824000
H	-2.58835100	-1.54109900	1.88537300
H	-1.81384100	-2.44301400	0.60556500
H	-0.84584300	-1.56675400	1.78333600
C	-3.42134800	0.04779700	-0.92388700
H	-3.52050600	-0.83638400	-1.54748900
H	-4.29512400	0.08713100	-0.27901500
H	-3.46140900	0.91686900	-1.57477600
Si	-1.84356300	0.00959800	0.09868700

E_0(CASSCF,vacuo) -676.113048

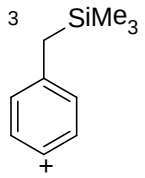
Zero-point correction= 0.228825
Thermal correction to Energy= 0.241967
Thermal correction to Enthalpy= 0.242911
Thermal correction to Gibbs Free Energy= **0.189645**

E_0(CASMP2,vacuo) -677.274106
ΔE_{CORR}(MP2) **-1.223110**

E_0(CASSCF,CPCM) **-676.190800**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1130379864
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611304E+03
 (    1) 0.9193143 (    3)-0.2051843 (   36)-0.0995631 (  351)-0.0800258 (   67)-0.0736410 (   38) 0.0689006 ( 1599)-0.0675384
 (   35)-0.0602416 ( 1663)-0.0552821 (    6)-0.0542191 (    5) 0.0515244 (   39) 0.0506746 ( 1711)-0.0504031 (   10)-0.0487321
 (   30)-0.0475850 (    9) 0.0447113 (   45)-0.0445609 (    8) 0.0431999 ( 1655)-0.0418101 (   55)-0.0411635 ( 1778)-0.0396838
 (   28)-0.0372303 ( 1772) 0.0370132 (   43)-0.0368369 ( 1606)-0.0366404 (   25) 0.0366101 (  121) 0.0361725 (   31)-0.0355889
 ( 1716) 0.0354378 ( 1721)-0.0346407 (   44)-0.0337397 ( 1770)-0.0333600 ( 1830)-0.0332745 ( 1779)-0.0331137 (   78) 0.0325430
 ( 1954) 0.0323063 (   79) 0.0322864 ( 1661) 0.0319276 ( 1605) 0.0300887 (   23) 0.0289239 ( 1601) 0.0288917 ( 1719) 0.0287126
 ( 1777)-0.0282861 (   26)-0.0277678 (   12) 0.0275321 (   24) 0.0260563 ( 1774) 0.0258916 ( 1892) 0.0257285 ( 1715)-0.0255374
 ( 1780)-0.0254619 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
      1  0.195064D+01
      2  0.294572D-06  0.198191D+01
      3  0.183804D-05 -0.964235D-07  0.190632D+01
      4 -0.987785D-06  0.625250D-06  0.276086D-05  0.183631D+01
      5 -0.156141D-04 -0.206660D-05  0.309813D-04 -0.260971D-04  0.145933D+00
      6 -0.673245D-06  0.506487D-05 -0.714567D-05 -0.147440D-04 -0.311509D-05
      7  0.923495D-05 -0.521464D-05 -0.412537D-05  0.293276D-04 -0.138820D-05
      8  0.298732D-05 -0.200886D-05 -0.570776D-05  0.194634D-04 -0.290662D-05
      9  0.343304D-06 -0.440850D-06 -0.718165D-06  0.541045D-06  0.736829D-08
                6             7             8             9
      6  0.835841D-01
      7  0.125482D-05  0.477029D-01
      8 -0.460178D-06 -0.138036D-05  0.306579D-01
      9  0.423480D-07  0.171705D-07  0.404874D-06  0.169416D-01
 MCSCF converged.
```



$^{3}2^{+}$a

GEOMETRY

C	-0.01648200	0.03047000	-0.00804200
C	-0.01710700	0.02453900	1.39964600
C	1.20061200	0.01134700	2.03183300
C	2.42556700	0.01085300	1.26989000
C	2.35329800	0.01058100	-0.17089000
C	1.13972900	0.02377000	-0.81100700
H	-0.93860100	0.03841500	1.94929900
H	1.26256300	0.01531900	3.10360000
H	3.26918800	0.01398800	-0.73095500
H	1.06603400	0.03708400	-1.88145300
C	3.69357300	-0.02439600	1.93345200
H	3.67672000	0.38594400	2.93534500
H	4.50724800	0.38538800	1.34825000
C	4.50451700	-2.80028200	0.59409600
H	4.93740400	-3.78806000	0.73198900
H	3.55302300	-2.93896100	0.08948200
H	5.16735200	-2.25482600	-0.07157600
C	3.05465100	-2.79935000	3.36473300
H	3.41445100	-3.78707600	3.64231500
H	2.88572700	-2.25335900	4.28850100
H	2.09761800	-2.93803700	2.87070900
C	5.96952200	-1.68449100	3.12502700
H	5.85603200	-1.13893300	4.05694500
H	6.42626600	-2.64154800	3.36444200
H	6.67069200	-1.13957900	2.50019300
Si	4.32609400	-1.96169600	2.26511900

E_0(CASSCF,vacuo) -676.126481

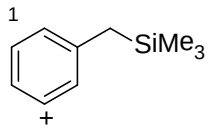
Zero-point correction= 0.230559
Thermal correction to Energy= 0.243532
Thermal correction to Enthalpy= 0.244477
Thermal correction to Gibbs Free Energy= **0.190413**

E_0(CASMP2,vacuo) -677.342505
ΔE_{CORR}(MP2) **-1.216024**

E_0(CASSCF,CPCM) **-676.198761**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1264813039
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612648E+03
 (     1) 0.9409963 ( 1264)-0.1251340 (  512) 0.1018127 ( 1268)-0.0830313 ( 3025) 0.0687073 ( 6166)-0.0685019 (  422)-0.0678901
 (    11)-0.0678794 ( 3035)-0.0603828 ( 2950)-0.0579712 ( 1430)-0.0547568 ( 2101)-0.0546844 ( 1354) 0.0520247 ( 2942)-0.0501832
 ( 1349)-0.0501189 ( 2945) 0.0500271 ( 1271) 0.0467267 ( 1261)-0.0400129 (    4) 0.0395639 ( 1272)-0.0391164 ( 1438)-0.0386045
 (  426)-0.0382038 ( 2946)-0.0380573 ( 1434)-0.0378752 ( 3028) 0.0351653 (  425)-0.0351040 (  177)-0.0347662 ( 3112)-0.0345144
 (   15) 0.0332333 ( 6081)-0.0321152 (  515) 0.0317435 ( 6077) 0.0314360 (  706) 0.0311555 ( 2185)-0.0300707 ( 1346) 0.0282313
 ( 5993) 0.0235706 ( 6080)-0.0228942 (  621)-0.0228541 ( 5997)-0.0223080 (  600)-0.0218535 ( 3226) 0.0217025 ( 3120)-0.0204390
 ( 2115)-0.0203103 ( 6145) 0.0196235 ( 1459)-0.0192377 ( 5996)-0.0179767 ( 4643) 0.0173570 ( 6161) 0.0152646 (  537)-0.0152044
 ( 5886)-0.0151150 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197301D+01
     2  0.336224D-06  0.192883D+01
     3  0.231703D-07 -0.778709D-07  0.190488D+01
     4  0.114405D-04 -0.225985D-04  0.845672D-06  0.100586D+01
     5 -0.220567D-05 -0.128498D-04 -0.274813D-06  0.189350D-06  0.999999D+00
     6  0.123060D-06 -0.248045D-06 -0.676127D-05  0.182446D-06 -0.394235D-07
     7  0.159822D-05  0.795336D-05  0.206079D-06 -0.107446D-04 -0.151866D-04
     8  0.204984D-05  0.265619D-05  0.238230D-06 -0.122563D-04 -0.352891D-05
     9 -0.776732D-06 -0.222679D-05 -0.393776D-07  0.181039D-05  0.159666D-05
                6             7             8             9
     6  0.863976D-01
     7  0.952380D-08  0.585571D-01
     8 -0.703633D-07  0.429624D-06  0.265412D-01
     9  0.215486D-08  0.293344D-06 -0.206816D-08  0.159363D-01
 MCSCF converged.
```



$^{1}2^{+}$b

GEOMETRY

C	-3.51988000	-0.04461900	0.48178600
C	-2.90740300	1.16677000	0.00752600
C	-1.61439800	1.11574300	-0.44280800
C	-0.91770800	-0.13734800	-0.62399400
C	-1.61740900	-1.36723800	-0.32112800
C	-2.87831900	-1.20854400	0.14898900
H	-3.39119200	2.11117300	0.17046800
H	-1.09254400	2.02107900	-0.68780100
H	-1.23726200	-2.30047400	-0.68857200
C	0.36350300	-0.17349300	-1.26179800
H	0.55063800	0.64415100	-1.94584000
H	0.61367000	-1.12755500	-1.70658400
C	1.68308600	-1.39954900	1.35932000
H	2.51673600	-1.38735500	2.05710700
H	0.77358600	-1.34290900	1.94997700
H	1.70316200	-2.36319600	0.85845700
C	1.65357600	1.70574900	0.97880900
H	2.49250300	1.87780100	1.64878400
H	1.65079400	2.52073600	0.26064500
H	0.75059600	1.77503800	1.57780500
C	3.39628700	-0.08011700	-0.90766100
H	3.43966200	0.71171800	-1.64925300
H	4.28018500	0.01485000	-0.28165800
H	3.46883400	-1.03120100	-1.42627900
Si	1.85467400	0.03040900	0.15473000
H	-4.33281000	-0.01370600	1.18228700

E_0(CASSCF,vacuo) -676.123672

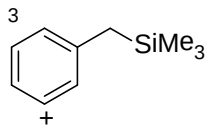
Zero-point correction= 0.229475
Thermal correction to Energy= 0.242716
Thermal correction to Enthalpy= 0.243660
Thermal correction to Gibbs Free Energy= **0.190039**

E_0(CASMP2,vacuo) -677.310704
ΔE_{CORR}(MP2) **-1.216635**

E_0(CASSCF,CPCM) **-676.195591**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1236721368
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67612367E+03
 (    1) 0.8553379 (    3)-0.3728142 (   25) 0.1079944 (   45)-0.1060115 (   38) 0.1013659 (  234)-0.0990800 (  284) 0.0666411
 (  276)-0.0625708 ( 1891)-0.0605755 (   91) 0.0593796 (  255)-0.0588052 (  240) 0.0548125 (  262) 0.0501157 (   52) 0.0481078
 (  239) 0.0455220 (  300)-0.0427959 (   30)-0.0426909 (   36)-0.0413583 (  352) 0.0402771 (  390)-0.0370880 (  121) 0.0370181
 (   49)-0.0355152 ( 1830)-0.0354431 (   28)-0.0354237 (  309)-0.0346702 (  286)-0.0344166 (  278) 0.0329176 (  378) 0.0320711
 (  283) 0.0318852 (   55)-0.0308335 (  235) 0.0305600 ( 1827)-0.0297715 (  260) 0.0291545 ( 1828)-0.0290743 ( 1836)-0.0288123
 (   10)-0.0278193 (  256) 0.0276006 (  364)-0.0274109 (    6)-0.0270533 ( 2145) 0.0262607 ( 1856)-0.0257752 (  253)-0.0257378
 (  244)-0.0255896 (  172)-0.0247108 (  261) 0.0244270 (   12)-0.0244177 (  298)-0.0242653 ( 1721) 0.0233602 (    9) 0.0230143
 (  704)-0.0229464 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197230D+01
     2 -0.142822D-05  0.193023D+01
     3 -0.207146D-06 -0.156700D-05  0.189239D+01
     4 -0.322786D-05 -0.114127D-05 -0.204745D-05  0.163276D+01
     5  0.826462D-05  0.714900D-05  0.380492D-05 -0.895591D-05  0.371592D+00
     6  0.608424D-05  0.990774D-06 -0.152339D-05 -0.103192D-04  0.252099D-05
     7 -0.223514D-05 -0.171852D-05 -0.824117D-06  0.295229D-05  0.145099D-06
     8  0.641963D-06 -0.346785D-05 -0.471150D-05  0.523352D-06 -0.275366D-05
     9  0.199681D-05  0.259962D-05 -0.127470D-05  0.325243D-06 -0.387916D-07
                6             7             8             9
     6  0.633743D-01
     7  0.158947D-05  0.955465D-01
     8 -0.657761D-06  0.774568D-06  0.263680D-01
     9 -0.387822D-06  0.738885D-06  0.195066D-06  0.154391D-01
 MCSCF converged.
```



$^{3}2^{+}$b

GEOMETRY

C	-3.52326400	-0.07293100	0.44995800
C	-2.90233600	1.14815100	0.11845000
C	-1.64313900	1.13876000	-0.44515700
C	-0.93725500	-0.09445000	-0.71716900
C	-1.57455000	-1.33368600	-0.36918800
C	-2.80999800	-1.26544600	0.18392900
H	-3.41004500	2.07638400	0.29834600
H	-1.16339600	2.06293600	-0.70623200
H	-1.08321800	-2.26834700	-0.56034800
C	0.37975600	-0.06558600	-1.28657100
H	0.57685800	0.81821100	-1.88098600
H	0.63794500	-0.96875200	-1.82561300
C	1.70454000	-1.52334300	1.20950000
H	2.52646100	-1.55095700	1.92072900
H	0.78504500	-1.55711500	1.78622100
H	1.76804800	-2.43170500	0.61718800
C	1.58617000	1.59924300	1.14637400
H	2.40611200	1.72088500	1.84992600
H	1.57558400	2.48514800	0.51773000
H	0.66962900	1.58328200	1.72885100
C	3.40974000	0.06467700	-0.87964800
H	3.44749600	0.93348400	-1.52988700
H	4.28045100	0.10917000	-0.23017700
H	3.51352000	-0.82187700	-1.49793100
Si	1.84535400	0.02431300	0.15454800
H	-4.50342500	-0.10345500	0.88565300

E_0(CASSCF,vacuo) -676.11965

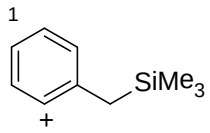
Zero-point correction= 0.229978
Thermal correction to Energy= 0.243046
Thermal correction to Enthalpy= 0.243990
Thermal correction to Gibbs Free Energy= **0.189717**

E_0(CASMP2,vacuo) -677.338034
ΔE_{CORR}(MP2) **-1.218381**

E_0(CASSCF,CPCM) **-676.191710**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1196530189
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611965E+03
(     1) 0.9393056 ( 1349)-0.1237242 (  428) 0.1006416 ( 1352)-0.0761566 (  506)-0.0742530 ( 6166)-0.0696861 ( 2950)-0.0598934
( 3035)-0.0583645 ( 2101) 0.0552609 ( 1430)-0.0537554 ( 1271) 0.0519485 (  171)-0.0516598 ( 1264)-0.0499332 ( 3028) 0.0491622
(  508)-0.0460955 ( 3026)-0.0457421 (   87) 0.0404868 ( 1434)-0.0403244 (  510)-0.0402176 (  430) 0.0400432 ( 3030)-0.0399234
( 1356)-0.0394796 (  512) 0.0394231 ( 1439)-0.0387680 ( 1354) 0.0373751 ( 1268) 0.0364723 ( 3025) 0.0359700 (   11)-0.0359576
( 3113)-0.0357696 ( 2941) 0.0341852 (   10)-0.0334266 (   16) 0.0332048 (   93) 0.0330241 (  177)-0.0325030 (  706)-0.0316709
( 2945) 0.0311682 ( 6077) 0.0296416 ( 2353)-0.0295032 ( 6081)-0.0287931 (  590) 0.0277436 (    4) 0.0247201 ( 1261)-0.0244766
(  600)-0.0232811 (  621) 0.0229965 ( 5909) 0.0224831 ( 3120)-0.0206813 ( 5913)-0.0205780 ( 1262) 0.0199607 ( 2116) 0.0197793
( 6079)-0.0194648 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197403D+01
     2 -0.374280D-06  0.193052D+01
     3  0.841438D-06  0.360590D-05  0.190041D+01
     4 -0.148905D-04 -0.106446D-04  0.988136D-06  0.100420D+01
     5  0.221024D-05 -0.378696D-05  0.592551D-05  0.141593D-06  0.999994D+00
     6 -0.216052D-05  0.215448D-05 -0.872717D-06 -0.714273D-05  0.112030D-05
     7 -0.192337D-05  0.239713D-05 -0.520107D-05  0.205726D-05 -0.245018D-05
     8  0.435748D-05 -0.116687D-05 -0.268846D-05 -0.719114D-05 -0.971799D-06
     9 -0.972311D-06  0.766175D-06 -0.208521D-05  0.257334D-05  0.932306D-07
                6             7             8             9
     6  0.564173D-01
     7 -0.116668D-05  0.899928D-01
     8 -0.750613D-06  0.147502D-05  0.283084D-01
     9 -0.236064D-06 -0.164416D-06 -0.257465D-06  0.161372D-01
MCSCF converged.
```



$^{1}2^{+}$c

GEOMETRY

C	-0.01196600	-0.02409700	0.01735800
C	-0.00425100	0.04254500	1.44157300
C	1.17211900	0.06415000	2.16080100
C	2.42386400	0.13537000	1.44386400
C	2.17853000	-0.17691800	0.15578000
C	1.17277300	-0.02724200	-0.74109900
H	-0.94567600	0.08542300	1.95511000
H	1.18041000	0.22801400	3.22209500
H	1.20229300	-0.25756300	-1.78710600
C	3.72246300	0.57280400	2.03302500
H	3.52461400	1.26633100	2.84186900
H	4.31872000	1.09146700	1.28862000
C	5.26203700	-2.03974500	1.29986600
H	5.92788500	-2.83233800	1.63097000
H	4.38647000	-2.52373300	0.87471000
H	5.77494400	-1.50929400	0.50153200
C	3.85151700	-1.81369400	4.06717200
H	4.45793600	-2.59946100	4.50982900
H	3.54919100	-1.15361000	4.87603600
H	2.95892100	-2.29058700	3.67043000
C	6.36134100	-0.06306900	3.45202500
H	6.10802700	0.62447800	4.25417900
H	7.04590800	-0.79987800	3.86365100
H	6.90593800	0.49557500	2.69599700
Si	4.83774800	-0.90536100	2.74367700
H	-0.92950400	-0.24545000	-0.49677000

E_0(CASSCF,vacuo) -676.121946

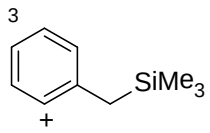
Zero-point correction= 0.229153
Thermal correction to Energy= 0.242431
Thermal correction to Enthalpy= 0.243375
Thermal correction to Gibbs Free Energy= **0.189575**

E_0(CASMP2,vacuo) -676.04106
ΔE_{CORR}(MP2) **-1.221225**

E_0(CASSCF,CPCM) **-676.197154**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1219456024
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67612195E+03
 (    1) 0.9259088 (    3)-0.1287454 (   30) 0.1032342 (    6)-0.1019432 (   28)-0.0987751 (    8)-0.0896044 (   43) 0.0833553
 (   67) 0.0819939 ( 1891)-0.0794772 (  257)-0.0638686 (  234)-0.0578904 (  240) 0.0559510 (  279)-0.0558734 (  241) 0.0540697
 (   10)-0.0511752 (  307) 0.0479392 (   55)-0.0470291 (  255)-0.0458426 (   36)-0.0427752 (  276)-0.0416199 (  310) 0.0406337
 (   35)-0.0405502 (   45)-0.0402324 (  253)-0.0358280 (    5) 0.0339770 (  286)-0.0330220 (  300)-0.0317082 (  325)-0.0316973
 (  283) 0.0314845 (  309)-0.0314159 (  258)-0.0309051 (   38) 0.0300772 (   92)-0.0296795 (   12) 0.0295540 (   78) 0.0280349
 (   31) 0.0273666 (  235) 0.0266977 (  704)-0.0244667 (  121) 0.0232824 (   79) 0.0232348 (   26) 0.0231706 (  285)-0.0227301
 (  238)-0.0226518 (   23)-0.0214880 (   24) 0.0212424 (   91) 0.0195607 (   15)-0.0191528 ( 1836)-0.0186821 (   13) 0.0176809
 (  239) 0.0171541 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.198238D+01
     2 -0.284469D-07  0.195024D+01
     3  0.594136D-06 -0.189618D-05  0.190144D+01
     4 -0.129126D-05 -0.450136D-06 -0.149386D-05  0.186714D+01
     5 -0.213803D-05  0.390611D-05  0.138788D-05  0.163361D-04  0.125574D+00
     6 -0.929241D-06 -0.359209D-06 -0.358336D-05 -0.254885D-05  0.352992D-05
     7 -0.313589D-05 -0.425975D-05 -0.902439D-05  0.253660D-04 -0.367587D-05
     8  0.153111D-05 -0.641984D-06  0.116821D-06 -0.279818D-04  0.485865D-05
     9  0.271508D-06 -0.130097D-05  0.801539D-07 -0.660776D-06  0.208538D-06
                6             7             8             9
     6  0.764504D-01
     7  0.198064D-05  0.518490D-01
     8  0.208318D-05  0.196992D-05  0.283999D-01
     9  0.942828D-07  0.369781D-07  0.521379D-07  0.165250D-01
 MCSCF converged.
```



$^{3}2^{+}$c

GEOMETRY

C	3.45697500	0.11481900	0.42044900
C	2.83636700	-1.15633400	0.19545500
C	1.59376900	-1.25266400	-0.37076200
C	0.88447400	-0.06171300	-0.76407000
C	1.55869500	1.17248100	-0.50847700
C	2.80275200	1.30015900	0.06238100
H	3.36761500	-2.04728900	0.47204500
H	1.13836500	-2.20933200	-0.54478900
C	-0.41321100	-0.09221500	-1.33646600
H	-0.67980800	-1.02536100	-1.81431600
H	-0.66967500	0.77637000	-1.92792700
C	-1.59589600	1.64732600	1.08050600
H	-2.41802300	1.80904700	1.77378600
H	-0.68075800	1.65221800	1.66420700
H	-1.57493900	2.49870900	0.40688600
C	-1.65938700	-1.48342900	1.26208600
H	-2.46531700	-1.51060200	1.99173400
H	-1.71278400	-2.40870000	0.69602500
H	-0.72687700	-1.47560800	1.81766400
C	-3.43430600	0.00035400	-0.85277700
H	-3.52710900	-0.91104100	-1.43519200
H	-4.29887800	0.05320500	-0.19528900
H	-3.49432700	0.84403200	-1.53323600
Si	-1.86625000	0.02922600	0.17275500
H	4.43428700	0.15146900	0.86303500
H	3.25434100	2.26101100	0.21684500

E_0(CASSCF,vacuo) -676.124686

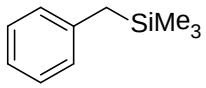
Zero-point correction= 0.230184
Thermal correction to Energy= 0.243262
Thermal correction to Enthalpy= 0.244206
Thermal correction to Gibbs Free Energy= **0.189918**

E_0(CASMP2,vacuo) -677.342114
ΔE_{CORR}(MP2) **-1.217428**

E_0(CASSCF,CPCM) **-676.195006**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1246856854
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612469E+03
(     1) 0.9344024 ( 1349)-0.1292945 (  506) 0.0909991 (  428) 0.0875272 ( 1345) 0.0692450 ( 2950)-0.0684505 (    5)-0.0679505
( 6166)-0.0603142 ( 3028)-0.0589611 ( 1352) 0.0589092 ( 1271)-0.0540874 ( 3035)-0.0539238 ( 2101)-0.0502870 ( 1430) 0.0487315
( 1264)-0.0472765 ( 2941) 0.0469148 (  171)-0.0461929 (   10)-0.0461663 (  508) 0.0451596 ( 1268)-0.0442748 ( 6081)-0.0411206
( 1354)-0.0409989 (  430) 0.0381265 ( 6077)-0.0363082 (  512) 0.0361473 (  706)-0.0345688 ( 1356)-0.0345088 ( 3113)-0.0342744
( 1439)-0.0340710 ( 1434)-0.0339365 ( 2945)-0.0337131 (  510)-0.0330828 ( 3030)-0.0325680 (   16)-0.0293190 ( 5909) 0.0289896
( 2942)-0.0281201 ( 3026) 0.0278113 ( 5913) 0.0275807 ( 6079) 0.0270443 ( 2353)-0.0268575 ( 3032)-0.0262878 (   11)-0.0251717
( 1429) 0.0242693 ( 3025) 0.0242565 ( 1460) 0.0242079 (  255)-0.0235730 (  590) 0.0234944 ( 3226)-0.0229235 (    6)-0.0227981
( 4621)-0.0226574 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.196706D+01
     2  0.741385D-07  0.193201D+01
     3 -0.492145D-06  0.336771D-05  0.189228D+01
     4 -0.667710D-05 -0.173773D-04  0.576024D-04  0.100363D+01
     5  0.284001D-06 -0.415511D-05  0.110319D-04 -0.178502D-06  0.999982D+00
     6 -0.395220D-05  0.740874D-05  0.712226D-05 -0.116894D-04 -0.427572D-06
     7 -0.481315D-05  0.261960D-05  0.265890D-05 -0.266175D-04 -0.500056D-05
     8 -0.289567D-05 -0.532041D-05 -0.166258D-05  0.772434D-05 -0.203194D-05
     9 -0.717169D-06  0.192916D-05  0.106491D-05 -0.974497D-06  0.406774D-06
                6             7             8             9
     6  0.593042D-01
     7  0.404897D-05  0.100599D+00
     8 -0.124114D-05 -0.767237D-06  0.300894D-01
     9 -0.719350D-06  0.742764D-06 -0.105541D-06  0.150477D-01
MCSCF converged.
```



GEOMETRY

C	-0.03044500	-0.05865000	0.00222100
C	-0.01500500	-0.05557300	1.39732900
C	1.19649200	0.01745500	2.08614900
C	2.41724600	0.08879400	1.40081300
C	2.38503100	0.08108900	-0.00058800
C	1.17632800	0.00920500	-0.69456700
H	-0.96273700	-0.11715400	-0.53046200
H	-0.93790500	-0.11361400	1.94692100
H	1.19305300	0.01200200	3.16257200
H	3.30857300	0.12621700	-0.55176500
H	1.17909700	0.00178900	-1.77024900
C	3.72799700	0.19198900	2.15051100
H	3.65823400	-0.34526800	3.09457800
H	4.51752600	-0.29899000	1.58463700
Si	4.32095600	1.99341800	2.54150200
C	5.96790600	1.87174900	3.47028400
H	6.35565900	2.85643100	3.72013700
H	5.86175400	1.31909200	4.40083300
H	6.72530300	1.36591100	2.87606900
C	3.05124300	2.88182800	3.62788700
H	2.08899100	2.96962800	3.13148900
H	2.88996700	2.35612900	4.56626000
H	3.38577500	3.88714000	3.87340600
C	4.57422000	2.96289400	0.93604400
H	5.30771500	2.48442000	0.29111100
H	3.65052600	3.05298200	0.37145700
H	4.93167000	3.96921500	1.14191100

E_0(CASSCF,vacuo) -677.043500

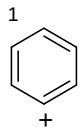
Zero-point correction= 0.243725
Thermal correction to Energy= 0.256542
Thermal correction to Enthalpy= 0.257486
Thermal correction to Gibbs Free Energy= **0.204645**

E_0(CASMP2,vacuo) -678.313641
ΔE_{CORR}(MP2) **-1.270141**

E_0(CASSCF,CPCM) **-677.047720**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.67704350E+03
(    1) 0.9361476 (   11)-0.1414799 (   14)-0.1408378 (   18)-0.1364358 (  147) 0.1071407 (  165) 0.1046980 (   13)-0.1008012
(  201)-0.0848002 (   89)-0.0425865 (    3)-0.0419124 (  190)-0.0398223 (  576)-0.0380749 (   38)-0.0377090 (   25) 0.0371819
(   22) 0.0363864 (    7)-0.0363513 (    6)-0.0359434 (  231)-0.0328446 (  102) 0.0326581 (  125)-0.0326498 (  186)-0.0315523
(  185)-0.0301594 (  112) 0.0257400 (  210)-0.0251813 (  504) 0.0244992 (  501) 0.0242499 (  115) 0.0148445 ( 1088) 0.0131568
(  612) 0.0129741 (  124)-0.0129155 (  605) 0.0128471 ( 1104) 0.0128303 (  616) 0.0124587 (  271)-0.0115804 (   86) 0.0112227
(  162) 0.0112215 ( 1101) 0.0105657 (  230)-0.0103144 (  107) 0.0101487 (  145)-0.0099109 (  517)-0.0098286 ( 1264)-0.0097194
( 1250)-0.0097059 (   69) 0.0096281 (  116)-0.0095819 ( 1113) 0.0094020 (  546)-0.0093723 (  608) 0.0091399 (  348) 0.0090659
(  563) 0.0086304 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.196003D+01
     2  0.295591D-08  0.198268D+01
     3 -0.828241D-05  0.114483D-04  0.190011D+01
     4  0.193360D-05 -0.266206D-05 -0.178119D-03  0.189974D+01
     5  0.960153D-05 -0.123115D-04  0.267208D-05  0.112076D-04  0.102023D+00
     6 -0.228696D-06  0.720388D-06  0.602468D-05 -0.178428D-05 -0.110929D-04
     7 -0.297330D-06  0.277712D-06  0.307449D-05 -0.113437D-05 -0.137135D-06
     8 -0.995179D-07  0.326538D-06  0.388628D-05 -0.107473D-05 -0.668371D-05
                6             7             8
     6  0.100607D+00
     7  0.287457D-07  0.174473D-01
     8  0.391496D-07  0.508204D-08  0.373530D-01
MCSCF converged.
```



GEOMETRY (C_{2v} point group)

C	0.00000000	0.00000000	1.29175000
C	0.00000000	1.22341000	0.61129000
C	0.00000000	1.27977700	-0.81293100
C	0.00000000	0.00000000	-1.19093600
C	0.00000000	-1.27977700	-0.81293100
C	0.00000000	-1.22341000	0.61129000
H	0.00000000	0.00000000	2.36427300
H	0.00000000	2.15985200	1.13695800
H	0.00000000	2.16830200	-1.41168900
H	0.00000000	-2.16830200	-1.41168900
H	0.00000000	-2.15985200	1.13695800

E_0(CASSCF,vacuo) -229.834034

Zero-point correction= 0.089924
Thermal correction to Energy= 0.094668
Thermal correction to Enthalpy= 0.095612
Thermal correction to Gibbs Free Energy= **0.062876**

E_0(CASMP2,vacuo) -230.456290
ΔE_{CORR}(MP2) **-0.622442**

E_0(CASSCF,CPCM) **-229.921782**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.22983403E+03
(    1) 0.9399176 (   34)-0.1547667 (   49)-0.1330210 (   44)-0.1322261 (   41)-0.1208722 (  114)-0.1069703 (  128)-0.1062222
(  143)-0.0423395 (   84)-0.0410789 (   14)-0.0404613 (  234)-0.0392839 (   74)-0.0355999 (  138) 0.0352126 (  100)-0.0342238
(  164)-0.0333822 (  253) 0.0329732 (   12)-0.0282954 (    3)-0.0268344 (  139) 0.0265774 (  372)-0.0248053 (  378)-0.0236280
(   69) 0.0185390 (   37) 0.0177974 (  187)-0.0164410 (  122)-0.0160538 (   32)-0.0149432 (  178)-0.0147719 (   66) 0.0139001
(  443) 0.0136165 (  454) 0.0134051 (  451) 0.0120409 (  211)-0.0116327 (  198)-0.0106625 (  163) 0.0104865 (  386) 0.0103886
(  387) 0.0095381 (  455) 0.0091390 (  258)-0.0090541 (  196) 0.0089186 (  383) 0.0087952 (  126)-0.0085124 (  345) 0.0082753
(   78)-0.0076233 (  318) 0.0073873 (  326)-0.0070960 (  306) 0.0070636 (  416) 0.0067629 (  172)-0.0063048 (  101) 0.0062008
(   73)-0.0060506 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195998D+01
     2  0.000000D+00  0.189387D+01
     3 -0.192284D-03  0.000000D+00  0.190491D+01
     4  0.000000D+00 -0.264293D-06  0.000000D+00  0.379359D-02
     5  0.000000D+00  0.215961D-03  0.000000D+00  0.432395D-08  0.106383D+00
     6 -0.228547D-03  0.000000D+00 -0.347992D-03  0.000000D+00  0.000000D+00
     7 -0.147064D-03  0.000000D+00 -0.261963D-03  0.000000D+00  0.000000D+00
                6             7
     6  0.938012D-01
     7 -0.528112D-04  0.372600D-01
MCSCF converged.
```

GEOMETRY

C	-0.00126700	0.00006500	-0.00068900
C	-0.00133800	0.00055000	1.39580200
C	1.20790400	-0.00005300	2.09403700
C	2.41733800	-0.00103200	1.39585000
C	2.41740900	-0.00147100	-0.00050300
C	1.20804900	-0.00096500	-0.69880800
H	-0.93269800	0.00047900	-0.53845200
H	-0.93282400	0.00128600	1.93347100
H	1.20791200	0.00024800	3.16956400
H	3.34871200	-0.00147800	1.93371500
H	3.34884000	-0.00222600	-0.53827100
H	1.20815900	-0.00131200	-1.77433300

E_0(CASSCF,vacuo) -230.776453

Zero-point correction= 0.105393
Thermal correction to Energy= 0.109655
Thermal correction to Enthalpy= 0.110600
Thermal correction to Gibbs Free Energy= **0.077987**

E_0(CASMP2,vacuo) -231.433520
ΔE_{CORR}(MP2) **-0.657066**

E_0(CASSCF,CPCM) **-230.779917**

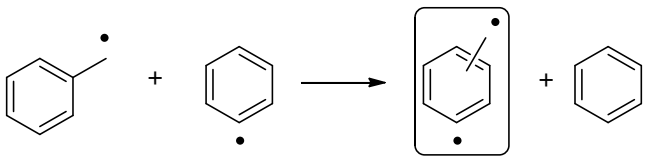
DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -230.7764534422
(    1) 0.9394554 (    3)-0.1472681 (   31)-0.1472657 (   17)-0.1379755 (   13) 0.1116288 (   36)-0.1094890 (   64) 0.1094888
(   60)-0.0416597 (   29)-0.0416594 (  101)-0.0386321 (   11)-0.0356381 (   14)-0.0356379 (   67) 0.0332762 (   69)-0.0329297
(   40)-0.0329295 (   42) 0.0319625 (   78)-0.0319619 (  105)-0.0254104 (  142) 0.0254102 (   20)-0.0205362 (    6) 0.0205361
(    7) 0.0205357 (   22)-0.0205351 (   47) 0.0140095 (   52) 0.0140094 (  135) 0.0137449 (  171) 0.0137448 (   53) 0.0121219
(  160)-0.0117394 (   57)-0.0115593 (  145)-0.0099986 (  116) 0.0099985 (   51)-0.0098975 (   84) 0.0098974 (  163) 0.0096136
(   50) 0.0094381 (   91)-0.0094380 (   98) 0.0090170 (  133) 0.0090169 (  110) 0.0071826 (  146) 0.0071824 (   46) 0.0069985
(  131) 0.0069002 (   55)-0.0066736 (   70)-0.0065062 (  122)-0.0060090 (  126)-0.0056341 (   93) 0.0056341 (   39)-0.0053122
(   77) 0.0053122 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195961D+01
     2  0.130189D-10  0.189860D+01
     3 -0.365267D-10 -0.869395D-06  0.189860D+01
     4 -0.208081D-10  0.215754D-10 -0.453858D-09  0.102745D+00
     5 -0.224188D-09  0.474367D-10  0.415532D-10  0.487741D-06  0.102744D+00
     6 -0.133192D-09 -0.315836D-09  0.192582D-10  0.866933D-11 -0.631325D-11
                6
     6  0.376954D-01
 MCSCF converged.
```

5. Cartesian coordinates and CASSCF output data for structures 3a-c

The level of theory chosen for optimizing these structures was the CASSCF(8,8)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring, the orbital at the benzylic position and the orbital at the dicoordinated carbon (see Fig. S6 for a graphical representation of the orbitals included in the active space in the case of $^{3}\mathbf{2}^{+}\mathbf{a}$, taken as a model). For all of the structures reported in this section, analytical frequency calculations have been adopted.

The energies reported in Fig. S1 have been calculated according to the equation reported below.



The level of theory of theory chosen for describing the compounds is as in the following:

- Benzyl radical: CASSCF(7,7)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring and the orbital at the benzylic position; analytical frequency calculations have been adopted.
- Phenyl radical: CASSCF(7,7)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring and the orbital at the dicoordinated carbon; analytical frequency calculations have been adopted.
- Ground state benzene: CASSCF(6,6)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring; analytical frequency calculations have been adopted. See previous section for details.

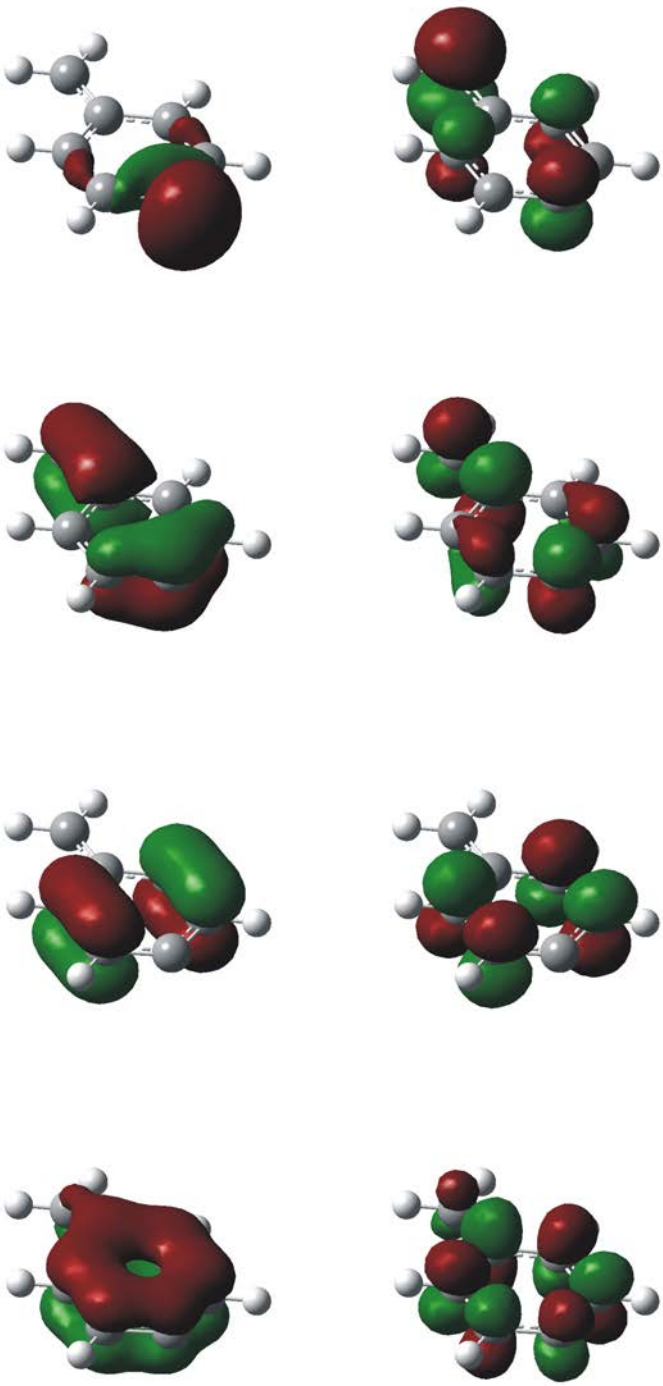
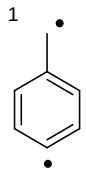


Fig. S6. Orbitals included in the active space for the CASSCF calculations in the case of ^{3}**3a**, taken as a model.



^{1}3a

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38180200
C	1.24333300	0.00000000	2.02685100
C	2.44708000	0.00030900	1.28839900
C	2.37468600	0.00079800	-0.12190700
C	1.13919800	0.00028200	-0.78196800
H	-0.91486900	-0.00055400	1.94515500
H	1.28501300	-0.00060100	3.10182900
H	3.28452000	0.00082700	-0.69594100
H	1.08598100	0.00006800	-1.85505800
C	3.72332100	0.00002500	1.96040200
H	3.78332200	-0.00042400	3.03135700
H	4.64027800	0.00021400	1.40386400

E_0(CASSCF,vacuo) -268.535904

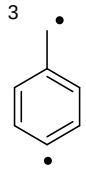
Zero-point correction= 0.105782
Thermal correction to Energy= 0.111572
Thermal correction to Enthalpy= 0.112516
Thermal correction to Gibbs Free Energy= **0.076737**

E_0(CASMP2,vacuo) -269.270175
ΔE_{CORR}(MP2) **-0.734271**

E_0(CASSCF,CPCM) **-268.540813**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.26853590E+03
(   16) 0.8175364 (    89) 0.3139717 (     1)-0.3138637 (   390) 0.1325992 (   108) 0.0995949 (   258) 0.0853261 (   636)-0.0823674
(  425)-0.0724913 (    96) 0.0689179 (   234) 0.0653808 (   146) 0.0653157 (   213) 0.0635786 (   208) 0.0632925 (    90)-0.0574609
(  112) 0.0546580 (    41) 0.0518447 (   818)-0.0509219 (   104) 0.0509089 (   363)-0.0471967 (   144) 0.0471154 (   184) 0.0451675
(  579) 0.0402170 (    56)-0.0402058 (   127) 0.0397508 (   348)-0.0382490 (    14) 0.0382357 (    69) 0.0377638 (   595)-0.0369845
(   68) 0.0359214 (   359) 0.0358344 (  1082) 0.0344963 (   221)-0.0344848 (   591) 0.0343593 (   565)-0.0338980 (    46) 0.0338859
(  126)-0.0332025 (   823) 0.0331718 (   116)-0.0331622 (   129) 0.0316577 (   869) 0.0310939 (   431) 0.0299467 (    51) 0.0299217
(  235) 0.0285460 (   641) 0.0257360 (   207) 0.0256620 (   272)-0.0246548 (   295)-0.0239189 (   686)-0.0228981 (   907) 0.0226904
(   30)-0.0226126 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.999982D+00
     2 -0.340207D-05  0.195577D+01
     3  0.150238D-06 -0.106451D-07  0.188719D+01
     4 -0.887008D-05 -0.751434D-06  0.882175D-09  0.190775D+01
     5  0.168901D-03  0.630963D-05 -0.989052D-07 -0.598624D-06  0.100094D+01
     6 -0.435591D-05  0.361361D-05 -0.998055D-07 -0.144747D-04  0.941476D-05
     7  0.534493D-07 -0.851797D-08  0.827936D-05 -0.736114D-07  0.328758D-07
     8  0.659686D-05 -0.160398D-05 -0.338831D-08  0.503563D-05 -0.380245D-05
                6             7             8
     6  0.928218D-01
     7  0.231435D-08  0.114862D+00
     8 -0.126398D-05  0.100745D-07  0.406822D-01
MCSCF converged.
```



^{3}3a

GEOMETRY

C	-1.85366700	0.00002100	0.00014200
C	-1.20989100	1.22269400	-0.00013100
C	0.19078500	1.21419500	-0.00011000
C	0.91186600	-0.00003700	-0.00012900
C	0.19075300	-1.21420400	-0.00034800
C	-1.20997500	-1.22264300	0.00015100
H	-1.75693900	2.14740500	0.00020200
H	0.72849300	2.14595900	0.00028400
H	0.72837000	-2.14602000	-0.00015500
H	-1.75701200	-2.14736200	0.00057000
C	2.35421800	-0.00001800	0.00017400
H	2.90626300	0.91965100	0.00039900
H	2.90628900	-0.91967200	0.00020500

E_0(CASSCF,vacuo) -268.549145

Zero-point correction=	0.106855
Thermal correction to Energy=	0.112295
Thermal correction to Enthalpy=	0.113240
Thermal correction to Gibbs Free Energy=	**0.076985**

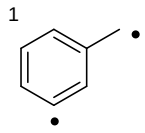
E_0(CASMP2,vacuo) -269.279533

ΔE_{CORR}(MP2) **-0.730388**

E_0(CASSCF,CPCM) **-268.553423**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.26854915E+03
(    1) 0.9063709 (   28) 0.1616177 (  182)-0.1376765 (   32) 0.1239191 (  191)-0.1125129 (   22)-0.1092125 (   26) 0.0986985
(  523) 0.0815127 (  538) 0.0722055 (  195)-0.0693996 (   33) 0.0692337 (  224)-0.0641320 (  131)-0.0624998 (  502) 0.0561805
(   20)-0.0556996 (  150) 0.0495012 (  179)-0.0482586 (  149)-0.0460106 (  497) 0.0431315 (   49)-0.0428459 (  674)-0.0424275
(  109) 0.0392660 (  181)-0.0375997 ( 1021)-0.0360191 (  166)-0.0351895 (   35) 0.0332915 (  370)-0.0332084 (  395)-0.0321334
(  210) 0.0302322 (  108) 0.0300589 (   88)-0.0295096 (  139)-0.0293893 (  254)-0.0292704 (  133) 0.0284567 (  644) 0.0284112
(  201)-0.0283361 (  659)-0.0269824 (  286)-0.0257695 (  381)-0.0246006 (  134)-0.0245613 (  185) 0.0244058 (  189) 0.0229930
(   75)-0.0228298 ( 1391) 0.0218916 (  387) 0.0214865 (  685) 0.0210537 (  573)-0.0198301 (   50)-0.0196622 (  572)-0.0196104
(  220)-0.0195874 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195119D+01
     2 -0.717053D-06  0.187749D+01
     3  0.275281D-07 -0.717717D-07  0.189100D+01
     4  0.312450D-04 -0.990314D-04 -0.558856D-07  0.100000D+01
     5 -0.171871D-04  0.436152D-05  0.163159D-06  0.499317D-06  0.100119D+01
     6  0.175887D-04  0.103070D-04 -0.865300D-07  0.355940D-04 -0.195238D-04
     7  0.110437D-06 -0.175237D-06 -0.134413D-04 -0.131721D-05 -0.165549D-06
     8  0.852189D-06 -0.117657D-04  0.616185D-07 -0.529079D-05  0.112137D-04
                6             7             8
     6  0.123162D+00
     7 -0.621903D-07  0.110926D+00
     8 -0.787827D-07  0.325145D-07  0.450343D-01
MCSCF converged.
```



^{1}3b

GEOMETRY

C	1.88497700	-0.18567300	0.00011400
C	1.25866200	1.07648100	-0.00008100
C	-0.12438200	1.17873200	-0.00004100
C	-0.96650100	0.01942400	0.00003900
C	-0.32248400	-1.25860500	-0.00011500
C	1.05308200	-1.30247200	0.00000200
H	1.85866300	1.96911300	-0.00011800
H	-0.58601000	2.15007000	-0.00005700
H	-0.91071100	-2.15827000	-0.00021000
C	-2.36349900	0.13269900	0.00008000
H	-2.84385100	1.09278200	0.00005100
H	-2.99186100	-0.73767200	0.00007800
H	2.95464300	-0.27953900	0.00026800

E_0(CASSCF,vacuo) -268.549658

Zero-point correction=	0.106107
Thermal correction to Energy=	0.111786
Thermal correction to Enthalpy=	0.112730
Thermal correction to Gibbs Free Energy=	**0.077078**

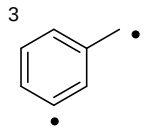
E_0(CASMP2,vacuo) -269.280197

ΔE_{CORR}(MP2) **-0.730539**

E_0(CASSCF,CPCM) **-268.553755**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.26854966E+03
(    2) 0.8718772 (   27) 0.1675807 (   24) 0.1659449 (    3) 0.1649837 (    1)-0.1648427 (  157)-0.1298612 (  138)-0.1051026
(   33)-0.0971422 (   31)-0.0962530 (  150)-0.0944692 (  394)-0.0914012 (  363)-0.0887038 (  112) 0.0799563 (  187)-0.0720858
(  175)-0.0527706 (  129)-0.0461978 (  117) 0.0431988 (   56) 0.0367478 (  705)-0.0358273 (  263)-0.0357266 (  455)-0.0344757
(  519) 0.0323334 (  155)-0.0311888 (   13)-0.0298351 (   64)-0.0297289 (  494)-0.0289780 (  109) 0.0287301 (  280)-0.0286492
(   95)-0.0282846 (  317)-0.0281066 (  484) 0.0258261 (  225)-0.0245709 (  104) 0.0245652 (  174) 0.0230785 (  146)-0.0230721
(   73) 0.0226353 (   86) 0.0223269 ( 1023) 0.0222981 (  449) 0.0218325 (  902)-0.0208019 (  196)-0.0207843 (  198)-0.0198885
(   91) 0.0198691 (  123) 0.0198286 (  447) 0.0195850 ( 1374)-0.0194289 (  911)-0.0191069 (  218)-0.0188583 (  863)-0.0186931
(   78) 0.0186865 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195116D+01
     2 -0.362618D-06  0.188780D+01
     3  0.311440D-06 -0.344363D-06  0.187044D+01
     4 -0.109309D-04 -0.585903D-05 -0.592705D-05  0.999975D+00
     5  0.382316D-05  0.317755D-05  0.608503D-05 -0.151750D-04  0.100154D+01
     6  0.246482D-05 -0.116683D-05 -0.374192D-05 -0.647718D-05 -0.206294D-05
     7  0.444622D-05 -0.262938D-05  0.657009D-05  0.112036D-05  0.240653D-05
     8  0.328987D-05 -0.229241D-05  0.265947D-05 -0.119192D-04 -0.779597D-07
                6             7             8
     6  0.113551D+00
     7 -0.240623D-06  0.129736D+00
     8 -0.153715D-07 -0.149960D-06  0.457910D-01
MCSCF converged.
```



^{3}3b

GEOMETRY

C	-1.88565700	-0.18437000	-0.00010500
C	-1.25950700	1.07459800	0.00007700
C	0.12620100	1.17469900	0.00003700
C	0.96200100	0.01953400	-0.00004100
C	0.32066000	-1.25742400	0.00011000
C	-1.05301700	-1.29814800	-0.00000900
H	-1.85807900	1.96826800	0.00009600
H	0.58831800	2.14594400	0.00005100
H	0.90794000	-2.15772200	0.00015600
C	2.36820100	0.13242700	-0.00008000
H	2.84831400	1.09245500	-0.00005300
H	2.99552400	-0.73848900	0.00001400
H	-2.95530700	-0.27834800	-0.00019700

E_0(CASSCF,vacuo) -268.544707

Zero-point correction=	0.106510
Thermal correction to Energy=	0.112000
Thermal correction to Enthalpy=	0.112944
Thermal correction to Gibbs Free Energy=	**0.076624**

E_0(CASMP2,vacuo) -269.276857

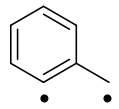
ΔE_{CORR}(MP2) **-0.732150**

E_0(CASSCF,CPCM) **-268.549360**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.26854471E+03
(    1) 0.9123548 (   28)-0.1536406 (   26) 0.1380368 (  182)-0.1247377 (  191)-0.1092693 (  523)-0.0812606 (   32)-0.0772258
(  538) 0.0727613 (  224) 0.0690587 (  195) 0.0668322 (  131) 0.0662331 (  181) 0.0567940 (   14)-0.0521909 (  502)-0.0514040
(  185)-0.0505617 (  497) 0.0503621 (  150)-0.0497252 (   49)-0.0450458 (   20) 0.0427110 (  674)-0.0401786 (   22) 0.0382451
(  271) 0.0372875 (  395)-0.0358310 ( 1021)-0.0352781 (  381)-0.0344990 (   75)-0.0325506 (  370)-0.0322269 (  171) 0.0313058
(   69)-0.0308437 (  179)-0.0295133 (   36)-0.0292948 (  659)-0.0291661 (  211) 0.0285681 (  644)-0.0275016 (  265) 0.0255799
(  121) 0.0253143 (   35) 0.0248007 (  114)-0.0236993 (  149) 0.0235598 (  218)-0.0234259 (   52) 0.0228876 (  201) 0.0224813
(   17)-0.0224413 ( 1391) 0.0224051 (   33) 0.0222951 (  122)-0.0222589 (   68)-0.0222070 (   85) 0.0218490 (  631) 0.0216101
(  139) 0.0210834 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195307D+01
     2 -0.121384D-05  0.188957D+01
     3  0.107085D-06  0.463828D-06  0.188502D+01
     4  0.258768D-06  0.115202D-04  0.145762D-04  0.100000D+01
     5  0.138718D-04 -0.489554D-04  0.553337D-04  0.274544D-05  0.100206D+01
     6  0.722969D-05  0.479359D-05 -0.462891D-05  0.621779D-06 -0.553310D-04
     7 -0.378783D-05  0.121423D-04 -0.298053D-05  0.946074D-05  0.257111D-04
     8 -0.107511D-06 -0.820737D-05  0.139635D-05 -0.183613D-05  0.106613D-04
                6             7             8
     6  0.111215D+00
     7 -0.119539D-05  0.115710D+00
     8  0.127582D-05 -0.540247D-06  0.433557D-01
MCSCF converged.
```

1



^{1}3c

GEOMETRY

C	1.83198100	0.01714000	0.00000800
C	1.09264100	1.18882400	-0.00000200
C	-0.31400100	1.15683200	-0.00002300
C	-1.01719400	-0.06432800	-0.00001300
C	-0.20264600	-1.22319200	0.00002600
C	1.15802500	-1.23781500	-0.00004100
H	1.59540800	2.13933000	0.00005600
H	-0.86690300	2.07996500	-0.00002500
C	-2.44240400	-0.13503600	0.00001900
H	-3.03641200	0.75844500	0.00000200
H	-2.94694600	-1.08074100	0.00001600
H	2.90644400	0.04842800	0.00012400
H	1.70999800	-2.15997300	-0.00000900

E_0(CASSCF,vacuo) -268.537328

Zero-point correction=	0.106216
Thermal correction to Energy=	0.111905
Thermal correction to Enthalpy=	0.112849
Thermal correction to Gibbs Free Energy=	**0.077216**

E_0(CASMP2,vacuo) -269.269839

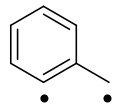
ΔE_{CORR}(MP2) **-0.732511**

E_0(CASSCF,CPCM) **-268.541709**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.26853733E+03
(   80) 0.9237452 (  179) 0.1487442 (  749) 0.1294215 (  342)-0.1116342 (  603)-0.0888597 (  182)-0.0857664 (  559) 0.0839655
(  524)-0.0796748 (  557) 0.0662595 (  449) 0.0655742 (  587)-0.0484552 (  177)-0.0435117 (  966) 0.0421359 (  394)-0.0413753
(  792)-0.0412414 (  155)-0.0388081 (  388) 0.0381090 ( 1232) 0.0373895 ( 1033) 0.0371157 (  427)-0.0369403 (  401) 0.0367065
(  461) 0.0353556 (  285) 0.0352339 (  173)-0.0338076 (  503) 0.0337354 (  122)-0.0332111 (  180)-0.0326169 (   81)-0.0295689
(   34)-0.0285671 (  654) 0.0277125 (  789) 0.0274978 (  419)-0.0272507 (    3) 0.0271331 (  214)-0.0270796 (   48)-0.0259283
(  534) 0.0253107 (  252)-0.0249857 (  129)-0.0245848 (  892) 0.0243685 ( 1291)-0.0237705 (  537) 0.0233515 (  237)-0.0232321
(  176)-0.0230411 (  373) 0.0229473 (  912)-0.0226176 ( 1007)-0.0223632 (  589)-0.0215574 (  435) 0.0214409 ( 1029)-0.0213962
(  418)-0.0212733 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195434D+01
     2 -0.467003D-06  0.190318D+01
     3 -0.208086D-05  0.544258D-05  0.100140D+01
     4 -0.836925D-06 -0.963850D-06 -0.240699D-06  0.414104D-01
     5  0.366629D-06 -0.410985D-06  0.353864D-04  0.503343D-05  0.189024D+01
     6 -0.355742D-05 -0.475193D-06 -0.767759D-06 -0.554064D-06 -0.104532D-04
     7  0.475686D-05  0.978321D-05 -0.241619D-04  0.125636D-06 -0.141042D-05
     8  0.574448D-04  0.870786D-04  0.389354D-03  0.841194D-04  0.124258D-03
                6             7             8
     6  0.977177D-01
     7  0.107517D-05  0.111712D+00
     8 -0.119842D-03 -0.223347D-04  0.100001D+01
MCSCF converged.
```

3



^{3}3c

GEOMETRY

C	-1.82926600	0.01061600	-0.00000100
C	-1.06944500	1.20104300	-0.00000200
C	0.31330400	1.16738000	0.00000400
C	1.02654100	-0.07789600	-0.00000900
C	0.20585500	-1.23009600	-0.00000400
C	-1.17608400	-1.22793800	0.00001000
H	-1.57588700	2.14967700	-0.00000500
H	0.87417100	2.08557800	0.00001300
C	2.42558900	-0.14401200	-0.00000100
H	3.02140400	0.74903700	0.00002300
H	2.93579900	-1.08776300	-0.00000200
H	-2.90314700	0.05698600	-0.00001100
H	-1.73131300	-2.14810400	0.00000400

E_0(CASSCF,vacuo) -268.549410

Zero-point correction=	0.106769
Thermal correction to Energy=	0.112242
Thermal correction to Enthalpy=	0.113186
Thermal correction to Gibbs Free Energy=	**0.076857**

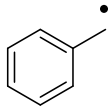
E_0(CASMP2,vacuo) -269.279010

ΔE_{CORR}(MP2) **-0.729600**

E_0(CASSCF,CPCM) **-268.553230**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.26854941E+03
(    1) 0.9069607 (   28) 0.1471042 (  182)-0.1304528 (  191)-0.1096388 (   26)-0.1059761 (   20) 0.0987345 (   33)-0.0980981
(   32) 0.0941607 (  523) 0.0857080 (  195) 0.0711297 (  538)-0.0701500 (  224) 0.0696215 (   22)-0.0691844 (  131) 0.0581613
(  181) 0.0577012 (  502) 0.0532812 (  497)-0.0494768 (  149) 0.0438183 (  150)-0.0435760 (   49) 0.0435118 (  674)-0.0409654
(  166) 0.0400159 (  109)-0.0381311 ( 1021)-0.0363429 (  395)-0.0342366 (  370)-0.0331386 (  179) 0.0327972 (  185)-0.0326737
(   75)-0.0307739 (   14) 0.0290300 (  381)-0.0286134 (  659)-0.0276687 (  644) 0.0253859 (   35)-0.0231782 (  211) 0.0229904
(  363) 0.0229620 ( 1391) 0.0222189 (  210) 0.0219152 (   48)-0.0217032 (  108)-0.0214771 (   88)-0.0214346 (  171) 0.0214083
(  573)-0.0210990 (  117) 0.0209798 (  254) 0.0205569 (  134)-0.0203545 (   69)-0.0203033 (   36) 0.0200723 (  189) 0.0199907
(  114)-0.0199559 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195140D+01
     2  0.267652D-05  0.189040D+01
     3  0.318170D-05  0.301657D-06  0.187676D+01
     4 -0.546026D-05  0.728120D-06  0.901481D-05  0.100000D+01
     5  0.646242D-05  0.293751D-04  0.785830D-05  0.158941D-05  0.100125D+01
     6  0.271841D-05  0.436771D-05  0.140035D-04 -0.158915D-05 -0.358742D-05
     7 -0.473821D-05  0.426095D-05 -0.593168D-05 -0.703353D-05  0.390048D-05
     8  0.101908D-05 -0.416108D-06 -0.306686D-05 -0.366590D-05  0.653406D-05
                6             7             8
     6  0.110955D+00
     7 -0.334804D-06  0.124148D+00
     8  0.252840D-05  0.360411D-05  0.450883D-01
MCSCF converged.
```



GEOMETRY

C	-0.02132400	-0.13152400	-0.01300400
C	0.00955600	-0.08380200	1.41078400
C	1.21060300	0.00598400	2.09851600
C	2.42734600	0.05163100	1.40171600
C	2.42327600	0.00570700	-0.00040300
C	1.22757100	-0.08401100	-0.69739600
H	-0.91861400	-0.11838600	1.95357700
H	1.20830000	0.04079500	3.17348100
H	3.35604700	0.12119600	1.93827600
H	3.35340700	0.04025800	-0.53931700
H	1.23422000	-0.11881000	-1.77260200
C	-1.23903800	-0.22300400	-0.71653700
H	-2.17881100	-0.25946600	-0.19901200
H	-1.26008800	-0.25953000	-1.78917800

E_0(CASSCF,vacuo) -269.195227

Zero-point correction=	0.119982
Thermal correction to Energy=	0.125507
Thermal correction to Enthalpy=	0.126451
Thermal correction to Gibbs Free Energy=	**0.090410**

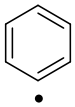
E_0(CASMP2,vacuo) -269.956812

ΔE_{CORR}(MP2) **-0.761585**

E_0(CASSCF,CPCM) **-269.199324**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.26919523E+03
(   1) 0.9157135 (   18) 0.1707392 (   21) 0.1410930 (  132) 0.1122689 (    5) 0.1050135 (   27) 0.0981938 (  153) 0.0902279
(  76) 0.0790767 (  252) 0.0764402 (   67) 0.0705168 (   51) 0.0625289 (    7) 0.0606186 (   26)-0.0542231 (   24) 0.0522048
(  60) 0.0480283 (  118) 0.0477091 (  146) 0.0420622 (  225) 0.0410685 (   38) 0.0407196 (   56) 0.0398228 (   75) 0.0360449
( 361) 0.0354926 (  247) 0.0343869 (   20) 0.0336101 (  123) 0.0333147 (  136) 0.0296903 (   19)-0.0287456 (   71)-0.0280084
( 229) 0.0279472 (   29) 0.0262467 (   41) 0.0260271 (   44) 0.0258714 (   64) 0.0246811 (   58) 0.0245569 (   85)-0.0242477
(  96)-0.0240629 (  116) 0.0240515 (   78)-0.0235103 (   31) 0.0227327 (  406) 0.0226082 (  162) 0.0224657 (  112)-0.0207183
(  87)-0.0205246 (  286) 0.0198238 (   54) 0.0190320 (  230) 0.0178719 (  125) 0.0175899 (  154) 0.0174949 (  549) 0.0174348
(   6)-0.0172070 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195457D+01
     2  0.551525D-06  0.188993D+01
     3 -0.170449D-06  0.414028D-05  0.189082D+01
     4 -0.119334D-04  0.657100D-04 -0.102013D-05  0.100155D+01
     5 -0.474764D-07 -0.754161D-06 -0.122893D-05 -0.594636D-06  0.110697D+00
     6  0.136663D-04 -0.382530D-05 -0.693613D-06 -0.568737D-04  0.968858D-06
     7 -0.398343D-05  0.908032D-05  0.375785D-07 -0.879292D-05  0.223917D-06
                6             7
     6  0.110515D+00
     7 -0.475735D-06  0.419280D-01
MCSCF converged.
```



GEOMETRY

C	-0.00669500	0.00005500	-0.00166100
C	-0.01738800	0.00044500	1.39831900
C	1.20794600	-0.00017200	2.04314000
C	2.43339100	-0.00113400	1.39839600
C	2.42282400	-0.00149300	-0.00151500
C	1.20806700	-0.00090100	-0.69409100
H	-0.93494600	0.00049500	-0.54519600
H	-0.94077300	0.00117600	1.94789000
H	3.35669800	-0.00158400	1.94809700
H	3.35109600	-0.00223700	-0.54501500
H	1.20814500	-0.00119600	-1.76936100

E_0(CASSCF,vacuo) -230.126993

Zero-point correction=	0.091937
Thermal correction to Energy=	0.096168
Thermal correction to Enthalpy=	0.097112
Thermal correction to Gibbs Free Energy=	**0.063955**

E_0(CASMP2,vacuo) -230.752803

ΔE_{CORR}(MP2) **-0.625810**

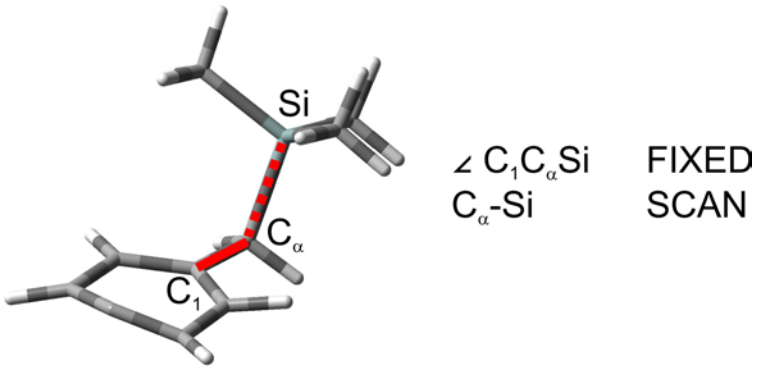
E_0(CASSCF,CPCM) **-230.131205**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.230126990E+03
(    1) 0.9329411 (   64) 0.1490489 (   58) 0.1485339 (   76) 0.1108671 (  195)-0.0973069 (   67)-0.0943451 (  208) 0.0934991
(    9) 0.0811669 (   60) 0.0747066 (   56)-0.0678452 (  165) 0.0572616 (  171)-0.0512829 (   15) 0.0470913 (  146) 0.0414904
(  247) 0.0406417 (  361) 0.0391055 (   21) 0.0352495 (  406) 0.0332366 (  123) 0.0332059 (  229) 0.0321168 (  132) 0.0317980
(   71)-0.0303329 (  220) 0.0265429 (  221)-0.0258676 (   34)-0.0237522 (  613) 0.0227896 (   16) 0.0227016 (  614)-0.0215894
(   51)-0.0211340 (   11)-0.0201652 (  178) 0.0179729 (  179)-0.0140841 (  711) 0.0139994 (  718) 0.0139898 (   28) 0.0137471
(  187)-0.0136194 (  581)-0.0136067 (   46)-0.0132660 (  202) 0.0127139 (   75)-0.0121406 (  336) 0.0119469 (   14)-0.0118204
(  579) 0.0117210 (  277)-0.0116989 (  235) 0.0101913 (  323)-0.0100226 (  716)-0.0099873 (  212)-0.0096773 (  402)-0.0095810
(  539) 0.0090529 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195762D+01
     2 -0.238321D-06  0.189732D+01
     3  0.767094D-06  0.271848D-06  0.188798D+01
     4 -0.153451D-06  0.499904D-07 -0.284986D-06  0.100000D+01
     5  0.764615D-06  0.236645D-04  0.996948D-05 -0.370313D-06  0.104612D+00
     6 -0.634909D-05 -0.100308D-04  0.124925D-04  0.128197D-07 -0.337543D-06
     7 -0.182417D-05  0.694356D-06  0.597515D-06  0.210948D-07 -0.289609D-06
                6             7
     6  0.112752D+00
     7  0.203631D-05  0.397092D-01
MCSCF converged.
```

6. Relaxed PES scans - TMS detachment from 2^+a-c

The level of theory chosen to carry out the analysis of the detachment of the TMS group from phenyl cations **2^+a-c** was the CASSCF(8,9)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π* orbitals of the aromatic ring, the σ/σ* couple of the C-Si bond and the orbital at the dicoordinated carbon (as in the case of the phenyl cations described above).
Two different variables were constrained via the OPT=MODREDUNDANT keyword. In particular, an elongation of the C_α-Si bond starting from the equilibrium distance found in the phenyl cation was performed up to > 3.5 Å (with a step size of + 0.1 Å). Moreover, the angle among C_1-C_α-Si was fixed in order to maintain the same trajectory when removing the TMS group and to avoid undesirable interactions between the Si atom and the carbon atoms of the aromatic ring (see figure below for a graphical representation applied to **^{1}2$^+$a**).



Solvent effect was again evaluated by single point calculations at the CPCM-CASSCF/6-31G(d) level of theory (methanol bulk) on the optimized geometries obtained in vacuo. Further notice that the occupancy of the σ* orbital of the C_α-Si (becoming a *p* orbital of the Si atom upon stretching of the bond) showed quite low values (< 0.01) for some of the structures reported below. Nevertheless, this orbital was kept in the active space for comparison purposes.

In the following, the optimized geometries for the relaxed PES scans are reported along with the most relevant data. The data reported in Table S7 have been reported in blue color for all of the structures reported below. Further notice that the geometries concerning steps 0 (see again Table S7) have not been reported since they correspond to the phenyl cations structures reported above.

Table S7. Total electronic energy (E_0(CASSCF,CPCM)) calculated at the CPCM-CASSCF(8,9)/6-31G(d) level of theory (MeOH bulk).

STEP	2^+**a**				2^+**b**				2^+**c**			
	SINGLET		TRIPLET		SINGLET		TRIPLET		SINGLET		TRIPLET	
	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [Hartree]	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [Hartree]	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [Hartree]	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [Hartree]	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [Hartree]	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [Hartree]
0	1.97617	-676.190800	2.06476	-676.198761	2.06681	-676.195591	2.05740	-676.191710	1.98339	-676.197154	2.09853	-676.195006
1	2.07617	-676.187404	2.16476	-676.196737	2.16681	-676.193713	2.15740	-676.189500	2.08339	-676.193854	2.19853	-676.193387
2	2.17617	-676.180951	2.26476	-676.194087	2.26681	-676.191632	2.25740	-676.187084	2.18339	-676.187768	2.29853	-676.191219
3	2.27617	-676.175168	2.36476	-676.190200	2.36681	-676.188314	2.35740	-676.183591	2.28339	-676.179996	2.39853	-676.187384
4	2.37617	-676.173176	2.46476	-676.187287	2.46681	-676.185961	2.45740	-676.181175	2.38339	-676.175372	2.49853	-676.184846
5	2.47617	-676.171719	2.56476	-676.184426	2.56681	-676.183501	2.55740	-676.178716	2.48339	-676.173094	2.59853	-676.182292
6	2.57617	-676.169825	2.66476	-676.181705	2.66681	-676.181060	2.65740	-676.176324	2.58339	-676.170740	2.69853	-676.179838
7	2.67617	-676.167755	2.76476	-676.179191	2.76681	-676.178750	2.75740	-676.174003	2.68339	-676.168426	2.79853	-676.177551
8	2.77617	-676.165627	2.86476	-676.176879	2.86681	-676.176632	2.85740	-676.171867	2.78339	-676.166172	2.89853	-676.175481
9	2.87617	-676.163564	2.96476	-676.174843	2.96681	-676.174732	2.95740	-676.169932	2.88339	-676.164082	2.99853	-676.173636
10	2.97617	-676.161666	3.06476	-676.173056	3.06681	-676.173054	3.05740	-676.168226	2.98339	-676.162176	3.09853	-676.171999
11	3.07617	-676.159950	3.16476	-676.171507	3.16681	-676.171568	3.15740	-676.166696	3.08339	-676.160460	3.19853	-676.170575
12	3.17617	-676.158425	3.26476	-676.170187	3.26681	-676.170295	3.25740	-676.165382	3.18339	-676.158953	3.29853	-676.169334
13	3.27617	-676.157091	3.36476	-676.169037	3.36681	-676.169168	3.35740	-676.164232	3.28339	-676.157630	3.39853	-676.168263
14	3.37617	-676.155928	3.46476	-676.168052	3.46681	-676.168167	3.45740	-676.163239	3.38339	-676.156464	3.49853	-676.167304
15	3.47617	-676.154924	3.56476	-676.166382	3.56681	-676.167306	3.55740	-676.162350	3.48339	-676.155404	3.59853	-676.165684
16	3.57617	-676.154013							3.58339	-676.154409[a]		

[a] The geometry was optimized in vacuo and the introduction of solvent effect was accomplished by applying a loose SCF convergence criterion (CONVER=4).

$^{1}2^{+}$a STEP 1

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36976654
C	1.29476463	0.00000000	1.90211200
C	2.36756931	0.31632064	1.05071981
C	2.10187271	0.54209687	-0.33952430
C	0.81712211	0.55776992	-0.92156854
H	-0.89689986	0.02324687	1.95960386
H	1.43954489	-0.10637987	2.96021032
H	2.93469753	0.56140225	-1.01943742
H	0.65794953	0.62150714	-1.97898616
C	3.76034787	0.40734175	1.54988306
H	3.77139307	0.71820778	2.58902046
H	4.33195983	1.12955332	0.97655255
C	4.92595842	-1.94971755	-0.29068917
H	5.54462199	-2.84037060	-0.36376853
H	3.94686028	-2.21484413	-0.68185268
H	5.36480664	-1.20550759	-0.95027886
C	3.97768626	-2.60728365	2.60141328
H	4.54444983	-3.53383847	2.64242708
H	3.88024933	-2.24844663	3.62248963
H	2.98509651	-2.85920203	2.23728933
C	6.54837776	-0.88538725	2.15610594
H	6.49435095	-0.49810670	3.16949569
H	7.20452987	-1.75163799	2.17559570
H	7.02683319	-0.13117807	1.53791278
Si	4.85324579	-1.35712160	1.49770220

E_0(CASSCF,vacuo) -676.111064

E_0(CASSCF,CPCM) **-676.187404**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1110636363
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67611106E+03
(     1) 0.9150152 (     3)-0.2246151 (    36)-0.1042497 (   351)-0.0862471 (    38) 0.0696460 ( 1599)-0.0682281 (    67)-0.0663226
( 1663)-0.0602027 (    39) 0.0549880 (    35)-0.0536244 ( 1711)-0.0520719 (    10)-0.0483436 (    45)-0.0476959 (     9) 0.0466638
(    6)-0.0459575 (    30)-0.0457969 ( 1778)-0.0452668 (     5) 0.0443254 (   121) 0.0404457 ( 1716) 0.0401114 ( 1655)-0.0398755
(   55)-0.0394546 (     8) 0.0382795 (    44)-0.0373810 ( 1661) 0.0364599 ( 1770)-0.0351214 ( 1721)-0.0349290 (    79) 0.0349109
(   25) 0.0347351 (    78) 0.0335877 ( 1606)-0.0334140 ( 1954) 0.0332242 (    43)-0.0331804 ( 1779)-0.0331728 ( 1772) 0.0327542
( 1830)-0.0324204 (    26)-0.0323269 ( 1774) 0.0302107 (    31)-0.0291923 (    28)-0.0291162 ( 1892) 0.0283526 ( 1601) 0.0269148
( 1605) 0.0267227 ( 1660)-0.0266153 ( 1604)-0.0263593 (   331) 0.0246715 ( 1777)-0.0245554 ( 1658)-0.0239643 (    23) 0.0230041
( 1713) 0.0228541 (
Final one electron symbolic density matrix:
                1              2              3              4              5
     1  0.195003D+01
     2 -0.372458D-06  0.197755D+01
     3  0.123624D-05 -0.410902D-06  0.190689D+01
     4  0.404987D-05  0.142749D-05  0.552272D-05  0.182319D+01
     5  0.311032D-05  0.287455D-05  0.168391D-04 -0.369740D-04  0.158434D+00
     6  0.289767D-05  0.607177D-06 -0.475894D-05  0.225735D-04 -0.905805D-06
     7 -0.234851D-05 -0.814066D-05 -0.140217D-04  0.442139D-04 -0.112025D-04
     8  0.288973D-05 -0.189594D-05 -0.876922D-05  0.270691D-04 -0.452741D-05
     9 -0.202959D-05 -0.342112D-05  0.281472D-06  0.149221D-05  0.136736D-05
                6              7              8              9
     6  0.829592D-01
     7  0.263128D-05  0.492340D-01
     8 -0.105755D-05  0.214512D-05  0.308032D-01
     9 -0.103546D-05  0.724403D-06  0.414105D-06  0.209070D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 2

GEOMETRY

C	3.37524600	0.06074000	0.59482200
C	3.01792300	-1.21098800	0.20072100
C	1.72548600	-1.28070600	-0.31332300
C	1.07389000	-0.07860100	-0.66259200
C	1.74139200	1.16499500	-0.40781600
C	3.05360100	1.27735800	0.09326200
H	3.67658200	-2.05428100	0.28934400
H	1.28803900	-2.23195900	-0.54938800
H	1.16764900	2.07200600	-0.47292800
H	3.49561500	2.21780200	0.35407700
C	-0.26577700	-0.07068600	-1.26711300
H	-0.44928500	-0.97637800	-1.83296700
H	-0.41250900	0.78768400	-1.91240800
C	-1.74826800	1.58966300	1.13912500
H	-2.59515900	1.70244100	1.81137600
H	-0.85379500	1.58465700	1.75634300
H	-1.72297700	2.47497300	0.50968600
C	-1.83110100	-1.53125300	1.20213900
H	-2.67149300	-1.56403200	1.89102000
H	-1.86919500	-2.44012100	0.60837500
H	-0.92609100	-1.55771400	1.80280100
C	-3.44045400	0.03264800	-0.98588900
H	-3.49441300	-0.85530400	-1.60864000
H	-4.35015600	0.06764700	-0.39171500
H	-3.44700900	0.89959900	-1.63979300
Si	-1.93195900	0.01099800	0.13034300

E_0(CASSCF,vacuo) -676.106328

E_0(CASSCF,CPCM) **-676.180951**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1063278597
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610633E+03
 (    1) 0.9079856 (    3)-0.2538437 (   36)-0.1124394 (  351)-0.0869381 (   38) 0.0666222 ( 1663)-0.0642341 ( 1599)-0.0633787
 (   39) 0.0614640 (   67)-0.0552373 ( 1711)-0.0532891 ( 1778)-0.0510726 (   45)-0.0489412 (   10)-0.0467859 (  121) 0.0453954
 (    9) 0.0444550 (   30)-0.0442349 ( 1716) 0.0422371 (   35)-0.0414631 ( 1661) 0.0399473 (   44)-0.0386496 ( 1770)-0.0386483
 (   78) 0.0364468 (   26)-0.0364100 (   55)-0.0362663 (   79) 0.0351138 ( 1954) 0.0350475 (    6)-0.0343947 ( 1655)-0.0335624
 ( 1713) 0.0334197 (    5) 0.0324083 ( 1774) 0.0319825 ( 1604)-0.0317213 (  331) 0.0316030 (   25) 0.0315085 ( 1660)-0.0313359
 ( 1721)-0.0308175 ( 1892) 0.0298164 ( 1830)-0.0296994 ( 1779)-0.0289071 (    8) 0.0284638 ( 1856) 0.0280544 ( 1606)-0.0261339
 ( 1720)-0.0259274 (   43)-0.0249507 ( 1772) 0.0247184 (  465) 0.0242250 ( 1605) 0.0228890 (   47)-0.0228270 ( 1601) 0.0213827
 (  122)-0.0201521 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.194914D+01
      2  0.274081D-06  0.197271D+01
      3 -0.663087D-07  0.791766D-06  0.190708D+01
      4 -0.224941D-05  0.541380D-06 -0.747887D-06  0.180021D+01
      5 -0.444280D-05  0.861758D-05 -0.315850D-04 -0.178849D-04  0.181414D+00
      6 -0.853191D-06 -0.806832D-06 -0.274466D-05  0.149257D-05 -0.246810D-05
      7  0.707938D-05 -0.737585D-06  0.209400D-04  0.843913D-05 -0.126181D-05
      8  0.907569D-06 -0.323460D-05  0.695376D-05 -0.324286D-05  0.101943D-06
      9 -0.102602D-05 -0.224632D-05 -0.410756D-06  0.127955D-05 -0.165419D-06
                   6             7             8             9
      6  0.832994D-01
      7 -0.745511D-06  0.507187D-01
      8  0.134545D-05  0.213675D-05  0.305776D-01
      9  0.231155D-07 -0.724191D-06 -0.441044D-06  0.248559D-01
 MCSCF converged.
```

$^{1}2^{+}$a STEP 3

GEOMETRY

C	-0.00629300	-0.00533000	-0.00137100
C	-0.00888200	0.01875200	1.38280200
C	1.23426700	0.01577300	2.01118500
C	2.43531600	0.04659900	1.24186200
C	2.34981400	0.07192900	-0.18199400
C	1.10978000	0.07505400	-0.81650600
H	-0.92133300	0.01242800	1.94710100
H	1.29661700	-0.00388100	3.08386300
H	3.25343000	0.09453000	-0.76326500
H	1.02818600	0.11047200	-1.88567800
C	3.70185900	0.05160700	1.88620800
H	3.72285200	0.35483300	2.92349700
H	4.54587500	0.39619900	1.30548500
C	4.80144300	-2.74960900	0.59922800
H	5.29227700	-3.71617100	0.69757400
H	3.84534900	-2.91988800	0.11644700
H	5.41886800	-2.14244300	-0.05464100
C	3.36860600	-2.82119100	3.41864500
H	3.75696200	-3.79315600	3.71746200
H	3.19285400	-2.25402200	4.32685300
H	2.41829000	-2.99056900	2.92427500
C	6.18825900	-1.42338000	3.11239200
H	6.00327100	-0.85923200	4.02046600
H	6.77562800	-2.29685200	3.38943800
H	6.80131200	-0.82041300	2.45082100
Si	4.60985100	-1.99504900	2.29572300

E_0(CASSCF,vacuo) -676.103244

E_0(CASSCF,CPCM) **-676.175168**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1032439509
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610324E+03
(     1) 0.7074211 (    3)-0.6121192 (   36)-0.1069304 (   78) 0.0951084 (   24)-0.0858371 ( 1662)-0.0668257 ( 1770)-0.0652656
( 2016) 0.0579174 ( 1904) 0.0578997 ( 2851) 0.0575894 (   39) 0.0546656 (  264)-0.0543935 ( 3323)-0.0514600 (   30)-0.0510628
(  366) 0.0477208 (   81)-0.0476626 ( 1854)-0.0420522 (  121) 0.0402075 ( 1715) 0.0398804 (  333)-0.0382968 ( 1957)-0.0376824
(  122)-0.0374457 ( 2108) 0.0366664 (  239)-0.0358230 (   67) 0.0347754 (  447) 0.0328974 (  235) 0.0326978 ( 1737)-0.0316858
(   62)-0.0314503 (   45)-0.0312229 (  237)-0.0312013 (  260)-0.0307283 (  243)-0.0307013 ( 1775)-0.0298563 (  300)-0.0294889
( 1600)-0.0283174 ( 1664)-0.0282467 ( 1983) 0.0279847 ( 1838)-0.0273046 (  358)-0.0270884 ( 2558) 0.0265599 (  112)-0.0263380
(   91) 0.0263175 (  406) 0.0259511 (  282) 0.0251743 (   66)-0.0251103 ( 1733) 0.0248325 (  305) 0.0245246 (  276)-0.0244074
(   2021) 0.0242445 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.193333D+01
     2  0.111744D-05  0.195808D+01
     3 -0.422301D-07  0.749201D-06  0.188888D+01
     4 -0.108859D-04  0.589018D-06 -0.820975D-05  0.113347D+01
     5 -0.949804D-05  0.333086D-05 -0.944297D-06  0.147028D-05  0.860783D+00
     6 -0.269085D-05 -0.173410D-06  0.290976D-05 -0.229216D-05 -0.181777D-05
     7 -0.347665D-05 -0.105113D-05  0.281668D-05 -0.779548D-05 -0.237153D-05
     8  0.270611D-05 -0.685688D-05 -0.318635D-06 -0.278347D-05  0.312272D-05
     9  0.304051D-06 -0.890586D-05 -0.517042D-08  0.360650D-05  0.107127D-05
                6             7             8             9
     6  0.106155D+00
     7  0.101063D-06  0.729175D-01
     8 -0.144514D-06 -0.144317D-05  0.121621D-01
     9  0.781730D-06 -0.173525D-05  0.694373D-06  0.342309D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 4

GEOMETRY

C	-0.09374800	0.13354000	0.05712900
C	0.06932600	-0.06371500	1.41704300
C	1.37278100	-0.00748200	1.90914800
C	2.46191600	0.27423100	1.03802400
C	2.21057100	0.49244400	-0.34522100
C	0.90996200	0.43794000	-0.84530500
H	-0.76394200	-0.26130200	2.06345000
H	1.56076300	-0.16733700	2.95536200
H	3.03185200	0.71056400	-1.00352400
H	0.70267000	0.61378200	-1.88325300
C	3.79144300	0.33533100	1.54565600
H	3.91482400	0.46285700	2.61086000
H	4.53514000	0.83342700	0.94155000
C	5.03222900	-2.16020200	-0.27162200
H	5.60707400	-3.07671600	-0.39448400
H	4.03968800	-2.34430900	-0.66752500
H	5.51320400	-1.39650800	-0.87350000
C	3.95617500	-2.80101800	2.64136900
H	4.44524700	-3.76878600	2.74017600
H	3.85010100	-2.39138400	3.64025400
H	2.96906600	-2.97724900	2.22863800
C	6.57886500	-1.05861700	2.26769900
H	6.43831300	-0.65144500	3.26324000
H	7.28913600	-1.87949900	2.35221600
H	7.03796800	-0.29919600	1.64388600
Si	4.99340200	-1.71440400	1.53782100

E_0(CASSCF,vacuo) -676.102116

E_0(CASSCF,CPCM) **-676.173176**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1021159143
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67610212E+03
(     1) 0.6862658 (     3)-0.6335392 (    36)-0.1053469 (    78) 0.0987947 (   24)-0.0782771 ( 1662)-0.0707016 ( 1770)-0.0684131
( 1904) 0.0653652 ( 2016) 0.0639218 ( 2851) 0.0607826 ( 3323)-0.0570330 (  264)-0.0566072 (  366) 0.0526641 (   39) 0.0513425
(   81)-0.0468557 ( 1854)-0.0464660 (    30)-0.0435512 ( 2108) 0.0431248 (  333)-0.0401075 ( 1715) 0.0397692 ( 1957)-0.0378600
(  121) 0.0373630 (  447) 0.0368542 (     2) 0.0367607 (  235) 0.0366387 (  122)-0.0354291 ( 1737)-0.0353246 (   67) 0.0347269
( 1983) 0.0330120 (  239)-0.0322861 ( 1775)-0.0311518 (  243)-0.0298847 (  300)-0.0296720 ( 1602) 0.0296302 (   45)-0.0293620
(  406) 0.0277204 (  237)-0.0276754 (  260)-0.0275194 ( 1600)-0.0272500 ( 2021) 0.0270372 (    91) 0.0267266 (   62)-0.0265602
( 2558) 0.0264700 (  276)-0.0261477 (  358)-0.0257642 (  282) 0.0243703 (  112)-0.0242507 ( 2557) 0.0241199 (   66)-0.0239345
( 1898) 0.0237985 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192765D+01
     2 -0.435064D-05  0.195723D+01
     3 -0.259159D-06  0.192325D-05  0.188914D+01
     4 -0.184608D-05 -0.519299D-05  0.223601D-05  0.107277D+01
     5 -0.144852D-04 -0.259849D-05  0.725239D-05  0.497339D-06  0.921333D+00
     6  0.183515D-05 -0.247806D-06 -0.150667D-05  0.297733D-05  0.542456D-06
     7  0.328840D-05  0.184920D-05  0.130000D-05 -0.446809D-05 -0.118555D-05
     8 -0.104581D-05  0.153572D-05  0.235340D-06  0.480369D-06 -0.422996D-05
     9  0.316828D-05  0.362939D-05 -0.178584D-05 -0.831354D-06 -0.266728D-05
                6             7             8             9
     6  0.106948D+00
     7  0.158969D-06  0.777283D-01
     8  0.136778D-06  0.253918D-05  0.118561D-01
     9  0.190173D-05  0.103545D-05 -0.484009D-06  0.353394D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 5

GEOMETRY

C	0.00585100	-0.00563300	0.00325500
C	0.00809600	-0.01340300	1.38664200
C	1.25361100	-0.01191900	2.01555500
C	2.44837800	0.02034400	1.24809500
C	2.36672200	0.04595800	-0.16970800
C	1.12569500	0.04472300	-0.80744000
H	-0.90319000	-0.02465700	1.95303000
H	1.31399700	-0.02319000	3.08889800
H	3.27019400	0.07851600	-0.75152800
H	1.04779000	0.07681600	-1.87714300
C	3.71995300	0.02411800	1.89590400
H	3.75484900	0.28413400	2.94258800
H	4.58110400	0.32708400	1.32058100
C	4.85848100	-2.89552400	0.61776500
H	5.31923800	-3.88063400	0.67468000
H	3.89159900	-3.01600400	0.14211100
H	5.48819400	-2.28176600	-0.01721900
C	3.42172100	-2.96686900	3.45027100
H	3.75868400	-3.95910800	3.74673800
H	3.27103500	-2.39328200	4.35841900
H	2.46853400	-3.08438000	2.94702200
C	6.26723000	-1.58540400	3.14689400
H	6.06787700	-1.01515500	4.04768100
H	6.87296500	-2.44330300	3.43525000
H	6.86651400	-0.97933900	2.47617000
Si	4.70646400	-2.20328400	2.33963000

E_0(CASSCF,vacuo) -676.100438

E_0(CASSCF,CPCM) **-676.171719**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1004379013
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67610044E+03
(     1) 0.6778110 (    3)-0.6406932 (   36)-0.1048921 (   78) 0.1002771 ( 1662)-0.0734143 (   24)-0.0727480 ( 1770)-0.0709210
( 1904) 0.0694835 ( 2016) 0.0675592 ( 2851) 0.0627036 ( 3323)-0.0599211 (  264)-0.0576143 (  366) 0.0547648 (    2) 0.0514962
(   39) 0.0493760 ( 1854)-0.0486775 ( 2108) 0.0462026 (   81)-0.0453766 (  333)-0.0408397 (   30)-0.0394340 ( 1715) 0.0393872
(  235) 0.0386906 (  447) 0.0384703 ( 1957)-0.0372589 ( 1737)-0.0370160 (  121) 0.0355610 ( 1983) 0.0353039 (  122)-0.0335974
(   67) 0.0333138 ( 1602) 0.0329960 ( 1775)-0.0317349 (  300)-0.0296786 (  239)-0.0295774 (  243)-0.0284289 (  406) 0.0283232
(   45)-0.0283130 ( 2021) 0.0279723 ( 1601) 0.0272676 ( 1898) 0.0268329 (  276)-0.0268214 (   91) 0.0264972 ( 2558) 0.0263550
(  260)-0.0252684 ( 1600)-0.0251015 (  237)-0.0250302 (  378) 0.0250001 (  358)-0.0244478 ( 1660) 0.0241758 ( 2557) 0.0238609
(   62)-0.0237115 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192363D+01
     2  0.131118D-06  0.195687D+01
     3  0.272304D-07 -0.122769D-07  0.188953D+01
     4  0.135188D-05  0.849174D-05 -0.281366D-07  0.105049D+01
     5  0.138070D-05  0.354619D-05 -0.980267D-06  0.108342D-06  0.943676D+00
     6 -0.290883D-06 -0.162139D-06 -0.401435D-05  0.233129D-06 -0.345923D-06
     7 -0.737953D-05 -0.155228D-06 -0.212231D-06 -0.475474D-05  0.128333D-04
     8 -0.373714D-05  0.119418D-05 -0.503192D-06 -0.863618D-06 -0.219803D-05
     9  0.234249D-05  0.118301D-05  0.160708D-06 -0.884556D-05  0.313250D-05
                6             7             8             9
     6  0.107267D+00
     7  0.241506D-07  0.805944D-01
     8  0.175579D-07  0.657746D-06  0.119598D-01
     9 -0.170302D-07  0.377597D-06 -0.115139D-06  0.359795D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 6

GEOMETRY

C	0.00541500	-0.00867800	0.00297200
C	0.00710800	-0.01215900	1.38616800
C	1.25245700	-0.01059800	2.01681000
C	2.44681300	0.01259400	1.25156100
C	2.36783200	0.03008100	-0.16480200
C	1.12741600	0.02871100	-0.80509100
H	-0.90462900	-0.01718600	1.95203600
H	1.31077300	-0.01397000	3.09046200
H	3.27213400	0.05755600	-0.74585600
H	1.05210200	0.05419700	-1.87521900
C	3.71936900	0.01432000	1.90220600
H	3.75849800	0.26514800	2.95025900
H	4.58785900	0.29540400	1.32811800
C	4.87064000	-2.98154300	0.65066600
H	5.30926900	-3.97750800	0.69697900
H	3.90045600	-3.07539900	0.17580300
H	5.51316800	-2.37469800	0.02220300
C	3.42703300	-3.03138500	3.48415400
H	3.73591400	-4.03232300	3.78281600
H	3.28875300	-2.45223700	4.39054000
H	2.47358400	-3.12349900	2.97619800
C	6.28902100	-1.67038100	3.18135900
H	6.08332000	-1.09229100	4.07556700
H	6.89950600	-2.52168100	3.47982000
H	6.88508400	-1.06793000	2.50470900
Si	4.73471300	-2.30497300	2.37823800

E_0(CASSCF,vacuo) -676.098372

E_0(CASSCF,CPCM) **-676.169825**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0983724394
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609837E+03
 (     1) 0.6727801 (     3)-0.6440758 (    36)-0.1046860 (    78) 0.1011250 ( 1662)-0.0753475 ( 1770)-0.0727843 ( 1904) 0.0722132
 (  2016) 0.0700642 (    24)-0.0687688 (     2) 0.0646388 ( 2851) 0.0639698 ( 3323)-0.0617406 (  264)-0.0581351 (  366) 0.0559063
 ( 1854)-0.0500502 ( 2108) 0.0480781 (    39) 0.0479499 (   81)-0.0439925 (  333)-0.0411708 (  235) 0.0400667 (  447) 0.0393076
 ( 1715) 0.0389084 ( 1737)-0.0380411 (    30)-0.0367262 ( 1983) 0.0366778 ( 1957)-0.0364693 ( 1602) 0.0352145 (  121) 0.0342510
 (  122)-0.0321140 (    67) 0.0320381 ( 1775)-0.0318674 ( 1601) 0.0314334 (  300)-0.0296244 ( 1898) 0.0287696 (  406) 0.0285973
 ( 2021) 0.0281721 (    45)-0.0275102 (   239)-0.0274678 (  276)-0.0271539 (  243)-0.0270692 ( 2558) 0.0263182 (   91) 0.0261354
 ( 1660) 0.0258624 (   378) 0.0256850 (   351)-0.0238170 ( 2557) 0.0236132 (  260)-0.0235893 (  358)-0.0233513 (  237)-0.0232048
 ( 1600)-0.0230947 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192056D+01
     2 -0.390378D-06  0.195666D+01
     3  0.107050D-07 -0.126802D-07  0.188982D+01
     4  0.378570D-04 -0.193559D-04 -0.148686D-06  0.103851D+01
     5 -0.289771D-04  0.204644D-04 -0.485661D-07 -0.281192D-06  0.955811D+00
     6  0.772502D-07  0.305780D-07  0.567033D-06 -0.711552D-07  0.131769D-06
     7  0.322291D-05 -0.561823D-06  0.302245D-06  0.654568D-05 -0.358464D-05
     8 -0.246061D-06  0.210337D-05  0.116882D-06 -0.772120D-05 -0.100556D-04
     9 -0.681500D-08  0.146468D-05 -0.438174D-07  0.230924D-05 -0.375265D-05
                6             7             8             9
     6  0.107517D+00
     7 -0.490305D-08  0.825416D-01
     8 -0.157317D-07 -0.357141D-07  0.121605D-01
     9  0.104100D-07 -0.249934D-06 -0.156068D-06  0.364224D-01
 MCSCF converged.
```

$^{1}2^{+}$a STEP 7

GEOMETRY

C	0.00564900	-0.00972800	0.00283000
C	0.00688500	-0.01162600	1.38588500
C	1.25205200	-0.00997700	2.01792300
C	2.44641000	0.00864400	1.25466700
C	2.36919800	0.02219700	-0.16069500
C	1.12929100	0.02076700	-0.80299100
H	-0.90521500	-0.01363600	1.95129100
H	1.30872300	-0.00920900	3.09177600
H	3.27412200	0.04742100	-0.74108000
H	1.05599300	0.04297400	-1.87338700
C	3.71967200	0.00809800	1.90756400
H	3.76186200	0.24891600	2.95730500
H	4.59370400	0.27285500	1.33511600
C	4.88772600	-3.06130200	0.67475800
H	5.30146700	-4.06854700	0.70797500
H	3.91487200	-3.12543200	0.20029000
H	5.54440100	-2.46182400	0.05415000
C	3.43962500	-3.10043400	3.50815900
H	3.71989500	-4.11151300	3.80140900
H	3.31511500	-2.52243400	4.41709500
H	2.48578700	-3.16350300	2.99639900
C	6.31368900	-1.75131200	3.20870300
H	6.10129800	-1.16890800	4.09841300
H	6.93105600	-2.59543200	3.51416300
H	6.90506000	-1.14936300	2.52766100
Si	4.76663600	-2.40319600	2.40897700

E_0(CASSCF,vacuo) -676.096081

E_0(CASSCF,CPCM) **-676.167755**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0960805397
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609608E+03
(     1) 0.6692040 (     3)-0.6458285 (    36)-0.1045595 (    78) 0.1016687 ( 1662)-0.0767175 (     2) 0.0764033 ( 1770)-0.0741116
( 1904) 0.0741046 ( 2016) 0.0718172 (    24)-0.0660499 ( 2851) 0.0648020 ( 3323)-0.0629402 (   264)-0.0583942 (  366) 0.0565715
( 1854)-0.0509706 ( 2108) 0.0493329 (    39) 0.0469148 (    81)-0.0428233 (  333)-0.0412967 (   235) 0.0411414 (  447) 0.0397668
( 1737)-0.0387401 ( 1715) 0.0384220 ( 1983) 0.0376078 ( 1602) 0.0370123 ( 1957)-0.0356848 ( 1601) 0.0352665 (   30)-0.0349244
(  121) 0.0333069 ( 1775)-0.0316665 (    67) 0.0311207 (  122)-0.0309541 ( 1898) 0.0301753 (  300)-0.0295606 (  406) 0.0287393
( 2021) 0.0279407 (  276)-0.0273411 ( 1660) 0.0269701 (    45)-0.0268314 ( 2558) 0.0263613 (  378) 0.0261089 (  243)-0.0259323
(  239)-0.0257907 (   91) 0.0257299 (  351)-0.0239144 ( 2557) 0.0234439 (  465) 0.0232023 (   66)-0.0226237 (  358)-0.0224632
(  282) 0.0224224 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191814D+01
     2 -0.656708D-06  0.195650D+01
     3  0.721544D-08 -0.217607D-07  0.188999D+01
     4  0.293899D-04 -0.858918D-05 -0.120730D-05  0.103096D+01
     5 -0.149614D-04  0.134950D-04  0.978992D-06 -0.142107D-05  0.963559D+00
     6  0.288062D-06  0.162847D-07  0.114570D-05 -0.154223D-05  0.138407D-05
     7  0.769012D-06  0.152182D-05  0.107430D-06  0.157353D-04 -0.136005D-04
     8 -0.338826D-05 -0.893067D-06  0.156427D-06 -0.118445D-04 -0.126117D-04
     9  0.356100D-05  0.173184D-05 -0.277801D-07  0.290681D-05 -0.653390D-05
                6             7             8             9
     6  0.107784D+00
     7 -0.117641D-07  0.839332D-01
     8 -0.157634D-07 -0.722958D-06  0.123578D-01
     9 -0.190934D-07  0.838351D-07  0.242830D-06  0.367701D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 8

GEOMETRY

C	0.00483500	-0.01011000	0.00243200
C	0.00592600	-0.01080300	1.38538000
C	1.25101700	-0.00896100	2.01843100
C	2.44543000	0.00663700	1.25684600
C	2.36932300	0.01781600	-0.15770600
C	1.12977400	0.01610300	-0.80154000
H	-0.90639800	-0.01096300	1.95053300
H	1.30641000	-0.00548900	3.09244000
H	3.27467600	0.04163100	-0.73765700
H	1.05805600	0.03606900	-1.87214300
C	3.71938600	0.00346200	1.91149200
H	3.76438600	0.23405800	2.96296900
H	4.59811000	0.25404900	1.34065800
C	4.90664500	-3.13669100	0.69375500
H	5.31159700	-4.14801700	0.71110600
H	3.93086300	-3.18519500	0.22340500
H	5.56559800	-2.53362800	0.07919500
C	3.45436400	-3.16910200	3.52877300
H	3.71416500	-4.18386700	3.82847600
H	3.33543300	-2.58372700	4.43363700
H	2.50287500	-3.21657900	3.01094000
C	6.34034400	-1.83783500	3.23276300
H	6.12438100	-1.25309800	4.11994800
H	6.96040200	-2.67887000	3.54223800
H	6.92990500	-1.23708700	2.54927100
Si	4.79847100	-2.50020300	2.43528600

E_0(CASSCF,vacuo) -676.093689

E_0(CASSCF,CPCM) **-676.165627**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0936887903
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609369E+03
 (     1) 0.6665184 (     3)-0.6467117 (    36)-0.1045011 (    78) 0.1020619 (     2) 0.0861807 ( 1662)-0.0777598 ( 1904) 0.0755042
 ( 1770)-0.0751022 ( 2016) 0.0730968 ( 2851) 0.0653885 (    24)-0.0642170 ( 3323)-0.0637781 (  264)-0.0585203 (  366) 0.0569760
 ( 1854)-0.0516469 ( 2108) 0.0502401 (   39) 0.0461037 (   235) 0.0421045 (   81)-0.0418569 (  333)-0.0413166 (  447) 0.0400156
 ( 1737)-0.0392717 ( 1601) 0.0387062 ( 1602) 0.0386983 ( 1983) 0.0382980 ( 1715) 0.0379326 ( 1957)-0.0349513 (   30)-0.0337206
 (  121) 0.0325862 ( 1898) 0.0313211 ( 1775)-0.0310984 (    67) 0.0304965 (  122)-0.0300486 (  300)-0.0295012 (  406) 0.0288186
 ( 1660) 0.0278094 (  276)-0.0274607 ( 2021) 0.0273515 ( 2558) 0.0264739 (  378) 0.0263905 (   45)-0.0262222 (   91) 0.0253027
 (  243)-0.0249386 (  239)-0.0244325 (  351)-0.0239650 (  465) 0.0233610 ( 2557) 0.0233479 (   66)-0.0222873 ( 2073) 0.0221616
 (  282) 0.0219372 (
 Final one electron symbolic density matrix:
                   1                  2                  3                  4                  5
      1  0.191618D+01
      2  0.617769D-06  0.195638D+01
      3  0.162098D-09  0.200164D-08  0.189005D+01
      4  0.195039D-04 -0.184824D-04 -0.598741D-07  0.102595D+01
      5 -0.389160D-04  0.136145D-04  0.746352D-07 -0.299693D-06  0.968811D+00
      6  0.276791D-07  0.290875D-08 -0.120387D-05  0.849550D-07 -0.613444D-07
      7  0.923600D-06 -0.119547D-05  0.825215D-08  0.165365D-04 -0.122663D-04
      8 -0.340345D-05 -0.797322D-06 -0.395114D-08  0.819539D-05  0.490813D-05
      9 -0.403863D-06 -0.813530D-08 -0.427802D-08  0.491981D-05 -0.415713D-05
                   6                  7                  8                  9
      6  0.108105D+00
      7 -0.751964D-10  0.850027D-01
      8 -0.953184D-09  0.470855D-06  0.124501D-01
      9  0.462812D-08  0.755015D-06  0.176766D-07  0.370784D-01
 MCSCF converged.
```

$^{1}2^{+}$a STEP 9

GEOMETRY

C	0.00409400	-0.01434800	0.00304900
C	0.00567500	-0.01353600	1.38588900
C	1.25098400	-0.01050400	2.01935800
C	2.44529900	0.00346700	1.25893200
C	2.36938400	0.01203200	-0.15492700
C	1.12986600	0.00914000	-0.79965400
H	-0.90660100	-0.01249700	1.95122400
H	1.30560200	-0.00438200	3.09348400
H	3.27483600	0.03533700	-0.73491100
H	1.05915700	0.02718700	-1.87041400
C	3.72032400	-0.00101800	1.91472500
H	3.76699400	0.22257500	2.96727800
H	4.60176100	0.23942700	1.34437900
C	4.92820700	-3.21031000	0.71172200
H	5.29097100	-4.23783100	0.71649100
H	3.95347800	-3.21296900	0.23648800
H	5.61425600	-2.62515500	0.10992300
C	3.47181700	-3.23899200	3.54521100
H	3.69526600	-4.26927900	3.82090000
H	3.37705600	-2.66923800	4.46261400
H	2.51805800	-3.24117500	3.02918100
C	6.36946600	-1.92137600	3.25675600
H	6.14739500	-1.33496700	4.14125700
H	6.99547900	-2.75670900	3.57026900
H	6.95474000	-1.31933800	2.57079900
Si	4.83391100	-2.59605900	2.46065100

E_0(CASSCF,vacuo) -676.091306

E_0(CASSCF,CPCM) **-676.163564**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0913063163
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67609131E+03
(     1) 0.6645016 (     3)-0.6472241 (    36)-0.1045095 (    78) 0.1023911 (     2) 0.0930908 ( 1662)-0.0786395 ( 1904) 0.0766329
( 1770)-0.0759102 ( 2016) 0.0741056 ( 2851) 0.0658557 ( 3323)-0.0644238 (    24)-0.0629197 (  264)-0.0585879 (  366) 0.0572444
( 1854)-0.0522015 ( 2108) 0.0509594 (   39) 0.0453792 (  235) 0.0430798 ( 1601) 0.0416527 (  333)-0.0412866 (   81)-0.0410481
( 1602) 0.0404267 (  447) 0.0401507 ( 1737)-0.0397210 ( 1983) 0.0388611 ( 1715) 0.0373859 ( 1957)-0.0342777 (   30)-0.0328749
( 1898) 0.0322893 (  121) 0.0319779 (   67) 0.0300443 ( 1775)-0.0300185 (  300)-0.0294550 (  122)-0.0293344 (  406) 0.0288702
( 1660) 0.0285350 (  276)-0.0275470 ( 2558) 0.0266142 (  378) 0.0265949 ( 2021) 0.0263404 (   45)-0.0256600 (   91) 0.0248681
(  243)-0.0240219 (  351)-0.0239923 (  465) 0.0234668 ( 2557) 0.0233391 (  239)-0.0232905 (  278) 0.0222807 ( 2073) 0.0219859
(   66)-0.0219655 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191455D+01
     2 -0.814324D-07  0.195628D+01
     3 -0.437114D-07  0.998438D-07  0.189005D+01
     4 -0.786089D-04  0.434352D-04  0.206834D-05  0.102245D+01
     5  0.833553D-04 -0.392738D-04 -0.123199D-06  0.364801D-05  0.972607D+00
     6  0.392509D-06  0.356632D-06 -0.894509D-06  0.488609D-06  0.253706D-06
     7 -0.585029D-05  0.378801D-06 -0.804634D-06 -0.400090D-04  0.397281D-04
     8 -0.240738D-05 -0.561479D-06 -0.508590D-06 -0.357306D-05  0.396620D-05
     9  0.784993D-06  0.366687D-06 -0.769996D-07 -0.175557D-04  0.133478D-04
                6             7             8             9
     6  0.108460D+00
     7  0.185595D-07  0.858933D-01
     8  0.162313D-07  0.555004D-06  0.123232D-01
     9  0.894644D-07  0.281676D-06 -0.542077D-07  0.373810D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 10

GEOMETRY

C	0.00426700	-0.01206800	0.00228000
C	0.00528800	-0.01171400	1.38502300
C	1.25032100	-0.00956800	2.01978800
C	2.44527100	0.00312600	1.26137500
C	2.37041200	0.01155300	-0.15198400
C	1.13139200	0.00957200	-0.79840700
H	-0.90736000	-0.00974300	1.94986000
H	1.30344600	-0.00285700	3.09406300
H	3.27638300	0.03440300	-0.73131700
H	1.06238800	0.02752200	-1.86933600
C	3.72070900	-0.00462500	1.91910300
H	3.76841700	0.21075500	2.97305000
H	4.60532200	0.22657500	1.35035500
C	4.94795700	-3.28314800	0.72731300
H	5.28805500	-4.31847000	0.71650400
H	3.97279000	-3.25780300	0.25345600
H	5.64598700	-2.70356300	0.13413600
C	3.48759300	-3.31049900	3.55977100
H	3.68420200	-4.34850800	3.82728000
H	3.40472900	-2.74553300	4.48116700
H	2.53578800	-3.28472300	3.04060400
C	6.39694200	-2.01041700	3.27951400
H	6.17061300	-1.42304600	4.16224200
H	7.02615000	-2.84247700	3.59594300
H	6.98013100	-1.40795400	2.59222500
Si	4.86627800	-2.69283100	2.48373300

E_0(CASSCF,vacuo) -676.088995

E_0(CASSCF,CPCM) **-676.161666**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0889945198
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608899E+03
 (     1) 0.6629811 (     3)-0.6475734 (    36)-0.1045682 (    78) 0.1026909 (     2) 0.0974791 ( 1662)-0.0793429 ( 1904) 0.0775328
 ( 1770)-0.0765259 ( 2016) 0.0748754 ( 2851) 0.0662033 ( 3323)-0.0649078 (    24)-0.0622170 (   264)-0.0586289 (   366) 0.0574359
 ( 1854)-0.0526464 ( 2108) 0.0515312 (    39) 0.0447794 (   235) 0.0440439 ( 1601) 0.0439252 ( 1602) 0.0420894 (   333)-0.0412375
 (    81)-0.0404250 (  447) 0.0402241 ( 1737)-0.0400945 ( 1983) 0.0393218 ( 1715) 0.0368500 ( 1957)-0.0336620 ( 1898) 0.0331531
 (    30)-0.0323780 (  121) 0.0315106 (    67) 0.0298385 (  300)-0.0294176 ( 1660) 0.0291944 (   406) 0.0289095 (   122)-0.0288077
 ( 1775)-0.0286365 (  276)-0.0276118 ( 2558) 0.0268045 (  378) 0.0267422 (    45)-0.0251404 ( 2021) 0.0251146 (    91) 0.0244469
 (  351)-0.0240050 (  465) 0.0235382 ( 2557) 0.0233958 (  243)-0.0231975 ( 1772) 0.0228560 (   278) 0.0227206 (   239)-0.0223682
 ( 1600)-0.0220835 (
 Final one electron symbolic density matrix:
                   1                   2                   3                   4                   5
      1  0.191325D+01
      2 -0.320068D-06  0.195620D+01
      3  0.443953D-07  0.128352D-06  0.188996D+01
      4  0.834325D-04 -0.395211D-04  0.117966D-05  0.101991D+01
      5 -0.715138D-04  0.394103D-04 -0.637573D-06 -0.125132D-05  0.975473D+00
      6  0.843981D-07  0.197037D-06 -0.133384D-05 -0.123539D-06  0.109712D-07
      7  0.294481D-05  0.823700D-06 -0.181005D-06  0.440895D-04 -0.336066D-04
      8  0.314470D-05 -0.831637D-06 -0.307111D-07  0.992301D-05 -0.592166D-06
      9  0.149745D-05 -0.114784D-05  0.157310D-06  0.155442D-04 -0.179871D-04
                   6                   7                   8                   9
      6  0.108874D+00
      7 -0.681476D-07  0.866305D-01
      8 -0.225781D-07  0.542232D-06  0.120255D-01
      9 -0.311944D-07  0.469910D-06  0.405832D-06  0.376753D-01
 MCSCF converged.
```

$^{1}2^{+}$a STEP 11

GEOMETRY

C	0.00406800	-0.01110800	0.00205300
C	0.00494000	-0.01069200	1.38470100
C	1.24988500	-0.00880600	2.02034600
C	2.44532600	0.00293600	1.26353000
C	2.37095300	0.01100300	-0.14940600
C	1.13221400	0.00925400	-0.79706300
H	-0.90789800	-0.00797800	1.94933000
H	1.30188600	-0.00132500	3.09474100
H	3.27722800	0.03358800	-0.72840400
H	1.06450900	0.02693300	-1.86813300
C	3.72129200	-0.00739800	1.92270800
H	3.76997200	0.20093200	2.97780600
H	4.60841500	0.21580700	1.35508500
C	4.96985300	-3.35712200	0.74340100
H	5.28783300	-4.39933500	0.71874000
H	3.99485700	-3.30552100	0.27108700
H	5.67936600	-2.78410900	0.15766900
C	3.50712500	-3.38288700	3.57500700
H	3.67879800	-4.42767100	3.83362200
H	3.43584400	-2.82362000	4.50073700
H	2.55730400	-3.33087300	3.05395500
C	6.42549500	-2.09671200	3.30054000
H	6.19492700	-1.50802800	4.18126200
H	7.05872800	-2.92471000	3.62014600
H	7.00591600	-1.49378000	2.61136100
Si	4.89982500	-2.78831500	2.50612400

E_0(CASSCF,vacuo) -676.086805

E_0(CASSCF,CPCM) **-676.159950**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0868047832
 Full Convergence on CI vector
          ( 1)        EIGENVALUE     -0.67608680E+03
 (     1) 0.6620202 (     3)-0.6479068 (    36)-0.1046964 (    78) 0.1029854 (     2) 0.0985361 ( 1662)-0.0799646 ( 1904) 0.0782822
 ( 1770)-0.0770473 ( 2016) 0.0754940 ( 2851) 0.0665036 ( 3323)-0.0652988 (    24)-0.0619036 (  264)-0.0586890 (  366) 0.0576014
 ( 1854)-0.0530376 ( 2108) 0.0520092 ( 1601) 0.0454784 (  235) 0.0450034 (    39) 0.0442282 ( 1602) 0.0436390 (  333)-0.0412045
 ( 1737)-0.0404253 (  447) 0.0402770 (    81)-0.0399684 ( 1983) 0.0397122 ( 1715) 0.0362527 ( 1898) 0.0338960 ( 1957)-0.0331453
 (   30)-0.0321294 (  121) 0.0311055 ( 1660) 0.0298520 (    67) 0.0297743 (  300)-0.0293969 (  406) 0.0289394 (  122)-0.0284504
 (  276)-0.0276645 ( 2558) 0.0269884 ( 1775)-0.0269828 (  378) 0.0268551 (   45)-0.0246720 (   91) 0.0240437 (  351)-0.0240231
 ( 2021) 0.0237062 (  465) 0.0235976 ( 1772) 0.0235703 ( 2557) 0.0235416 ( 1600)-0.0234183 (  278) 0.0231651 (  243)-0.0224413
 ( 1891)-0.0221635 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.191223D+01
      2 -0.164748D-06  0.195613D+01
      3  0.371136D-07 -0.229586D-07  0.188982D+01
      4  0.513054D-04 -0.255552D-04 -0.121509D-05  0.101821D+01
      5 -0.464339D-04  0.229490D-04  0.983851D-06  0.245214D-05  0.977526D+00
      6  0.380678D-06 -0.582780D-07 -0.390268D-06  0.107566D-05 -0.469492D-06
      7  0.195432D-05  0.464186D-06  0.359506D-06  0.256131D-04 -0.199251D-04
      8  0.230802D-05 -0.539297D-07  0.253301D-07  0.397557D-05  0.239075D-05
      9 -0.447588D-06 -0.797181D-07 -0.112408D-07  0.752811D-05 -0.722146D-05
                   6             7             8             9
      6  0.109321D+00
      7 -0.104181D-08  0.872683D-01
      8 -0.974507D-08  0.201076D-06  0.115434D-01
      9  0.299779D-07 -0.363640D-07  0.125526D-06  0.379621D-01
 MCSCF converged.
```

$^{1}2^{+}$a STEP 12

GEOMETRY

C	0.00333800	-0.01234000	0.00239500
C	0.00451500	-0.01086600	1.38495000
C	1.24958200	-0.00826300	2.02101500
C	2.44530600	0.00273300	1.26533100
C	2.37084500	0.00971400	-0.14723600
C	1.13215700	0.00721500	-0.79563400
H	-0.90832300	-0.00762400	1.94967700
H	1.30088200	0.00045100	3.09549900
H	3.27720600	0.03212700	-0.72622800
H	1.06529800	0.02399800	-1.86682500
C	3.72197100	-0.00955600	1.92542900
H	3.77169400	0.19297900	2.98143200
H	4.61101900	0.20651900	1.35838100
C	4.99352500	-3.43044300	0.75942400
H	5.28562100	-4.47987900	0.72134000
H	4.01999200	-3.34948400	0.28788100
H	5.71681400	-2.86684300	0.18160800
C	3.52802100	-3.45537700	3.58930700
H	3.67304100	-4.50731200	3.83525400
H	3.46948000	-2.90506500	4.52118300
H	2.58054400	-3.37398100	3.06745100
C	6.45542000	-2.18380800	3.32198900
H	6.22098700	-1.59425100	4.20109900
H	7.09185800	-3.00848300	3.64428000
H	7.03379000	-1.58038000	2.63152800
Si	4.93426100	-2.88274500	2.52808000

E_0(CASSCF,vacuo) -676.084765

E_0(CASSCF,CPCM) **-676.158425**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0847652825
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67608477E+03
(     1) 0.6616234 (     3)-0.6483406 (    36)-0.1048897 (    78) 0.1032882 (     2) 0.0957080 ( 1662)-0.0805429 ( 1904) 0.0789418
( 1770)-0.0775201 ( 2016) 0.0760257 ( 2851) 0.0667878 ( 3323)-0.0656411 (    24)-0.0618314 (  264)-0.0587925 (  366) 0.0577733
( 1854)-0.0534021 ( 2108) 0.0524294 ( 1601) 0.0463097 (  235) 0.0459470 ( 1602) 0.0450071 (   39) 0.0436817 (  333)-0.0412100
( 1737)-0.0407272 (  447) 0.0403369 ( 1983) 0.0400525 (   81)-0.0396592 ( 1715) 0.0356014 ( 1898) 0.0345197 ( 1957)-0.0327020
(   30)-0.0320394 (  121) 0.0307280 ( 1660) 0.0305169 (   67) 0.0297911 (  300)-0.0293887 (  406) 0.0289658 (  122)-0.0282246
(  276)-0.0277172 ( 2558) 0.0271567 (  378) 0.0269440 ( 1775)-0.0251118 ( 1600)-0.0250936 (   45)-0.0242566 (  351)-0.0240594
( 1772) 0.0239457 ( 2557) 0.0237536 (   91) 0.0236710 (  465) 0.0236611 (  278) 0.0236198 ( 1832) 0.0227056 ( 1891)-0.0223864
( 2017)-0.0223641 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191143D+01
     2 -0.540529D-06  0.195608D+01
     3  0.130769D-08 -0.805040D-08  0.188965D+01
     4  0.733872D-04 -0.346827D-04 -0.930356D-07  0.101717D+01
     5 -0.679173D-04  0.336412D-04 -0.273043D-07 -0.162519D-05  0.978926D+00
     6  0.109836D-07 -0.184439D-07 -0.926438D-06  0.993553D-07 -0.734733D-07
     7  0.205044D-05 -0.675789D-07  0.358021D-07  0.368224D-04 -0.318264D-04
     8  0.197639D-05  0.501511D-06 -0.880369D-08  0.374953D-05 -0.120513D-05
     9  0.265181D-06 -0.440203D-06 -0.885977D-08  0.154745D-04 -0.146867D-04
                6             7             8             9
     6  0.109774D+00
     7  0.403206D-08  0.878397D-01
     8  0.562055D-08  0.234191D-06  0.108948D-01
     9  0.161679D-07  0.190775D-06  0.286863D-06  0.382362D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 13

GEOMETRY

C	0.00350800	-0.01115100	0.00104200
C	0.00389900	-0.01079300	1.38351000
C	1.24858700	-0.00875700	2.02093300
C	2.44520900	0.00256600	1.26726700
C	2.37170600	0.01073900	-0.14502900
C	1.13356200	0.00875700	-0.79507300
H	-0.90937500	-0.00777200	1.94763400
H	1.29840200	-0.00064500	3.09555100
H	3.27858900	0.03368600	-0.72328900
H	1.06832200	0.02643500	-1.86640100
C	3.72198300	-0.01230700	1.92918000
H	3.77173000	0.18353800	2.98629100
H	4.61314400	0.19807400	1.36359600
C	5.01618600	-3.50557000	0.77432600
H	5.28161200	-4.56156500	0.72304000
H	4.04478900	-3.39502700	0.30400800
H	5.75315900	-2.95244900	0.20385400
C	3.54947500	-3.53097000	3.60282300
H	3.66815500	-4.58954400	3.83420900
H	3.50392200	-2.99151200	4.54166300
H	2.60454900	-3.41981700	3.08148700
C	6.48502000	-2.27329900	3.34167700
H	6.24744500	-1.68334300	4.21968800
H	7.12453700	-3.09501900	3.66582300
H	7.06128200	-1.66913200	2.65008600
Si	4.96763600	-2.97845800	2.54852400

E_0(CASSCF,vacuo) -676.082889

E_0(CASSCF,CPCM) **-676.157091**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0828889567
Full Convergence on CI vector      -0.67608289E+03
          ( 1)        EIGENVALUE
(     1) 0.6615947 (     3)-0.6488339 (    36)-0.1051234 (    78) 0.1035893 (     2) 0.0903702 ( 1662)-0.0810805 ( 1904) 0.0795192
( 1770)-0.0779527 ( 2016) 0.0764825 ( 2851) 0.0670590 ( 3323)-0.0659430 (    24)-0.0619300 (  264)-0.0589329 (  366) 0.0579565
( 1854)-0.0537391 ( 2108) 0.0527987 (  235) 0.0468449 ( 1601) 0.0464599 ( 1602) 0.0461477 (   39) 0.0431532 (  333)-0.0412495
( 1737)-0.0409987 (  447) 0.0404105 ( 1983) 0.0403461 (   81)-0.0394597 ( 1898) 0.0350392 ( 1715) 0.0349094 ( 1957)-0.0323316
(   30)-0.0320637 ( 1660) 0.0311814 (  121) 0.0303723 (   67) 0.0298663 (  300)-0.0293881 (  406) 0.0289849 (  122)-0.0281006
(  276)-0.0277631 ( 2558) 0.0272985 (  378) 0.0270155 ( 1600)-0.0269532 (  351)-0.0241122 (  278) 0.0240532 ( 2557) 0.0240197
( 1772) 0.0239892 (   45)-0.0238920 (  465) 0.0237311 (   91) 0.0233304 ( 1832) 0.0232828 ( 1775)-0.0231623 ( 2081)-0.0228650
(  379)-0.0227917 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191084D+01
     2 -0.215132D-06  0.195604D+01
     3  0.657529D-08  0.139650D-07  0.188946D+01
     4 -0.712166D-04  0.269198D-04  0.236046D-08  0.101659D+01
     5  0.632861D-04 -0.258414D-04  0.119851D-06  0.369595D-05  0.979881D+00
     6  0.147550D-06 -0.174286D-07  0.853051D-06  0.169711D-07  0.136039D-06
     7 -0.115638D-05  0.713472D-06  0.109147D-07 -0.411114D-04  0.357249D-04
     8 -0.719574D-06  0.181988D-06  0.454919D-07  0.631920D-05 -0.708456D-05
     9 -0.172149D-06 -0.203970D-06 -0.175086D-07 -0.171465D-04  0.159832D-04
                6             7             8             9
     6  0.110221D+00
     7 -0.240654D-08  0.883546D-01
     8 -0.386575D-08 -0.195288D-06  0.101284D-01
     9  0.149170D-07 -0.137401D-06  0.828309D-07  0.384900D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 14

GEOMETRY

C	0.00310000	-0.01226300	0.00117900
C	0.00357800	-0.01105500	1.38356600
C	1.24829000	-0.00826000	2.02150300
C	2.44532900	0.00280800	1.26899000
C	2.37183400	0.01045000	-0.14304500
C	1.13380800	0.00780700	-0.79386300
H	-0.90976900	-0.00787900	1.94766600
H	1.29736700	0.00056800	3.09620400
H	3.27885100	0.03356100	-0.72119200
H	1.06941300	0.02514800	-1.86529900
C	3.72256600	-0.01378600	1.93181600
H	3.77289100	0.17685200	2.98972700
H	4.61528700	0.19086900	1.36682600
C	5.04000600	-3.58196800	0.79112500
H	5.26872700	-4.64590300	0.72859000
H	4.07350800	-3.43393800	0.32045100
H	5.79602400	-3.04728200	0.22820800
C	3.57356100	-3.60571900	3.61818300
H	3.66150700	-4.67192800	3.82709400
H	3.54518100	-3.08372200	4.56741500
H	2.63111500	-3.45733200	3.10113400
C	6.51614700	-2.35986300	3.36106800
H	6.27556600	-1.76860700	4.23741500
H	7.15903100	-3.17807100	3.68773400
H	7.08993300	-1.75549400	2.66756000
Si	5.00226900	-3.07219500	2.56979700

E_0(CASSCF,vacuo) -676.081178

E_0(CASSCF,CPCM) **-676.155928**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0811780307
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608118E+03
(     1) 0.6619891 (     3)-0.6493617 (    36)-0.1053942 (    78) 0.1038842 (     2) 0.0817627 ( 1662)-0.0815901 ( 1904) 0.0800347
( 1770)-0.0783625 ( 2016) 0.0768866 ( 2851) 0.0673272 ( 3323)-0.0662163 (   24)-0.0621334 (  264)-0.0591134 (  366) 0.0581509
( 1854)-0.0540598 ( 2108) 0.0531282 (  235) 0.0476856 ( 1602) 0.0470506 ( 1601) 0.0459974 (   39) 0.0426061 (  333)-0.0413283
( 1737)-0.0412481 ( 1983) 0.0406011 (  447) 0.0404970 (   81)-0.0393751 ( 1898) 0.0354479 ( 1715) 0.0341864 (   30)-0.0321737
( 1957)-0.0320250 ( 1660) 0.0318549 (  121) 0.0300100 (   67) 0.0299593 (  300)-0.0293940 (  406) 0.0289992 ( 1600)-0.0288701
(  122)-0.0280685 (  276)-0.0278154 ( 2558) 0.0274124 (  378) 0.0270680 (  278) 0.0244803 ( 2557) 0.0243252 (  351)-0.0241846
(  465) 0.0238101 ( 1772) 0.0237527 ( 1832) 0.0237393 (   45)-0.0235783 ( 2081)-0.0233113 (  379)-0.0232054 (   91) 0.0230244
( 2010) 0.0227802 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191040D+01
     2 -0.218240D-06  0.195601D+01
     3  0.347707D-07 -0.469156D-07  0.188927D+01
     4 -0.412887D-04  0.334499D-04 -0.206748D-06  0.101656D+01
     5  0.438419D-04 -0.305162D-04  0.613768D-08 -0.457464D-05  0.980283D+00
     6  0.638109D-06  0.401121D-07 -0.535314D-06  0.637397D-06 -0.171299D-06
     7 -0.469550D-06  0.453658D-06  0.555508D-06 -0.117626D-04  0.124566D-04
     8  0.814256D-06 -0.228492D-06  0.251120D-07 -0.899662D-05  0.140714D-04
     9  0.209303D-06 -0.103512D-06  0.971702D-09 -0.905327D-05  0.711675D-05
                6             7             8             9
     6  0.110647D+00
     7 -0.448487D-08  0.888222D-01
     8  0.105753D-07  0.161420D-06  0.928276D-02
     9 -0.102893D-07 -0.312423D-06 -0.144689D-06  0.387189D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 15

GEOMETRY

C	0.00221600	-0.00725500	0.00157000
C	0.00303800	-0.00641800	1.38388200
C	1.24789500	-0.00583200	2.02201500
C	2.44522100	0.00364500	1.27032500
C	2.37141100	0.01212100	-0.14148000
C	1.13336900	0.01162400	-0.79273700
H	-0.91028100	-0.00179100	1.94810500
H	1.29659300	0.00256100	3.09677800
H	3.27848400	0.03424100	-0.71965600
H	1.06948900	0.02980700	-1.86423600
C	3.72295200	-0.01604300	1.93371000
H	3.77408300	0.16975100	2.99234500
H	4.61704300	0.18331200	1.36917600
C	5.06446800	-3.66161700	0.80548800
H	5.27842100	-4.72789700	0.73211300
H	4.09927900	-3.49616900	0.33757700
H	5.82673400	-3.13117000	0.24703300
C	3.59644100	-3.68536500	3.63144900
H	3.66684400	-4.75394800	3.83464700
H	3.57415400	-3.16754200	4.58311000
H	2.65750600	-3.51961600	3.11296100
C	6.54540100	-2.45184400	3.37936100
H	6.30232200	-1.86003400	4.25470500
H	7.19032400	-3.26783200	3.70758100
H	7.11775100	-1.84690600	2.68508400
Si	5.03413800	-3.16820200	2.58826400

E_0(CASSCF,vacuo) -676.079627

E_0(CASSCF,CPCM) **-676.154924**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0796264537
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67607963E+03
(     1) 0.6624709 (     3)-0.6497679 (    36)-0.1056532 (    78) 0.1041396 ( 1662)-0.0820343 ( 1904) 0.0804602 ( 1770)-0.0787242
( 2016) 0.0772178 (     2) 0.0729637 ( 2851) 0.0675661 ( 3323)-0.0664412 (   24)-0.0623981 (  264)-0.0593022 (  366) 0.0583358
( 1854)-0.0543411 ( 2108) 0.0534026 (  235) 0.0484144 ( 1602) 0.0477202 ( 1601) 0.0451217 (   39) 0.0421156 ( 1737)-0.0414599
(  333)-0.0414235 ( 1983) 0.0408074 (  447) 0.0405857 (   81)-0.0393414 ( 1898) 0.0357972 ( 1715) 0.0335275 ( 1660) 0.0324679
(   30)-0.0323292 ( 1957)-0.0317543 ( 1600)-0.0306852 (   67) 0.0300682 (  121) 0.0296890 (  300)-0.0293974 (  406) 0.0290060
(  122)-0.0280764 (  276)-0.0278641 ( 2558) 0.0275176 (  378) 0.0271039 (  278) 0.0248627 ( 2557) 0.0246089 (  351)-0.0242636
( 1832) 0.0240798 (  465) 0.0238881 ( 2081)-0.0236404 (  379)-0.0235517 ( 1772) 0.0233212 (   45)-0.0233130 ( 2010) 0.0230906
( 1891)-0.0229288 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191009D+01
     2  0.388570D-05  0.195599D+01
     3 -0.137176D-07 -0.355160D-06  0.188909D+01
     4  0.205083D-04 -0.194938D-04 -0.832179D-06  0.101681D+01
     5 -0.311040D-04  0.171897D-04  0.512292D-06  0.267257D-05  0.980366D+00
     6 -0.159632D-06  0.295455D-07  0.736827D-06 -0.708842D-08 -0.217173D-06
     7  0.305906D-06 -0.346022D-05  0.194678D-06  0.324128D-05 -0.566896D-05
     8 -0.321762D-05  0.306712D-05 -0.626772D-07  0.786842D-05 -0.798045D-05
     9 -0.368814D-05 -0.379999D-06  0.333551D-07  0.657918D-05  0.512053D-06
                6             7             8             9
     6  0.111040D+00
     7  0.215233D-07  0.892394D-01
     8 -0.235217D-07 -0.242757D-06  0.845876D-02
     9 -0.437457D-06  0.391937D-05  0.613175D-06  0.389172D-01
MCSCF converged.
```

$^{1}2^{+}$a STEP 16

GEOMETRY

C	0.00054900	-0.01673000	0.00223700
C	0.00215100	-0.01268900	1.38447400
C	1.24735300	-0.00799800	2.02242300
C	2.44464700	0.00245000	1.27110700
C	2.37009800	0.00822800	-0.14045500
C	1.13182200	0.00365800	-0.79174400
H	-0.91093000	-0.00888400	1.94917800
H	1.29590000	0.00257800	3.09722200
H	3.27692700	0.03125700	-0.71907100
H	1.06813700	0.01975100	-1.86333600
C	3.72307700	-0.01556100	1.93460300
H	3.77489600	0.16650800	2.99372500
H	4.61788700	0.17906900	1.36979200
C	5.09694200	-3.73169800	0.82301200
H	5.25212300	-4.80717500	0.73793900
H	4.14483400	-3.50963400	0.35087000
H	5.88982400	-3.23573600	0.27587000
C	3.62570700	-3.75769300	3.64386600
H	3.65289600	-4.83543500	3.80420100
H	3.62710700	-3.27571900	4.61427900
H	2.69195400	-3.53529200	3.13654000
C	6.58291300	-2.53749300	3.40323700
H	6.33707900	-1.94643000	4.27834300
H	7.22913300	-3.35216200	3.73269400
H	7.15525800	-1.93187400	2.70951600
Si	5.07504600	-3.25666400	2.61018800

E_0(CASSCF,vacuo) -676.078229

E_0(CASSCF,CPCM) **-676.154013**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0782289960
Full Convergence on CI vector     -0.67607823E+03
          ( 1)        EIGENVALUE
(     1) 0.6633081 (     3)-0.6500519 (    36)-0.1059460 (    78) 0.1043704 ( 1662)-0.0824909 ( 1904) 0.0808402 ( 1770)-0.0790941
( 2016) 0.0775082 ( 2851) 0.0678218 ( 3323)-0.0666439 (    24)-0.0626907 (     2) 0.0614149 (  264)-0.0595206 (  366) 0.0585139
( 1854)-0.0546260 ( 2108) 0.0536473 (  235) 0.0491247 ( 1602) 0.0482056 ( 1601) 0.0436459 ( 1737)-0.0416683 (   39) 0.0415693
(  333)-0.0415452 ( 1983) 0.0409861 (  447) 0.0406691 (   81)-0.0393690 ( 1898) 0.0360538 ( 1660) 0.0331088 ( 1715) 0.0327903
(   30)-0.0325466 ( 1600)-0.0324589 ( 1957)-0.0315267 (   67) 0.0301434 (  300)-0.0294051 (  121) 0.0293212 (  406) 0.0289977
(  122)-0.0281378 (  276)-0.0279144 ( 2558) 0.0275978 (  378) 0.0271180 (  278) 0.0252539 ( 2557) 0.0249392 (  351)-0.0243581
( 1832) 0.0243448 (  465) 0.0239682 (  379)-0.0238709 ( 2081)-0.0238608 ( 2010) 0.0234474 (   45)-0.0230852 ( 1891)-0.0230825
( 1772) 0.0226311 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190990D+01
     2  0.111741D-05  0.195598D+01
     3  0.414018D-08  0.295623D-07  0.188892D+01
     4  0.127180D-04 -0.126722D-04 -0.450175D-06  0.101776D+01
     5 -0.124951D-04  0.125405D-04  0.479585D-06  0.230061D-05  0.979770D+00
     6  0.598692D-07  0.601888D-08  0.435402D-06  0.846065D-08  0.480627D-08
     7 -0.157258D-06 -0.126004D-05 -0.147689D-07 -0.127396D-05  0.482926D-05
     8 -0.255762D-06  0.302645D-06 -0.410804D-07  0.105603D-04 -0.916721D-05
     9 -0.189261D-05 -0.884230D-06 -0.664704D-08  0.344041D-05 -0.169852D-05
                6             7             8             9
     6  0.111407D+00
     7 -0.548576D-08  0.896217D-01
     8  0.814211D-08  0.222763D-06  0.754659D-02
     9  0.172174D-07  0.110480D-05  0.347016D-06  0.390925D-01
MCSCF converged.
```

$^{3}2^{+}$a STEP 1

GEOMETRY

C	-3.47277600	0.00001500	0.48037200
C	-2.88443000	1.24540900	0.19832000
C	-1.64582500	1.24251800	-0.39529000
C	-0.98752100	-0.00001400	-0.71915100
C	-1.64584700	-1.24253000	-0.39527500
C	-2.88445700	-1.24539200	0.19832600
H	-3.39345900	2.16065400	0.43222800
H	-1.15436000	2.16462900	-0.64262200
H	-1.15439200	-2.16465300	-0.64258500
H	-3.39350600	-2.16062600	0.43223400
C	0.29799600	-0.00003000	-1.31542300
H	0.56049600	0.90144400	-1.85214200
H	0.56049100	-0.90152600	-1.85210600
C	1.66265400	-1.57005600	1.17549600
H	2.49444500	-1.66211500	1.87025500
H	0.75188400	-1.57064200	1.76586100
H	1.66922700	-2.45951600	0.55281800
C	1.66274500	1.57018100	1.17532200
H	2.49454200	1.66226900	1.87007000
H	1.66937100	2.45957200	0.55254500
H	0.75197600	1.57088600	1.76568700
C	3.37536900	-0.00010400	-0.93814900
H	3.41688800	0.87910900	-1.57325000
H	4.27501400	-0.00005700	-0.32689700
H	3.41687500	-0.87942700	-1.57309800
Si	1.86907500	0.00000100	0.17383700

E_0(CASSCF,vacuo) -676.125595

E_0(CASSCF,CPCM) **-676.196737**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1255951563
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612560E+03
 ( 7764) 0.9365302 ( 7933)-0.1271644 ( 6449) 0.1062338 ( 8183) 0.0786101 ( 7961)-0.0741957 ( 9024)-0.0725537 ( 7779) 0.0715562
 ( 9039)-0.0643580 ( 8613) 0.0581596 ( 6201) 0.0555204 ( 6588) 0.0536148 ( 1547)-0.0533991 (10233) 0.0531479 (10193) 0.0514828
 ( 6161) 0.0463372 ( 7932) 0.0461507 ( 7765)-0.0457920 ( 7947) 0.0433391 ( 2272)-0.0424406 (10199)-0.0420553 ( 7911)-0.0383430
 ( 5951)-0.0378760 ( 8150)-0.0365711 ( 8277) 0.0359109 ( 1514) 0.0357495 (10166) 0.0348972 ( 4825)-0.0343019 ( 1581) 0.0342150
 ( 8177) 0.0337294 ( 6435) 0.0335874 ( 9025) 0.0332484 ( 7794)-0.0330249 ( 2308) 0.0316954 (10293)-0.0300999 ( 6928)-0.0298197
 ( 6892) 0.0292768 ( 2299) 0.0288528 ( 1556) 0.0286673 ( 8638)-0.0280496 ( 7936)-0.0252510 ( 1968)-0.0250109 ( 6919)-0.0248557
 ( 8486) 0.0241544 ( 8519)-0.0236862 ( 1768) 0.0236531 ( 6167)-0.0233185 ( 1804) 0.0216590 ( 6618)-0.0213902 ( 4828)-0.0204486
 ( 8553) 0.0179658 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.291258D-01
     2 -0.487703D-05  0.192657D+01
     3  0.622820D-06 -0.738600D-06  0.641102D-01
     4 -0.142034D-05 -0.119188D-06  0.555696D-06  0.196498D+01
     5  0.891011D-05  0.952575D-05  0.134618D-04  0.363893D-05  0.100535D+01
     6  0.162751D-07 -0.963506D-07 -0.370312D-07  0.538491D-07 -0.266194D-06
     7  0.551432D-07  0.141181D-08 -0.336872D-07 -0.139742D-07  0.159544D-07
     8 -0.925940D-06  0.111512D-05 -0.897571D-06  0.155749D-05 -0.404072D-05
     9  0.881861D-06 -0.905751D-05 -0.587780D-05  0.646528D-06  0.317961D-06
                6             7             8             9
     6  0.190278D+01
     7 -0.912080D-06  0.903892D-01
     8 -0.152444D-07  0.492064D-08  0.166872D-01
     9 -0.472345D-06  0.220665D-07 -0.683318D-06  0.999999D+00
 MCSCF converged.
```

$^{3}2^{+}$a STEP 2

GEOMETRY

C	3.48930600	0.00000000	0.50022600
C	2.90477800	-1.24344700	0.21089400
C	1.67184600	-1.24141300	-0.39819600
C	1.01687300	0.00000000	-0.72951300
C	1.67184700	1.24141300	-0.39819600
C	2.90477900	1.24344600	0.21089400
H	3.41031300	-2.15938700	0.44974900
H	1.18551000	-2.16470900	-0.65220000
H	1.18551200	2.16471000	-0.65220000
H	3.41031100	2.15938600	0.44975500
C	-0.25284000	0.00000100	-1.33970200
H	-0.54036500	-0.90546500	-1.85425600
H	-0.54036600	0.90546600	-1.85425600
C	-1.69571000	1.57619700	1.17719400
H	-2.52545700	1.68064600	1.87321600
H	-0.78271600	1.57316600	1.76325500
H	-1.69741800	2.45786400	0.54418700
C	-1.69570800	-1.57619500	1.17719800
H	-2.52546200	-1.68064700	1.87321200
H	-1.69740400	-2.45786300	0.54419400
H	-0.78272000	-1.57315600	1.76326800
C	-3.37634500	-0.00000300	-0.97352800
H	-3.39385500	-0.87983700	-1.60835300
H	-4.29773600	-0.00002000	-0.39491500
H	-3.39387400	0.87984600	-1.60833200
Si	-1.91765800	0.00000000	0.19571800

E_0(CASSCF,vacuo) -676.123535

E_0(CASSCF,CPCM) **-676.194087**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1235353635
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67612354E+03
 ( 8693) 0.9319456 ( 8780)-0.1289653 ( 7855)-0.1118942 ( 8448) 0.0852577 ( 8021) 0.0769124 ( 8687)-0.0758806 ( 8015)-0.0695576
 ( 8779) 0.0627550 ( 8356) 0.0574947 ( 8105) 0.0531448 ( 2904)-0.0524820 ( 8605) 0.0505894 ( 8777) 0.0500536 ( 8696)-0.0497631
 ( 8608)-0.0453418 ( 5732)-0.0444734 ( 9968)-0.0438554 ( 8353)-0.0421630 ( 7938) 0.0408989 ( 8739) 0.0375138 ( 2931) 0.0372345
 ( 7028) 0.0368529 ( 8771)-0.0368454 ( 8815) 0.0368383 ( 2861)-0.0354997 ( 8437) 0.0345139 ( 8405) 0.0341926 ( 7196)-0.0341259
 ( 7847)-0.0339512 ( 2431) 0.0339040 (10548) 0.0334131 ( 8698) 0.0333718 (10505) 0.0333173 ( 2564) 0.0331966 ( 9942)-0.0323137
 ( 8573)-0.0315173 (10398)-0.0307938 ( 8616)-0.0306541 (10352) 0.0306511 (10411)-0.0305579 ( 2896)-0.0298303 ( 5778) 0.0290749
 ( 8024)-0.0285636 ( 2599)-0.0271424 ( 7170)-0.0253501 ( 7002) 0.0249336 (10540) 0.0244119 ( 8273) 0.0240700 ( 8688) 0.0228647
 ( 2372) 0.0228309 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.322936D-01
      2  0.133438D-05  0.195915D+01
      3 -0.408969D-06 -0.237203D-05  0.169573D-01
      4  0.155284D-06 -0.313464D-05  0.993630D-06  0.704308D-01
      5  0.228820D-07  0.952057D-07 -0.427713D-07 -0.148968D-07  0.190087D+01
      6  0.632443D-07  0.244444D-07  0.130668D-07  0.656299D-07  0.149433D-05
      7  0.507815D-06  0.819670D-06  0.211532D-05  0.179051D-05  0.122075D-06
      8  0.180687D-05 -0.318348D-06 -0.191428D-05 -0.833584D-05 -0.734449D-07
      9 -0.757443D-06 -0.675176D-05 -0.300928D-05  0.671740D-05 -0.193430D-06
                   6             7             8             9
      6  0.937204D-01
      7 -0.904331D-08  0.192217D+01
      8 -0.123200D-07 -0.892847D-05  0.999999D+00
      9 -0.297530D-08  0.122913D-04  0.495535D-07  0.100440D+01
 MCSCF converged.
```

$^{3}2^{+}$a STEP 3

GEOMETRY

C	3.50689700	0.00000000	-0.52105500
C	2.92666600	1.24163400	-0.22416500
C	1.69990900	1.23994500	0.40109000
C	1.04885400	-0.00000100	0.73928000
C	1.69991200	-1.23994600	0.40109300
C	2.92666900	-1.24163400	-0.22416200
H	3.42852300	2.15820900	-0.46847200
H	1.21866800	2.16434400	0.66174600
H	1.21867100	-2.16434600	0.66174900
H	3.42852700	-2.15820800	-0.46846900
C	-0.20847700	-0.00000200	1.36486000
H	-0.51548000	0.90822800	1.86107300
H	-0.51547700	-0.90823100	1.86107600
C	-1.72787600	-1.58097400	-1.17756500
H	-2.55494400	-1.69957900	-1.87506800
H	-0.81286900	-1.57144900	-1.75983500
H	-1.72252000	-2.45567700	-0.53556000
C	-1.72791200	1.58101800	-1.17750100
H	-2.55498500	1.69963500	-1.87499600
H	-1.72257200	2.45569500	-0.53545900
H	-0.81290700	1.57153600	-1.75977500
C	-3.38406400	-0.00004100	1.00276200
H	-3.38122200	0.88039200	1.63653500
H	-4.32324600	-0.00003000	0.45270000
H	-3.38121400	-0.88051000	1.63648500
Si	-1.96860200	0.00000000	-0.21439600

E_0(CASSCF,vacuo) -676.120856

E_0(CASSCF,CPCM) **-676.190200**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1208556510
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67612086E+03
( 6423) 0.9279790 ( 9056) 0.1305203 ( 1798)-0.1171772 ( 7782)-0.0887203 (  963)-0.0806850 ( 6391)-0.0797903 (  931) 0.0754286
( 3487)-0.0590620 ( 4827) 0.0525463 ( 9027)-0.0522050 ( 6452)-0.0519563 ( 9022)-0.0514109 ( 9546)-0.0511767 ( 6906)-0.0495033
( 9017) 0.0438764 ( 9527)-0.0435574 (  382)-0.0432980 ( 6338)-0.0426847 ( 8261) 0.0420307 ( 5954) 0.0406005 ( 5934) 0.0389418
( 3462)-0.0384931 ( 6931)-0.0379602 ( 7746) 0.0360402 ( 9566)-0.0360116 ( 9037) 0.0355138 ( 8185)-0.0354826 (   86)-0.0343379
( 6442) 0.0339530 ( 7356) 0.0336800 ( 1771)-0.0333728 ( 7345)-0.0330963 ( 8196) 0.0328318 ( 7802)-0.0320928 ( 6264) 0.0315825
( 6253)-0.0315326 (  133) 0.0308681 ( 7460) 0.0307617 ( 8995) 0.0304091 ( 3987)-0.0302964 (  953)-0.0295262 ( 6406)-0.0287293
(  122)-0.0278191 ( 9026) 0.0277472 ( 6962)-0.0277005 ( 5923) 0.0268745 (  113) 0.0264861 ( 7421) 0.0262715 ( 7394)-0.0262014
( 9535)-0.0256775 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.767250D-01
     2 -0.116879D-07  0.189930D+01
     3  0.166277D-05 -0.118848D-06  0.100316D+01
     4 -0.173837D-05  0.292490D-08 -0.406244D-05  0.191679D+01
     5 -0.544351D-08  0.397540D-06 -0.219705D-07  0.630001D-09  0.963281D-01
     6 -0.238848D-04  0.105281D-06  0.464320D-05 -0.369473D-04  0.923319D-08
     7  0.175396D-06 -0.327172D-08  0.375481D-05 -0.118388D-05 -0.142341D-08
     8 -0.578536D-06 -0.361867D-08  0.173153D-05 -0.131473D-05 -0.108698D-08
     9  0.250168D-05  0.313314D-09  0.435284D-05 -0.916514D-06  0.430591D-08
                6             7             8             9
     6  0.999998D+00
     7 -0.222276D-05  0.169756D-01
     8  0.692723D-05  0.118253D-06  0.348936D-01
     9 -0.628357D-05  0.299952D-06  0.165427D-05  0.195583D+01
MCSCF converged.
```

$^{3}2^{+}$a STEP 4

GEOMETRY

C	3.52543100	0.00000000	-0.54276200
C	2.94968300	1.24004000	-0.23822600
C	1.72967700	1.23838200	0.40361600
C	1.08295100	-0.00000100	0.74863000
C	1.72967800	-1.23838300	0.40361800
C	2.94968400	-1.24004000	-0.23822500
H	3.44782900	2.15720400	-0.48806100
H	1.25355300	2.16375100	0.67108100
H	1.25355600	-2.16375200	0.67108300
H	3.44783200	-2.15720400	-0.48805800
C	-0.16416100	-0.00000100	1.39036000
H	-0.48515700	0.91009000	1.87253900
H	-0.48515600	-0.91009100	1.87254000
C	-1.76094800	-1.58473800	-1.17722300
H	-2.58507100	-1.71683700	-1.87637400
H	-0.84415700	-1.56845700	-1.75609300
H	-1.74883500	-2.45318800	-0.52736900
C	-1.76098200	1.58477600	-1.17716800
H	-2.58510800	1.71688300	-1.87631300
H	-1.74888300	2.45320300	-0.52728400
H	-0.84419100	1.56853200	-1.75604100
C	-3.39541400	-0.00003600	1.02894500
H	-3.37366300	0.88099500	1.66111900
H	-4.35044300	-0.00002800	0.50603800
H	-3.37365500	-0.88109600	1.66107700
Si	-2.02086000	0.00000000	-0.23066200

E_0(CASSCF,vacuo) -676.117875

E_0(CASSCF,CPCM) **-676.187287**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1178754081
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67611788E+03
( 6423) 0.9248188 ( 9056) 0.1318507 ( 1798)-0.1215469 ( 7782)-0.0902407 (  963)-0.0836708 ( 6391)-0.0830118 (  931) 0.0810816
( 3487)-0.0607449 ( 9027)-0.0532933 ( 6452)-0.0530708 ( 4827) 0.0516638 ( 9546)-0.0493435 ( 6906)-0.0492669 ( 9527)-0.0476740
( 9017) 0.0469278 ( 8261) 0.0468964 ( 5954) 0.0455715 (  382)-0.0451358 ( 9022)-0.0420368 ( 5934) 0.0411861 ( 6338)-0.0407246
( 8196) 0.0382686 ( 7356) 0.0379531 ( 7746) 0.0373565 (  133) 0.0369156 ( 9566)-0.0363751 (   86)-0.0358826 ( 3462)-0.0356878
( 3987)-0.0353911 ( 6442) 0.0346140 (  953)-0.0341402 ( 6406)-0.0335373 ( 8185)-0.0333204 ( 9037) 0.0330032 ( 6931)-0.0328264
( 9026) 0.0326986 ( 1771)-0.0325700 ( 6368)-0.0304735 ( 7394)-0.0304654 ( 7802)-0.0304240 ( 7345)-0.0298109 ( 5915) 0.0297238
( 6264) 0.0285828 ( 7460) 0.0278773 ( 6422)-0.0271727 ( 6339) 0.0270910 ( 5923) 0.0268667 ( 8995) 0.0256511 ( 6962)-0.0241494
(  122)-0.0239783 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.824358D-01
     2 -0.368514D-08  0.189807D+01
     3  0.436557D-05  0.101764D-07  0.100198D+01
     4 -0.332143D-05  0.357499D-09 -0.632016D-06  0.191151D+01
     5 -0.411119D-09  0.685532D-06  0.650762D-08  0.198815D-08  0.983624D-01
     6  0.248619D-04 -0.177853D-09 -0.536136D-05  0.422605D-04  0.398957D-08
     7  0.455350D-06  0.670398D-08  0.879622D-05 -0.247000D-05 -0.103886D-09
     8 -0.100147D-05  0.107493D-08  0.521427D-05 -0.378646D-05 -0.783189D-10
     9  0.333005D-05 -0.186289D-09 -0.143009D-06 -0.104850D-05  0.526751D-08
                6             7             8             9
     6  0.999997D+00
     7  0.398784D-05  0.167900D-01
     8 -0.925146D-05  0.157345D-06  0.367249D-01
     9  0.899674D-05 -0.190593D-06  0.323533D-05  0.195412D+01
MCSCF converged.
```

$^{3}2^{+}$a STEP 5

GEOMETRY

C	3.54486900	0.00000100	-0.56501700
C	2.97354000	1.23870700	-0.25280100
C	1.76079200	1.23694000	0.40555300
C	1.11860300	-0.00000100	0.75759100
C	1.76079400	-1.23694100	0.40555300
C	2.97354200	-1.23870600	-0.25280100
H	3.46801300	2.15634900	-0.50833500
H	1.28951900	2.16307300	0.67970800
H	1.28952200	-2.16307500	0.67970900
H	3.46801700	-2.15634700	-0.50833400
C	-0.11923100	-0.00000200	1.41580300
H	-0.45047200	0.91135600	1.88724800
H	-0.45047100	-0.91136000	1.88724800
C	-1.79526000	-1.58774500	-1.17633400
H	-2.60916400	-1.72635500	-1.88652500
H	-0.87020500	-1.57023400	-1.74160900
H	-1.78939100	-2.45128800	-0.52021900
C	-1.79528800	1.58777800	-1.17628600
H	-2.60919500	1.72639500	-1.88647300
H	-1.78943600	2.45130100	-0.52014500
H	-0.87023400	1.57030100	-1.74156100
C	-3.40992100	-0.00003100	1.05259400
H	-3.36897100	0.88134400	1.68309500
H	-4.37965900	-0.00002400	0.55702400
H	-3.36896500	-0.88143300	1.68305900
Si	-2.07382500	0.00000000	-0.24478700

E_0(CASSCF,vacuo) -676.114790

E_0(CASSCF,CPCM) **-676.184426**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1147899099
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67611479E+03
 ( 6423) 0.9223921 ( 9056) 0.1329464 ( 1798)-0.1248393 ( 7782)-0.0905700 (  963)-0.0859786 (  931) 0.0859366 ( 6391)-0.0855629
 ( 3487)-0.0624325 ( 9027)-0.0538016 ( 6452)-0.0535982 ( 4827) 0.0505864 ( 9527)-0.0502510 ( 6906)-0.0497294 ( 8261) 0.0496403
 ( 5954) 0.0487872 ( 9017) 0.0476309 ( 9546)-0.0472485 (  382)-0.0467022 ( 5934) 0.0416163 ( 8196) 0.0414040 (  133) 0.0408964
 ( 6338)-0.0393755 ( 3987)-0.0392647 ( 7356) 0.0392227 ( 7746) 0.0381561 ( 6406)-0.0372440 ( 9566)-0.0364322 (   86)-0.0363674
 (  953)-0.0359827 ( 9026) 0.0358279 ( 6442) 0.0352293 ( 9022)-0.0348292 ( 6368)-0.0337431 ( 3462)-0.0336196 ( 7394)-0.0332514
 ( 5915) 0.0332182 ( 1771)-0.0317124 ( 8185)-0.0310074 ( 9037) 0.0306319 ( 6931)-0.0296837 ( 6422)-0.0292010 ( 6339) 0.0291764
 ( 7802)-0.0291212 ( 7342)-0.0273413 ( 6307)-0.0264950 ( 7345)-0.0262365 ( 5923) 0.0259709 (  962) 0.0255430 ( 6264) 0.0252512
 ( 7460) 0.0252191 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.872963D-01
     2 -0.460048D-08  0.189715D+01
     3 -0.102886D-04  0.252681D-08  0.100106D+01
     4 -0.201996D-05  0.909405D-09 -0.202923D-04  0.190690D+01
     5 -0.805789D-09  0.378745D-06  0.320840D-08 -0.578494D-08  0.999439D-01
     6  0.679560D-04  0.432589D-08 -0.708880D-05  0.112956D-03  0.112232D-07
     7 -0.191410D-06 -0.782505D-08 -0.108461D-05 -0.132607D-05  0.747226D-09
     8 -0.698209D-06 -0.107055D-08  0.413409D-06  0.655986D-06 -0.690215D-09
     9  0.245214D-05 -0.889892D-09  0.243685D-05 -0.648332D-06  0.598554D-08
                6             7             8             9
     6  0.999995D+00
     7  0.970111D-05  0.164330D-01
     8 -0.168721D-04  0.286670D-07  0.379743D-01
     9  0.252945D-04  0.822641D-06  0.754792D-06  0.195326D+01
 MCSCF converged.
```

$^{3}2^{+}$a STEP 6

GEOMETRY

C	-3.56437600	0.00005300	-0.58816700
C	-2.99764100	-1.23755200	-0.26788800
C	-1.79295200	-1.23568900	0.40745500
C	-1.15537100	-0.00006200	0.76706200
C	-1.79283100	1.23562600	0.40745000
C	-2.99751700	1.23760400	-0.26789300
H	-3.48820900	-2.15563100	-0.52953600
H	-1.32659500	-2.16251300	0.68830400
H	-1.32640500	2.16240500	0.68833300
H	-3.48802000	2.15573000	-0.52949900
C	0.07370500	-0.00012300	1.44152000
H	0.41238800	-0.91246100	1.90462200
H	0.41244300	0.91218000	1.90466600
C	1.83020300	1.59057700	-1.17381400
H	2.63204100	1.73498500	-1.89681400
H	0.89601500	1.57187800	-1.72372800
H	1.83233300	2.44982800	-0.51236000
C	1.82903200	-1.58908300	-1.17600200
H	2.63076000	-1.73307200	-1.89920900
H	1.83054800	-2.44924800	-0.51573600
H	0.89485300	-1.56895100	-1.72587800
C	3.42744500	-0.00138500	1.07341700
H	3.37058100	-0.88373900	1.70106700
H	4.40932400	-0.00133000	0.60158100
H	3.37112600	0.88006300	1.70238900
Si	2.12704500	0.00000600	-0.25693200

E_0(CASSCF,vacuo) -676.111719

E_0(CASSCF,CPCM) **-676.181705**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1117188940
Full Convergence on CI vector
         ( 1)      EIGENVALUE     -0.67611172E+03
( 2949) 0.9204983 ( 1263)-0.0872869 ( 3247) 0.0852031 ( 4810)-0.0786036 (   55)-0.0782235 ( 8997)-0.0646841 ( 2998) 0.0645317
( 9046)-0.0615204 ( 5889)-0.0593859 ( 2970) 0.0592449 (   19) 0.0587964 ( 5910)-0.0562235 ( 3211) 0.0539820 ( 4791)-0.0507196
( 1282)-0.0507187 ( 1521)-0.0457905 ( 3118)-0.0452174 ( 3998)-0.0440145 ( 7737) 0.0421329 ( 1290)-0.0420770 ( 4846)-0.0420753
( 4723) 0.0417924 (  470) 0.0404084 ( 2983) 0.0400506 ( 1269)-0.0398383 ( 2943) 0.0396968 ( 3080)-0.0394066 ( 8876)-0.0386885
( 3372) 0.0385020 ( 4705) 0.0382190 (  105)-0.0374833 ( 4797)-0.0365760 ( 2962) 0.0364471 ( 4725)-0.0362543 ( 3457) 0.0359668
(   85) 0.0358853 ( 4717) 0.0350861 ( 3465)-0.0344114 ( 5883)-0.0336867 ( 9010)-0.0336864 ( 1270)-0.0321928 ( 3501)-0.0321362
( 5938)-0.0309508 ( 9018)-0.0309508 ( 3369)-0.0306219 ( 2952)-0.0306022 ( 4798)-0.0295536 (  141) 0.0295018 ( 8875)-0.0281913
(  103) 0.0281259 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190303D+01
     2  0.494495D-05  0.967199D-01
     3  0.560412D-06 -0.498434D-05  0.189641D+01
     4 -0.973337D-05 -0.817329D-05 -0.209417D-05  0.100012D+01
     5 -0.117208D-06 -0.227853D-05  0.393816D-06  0.228288D-05  0.195280D+01
     6  0.835994D-05  0.119978D-04  0.412676D-05 -0.401845D-03  0.294167D-05
     7  0.533161D-05 -0.464032D-06 -0.288938D-05 -0.128650D-05  0.185984D-05
     8 -0.780850D-05  0.447497D-06  0.699711D-06 -0.289460D-06  0.104988D-07
     9  0.747165D-05 -0.982880D-02  0.290995D-05 -0.456497D-05 -0.336535D-05
                6             7             8             9
     6  0.100030D+01
     7  0.336319D-08  0.158854D-01
     8 -0.264797D-05 -0.410609D-07  0.388669D-01
     9  0.462209D-05 -0.318382D-06 -0.800827D-06  0.958778D-01
MCSCF converged.
```

$^{3}2^{+}$a STEP 7

GEOMETRY

C	-3.58444800	0.00024200	-0.61164300
C	-3.02220500	-1.23650200	-0.28350500
C	-1.82600600	-1.23463100	0.40856800
C	-1.19300100	-0.00017500	0.77618200
C	-1.82575400	1.23449700	0.40888400
C	-3.02197100	1.23678600	-0.28316300
H	-3.50886500	-2.15492400	-0.55140500
H	-1.36442400	-2.16207000	0.69580600
H	-1.36403600	2.16176800	0.69644700
H	-3.50848000	2.15537500	-0.55077200
C	0.02747700	-0.00039500	1.46660200
H	0.37153200	-0.91357100	1.92324600
H	0.37168700	0.91254600	1.92359500
C	1.86648500	1.59248800	-1.17201400
H	2.65958700	1.74438300	-1.90337300
H	0.92632200	1.57068000	-1.71151300
H	1.87145900	2.44763300	-0.50550500
C	1.86491700	-1.59075600	-1.17440700
H	2.65790400	-1.74233800	-1.90595300
H	1.86899000	-2.44691400	-0.50919300
H	0.92481400	-1.56717000	-1.71393400
C	3.44518900	-0.00157100	1.09392500
H	3.37163300	-0.88430200	1.71914500
H	4.43893800	-0.00162200	0.64708900
H	3.37233800	0.88023700	1.72052800
Si	2.18046400	0.00002800	-0.26791200

E_0(CASSCF,vacuo) -676.108746

E_0(CASSCF,CPCM) **-676.179191**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1087463087
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67610875E+03
( 5567) 0.9189709 (10581) 0.1345722 ( 4387) 0.1289727 ( 3958) 0.0931745 ( 5871)-0.0897204 ( 3971) 0.0893742 ( 5554) 0.0893095
( 9768)-0.0651910 (10523)-0.0543053 ( 5625)-0.0541305 (10190)-0.0529186 ( 5781)-0.0522693 ( 5228) 0.0520570 ( 5687)-0.0513321
( 3805) 0.0497111 (10019) 0.0482869 (10520) 0.0461897 ( 4131) 0.0455618 ( 9851)-0.0441855 (10239) 0.0431058 ( 2692) 0.0423174
( 5604)-0.0421187 ( 5787) 0.0404081 (10516)-0.0390238 ( 5855) 0.0384135 ( 4972) 0.0379135 ( 5037)-0.0372633 ( 2272) 0.0371564
( 5738)-0.0369230 ( 4799) 0.0367599 ( 4127) 0.0362534 ( 5620) 0.0360903 ( 3968) 0.0360257 (10233)-0.0359415 ( 2287)-0.0325558
( 4979) 0.0317180 ( 5560) 0.0316660 ( 9803)-0.0307811 ( 4966) 0.0298817 ( 3964) 0.0293597 ( 4378)-0.0293143 ( 5865) 0.0271873
( 4807) 0.0270966 (10515) 0.0269210 ( 5652)-0.0266872 ( 2693) 0.0262549 (10519)-0.0251647 ( 5736) 0.0239117 ( 5822) 0.0237387
(10072) 0.0236387 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189581D+01
     2 -0.714198D-05  0.151546D-01
     3  0.247933D-04 -0.121375D-05  0.947840D-01
     4 -0.561778D-05 -0.521567D-06  0.127513D-06  0.395503D-01
     5 -0.228764D-04 -0.824456D-05 -0.354298D-05 -0.334341D-05  0.100002D+01
     6  0.739053D-05  0.378820D-06  0.661220D-06  0.195092D-06  0.269997D-05
     7 -0.169711D-04 -0.180948D-05 -0.209323D-05 -0.960797D-06 -0.699230D-05
     8  0.106949D-05  0.449402D-05  0.499465D-05  0.830785D-05  0.198309D-04
     9  0.498010D-05  0.721279D-06 -0.343470D-05  0.310957D-05 -0.170428D-03
                6             7             8             9
     6  0.195254D+01
     7  0.567287D-06  0.189982D+01
     8 -0.132634D-05  0.174343D-05  0.102304D+00
     9  0.316448D-05  0.632944D-05 -0.526836D-05  0.100002D+01
MCSCF converged.
```

$^{3}2^{+}$a STEP 8

GEOMETRY

C	-3.60490000	0.00000500	-0.63545800
C	-3.04701200	-1.23585000	-0.29905900
C	-1.85981200	-1.23364100	0.40977000
C	-1.23159800	-0.00000500	0.78537300
C	-1.85979700	1.23363600	0.40976800
C	-3.04700100	1.23585800	-0.29906400
H	-3.52953600	-2.15474900	-0.57296200
H	-1.40300200	-2.16150400	0.70368500
H	-1.40297000	2.16149300	0.70368600
H	-3.52952400	2.15475900	-0.57297300
C	-0.01982800	-0.00000900	1.49147200
H	0.32802700	-0.91366900	1.94358200
H	0.32803700	0.91364700	1.94357900
C	1.90191600	1.59291200	-1.17045600
H	2.68637300	1.75258600	-1.90972300
H	0.95634400	1.56622900	-1.70023700
H	1.90829500	2.44493900	-0.50016300
C	1.90179400	-1.59276700	-1.17067600
H	2.68622200	-1.75238400	-1.90998700
H	1.90813500	-2.44489100	-0.50050700
H	0.95621000	-1.56594700	-1.70043000
C	3.46684500	-0.00013800	1.11118800
H	3.38001000	-0.88287700	1.73456000
H	4.47019800	-0.00010000	0.68564500
H	3.38001400	0.88248400	1.73472600
Si	2.23382300	-0.00000200	-0.27711600

E_0(CASSCF,vacuo) -676.105931

E_0(CASSCF,CPCM) **-676.176879**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1059304558
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610593E+03
 ( 5567) 0.9176807 (10581) 0.1351587 ( 4387) 0.1315595 ( 3958) 0.0958345 ( 5554) 0.0908348 ( 3971) 0.0908011 ( 5871)-0.0900194
 ( 9768)-0.0661638 (10523)-0.0545660 ( 5625)-0.0544039 (10190)-0.0535987 ( 5781)-0.0532247 ( 5228) 0.0531622 ( 5687)-0.0520785
 ( 3805) 0.0500764 (10019) 0.0475004 ( 4131) 0.0469837 ( 9851)-0.0456637 (10520) 0.0452972 ( 5604)-0.0436587 (10239) 0.0415259
 ( 2692) 0.0411646 (10516)-0.0398344 ( 5787) 0.0397381 ( 5855) 0.0383082 ( 5037)-0.0382176 ( 4799) 0.0379497 ( 5738)-0.0379386
 ( 4972) 0.0374863 ( 5620) 0.0366179 ( 4127) 0.0360288 ( 3968) 0.0356472 (10233)-0.0355819 ( 2272) 0.0350678 ( 2287)-0.0338524
 ( 4979) 0.0326300 ( 5560) 0.0325547 ( 4966) 0.0309907 ( 3964) 0.0305890 ( 9803)-0.0297292 ( 4807) 0.0280013 ( 4378)-0.0278926
 ( 5865) 0.0266180 ( 5652)-0.0260011 (10515) 0.0255514 ( 2693) 0.0240636 ( 5822) 0.0240322 (10072) 0.0239912 ( 5736) 0.0230518
 ( 5289) 0.0220922 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189530D+01
     2  0.564575D-05  0.142486D-01
     3  0.519290D-04  0.122027D-06  0.977282D-01
     4  0.237732D-05  0.172666D-07  0.515157D-07  0.401165D-01
     5 -0.440401D-04  0.186953D-05  0.177821D-05  0.101153D-06  0.999849D+00
     6  0.437718D-05  0.554539D-06  0.129622D-06  0.166919D-06 -0.520681D-06
     7 -0.213993D-04 -0.258966D-06 -0.965974D-07  0.257472D-06 -0.130601D-05
     8 -0.170118D-06  0.705013D-05  0.965844D-05  0.289962D-05  0.289144D-04
     9  0.630973D-05 -0.586837D-06 -0.400002D-06 -0.532529D-06 -0.137398D-03
                6             7             8             9
     6  0.195237D+01
     7  0.562808D-07  0.189713D+01
     8  0.181459D-04 -0.120479D-04  0.103240D+00
     9  0.587570D-06  0.157171D-05 -0.410409D-05  0.100002D+01
 MCSCF converged.
```

$^{3}2^{+}$a STEP 9

GEOMETRY

C	3.62530600	0.00026900	-0.65955100
C	3.07179800	1.23533500	-0.31478600
C	1.89407200	1.23275800	0.41078900
C	1.27070300	-0.00023400	0.79455200
C	1.89433500	-1.23296100	0.41036700
C	3.07210600	-1.23503200	-0.31512900
H	3.54993100	2.15468700	-0.59502700
H	1.44189900	2.16095900	0.71118700
H	1.44247700	-2.16135900	0.71063200
H	3.55058700	-2.15418700	-0.59543900
C	0.06767300	-0.00047200	1.51581800
H	-0.28307600	0.91358400	1.96436300
H	-0.28299300	-0.91477200	1.96392600
C	-1.93912800	-1.59319600	-1.16860800
H	-2.71072900	-1.75590600	-1.92084800
H	-0.98502500	-1.56451300	-1.68296100
H	-1.95439200	-2.44341600	-0.49634100
C	-1.93910600	1.59371200	-1.16788100
H	-2.71073500	1.75680600	-1.92000900
H	-1.95429600	2.44361700	-0.49521500
H	-0.98502700	1.56521800	-1.68228800
C	-3.48806000	-0.00027000	1.12891700
H	-3.38700100	0.88261600	1.74985700
H	-4.50086600	-0.00017500	0.72583600
H	-3.38700400	-0.88345200	1.74943800
Si	-2.28728200	0.00006000	-0.28528800

E_0(CASSCF,vacuo) -676.103309

E_0(CASSCF,CPCM) **-676.174843**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1033089971
Full Convergence on CI vector
         ( 1)      EIGENVALUE     -0.67610331E+03
( 2205) 0.9165383 ( 5670) 0.0976637 ( 2630) 0.0916487 ( 5634)-0.0797009 ( 2264)-0.0715038 ( 8589) 0.0714259 ( 8648)-0.0704184
( 8478)-0.0695515 ( 5466)-0.0648075 ( 2212)-0.0583577 ( 2793)-0.0583012 ( 2800) 0.0564709 ( 8426) 0.0539137 ( 2682)-0.0539037
( 5502)-0.0528252 ( 3867)-0.0501684 ( 8757)-0.0467254 ( 2596)-0.0452659 ( 2268) 0.0448079 ( 2625)-0.0425590 ( 2210)-0.0424286
(  860) 0.0418855 ( 2112) 0.0417759 ( 8646) 0.0405790 ( 2798) 0.0405547 ( 2120)-0.0386760 ( 2325) 0.0372496 (  429) 0.0371612
( 2544)-0.0369580 ( 2290)-0.0357704 ( 2231) 0.0352880 ( 8421)-0.0346704 ( 2262) 0.0345932 ( 8480) 0.0345553 ( 5817) 0.0345309
( 2632) 0.0345260 ( 6824)-0.0341740 ( 2157) 0.0340784 ( 8596)-0.0339264 ( 2852) 0.0339109 ( 2850) 0.0338290 (  441)-0.0334467
( 2193)-0.0333548 ( 2607)-0.0327172 (  882) 0.0320829 ( 6810)-0.0320827 ( 2613) 0.0312956 ( 2280)-0.0303722 ( 6826)-0.0301603
(  446) 0.0301410 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189484D+01
     2  0.788965D-05  0.999811D+00
     3  0.119988D-04 -0.127069D-05  0.406208D-01
     4 -0.270861D-05 -0.192664D-05 -0.163950D-06  0.131726D-01
     5  0.576517D-05  0.926707D-05  0.142467D-04 -0.387309D-05  0.189484D+01
     6 -0.979026D-06 -0.629521D-04 -0.167521D-05  0.517454D-06 -0.117025D-04
     7 -0.326662D-04  0.282699D-04  0.137507D-04  0.603352D-05  0.266868D-04
     8  0.602173D-05 -0.119244D-05 -0.928845D-07 -0.326496D-07  0.710220D-05
     9 -0.505304D-05 -0.373048D-06  0.114296D-06  0.292822D-06 -0.593668D-05
                6             7             8             9
     6  0.100005D+01
     7 -0.616861D-05  0.104075D+00
     8 -0.149347D-05 -0.150077D-04  0.195224D+01
     9 -0.602125D-05  0.118480D-04  0.281206D-06  0.100361D+00
MCSCF converged.
```

$^{3}2^{+}$a STEP 10

GEOMETRY

C	3.64647300	-0.00000700	-0.68340700
C	3.09757900	1.23459300	-0.33090500
C	1.92950300	1.23220300	0.41087200
C	1.31068600	0.00002400	0.80334700
C	1.92948400	-1.23221400	0.41092700
C	3.09755600	-1.23463500	-0.33084300
H	3.57175500	2.15415900	-0.61732200
H	1.48222300	2.16089200	0.71738500
H	1.48218700	-2.16088200	0.71749000
H	3.57175200	-2.15421200	-0.61720100
C	0.11667100	0.00007200	1.53953500
H	-0.23587200	0.91472500	1.98505200
H	-0.23588300	-0.91453700	1.98513700
C	-1.97681200	-1.59363200	-1.16541800
H	-2.73640100	-1.76012300	-1.92912400
H	-1.01524500	-1.56261500	-1.66579200
H	-1.99939800	-2.44202600	-0.49116900
C	-1.97714900	1.59395700	-1.16492100
H	-2.73677800	1.76049900	-1.92857900
H	-1.99994300	2.44214400	-0.49041900
H	-1.01561200	1.56330100	-1.66528600
C	-3.51264000	-0.00035100	1.14435100
H	-3.39940600	0.88294500	1.76259000
H	-4.53331300	-0.00041200	0.76111600
H	-3.39920400	-0.88380100	1.76233200
Si	-2.34064000	-0.00000800	-0.29195900

E_0(CASSCF,vacuo) -676.100901

E_0(CASSCF,CPCM) **-676.173056**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1009012864
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610090E+03
 ( 3117) 0.9155200 (  253) 0.1359900 ( 4214) 0.1032890 ( 5062)-0.0999496 ( 3130)-0.0936992 ( 5049) 0.0935642 ( 3213)-0.0839741
 ( 3699) 0.0674544 (  596)-0.0630012 (  261)-0.0552751 ( 3109)-0.0551349 ( 6059) 0.0544201 ( 3558) 0.0543743 ( 1441)-0.0532105
 ( 9260)-0.0488810 ( 2025) 0.0474779 (   12)-0.0474085 ( 3115)-0.0456548 ( 3206)-0.0443731 ( 4221) 0.0438296 (  308) 0.0407817
 ( 4930) 0.0396658 ( 9073) 0.0393998 ( 6078)-0.0392259 ( 4082)-0.0387416 ( 9128) 0.0369125 (    8) 0.0366899 (  600) 0.0362896
 ( 1185)-0.0362193 ( 9298)-0.0355010 ( 3539)-0.0349047 ( 9081)-0.0341824 ( 3164)-0.0340804 (  302) 0.0340715 ( 9094) 0.0325523
 ( 5096)-0.0323005 ( 3536) 0.0305375 ( 4723) 0.0302389 ( 6056)-0.0300719 ( 3110) 0.0296651 ( 3081)-0.0295212 (  345)-0.0294732
 (  601) 0.0294306 ( 3883) 0.0288987 ( 3709) 0.0280300 (  309) 0.0277508 ( 5090) 0.0273425 ( 4718)-0.0268839 ( 1431)-0.0252981
 ( 3540)-0.0248122 (
 Final one electron symbolic density matrix:
                   1                 2                 3                 4                 5
      1  0.195213D+01
      2 -0.731108D-06  0.104811D+00
      3  0.102743D-05 -0.106623D-04  0.189287D+01
      4  0.505232D-05  0.259051D-04  0.832644D-05  0.100007D+01
      5  0.572027D-05 -0.551231D-05 -0.136811D-04  0.106303D-04  0.189444D+01
      6  0.228922D-05 -0.550389D-05 -0.865742D-05  0.721001D-06 -0.766668D-05
      7 -0.204361D-05  0.724743D-05  0.379192D-05 -0.261765D-05  0.153292D-05
      8 -0.414396D-05 -0.211221D-04 -0.670151D-05  0.988592D-04 -0.911003D-05
      9 -0.111180D-05  0.153481D-05  0.803783D-05 -0.374492D-06 -0.372095D-04
                   6                 7                 8                 9
      6  0.120070D-01
      7  0.165739D-06  0.410762D-01
      8 -0.888605D-06  0.211465D-05  0.999875D+00
      9 -0.142152D-06  0.107329D-05  0.436894D-06  0.102715D+00
 MCSCF converged.
```

$^{3}2^{+}$a STEP 11

GEOMETRY

C	3.66817300	0.00000900	-0.70736200
C	3.12373700	1.23415100	-0.34703000
C	1.96552900	1.23166000	0.41074300
C	1.35151200	-0.00000600	0.81160200
C	1.96554100	-1.23167000	0.41073800
C	3.12374400	-1.23414700	-0.34702800
H	3.59383600	2.15400700	-0.63940000
H	1.52302400	2.16067200	0.72349700
H	1.52304200	-2.16068700	0.72348600
H	3.59384400	-2.15399700	-0.63941600
C	0.16669800	-0.00000900	1.56249900
H	-0.18725200	0.91504100	2.00570800
H	-0.18724800	-0.91506100	2.00570700
C	-2.01761900	-1.59359800	-1.16289400
H	-2.76227200	-1.75877000	-1.94158400
H	-1.04671500	-1.56277400	-1.64526700
H	-2.05353000	-2.44180900	-0.48914800
C	-2.01761600	1.59362300	-1.16285200
H	-2.76228600	1.75882700	-1.94152000
H	-2.05350300	2.44181500	-0.48908100
H	-1.04672500	1.56280500	-1.64525200
C	-3.53566300	-0.00001700	1.16166600
H	-3.40929200	0.88365300	1.77680800
H	-4.56422700	-0.00000700	0.79968700
H	-3.40929900	-0.88370600	1.77678100
Si	-2.39397300	0.00000100	-0.29725000

E_0(CASSCF,vacuo) -676.098713

E_0(CASSCF,CPCM) **-676.171507**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0987129417
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609871E+03
( 5393) 0.9145911 ( 1934) 0.1210468 ( 3722) 0.1103588 ( 4548)-0.0908307 ( 5388)-0.0881537 ( 4553) 0.0880177 ( 2032) 0.0693958
( 3556)-0.0658126 ( 3618)-0.0559390 ( 1949) 0.0516319 ( 5378) 0.0515120 ( 8330)-0.0508302 ( 4994) 0.0506417 ( 1109) 0.0480332
( 5377)-0.0463006 ( 5112) 0.0461527 ( 9597)-0.0459111 ( 2042) 0.0444902 ( 2864) 0.0438613 ( 3620) 0.0425926 (  353)-0.0401067
( 8354)-0.0390343 ( 1999) 0.0380874 ( 3614)-0.0378072 ( 1940)-0.0377864 ( 5765)-0.0373382 ( 3554) 0.0372321 (10334)-0.0368948
(10399)-0.0367265 ( 3724)-0.0367179 ( 2862)-0.0358491 ( 9629)-0.0358447 ( 5382)-0.0355321 ( 2873) 0.0354760 (10349)-0.0348536
( 2004)-0.0347488 ( 5443) 0.0347432 ( 4970) 0.0346314 ( 1866) 0.0337482 ( 4972)-0.0332843 ( 5381)-0.0311083 ( 8332) 0.0307934
(10344) 0.0306799 ( 4603) 0.0304957 ( 1864) 0.0301166 ( 5316) 0.0298819 ( 2034) 0.0297401 ( 1938)-0.0295661 ( 3624) 0.0295059
( 5822) 0.0292943 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195204D+01
     2  0.921360D-05  0.105405D+00
     3 -0.428440D-05 -0.442480D-03  0.104940D+00
     4 -0.205677D-06 -0.777781D-05  0.313101D-05  0.189117D+01
     5  0.110389D-07  0.151515D-05 -0.423344D-06  0.261833D-06  0.414973D-01
     6  0.650420D-06 -0.109942D-05  0.775724D-06 -0.186746D-06 -0.687500D-07
     7  0.213126D-05 -0.788688D-05  0.386822D-05 -0.251989D-05 -0.106323D-05
     8 -0.315231D-06  0.647005D-05  0.165733D-04 -0.131880D-05  0.962106D-06
     9 -0.188462D-06 -0.441863D-05  0.336078D-05 -0.147746D-05  0.839583D-06
                6             7             8             9
     6  0.107944D-01
     7 -0.109744D-05  0.100016D+01
     8 -0.722169D-05  0.968909D-05  0.189407D+01
     9 -0.756341D-06 -0.364269D-04  0.786757D-05  0.999927D+00
MCSCF converged.
```

$^{3}2^{+}$a STEP 12

GEOMETRY

C	-3.69053200	0.00003600	-0.73128400
C	-3.15065600	-1.23373000	-0.36328900
C	-2.00253200	-1.23123400	0.41013800
C	-1.39328000	-0.00003600	0.81937700
C	-2.00249400	1.23120500	0.41019100
C	-3.15061300	1.23377500	-0.36323200
H	-3.61661200	-2.15382300	-0.66168700
H	-1.56473600	-2.16055800	0.72881900
H	-1.56465900	2.16049900	0.72890600
H	-3.61654500	2.15389600	-0.66158100
C	-0.21790300	-0.00006500	1.58471300
H	0.13693900	-0.91550200	2.02609500
H	0.13694500	0.91534600	2.02614600
C	2.06028300	1.59335300	-1.16046200
H	2.79070100	1.75652400	-1.95300100
H	1.08094200	1.56291800	-1.62594900
H	2.10886500	2.44187100	-0.48801800
C	2.06015400	-1.59313500	-1.16077800
H	2.79056300	-1.75622100	-1.95334100
H	2.10865200	-2.44178500	-0.48849500
H	1.08081700	-1.56252200	-1.62626200
C	3.55955500	-0.00018500	1.17881300
H	3.42079600	-0.88419200	1.79083100
H	4.59526700	-0.00019800	0.83744400
H	3.42087600	0.88371700	1.79100200
Si	2.44709300	0.00000800	-0.30114500

E_0(CASSCF,vacuo) -676.096739

E_0(CASSCF,CPCM) **-676.170187**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0967385684
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609674E+03
(  815) 0.9137564 ( 1665)-0.1365207 ( 4316) 0.1171469 ( 1070)-0.1028990 (  818)-0.0963118 ( 1067) 0.0961621 ( 7235)-0.0753268
( 3320)-0.0724584 ( 2656)-0.0681724 ( 1655)-0.0561548 (  825) 0.0560407 (  159) 0.0551210 ( 2151) 0.0547762 (  249)-0.0539429
(  896)-0.0500122 ( 1907)-0.0484288 (  828)-0.0467751 ( 3811)-0.0450968 ( 7256) 0.0434065 ( 4295)-0.0428419 ( 1651) 0.0412860
(  564)-0.0407623 (  489) 0.0400868 (  135)-0.0399798 ( 6239) 0.0397370 ( 5183)-0.0386893 (  475)-0.0365900 ( 1627)-0.0358261
(  479) 0.0354572 (  811)-0.0353423 (  900)-0.0349721 ( 2175)-0.0344082 ( 6260)-0.0343748 ( 3299) 0.0339604 (  482)-0.0335111
( 1063)-0.0333593 (  793) 0.0330046 (  128) 0.0318793 ( 2144)-0.0316770 ( 3357) 0.0314966 ( 1039)-0.0288529 ( 1124) 0.0274287
( 2685)-0.0267632 ( 4431) 0.0267148 ( 6730) 0.0257027 ( 1155)-0.0256978 (  536)-0.0256665 (  220)-0.0250207 ( 8123)-0.0245521
(  560)-0.0237862 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.999971D+00
     2 -0.137814D-03  0.100029D+01
     3 -0.399214D-05  0.584445D-05  0.189374D+01
     4 -0.166883D-05  0.266428D-05  0.355545D-08  0.106099D+00
     5 -0.560699D-06  0.869455D-06  0.159453D-05  0.166933D-05  0.418806D-01
     6  0.449869D-05 -0.817253D-05  0.317201D-05  0.839976D-05 -0.896370D-06
     7 -0.165186D-05  0.226854D-05 -0.157779D-05 -0.331753D-05 -0.484516D-07
     8  0.279108D-05 -0.475887D-05 -0.208135D-05 -0.539521D-05  0.250317D-06
     9 -0.154932D-05  0.256824D-05 -0.615724D-05 -0.493883D-06  0.831138D-07
                6             7             8             9
     6  0.188971D+01
     7 -0.214824D-06  0.195195D+01
     8 -0.952375D-06  0.177569D-05  0.106760D+00
     9 -0.642088D-06 -0.548113D-06 -0.290974D-06  0.960463D-02
MCSCF converged.
```

$^{3}2^{+}$a STEP 13

GEOMETRY

C	3.71310100	0.00029000	-0.75478700
C	3.17766700	1.23358700	-0.37898900
C	2.03980300	1.23075900	0.40979900
C	1.43557300	-0.00023600	0.82709000
C	2.04006700	-1.23095100	0.40935900
C	3.17793100	-1.23325400	-0.37943000
H	3.63932800	2.15402200	-0.68314500
H	1.60657100	2.16022000	0.73451000
H	1.60703600	-2.16062100	0.73373600
H	3.63978700	-2.15348200	-0.68391500
C	0.26974000	-0.00050100	1.60644200
H	-0.08584900	0.91514900	2.04650500
H	-0.08568700	-0.91638500	2.04614000
C	-2.10183800	-1.59179400	-1.15887000
H	-2.80966900	-1.74659300	-1.97326000
H	-1.10954900	-1.56409900	-1.59695900
H	-2.17327300	-2.44306600	-0.49211500
C	-2.10253600	1.59300600	-1.15713700
H	-2.81048700	1.74839700	-1.97131000
H	-2.17429600	2.44352200	-0.48945200
H	-1.11027000	1.56621600	-1.59533600
C	-3.58724900	-0.00098000	1.19363900
H	-3.43825500	0.88294700	1.80342900
H	-4.62877000	-0.00100700	0.87005100
H	-3.43790600	-0.88550900	1.80246800
Si	-2.50016200	0.00005200	-0.30386000

E_0(CASSCF,vacuo) -676.094968

E_0(CASSCF,CPCM) **-676.169037**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0949674684
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67609497E+03
( 6161) 0.9130025 ( 6414) 0.1083487 ( 1514)-0.0980263 (  366) 0.0795159 ( 6163) 0.0786100 ( 6917) 0.0784889 ( 6919) 0.0763463
(  371) 0.0687933 ( 7764) 0.0649280 ( 6133)-0.0576844 (  701) 0.0576046 ( 6602) 0.0529741 ( 7730) 0.0526878 ( 1548)-0.0526813
(  673)-0.0526683 ( 6419)-0.0505396 ( 5914) 0.0487501 ( 2297) 0.0487253 ( 6136)-0.0471358 ( 1541) 0.0456250 ( 6134)-0.0455405
( 3229) 0.0446272 ( 7904)-0.0442585 ( 1793)-0.0426546 ( 1513)-0.0406727 ( 7759)-0.0406544 ( 9020) 0.0406259 ( 7729)-0.0385339
( 3200)-0.0383169 ( 6889)-0.0377459 (  703) 0.0377348 ( 9039) 0.0366580 ( 9208) 0.0364915 ( 9185) 0.0360006 ( 6184) 0.0358829
(   34)-0.0357731 ( 7931)-0.0344861 ( 7933) 0.0342279 ( 7757)-0.0335179 ( 6168)-0.0334590 (  674)-0.0334368 ( 1564) 0.0334125
( 6924)-0.0334062 ( 7107) 0.0331624 ( 9025)-0.0327724 ( 9158)-0.0325098 ( 7947)-0.0324959 ( 1562)-0.0316361 ( 3224) 0.0298442
(  708) 0.0296408 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.107286D+00
     2  0.297265D-05  0.195186D+01
     3  0.777670D-06  0.563039D-07  0.189344D+01
     4  0.133920D-04  0.771477D-06  0.438583D-05  0.188843D+01
     5  0.803397D-05 -0.826821D-06  0.322547D-04  0.850677D-06  0.100032D+01
     6 -0.175941D-02  0.155053D-05 -0.844102D-06  0.882053D-05  0.541436D-05
     7  0.367930D-06 -0.380900D-06 -0.842755D-06  0.450361D-06 -0.877513D-06
     8  0.629426D-06 -0.123942D-05  0.449530D-05 -0.382559D-06 -0.194975D-06
     9  0.609490D-05  0.357507D-05  0.141027D-04 -0.842587D-05  0.479356D-03
                6             7             8             9
     6  0.107839D+00
     7 -0.116380D-05  0.422314D-01
     8  0.174618D-07  0.136324D-06  0.845167D-02
     9 -0.209997D-05  0.527471D-06  0.454517D-06  0.100014D+01
MCSCF converged.
```

$^{3}2^{+}$a STEP 14

GEOMETRY

C	-3.73646300	-0.00010800	-0.77753700
C	-3.20565200	-1.23323600	-0.39464200
C	-2.07800100	-1.23056600	0.40887100
C	-1.47852500	0.00007700	0.83437200
C	-2.07807200	1.23061800	0.40869900
C	-3.20570800	1.23310000	-0.39484200
H	-3.66330500	-2.15380000	-0.70457900
H	-1.64945100	-2.16030600	0.73915700
H	-1.64952700	2.16043300	0.73877600
H	-3.66337500	2.15359100	-0.70497700
C	-0.32244400	0.00015200	1.62734500
H	0.03363900	-0.91588000	2.06592200
H	0.03363000	0.91626300	2.06576600
C	2.14397200	1.59170300	-1.15415400
H	2.82772400	1.73862900	-1.99024000
H	1.13904600	1.56813700	-1.56346900
H	2.23933800	2.44487900	-0.49298700
C	2.14364100	-1.59127800	-1.15485500
H	2.82731200	-1.73794700	-1.99105100
H	2.23889300	-2.44477300	-0.49408400
H	1.13869400	-1.56734400	-1.56409900
C	3.61967700	-0.00046100	1.20553700
H	3.46226300	-0.88507400	1.81228000
H	4.66564800	-0.00050000	0.89623400
H	3.46244400	0.88391400	1.81267400
Si	2.55303300	-0.00001600	-0.30557700

E_0(CASSCF,vacuo) -676.093385

E_0(CASSCF,CPCM) **-676.168052**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0933849644
Full Convergence on CI vector     -0.67609338E+03
          ( 1)      EIGENVALUE
( 5564) 0.9123231 ( 2459)-0.1122836 ( 5735)-0.0978110 (10578) 0.0889231 ( 5549) 0.0743489 ( 2708)-0.0742458 ( 8525)-0.0737170
( 5787)-0.0720000 ( 2693)-0.0704588 ( 5570)-0.0647622 ( 5816)-0.0646788 ( 2511) 0.0627377 ( 5822) 0.0594940 ( 4135)-0.0592429
( 8562) 0.0549770 (10541)-0.0549762 ( 8756) 0.0489262 ( 5591)-0.0473834 ( 8672) 0.0451790 (10520)-0.0430374 ( 5622)-0.0429639
(10526) 0.0422444 ( 8489)-0.0422393 ( 5684) 0.0418842 ( 9765) 0.0414644 ( 2714) 0.0396876 ( 5801)-0.0396824 ( 2279)-0.0382407
( 5649)-0.0378925 ( 8504)-0.0374962 ( 5585) 0.0374392 ( 2271) 0.0370737 ( 2324)-0.0364995 ( 3968)-0.0364909 ( 3957) 0.0364237
( 5553)-0.0363715 ( 2127) 0.0363112 ( 9819) 0.0361759 ( 9747) 0.0361321 ( 5874) 0.0348030 ( 2729)-0.0347896 ( 9800)-0.0340817
( 5639)-0.0333285 ( 8510)-0.0317376 ( 5487)-0.0316302 (10509) 0.0313452 ( 4371) 0.0312592 (10519)-0.0311032 ( 4026) 0.0305538
( 4391) 0.0304864 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189319D+01
     2  0.526119D-05  0.108762D+00
     3 -0.772846D-06 -0.222713D-05  0.425513D-01
     4 -0.822579D-05 -0.120237D-05 -0.181272D-06  0.737967D-02
     5  0.504657D-05  0.486984D-05  0.295284D-05 -0.427435D-05  0.188733D+01
     6 -0.157939D-04  0.130403D-04  0.283645D-05  0.901409D-06  0.257611D-04
     7  0.190357D-05 -0.104648D-05 -0.269842D-06 -0.207897D-05  0.725629D-06
     8  0.417353D-05  0.286834D-02  0.164297D-05  0.240005D-07 -0.783759D-05
     9 -0.507219D-06 -0.139973D-06  0.491774D-06  0.459209D-07 -0.143335D-05
                6             7             8             9
     6  0.100065D+01
     7  0.614668D-05  0.195178D+01
     8  0.798484D-05 -0.527475D-05  0.108366D+00
     9 -0.197026D-03  0.137295D-05 -0.251531D-06  0.999992D+00
MCSCF converged.
```

$^{3}2^{+}$a STEP 15

GEOMETRY

C	-3.75969400	0.00002400	-0.80070500
C	-3.23365500	-1.23291500	-0.41067500
C	-2.11647000	-1.23033700	0.40754500
C	-1.52193700	-0.00001500	0.84113500
C	-2.11645400	1.23032400	0.40758600
C	-3.23364200	1.23294000	-0.41063500
H	-3.68711400	-2.15361000	-0.72650100
H	-1.69258100	-2.16033200	0.74327800
H	-1.69255500	2.16030400	0.74334700
H	-3.68708900	2.15365200	-0.72643100
C	-0.37552000	-0.00004100	1.64747900
H	-0.01911300	-0.91642000	2.08482500
H	-0.01909600	0.91631600	2.08486100
C	2.18992600	1.59018300	-1.15318300
H	2.83822800	1.71817600	-2.01981700
H	1.16808300	1.57658300	-1.52010600
H	2.32351400	2.44825100	-0.50528700
C	2.18978300	-1.59000300	-1.15344400
H	2.83794700	-1.71783200	-2.02020400
H	2.32344700	-2.44820300	-0.50574000
H	1.16788300	-1.57630700	-1.52020800
C	3.64496800	-0.00016300	1.22316200
H	3.47622000	-0.88492500	1.82673000
H	4.69660400	-0.00016700	0.93348500
H	3.47627000	0.88450000	1.82688700
Si	2.60610900	0.00000200	-0.30633600

E_0(CASSCF,vacuo) -676.091977

E_0(CASSCF,CPCM) **-676.166382**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0919774397
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67609198E+03
( 5564) 0.9116969 ( 2459)-0.1139824 ( 5735)-0.0991991 (10578) 0.0888863 ( 5549) 0.0751402 ( 2708)-0.0750521 ( 8525)-0.0734759
( 5787)-0.0727093 ( 2693)-0.0710053 ( 5570)-0.0654005 ( 5816)-0.0653233 ( 2511) 0.0632067 ( 4135)-0.0599196 ( 5822) 0.0597806
(10541)-0.0552064 ( 8562) 0.0551991 ( 8756) 0.0490822 ( 5591)-0.0475703 ( 8672) 0.0449375 (10520)-0.0434328 ( 5622)-0.0433749
( 8489)-0.0422520 (10526) 0.0422324 ( 5684) 0.0420333 ( 9765) 0.0415449 ( 5801)-0.0401076 ( 2714) 0.0400950 ( 2279)-0.0384771
( 5649)-0.0379052 ( 8504)-0.0377532 ( 5585) 0.0376986 ( 2271) 0.0370342 ( 3968)-0.0369354 ( 5553)-0.0368152 ( 2324)-0.0365599
( 3957) 0.0363731 ( 2127) 0.0362095 ( 9747) 0.0361409 ( 9819) 0.0356750 ( 2729)-0.0348807 ( 5874) 0.0348526 ( 9800)-0.0339577
( 5639)-0.0334537 ( 8510)-0.0319123 ( 5487)-0.0315244 ( 4371) 0.0314981 (10509) 0.0314432 (10519)-0.0307217 ( 4026) 0.0306972
( 4391) 0.0305609 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189294D+01
     2  0.391222D-05  0.109739D+00
     3 -0.451893D-06 -0.952630D-06  0.428456D-01
     4  0.117480D-05  0.577927D-06  0.175185D-07  0.638087D-02
     5  0.555020D-06 -0.125582D-05 -0.324221D-06 -0.182906D-05  0.188635D+01
     6  0.165434D-05 -0.716008D-05 -0.396708D-05  0.649505D-06  0.539174D-05
     7  0.434001D-06  0.201838D-05  0.566392D-06  0.237424D-05  0.825478D-06
     8 -0.984714D-05  0.380086D-02 -0.470416D-06  0.253171D-06 -0.187430D-05
     9  0.320782D-06 -0.124325D-05  0.342592D-06  0.138634D-06 -0.406168D-05
                6             7             8             9
     6  0.100084D+01
     7 -0.105597D-04  0.195170D+01
     8 -0.166821D-05 -0.591948D-06  0.109212D+00
     9 -0.187731D-03  0.770680D-06 -0.814693D-06  0.999991D+00
MCSCF converged.
```

$^{1}2^{+}$b STEP 1

GEOMETRY

C	-3.51797300	-0.05045000	0.50778600
C	-2.91369500	1.16135400	0.03856300
C	-1.63749300	1.12656200	-0.46104900
C	-0.93898800	-0.12207600	-0.66860300
C	-1.63145500	-1.35346000	-0.35173200
C	-2.87742300	-1.22727100	0.18111500
H	-3.40249200	2.10203200	0.20857200
H	-1.13343100	2.03787600	-0.72173300
H	-1.24382900	-2.28914000	-0.70622900
C	0.32562800	-0.15130500	-1.30104600
H	0.55923300	0.69110900	-1.93721100
H	0.61480300	-1.09895100	-1.73292300
C	1.70035600	-1.43375600	1.33686500
H	2.53027900	-1.44720400	2.03975700
H	0.78673400	-1.38687100	1.92077300
H	1.71863100	-2.37996000	0.80478800
C	1.66313600	1.69321600	1.01651400
H	2.49545200	1.86815000	1.69464100
H	1.65671000	2.51248400	0.30406900
H	0.75390500	1.74319200	1.60680100
C	3.39154700	-0.06223200	-0.93128000
H	3.41442800	0.74512300	-1.65626900
H	4.29351200	0.01875500	-0.32875800
H	3.44608700	-1.00345500	-1.46889600
Si	1.89180500	0.03056800	0.18525100
H	-4.35712400	-0.02457800	1.17629600

E_0(CASSCF,vacuo) -676.122923

E_0(CASSCF,CPCM) **-676.193713**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1229225730
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612292E+03
 (     1) 0.8175554 (     3)-0.4371353 (    25) 0.1270226 (   234)-0.1079324 (    45)-0.1056131 (    38) 0.1045562 (    91) 0.0708460
 (   284) 0.0678878 (   276)-0.0656855 (   255)-0.0595913 (   352) 0.0483411 (  1891)-0.0474620 (    52) 0.0455262 (   240) 0.0441880
 (   390)-0.0438014 (   262) 0.0436273 (  1830)-0.0432427 (   239) 0.0417009 (   378) 0.0392216 (   300)-0.0375339 (    36)-0.0363242
 (  1828)-0.0352714 (  1856)-0.0344108 (   121) 0.0337306 (    30)-0.0337114 (  1721) 0.0333026 (  1836)-0.0326286 (  1601)-0.0325994
 (    28)-0.0325914 (   309)-0.0325105 (  1827)-0.0302903 (    49)-0.0300986 (   364)-0.0280433 (   286)-0.0277519 (   278) 0.0275050
 (    55)-0.0273816 (   235) 0.0270070 (   256) 0.0267309 (   260) 0.0260089 (  2145) 0.0254938 (   244)-0.0254345 (   298)-0.0248199
 (  1710)-0.0243548 (   821) 0.0242604 (    10)-0.0240228 (  2080) 0.0235035 (   406) 0.0229723 (   719)-0.0229217 (    78) 0.0225891
 (    79)-0.0224664 (
 Final one electron symbolic density matrix:
                   1                 2                 3                 4                 5
      1  0.196292D+01
      2  0.365534D-05  0.192608D+01
      3  0.146972D-06  0.598762D-06  0.188689D+01
      4  0.613351D-05 -0.502778D-05  0.663284D-05  0.151309D+01
      5 -0.111499D-04  0.125090D-04 -0.299231D-05  0.260355D-04  0.493410D+00
      6 -0.619674D-05  0.332619D-05 -0.167494D-05 -0.150228D-06  0.187135D-05
      7  0.179249D-05 -0.638754D-06 -0.105274D-05 -0.129155D-04 -0.976997D-05
      8 -0.709218D-05  0.343025D-05  0.520234D-06 -0.192949D-05  0.112572D-06
      9 -0.396430D-05  0.705093D-06 -0.568613D-06  0.188892D-05  0.125829D-05
                   6                 7                 8                 9
      6  0.680391D-01
      7 -0.439400D-06  0.103967D+00
      8  0.257828D-05 -0.463645D-06  0.299266D-01
      9 -0.344282D-06 -0.535492D-07  0.289832D-06  0.156741D-01
 MCSCF converged.
```

$^{1}2^{+}$b STEP 2

GEOMETRY

C	-3.52743100	-0.05964400	0.51903800
C	-2.92364700	1.15406800	0.07895100
C	-1.66349200	1.13546900	-0.46844800
C	-0.96673900	-0.10580400	-0.70796900
C	-1.63876300	-1.33928900	-0.37040000
C	-2.87501400	-1.24335800	0.20372700
H	-3.41721600	2.09008300	0.26093300
H	-1.17752400	2.05375400	-0.73995100
H	-1.22533900	-2.27881400	-0.68456500
C	0.28836500	-0.12400700	-1.34179300
H	0.55596200	0.74132000	-1.93034400
H	0.60684800	-1.06279800	-1.77016700
C	1.72037300	-1.47123800	1.30342600
H	2.54423700	-1.51200400	2.01306200
H	0.80108500	-1.43737100	1.87831500
H	1.74018400	-2.39721000	0.73772800
C	1.66939100	1.67470600	1.05817000
H	2.49202100	1.85097300	1.74833800
H	1.65940700	2.50226500	0.35608400
H	0.75234000	1.70013700	1.63693600
C	3.39569500	-0.03458700	-0.95029000
H	3.39954200	0.79124100	-1.65401900
H	4.31275700	0.03219000	-0.36837000
H	3.43614500	-0.96278200	-1.51066700
Si	1.93271800	0.02994800	0.21089200
H	-4.41092400	-0.04815200	1.12773000

E_0(CASSCF,vacuo) -676.121207

E_0(CASSCF,CPCM) **-676.191632**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1212070893
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612121E+03
 (     1) 0.7660206 (     3)-0.5125833 (    25) 0.1391981 (   234)-0.1185065 (    45)-0.1046652 (    38) 0.0986554 (    91) 0.0820284
 (   284) 0.0665054 (   276)-0.0657642 (   255)-0.0616167 (   352) 0.0568898 (   390)-0.0503316 ( 1601)-0.0475578 (   378) 0.0471207
 ( 1721) 0.0419101 (    52) 0.0418647 (    79)-0.0405428 ( 1830)-0.0390760 ( 1856)-0.0354507 (   262) 0.0339422 (   240) 0.0334559
 (   821) 0.0325632 ( 1828)-0.0321374 ( 1891)-0.0320353 (   121) 0.0319014 (    36)-0.0313087 (   239) 0.0312372 ( 1836)-0.0311014
 ( 1678)-0.0306616 (   309)-0.0305557 (   300)-0.0304446 ( 1967)-0.0302631 ( 1605)-0.0268981 ( 2080) 0.0267419 (   256) 0.0263887
 (    55)-0.0262085 (   364)-0.0259444 (    49)-0.0249265 (   244)-0.0248426 ( 2017) 0.0248132 (   719)-0.0246628 (    30)-0.0244451
 ( 1083)-0.0243872 (   122) 0.0241443 ( 1711)-0.0240599 ( 2110) 0.0239812 (    98)-0.0239541 ( 1621)-0.0237655 ( 1710)-0.0237395
 (    28)-0.0235680 (
 Final one electron symbolic density matrix:
                 1             2             3             4             5
     1  0.195713D+01
     2  0.338599D-05  0.192105D+01
     3  0.366604D-06 -0.139739D-06  0.188211D+01
     4  0.231775D-05 -0.263722D-06  0.965403D-05  0.134989D+01
     5 -0.305372D-05  0.976481D-05 -0.471692D-07  0.166237D-04  0.655367D+00
     6 -0.407280D-05  0.339330D-05 -0.116165D-05 -0.152331D-05  0.198045D-06
     7  0.249475D-06  0.147027D-06 -0.198818D-05 -0.153141D-04 -0.138721D-04
     8 -0.407356D-05  0.110043D-06 -0.630778D-06 -0.279266D-05 -0.222973D-05
     9 -0.506197D-05 -0.893939D-06 -0.402201D-06  0.115617D-05  0.819889D-06
                 6             7             8             9
     6  0.737415D-01
     7  0.155096D-06  0.111031D+00
     8  0.210172D-05  0.161248D-06  0.342250D-01
     9 -0.553908D-07  0.119081D-06  0.670190D-08  0.154469D-01
 MCSCF converged.
```

$^{1}2^{+}$b STEP 3

GEOMETRY

C	-3.54031000	-0.06784600	0.53166100
C	-2.93746500	1.14775400	0.11544100
C	-1.69224100	1.14005100	-0.47322700
C	-0.99931400	-0.09446500	-0.74028500
C	-1.64980600	-1.32929500	-0.38201600
C	-2.87632800	-1.25184000	0.22224600
H	-3.43392600	2.08026400	0.30764100
H	-1.22251800	2.06353700	-0.75649000
H	-1.21285900	-2.26982800	-0.66044300
C	0.24942300	-0.10233500	-1.38094100
H	0.53970500	0.77977000	-1.93104800
H	0.58837000	-1.03341600	-1.80861400
C	1.74390500	-1.50054500	1.27397100
H	2.55991300	-1.56416800	1.99158800
H	0.81793700	-1.47725700	1.83790300
H	1.76747200	-2.40883200	0.68102400
C	1.67913100	1.65870200	1.09081400
H	2.49042500	1.83729500	1.79426900
H	1.66758200	2.49279800	0.39706100
H	0.75375400	1.66273500	1.65611600
C	3.40673700	-0.00963700	-0.96616500
H	3.39332500	0.83118800	-1.65137900
H	4.33704400	0.04616300	-0.40369100
H	3.43440400	-0.92655500	-1.54509900
Si	1.97650000	0.02941200	0.23201900
H	-4.45402700	-0.06872700	1.09391400

E_0(CASSCF,vacuo) -676.118996

E_0(CASSCF,CPCM) **-676.188314**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1189959448
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611900E+03
 (     1) 0.7207504 (     3)-0.5685614 (    25) 0.1440997 (   234)-0.1255791 (    45)-0.1029710 (    38) 0.0900676 (    91) 0.0894664
 (   276)-0.0657669 (   284) 0.0653763 (   255)-0.0633322 (   352) 0.0622470 (  1601)-0.0563829 (   390)-0.0554228 (    79)-0.0540324
 (   378) 0.0539132 (  1721) 0.0472012 (  1967)-0.0391042 (   821) 0.0385274 (  1678)-0.0375757 (    52) 0.0373456 (  1830)-0.0338793
 (  1083)-0.0323273 (  1856)-0.0314054 (  1920) 0.0305464 (   121) 0.0305220 (  1779) 0.0297403 (  1605)-0.0286369 (  2017) 0.0281931
 (  1772)-0.0281898 (    36)-0.0278892 (  1836)-0.0276465 (  2080) 0.0273242 (   309)-0.0270438 (   122) 0.0269872 (   262) 0.0268489
 (   331)-0.0265387 (  1711)-0.0264923 (    98)-0.0259419 (   719)-0.0256658 (   256) 0.0255895 (  1828)-0.0255564 (  1793)-0.0255291
 (   240) 0.0254026 (    55)-0.0253314 (  2110) 0.0250076 (   300)-0.0249824 (  2029)-0.0244186 (    32)-0.0237386 (  1718)-0.0236166
 (   351)-0.0233117 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195444D+01
     2 -0.191795D-05  0.191600D+01
     3 -0.163143D-05 -0.671544D-06  0.187936D+01
     4  0.355749D-05  0.135381D-05  0.985247D-05  0.121247D+01
     5 -0.640999D-05  0.132638D-04 -0.187323D-05  0.619936D-05  0.790806D+00
     6 -0.240158D-05  0.258409D-05 -0.140148D-05 -0.752351D-05 -0.273854D-05
     7  0.186114D-05  0.719640D-07  0.141330D-06 -0.100633D-04 -0.969162D-05
     8 -0.123983D-05  0.441896D-05  0.502173D-06 -0.308420D-05 -0.789859D-06
     9 -0.118754D-05 -0.111454D-05  0.143390D-06  0.239775D-05  0.116132D-05
                6             7             8             9
     6  0.793410D-01
     7  0.607618D-06  0.115315D+00
     8 -0.153166D-05 -0.160638D-05  0.371220D-01
     9  0.119339D-06  0.122272D-06 -0.279099D-06  0.151460D-01
 MCSCF converged.
```

$^{1}2^{+}$b STEP 4

GEOMETRY

C	3.55512600	-0.07007400	-0.55079600
C	2.95583000	1.14502000	-0.13872500
C	1.72243500	1.14021300	0.47951900
C	1.03421400	-0.09111200	0.76178500
C	1.67115900	-1.32492500	0.38685000
C	2.88791000	-1.25327100	-0.24070500
H	3.45164800	2.07666100	-0.33710100
H	1.26335600	2.06562300	0.77458100
H	1.22529100	-2.26594300	0.64994300
C	-0.20757400	-0.09490800	1.41455800
H	-0.51153200	0.79486100	1.94318600
H	-0.56011600	-1.02288900	1.83634000
C	-1.77310800	-1.51536600	-1.25935200
H	-2.57969300	-1.59351900	-1.98662100
H	-0.83969500	-1.49671300	-1.81066400
H	-1.80178500	-2.41249300	-0.65031200
C	-1.69925800	1.65216400	-1.10631900
H	-2.49837900	1.83557300	-1.82285000
H	-1.69044000	2.48724500	-0.41412400
H	-0.76526300	1.64381100	-1.65686100
C	-3.42066900	0.00326200	0.98475800
H	-3.38921000	0.85105400	1.66042000
H	-4.36494600	0.05424000	0.44492200
H	-3.43352200	-0.90860000	1.57179200
Si	-2.02426000	0.03004000	-0.24953100
H	4.47753400	-0.07549400	-1.09865900

E_0(CASSCF,vacuo) -676.116460

E_0(CASSCF,CPCM) **-676.185961**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1164603751
 Full Convergence on CI vector
          ( 1)        EIGENVALUE     -0.67611646E+03
 (     1) 0.6972623 (     3)-0.5935388 (    25) 0.1451195 (   234)-0.1295133 (    45)-0.1018499 (    91) 0.0927097 (    38) 0.0850902
 (   276)-0.0668846 (   284) 0.0656125 (   352) 0.0648931 (   255)-0.0646185 (  1601)-0.0608480 (    79)-0.0600261 (   390)-0.0585641
 (   378) 0.0583387 (  1721) 0.0502041 (  1967)-0.0442628 (   821) 0.0424065 (  1678)-0.0415636 (  1083)-0.0375605 (  1920) 0.0360481
 (    52) 0.0337977 (  1779) 0.0333126 (  1830)-0.0310855 (  1772)-0.0307056 (  2017) 0.0301418 (   121) 0.0293690 (  2029)-0.0292066
 (  1793)-0.0290670 (   331)-0.0287243 (  1605)-0.0283206 (   122) 0.0276208 (  1711)-0.0273731 (  1856)-0.0272443 (  2080) 0.0269920
 (   719)-0.0261815 (    36)-0.0260750 (    98)-0.0258415 (  1836)-0.0250112 (  2043) 0.0248332 (   256) 0.0247583 (    55)-0.0246961
 (   351)-0.0244896 (    32)-0.0240379 (   309)-0.0237268 (   441)-0.0234673 (  2110) 0.0234089 (   705) 0.0232138 (   262) 0.0232056
 (  1953) 0.0231522 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195320D+01
     2  0.184643D-05  0.191174D+01
     3  0.204615D-05  0.484579D-05  0.187804D+01
     4  0.435478D-05 -0.257938D-05  0.746104D-05  0.114512D+01
     5  0.267529D-05  0.860745D-05 -0.184421D-04  0.564474D-06  0.856833D+00
     6  0.347612D-05 -0.562473D-05  0.313683D-05 -0.226176D-04  0.122649D-04
     7 -0.255063D-05  0.217736D-05  0.135644D-05  0.891043D-05 -0.556528D-05
     8 -0.380875D-05 -0.120146D-05  0.192847D-05 -0.104382D-04  0.569378D-05
     9  0.728692D-06 -0.412336D-06 -0.235867D-05 -0.191881D-04  0.108893D-04
                6             7             8             9
     6  0.838412D-01
     7 -0.387350D-05  0.117490D+00
     8 -0.135137D-05  0.246475D-05  0.388275D-01
     9  0.127049D-05  0.130741D-06  0.216134D-05  0.149055D-01
 MCSCF converged.
```

$^{1}2^{+}$b STEP 5

GEOMETRY

C	3.57175800	-0.06915200	-0.57273700
C	2.97656700	1.14422100	-0.15644000
C	1.75338500	1.13874800	0.48537100
C	1.07054300	-0.09128800	0.77768200
C	1.69857200	-1.32296500	0.38876500
C	2.90581900	-1.25220000	-0.25900200
H	3.46981700	2.07625600	-0.35971700
H	1.30171100	2.06458300	0.79106300
H	1.25103300	-2.26487800	0.64647700
C	-0.16365900	-0.09464200	1.44507900
H	-0.47685700	0.79853000	1.96130300
H	-0.52486600	-1.02192700	1.85967800
C	-1.80421100	-1.52171700	-1.25391800
H	-2.60483100	-1.61300000	-1.98668000
H	-0.86652100	-1.50049300	-1.79757800
H	-1.83128400	-2.41179600	-0.63489700
C	-1.72576000	1.65194300	-1.10923700
H	-2.51722200	1.84712600	-1.83154800
H	-1.71365600	2.48264400	-0.41214100
H	-0.78725200	1.63457900	-1.65161300
C	-3.43844600	0.00712700	1.00240200
H	-3.39029700	0.85724400	1.67392100
H	-4.39545300	0.05641300	0.48473900
H	-3.43626600	-0.90343900	1.59131200
Si	-2.07426600	0.03093700	-0.26440100
H	4.49425700	-0.07540500	-1.12049300

E_0(CASSCF,vacuo) -676.113744

E_0(CASSCF,CPCM) **-676.183501**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1137434577
 Full Convergence on CI vector
          ( 1)        EIGENVALUE     -0.67611374E+03
 (    1) 0.6848873 (    3)-0.6053320 (   25) 0.1451748 (  234)-0.1320032 (   45)-0.1011987 (   91) 0.0942604 (   38) 0.0823684
 (  276)-0.0683676 (  284) 0.0664927 (  352) 0.0664302 (  255)-0.0655676 ( 1601)-0.0633205 (   79)-0.0627987 (  378) 0.0614785
 (  390)-0.0608661 ( 1721) 0.0520771 ( 1967)-0.0473369 (  821) 0.0452175 ( 1678)-0.0442021 ( 1083)-0.0411491 ( 1920) 0.0396007
 ( 1779) 0.0354827 ( 2029)-0.0321186 ( 1772)-0.0320251 ( 1793)-0.0313232 ( 2017) 0.0312935 (   52) 0.0309807 (  331)-0.0297349
 ( 1830)-0.0295724 (  121) 0.0283589 ( 2043) 0.0277356 ( 1711)-0.0276948 (  122) 0.0274558 ( 1605)-0.0273875 ( 2080) 0.0266122
 (  719)-0.0265211 (  441)-0.0254666 (   36)-0.0249890 (   98)-0.0248633 (  351)-0.0243043 ( 1953) 0.0242929 (   55)-0.0241862
 (  256) 0.0240539 (   32)-0.0239598 ( 1856)-0.0236826 (  705) 0.0236591 (  704)-0.0231665 ( 1619)-0.0230988 ( 1836)-0.0229342
 ( 1770)-0.0228324 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195259D+01
     2 -0.148008D-05  0.190825D+01
     3  0.247503D-06 -0.960194D-06  0.187724D+01
     4 -0.689820D-06  0.761938D-05 -0.109634D-04  0.111122D+01
     5  0.178697D-05 -0.264751D-04  0.587418D-05  0.313470D-06  0.889880D+00
     6  0.947143D-06 -0.908867D-05  0.710039D-05  0.110618D-04 -0.449642D-05
     7 -0.520535D-05  0.227471D-05  0.681793D-05 -0.626779D-06  0.665805D-05
     8  0.815939D-06  0.742144D-06  0.160396D-05 -0.294627D-06  0.135465D-05
     9 -0.663923D-05  0.381262D-05  0.144660D-05 -0.253557D-05  0.262727D-05
                6             7             8             9
     6  0.874507D-01
     7  0.993693D-06  0.118879D+00
     8 -0.166473D-05  0.315991D-06  0.399145D-01
     9 -0.501975D-06  0.407197D-06 -0.894683D-07  0.145712D-01
 MCSCF converged.
```

$^{1}2^{+}$b STEP 6

GEOMETRY

C	3.58898200	-0.06638100	-0.59640600
C	2.99854300	1.14456800	-0.17090800
C	1.78540100	1.13667100	0.49224600
C	1.10785500	-0.09315400	0.79152500
C	1.72853700	-1.32210700	0.38800700
C	2.92599500	-1.24996700	-0.27900500
H	3.48864300	2.07757200	-0.37773200
H	1.34011800	2.06202900	0.80915300
H	1.28203200	-2.26531800	0.64337600
C	-0.11841000	-0.09795300	1.47423700
H	-0.43795800	0.79646200	1.98343200
H	-0.48589700	-1.02570800	1.88106700
C	-1.83868600	-1.52546200	-1.25040400
H	-2.62522000	-1.62076800	-1.99809100
H	-0.89076300	-1.50640300	-1.77606300
H	-1.87757200	-2.41095300	-0.62575700
C	-1.75590400	1.65183600	-1.11160000
H	-2.53369600	1.85180600	-1.84767100
H	-1.75174300	2.48045000	-0.41220500
H	-0.80817400	1.62950200	-1.63746000
C	-3.45561200	0.01035900	1.02224900
H	-3.39133800	0.86243100	1.68971000
H	-4.42525300	0.05799100	0.52779800
H	-3.43822300	-0.89941300	1.61189300
Si	-2.12522800	0.03224400	-0.27722200
H	4.50803800	-0.07156900	-1.14998600

E_0(CASSCF,vacuo) -676.110974

E_0(CASSCF,CPCM) **-676.181060**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1109742533
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67611097E+03
( 2485) 0.6773406 ( 2211)-0.6119365 ( 2414)-0.1451288 ( 5945) 0.1338533 ( 2556)-0.1007359 ( 2278) 0.0951056 ( 2551) 0.0807460
( 5050)-0.0697573 ( 4630)-0.0674922 ( 6166) 0.0674902 ( 5016) 0.0663604 ( 3979) 0.0648706 ( 2482)-0.0643847 ( 4656) 0.0638566
( 5836)-0.0626987 ( 4160) 0.0532493 ( 3890)-0.0492700 ( 5120) 0.0472476 ( 5645)-0.0460555 ( 4722)-0.0436868 ( 5227) 0.0420574
( 3726)-0.0368136 ( 3388) 0.0339468 ( 5036)-0.0328837 ( 3721) 0.0328253 ( 3391)-0.0320462 (  599)-0.0297974 ( 4642) 0.0297372
( 3741)-0.0286809 ( 2343) 0.0286329 ( 3240)-0.0277694 ( 2475) 0.0274659 ( 2205)-0.0270351 ( 6055)-0.0267928 ( 3403) 0.0263435
( 3987) 0.0262526 (  469) 0.0262126 ( 2926) 0.0248884 ( 1891)-0.0242375 ( 6061)-0.0239604 ( 4186)-0.0238266 ( 2145)-0.0237176
( 2407) 0.0236522 ( 2340)-0.0236416 (  630)-0.0233742 ( 5009)-0.0233095 ( 6065)-0.0232656 ( 5039)-0.0224565 ( 2404) 0.0223303
( 1711) 0.0221492 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.140968D-01
     2 -0.179676D-05  0.190541D+01
     3 -0.166260D-05  0.127724D-05  0.195227D+01
     4 -0.334789D-06  0.685994D-06 -0.591078D-05  0.903881D-01
     5  0.501083D-06 -0.647054D-05  0.596820D-06  0.122443D-05  0.406627D-01
     6  0.123906D-04  0.240309D-04 -0.411888D-05 -0.767988D-05  0.538964D-06
     7 -0.355615D-05  0.120449D-05  0.314728D-06 -0.627635D-05 -0.346817D-05
     8 -0.701021D-07 -0.589928D-05  0.437351D-05  0.109932D-05 -0.798201D-07
     9 -0.146816D-04 -0.157386D-04  0.483124D-05  0.757709D-05 -0.222118D-05
                6             7             8             9
     6  0.909279D+00
     7 -0.171073D-04  0.187665D+01
     8 -0.644661D-05  0.514184D-06  0.119927D+00
     9  0.535900D-06  0.230934D-05  0.592498D-05  0.109131D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 7

GEOMETRY

C	3.60676300	-0.06334300	-0.62049100
C	3.02097200	1.14516800	-0.18495300
C	1.81781700	1.13438100	0.49805400
C	1.14581400	-0.09570900	0.80417200
C	1.76017400	-1.32193300	0.38691100
C	2.94776400	-1.24770900	-0.29841100
H	3.50746300	2.07930700	-0.39553900
H	1.37820900	2.05899400	0.82537500
H	1.31617500	-2.26647600	0.64225300
C	-0.07225000	-0.10245000	1.50231500
H	-0.39602800	0.79262800	2.00697000
H	-0.44394500	-1.03079100	1.90310600
C	-1.88035800	-1.53293200	-1.24091900
H	-2.65499700	-1.63354600	-2.00049500
H	-0.92398700	-1.52019700	-1.75128400
H	-1.93119900	-2.41148500	-0.60761100
C	-1.77963200	1.64749000	-1.11759000
H	-2.54245200	1.85413800	-1.86758700
H	-1.77893300	2.47614300	-0.41842900
H	-0.82314200	1.61375000	-1.62682400
C	-3.47607000	0.02302700	1.03969900
H	-3.39289400	0.87821500	1.70091800
H	-4.45665600	0.07224900	0.56695300
H	-3.44830900	-0.88452200	1.63221900
Si	-2.17685400	0.03375200	-0.28858400
H	4.52068300	-0.06687300	-1.18257400

E_0(CASSCF,vacuo) -676.108249

E_0(CASSCF,CPCM) **-676.178750**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1082491921
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67610825E+03
( 2485) 0.6722516 ( 2211)-0.6160437 ( 2414)-0.1452245 ( 5945) 0.1354429 ( 2556)-0.1003487 ( 2278) 0.0955855 ( 2551) 0.0797600
( 5050)-0.0709592 ( 6166) 0.0684254 ( 4630)-0.0683532 ( 5016) 0.0670897 ( 3979) 0.0660071 ( 4656) 0.0657166 ( 2482)-0.0654646
( 5836)-0.0641858 ( 4160) 0.0540023 ( 3890)-0.0505465 ( 5120) 0.0487278 ( 5645)-0.0474369 ( 4722)-0.0455273 ( 5227) 0.0438634
( 3726)-0.0376560 ( 3388) 0.0351432 ( 5036)-0.0340445 ( 3721) 0.0333978 ( 3391)-0.0326093 ( 4642) 0.0312137 (  599)-0.0290987
( 3741)-0.0281011 ( 3240)-0.0277443 ( 6055)-0.0270363 ( 2475) 0.0266812 ( 2343) 0.0266158 ( 2205)-0.0265511 ( 3403) 0.0261516
(  469) 0.0260397 ( 2926) 0.0252192 ( 3987) 0.0250900 ( 4186)-0.0244767 ( 6061)-0.0241932 ( 1891)-0.0236722 ( 6065)-0.0233753
( 2145)-0.0232824 ( 2407) 0.0232148 ( 3916) 0.0225527 ( 5009)-0.0224665 ( 2340)-0.0223681 ( 2404) 0.0221010 (  630)-0.0220315
( 1711) 0.0218667 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.134504D-01
     2  0.197901D-05  0.190308D+01
     3 -0.969225D-06 -0.167233D-05  0.195209D+01
     4  0.643329D-06  0.255062D-05 -0.954035D-06  0.928556D-01
     5 -0.204663D-06  0.724431D-06  0.184363D-05 -0.192431D-05  0.412309D-01
     6  0.102076D-04  0.113510D-04 -0.517223D-06 -0.363641D-05 -0.107849D-04
     7 -0.147530D-05 -0.526922D-06 -0.128648D-05 -0.354050D-05 -0.119041D-05
     8  0.436756D-06  0.253114D-05 -0.241079D-05 -0.711249D-06  0.155722D-05
     9  0.396250D-05 -0.588908D-05  0.736285D-05  0.214208D-05 -0.765566D-05
                6             7             8             9
     6  0.921946D+00
     7 -0.101663D-04  0.187616D+01
     8 -0.146547D-06  0.150596D-06  0.120803D+00
     9  0.102761D-05  0.171461D-05  0.492863D-05  0.107838D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 8

GEOMETRY

C	3.62512600	-0.05912100	-0.64547100
C	3.04485800	1.14654800	-0.19703700
C	1.85189800	1.13208400	0.50496400
C	1.18471900	-0.09871600	0.81564400
C	1.79288300	-1.32193900	0.38339800
C	2.97030800	-1.24464300	-0.31980500
H	3.52790500	2.08202700	-0.40998900
H	1.41803400	2.05547600	0.84362700
H	1.35200600	-2.26805600	0.63877400
C	-0.02473600	-0.10846800	1.52924100
H	-0.35118900	0.78585700	2.03288900
H	-0.39963100	-1.03827800	1.92286400
C	-1.90666700	-1.52469600	-1.25032100
H	-2.67188800	-1.63171400	-2.01878900
H	-0.94501900	-1.49911000	-1.75028000
H	-1.95454000	-2.40487400	-0.61923500
C	-1.82289600	1.65737100	-1.10286800
H	-2.57608400	1.87241200	-1.86047500
H	-1.83116100	2.47740700	-0.39384000
H	-0.86003000	1.62865100	-1.60033000
C	-3.49770900	0.00575100	1.05623000
H	-3.40536700	0.85669400	1.72158800
H	-4.48867500	0.05237800	0.60478500
H	-3.45131400	-0.90652700	1.64013300
Si	-2.22874500	0.03520000	-0.29840800
H	4.53266900	-0.06015700	-1.21784700

E_0(CASSCF,vacuo) -676.105639

E_0(CASSCF,CPCM) **-676.176632**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1056393237
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610564E+03
( 2485) 0.6687501 ( 2211)-0.6185376 ( 2414)-0.1455420 ( 5945) 0.1370616 ( 2556)-0.1000272 ( 2278) 0.0958358 ( 2551) 0.0792482
( 5050)-0.0719818 ( 6166) 0.0692530 ( 4630)-0.0691861 ( 5016) 0.0678747 ( 4656) 0.0671768 ( 3979) 0.0669900 ( 2482)-0.0662937
( 5836)-0.0653771 ( 4160) 0.0545022 ( 3890)-0.0514004 ( 5120) 0.0498011 ( 5645)-0.0485049 ( 4722)-0.0468469 ( 5227) 0.0452194
( 3726)-0.0382022 ( 3388) 0.0359345 ( 5036)-0.0349460 ( 3721) 0.0338899 ( 3391)-0.0331002 ( 4642) 0.0323298 (  599)-0.0278305
( 3741)-0.0277102 ( 3240)-0.0276778 ( 6055)-0.0272874 ( 2205)-0.0260858 ( 3403) 0.0260077 ( 2475) 0.0259938 ( 2926) 0.0253909
(  469) 0.0251884 ( 4186)-0.0249156 ( 2343) 0.0248978 ( 6061)-0.0243917 ( 3987) 0.0240044 ( 6065)-0.0235016 ( 1891)-0.0232254
( 3916) 0.0231585 ( 2145)-0.0228948 ( 2407) 0.0227072 ( 2337) 0.0219603 ( 5921)-0.0218370 ( 2404) 0.0217466 ( 1711) 0.0216057
( 5009)-0.0214974 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.126436D-01
     2  0.515163D-05  0.190113D+01
     3 -0.686067D-05  0.306453D-05  0.195197D+01
     4  0.626402D-06  0.203875D-05 -0.867138D-07  0.950058D-01
     5  0.167830D-06  0.244441D-05  0.224318D-06  0.431981D-05  0.417056D-01
     6  0.114131D-04  0.354502D-05 -0.921892D-05 -0.154441D-05  0.654524D-05
     7 -0.585526D-05 -0.530994D-06  0.275864D-06 -0.151234D-05 -0.182133D-05
     8 -0.481220D-06 -0.603496D-08 -0.698994D-06 -0.380854D-06 -0.255792D-06
     9 -0.165550D-04 -0.748175D-05 -0.278020D-05 -0.776410D-05  0.201913D-05
                6             7             8             9
     6  0.930266D+00
     7  0.653782D-05  0.187571D+01
     8 -0.137933D-04 -0.228283D-05  0.121598D+00
     9  0.246632D-06  0.144618D-04 -0.107906D-04  0.106997D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 9

GEOMETRY

C	3.64400400	-0.05496100	-0.67039000
C	3.06927600	1.14795400	-0.20914700
C	1.88657900	1.12979100	0.51099300
C	1.22425300	-0.10190900	0.82640700
C	1.82637300	-1.32220200	0.37947500
C	2.99359000	-1.24170100	-0.34090600
H	3.54887800	2.08474900	-0.42447900
H	1.45830100	2.05187500	0.86051700
H	1.38909900	-2.26985300	0.63576600
C	0.02369600	-0.11474800	1.55531500
H	-0.30431100	0.77877700	2.05891900
H	-0.35341300	-1.04592400	1.94300300
C	-1.94344700	-1.52331500	-1.25028300
H	-2.69423300	-1.63097800	-2.03295500
H	-0.97283500	-1.49699700	-1.73281700
H	-2.00227600	-2.40251500	-0.61893100
C	-1.85861700	1.65939600	-1.09829000
H	-2.59677800	1.87819700	-1.86966800
H	-1.87762600	2.47704000	-0.38686800
H	-0.88675400	1.62861800	-1.57806700
C	-3.51983100	0.00370300	1.07335900
H	-3.41314900	0.85352300	1.73795200
H	-4.52044900	0.05099300	0.64332200
H	-3.46024400	-0.91020700	1.65343300
Si	-2.28100900	0.03671600	-0.30676700
H	4.54466000	-0.05336300	-1.25358300

E_0(CASSCF,vacuo) -676.103191

E_0(CASSCF,CPCM) **-676.174732**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1031905674
 Full Convergence on CI vector      -0.67610319E+03
          ( 1)        EIGENVALUE
 ( 2485) 0.6660956 ( 2211)-0.6202139 ( 2414)-0.1460562 ( 5945) 0.1387275 ( 2556)-0.0997205 ( 2278) 0.0959548 ( 2551) 0.0790312
 ( 5050)-0.0728434 ( 4630)-0.0700250 ( 6166) 0.0699755 ( 5016) 0.0687008 ( 4656) 0.0683612 ( 3979) 0.0678830 ( 2482)-0.0670243
 ( 5836)-0.0663682 ( 4160) 0.0548441 ( 3890)-0.0520066 ( 5120) 0.0505952 ( 5645)-0.0493517 ( 4722)-0.0478287 ( 5227) 0.0462834
 ( 3726)-0.0385695 ( 3388) 0.0364871 ( 5036)-0.0356613 ( 3721) 0.0343353 ( 3391)-0.0335477 ( 4642) 0.0332079 ( 3240)-0.0275928
 ( 6055)-0.0275436 ( 3741)-0.0274262 (  599)-0.0261645 ( 3403) 0.0258990 ( 2205)-0.0256645 ( 2926) 0.0254819 ( 2475) 0.0253924
 ( 4186)-0.0252159 ( 6061)-0.0245653 (  469) 0.0238820 ( 6065)-0.0236384 ( 3916) 0.0235861 ( 2343) 0.0233993 ( 2337) 0.0230700
 ( 3987) 0.0229925 ( 1891)-0.0228691 ( 2145)-0.0225568 ( 2407) 0.0221685 ( 5921)-0.0217401 ( 1711) 0.0213851 ( 2404) 0.0213389
 ( 1953) 0.0210415 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.117030D-01
     2 -0.747149D-05  0.189949D+01
     3  0.204787D-05  0.786863D-06  0.195188D+01
     4  0.930825D-06 -0.285737D-05 -0.199593D-05  0.969289D-01
     5  0.454599D-06 -0.373872D-05  0.543253D-06  0.101043D-05  0.421238D-01
     6  0.106366D-04 -0.897539D-05  0.431340D-06 -0.948991D-06  0.847662D-06
     7 -0.215218D-05  0.161740D-05 -0.583040D-06 -0.237648D-05 -0.196797D-05
     8  0.153204D-06 -0.635459D-05  0.524416D-05  0.146847D-05  0.523382D-06
     9 -0.114960D-04  0.359989D-05 -0.457924D-06 -0.294157D-05 -0.309191D-05
                6             7             8             9
     6  0.936336D+00
     7 -0.102695D-04  0.187528D+01
     8 -0.243280D-05  0.350411D-06  0.122334D+00
     9  0.558386D-06 -0.578632D-06  0.154695D-05  0.106393D+01
 MCSCF converged.
```

$^{1}2^{+}$b STEP 10

GEOMETRY

C	3.66304700	-0.05034700	-0.69574500
C	3.09422900	1.14962300	-0.22076400
C	1.92215500	1.12736700	0.51721500
C	1.26466400	-0.10552700	0.83678100
C	1.86077800	-1.32273500	0.37483200
C	3.01732200	-1.23853500	-0.36271800
H	3.57020200	2.08784000	-0.43831100
H	1.49941100	2.04789700	0.87770800
H	1.42724600	-2.27200600	0.63184400
C	0.07319600	-0.12196400	1.58067200
H	-0.25555500	0.77028700	2.08567900
H	-0.30527900	-1.05475600	1.96266300
C	-1.97930500	-1.51878900	-1.25372500
H	-2.71520200	-1.62528500	-2.05068500
H	-1.00006300	-1.48951600	-1.71868000
H	-2.04820800	-2.39910100	-0.62509200
C	-1.89757400	1.66374400	-1.08943300
H	-2.62076500	1.88673800	-1.87377200
H	-1.92840000	2.47768100	-0.37430600
H	-0.91700700	1.63331000	-1.55156900
C	-3.54350400	-0.00317600	1.08944400
H	-3.42450800	0.84413400	1.75514100
H	-4.55286000	0.04424700	0.67997000
H	-3.47026100	-0.91988000	1.66350400
Si	-2.33319900	0.03829500	-0.31376700
H	4.55598900	-0.04568200	-1.29070200

E_0(CASSCF,vacuo) -676.100929

E_0(CASSCF,CPCM) **-676.173054**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1009286639
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610093E+03
( 2485) 0.6640481 ( 2211)-0.6213165 ( 2414)-0.1467359 ( 5945) 0.1404316 ( 2556)-0.0994281 ( 2278) 0.0959803 ( 2551) 0.0790358
( 5050)-0.0735701 ( 4630)-0.0708733 ( 6166) 0.0706101 ( 5016) 0.0695571 ( 4656) 0.0693258 ( 3979) 0.0687178 ( 2482)-0.0676996
( 5836)-0.0672000 ( 4160) 0.0550820 ( 3890)-0.0524417 ( 5120) 0.0511829 ( 5645)-0.0500328 ( 4722)-0.0485568 ( 5227) 0.0471263
( 3726)-0.0388192 ( 3388) 0.0368764 ( 5036)-0.0362347 ( 3721) 0.0347510 ( 3391)-0.0339666 ( 4642) 0.0339026 ( 6055)-0.0278029
( 3240)-0.0275045 ( 3741)-0.0272212 ( 3403) 0.0258200 ( 2926) 0.0255225 ( 4186)-0.0254209 ( 2205)-0.0252983 ( 2475) 0.0248687
( 6061)-0.0247187 (  599)-0.0242866 ( 2337) 0.0240418 ( 3916) 0.0238880 ( 6065)-0.0237788 ( 1891)-0.0225894 (  469) 0.0223119
( 2145)-0.0222721 ( 2343) 0.0220991 ( 3987) 0.0220660 ( 2407) 0.0216241 ( 5921)-0.0212527 ( 1711) 0.0212044 ( 2404) 0.0209043
( 1953) 0.0208753 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.106858D-01
     2 -0.298614D-05  0.189809D+01
     3  0.686028D-06 -0.131837D-05  0.195180D+01
     4  0.380610D-06 -0.131706D-05  0.846137D-06  0.986632D-01
     5 -0.410365D-06 -0.134809D-05  0.142541D-05 -0.200858D-05  0.425032D-01
     6  0.395089D-05 -0.304537D-05 -0.108515D-04 -0.457201D-05  0.376406D-05
     7  0.275642D-05 -0.174857D-06 -0.159604D-05  0.446170D-05  0.650074D-06
     8  0.405484D-06  0.385029D-05 -0.269853D-05 -0.689065D-06  0.135480D-05
     9 -0.602171D-05 -0.154880D-05 -0.576221D-05  0.219957D-05  0.889824D-05
                6             7             8             9
     6  0.940803D+00
     7  0.121584D-04  0.187487D+01
     8 -0.168881D-04 -0.319783D-05  0.123024D+00
     9 -0.120794D-05  0.275830D-04 -0.142332D-04  0.105956D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 11

GEOMETRY

C	3.68322800	-0.04500000	-0.72103800
C	3.12050600	1.15170000	-0.23144100
C	1.95905700	1.12477500	0.52355200
C	1.30612700	-0.10966400	0.84596800
C	1.89627200	-1.32350100	0.36839300
C	3.04214000	-1.23493300	-0.38558200
H	3.59301300	2.09147300	-0.45018200
H	1.54182500	2.04338800	0.89543400
H	1.46663900	-2.27456300	0.62564400
C	0.12426800	-0.13022900	1.60485200
H	-0.20455400	0.76037900	2.11235900
H	-0.25554700	-1.06478300	1.98073500
C	-2.01915400	-1.51519300	-1.25513500
H	-2.74310800	-1.62103200	-2.06318400
H	-1.03339000	-1.48381000	-1.70632200
H	-2.09599700	-2.39620200	-0.62853100
C	-1.93813200	1.66660300	-1.08266500
H	-2.64840600	1.89219400	-1.87814800
H	-1.97888100	2.47854900	-0.36590200
H	-0.95062200	1.63558800	-1.53010800
C	-3.56761100	-0.00730300	1.10615900
H	-3.43661600	0.83845800	1.77157600
H	-4.58498900	0.04010700	0.71656400
H	-3.48204600	-0.92595400	1.67538300
Si	-2.38541400	0.03996000	-0.31900300
H	4.56828100	-0.03676200	-1.32766400

E_0(CASSCF,vacuo) -676.098863

E_0(CASSCF,CPCM) **-676.171568**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0988631823
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609886E+03
( 2485) 0.6624909 ( 2211)-0.6219529 ( 2414)-0.1475537 ( 5945) 0.1421642 ( 2556)-0.0991657 ( 2278) 0.0959509 ( 2551) 0.0792229
( 5050)-0.0741860 ( 4630)-0.0717299 ( 6166) 0.0711695 ( 5016) 0.0704306 ( 4656) 0.0701062 ( 3979) 0.0695156 ( 2482)-0.0683299
( 5836)-0.0678966 ( 4160) 0.0552571 ( 3890)-0.0527579 ( 5120) 0.0516175 ( 5645)-0.0505874 ( 4722)-0.0490900 ( 5227) 0.0477940
( 3726)-0.0389955 ( 3388) 0.0371527 ( 5036)-0.0366988 ( 3721) 0.0351504 ( 4642) 0.0344513 ( 3391)-0.0343646 ( 6055)-0.0280655
( 3240)-0.0274198 ( 3741)-0.0270773 ( 3403) 0.0257639 ( 4186)-0.0255610 ( 2926) 0.0255276 ( 2205)-0.0249878 ( 6061)-0.0248608
( 2337) 0.0248418 ( 2475) 0.0244165 ( 3916) 0.0240971 ( 6065)-0.0239187 ( 1891)-0.0223715 (  599)-0.0223456 ( 2145)-0.0220419
( 3987) 0.0212448 ( 2407) 0.0210907 ( 1711) 0.0210561 ( 2343) 0.0209989 ( 4949) 0.0208332 ( 1953) 0.0207289 (  469) 0.0206255
( 2404) 0.0204691 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.963904D-02
     2  0.101530D-05  0.189689D+01
     3 -0.804977D-06  0.435499D-06  0.195173D+01
     4  0.854552D-06 -0.489105D-06 -0.278046D-05  0.100230D+00
     5  0.377797D-06 -0.118669D-05  0.136377D-06  0.560575D-06  0.428545D-01
     6  0.118938D-04  0.332020D-05 -0.158219D-05 -0.310629D-05  0.214110D-05
     7 -0.518196D-05  0.976920D-06  0.559997D-07 -0.424622D-05 -0.162141D-05
     8  0.118730D-06 -0.138085D-05  0.186338D-05  0.824460D-06  0.579957D-09
     9 -0.141705D-04 -0.281070D-05 -0.231894D-05 -0.415129D-06 -0.447299D-06
                6             7             8             9
     6  0.943960D+00
     7 -0.691600D-05  0.187447D+01
     8 -0.757824D-05  0.289714D-05  0.123684D+00
     9  0.670223D-06  0.508539D-05 -0.121025D-05  0.105655D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 12

GEOMETRY

C	3.70355600	-0.03946500	-0.74617500
C	3.14731700	1.15386400	-0.24163500
C	1.99670300	1.12211400	0.53002500
C	1.34820100	-0.11396900	0.85481800
C	1.93206200	-1.32435600	0.36139800
C	3.06707600	-1.23122400	-0.40864900
H	3.61646500	2.09518400	-0.46128600
H	1.58516400	2.03865500	0.91340700
H	1.50631900	-2.27721100	0.61876600
C	0.17606700	-0.13891100	1.62832700
H	-0.15223500	0.74977200	2.13923900
H	-0.20474200	-1.07533000	1.99815700
C	-2.05789200	-1.50921700	-1.25897800
H	-2.76140300	-1.60667000	-2.08595100
H	-1.06113600	-1.47828900	-1.68598500
H	-2.15292500	-2.39364200	-0.63987600
C	-1.98038300	1.67067100	-1.07316400
H	-2.66972600	1.89356700	-1.88761800
H	-2.04236600	2.48183200	-0.35717300
H	-0.98135400	1.64309200	-1.49515200
C	-3.59391200	-0.01470100	1.12169400
H	-3.45223100	0.82832400	1.78843600
H	-4.61838100	0.03282400	0.75080200
H	-3.49641000	-0.93623200	1.68434700
Si	-2.43772700	0.04162500	-0.32296100
H	4.58037200	-0.02747100	-1.36461600

E_0(CASSCF,vacuo) -676.096993

E_0(CASSCF,CPCM) **-676.170295**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0969930773
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609699E+03
( 2485) 0.6612169 ( 2211)-0.6223713 ( 2414)-0.1484241 ( 5945) 0.1438369 ( 2556)-0.0989195 ( 2278) 0.0958903 ( 2551) 0.0794948
( 5050)-0.0747198 ( 4630)-0.0725554 ( 6166) 0.0716783 ( 5016) 0.0712755 ( 4656) 0.0707661 ( 3979) 0.0702443 ( 2482)-0.0689283
( 5836)-0.0685106 ( 4160) 0.0553911 ( 3890)-0.0530025 ( 5120) 0.0519604 ( 5645)-0.0510508 ( 4722)-0.0495091 ( 5227) 0.0483453
( 3726)-0.0391254 ( 3388) 0.0373611 ( 5036)-0.0370811 ( 3721) 0.0355151 ( 4642) 0.0348994 ( 3391)-0.0347283 ( 6055)-0.0283168
( 3240)-0.0273415 ( 3741)-0.0269732 ( 3403) 0.0257270 ( 4186)-0.0256544 ( 2926) 0.0255183 ( 2337) 0.0254847 ( 6061)-0.0249878
( 2205)-0.0247217 ( 3916) 0.0242455 ( 6065)-0.0240539 ( 2475) 0.0240200 ( 1891)-0.0222050 ( 2145)-0.0218561 ( 4949) 0.0211383
( 1711) 0.0209426 ( 1953) 0.0206080 ( 2407) 0.0205812 ( 3987) 0.0205018 (  599)-0.0204249 ( 2404) 0.0200481 ( 2343) 0.0200473
( 5671)-0.0199051 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.859437D-02
     2  0.111626D-05  0.189586D+01
     3  0.137550D-05 -0.178168D-05  0.195166D+01
     4  0.134790D-06  0.284751D-06 -0.120065D-04  0.101651D+00
     5  0.463602D-06 -0.935497D-05  0.108747D-05 -0.361541D-05  0.431745D-01
     6  0.923370D-05  0.181365D-05  0.133757D-05 -0.923594D-05  0.832687D-05
     7  0.107434D-05  0.487133D-05 -0.126838D-05 -0.922613D-05 -0.328001D-05
     8  0.221944D-05 -0.563629D-05  0.767895D-05  0.390972D-05  0.143567D-05
     9 -0.949761D-05 -0.442178D-05 -0.113286D-04 -0.348174D-05  0.485834D-05
                6             7             8             9
     6  0.946425D+00
     7 -0.103263D-04  0.187410D+01
     8 -0.734614D-05  0.937639D-05  0.124293D+00
     9 -0.117449D-06  0.298606D-05  0.245240D-05  0.105425D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 13

GEOMETRY

C	3.72411000	-0.03325800	-0.77107800
C	3.17445900	1.15630900	-0.25098500
C	2.03484400	1.11909900	0.53691800
C	1.39079800	-0.11895400	0.86314900
C	1.96828400	-1.32552100	0.35326200
C	3.09233200	-1.22714600	-0.43237200
H	3.64023300	2.09932300	-0.47086900
H	1.62902800	2.03319900	0.93224000
H	1.54645600	-2.28032800	0.61009100
C	0.22852800	-0.14891400	1.65089800
H	-0.09902200	0.73746400	2.16601900
H	-0.15308000	-1.08738400	2.01432400
C	-2.09759800	-1.50116600	-1.26527300
H	-2.77100700	-1.58124900	-2.11866300
H	-1.08584600	-1.47505300	-1.65675200
H	-2.22237900	-2.39140500	-0.66013300
C	-2.02401000	1.67548100	-1.06198700
H	-2.68289000	1.88977900	-1.90341600
H	-2.11888400	2.48756900	-0.35083300
H	-1.00943000	1.65503400	-1.44654700
C	-3.62045700	-0.02401500	1.13765500
H	-3.46777900	0.81511100	1.80695500
H	-4.65162400	0.02452000	0.78565500
H	-3.51151000	-0.94930600	1.69204200
Si	-2.49018300	0.04344400	-0.32571900
H	4.59254400	-0.01699200	-1.40117000

E_0(CASSCF,vacuo) -676.095310

E_0(CASSCF,CPCM) **-676.169168**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0953099079
Full Convergence on CI vector     -0.67609531E+03
          ( 1)      EIGENVALUE
( 2485) 0.6601070 ( 2211)-0.6226875 ( 2414)-0.1493415 ( 5945) 0.1454186 ( 2556)-0.0986764 ( 2278) 0.0958069 ( 2551) 0.0798200
( 5050)-0.0751778 ( 4630)-0.0733366 ( 6166) 0.0721403 ( 5016) 0.0720796 ( 4656) 0.0713316 ( 3979) 0.0709129 ( 2482)-0.0695210
( 5836)-0.0690621 ( 4160) 0.0554867 ( 3890)-0.0531924 ( 5120) 0.0522284 ( 5645)-0.0514402 ( 4722)-0.0498434 ( 5227) 0.0488105
( 3726)-0.0392156 ( 3388) 0.0375185 ( 5036)-0.0373983 ( 3721) 0.0358492 ( 4642) 0.0352739 ( 3391)-0.0350633 ( 6055)-0.0285515
( 3240)-0.0272682 ( 3741)-0.0268998 ( 2337) 0.0259868 ( 4186)-0.0257117 ( 3403) 0.0257086 ( 2926) 0.0255035 ( 6061)-0.0251026
( 2205)-0.0244880 ( 3916) 0.0243509 ( 6065)-0.0241832 ( 2475) 0.0236687 ( 1891)-0.0220808 ( 2145)-0.0217026 ( 4949) 0.0214302
( 1711) 0.0208630 ( 1953) 0.0205083 ( 5671)-0.0201478 ( 2407) 0.0200876 ( 6216)-0.0200073 ( 5021)-0.0199116 ( 3977)-0.0198323
( 3987) 0.0198177 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.758044D-02
     2 -0.898510D-06  0.189497D+01
     3 -0.389140D-06  0.335038D-05  0.195160D+01
     4  0.689437D-07 -0.368218D-05 -0.267779D-05  0.102935D+00
     5  0.444990D-06 -0.136365D-05 -0.227793D-05  0.461853D-05  0.434677D-01
     6  0.501462D-05  0.965805D-05  0.437489D-05 -0.230664D-05  0.333557D-06
     7 -0.439199D-05  0.260407D-06  0.342497D-05 -0.466187D-05 -0.810124D-06
     8 -0.344121D-06 -0.115655D-05  0.282693D-05  0.190876D-06 -0.340684D-05
     9 -0.146440D-05  0.577269D-05 -0.175754D-05  0.267654D-05 -0.123001D-05
                6             7             8             9
     6  0.948519D+00
     7 -0.237515D-05  0.187375D+01
     8 -0.600471D-05  0.367155D-05  0.124860D+00
     9  0.985839D-06  0.436762D-05  0.657327D-05  0.105232D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 14

GEOMETRY

C	3.74517500	-0.02662100	-0.79558700
C	3.20266900	1.15894600	-0.25925800
C	2.07407000	1.11601300	0.54428300
C	1.43399600	-0.12410300	0.87084200
C	2.00466200	-1.32664400	0.34397200
C	3.11770500	-1.22271000	-0.45671700
H	3.66545400	2.10363200	-0.47857000
H	1.67427200	2.02741400	0.95193700
H	1.58646800	-2.28342600	0.59963200
C	0.28174900	-0.15939800	1.67245400
H	-0.04454000	0.72429700	2.19271000
H	-0.10086800	-1.10001400	2.02889200
C	-2.14021600	-1.49627100	-1.26654800
H	-2.78012900	-1.55860300	-2.14661800
H	-1.11372000	-1.47940800	-1.61937600
H	-2.29838600	-2.39034400	-0.67521700
C	-2.06615300	1.67734200	-1.05550100
H	-2.68723100	1.87752400	-1.92837400
H	-2.19945100	2.49381400	-0.35580400
H	-1.03491000	1.66371600	-1.39459600
C	-3.64906200	-0.02731600	1.15282800
H	-3.48550800	0.80987700	1.82206500
H	-4.68599600	0.02223500	0.81805600
H	-3.53084600	-0.95465400	1.70195000
Si	-2.54266100	0.04530900	-0.32743800
H	4.60507700	-0.00581800	-1.43717000

E_0(CASSCF,vacuo) -676.093802

E_0(CASSCF,CPCM) **-676.168167**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0938024361
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67609380E+03
( 2485) 0.6591929 ( 2211)-0.6228524 ( 2414)-0.1502813 ( 5945) 0.1469349 ( 2556)-0.0984592 ( 2278) 0.0957131 ( 2551) 0.0801925
( 5050)-0.0755648 ( 4630)-0.0740817 ( 5016) 0.0728508 ( 6166) 0.0725428 ( 4656) 0.0718006 ( 3979) 0.0715349 ( 2482)-0.0700885
( 5836)-0.0695309 ( 4160) 0.0555559 ( 3890)-0.0533326 ( 5120) 0.0524258 ( 5645)-0.0517706 ( 4722)-0.0500916 ( 5227) 0.0491969
( 3726)-0.0392792 ( 5036)-0.0376668 ( 3388) 0.0376336 ( 3721) 0.0361601 ( 4642) 0.0355840 ( 3391)-0.0353744 ( 6055)-0.0287748
( 3240)-0.0272071 ( 3741)-0.0268495 ( 2337) 0.0263478 ( 4186)-0.0257441 ( 3403) 0.0256989 ( 2926) 0.0254857 ( 6061)-0.0252055
( 3916) 0.0244213 ( 6065)-0.0243132 ( 2205)-0.0242897 ( 2475) 0.0233641 ( 1891)-0.0219894 ( 4949) 0.0217038 ( 2145)-0.0215791
( 1711) 0.0208045 ( 1953) 0.0204266 ( 5671)-0.0203594 ( 6216)-0.0201391 ( 5021)-0.0201166 ( 3977)-0.0199388 ( 2407) 0.0196277
( 4627) 0.0194390 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.662660D-02
     2 -0.171230D-05  0.189419D+01
     3  0.895095D-06 -0.160714D-05  0.195154D+01
     4  0.106123D-06 -0.122554D-05 -0.195525D-05  0.104087D+00
     5 -0.512431D-07 -0.245518D-05  0.912825D-06 -0.196927D-05  0.437383D-01
     6  0.709328D-06  0.151417D-05 -0.450977D-05 -0.441054D-05 -0.648688D-07
     7 -0.363523D-05  0.117704D-05 -0.107869D-05 -0.178949D-05 -0.537253D-06
     8  0.166890D-06 -0.234155D-05 -0.107024D-06  0.965462D-06  0.112551D-05
     9 -0.191517D-05 -0.736566D-05 -0.464364D-05  0.254412D-05 -0.528508D-07
                6             7             8             9
     6  0.950125D+00
     7 -0.280927D-06  0.187342D+01
     8 -0.117348D-04  0.157038D-05  0.125385D+00
     9  0.431760D-07  0.157367D-04 -0.853816D-05  0.105088D+01
MCSCF converged.
```

$^{1}2^{+}$b STEP 15

GEOMETRY

C	3.76675700	-0.01688800	-0.81935600
C	3.23008700	1.16287300	-0.26490700
C	2.11271900	1.11136300	0.55410500
C	1.47749300	-0.13200300	0.87773100
C	2.04172600	-1.32850100	0.33074200
C	3.14425400	-1.21637700	-0.48349900
H	3.68915400	2.11007900	-0.48139500
H	1.71844500	2.01875300	0.97605600
H	1.62777300	-2.28814500	0.58271600
C	0.33494200	-0.17564600	1.69259700
H	0.00933300	0.70404100	2.21978500
H	-0.04733100	-1.11940900	2.04080300
C	-2.18484400	-1.48877700	-1.27128200
H	-2.77522700	-1.51945500	-2.18660300
H	-1.14010600	-1.49069500	-1.56840700
H	-2.39419000	-2.38853800	-0.70529300
C	-2.10887500	1.68100700	-1.04593900
H	-2.66978100	1.85653900	-1.96329100
H	-2.30260200	2.50368100	-0.36816400
H	-1.05608200	1.68204200	-1.31384400
C	-3.67643400	-0.03218500	1.16914200
H	-3.49977300	0.80068900	1.84056800
H	-4.71889400	0.02170800	0.85236600
H	-3.55086900	-0.96348800	1.70996500
Si	-2.59540400	0.04803000	-0.32858500
H	4.61885300	0.01057600	-1.47107700

E_0(CASSCF,vacuo) -676.092459

E_0(CASSCF,CPCM) **-676.167306**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0924588696
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609246E+03
( 2485) 0.6579341 ( 2211)-0.6234374 ( 2414)-0.1511991 ( 5945) 0.1483358 ( 2556)-0.0982350 ( 2278) 0.0956683 ( 2551) 0.0804465
( 5050)-0.0758777 ( 4630)-0.0747582 ( 5016) 0.0735776 ( 6166) 0.0728931 ( 4656) 0.0722728 ( 3979) 0.0720883 ( 2482)-0.0707526
( 5836)-0.0700123 ( 4160) 0.0555914 ( 3890)-0.0534857 ( 5120) 0.0525900 ( 5645)-0.0520287 ( 4722)-0.0503562 ( 5227) 0.0495672
( 3726)-0.0393128 ( 5036)-0.0378741 ( 3388) 0.0377529 ( 3721) 0.0364268 ( 4642) 0.0358797 ( 3391)-0.0356616 ( 6055)-0.0289821
( 3240)-0.0271263 ( 3741)-0.0267966 ( 2337) 0.0265952 ( 4186)-0.0257476 ( 3403) 0.0257092 ( 2926) 0.0254860 ( 6061)-0.0252921
( 3916) 0.0244913 ( 6065)-0.0244481 ( 2205)-0.0241067 ( 2475) 0.0230922 ( 4949) 0.0219618 ( 1891)-0.0219106 ( 2145)-0.0214671
( 1711) 0.0207854 ( 5671)-0.0205330 ( 1953) 0.0203782 ( 5021)-0.0203031 ( 6216)-0.0202553 ( 3977)-0.0199747 ( 4627) 0.0196561
( 5253) 0.0193020 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.572465D-02
     2  0.122870D-05  0.189349D+01
     3 -0.128968D-05 -0.606663D-07  0.195150D+01
     4 -0.202883D-06 -0.147242D-06 -0.577266D-06  0.105148D+00
     5  0.451537D-08 -0.209413D-06 -0.219327D-06  0.143407D-06  0.439841D-01
     6 -0.142618D-05 -0.908212D-07 -0.265493D-06  0.522537D-05 -0.326914D-05
     7 -0.224997D-05  0.250001D-06 -0.267801D-06  0.343332D-05 -0.339611D-07
     8 -0.954846D-07  0.467609D-06  0.493413D-06  0.193406D-06  0.436397D-06
     9 -0.456795D-05  0.478892D-05 -0.101252D-06  0.232096D-05 -0.349574D-05
                6             7             8             9
     6  0.952781D+00
     7 -0.689208D-05  0.187310D+01
     8  0.128012D-05 -0.612268D-06  0.125886D+00
     9  0.293611D-06 -0.400117D-06  0.421529D-05  0.104838D+01
MCSCF converged.
```

$^{3}2^{+}$b STEP 1

GEOMETRY

C	-3.53728800	-0.07577200	0.46732000
C	-2.91848200	1.14569400	0.12836500
C	-1.66485400	1.14187900	-0.44873200
C	-0.96253700	-0.08844800	-0.72887300
C	-1.59804100	-1.33004200	-0.37183000
C	-2.82905900	-1.26390200	0.19493800
H	-3.42589600	2.07338100	0.31270600
H	-1.19208900	2.06817000	-0.71572300
H	-1.10856300	-2.26456700	-0.56954700
C	0.33190900	-0.06370900	-1.30964100
H	0.56804200	0.82907300	-1.87304600
H	0.62513800	-0.97148500	-1.81957300
C	1.72789700	-1.52814000	1.21624600
H	2.55420700	-1.57508400	1.92196900
H	0.81068800	-1.54799900	1.79620600
H	1.77263600	-2.43058600	0.61415600
C	1.62782200	1.60954500	1.14632200
H	2.45210300	1.74363300	1.84315600
H	1.60949200	2.48498200	0.50424000
H	0.71407800	1.59357900	1.73198700
C	3.40311900	0.05027100	-0.92178700
H	3.42108600	0.91716900	-1.57471900
H	4.29803700	0.09159000	-0.30501900
H	3.47713000	-0.84007800	-1.53816300
Si	1.88959200	0.02481700	0.18038000
H	-4.51330000	-0.10347100	0.91208200

E_0(CASSCF,vacuo) -676.118808

E_0(CASSCF,CPCM) **-676.189500**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1188080850
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611881E+03
 (     1) 0.9349836 ( 1349)-0.1264209 (  428) 0.1103738 (  506)-0.0895630 ( 1352)-0.0704058 ( 2950)-0.0647319 ( 6166)-0.0582395
 (   171)-0.0570163 ( 1430)-0.0550548 ( 1271) 0.0547777 ( 2101) 0.0543908 ( 3035)-0.0533088 ( 3028) 0.0525623 ( 1264)-0.0455526
 (   508)-0.0452305 (  430) 0.0427424 ( 6081)-0.0397283 ( 2941) 0.0393781 (   87) 0.0392515 ( 1356)-0.0386119 (   10)-0.0385059
 (   510)-0.0382868 ( 1434)-0.0379942 ( 3026)-0.0376309 (  706)-0.0373046 ( 3030)-0.0367786 ( 3113)-0.0357928 (   16) 0.0354688
 ( 1439)-0.0353312 ( 1354) 0.0342578 (  177)-0.0336781 (   93) 0.0324897 ( 6077) 0.0305842 ( 5909) 0.0303880 ( 5913)-0.0290389
 (  3025) 0.0287613 (   11)-0.0286672 ( 2945) 0.0281963 ( 3226)-0.0277236 ( 6079)-0.0273785 ( 1460) 0.0268066 ( 6145)-0.0267528
 (  5970) 0.0256032 ( 5966) 0.0248431 (  621) 0.0242352 ( 5911)-0.0242008 (  617) 0.0241311 ( 1373) 0.0239059 (  512) 0.0237505
 ( 2353)-0.0234072 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.196539D+01
     2 -0.677824D-06  0.192925D+01
     3  0.414306D-06 -0.173059D-05  0.189758D+01
     4 -0.114036D-04  0.901446D-05 -0.666294D-04  0.100377D+01
     5  0.355709D-05  0.145235D-04  0.309579D-04  0.109542D-04  0.999986D+00
     6  0.144671D-05 -0.914518D-06 -0.436149D-06  0.182564D-05  0.505012D-05
     7 -0.269141D-05  0.360659D-05  0.257720D-05 -0.136999D-04  0.999547D-05
     8  0.957312D-06 -0.316337D-06  0.527056D-05  0.450962D-05  0.152317D-05
     9  0.795290D-05 -0.360133D-05  0.160372D-05 -0.273457D-05  0.366790D-06
                6             7             8             9
     6  0.622359D-01
     7  0.299404D-05  0.945285D-01
     8 -0.448525D-06  0.625652D-06  0.306390D-01
     9  0.463120D-06  0.384019D-06  0.609648D-06  0.166127D-01
 MCSCF converged.
```

$^{3}2^{+}$b STEP 2

GEOMETRY

C	-3.55320800	-0.07702000	0.48520300
C	-2.93728200	1.14351300	0.13842600
C	-1.68887600	1.14254800	-0.45294100
C	-0.99096300	-0.08520300	-0.73897900
C	-1.62322000	-1.32661400	-0.37451600
C	-2.85027800	-1.26158700	0.20690900
H	-3.44321700	2.07127900	0.32716000
H	-1.22246700	2.07041600	-0.72647700
H	-1.13690000	-2.26189000	-0.57769200
C	0.28764900	-0.06373100	-1.33312000
H	0.55442100	0.83507800	-1.87037400
H	0.60860100	-0.97488600	-1.81726800
C	1.75303600	-1.53235300	1.22116200
H	2.57935700	-1.59643300	1.92615600
H	0.83508600	-1.54143000	1.79929400
H	1.78510700	-2.42846700	0.60965600
C	1.66405600	1.61868200	1.14420200
H	2.48792400	1.76686400	1.83931000
H	1.64008100	2.48370900	0.48908500
H	0.74971700	1.60117900	1.72788700
C	3.40269700	0.03989100	-0.95767000
H	3.39952800	0.90495600	-1.61270800
H	4.32003900	0.07961800	-0.37389300
H	3.44948500	-0.85372000	-1.57139900
Si	1.93827800	0.02551300	0.20418800
H	-4.52432800	-0.10221100	0.94056500

E_0(CASSCF,vacuo) -676.116967

E_0(CASSCF,CPCM) **-676.187084**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1169666135
Full Convergence on CI vector      -0.67611697E+03
          ( 1)        EIGENVALUE
(     1) 0.9302457 ( 1349)-0.1288557 (  428) 0.1175548 (  506)-0.0977673 ( 2950)-0.0712936 (  171)-0.0600039 ( 1352)-0.0571258
( 1271) 0.0560551 ( 1430)-0.0540228 ( 3028) 0.0535973 ( 2101) 0.0535591 (  508)-0.0467241 ( 2941) 0.0444179 (  430) 0.0439376
( 3035)-0.0438694 (   10)-0.0435942 ( 6081)-0.0414288 ( 1264)-0.0409429 ( 6166)-0.0408309 (  617) 0.0389416 ( 1373) 0.0376708
(  706)-0.0375584 ( 1434)-0.0373499 ( 5970) 0.0372859 (   16) 0.0371429 ( 1460) 0.0369413 ( 5966) 0.0367591 ( 1356)-0.0365985
(   87) 0.0365163 (  510)-0.0343456 ( 3113)-0.0338831 (  177)-0.0326320 ( 3030)-0.0323730 ( 5911)-0.0318491 ( 3226)-0.0315750
( 6145)-0.0310004 ( 1439)-0.0307824 ( 5909) 0.0304930 ( 5913)-0.0304547 (   93) 0.0295426 ( 6079)-0.0284915 ( 1354) 0.0269281
(  685)-0.0263939 (   23) 0.0257074 ( 4621) 0.0249047 ( 3137) 0.0246146 ( 3205)-0.0243911 ( 5975) 0.0236850 ( 2969) 0.0234576
( 3025) 0.0231331 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195879D+01
     2 -0.296367D-06  0.192532D+01
     3  0.147553D-06  0.616859D-06  0.189501D+01
     4 -0.144356D-06 -0.465587D-06  0.203777D-04  0.100267D+01
     5 -0.529558D-05 -0.310689D-04 -0.273385D-04 -0.118292D-04  0.999970D+00
     6  0.477269D-05 -0.323780D-05 -0.260291D-06 -0.393688D-05  0.138259D-05
     7  0.156350D-05 -0.126913D-05 -0.100285D-05  0.404891D-05 -0.136066D-04
     8  0.412672D-05 -0.304989D-05 -0.238816D-05 -0.445540D-05  0.717282D-06
     9  0.621471D-06 -0.996268D-06 -0.583314D-06 -0.181543D-05 -0.693967D-07
                6             7             8             9
     6  0.693086D-01
     7 -0.881514D-06  0.986595D-01
     8 -0.221315D-06  0.642298D-07  0.339020D-01
     9  0.616610D-07 -0.211467D-06  0.126331D-08  0.163753D-01
MCSCF converged.
```

$^{3}2^{+}$b STEP 3

GEOMETRY

C	-3.57088900	-0.07660900	0.50510500
C	-2.95871800	1.14209000	0.14886800
C	-1.71594000	1.14159300	-0.45783200
C	-1.02306300	-0.08409100	-0.74842900
C	-1.65119400	-1.32374400	-0.37650400
C	-2.87366600	-1.25885300	0.22054100
H	-3.46242700	2.07043400	0.34136600
H	-1.25527400	2.07031800	-0.73907700
H	-1.16882100	-2.26016200	-0.58497100
C	0.24470500	-0.06561500	-1.35816700
H	0.53252300	0.83645600	-1.87692000
H	0.58463600	-0.97920900	-1.82235100
C	1.77985100	-1.53487900	1.22487600
H	2.59980300	-1.61044600	1.93674900
H	0.85639900	-1.53699100	1.79358200
H	1.80936200	-2.42588800	0.60644100
C	1.69810700	1.62630800	1.14022900
H	2.51529000	1.78520000	1.84145800
H	1.67647900	2.48263500	0.47428100
H	0.77811800	1.60839300	1.71424800
C	3.41114600	0.03187000	-0.98597200
H	3.38912600	0.89500300	-1.64273600
H	4.34654800	0.07131900	-0.43081000
H	3.43564900	-0.86484900	-1.59596800
Si	1.98981500	0.02635100	0.22406900
H	-4.53685800	-0.09954300	0.97144900

E_0(CASSCF,vacuo) -676.114607

E_0(CASSCF,CPCM) **-676.183591**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1146071236
Full Convergence on CI vector
         ( 1)        EIGENVALUE     -0.67611461E+03
(     1) 0.9265659 ( 1349)-0.1307635 (  428) 0.1154442 (  506)-0.0930133 ( 2950)-0.0783801 ( 1271) 0.0571391 ( 3028) 0.0547672
(  171)-0.0545521 ( 2101) 0.0511720 ( 1430)-0.0503573 ( 2941) 0.0482888 (   10)-0.0477050 (  508)-0.0476180 ( 5970) 0.0458882
(  617) 0.0443562 ( 1460) 0.0439706 ( 1373) 0.0438317 (  430) 0.0428249 ( 1352)-0.0422302 (  170)-0.0413769 ( 5966) 0.0409570
(  507) 0.0401919 ( 6081)-0.0390485 ( 1264)-0.0375613 (   92) 0.0374388 ( 1434)-0.0374029 (   16) 0.0373573 (  429)-0.0367599
( 5911)-0.0358041 ( 3035)-0.0353236 (  685)-0.0341521 (  706)-0.0339938 ( 5892)-0.0329240 (   23) 0.0328409 ( 1356)-0.0327143
( 3205)-0.0323950 (  4621) 0.0323871 ( 2969) 0.0321526 (   87) 0.0315682 (  510)-0.0302686 ( 3113)-0.0298590 ( 1377) 0.0295017
( 3226)-0.0292829 (  177)-0.0291955 ( 6145)-0.0290658 ( 3139)-0.0286552 ( 6053) 0.0276533 ( 6166)-0.0270304 ( 3030)-0.0270114
( 5996)-0.0260917 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195551D+01
     2  0.123862D-05  0.192022D+01
     3 -0.896761D-07  0.617639D-07  0.189307D+01
     4  0.725933D-05 -0.241941D-04 -0.890338D-05  0.100128D+01
     5 -0.109140D-04 -0.384270D-04 -0.332978D-04 -0.796919D-05  0.999917D+00
     6 -0.325306D-05  0.208595D-05  0.216225D-06 -0.311781D-05  0.390483D-05
     7 -0.254653D-06  0.710498D-07 -0.783543D-06 -0.390624D-05 -0.159952D-04
     8 -0.183768D-05  0.103489D-05  0.338135D-06 -0.514567D-06  0.270087D-06
     9 -0.216552D-05  0.173073D-05 -0.214540D-06  0.966770D-06 -0.309425D-05
                6             7             8             9
     6  0.759294D-01
     7 -0.715234D-07  0.101708D+00
     8  0.116242D-05 -0.642133D-07  0.363097D-01
     9 -0.886620D-07 -0.842673D-07 -0.171573D-06  0.160500D-01
MCSCF converged.
```

$^{3}2^{+}$b STEP 4

GEOMETRY

C	3.58959900	-0.07547600	-0.52628400
C	2.98153500	1.14125900	-0.15985300
C	1.74528800	1.14010000	0.46319100
C	1.05766400	-0.08399700	0.75818100
C	1.68071900	-1.32129600	0.37766100
C	2.89769200	-1.25610300	-0.23581100
H	3.48247000	2.07039600	-0.35632600
H	1.29009000	2.06926500	0.75265500
H	1.20236700	-2.25894700	0.59082200
C	-0.20165700	-0.06836400	1.38429600
H	-0.50435500	0.83540900	1.88985400
H	-0.55499400	-0.98392000	1.83256800
C	-1.80948500	-1.53708500	-1.22664200
H	-2.62633700	-1.62760500	-1.94089400
H	-0.88396300	-1.52939000	-1.79153700
H	-1.83003800	-2.42312600	-0.60124700
C	-1.73139100	1.63145700	-1.13750700
H	-2.54492000	1.80505300	-1.84007600
H	-1.70341100	2.48013800	-0.46254500
H	-0.80959000	1.60741800	-1.70797700
C	-3.42406900	0.02713400	1.01051900
H	-3.38480900	0.88954900	1.66705300
H	-4.37514100	0.06591600	0.48174500
H	-3.42924000	-0.87153800	1.61771200
Si	-2.04236800	0.02726900	-0.24095900
H	4.54965200	-0.09616400	-1.00488300

E_0(CASSCF,vacuo) -676.111964

E_0(CASSCF,CPCM) **-676.181175**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1119642109
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611196E+03
(     1) 0.9240147 ( 1349)-0.1322208 (  428) 0.1187815 (  506)-0.0938019 ( 2950)-0.0847756 ( 1271) 0.0586049 ( 3028) 0.0569609
(   171)-0.0568243 ( 5970) 0.0511726 ( 2941) 0.0507988 (   10)-0.0504892 ( 2101) 0.0498547 (  508)-0.0490389 ( 1460) 0.0480772
(   617) 0.0479667 ( 1430)-0.0473713 ( 1373) 0.0458433 (  430) 0.0424964 (  170)-0.0419380 ( 5966) 0.0418360 (  507) 0.0407489
(   685)-0.0393237 ( 5892)-0.0390880 (   23) 0.0382833 (   16) 0.0381334 ( 4621) 0.0380708 (   92) 0.0375642 ( 5911)-0.0372768
( 1434)-0.0372435 ( 6081)-0.0371986 (  429)-0.0368934 ( 2969) 0.0355412 ( 1264)-0.0354165 ( 3205)-0.0353713 ( 3139)-0.0343557
( 1377) 0.0341906 ( 6053) 0.0326444 ( 5996)-0.0316434 ( 1352)-0.0316044 (  706)-0.0309695 ( 3035)-0.0301066 (   87) 0.0292380
( 1356)-0.0286344 (  510)-0.0279869 (  177)-0.0268178 ( 3113)-0.0256505 ( 3200)-0.0255435 ( 6145)-0.0251321 ( 3226)-0.0250850
( 5975) 0.0245203 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195412D+01
     2 -0.195519D-05  0.191538D+01
     3  0.102191D-05 -0.159579D-05  0.189169D+01
     4 -0.204865D-04  0.336964D-04  0.246258D-04  0.100014D+01
     5  0.321370D-05 -0.880285D-05 -0.445460D-05  0.615405D-03  0.999833D+00
     6  0.197430D-04 -0.144912D-04  0.221504D-05 -0.145918D-04  0.510513D-06
     7  0.330906D-05 -0.316132D-05  0.186110D-06  0.717119D-05 -0.748541D-05
     8  0.835252D-05 -0.112089D-04 -0.277124D-05 -0.890901D-05 -0.275930D-06
     9  0.100437D-04 -0.120584D-04  0.136108D-05 -0.222068D-04  0.716331D-05
                6             7             8             9
     6  0.814252D-01
     7 -0.385447D-07  0.103938D+00
     8 -0.185490D-05  0.440857D-06  0.377953D-01
     9  0.160813D-05 -0.255383D-06  0.987778D-06  0.156897D-01
MCSCF converged.
```

$^{3}2^{+}$b STEP 5

GEOMETRY

C	3.60902800	-0.07333000	-0.54901300
C	3.00540300	1.14112700	-0.17094000
C	1.77632400	1.13820600	0.46869000
C	1.09394200	-0.08503300	0.76777200
C	1.71222300	-1.31971700	0.37789800
C	2.92261400	-1.25331500	-0.25229600
H	3.50328000	2.07126400	-0.37095900
H	1.32602000	2.06718000	0.76703000
H	1.23813000	-2.25865900	0.59571400
C	-0.15769400	-0.07242600	1.41065200
H	-0.47071200	0.83186200	1.90763300
H	-0.52004800	-0.98973400	1.84652200
C	-1.84091200	-1.53730600	-1.22940200
H	-2.64489200	-1.63262900	-1.95785500
H	-0.90541300	-1.52717500	-1.77738900
H	-1.86947400	-2.42021300	-0.60022600
C	-1.76605500	1.63677000	-1.13274300
H	-2.56638100	1.81662500	-1.84913400
H	-1.74884300	2.47941000	-0.45019800
H	-0.83381700	1.61369000	-1.68582600
C	-3.44096200	0.02172100	1.03198500
H	-3.38500800	0.88268500	1.68898500
H	-4.40607400	0.06016300	0.52873900
H	-3.42741000	-0.87912900	1.63557000
Si	-2.09540900	0.02830200	-0.25530300
H	4.56290700	-0.09174500	-1.03996700

E_0(CASSCF,vacuo) -676.109188

E_0(CASSCF,CPCM) **-676.178716**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1091879233
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610919E+03
 (     1) 0.9223264 ( 1349)-0.1332533 (  428) 0.1204870 (  506)-0.0932772 ( 2950)-0.0898755 ( 1271) 0.0601268 ( 3028) 0.0595328
 (   171)-0.0585187 ( 5970) 0.0542865 ( 2941) 0.0522991 (   10)-0.0522216 ( 1460) 0.0503839 (  508)-0.0496727 (  617) 0.0493294
 ( 2101) 0.0484721 ( 1373) 0.0453577 ( 1430)-0.0443271 ( 5892)-0.0427785 (  170)-0.0422469 (   23) 0.0421961 ( 4621) 0.0420981
 (   430) 0.0420770 (  685)-0.0419112 (  507) 0.0410600 ( 5966) 0.0409255 (   16) 0.0386392 ( 3139)-0.0380845 ( 5911)-0.0377110
 (    92) 0.0375970 (  429)-0.0369265 ( 1434)-0.0368742 ( 1377) 0.0367830 ( 6081)-0.0362337 ( 2969) 0.0358003 ( 6053) 0.0355115
 ( 3205)-0.0353604 ( 5996)-0.0347947 ( 1264)-0.0340554 ( 3200)-0.0296044 (  706)-0.0282953 ( 2973)-0.0275543 ( 6058)-0.0274375
 ( 3035)-0.0274116 (   87) 0.0273688 (  510)-0.0264187 ( 1356)-0.0252396 ( 3116) 0.0250380 (  177)-0.0247385 ( 1352)-0.0239818
 ( 5975) 0.0228542 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195357D+01
     2 -0.197804D-06  0.191137D+01
     3  0.106850D-05  0.170705D-05  0.189075D+01
     4  0.862978D-05 -0.205564D-04  0.766423D-05  0.999364D+00
     5 -0.426529D-05 -0.161819D-05  0.147691D-04  0.103652D-02  0.999776D+00
     6 -0.344031D-05  0.161445D-05  0.582902D-05 -0.749578D-05  0.113222D-05
     7  0.867508D-06 -0.481093D-05 -0.175443D-05  0.548677D-05 -0.325517D-05
     8  0.925583D-06 -0.113302D-05  0.246642D-05 -0.221459D-05 -0.125395D-05
     9 -0.218689D-05  0.282748D-06  0.361615D-06  0.358298D-05 -0.886103D-06
                6             7             8             9
     6  0.856323D-01
     7 -0.159915D-05  0.105542D+00
     8  0.240605D-06  0.876727D-06  0.386868D-01
     9  0.551093D-06 -0.320972D-06 -0.411521D-06  0.153148D-01
 MCSCF converged.
```

$^{3}2^{+}$b STEP 6

GEOMETRY

C	3.62896800	-0.07075700	-0.57225700
C	3.02980100	1.14142700	-0.18235100
C	1.80857100	1.13627800	0.47413400
C	1.13137800	-0.08655800	0.77765700
C	1.74463600	-1.31858400	0.37718900
C	2.94771200	-1.25055300	-0.26978200
H	3.52437300	2.07266300	-0.38593200
H	1.36303700	2.06480900	0.78150300
H	1.27462500	-2.25881400	0.59898100
C	-0.11283800	-0.07705300	1.43709300
H	-0.43292600	0.82720200	1.92853400
H	-0.48125700	-0.99606000	1.86298400
C	-1.87190800	-1.53530700	-1.23346400
H	-2.66560900	-1.63691900	-1.97263000
H	-0.92918500	-1.51899200	-1.76866400
H	-1.90312300	-2.41637000	-0.60212700
C	-1.80263700	1.64278200	-1.12525500
H	-2.59266900	1.83130100	-1.85115900
H	-1.79173600	2.47868800	-0.43462100
H	-0.86302100	1.61981800	-1.66559700
C	-3.46057900	0.01390100	1.05092300
H	-3.39032300	0.87262000	1.70929000
H	-4.43777400	0.05211000	0.57095600
H	-3.42983100	-0.88988800	1.64925200
Si	-2.14853200	0.02937200	-0.26772300
H	4.57625300	-0.08684000	-1.07596400

E_0(CASSCF,vacuo) -676.106379

E_0(CASSCF,CPCM) **-676.176324**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1063786830
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67610638E+03
 (     1) 0.9211470 ( 1349)-0.1339784 (  428) 0.1214750 ( 2950)-0.0937977 (  506)-0.0924991 ( 3028) 0.0619820 ( 1271) 0.0614663
 (  171)-0.0598724 ( 5970) 0.0561933 (   10)-0.0533730 ( 2941) 0.0532990 ( 1460) 0.0517227 (  617) 0.0498122 (  508)-0.0497590
 ( 2101) 0.0471893 ( 5892)-0.0451494 (   23) 0.0450018 ( 4621) 0.0449406 ( 1373) 0.0439538 (  685)-0.0427206 (  170)-0.0423655
 ( 1430)-0.0415255 (  430) 0.0414404 (  507) 0.0412093 ( 3139)-0.0407135 ( 5966) 0.0394844 (   16) 0.0390049 ( 1377) 0.0382369
 ( 5911)-0.0377824 (   92) 0.0375097 ( 6053) 0.0371972 (  429)-0.0368545 ( 5996)-0.0366296 ( 1434)-0.0363972 ( 6081)-0.0357517
 ( 2969) 0.0348821 ( 3205)-0.0339450 ( 1264)-0.0330989 ( 3200)-0.0322833 ( 2973)-0.0295644 ( 6058)-0.0293937 ( 3035)-0.0261020
 (  706)-0.0259531 (   87) 0.0259143 ( 3116) 0.0254242 (  510)-0.0253134 (  177)-0.0229212 (  619) 0.0225767 ( 1356)-0.0225430
 ( 2116) 0.0223410 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195336D+01
     2  0.176899D-05  0.190816D+01
     3  0.192855D-06  0.157362D-05  0.189006D+01
     4  0.611158D-05 -0.236263D-04  0.945380D-05  0.998920D+00
     5  0.295363D-05  0.174116D-04  0.126306D-05  0.125901D-02  0.999748D+00
     6  0.379488D-05  0.187301D-04 -0.191244D-05 -0.231375D-05 -0.610630D-05
     7 -0.688520D-06  0.105682D-05 -0.336398D-05 -0.184571D-05  0.100916D-05
     8 -0.107099D-05  0.150111D-04  0.740213D-05 -0.462933D-05  0.310273D-05
     9 -0.260617D-06  0.156057D-04  0.624563D-05  0.988476D-06 -0.536285D-06
                6             7             8             9
     6  0.888379D-01
     7 -0.337239D-05  0.106773D+00
     8  0.162260D-05 -0.169937D-05  0.392631D-01
     9  0.200925D-06 -0.227307D-05 -0.128482D-06  0.148701D-01
 MCSCF converged.
```

$^{3}2^{+}$b STEP 7

GEOMETRY

C	3.64915800	-0.06823000	-0.59605200
C	3.05489800	1.14187900	-0.19401900
C	1.84205200	1.13453600	0.47933100
C	1.16959100	-0.08810500	0.78748400
C	1.77755600	-1.31767300	0.37594700
C	2.97272900	-1.24800000	-0.28780600
H	3.54629400	2.07411900	-0.40112800
H	1.40145800	2.06253700	0.79578900
H	1.31155600	-2.25910300	0.60166800
C	-0.06715500	-0.08140600	1.46316700
H	-0.39208900	0.82253500	1.95114500
H	-0.43996700	-1.00191600	1.88093600
C	-1.90705900	-1.53558200	-1.23347200
H	-2.68850000	-1.64191500	-1.98519200
H	-0.95593500	-1.51710200	-1.75358800
H	-1.94542600	-2.41392600	-0.59898000
C	-1.83793000	1.64546600	-1.12176300
H	-2.61515200	1.84014600	-1.86002800
H	-1.83507500	2.47732900	-0.42639900
H	-0.88962600	1.62044500	-1.64666700
C	-3.48084200	0.01160500	1.06942500
H	-3.39558400	0.86962400	1.72676500
H	-4.46916300	0.04997900	0.61213300
H	-3.43523300	-0.89363500	1.66441600
Si	-2.20179200	0.03043400	-0.27869100
H	4.58954400	-0.08213300	-1.11265100

E_0(CASSCF,vacuo) -676.103619

E_0(CASSCF,CPCM) **-676.174003**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1036185123
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610362E+03
 (     1) 0.9202424 ( 1349)-0.1344506 (   428) 0.1245180 ( 2950)-0.0968018 (  506)-0.0945121 ( 3028) 0.0640877 (  171)-0.0636299
 ( 1271) 0.0625277 ( 5970) 0.0574121 (    10)-0.0543208 ( 2941) 0.0541822 ( 1460) 0.0525172 (  617) 0.0510765 (  508)-0.0498644
 (   23) 0.0470062 ( 4621) 0.0469390 ( 5892)-0.0467674 ( 2101) 0.0464153 ( 1373) 0.0427121 ( 3139)-0.0426604 (  685)-0.0426179
 (  430) 0.0407186 (   16) 0.0395272 ( 1430)-0.0394078 ( 1377) 0.0390739 ( 5966) 0.0384219 ( 6053) 0.0382187 ( 5996)-0.0377630
 ( 5911)-0.0377198 (  507)-0.0372302 (  170) 0.0360941 ( 1434)-0.0358893 ( 6081)-0.0354895 ( 3200)-0.0340082 ( 2969) 0.0337967
 (  429) 0.0331038 (   92)-0.0324593 ( 1264)-0.0323458 ( 3205)-0.0318938 ( 2973)-0.0309821 ( 6058)-0.0307926 ( 3035)-0.0255329
 ( 3116) 0.0253687 (   87) 0.0253640 ( 3026) 0.0250838 (  510)-0.0247252 (  706)-0.0239976 (  619) 0.0229798 ( 2116) 0.0228530
 ( 3120)-0.0226995 (
 Final one electron symbolic density matrix:
                 1             2             3             4             5
     1  0.195328D+01
     2 -0.120804D-06  0.190559D+01
     3 -0.838242D-07  0.486533D-07  0.188953D+01
     4 -0.108107D-05 -0.408668D-05 -0.103306D-04  0.998397D+00
     5  0.449317D-05  0.333265D-04  0.204672D-04 -0.315641D-05  0.100008D+01
     6 -0.116048D-06 -0.589433D-06 -0.179135D-05 -0.178670D-05  0.572637D-06
     7 -0.896888D-07  0.204687D-05  0.949482D-06 -0.501759D-05  0.965796D-05
     8 -0.949793D-07  0.162572D-06 -0.247240D-06 -0.121494D-05  0.254581D-05
     9  0.272751D-06 -0.113527D-05  0.998113D-07 -0.359691D-05  0.361818D-05
                 6             7             8             9
     6  0.913619D-01
     7  0.167061D-06  0.107767D+00
     8  0.259424D-07 -0.580110D-08  0.396811D-01
     9  0.365659D-07  0.215268D-06  0.838310D-07  0.143127D-01
 MCSCF converged.
```

$^{3}2^{+}$b STEP 8

GEOMETRY

C	3.66969400	-0.06525300	-0.62024600
C	3.08046000	1.14267500	-0.20564600
C	1.87645200	1.13275500	0.48450000
C	1.20862100	-0.09006700	0.79723900
C	1.81138400	-1.31714800	0.37391700
C	2.99806900	-1.24537200	-0.30651100
H	3.56857900	2.07600800	-0.41599700
H	1.44075000	2.05998800	0.81026900
H	1.34936800	-2.25982000	0.60313200
C	-0.02040400	-0.08638200	1.48881000
H	-0.34853100	0.81692200	1.97515800
H	-0.39608900	-1.00844500	1.89974600
C	-1.94170700	-1.53383300	-1.23490300
H	-2.71279100	-1.64533700	-1.99676300
H	-0.98406000	-1.51057600	-1.74280500
H	-1.98368400	-2.41063600	-0.59871300
C	-1.87515700	1.64917200	-1.11543200
H	-2.64191700	1.85158800	-1.86277000
H	-1.87759300	2.47613000	-0.41442500
H	-0.92029700	1.62234600	-1.62830800
C	-3.50354200	0.00670300	1.08591300
H	-3.40526900	0.86335200	1.74310800
H	-4.50164200	0.04477800	0.64976300
H	-3.44347200	-0.90053100	1.67644200
Si	-2.25496600	0.03154000	-0.28814100
H	4.60295200	-0.07683100	-1.14971600

E_0(CASSCF,vacuo) -676.100970

E_0(CASSCF,CPCM) **-676.171867**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1009695169
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67610097E+03
 (     1) 0.9194793 ( 1349)-0.1347172 (   428) 0.1258803 ( 2950)-0.0991126 (  506)-0.0945940 ( 3028) 0.0658090 (  171)-0.0649325
 ( 1271) 0.0633166 ( 5970) 0.0582197 (    10)-0.0552760 ( 2941) 0.0551096 ( 1460) 0.0529928 (  617) 0.0514855 (  508)-0.0494716
 (   23) 0.0484373 ( 4621) 0.0483412 ( 5892)-0.0479116 ( 2101) 0.0454914 ( 3139)-0.0441347 (  685)-0.0412231 ( 1373) 0.0411094
 (   16) 0.0398381 (  430) 0.0395931 ( 1377) 0.0395637 ( 6053) 0.0388503 ( 5996)-0.0385021 ( 5911)-0.0375982 ( 1430)-0.0372413
 ( 5966) 0.0370514 (  507)-0.0364887 ( 1434)-0.0353987 (  170) 0.0353967 ( 6081)-0.0353288 ( 3200)-0.0347196 ( 2969) 0.0325152
 (  429) 0.0323613 ( 2973)-0.0320167 ( 6058)-0.0318291 (   92)-0.0317395 ( 1264)-0.0317184 ( 3205)-0.0295745 ( 3026) 0.0284808
 ( 3035)-0.0253753 ( 3116) 0.0250632 (   87) 0.0245376 (  510)-0.0241126 ( 3120)-0.0235224 ( 2116) 0.0230252 (  619) 0.0229322
 (  706)-0.0219845 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195325D+01
     2  0.708557D-07  0.190348D+01
     3 -0.230336D-06  0.352127D-08  0.188909D+01
     4 -0.290494D-06 -0.483217D-05 -0.415374D-05  0.998402D+00
     5  0.381516D-05 -0.841789D-05 -0.236515D-04  0.671204D-06  0.100007D+01
     6 -0.119958D-05  0.965026D-07 -0.200733D-05 -0.643745D-05 -0.712590D-06
     7 -0.215018D-07  0.247328D-05  0.207903D-06 -0.313252D-05  0.480938D-06
     8 -0.321687D-06 -0.509683D-06  0.845438D-07 -0.849563D-06  0.722833D-06
     9 -0.434332D-06  0.213356D-06  0.505970D-06 -0.371135D-05  0.247760D-06
                6             7             8             9
     6  0.934465D-01
     7  0.130690D-06  0.108607D+00
     8  0.224398D-06 -0.130261D-06  0.400232D-01
     9  0.381749D-06  0.215109D-06  0.530322D-07  0.136207D-01
 MCSCF converged.
```

$^{3}2^{+}$b STEP 9

GEOMETRY

C	3.69062500	-0.06237800	-0.64443800
C	3.10667200	1.14352100	-0.21747500
C	1.91181100	1.13114200	0.48922100
C	1.24826600	-0.09195200	0.80670400
C	1.84556200	-1.31673900	0.37132600
C	3.02346800	-1.24290200	-0.32538100
H	3.59166600	2.07785500	-0.43100800
H	1.48116200	2.05758200	0.82419600
H	1.38736100	-2.26054400	0.60394900
C	0.02724600	-0.09102500	1.51382200
H	-0.30278100	0.81160600	1.99959100
H	-0.35046400	-1.01449900	1.91907000
C	-1.97750800	-1.53155200	-1.23632900
H	-2.73598600	-1.64544800	-2.01058700
H	-1.01206400	-1.50478600	-1.72927800
H	-2.02661500	-2.40778000	-0.60002900
C	-1.91379100	1.65237200	-1.10908200
H	-2.66812900	1.85988000	-1.86778800
H	-1.92500900	2.47560400	-0.40394800
H	-0.95113900	1.62479100	-1.60733300
C	-3.52684300	0.00165300	1.10223600
H	-3.41590100	0.85692300	1.75914200
H	-4.53409600	0.03930700	0.68710000
H	-3.45262200	-0.90751100	1.68809200
Si	-2.30821800	0.03257100	-0.29630000
H	4.61662100	-0.07180800	-1.18658900

E_0(CASSCF,vacuo) -676.098476

E_0(CASSCF,CPCM) **-676.169932**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0984761938
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609848E+03
(     1) 0.9187920 ( 1349)-0.1348159 (  428) 0.1261478 ( 2950)-0.1009227 (  506)-0.0934745 ( 3028) 0.0672022 (  171)-0.0645661
( 1271) 0.0638818 ( 5970) 0.0587769 (   10)-0.0563231 ( 2941) 0.0561595 ( 1460) 0.0532750 (  617) 0.0513449 (   23) 0.0494660
( 4621) 0.0493327 (  508)-0.0487494 ( 5892)-0.0487460 ( 3139)-0.0452775 ( 2101) 0.0444976 (   16) 0.0399625 ( 1377) 0.0398534
( 1373) 0.0394217 ( 6053) 0.0392484 (  507)-0.0390906 ( 5996)-0.0390110 (  685)-0.0389470 (  430) 0.0380921 (  170) 0.0380230
( 5911)-0.0374456 ( 5966) 0.0356537 ( 6081)-0.0352190 ( 1430)-0.0351588 ( 1434)-0.0349481 (  429) 0.0346266 ( 3200)-0.0345089
(   92)-0.0340137 ( 2973)-0.0327925 ( 6058)-0.0326164 ( 1264)-0.0311836 ( 2969) 0.0311320 ( 3026) 0.0309400 ( 3205)-0.0271597
( 3035)-0.0254587 ( 3116) 0.0245820 ( 3120)-0.0242213 (  510)-0.0235072 (   87) 0.0234373 ( 2116) 0.0229722 (  619) 0.0226154
(  198) 0.0220715 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195324D+01
     2  0.133397D-06  0.190172D+01
     3 -0.115918D-06  0.316939D-07  0.188871D+01
     4  0.452290D-06 -0.112982D-04 -0.455569D-05  0.998533D+00
     5  0.287042D-05  0.103436D-05 -0.126507D-04  0.456749D-05  0.100008D+01
     6 -0.184111D-05  0.299772D-06 -0.183574D-05 -0.899575D-05 -0.184648D-06
     7  0.106586D-06  0.266260D-05  0.280662D-06 -0.363384D-05  0.425232D-05
     8 -0.391002D-06 -0.939173D-06  0.145264D-06 -0.122377D-05 -0.112962D-05
     9 -0.743425D-06  0.104954D-05  0.567866D-06 -0.558713D-05  0.182044D-06
                6             7             8             9
     6  0.952628D-01
     7  0.518999D-07  0.109343D+00
     8  0.255667D-06 -0.684643D-08  0.403303D-01
     9  0.616177D-06  0.179632D-06  0.572877D-07  0.127834D-01
MCSCF converged.
```

$^{3}2^{+}$b STEP 10

GEOMETRY

C	3.71192100	-0.05888000	-0.66891300
C	3.13339800	1.14473200	-0.22886700
C	1.94799900	1.12935700	0.49418700
C	1.28873600	-0.09438400	0.81582200
C	1.88066300	-1.31667100	0.36773500
C	3.04933900	-1.24017000	-0.34515000
H	3.61513100	2.08021800	-0.44512600
H	1.52233300	2.05471400	0.83869800
H	1.42626600	-2.26174200	0.60304900
C	0.07598600	-0.09668900	1.53815700
H	-0.25512600	0.80486500	2.02474800
H	-0.30301400	-1.02180400	1.93790900
C	-2.01442400	-1.52797900	-1.23878000
H	-2.76052400	-1.64278100	-2.02499600
H	-1.04171800	-1.49738200	-1.71729200
H	-2.07054600	-2.40469300	-0.60388000
C	-1.95440300	1.65608200	-1.10144200
H	-2.69680800	1.86815900	-1.87074700
H	-1.97453800	2.47565500	-0.39238800
H	-0.98454600	1.62854400	-1.58579100
C	-3.55100800	-0.00459400	1.11817000
H	-3.42826200	0.84887500	1.77528900
H	-4.56662700	0.03256800	0.72342200
H	-3.46306400	-0.91600100	1.69858100
Si	-2.36133000	0.03369700	-0.30308800
H	4.63041000	-0.06578400	-1.22375600

E_0(CASSCF,vacuo) -676.096165

E_0(CASSCF,CPCM) **-676.168226**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0961653562
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609617E+03
 (     1) 0.9181596 ( 1349)-0.1347836 (  428) 0.1249360 ( 2950)-0.1023541 (  506)-0.0907234 ( 3028) 0.0683340 ( 1271) 0.0642787
 (   171)-0.0621802 ( 5970) 0.0591753 (   10)-0.0574454 ( 2941) 0.0573031 ( 1460) 0.0534395 (  617) 0.0504801 (   23) 0.0502100
 (  4621) 0.0500402 ( 5892)-0.0493632 (  508)-0.0477212 ( 3139)-0.0461720 (  507)-0.0450247 (  170) 0.0439863 ( 2101) 0.0433849
 (  1377) 0.0400246 (   16) 0.0398534 (  429) 0.0398478 ( 6053) 0.0395029 ( 5996)-0.0393735 (   92)-0.0392502 ( 1373) 0.0376652
 (  5911)-0.0372772 (  430) 0.0363042 (  685)-0.0360578 ( 6081)-0.0351418 ( 1434)-0.0345553 ( 5966) 0.0342187 ( 3200)-0.0335014
 (  2973)-0.0333790 ( 6058)-0.0332164 ( 1430)-0.0331257 ( 3026) 0.0326072 ( 1264)-0.0307383 ( 2969) 0.0296579 ( 3035)-0.0256846
 (  3120)-0.0248131 ( 3205)-0.0247956 ( 3116) 0.0239273 (  510)-0.0228648 ( 2116) 0.0226184 (  433) 0.0222032 (  619) 0.0220951
 (   198) 0.0220928 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.195322D+01
      2 -0.779440D-06  0.190024D+01
      3  0.551864D-06 -0.585888D-06  0.188837D+01
      4 -0.162135D-05  0.342703D-04  0.259319D-05  0.998739D+00
      5 -0.682439D-05 -0.469609D-04 -0.205451D-04 -0.757130D-05  0.100009D+01
      6  0.243525D-05 -0.484800D-06  0.247779D-05  0.124951D-04 -0.195727D-05
      7 -0.257390D-06 -0.150448D-05  0.137502D-05  0.622116D-05 -0.213783D-04
      8  0.301122D-07  0.160890D-05  0.770516D-07  0.110742D-05  0.303553D-05
      9  0.534797D-07 -0.191805D-05  0.186616D-05 -0.176670D-05  0.709147D-05
                   6             7             8             9
      6  0.968876D-01
      7  0.269935D-06  0.110001D+00
      8 -0.655369D-06  0.262340D-06  0.406166D-01
      9 -0.514502D-06  0.903395D-07 -0.281868D-07  0.118370D-01
 MCSCF converged.
```

$^{3}2^{+}$b STEP 11

GEOMETRY

C	3.73388300	-0.05506600	-0.69328800
C	3.16090300	1.14615700	-0.24002900
C	1.98514100	1.12752900	0.49901600
C	1.33004700	-0.09707100	0.82438800
C	1.91647100	-1.31677900	0.36318500
C	3.07574900	-1.23731400	-0.36540900
H	3.63946600	2.08282900	-0.45855900
H	1.56448900	2.05162700	0.85319000
H	1.46575700	-2.26314700	0.60069200
C	0.12587900	-0.10280100	1.56169700
H	-0.20562600	0.79747500	2.05001400
H	-0.25396000	-1.02962400	1.95623100
C	-2.05356300	-1.52445400	-1.24061200
H	-2.78761600	-1.63897100	-2.03824800
H	-1.07407200	-1.49089700	-1.70522700
H	-2.11717000	-2.40200100	-0.60770000
C	-1.99624800	1.65917000	-1.09431800
H	-2.72704100	1.87472300	-1.87383700
H	-2.02517500	2.47596400	-0.38248100
H	-1.01968200	1.63152400	-1.56532500
C	-3.57608000	-0.00993200	1.13393600
H	-3.44196100	0.84198100	1.79085200
H	-4.59931100	0.02674100	0.75888000
H	-3.47532600	-0.92329200	1.70917400
Si	-2.41433700	0.03483800	-0.30847200
H	4.64485000	-0.05929400	-1.26045000

E_0(CASSCF,vacuo) -676.094049

E_0(CASSCF,CPCM) **-676.166696**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.09404879l9
Full Convergence on CI vector      -0.67609405E+03
          ( 1)        EIGENVALUE
(     1) 0.9175760 ( 1349)-0.1346549 (  428) 0.1217387 ( 2950)-0.1035018 (  506)-0.0858236 ( 3028) 0.0692706 ( 1271) 0.0645637
( 5970) 0.0594704 (   10)-0.0585965 ( 2941) 0.0584852 (  171)-0.0573378 ( 1460) 0.0535338 (  507)-0.0535285 (  170) 0.0525126
(   23) 0.0507556 ( 4621) 0.0505549 ( 5892)-0.0498289 (  617) 0.0486607 (  429) 0.0473450 ( 3139)-0.0468811 (   92)-0.0467546
(  508)-0.0463626 ( 2101) 0.0420808 ( 1377) 0.0401245 ( 6053) 0.0396698 ( 5996)-0.0396368 (   16) 0.0394446 ( 5911)-0.0371041
( 1373) 0.0358054 ( 6081)-0.0350907 (  430) 0.0342958 ( 1434)-0.0342259 ( 2973)-0.0338270 ( 6058)-0.0336759 ( 3026) 0.0335623
(  685)-0.0327829 ( 5966) 0.0327005 ( 3200)-0.0318163 ( 1430)-0.0310954 ( 1264)-0.0303781 ( 2969) 0.0280712 ( 3035)-0.0259916
( 3120)-0.0253118 ( 3116) 0.0230744 ( 3205)-0.0225735 (  618) 0.0223128 (  281)-0.0221745 (  510)-0.0221408 (  433) 0.0219433
( 2116) 0.0218667 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195321D+01
     2 -0.384237D-06  0.189898D+01
     3 -0.363147D-06  0.501990D-06  0.188806D+01
     4 -0.333760D-06  0.352341D-04  0.643458D-05  0.998980D+00
     5 -0.574860D-05 -0.324651D-04 -0.109771D-04 -0.512846D-05  0.100011D+01
     6  0.311522D-05 -0.162567D-05  0.484935D-05  0.121970D-04 -0.208044D-05
     7 -0.160152D-06 -0.199070D-05  0.228806D-05  0.820884D-05 -0.166124D-04
     8  0.344818D-06  0.122059D-05 -0.231180D-06  0.763221D-06  0.318678D-05
     9  0.140572D-05 -0.559606D-05 -0.840759D-06 -0.234964D-05  0.109509D-04
                6             7             8             9
     6  0.983617D-01
     7  0.451960D-08  0.110596D+00
     8 -0.372674D-06 -0.349608D-06  0.408862D-01
     9 -0.853251D-06 -0.293429D-06  0.393414D-07  0.108223D-01
MCSCF converged.
```

$^{3}2^{+}$b STEP 12

GEOMETRY

C	3.75615200	-0.05122600	-0.71747900
C	3.18913200	1.14762500	-0.25090400
C	2.02322700	1.12577400	0.50391300
C	1.37201700	-0.09970800	0.83271300
C	1.95254700	-1.31688900	0.35817000
C	3.10220600	-1.23445400	-0.38585700
H	3.66470000	2.08542300	-0.47149200
H	1.60785100	2.04856100	0.86782200
H	1.50528700	-2.26449000	0.59758200
C	0.17661700	-0.10881600	1.58465200
H	-0.15461300	0.79008000	2.07536700
H	-0.20386900	-1.03733000	1.97417700
C	-2.09201100	-1.51975700	-1.24310300
H	-2.80827400	-1.62890100	-2.05754000
H	-1.10263700	-1.48521200	-1.68672700
H	-2.17024400	-2.39988600	-0.61557800
C	-2.03955000	1.66253800	-1.08606900
H	-2.75362500	1.87718700	-1.88122600
H	-2.08511200	2.47789800	-0.37357800
H	-1.05314400	1.63748700	-1.53675800
C	-3.60360700	-0.01683600	1.14831700
H	-3.45992400	0.83324100	1.80561900
H	-4.63338400	0.01887500	0.79114300
H	-3.49074900	-0.93234800	1.71789200
Si	-2.46729100	0.03590900	-0.31257100
H	4.65944100	-0.05282300	-1.29683100

E_0(CASSCF,vacuo) -676.092127

E_0(CASSCF,CPCM) **-676.165382**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0921273483
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609213E+03
(     1) 0.9170470 ( 1349)-0.1344552 (  428) 0.1151242 ( 2950)-0.1044459 (  506)-0.0771850 ( 3028) 0.0700747 ( 1271) 0.0647813
(   507)-0.0645334 (  170) 0.0635365 (   10)-0.0597243 ( 5970) 0.0596991 ( 2941) 0.0596483 (  429) 0.0570270 (   92)-0.0564391
( 1460) 0.0535876 (   23) 0.0511722 ( 4621) 0.0509492 ( 5892)-0.0501909 (  171)-0.0485646 ( 3139)-0.0474574 (  617) 0.0452097
(  508)-0.0444769 ( 2101) 0.0403640 ( 1377) 0.0401827 ( 5996)-0.0398322 ( 6053) 0.0397844 (   16) 0.0385224 ( 5911)-0.0369346
( 6081)-0.0350611 ( 2973)-0.0341766 ( 6058)-0.0340324 ( 1434)-0.0339560 ( 3026) 0.0337156 ( 1373) 0.0336771 (  430) 0.0320014
( 5966) 0.0309417 ( 1264)-0.0300978 ( 3200)-0.0294620 (  685)-0.0291864 ( 1430)-0.0289124 (  618) 0.0269719 (  281)-0.0268263
( 3035)-0.0263458 ( 2969) 0.0262403 ( 3120)-0.0257346 ( 3116) 0.0219148 (  510)-0.0212121 ( 4643) 0.0210441 (  433) 0.0209901
(  198) 0.0209814 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195319D+01
     2 -0.152728D-06  0.189791D+01
     3 -0.148937D-06  0.428987D-06  0.188778D+01
     4 -0.666481D-05  0.111372D-04  0.249034D-05  0.999225D+00
     5 -0.669077D-05 -0.299630D-05  0.100150D-04  0.154100D-04  0.100014D+01
     6 -0.154663D-06 -0.248715D-05  0.467233D-05  0.127165D-04  0.634589D-05
     7 -0.917500D-06 -0.536107D-05 -0.646131D-05  0.509729D-05  0.955029D-06
     8  0.612196D-06  0.950690D-06  0.682332D-06  0.106911D-05 -0.357470D-06
     9  0.232015D-05  0.440748D-06  0.138663D-05  0.450072D-05  0.270910D-05
                6             7             8             9
     6  0.997058D-01
     7 -0.545968D-06  0.111134D+00
     8 -0.251030D-06 -0.383206D-06  0.411376D-01
     9 -0.818699D-06 -0.710160D-06 -0.185675D-07  0.977459D-02
MCSCF converged.
```

$^{3}2^{+}$b STEP 13

GEOMETRY

C	3.77875800	-0.04742400	-0.74143300
C	3.21798500	1.14909200	-0.26162300
C	2.06204300	1.12404800	0.50854800
C	1.41448100	-0.10237300	0.84054200
C	1.98883000	-1.31708100	0.35261000
C	3.12878400	-1.23165100	-0.40639500
H	3.69078300	2.08794300	-0.48400600
H	1.65212300	2.04545600	0.88219300
H	1.54488600	-2.26586500	0.59376700
C	0.22809300	-0.11475000	1.60677200
H	-0.10252300	0.78277800	2.10009800
H	-0.15315300	-1.04484000	1.99141300
C	-2.13111600	-1.51294500	-1.24837900
H	-2.81955200	-1.60722000	-2.08821100
H	-1.12709000	-1.48160100	-1.65889500
H	-2.23644600	-2.39852400	-0.63278100
C	-2.08577100	1.66674300	-1.07633600
H	-2.77502300	1.87416700	-1.89492200
H	-2.15975400	2.48225000	-0.36655600
H	-1.08530600	1.64880700	-1.49606900
C	-3.63036800	-0.02657100	1.16387700
H	-3.47707000	0.82076000	1.82261000
H	-4.66663200	0.00812700	0.82555600
H	-3.50470100	-0.94495000	1.72616900
Si	-2.52037200	0.03690100	-0.31548700
H	4.67434600	-0.04643500	-1.33264800

E_0(CASSCF,vacuo) -676.090394

E_0(CASSCF,CPCM) **-676.164232**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0903935467
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609039E+03
(     1) 0.9165653 ( 1349)-0.1341982 (  428) 0.1166122 ( 2950)-0.1052158 (  506)-0.0778193 ( 3028) 0.0707583 (  507)-0.0650419
( 1271) 0.0649488 (  170) 0.0640669 (   10)-0.0608207 ( 2941) 0.0607881 ( 5970) 0.0598725 (  429) 0.0574371 (   92)-0.0568514
( 1460) 0.0536115 (   23) 0.0514729 ( 4621) 0.0512393 ( 5892)-0.0504762 (  171)-0.0488630 ( 3139)-0.0479243 (  617) 0.0456149
(  508)-0.0439531 ( 1377) 0.0402106 ( 5996)-0.0399785 ( 2101) 0.0399268 ( 6053) 0.0398619 (   16) 0.0387609 ( 5911)-0.0367731
( 6081)-0.0350466 ( 3026) 0.0346384 ( 2973)-0.0344522 ( 6058)-0.0343092 ( 1434)-0.0337366 ( 1373) 0.0326742 (  430) 0.0307822
( 5966) 0.0301968 ( 1264)-0.0298805 ( 3200)-0.0278037 ( 1430)-0.0277606 (  618) 0.0272267 (  281)-0.0270752 ( 3035)-0.0267149
(  685)-0.0266124 ( 3120)-0.0260936 ( 2969) 0.0253034 ( 3116) 0.0214229 (  198) 0.0212035 ( 4643) 0.0212025 (  510)-0.0209591
(  255)-0.0206631 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195318D+01
     2 -0.381921D-05  0.189700D+01
     3  0.108498D-05  0.919424D-06  0.188754D+01
     4  0.739173D-06  0.111380D-04  0.147164D-04  0.999467D+00
     5 -0.132927D-04  0.249702D-05 -0.720736D-05  0.215747D-03  0.100018D+01
     6 -0.316203D-04 -0.144962D-04  0.834426D-05  0.776672D-06  0.510398D-05
     7  0.123389D-04 -0.220115D-04 -0.188013D-04  0.364010D-05 -0.321872D-05
     8 -0.286094D-05 -0.275490D-04  0.120922D-04 -0.196297D-04 -0.191529D-04
     9  0.690474D-05 -0.685576D-05  0.112759D-04  0.151845D-04  0.669494D-05
                6             7             8             9
     6  0.100927D+00
     7 -0.120550D-05  0.111615D+00
     8 -0.254481D-05  0.201386D-06  0.413718D-01
     9 -0.328876D-05 -0.104120D-05  0.120022D-05  0.872743D-02
MCSCF converged.
```

$^{3}2^{+}$b STEP 14

GEOMETRY

C	3.80177600	-0.04250800	-0.76512400
C	3.24723200	1.15107100	-0.27105400
C	2.10136900	1.12180900	0.51412500
C	1.45763300	-0.10602900	0.84794700
C	2.02587500	-1.31767400	0.34562700
C	3.15596000	-1.22823500	-0.42797200
H	3.71710300	2.09126800	-0.49425800
H	1.69674100	2.04134000	0.89818900
H	1.58526400	-2.26792000	0.58737800
C	0.28034400	-0.12267200	1.62807500
H	-0.04947400	0.77288000	2.12523900
H	-0.10136800	-1.05474700	2.00708400
C	-2.16924700	-1.50342000	-1.25634500
H	-2.82737300	-1.57996700	-2.12177100
H	-1.15101900	-1.47491000	-1.63151100
H	-2.30234800	-2.39595200	-0.65655000
C	-2.13357000	1.67297200	-1.06274400
H	-2.79686600	1.87411400	-1.90392800
H	-2.23676200	2.48726200	-0.35536000
H	-1.11984000	1.66379600	-1.45057500
C	-3.65988800	-0.03992000	1.17756100
H	-3.49942600	0.80366000	1.83946400
H	-4.70158700	-0.00695900	0.85588700
H	-3.52181800	-0.96191300	1.73104300
Si	-2.57326400	0.03813100	-0.31734900
H	4.68955200	-0.03815900	-1.36801300

E_0(CASSCF,vacuo) -676.088836

E_0(CASSCF,CPCM) **-676.163239**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0888364388
 Full Convergence on CI vector      -0.67608884E+03
          ( 1)        EIGENVALUE
 (     1) 0.9161372 ( 1349)-0.1339180 (   428) 0.1179932 ( 2950)-0.1058552 (  506)-0.0785183 ( 3028) 0.0713724 (  507)-0.0655591
 ( 1271) 0.0651063 (  170) 0.0646022 (    10)-0.0618385 ( 2941) 0.0618339 ( 5970) 0.0600096 (  429) 0.0578238 (   92)-0.0572392
 ( 1460) 0.0536198 (   23) 0.0517053 ( 4621) 0.0514681 ( 5892)-0.0507112 (  171)-0.0491064 ( 3139)-0.0483120 (  617) 0.0459988
 (  508)-0.0434520 ( 1377) 0.0402195 ( 5996)-0.0400827 ( 6053) 0.0399145 ( 2101) 0.0395446 (   16) 0.0389824 ( 5911)-0.0366277
 ( 3026) 0.0353682 ( 6081)-0.0350464 ( 2973)-0.0346757 ( 6058)-0.0345307 ( 1434)-0.0335608 ( 1373) 0.0317624 ( 1264)-0.0297246
 (  430) 0.0296897 ( 5966) 0.0295349 (  618) 0.0274605 (  281)-0.0273032 ( 3035)-0.0270799 ( 1430)-0.0267419 ( 3120)-0.0263979
 ( 3200)-0.0259810 ( 2969) 0.0244254 (  685)-0.0242177 (  198) 0.0214076 ( 4643) 0.0213372 (  422) 0.0211323 ( 3116) 0.0209164
 (  255)-0.0208656 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195316D+01
     2 -0.705307D-07  0.189622D+01
     3 -0.192997D-06  0.259974D-06  0.188732D+01
     4  0.142244D-07  0.326911D-06  0.338189D-05  0.999700D+00
     5  0.581297D-05  0.616189D-05 -0.291829D-05  0.409728D-03  0.100022D+01
     6  0.938378D-06  0.774557D-06  0.295367D-06  0.355915D-05 -0.308294D-05
     7  0.378138D-06 -0.294724D-05 -0.473245D-06 -0.146011D-05  0.135474D-04
     8 -0.113728D-06  0.196400D-06 -0.761096D-06 -0.307909D-06  0.957037D-06
     9  0.108238D-06  0.125292D-06  0.291531D-06  0.332207D-05  0.167195D-06
                6             7             8             9
     6  0.102023D+00
     7 -0.563584D-07  0.112048D+00
     8  0.141511D-06 -0.823111D-07  0.415841D-01
     9 -0.193702D-06  0.728017D-07 -0.187655D-07  0.772183D-02
 MCSCF converged.
```

$^{3}2^{+}$b STEP 15

GEOMETRY

C	3.82588100	-0.05012800	-0.78772500
C	3.28177500	1.14726400	-0.29160300
C	2.14582500	1.12547500	0.50813600
C	1.50115800	-0.09823000	0.85578900
C	2.05937300	-1.31395900	0.35106100
C	3.17985800	-1.23181300	-0.43734600
H	3.75257000	2.08484000	-0.52402600
H	1.75005700	2.04812600	0.89406600
H	1.61976500	-2.26190600	0.60364700
C	0.33313900	-0.10696400	1.64994100
H	0.00722700	0.79299000	2.14138000
H	-0.05162700	-1.03562400	2.03379200
C	-2.21572400	-1.51515100	-1.23735300
H	-2.83636900	-1.58029600	-2.13086300
H	-1.18210000	-1.50478300	-1.56949400
H	-2.38894900	-2.40432000	-0.64307500
C	-2.17532400	1.66016700	-1.07829800
H	-2.80363800	1.83928400	-1.95039400
H	-2.31133600	2.48711400	-0.39162800
H	-1.14689900	1.65099900	-1.42479100
C	-3.69220400	-0.02557200	1.19143200
H	-3.52140900	0.82525700	1.84151700
H	-4.73874300	0.00450200	0.88554100
H	-3.54603300	-0.94171700	1.75260000
Si	-2.62650300	0.03574500	-0.31862100
H	4.70598500	-0.05143700	-1.40178300

E_0(CASSCF,vacuo) -676.087442

E_0(CASSCF,CPCM) **-676.162350**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0874424220
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608744E+03
(     1) 0.9157276 ( 1349)-0.1335262 (  428) 0.1192998 ( 2950)-0.1063918 (  506)-0.0793416 ( 3028) 0.0718862 (  507)-0.0661305
( 1271) 0.0652049 (  170) 0.0651634 ( 2941) 0.0628444 (   10)-0.0628122 ( 5970) 0.0601066 (  429) 0.0581919 (   92)-0.0575754
( 1460) 0.0536070 (   23) 0.0518578 ( 4621) 0.0516311 ( 5892)-0.0509074 (  171)-0.0493247 ( 3139)-0.0486431 (  617) 0.0463928
(  508)-0.0429637 ( 1377) 0.0402159 ( 5996)-0.0401725 ( 6053) 0.0399503 ( 2101) 0.0391966 (   16) 0.0391732 ( 5911)-0.0365006
( 3026) 0.0359254 ( 6081)-0.0350543 ( 2973)-0.0348623 ( 6058)-0.0347108 ( 1434)-0.0334206 ( 1373) 0.0309332 ( 1264)-0.0296307
( 5966) 0.0289350 (  430) 0.0286931 (  618) 0.0276970 (  281)-0.0275251 ( 3035)-0.0274617 ( 3120)-0.0266715 ( 1430)-0.0258087
( 3200)-0.0239976 ( 2969) 0.0235995 (  422) 0.0225507 (  685)-0.0220174 (  198) 0.0216226 ( 4643) 0.0214449 (  255)-0.0210808
( 2116) 0.0209866 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195313D+01
     2  0.460236D-06  0.189553D+01
     3 -0.554424D-06  0.181018D-06  0.188712D+01
     4  0.477671D-05 -0.438160D-05 -0.112595D-04  0.999914D+00
     5 -0.667475D-05 -0.142904D-05  0.173843D-04  0.616915D-03  0.100027D+01
     6  0.607876D-06  0.325455D-06 -0.404175D-05 -0.409055D-05  0.142762D-05
     7 -0.179562D-06 -0.162132D-05 -0.653898D-06  0.466564D-05 -0.898069D-05
     8  0.130545D-05 -0.196096D-06  0.455067D-06  0.467116D-06 -0.357250D-05
     9 -0.311044D-05  0.788389D-05 -0.692083D-06 -0.119026D-04 -0.891475D-05
                6             7             8             9
     6  0.103041D+00
     7 -0.285310D-06  0.112429D+00
     8  0.594285D-06 -0.105685D-06  0.417937D-01
     9  0.300131D-06  0.754808D-06  0.164985D-06  0.676861D-02
MCSCF converged.
```

$^{1}2^{+}$c STEP 1

GEOMETRY

C	0.01384700	0.01871600	0.00837700
C	0.01539300	-0.01312200	1.43646400
C	1.18720000	-0.03935200	2.15830100
C	2.43385400	0.09304200	1.44049200
C	2.21545800	-0.14340500	0.12537400
C	1.19947300	0.07601000	-0.74679600
H	-0.92926700	-0.00421600	1.94599200
H	1.19274300	0.05979900	3.22750900
H	1.22293900	-0.07928400	-1.80680700
C	3.71537800	0.52224600	2.04980900
H	3.51902400	1.17064800	2.89463600
H	4.32606100	1.06045900	1.33250100
C	5.33373800	-2.10671000	1.25358600
H	6.00324000	-2.91019600	1.54990500
H	4.45884900	-2.57280500	0.80836500
H	5.84306300	-1.53750100	0.48066400
C	3.91115200	-1.99278700	4.02999500
H	4.51612000	-2.79131400	4.45174900
H	3.60209400	-1.35823000	4.85613900
H	3.02323000	-2.45733800	3.60956900
C	6.40284800	-0.18309100	3.47862200
H	6.13118600	0.47513500	4.29874600
H	7.10343000	-0.91572300	3.87094100
H	6.93468200	0.40809500	2.73882500
Si	4.90335800	-1.04206900	2.74419800
H	-0.90071800	-0.18268600	-0.51946100

E_0(CASSCF,vacuo) -676.120018

E_0(CASSCF,CPCM) **-676.193854**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1200177789
 Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.676120O2E+03
 (     1) 0.9210014 (     3)-0.1640271 (    30) 0.0974041 (     8)-0.0950135 (     6)-0.0932649 (    43) 0.0932000 ( 1891)-0.0851740
 (    28)-0.0789479 (    67) 0.0727350 (   234)-0.0678281 (    45)-0.0576203 (   255)-0.0530559 (   241) 0.0526581 (   240) 0.0509341
 (   257)-0.0506874 (   286)-0.0497207 (    55)-0.0487522 (   309)-0.0462592 (   307) 0.0456843 (   279)-0.0456792 (    10)-0.0432609
 (    36)-0.0420301 (   276)-0.0416626 (   258)-0.0389373 (   310) 0.0357097 (   300)-0.0342569 (   325)-0.0338571 (   121) 0.0323171
 (   253)-0.0317819 (    35)-0.0315194 (    79) 0.0297036 (    38) 0.0295908 (    92)-0.0281071 (    32)-0.0265649 (   283) 0.0263328
 (    78) 0.0262773 (     5) 0.0260022 (    24) 0.0246700 (   704)-0.0246017 ( 1836)-0.0245159 (   238)-0.0240655 (    91) 0.0235806
 (   303)-0.0227173 ( 1856) 0.0210539 (    31) 0.0206398 ( 1656) 0.0204587 (   285)-0.0192570 (    26) 0.0191314 (   298) 0.0183478
 (     9)-0.0183298 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.197832D+01
      2 -0.477373D-06  0.194831D+01
      3  0.630269D-06  0.771011D-06  0.190294D+01
      4  0.271685D-05  0.492818D-05 -0.469675D-05  0.185173D+01
      5  0.228727D-04  0.307923D-04  0.105899D-05 -0.551514D-04  0.138790D+00
      6 -0.483573D-05  0.303377D-06  0.182518D-04 -0.157843D-04 -0.375414D-05
      7  0.146133D-04  0.279834D-04  0.144465D-04 -0.534502D-04  0.842197D-05
      8 -0.105137D-04 -0.174784D-04 -0.844115D-05  0.401629D-04 -0.400975D-05
      9 -0.192514D-05  0.236384D-06 -0.804517D-07  0.416283D-05 -0.222425D-06
                   6             7             8             9
      6  0.709710D-01
      7 -0.621231D-05  0.579898D-01
      8 -0.447476D-05 -0.600869D-06  0.307417D-01
      9 -0.532419D-06  0.240085D-06 -0.443656D-06  0.202017D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 2

GEOMETRY

C	0.01268000	0.00733800	0.00974200
C	0.01425200	-0.00626600	1.43937800
C	1.18536100	-0.01900500	2.15886600
C	2.42747500	0.10909700	1.43104500
C	2.23072800	-0.15160700	0.10998700
C	1.19900500	0.06032100	-0.74630700
H	-0.93071600	0.01017200	1.94833600
H	1.19203900	0.10239800	3.22576600
H	1.21475400	-0.10000900	-1.80588700
C	3.69323500	0.56349000	2.02835400
H	3.50568600	1.21851000	2.86888700
H	4.32103900	1.06999800	1.30395500
C	5.38668000	-2.12701400	1.32849400
H	6.05962500	-2.92322000	1.63722500
H	4.51204800	-2.60124900	0.89231400
H	5.89235300	-1.56627800	0.54758000
C	3.95457700	-1.95769000	4.10581600
H	4.55913900	-2.74233300	4.55399000
H	3.63877700	-1.29966200	4.91030100
H	3.07141600	-2.43515600	3.69069600
C	6.42705200	-0.12437600	3.50798600
H	6.13712100	0.55221700	4.30623600
H	7.14396700	-0.82789600	3.92403700
H	6.94501700	0.45473000	2.74946200
Si	4.95264200	-1.04390100	2.80128500
H	-0.90133000	-0.20937100	-0.51316500

E_0(CASSCF,vacuo) -676.115345

E_0(CASSCF,CPCM) **-676.187768**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1153446462
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611534E+03
(     1) 0.9146554 (    3)-0.2024086 (   43) 0.0941839 (   30) 0.0909203 (    8)-0.0896528 ( 1891)-0.0871678 (    6)-0.0859681
(    45)-0.0778475 (  234)-0.0745903 (   67) 0.0653564 (  286)-0.0624317 (   28)-0.0596407 (  255)-0.0584201 (  309)-0.0573943
(   240) 0.0488748 (   55)-0.0479418 (  241) 0.0461975 (  258)-0.0424527 (  276)-0.0416612 (  307) 0.0398568 (   32)-0.0395243
(   121) 0.0394457 (   36)-0.0388278 (  257)-0.0383192 (  300)-0.0376762 (  279)-0.0348949 (  325)-0.0340283 ( 1836)-0.0312985
(    10)-0.0307339 (  310) 0.0295869 (   79) 0.0294545 ( 1856) 0.0287299 (   91) 0.0278849 (  253)-0.0275726 (   92)-0.0260800
(   303)-0.0258544 (   24) 0.0255639 (  704)-0.0249373 ( 1656) 0.0244086 (   78) 0.0242606 (  283) 0.0239375 (  238)-0.0237467
(    38) 0.0194167 (  298) 0.0192407 ( 2145) 0.0190914 ( 1890) 0.0187250 (  407) 0.0174609 (  244) 0.0171866 (  497) 0.0165984
(    13) 0.0165107 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.197385D+01
     2  0.342325D-06  0.194629D+01
     3 -0.155858D-05  0.291271D-05  0.190438D+01
     4  0.167590D-05  0.629248D-05 -0.884657D-05  0.183117D+01
     5  0.115812D-04  0.963935D-05 -0.303250D-04 -0.300980D-04  0.158341D+00
     6 -0.184286D-05  0.146186D-04  0.752432D-05 -0.151785D-05 -0.374291D-05
     7  0.830976D-05  0.133340D-04 -0.950517D-05 -0.386733D-04  0.262452D-05
     8  0.182793D-05 -0.303659D-05 -0.690895D-05  0.186722D-04 -0.330139D-05
     9 -0.912331D-06 -0.587547D-06 -0.985041D-07  0.314113D-05 -0.214942D-06
                6             7             8             9
     6  0.660540D-01
     7 -0.443575D-05  0.636119D-01
     8 -0.775973D-05  0.120474D-05  0.322917D-01
     9 -0.661990D-06  0.104616D-06 -0.511499D-06  0.240126D-01
MCSCF converged.
```

$^{1}2^{+}$c STEP 3

GEOMETRY

C	0.01286400	-0.00766100	0.01759900
C	0.01735000	-0.00278300	1.44608500
C	1.19053500	0.00439000	2.15883900
C	2.42990000	0.11797800	1.42229100
C	2.26378500	-0.15607900	0.08764300
C	1.20377700	0.03788500	-0.73792300
H	-0.92590200	0.01890600	1.95818600
H	1.19927500	0.15159800	3.22252600
H	1.20971100	-0.11465900	-1.79906900
C	3.67714600	0.57799900	2.01275600
H	3.51228400	1.22256500	2.86471400
H	4.33659100	1.04759100	1.29286600
C	5.43251300	-2.16343000	1.36859300
H	6.10556600	-2.96049100	1.67589900
H	4.55704400	-2.63418300	0.93144700
H	5.93781700	-1.59823900	0.59127200
C	3.98455900	-1.98111900	4.14786900
H	4.58487400	-2.75942500	4.61321200
H	3.66079400	-1.31091100	4.93848100
H	3.10686100	-2.46298700	3.72744200
C	6.44239400	-0.11885300	3.53669500
H	6.13247000	0.56192600	4.32334300
H	7.17500100	-0.79863700	3.96552200
H	6.94729700	0.45961600	2.76940900
Si	4.99739400	-1.08950600	2.84359200
H	-0.90253900	-0.23025800	-0.50034400

E_0(CASSCF,vacuo) -676.109307

E_0(CASSCF,CPCM) **-676.179996**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1093065896
Full Convergence on CI vector
         ( 1)      EIGENVALUE     -0.67610931E+03
(    1) 0.9009897 (    3)-0.2643994 (   45)-0.0940873 (  234)-0.0825706 ( 1891)-0.0788000 (   43) 0.0772517 (   30) 0.0709593
(  286)-0.0686851 (    6)-0.0671015 (    8)-0.0644835 (  309)-0.0630432 (  255)-0.0600801 (   32)-0.0514124 (  240) 0.0511162
(   67) 0.0457737 (  121) 0.0457294 (   55)-0.0444935 (  300)-0.0433401 (   79) 0.0427982 (   36)-0.0414144 (  276)-0.0406509
(  258)-0.0401604 ( 1836)-0.0378556 ( 1856) 0.0371504 (   28)-0.0362437 (   91) 0.0342103 (  241) 0.0329597 (  325)-0.0316060
( 1890) 0.0295887 (  307) 0.0288117 ( 1656) 0.0285251 (   52) 0.0272432 (   47)-0.0266172 (   38) 0.0262886 (  704)-0.0261516
( 1711)-0.0259449 (   24) 0.0251845 (  283) 0.0249643 (  303)-0.0248506 (  244) 0.0245523 ( 2145) 0.0229996 (   78) 0.0229102
(  352) 0.0224909 (  257)-0.0223869 (  253)-0.0223226 (  238)-0.0222420 (   92)-0.0219705 (  392) 0.0218255 (   44) 0.0215437
(   10)-0.0212831 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.196899D+01
     2  0.638597D-06  0.194274D+01
     3  0.370002D-06 -0.156383D-05  0.190639D+01
     4 -0.426755D-05  0.425244D-06  0.305218D-05  0.178315D+01
     5 -0.184809D-04  0.118485D-04  0.129050D-04  0.344167D-04  0.207033D+00
     6  0.737148D-05  0.713196D-05 -0.187170D-05 -0.208859D-04  0.399973D-06
     7 -0.561589D-05  0.384830D-05 -0.140289D-05  0.161185D-04 -0.845034D-05
     8  0.102435D-05 -0.189927D-05 -0.183988D-05 -0.122120D-04  0.409839D-05
     9  0.271440D-05 -0.107143D-05 -0.462175D-06 -0.385324D-05  0.116703D-05
                6             7             8             9
     6  0.604533D-01
     7  0.470341D-06  0.703802D-01
     8 -0.883036D-06  0.870093D-06  0.341269D-01
     9 -0.333212D-07  0.116235D-06 -0.124632D-06  0.267416D-01
MCSCF converged.
```

$^{1}2^{+}$c STEP 4

GEOMETRY

C	0.07926900	-0.28229900	0.10222400
C	0.08389400	-0.07263300	1.47716100
C	1.27562000	0.21769800	2.14367400
C	2.51142500	0.30189500	1.43286800
C	2.44182500	0.03141200	0.04290900
C	1.30076200	-0.20815400	-0.64690000
H	-0.83492400	-0.12008300	2.02992200
H	1.26450400	0.43519900	3.19618700
H	1.30304200	-0.37700800	-1.70703000
C	3.72033900	0.64875400	2.07545100
H	3.64622300	1.12833000	3.03967800
H	4.51948100	1.01342600	1.44715100
C	5.34090000	-2.16130600	1.28289400
H	5.97442800	-3.01492000	1.51737600
H	4.43390000	-2.54444600	0.82829900
H	5.86712700	-1.55944300	0.54964300
C	3.86277700	-2.04359800	4.08236700
H	4.38916000	-2.88130100	4.53645800
H	3.56959600	-1.37528500	4.88515700
H	2.96818500	-2.43893700	3.61366600
C	6.41716900	-0.24629700	3.56757900
H	6.10462100	0.41229200	4.37091900
H	7.14154500	-0.94386600	3.98433600
H	6.93244800	0.34397500	2.81741900
Si	4.99137300	-1.21273400	2.85000200
H	-0.83450400	-0.52830500	-0.40488400

E_0(CASSCF,vacuo) -676.107967

E_0(CASSCF,CPCM) **-676.175372**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1079669114
 Full Convergence on CI vector
          ( 1)        EIGENVALUE     -0.67610797E+03
 (     1) 0.7136998 (     3)-0.6007733 (   234)-0.0929341 (    45)-0.0871892 (    91) 0.0745894 (    26)-0.0616310 (   235)-0.0536461
 (   276)-0.0525571 (   255)-0.0485814 ( 1600)-0.0480795 ( 1721)-0.0464224 (   378) 0.0459882 (   284)-0.0459327 (   352) 0.0443522
 (   821)-0.0416801 ( 1967) 0.0404257 (   390) 0.0394501 (    36)-0.0388368 (    24) 0.0387066 (    47)-0.0375994 (   121) 0.0375808
 (   300)-0.0364767 ( 1083) 0.0360648 (    44) 0.0353627 (    32)-0.0342076 ( 1779)-0.0338833 (    78) 0.0330221 (   122)-0.0326692
 ( 1711)-0.0322050 (   309)-0.0314487 (   406) 0.0309328 (    55)-0.0300044 ( 2029) 0.0299256 ( 1678)-0.0298034 ( 1713)-0.0296593
 (   379) 0.0291154 (   286)-0.0290412 (    90)-0.0290264 ( 1599) 0.0289614 (   331) 0.0286876 (   299)-0.0285678 (   285)-0.0284462
 (   256)-0.0277176 ( 1953) 0.0273068 (   419) 0.0264625 (    70) 0.0263478 (   105) 0.0263342 (    30) 0.0260052 ( 1605) 0.0259532
 (    98) 0.0257080 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195411D+01
     2 -0.223645D-06  0.192077D+01
     3 -0.446903D-07 -0.546188D-06  0.190508D+01
     4 -0.508782D-05 -0.541036D-05  0.202532D-04  0.115921D+01
     5  0.168216D-04  0.474461D-05 -0.121654D-05  0.524909D-05  0.839622D+00
     6  0.123061D-05  0.425717D-07  0.987427D-06 -0.832133D-05 -0.239716D-05
     7  0.200222D-05  0.384815D-05  0.943620D-06  0.870841D-05 -0.413090D-05
     8 -0.226956D-05 -0.173575D-05  0.142381D-05  0.567366D-05  0.148196D-05
     9  0.231172D-06  0.583105D-06 -0.110580D-05  0.131814D-06 -0.691822D-06
                6             7             8             9
     6  0.766037D-01
     7  0.329257D-06  0.894999D-01
     8 -0.171190D-06 -0.357650D-06  0.395395D-01
     9  0.106393D-06  0.148241D-06 -0.950803D-07  0.155592D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 5

GEOMETRY

C	0.01464400	-0.02393800	0.00150700
C	0.01201000	-0.01544300	1.39182200
C	1.21533100	-0.00673400	2.10259000
C	2.46517400	-0.01160600	1.42094700
C	2.39657000	-0.05817000	0.00634500
C	1.25111500	-0.02716900	-0.71938500
H	-0.91887900	-0.00231600	1.92617300
H	1.20510800	0.05029500	3.17607200
H	1.25967100	-0.03462500	-1.79284800
C	3.69618300	0.04088600	2.11445700
H	3.67860300	0.35147400	3.14732200
H	4.56973900	0.34090700	1.55652900
C	4.90034300	-2.89186600	0.90931600
H	5.37346400	-3.86935900	0.98866900
H	3.95041100	-3.02925500	0.40484300
H	5.53738200	-2.27261100	0.28718800
C	3.38692500	-2.96667500	3.69998300
H	3.73857100	-3.94659700	4.01904900
H	3.19512500	-2.38581700	4.59572300
H	2.45187500	-3.11369100	3.17093400
C	6.21433900	-1.54374200	3.46901900
H	5.98030600	-0.96849600	4.35822800
H	6.82003700	-2.39255600	3.78274300
H	6.82685800	-0.93548400	2.81242800
Si	4.68437600	-2.18128200	2.61716900
H	-0.91160900	-0.04665800	-0.54102000

E_0(CASSCF,vacuo) -676.105327

E_0(CASSCF,CPCM) **-676.173094**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1053273259
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610533E+03
 (     1) 0.7038478 (     3)-0.6096242 (   234)-0.0947351 (    45)-0.0822855 (    91) 0.0721807 (    26)-0.0554111 (   276)-0.0549191
 (    24) 0.0548306 ( 1600)-0.0493154 (   378) 0.0491122 ( 1721)-0.0488164 (   255)-0.0487441 (   821)-0.0480153 (   352) 0.0459878
 ( 1967) 0.0433845 ( 1083) 0.0426120 (   284)-0.0413838 (    36)-0.0399138 (   235)-0.0394203 (    44) 0.0391390 (   285)-0.0382914
 (  300)-0.0380978 ( 1779)-0.0369522 (   390) 0.0367528 (   299)-0.0352066 (   121) 0.0349776 (    78) 0.0349769 (    30) 0.0337447
 ( 1678)-0.0337083 (   90)-0.0333319 (   391) 0.0332455 ( 2029) 0.0331532 (   406) 0.0331360 (    47)-0.0327890 ( 1711)-0.0314862
 (  122)-0.0312414 (  405) 0.0311821 (    32)-0.0310091 (   331) 0.0303969 ( 1920) 0.0297257 ( 1713)-0.0293978 (    55)-0.0291461
 ( 1605) 0.0277473 ( 1609) 0.0275923 (   256)-0.0274407 ( 1953) 0.0272461 ( 1770)-0.0265681 (   105) 0.0259447 ( 1619)-0.0258328
 (  441)-0.0255978 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195347D+01
     2 -0.721237D-06  0.191622D+01
     3 -0.835867D-06 -0.192320D-06  0.190342D+01
     4  0.311876D-05  0.723189D-05  0.101369D-04  0.113255D+01
     5  0.266749D-05  0.945375D-05  0.249825D-06 -0.198857D-05  0.865234D+00
     6 -0.208767D-05 -0.100524D-05  0.195511D-05 -0.581890D-05 -0.907627D-05
     7 -0.786529D-06 -0.771958D-07  0.206684D-05 -0.718977D-05  0.395242D-05
     8  0.165370D-06 -0.152479D-05 -0.105880D-05  0.269586D-05  0.120629D-05
     9 -0.486978D-06 -0.236305D-06  0.149418D-06 -0.815771D-06 -0.177107D-05
                6             7             8             9
     6  0.832735D-01
     7 -0.440086D-07  0.911216D-01
     8 -0.201745D-05  0.184627D-06  0.398380D-01
     9 -0.200157D-06  0.380632D-06 -0.165256D-06  0.148586D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 6

GEOMETRY

C	0.01022800	-0.01976600	0.00304400
C	0.00966400	-0.01116800	1.39311700
C	1.21448600	-0.00528100	2.10352800
C	2.46049300	-0.01352900	1.42155400
C	2.39086900	-0.05396800	0.00777300
C	1.24359400	-0.02463500	-0.71785900
H	-0.92057100	0.00369500	1.92875000
H	1.20423200	0.04672300	3.17745100
H	1.25217000	-0.02824000	-1.79137100
C	3.69527700	0.02799300	2.11364200
H	3.68759100	0.31474200	3.15285300
H	4.57648800	0.30698200	1.55829100
C	4.90360500	-2.96027000	0.89098300
H	5.34882100	-3.95292300	0.94172600
H	3.94763200	-3.05667300	0.38853100
H	5.55557800	-2.34189900	0.28394600
C	3.39438800	-3.05118900	3.68864600
H	3.71523300	-4.04684400	3.99196300
H	3.22227100	-2.47763900	4.59281300
H	2.45552400	-3.16014200	3.15732100
C	6.23937300	-1.64699800	3.46572400
H	6.00295200	-1.07579200	4.35673300
H	6.85078900	-2.49324700	3.77629600
H	6.84645300	-1.03431800	2.80841500
Si	4.71347700	-2.29235700	2.61683300
H	-0.91722200	-0.03565200	-0.53781100

E_0(CASSCF,vacuo) -676.102623

E_0(CASSCF,CPCM) **-676.170740**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1026233656
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610262E+03
 (     1) 0.6971192 (     3)-0.6157505 (   234)-0.0924150 (    45)-0.0788405 (    91) 0.0703433 (    24) 0.0664517 (   276)-0.0572073
 (   821)-0.0519845 (   378) 0.0517967 (    26)-0.0503631 ( 1721)-0.0494299 ( 1600)-0.0490347 ( 1083) 0.0468920 (   255)-0.0467222
 (   352) 0.0456900 ( 1967) 0.0445816 (   285)-0.0445032 (    36)-0.0403148 (   300)-0.0403038 (    44) 0.0398786 (   391) 0.0395036
 (    30) 0.0392771 (   284)-0.0389109 (   299)-0.0384007 ( 1779)-0.0378131 (    78) 0.0361370 (   406) 0.0357355 ( 1678)-0.0356456
 (   390) 0.0353621 (    90)-0.0348484 (   405) 0.0344191 ( 2029) 0.0343277 (   121) 0.0325670 ( 1920) 0.0319544 ( 1711)-0.0304991
 (   331) 0.0298988 (   122)-0.0297429 (    47)-0.0291712 (    32)-0.0289414 ( 1770)-0.0285874 ( 1713)-0.0285609 ( 1736)-0.0282963
 ( 1609) 0.0282788 ( 1605) 0.0282629 (    55)-0.0280428 (   256)-0.0277859 (    67)-0.0271692 ( 1663) 0.0270936 ( 1953) 0.0267927
 ( 2016) 0.0260153 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195350D+01
     2 -0.129458D-07  0.191289D+01
     3 -0.432902D-06  0.182539D-05  0.190210D+01
     4 -0.178913D-05  0.655547D-05  0.200975D-04  0.111424D+01
     5  0.899074D-05  0.166612D-04 -0.106244D-04 -0.245529D-05  0.882927D+00
     6 -0.551723D-05 -0.887975D-05  0.556792D-05 -0.121667D-04 -0.143686D-04
     7  0.208920D-05  0.334933D-05  0.246634D-05 -0.104277D-04  0.648886D-05
     8  0.503484D-06  0.317293D-06  0.866657D-06 -0.114538D-05  0.192065D-05
     9 -0.464550D-06 -0.329548D-05  0.474583D-05 -0.609232D-06 -0.225984D-05
                6             7             8             9
     6  0.876301D-01
     7  0.789986D-06  0.923833D-01
     8 -0.435232D-07  0.315443D-06  0.398993D-01
     9  0.101709D-05 -0.602304D-06 -0.695405D-09  0.144271D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 7

GEOMETRY

C	0.00762400	-0.01820900	0.00441900
C	0.00844100	-0.00818100	1.39431700
C	1.21421800	-0.00327600	2.10467900
C	2.45775100	-0.01398400	1.42294000
C	2.38748200	-0.05153300	0.00991300
C	1.23901200	-0.02455600	-0.71605500
H	-0.92140700	0.00818100	1.93074900
H	1.20367100	0.04620900	3.17886500
H	1.24793600	-0.02667400	-1.78960200
C	3.69553800	0.02003000	2.11439600
H	3.69463500	0.28863200	3.15795800
H	4.58220700	0.28273000	1.56094300
C	4.92069200	-3.02185400	0.87810700
H	5.34009300	-4.02689400	0.90177900
H	3.96159100	-3.08029200	0.37573700
H	5.58764600	-2.40381600	0.28748800
C	3.40823000	-3.13399900	3.67713100
H	3.70115100	-4.14270900	3.96594000
H	3.25000500	-2.56880200	4.58887800
H	2.46862400	-3.20922200	3.14133700
C	6.26673300	-1.74222400	3.47100000
H	6.02450100	-1.17713700	4.36421600
H	6.88488600	-2.58506900	3.77835800
H	6.86866800	-1.12246100	2.81577000
Si	4.74800300	-2.39609300	2.61967000
H	-0.92052600	-0.03024300	-0.53544100

E_0(CASSCF,vacuo) -676.099899

E_0(CASSCF,CPCM) **-676.168426**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0998991743
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609990E+03
(     1) 0.6921734 (     3)-0.6202593 (   234)-0.0884158 (    45)-0.0788855 (    24) 0.0753141 (    91) 0.0712441 (   276)-0.0620694
(   378) 0.0566508 (   821)-0.0545467 (  1721)-0.0508501 (  1083) 0.0497827 (  1600)-0.0491651 (   285)-0.0475044 (  1967) 0.0463630
(    26)-0.0462818 (   352) 0.0447247 (   255)-0.0436897 (    30) 0.0435515 (   391) 0.0426934 (   284)-0.0418500 (   300)-0.0395704
(  1779)-0.0388979 (   390) 0.0385987 (  1678)-0.0385928 (   299)-0.0384055 (    36)-0.0375715 (    44) 0.0365213 (  2029) 0.0356040
(   406) 0.0355822 (  1920) 0.0350272 (   405) 0.0347552 (    78) 0.0343015 (    90)-0.0325565 (    67)-0.0317610 (   121) 0.0303690
(  1770)-0.0299831 (   256)-0.0298503 (  1736)-0.0294478 (  1711)-0.0294033 (    32)-0.0286301 (  1609) 0.0283424 (   331) 0.0282901
(   122)-0.0282686 (  1605) 0.0281781 (  1713)-0.0280382 (   354) 0.0276850 (  2016) 0.0275316 (    55)-0.0269285 (  1982) 0.0266636
(   704)-0.0263982 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195367D+01
     2 -0.750019D-06  0.191042D+01
     3  0.651526D-06 -0.372117D-06  0.190106D+01
     4  0.561571D-05  0.145330D-04 -0.247071D-05  0.110080D+01
     5  0.177838D-05  0.713884D-05  0.345895D-05 -0.246741D-05  0.896073D+00
     6 -0.443757D-05 -0.278771D-06  0.104515D-05 -0.127894D-04 -0.104717D-04
     7  0.842859D-06 -0.363885D-05  0.120666D-06 -0.132433D-05 -0.147153D-05
     8  0.348145D-06 -0.229053D-05  0.383605D-06 -0.299950D-05  0.475461D-05
     9 -0.825440D-06 -0.121100D-05  0.333017D-05 -0.538200D-05 -0.781749D-05
                6             7             8             9
     6  0.905558D-01
     7 -0.470490D-06  0.934230D-01
     8 -0.551271D-06 -0.118360D-05  0.399059D-01
     9  0.843576D-06  0.937918D-06 -0.623672D-07  0.140857D-01
MCSCF converged.
```

$^{1}2^{+}$c STEP 8

GEOMETRY

C	0.00799400	-0.01662100	0.00181700
C	0.00705100	-0.00848300	1.39156900
C	1.21207100	-0.00414000	2.10442800
C	2.45540300	-0.01363800	1.42571200
C	2.38743500	-0.04649800	0.01306900
C	1.23962400	-0.02085600	-0.71558300
H	-0.92364100	0.00655800	1.92675100
H	1.19896700	0.04139700	3.17888800
H	1.25111700	-0.01960600	-1.78914800
C	3.69417700	0.01408600	2.11958000
H	3.69550700	0.26617800	3.16685300
H	4.58569800	0.26652200	1.57005100
C	4.94121900	-3.07929600	0.86566800
H	5.33965200	-4.09326400	0.86171800
H	3.97934100	-3.10473000	0.36577900
H	5.61902200	-2.45912100	0.29004400
C	3.42830300	-3.21782600	3.66635500
H	3.69708900	-4.23740700	3.94070200
H	3.28197900	-2.66160800	4.58543500
H	2.48863700	-3.26308000	3.12728900
C	6.29762700	-1.83635900	3.47598800
H	6.05052700	-1.27884300	4.37251400
H	6.92232400	-2.67656000	3.77808200
H	6.89403400	-1.20843800	2.82361300
Si	4.78520700	-2.49678100	2.62209300
H	-0.91946400	-0.02628900	-0.53936500

E_0(CASSCF,vacuo) -676.097213

E_0(CASSCF,CPCM) **-676.166172**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0972137919
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609721E+03
(     1) 0.6885010 (    3)-0.6235104 (   45)-0.0837865 (  234)-0.0804663 (   24) 0.0794333 (   91) 0.0763850 (  276)-0.0726415
(   378) 0.0666581 (  821)-0.0562491 (  284)-0.0551967 ( 1721)-0.0544438 ( 1083) 0.0517745 (  390) 0.0511838 ( 1967) 0.0500096
( 1600)-0.0490927 (   30) 0.0454567 ( 1678)-0.0448126 (  285)-0.0433805 (   26)-0.0428127 (  352) 0.0421875 ( 1779)-0.0412732
( 1920) 0.0410464 (  391) 0.0390758 (  255)-0.0382786 ( 2029) 0.0379463 (  256)-0.0345001 (   67)-0.0339765 (  300)-0.0327825
(  354) 0.0324150 ( 1770)-0.0312782 (  299)-0.0312575 ( 1793)-0.0312237 (   36)-0.0300697 (  406) 0.0297545 (   32)-0.0297513
( 2016) 0.0288620 ( 2043) 0.0285206 (  405) 0.0284478 (  121) 0.0282754 (   70) 0.0282490 ( 1711)-0.0281543 (   78) 0.0278942
( 1713)-0.0273272 ( 1609) 0.0268562 (  122)-0.0267710 (  704)-0.0266973 ( 1605) 0.0264361 (  331) 0.0259662 (   55)-0.0258333
( 1830)-0.0253781 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195384D+01
     2  0.283817D-05  0.190855D+01
     3 -0.490100D-06  0.691899D-05  0.190019D+01
     4  0.264006D-04  0.299479D-04 -0.604395D-04  0.109099D+01
     5 -0.138146D-04 -0.284346D-04 -0.136010D-04 -0.250850D-05  0.905813D+00
     6  0.151729D-05 -0.905023D-05 -0.423004D-04  0.413493D-04  0.413935D-04
     7 -0.291408D-04 -0.743112D-04 -0.457910D-04  0.126332D-04  0.318058D-04
     8 -0.366946D-05  0.148631D-04 -0.107279D-04  0.234657D-05 -0.112487D-04
     9 -0.748659D-05 -0.364540D-05  0.105544D-06 -0.410270D-05 -0.951741D-06
                6             7             8             9
     6  0.925650D-01
     7  0.155047D-04  0.944156D-01
     8  0.495594D-06  0.452824D-05  0.399138D-01
     9 -0.187058D-05 -0.105068D-04 -0.187360D-05  0.137148D-01
MCSCF converged.
```

$^{1}2^{+}$c STEP 9

GEOMETRY

C	0.00253700	-0.01626400	0.00914400
C	0.00755300	-0.00266900	1.39866800
C	1.21574200	0.00120300	2.10734000
C	2.45546900	-0.01409400	1.42484100
C	2.38173500	-0.05013800	0.01292600
C	1.23078900	-0.02620200	-0.71206900
H	-0.92094600	0.01687400	1.93765300
H	1.20612300	0.04910600	3.18183000
H	1.23896000	-0.02798400	-1.78571200
C	3.69885000	0.00849000	2.11378600
H	3.70889500	0.25050200	3.16304200
H	4.59224900	0.24565600	1.56129700
C	4.97348800	-3.14031100	0.85347900
H	5.34082200	-4.16576700	0.82601500
H	4.01304500	-3.12505100	0.35017800
H	5.67201100	-2.52647500	0.29638200
C	3.44802300	-3.30288500	3.64704900
H	3.69058100	-4.33371700	3.90397300
H	3.31094500	-2.75928400	4.57490900
H	2.51058900	-3.31597400	3.10227600
C	6.32599200	-1.92685700	3.48438200
H	6.06897200	-1.37685500	4.38267300
H	6.95799600	-2.76243400	3.78490900
H	6.91846400	-1.29020100	2.83700100
Si	4.82485600	-2.59694700	2.62153000
H	-0.92721000	-0.02395000	-0.52821100

E_0(CASSCF,vacuo) -676.094624

E_0(CASSCF,CPCM) **-676.164082**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.09462412 12
 Full Convergence on CI vector
          ( 1)        EIGENVALUE     -0.67609462E+03
 (     1) 0.6855861 (     3)-0.6259961 (    45)-0.0860054 (   276)-0.0827998 (    91) 0.0791808 (   378) 0.0763497 (    24) 0.0718978
 (   284)-0.0707431 (   390) 0.0656303 (   234)-0.0634856 (   821)-0.0573943 (  1721)-0.0566678 (    25)-0.0546146 (  1083) 0.0531813
 (  1967) 0.0523412 (  1678)-0.0512979 (  1920) 0.0473303 (  1600)-0.0449453 (  1779)-0.0423273 (    30) 0.0408929 (    26)-0.0397358
 (   235) 0.0391984 (  2029) 0.0390189 (  1793)-0.0366177 (   256)-0.0361292 (   352) 0.0351017 (   354) 0.0349514 (  2043) 0.0337699
 (  1770)-0.0316980 (    67)-0.0310052 (  2016) 0.0292296 (    38)-0.0285416 (   255)-0.0283836 (  1711)-0.0276673 (    32)-0.0276530
 (    70) 0.0273978 (   237) 0.0273934 (   373)-0.0265248 (   121) 0.0262105 (    79) 0.0260724 (   300)-0.0260573 (   285)-0.0259714
 (  1830)-0.0254431 (    36)-0.0253248 (  1953) 0.0252404 (   122)-0.0252278 (   236)-0.0249054 (    55)-0.0247866 (  1713)-0.0243337
 (   704)-0.0242359 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.195398D+01
      2 -0.206064D-06  0.190711D+01
      3  0.166851D-05 -0.249211D-05  0.189942D+01
      4  0.918806D-06 -0.105064D-04 -0.333877D-04  0.108337D+01
      5 -0.213476D-04 -0.367114D-04 -0.106142D-04 -0.233039D-05  0.913511D+00
      6  0.373943D-05  0.665245D-05  0.605396D-05 -0.709453D-05  0.764032D-05
      7  0.381279D-05  0.133400D-05  0.719319D-05 -0.219179D-04 -0.108184D-04
      8 -0.644460D-05 -0.197112D-05  0.558347D-05  0.373569D-05 -0.521859D-05
      9  0.436073D-05  0.111450D-04  0.408046D-05  0.176165D-05  0.954118D-06
                   6             7             8             9
      6  0.938385D-01
      7 -0.434457D-05  0.955974D-01
      8 -0.382577D-06 -0.341409D-05  0.399370D-01
      9  0.166423D-05  0.615619D-05  0.499571D-06  0.132324D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 10

GEOMETRY

C	0.00771900	-0.01441300	-0.00089100
C	0.00498600	-0.00653400	1.38848600
C	1.20928700	-0.00334800	2.10476300
C	2.45251700	-0.01347200	1.43057700
C	2.38687500	-0.04236200	0.01832300
C	1.23999300	-0.01874100	-0.71397700
H	-0.92667000	0.00893300	1.92228500
H	1.19252600	0.03872900	3.17949100
H	1.25525200	-0.01498300	-1.78758500
C	3.69323900	0.00458000	2.12711800
H	3.69937400	0.23076600	3.17966200
H	4.59212500	0.23715800	1.58220300
C	5.00246200	-3.19005100	0.84286500
H	5.35061800	-4.22113100	0.78614800
H	4.04131300	-3.14360900	0.34263200
H	5.71117000	-2.57344200	0.30211400
C	3.47439900	-3.39203900	3.63370300
H	3.69726700	-4.43178100	3.87259700
H	3.34504100	-2.86222200	4.57049600
H	2.53867000	-3.37843800	3.08590800
C	6.35784100	-2.01896800	3.49451700
H	6.09443300	-1.48082800	4.39807000
H	6.99723600	-2.85196300	3.78723300
H	6.94484600	-1.37085400	2.85362400
Si	4.86494700	-2.69369800	2.62418500
H	-0.91889900	-0.02049900	-0.54371500

E_0(CASSCF,vacuo) -676.092173

E_0(CASSCF,CPCM) **-676.162176**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0921725215
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67609217E+03
 (    1) 0.6833648 (    3)-0.6277716 (  276)-0.0860146 (   45)-0.0827934 (  378) 0.0796654 (   91) 0.0768960 (   25)-0.0760164
 (  284)-0.0757672 (  390) 0.0703562 (   24) 0.0604586 (  821)-0.0581829 ( 1721)-0.0558777 ( 1083) 0.0541772 ( 1678)-0.0541558
 ( 1967) 0.0518354 ( 1920) 0.0502423 (  235) 0.0489937 (  234)-0.0462761 ( 1779)-0.0412253 (   38)-0.0404445 ( 1793)-0.0392854
 ( 1600)-0.0391817 ( 2029) 0.0381038 (   26)-0.0369598 ( 2043) 0.0364706 (   79) 0.0355703 (   30) 0.0340201 (  354) 0.0329320
 (  256)-0.0328005 ( 1770)-0.0311143 ( 2016) 0.0286619 (  237) 0.0284624 ( 1711)-0.0281489 (  352) 0.0271593 (  373)-0.0271425
 (  236)-0.0271213 (   67)-0.0264392 ( 1599)-0.0263351 (   36)-0.0261831 ( 1953) 0.0259910 (  300)-0.0259211 (  278) 0.0258376
 ( 1830)-0.0254904 (   78) 0.0244160 (  121) 0.0241525 (   55)-0.0238144 (  406) 0.0237640 ( 2080) 0.0236458 (  122)-0.0236310
 (   70) 0.0235430 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195409D+01
     2  0.348023D-06  0.190602D+01
     3  0.109300D-05 -0.792927D-06  0.189868D+01
     4 -0.758490D-05 -0.180985D-04 -0.264616D-04  0.107777D+01
     5 -0.353598D-05 -0.962918D-05 -0.342234D-04  0.105292D-05  0.919292D+00
     6  0.441276D-05  0.498318D-05 -0.771099D-05  0.759123D-05  0.663193D-05
     7 -0.107246D-05 -0.137510D-04 -0.111515D-05 -0.895760D-05 -0.105247D-04
     8 -0.400200D-05 -0.150300D-05  0.283876D-05 -0.278178D-05 -0.584741D-06
     9  0.389998D-05  0.128865D-04  0.378808D-05  0.485878D-05  0.613810D-05
                6             7             8             9
     6  0.946152D-01
     7 -0.819385D-06  0.969309D-01
     8 -0.164628D-06 -0.167727D-05  0.399828D-01
     9  0.366748D-06  0.319481D-05  0.190410D-06  0.126181D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 11

GEOMETRY

C	0.00170000	-0.01551500	0.00797400
C	0.00609500	-0.00095200	1.39708400
C	1.21410400	0.00274900	2.10802400
C	2.45379000	-0.01374000	1.42901400
C	2.38089400	-0.04836100	0.01734900
C	1.23052400	-0.02609100	-0.71013200
H	-0.92291500	0.01928800	1.93546700
H	1.20194100	0.04919000	3.18270800
H	1.24130200	-0.02683600	-1.78385300
C	3.69917800	0.00098500	2.11960200
H	3.71331200	0.22254100	3.17283800
H	4.59805200	0.22135000	1.57006200
C	5.03930900	-3.24848100	0.82669600
H	5.35112600	-4.28957900	0.74581800
H	4.08137100	-3.15739900	0.32597300
H	5.77003800	-2.64320400	0.30293400
C	3.50517000	-3.47791300	3.61176400
H	3.70419900	-4.52716300	3.82959100
H	3.38593800	-2.96370700	4.55844800
H	2.57117200	-3.43271300	3.06246400
C	6.39373400	-2.10748200	3.49531500
H	6.12221400	-1.57772300	4.40139100
H	7.04078100	-2.93594300	3.78459100
H	6.97550500	-1.44996100	2.85926000
Si	4.91048600	-2.79042800	2.61770000
H	-0.92752800	-0.02125300	-0.53043500

E_0(CASSCF,vacuo) -676.089889

E_0(CASSCF,CPCM) **-676.160460**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0898888717
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608989E+03
 (     1) 0.6818069 (     3)-0.6288922 (    25)-0.0890644 (   276)-0.0876278 (   378) 0.0814225 (    45)-0.0804388 (   284)-0.0771210
 (    91) 0.0751748 (   390) 0.0717191 (   821)-0.0587638 (  1678)-0.0556128 (  1721)-0.0550448 (  1083) 0.0548974 (    24) 0.0525425
 (  1920) 0.0517865 (  1967) 0.0512212 (   235) 0.0493284 (    38)-0.0474178 (    79) 0.0416429 (  1793)-0.0407176 (  1779)-0.0402808
 (  2043) 0.0379588 (  2029) 0.0373159 (  1600)-0.0353500 (   234)-0.0348887 (    26)-0.0344960 (   354) 0.0306508 (  1599)-0.0304999
 (  1770)-0.0304775 (   256)-0.0295304 (    30) 0.0291224 (   236)-0.0289904 (  1711)-0.0286810 (   237) 0.0285570 (  2016) 0.0280811
 (   373)-0.0269502 (   300)-0.0269203 (  1953) 0.0266569 (    36)-0.0265867 (  1830)-0.0255317 (   278) 0.0252001 (    78) 0.0247894
 (   406) 0.0247096 (    40) 0.0246427 (   379)-0.0241291 (  2080) 0.0237702 (    67)-0.0234210 (    55)-0.0229865 (   325)-0.0229422
 (   279) 0.0224880 (
 Final one electron symbolic density matrix:
                   1                   2                   3                   4                   5
      1  0.195418D+01
      2  0.119899D-05  0.190522D+01
      3  0.215773D-06  0.824760D-06  0.189796D+01
      4 -0.529185D-05 -0.845299D-05 -0.319214D-04  0.107406D+01
      5 -0.492370D-05 -0.934788D-05 -0.363704D-04  0.605116D-07  0.923248D+00
      6 -0.191559D-06 -0.370103D-05 -0.107888D-04  0.788150D-05  0.792698D-05
      7 -0.342488D-05 -0.110002D-04 -0.355007D-05 -0.132820D-04 -0.168863D-04
      8 -0.223943D-05  0.144075D-05  0.844107D-06 -0.336010D-05 -0.255233D-05
      9  0.157600D-05  0.475484D-05  0.107036D-04  0.412725D-05  0.446676D-05
                   6                   7                   8                   9
      6  0.951593D-01
      7  0.573303D-06  0.982836D-01
      8  0.754480D-06  0.777053D-07  0.400425D-01
      9 -0.827031D-07  0.235178D-05  0.264650D-06  0.118519D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 12

GEOMETRY

C	0.00735800	-0.01349100	-0.00225500
C	0.00378400	-0.00527700	1.38667100
C	1.20776500	-0.00235200	2.10531900
C	2.45140600	-0.01323200	1.43474500
C	2.38665700	-0.04083300	0.02249500
C	1.24066600	-0.01779200	-0.71224200
H	-0.92844300	0.01057300	1.91975600
H	1.18841100	0.03861200	3.18017900
H	1.25852300	-0.01265400	-1.78590800
C	3.69356600	-0.00241200	2.13296000
H	3.70284600	0.20533800	3.18887600
H	4.59719400	0.21556900	1.59067300
C	5.07195000	-3.29746900	0.81201200
H	5.34797400	-4.34594400	0.70138000
H	4.11719400	-3.16090200	0.31504400
H	5.82213100	-2.70175700	0.30527100
C	3.54040100	-3.57141600	3.59383700
H	3.72093200	-4.62896200	3.78669300
H	3.43073500	-3.07703600	4.55208900
H	2.60715400	-3.49761600	3.04610200
C	6.43018700	-2.19771300	3.49854800
H	6.15296400	-1.68233200	4.41115400
H	7.08673900	-3.02245200	3.77741000
H	7.00409400	-1.52644700	2.86973300
Si	4.95485200	-2.88545000	2.61388400
H	-0.91859100	-0.01820700	-0.54635100

E_0(CASSCF,vacuo) -676.087787

E_0(CASSCF,CPCM) **-676.158953**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0877874395
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608779E+03
 (     1) 0.6806966 (     3)-0.6295867 (    25)-0.0980207 (   276)-0.0891649 (   378) 0.0830311 (    45)-0.0794600 (   284)-0.0778571
 (    91) 0.0745750 (   390) 0.0725098 (   821)-0.0591793 (  1678)-0.0566484 (  1083) 0.0554062 (  1721)-0.0546370 (  1920) 0.0528835
 (    38)-0.0520487 (  1967) 0.0509532 (    24) 0.0473210 (   235) 0.0466374 (    79) 0.0459539 (  1793)-0.0417047 (  1779)-0.0397726
 (  2043) 0.0389841 (  2029) 0.0369105 (  1600)-0.0331310 (    26)-0.0324989 (  1599)-0.0324633 (   236)-0.0304362 (  1770)-0.0299846
 (  1711)-0.0290725 (   354) 0.0289870 (   237) 0.0279617 (   234)-0.0277659 (  2016) 0.0276411 (   300)-0.0273934 (   256)-0.0271523
 (  1953) 0.0271215 (   373)-0.0265937 (    36)-0.0261305 (    30) 0.0258098 (  1830)-0.0255663 (    40) 0.0251780 (   406) 0.0251488
 (    78) 0.0243835 (   279) 0.0242819 (  2080) 0.0238614 (   325)-0.0235648 (   379)-0.0233360 (   278) 0.0233016 (   466) 0.0230789
 (    55)-0.0223513 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195424D+01
     2  0.568012D-06  0.190465D+01
     3 -0.849798D-06  0.161944D-05  0.189726D+01
     4 -0.878167D-05  0.163631D-05 -0.153001D-04  0.107161D+01
     5 -0.188655D-04 -0.868951D-05 -0.119828D-04 -0.145970D-05  0.925989D+00
     6 -0.114410D-05  0.332754D-05  0.986324D-05 -0.260658D-05  0.521912D-05
     7 -0.963764D-06  0.158155D-04 -0.304494D-05 -0.146476D-04 -0.125155D-04
     8 -0.543002D-06  0.464596D-06  0.135119D-05 -0.107243D-05 -0.588394D-05
     9  0.314789D-05  0.326285D-05 -0.309655D-05 -0.220064D-05 -0.207510D-05
                6             7             8             9
     6  0.955812D-01
     7  0.111335D-05  0.995678D-01
     8  0.261715D-06  0.672617D-06  0.401208D-01
     9  0.565472D-06  0.225899D-05  0.118879D-06  0.109868D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 13

GEOMETRY

C	0.00645900	-0.01288700	-0.00252200
C	0.00288600	-0.00226300	1.38615000
C	1.20691300	0.00055100	2.10555100
C	2.45072600	-0.01316300	1.43635300
C	2.38588500	-0.04263800	0.02404100
C	1.24022100	-0.01964500	-0.71146200
H	-0.92943600	0.01552400	1.91913900
H	1.18672800	0.04300700	3.18038200
H	1.25894600	-0.01585500	-1.78517100
C	3.69343100	-0.00522600	2.13494400
H	3.70441500	0.19544800	3.19203100
H	4.59925100	0.20435200	1.59332400
C	5.09789100	-3.35326700	0.79258900
H	5.33382900	-4.40830300	0.65497600
H	4.14523600	-3.17075100	0.30582800
H	5.86570100	-2.77256600	0.29511100
C	3.58527300	-3.65993300	3.58024600
H	3.74932600	-4.72378300	3.75255100
H	3.48948600	-3.18110100	4.54777400
H	2.65015700	-3.56150800	3.03934900
C	6.47743800	-2.28834100	3.48450200
H	6.20128600	-1.78345500	4.40329000
H	7.14250100	-3.11011900	3.75222500
H	7.04200600	-1.60730600	2.85769500
Si	5.00306100	-2.97951000	2.60315200
H	-0.91930500	-0.01719800	-0.54699000

E_0(CASSCF,vacuo) -676.085872

E_0(CASSCF,CPCM) **-676.157630**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0858721935
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608587E+03
 (     1) 0.6799088 (     3)-0.6299882 (    25)-0.1047253 (   276)-0.0905089 (   378) 0.0844009 (    45)-0.0791870 (   284)-0.0783114
 (    91) 0.0745335 (   390) 0.0730214 (   821)-0.0594813 (  1678)-0.0574122 (  1083) 0.0557695 (    38)-0.0554596 (  1721)-0.0544590
 (  1920) 0.0536863 (  1967) 0.0508633 (    79) 0.0492574 (    24) 0.0435633 (   235) 0.0434123 (  1793)-0.0424105 (  2043) 0.0397131
 (  1779)-0.0395082 (  2029) 0.0367108 (  1599)-0.0335237 (  1600)-0.0318375 (   236)-0.0314741 (    26)-0.0309980 (  1770)-0.0296054
 (  1711)-0.0293579 (   354) 0.0277727 (   300)-0.0274895 (  1953) 0.0274492 (  2016) 0.0272980 (   237) 0.0269734 (   373)-0.0262055
 (  1830)-0.0255950 (    36)-0.0254611 (   256)-0.0254043 (   279) 0.0252525 (   406) 0.0252301 (    40) 0.0251308 (    27)-0.0240424
 (   325)-0.0240137 (  2080) 0.0239286 (   466) 0.0239043 (    78) 0.0237832 (    30) 0.0234090 (   234)-0.0232681 (   667)-0.0226305
 (    82)-0.0223265 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.195428D+01
      2 -0.196823D-06  0.190425D+01
      3 -0.459111D-06  0.472339D-06  0.189660D+01
      4 -0.381652D-05  0.620483D-05  0.676659D-05  0.107003D+01
      5 -0.473498D-07  0.509181D-05  0.167335D-05 -0.680802D-07  0.927868D+00
      6 -0.312742D-05 -0.355981D-05  0.929467D-05 -0.632472D-06 -0.122301D-04
      7  0.655819D-05  0.155577D-04 -0.560830D-06  0.845801D-05  0.405674D-05
      8  0.928545D-06  0.555657D-06 -0.306179D-05 -0.448533D-05 -0.930123D-06
      9 -0.223536D-05 -0.765684D-05 -0.255017D-06 -0.636760D-06 -0.226979D-06
                   6             7             8             9
      6  0.959230D-01
      7  0.391001D-06  0.100770D+00
      8 -0.130347D-06  0.862338D-06  0.402111D-01
      9 -0.262796D-06 -0.940516D-06  0.130458D-06  0.100607D-01
 MCSCF converged.
```

$^{1}2^{+}$c STEP 14

GEOMETRY

C	0.01500400	-0.01015100	-0.01526700
C	0.00075100	-0.00998500	1.37318500
C	1.19919300	-0.00875600	2.10253400
C	2.44836600	-0.01400800	1.44411600
C	2.39435200	-0.03327300	0.03107200
C	1.25462100	-0.00743500	-0.71374100
H	-0.93581400	0.00091200	1.89900400
H	1.16985200	0.02580600	3.17747800
H	1.28236200	0.00535200	-1.78723700
C	3.68623000	-0.00985000	2.15255100
H	3.68976100	0.17653300	3.21215500
H	4.59689500	0.20120500	1.61992000
C	5.11071800	-3.40713600	0.76737100
H	5.25743400	-4.47353500	0.59889100
H	4.17043200	-3.13593600	0.29681700
H	5.91652100	-2.87450000	0.27656400
C	3.64761200	-3.75366300	3.57489500
H	3.80730500	-4.81992600	3.73634800
H	3.56606700	-3.28229500	4.54737300
H	2.70678500	-3.64563400	3.04562300
C	6.53589400	-2.37389100	3.45084100
H	6.26946300	-1.88714600	4.38219200
H	7.21840200	-3.18935700	3.69307800
H	7.07811300	-1.67527800	2.82350700
Si	5.05626800	-3.07286000	2.58655900
H	-0.90635100	-0.01332900	-0.56722100

E_0(CASSCF,vacuo) -676.084141

E_0(CASSCF,CPCM) **-676.156464**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0841408412
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67608414E+03
(     1) 0.6799904 (    3)-0.6295417 (   25)-0.1101076 (  276)-0.0916960 (  378) 0.0854303 (   45)-0.0793123 (  284)-0.0786419
(    91) 0.0746921 (  390) 0.0732674 (  821)-0.0597991 (   38)-0.0582548 ( 1678)-0.0580410 ( 1083) 0.0560281 ( 1721)-0.0544289
( 1920) 0.0542427 (   79) 0.0518463 ( 1967) 0.0507977 ( 1793)-0.0429700 (  235) 0.0404143 (   24) 0.0403914 ( 2043) 0.0402147
( 1779)-0.0393928 ( 2029) 0.0365623 ( 1599)-0.0342025 (  236)-0.0321811 ( 1600)-0.0309425 (   26)-0.0298576 ( 1711)-0.0296134
( 1770)-0.0293147 ( 1953) 0.0276746 (  300)-0.0274263 ( 2016) 0.0269690 (  354) 0.0267896 (  279) 0.0259225 (  373)-0.0259018
(  237) 0.0257634 ( 1830)-0.0256456 (  406) 0.0251048 (   27)-0.0250304 (   40) 0.0249312 (   36)-0.0248890 (  466) 0.0245088
(  325)-0.0243529 ( 2080) 0.0239631 (  256)-0.0238878 (  667)-0.0234934 (   78) 0.0232283 (  381)-0.0229484 (  435) 0.0225574
(   82)-0.0224014 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195433D+01
     2  0.219955D-05  0.190397D+01
     3 -0.170755D-05  0.474909D-05  0.189599D+01
     4 -0.233948D-05  0.105199D-04 -0.808311D-05  0.107091D+01
     5 -0.163343D-04 -0.418009D-05  0.273636D-06 -0.164568D-05  0.927318D+00
     6 -0.453772D-05 -0.129192D-05  0.200061D-04 -0.119935D-04 -0.229241D-05
     7  0.436589D-05  0.241650D-04 -0.564523D-05  0.397261D-05  0.336574D-05
     8  0.828165D-06 -0.143727D-05 -0.444383D-05 -0.491235D-06 -0.338548D-05
     9  0.148050D-05  0.433387D-05  0.528043D-05 -0.149099D-05 -0.698709D-05
                6             7             8             9
     6  0.962046D-01
     7  0.250260D-05  0.101915D+00
     8  0.144294D-05  0.255083D-05  0.402976D-01
     9  0.209218D-05  0.591801D-06  0.555340D-07  0.905889D-02
MCSCF converged.
```

$^{1}2^{+}$c STEP 15

GEOMETRY

C	0.02189700	-0.00735800	-0.02630100
C	-0.00127800	-0.01075300	1.36190400
C	1.19236700	-0.01123100	2.09959400
C	2.44598200	-0.01543800	1.45030900
C	2.40096000	-0.03190600	0.03684400
C	1.26632400	-0.00240100	-0.71588200
H	-0.94133500	-0.00109800	1.88159900
H	1.15542700	0.02160800	3.17438600
H	1.30168700	0.01397300	-1.78915600
C	3.67979600	-0.01473500	2.16685100
H	3.67764700	0.16381600	3.22766600
H	4.59501200	0.19277900	1.64080700
C	5.09505800	-3.47314800	0.74250000
H	5.11617500	-4.54494900	0.55083900
H	4.17909400	-3.08998300	0.30070200
H	5.94133900	-3.01920800	0.24109200
C	3.73039600	-3.84313200	3.59389700
H	3.88478400	-4.91256100	3.73899100
H	3.68439300	-3.38099700	4.57306900
H	2.77405800	-3.72167500	3.09588400
C	6.60919000	-2.45143000	3.38404000
H	6.36821600	-1.97434800	4.32724400
H	7.31140900	-3.25846100	3.59678100
H	7.11934300	-1.74157800	2.74243000
Si	5.11122200	-3.16519300	2.56648700
H	-0.89572400	-0.00972800	-0.58449500

E_0(CASSCF,vacuo) -676.082588

E_0(CASSCF,CPCM) **-676.155404**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0825881599
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608259E+03
 (     1) 0.6809729 (     3)-0.6281835 (    25)-0.1143713 (   276)-0.0927077 (   378) 0.0860796 (    45)-0.0796824 (   284)-0.0789343
 (    91) 0.0749161 (   390) 0.0733085 (    38)-0.0605901 (   821)-0.0601392 (  1678)-0.0585620 (  1083) 0.0561792 (  1920) 0.0545674
 ( 1721)-0.0545200 (    79) 0.0537809 ( 1967) 0.0507254 ( 1793)-0.0434111 ( 2043) 0.0405077 ( 1779)-0.0394016 (   235) 0.0380765
 (    24) 0.0378189 ( 2029) 0.0364357 ( 1599)-0.0345863 (   236)-0.0325777 ( 1600)-0.0303714 ( 1711)-0.0298430 ( 1770)-0.0291167
 (    26)-0.0290799 ( 1953) 0.0278007 (  300)-0.0273044 ( 2016) 0.0266444 (   279) 0.0263576 (   354) 0.0260655 (   373)-0.0258441
 ( 1830)-0.0257196 (    27)-0.0252336 (  466) 0.0248964 (  406) 0.0248498 (    40) 0.0246231 (   325)-0.0246031 (   237) 0.0245087
 (    36)-0.0244837 (   667)-0.0242720 ( 2080) 0.0239647 (  381)-0.0235345 (   239) 0.0228409 (    78) 0.0227851 (   435) 0.0226950
 (   256)-0.0225889 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195439D+01
     2  0.102738D-06  0.190378D+01
     3  0.146130D-05 -0.114092D-05  0.189543D+01
     4 -0.869291D-05 -0.208565D-04 -0.510220D-05  0.107437D+01
     5  0.906035D-05  0.233015D-04 -0.140749D-04  0.295710D-05  0.924209D+00
     6 -0.732664D-06 -0.496121D-06 -0.118638D-04  0.112220D-04  0.519622D-06
     7 -0.502613D-05 -0.980565D-05 -0.109570D-05 -0.651201D-05 -0.565985D-05
     8  0.382936D-06  0.204346D-05  0.116300D-05 -0.159203D-05  0.127161D-05
     9 -0.120371D-05 -0.431856D-05  0.254482D-05  0.309067D-05  0.177002D-05
                6             7             8             9
     6  0.964363D-01
     7 -0.649838D-06  0.102984D+00
     8  0.219203D-07 -0.160291D-05  0.403785D-01
     9  0.668326D-08  0.643086D-06  0.119093D-06  0.802823D-02
 MCSCF converged.
```

$^{1}2^{+}$c STEP 16

GEOMETRY

C	0.09428900	0.03222700	-0.11990200
C	-0.01244600	-0.05539300	1.26154800
C	1.13401900	-0.07865200	2.07061300
C	2.42457200	-0.02239000	1.50158500
C	2.46518200	0.04403100	0.08929600
C	1.37788200	0.10164800	-0.72920100
H	-0.98224700	-0.09410200	1.72196100
H	1.03088600	-0.10975000	3.14114300
H	1.47827600	0.18452100	-1.79531500
C	3.61317200	-0.04370500	2.29126800
H	3.54478400	0.06386900	3.35925100
H	4.55491900	0.20682800	1.83555000
C	4.93446700	-3.56593100	0.72345200
H	4.66096000	-4.60281000	0.54389700
H	4.11441200	-2.95338900	0.35276000
H	5.82186200	-3.33000200	0.14815600
C	3.92747400	-3.93723200	3.72320800
H	4.16310000	-4.98168300	3.92996700
H	3.93900700	-3.40694900	4.66852900
H	2.92571900	-3.90907300	3.30785500
C	6.73209000	-2.49770400	3.16110300
H	6.58824800	-2.00847200	4.11782800
H	7.47553400	-3.28285100	3.30465400
H	7.14628700	-1.78850600	2.45288500
Si	5.17029700	-3.26209800	2.53222600
H	-0.78751900	0.04572100	-0.73300600

E_0(CASSCF,vacuo) -676.081225

E_0(CASSCF,CPCM) **-676.154409**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.0812246267
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67608122E+03
 (     1) 0.6832321 (     3)-0.6254805 (    25)-0.1181988 (   276)-0.0936004 (   378) 0.0863144 (    45)-0.0802326 (   284)-0.0792130
 (    91) 0.0751090 (   390) 0.0730934 (    38)-0.0628978 (   821)-0.0605347 (  1678)-0.0590242 (  1083) 0.0562042 (    79) 0.0552969
 ( 1721)-0.0547139 (  1920) 0.0546558 (  1967) 0.0505796 (  1793)-0.0437878 (  2043) 0.0406041 (  1779)-0.0395096 (   235) 0.0365800
 ( 2029) 0.0362613 (    24) 0.0351921 (  1599)-0.0348557 (   236)-0.0327020 (  1711)-0.0300919 (  1600)-0.0299468 (  1770)-0.0289876
 (   26)-0.0286618 (  1953) 0.0278347 (   300)-0.0271653 (   279) 0.0267584 (  2016) 0.0262557 (   373)-0.0261025 (  1830)-0.0258290
 (  354) 0.0254037 (   667)-0.0251636 (   466) 0.0250909 (   325)-0.0247926 (   406) 0.0244639 (    27)-0.0244145 (    36)-0.0243151
 (   40) 0.0242915 (   381)-0.0241287 (   239) 0.0240370 (  2080) 0.0239234 (   237) 0.0232311 (   467)-0.0227988 (  1601)-0.0227181
 (   435) 0.0226825 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195447D+01
     2 -0.520157D-06  0.190369D+01
     3 -0.220937D-06  0.131644D-05  0.189490D+01
     4  0.502087D-05  0.816860D-05  0.505318D-05  0.108154D+01
     5 -0.575918D-05 -0.239997D-05  0.780537D-05 -0.150814D-05  0.917431D+00
     6 -0.220196D-05 -0.169519D-05  0.518488D-05 -0.124565D-04  0.297021D-05
     7  0.340827D-05  0.475936D-05 -0.413665D-06  0.514555D-05  0.614050D-05
     8 -0.239082D-06 -0.845161D-06 -0.292694D-05  0.343413D-05 -0.315447D-05
     9 -0.161046D-06 -0.158264D-07  0.805035D-07  0.176987D-05  0.182528D-06
                6             7             8             9
     6  0.965914D-01
     7  0.101345D-05  0.104070D+00
     8 -0.749317D-06  0.356056D-06  0.404553D-01
     9  0.354640D-06 -0.406090D-06 -0.768735D-07  0.685297D-02
 MCSCF converged.
```

$^{3}2^{+}$c STEP 1

GEOMETRY

C	3.47321100	0.11704700	0.43698300
C	2.85898800	-1.15263900	0.20959100
C	1.62110600	-1.25148700	-0.37017800
C	0.91286300	-0.06215100	-0.77505500
C	1.58066700	1.17192000	-0.51552600
C	2.81942300	1.30009800	0.06860000
H	3.38744200	-2.04311300	0.49301900
H	1.16995400	-2.20989200	-0.54741600
C	-0.36748600	-0.09943700	-1.36151800
H	-0.65926300	-1.03765700	-1.81132700
H	-0.65425200	0.77270700	-1.93125700
C	-1.63661600	1.66263200	1.06958600
H	-2.46116300	1.84113400	1.75646200
H	-0.72289100	1.67134300	1.65444600
H	-1.60936600	2.49893900	0.37822500
C	-1.68370900	-1.47998300	1.27755500
H	-2.49078600	-1.52050600	2.00591100
H	-1.72265400	-2.40296800	0.70745900
H	-0.75156200	-1.45669100	1.83235700
C	-3.43371800	-0.01936200	-0.89049400
H	-3.49707400	-0.93640700	-1.46729900
H	-4.32226900	0.03121400	-0.26488200
H	-3.47486200	0.81942000	-1.57781600
Si	-1.91245000	0.03088000	0.19721100
H	4.44603200	0.15849000	0.88889100
H	3.26863900	2.26184000	0.22500700

E_0(CASSCF,vacuo) -676.123964

E_0(CASSCF,CPCM) **-676.193387**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1239637563
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612396E+03
 (     1) 0.9297921 ( 1349)-0.1316107 (  428) 0.0973640 (  506) 0.0960373 ( 1345) 0.0725192 ( 2950)-0.0716270 (    5)-0.0713473
 ( 3028)-0.0595601 ( 1271)-0.0546503 ( 2941) 0.0529213 (   10)-0.0521468 ( 1352) 0.0518761 ( 2101)-0.0504453 ( 1430) 0.0484085
 (  171)-0.0478266 ( 6166)-0.0467928 ( 3035)-0.0467704 (  508) 0.0454990 ( 6081)-0.0439356 ( 1264)-0.0435694 (  430) 0.0390389
 (  706)-0.0367231 ( 1354)-0.0354787 ( 1356)-0.0351283 ( 1268)-0.0346582 ( 1460) 0.0342004 ( 3113)-0.0341931 (  617)-0.0339073
 ( 1434)-0.0334976 ( 5909) 0.0324790 ( 3030)-0.0319904 ( 1373)-0.0311251 ( 1439)-0.0310623 (   16)-0.0309497 ( 5913) 0.0307214
 ( 3226)-0.0294806 ( 6079) 0.0294230 (  510)-0.0292564 ( 5911)-0.0292156 ( 5970) 0.0291227 ( 2945)-0.0290508 ( 6145)-0.0288859
 ( 4621)-0.0285240 ( 5966)-0.0282279 ( 6077)-0.0277874 (   23)-0.0267352 (  512) 0.0259451 ( 3137)-0.0248338 (   33) 0.0231606
 ( 6049)-0.0227663 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195950D+01
     2 -0.274881D-05  0.192939D+01
     3 -0.644407D-06  0.354816D-06  0.188934D+01
     4 -0.321016D-04  0.188500D-04  0.382245D-05  0.100316D+01
     5  0.197442D-05 -0.707603D-05  0.133356D-04 -0.115616D-05  0.999969D+00
     6  0.900228D-05 -0.716810D-06  0.267836D-05 -0.716607D-05  0.109434D-04
     7 -0.129290D-05  0.245721D-05 -0.335310D-05 -0.257503D-06 -0.132841D-05
     8 -0.832372D-05  0.336311D-05  0.559345D-06  0.547834D-05 -0.236696D-05
     9  0.566877D-06 -0.198240D-05  0.211719D-06 -0.118609D-05  0.175113D-06
                6             7             8             9
     6  0.651073D-01
     7  0.237568D-06  0.104731D+00
     8  0.216111D-05 -0.538412D-06  0.334662D-01
     9 -0.101799D-06 -0.792053D-07 -0.217164D-06  0.153310D-01
 MCSCF converged.
```

$^{3}2^{+}$c STEP 2

GEOMETRY

C	3.49078200	0.12063300	0.45500200
C	2.88350400	-1.14837700	0.22535200
C	1.65085700	-1.25076200	-0.36915400
C	0.94440000	-0.06475300	-0.78544400
C	1.60511100	1.16957300	-0.52317800
C	2.83796000	1.30056400	0.07490400
H	3.40944800	-2.03771400	0.51703800
H	1.20481600	-2.21137100	-0.54905100
C	-0.32324000	-0.10894800	-1.38763800
H	-0.63236200	-1.05122600	-1.81458800
H	-0.63203600	0.76434800	-1.94208000
C	-1.67475600	1.67726700	1.05504700
H	-2.49614000	1.87134200	1.74209500
H	-0.75794800	1.69075300	1.63422100
H	-1.64762400	2.49884900	0.34677200
C	-1.70907800	-1.47415000	1.29298000
H	-2.51175700	-1.52306500	2.02623000
H	-1.74137900	-2.39614500	0.72156300
H	-0.77346400	-1.43812100	1.84050300
C	-3.44041500	-0.03808400	-0.92095700
H	-3.47844500	-0.96132300	-1.48950600
H	-4.34919000	0.01230600	-0.32438800
H	-3.46394000	0.79469800	-1.61591300
Si	-1.96164400	0.03272400	0.21822700
H	4.45846900	0.16707900	0.91740400
H	3.28381200	2.26367800	0.23303900

E_0(CASSCF,vacuo) -676.122195

E_0(CASSCF,CPCM) **-676.191219**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1221954284
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67612220E+03
(     1) 0.9259693 ( 1349)-0.1333642 (  428) 0.1042861 (  506) 0.0974201 ( 2950)-0.0759588 ( 1345) 0.0740284 (    5)-0.0729548
( 3028)-0.0587578 ( 2941) 0.0577232 (   10)-0.0570960 ( 1271)-0.0546195 ( 2101)-0.0500286 (  171)-0.0495602 ( 1430) 0.0473466
(  508) 0.0464051 ( 1460) 0.0423752 (  617)-0.0419835 ( 1352) 0.0419060 ( 6081)-0.0412914 ( 1264)-0.0400884 ( 1373)-0.0399942
( 5970) 0.0385784 (  430) 0.0384035 ( 3035)-0.0380458 (  706)-0.0350068 ( 5911)-0.0347190 ( 4621)-0.0345692 ( 1434)-0.0342757
( 5966)-0.0337645 ( 1356)-0.0332973 (   23)-0.0328160 ( 6166)-0.0327520 (   16)-0.0318778 ( 3113)-0.0314993 ( 3226)-0.0303803
(  685)-0.0300801 ( 6145)-0.0300457 ( 3030)-0.0295621 ( 5892) 0.0294615 ( 2969) 0.0293612 ( 1354)-0.0287284 (   33) 0.0284863
( 3205)-0.0284575 ( 6049)-0.0281762 ( 5909) 0.0280311 ( 3139) 0.0274647 ( 5913) 0.0270826 ( 1268)-0.0264937 ( 1439)-0.0264576
( 1377) 0.0263642 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195519D+01
     2  0.151081D-05  0.192531D+01
     3  0.169168D-06 -0.157169D-06  0.188714D+01
     4  0.264462D-04 -0.106464D-04 -0.675256D-05  0.100218D+01
     5  0.373233D-05 -0.123152D-04  0.166042D-04 -0.146016D-06  0.999950D+00
     6 -0.541261D-05  0.573699D-05  0.442250D-05 -0.353927D-05  0.603989D-05
     7  0.203186D-05 -0.332674D-05 -0.428946D-05 -0.598512D-06 -0.596623D-05
     8  0.100950D-05 -0.146618D-05 -0.122532D-05  0.352193D-05 -0.203191D-05
     9 -0.501587D-05  0.268752D-05  0.212594D-05  0.737163D-05  0.286515D-05
                6             7             8             9
     6  0.708663D-01
     7  0.240009D-07  0.107665D+00
     8 -0.174241D-05 -0.537933D-07  0.362496D-01
     9 -0.738879D-06  0.195337D-06  0.829996D-06  0.154454D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 3

GEOMETRY

C	-3.50947000	0.12521900	-0.47418100
C	-2.90911800	-1.14373700	-0.24287200
C	-1.68231500	-1.25041100	0.36696800
C	-0.97830600	-0.06864300	0.79552800
C	-1.63177100	1.16628100	0.53146300
C	-2.85807100	1.30151400	-0.08103900
H	-3.43257200	-2.03149100	-0.54389700
H	-1.24170000	-2.21341700	0.54889700
C	0.27892900	-0.11997600	1.41425100
H	0.60079800	-1.06584300	1.82143600
H	0.60453500	0.75287600	1.95809500
C	1.71058500	1.68905600	-1.04197800
H	2.52706300	1.89858800	-1.73084500
H	0.78978500	1.70463300	-1.61423200
H	1.68339500	2.49757300	-0.31921200
C	1.73843900	-1.46914800	-1.30504100
H	2.53600500	-1.52566500	-2.04378500
H	1.76617500	-2.38978200	-0.73172700
H	0.79913500	-1.42298600	-1.84495600
C	3.45163900	-0.05183200	0.94732900
H	3.46822400	-0.98012700	1.50820600
H	4.37801500	-0.00081200	0.37787000
H	3.45752000	0.77589700	1.64833200
Si	2.01228800	0.03481900	-0.23633900
H	-4.47156800	0.17684600	-0.94768800
H	-3.30008500	2.26629300	-0.24031800

E_0(CASSCF,vacuo) -676.119827

E_0(CASSCF,CPCM) **-676.187384**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1198268166
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611983E+03
(     1) 0.9230082 ( 1349)-0.1346792 (  428) 0.1050638 (  506) 0.0953237 ( 2950)-0.0810686 ( 1345) 0.0746852 (    5)-0.0737008
( 2941) 0.0613182 (   10)-0.0609394 ( 3028)-0.0584883 ( 1271)-0.0550917 (  171)-0.0530631 ( 2101)-0.0480571 ( 1460) 0.0476896
(  508) 0.0461132 ( 5970) 0.0455486 (  617)-0.0449746 ( 1430) 0.0447351 ( 1373)-0.0433880 ( 4621)-0.0396118 ( 6081)-0.0385906
(   23)-0.0378261 ( 1264)-0.0373654 ( 5911)-0.0372075 (  430) 0.0365260 ( 5892) 0.0363811 (  685)-0.0357394 ( 2969) 0.0352011
( 1434)-0.0349843 ( 5966)-0.0348938 ( 3205)-0.0344239 ( 3139) 0.0333124 ( 1377) 0.0328537 ( 6053) 0.0322994 ( 1352) 0.0321076
(   16)-0.0317865 (   33) 0.0314406 ( 3035)-0.0313712 (  706)-0.0312971 ( 6049)-0.0312525 ( 1356)-0.0299924 ( 5996)-0.0295004
( 3113)-0.0274619 ( 3226)-0.0274561 ( 6145)-0.0273522 (   92)-0.0266204 ( 3030)-0.0261799 (  429) 0.0252461 ( 2973) 0.0250360
( 6058) 0.0249025 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195311D+01
     2  0.232688D-05  0.192075D+01
     3  0.164425D-06 -0.629637D-06  0.188554D+01
     4  0.262292D-04 -0.420139D-04 -0.116941D-04  0.100116D+01
     5  0.773095D-05 -0.133595D-04  0.128770D-04 -0.106707D-05  0.999906D+00
     6 -0.843723D-05  0.706059D-05  0.420437D-05 -0.182599D-04  0.132641D-05
     7  0.510519D-07 -0.202142D-05 -0.133411D-05 -0.994352D-06  0.141814D-05
     8  0.401429D-05 -0.166256D-05 -0.178676D-05  0.421693D-05  0.203879D-05
     9 -0.764751D-05  0.766710D-05  0.192349D-05  0.361432D-05  0.253875D-05
                6             7             8             9
     6  0.761718D-01
     7 -0.651419D-06  0.109840D+00
     8 -0.268149D-05 -0.877206D-07  0.381317D-01
     9 -0.500857D-07  0.581898D-07  0.418577D-06  0.153924D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 4

GEOMETRY

C	-3.52845700	0.13151000	-0.49409400
C	-2.93574400	-1.13841900	-0.26221100
C	-1.71552100	-1.25111100	0.36327500
C	-1.01357000	-0.07482300	0.80570400
C	-1.65911100	1.16170800	0.54092600
C	-2.87805300	1.30325000	-0.08625100
H	-3.45714600	-2.02378500	-0.57384900
H	-1.28111100	-2.21699300	0.54614200
C	0.23457600	-0.13475400	1.44094100
H	0.56422200	-1.08454200	1.83074000
H	0.57281500	0.73588800	1.97929900
C	1.74678100	1.70230200	-1.02335900
H	2.55467400	1.92694000	-1.71808300
H	0.81934700	1.72165700	-1.58436600
H	1.72459100	2.49727300	-0.28590000
C	1.76770600	-1.45857600	-1.32181200
H	2.55664500	-1.51722300	-2.07007400
H	1.79490300	-2.38125300	-0.75226300
H	0.82265500	-1.40085800	-1.85017100
C	3.46585200	-0.06938300	0.97083100
H	3.46126700	-1.00398600	1.52099800
H	4.40841400	-0.01745300	0.42799300
H	3.45557200	0.75154900	1.67944500
Si	2.06401400	0.03735100	-0.25204200
H	-4.48447900	0.18944000	-0.97916800
H	-3.31531400	2.27022200	-0.24584900

E_0(CASSCF,vacuo) -676.117140

E_0(CASSCF,CPCM) **-676.184846**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1171395069
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67611714E+03
(     1) 0.9207981 ( 1349)-0.1356183 (  428) 0.1064636 (  506) 0.0939029 ( 2950)-0.0858727 ( 1345) 0.0749682 (    5)-0.0740679
( 2941) 0.0638853 (   10)-0.0637468 ( 3028)-0.0591089 ( 1271)-0.0560538 (  171)-0.0551325 ( 1460) 0.0507337 ( 5970) 0.0500936
(  617)-0.0465565 ( 2101)-0.0463907 (  508) 0.0458504 ( 1373)-0.0441385 ( 4621)-0.0434033 ( 1430) 0.0423617 (   23)-0.0416058
( 5892) 0.0403874 (  685)-0.0389589 ( 5911)-0.0379923 ( 2969) 0.0370454 ( 6081)-0.0370405 ( 3139) 0.0368325 ( 1377) 0.0368171
( 3205)-0.0364959 ( 6053) 0.0363205 ( 1264)-0.0354060 ( 1434)-0.0353155 (  430) 0.0351170 ( 5966)-0.0344430 ( 5996)-0.0338751
(   33) 0.0329552 ( 6049)-0.0328704 (   16)-0.0318881 (   92)-0.0313468 (  429) 0.0298416 ( 2973) 0.0283987 (  706)-0.0281320
( 6058) 0.0279988 ( 3035)-0.0274282 ( 1356)-0.0266957 ( 3200)-0.0252558 ( 1352) 0.0249910 ( 3116)-0.0249848 ( 6145)-0.0238121
( 3226)-0.0237377 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195221D+01
     2 -0.308761D-05  0.191652D+01
     3  0.932796D-06 -0.831173D-06  0.188437D+01
     4  0.877225D-05 -0.117560D-04  0.400178D-06  0.100038D+01
     5 -0.329131D-05 -0.353014D-05  0.177247D-04 -0.398396D-03  0.999825D+00
     6  0.104486D-04 -0.699809D-05  0.203650D-05 -0.104367D-04 -0.458950D-05
     7  0.172868D-05  0.209635D-05  0.464341D-06 -0.289162D-07 -0.114932D-05
     8  0.439554D-05  0.874233D-06 -0.106880D-05 -0.115660D-06 -0.457213D-05
     9 -0.136344D-04  0.188585D-05 -0.110382D-05  0.138136D-06 -0.159519D-05
                6             7             8             9
     6  0.806835D-01
     7 -0.467564D-07  0.111494D+00
     8  0.349145D-05 -0.604188D-06  0.393322D-01
     9  0.268443D-05  0.925010D-06 -0.327037D-06  0.151903D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 5

GEOMETRY

C	-3.54822300	0.13780900	-0.51481800
C	-2.96231800	-1.13331800	-0.28238000
C	-1.74938900	-1.25184800	0.35888600
C	-1.05024100	-0.08083700	0.81578300
C	-1.68850700	1.15732100	0.55002400
C	-2.89966700	1.30507700	-0.09202600
H	-3.48126400	-2.01623900	-0.60507400
H	-1.32068600	-2.22034100	0.54250700
C	0.18925300	-0.14862100	1.46742700
H	0.52435500	-1.10163100	1.84303600
H	0.53665100	0.71967100	2.00268000
C	1.78177500	1.71290400	-1.00745900
H	2.58484300	1.95681600	-1.70158500
H	0.85166400	1.73145600	-1.56388500
H	1.75504900	2.49416700	-0.25584100
C	1.80041700	-1.45138700	-1.33299400
H	2.58506100	-1.51853100	-2.08532900
H	1.82047300	-2.37333900	-0.76228100
H	0.85314300	-1.38240700	-1.85583900
C	3.48322100	-0.08190000	0.99096500
H	3.46219500	-1.02148900	1.53186200
H	4.43906200	-0.02881100	0.47118400
H	3.45862300	0.73378300	1.70501900
Si	2.11594300	0.04000800	-0.26596300
H	-4.49787600	0.20143900	-1.01166100
H	-3.33242000	2.27413400	-0.25175400

E_0(CASSCF,vacuo) -676.114314

E_0(CASSCF,CPCM) **-676.182292**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1143138687
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67611431E+03
(     1) 0.9191446 ( 1349)-0.1362483 (  428) 0.1092760 (  506) 0.0935503 ( 2950)-0.0898993 ( 1345) 0.0751122 (    5)-0.0742915
(    10)-0.0657809 ( 2941) 0.0657243 ( 3028)-0.0602346 ( 1271)-0.0571882 (  171)-0.0558541 ( 5970) 0.0530206 ( 1460) 0.0524391
(   617)-0.0478524 ( 4621)-0.0461718 (  508) 0.0457832 ( 2101)-0.0452774 (   23)-0.0444084 ( 1373)-0.0439092 ( 5892) 0.0428044
(   685)-0.0406463 ( 1430) 0.0404675 ( 1377) 0.0391560 ( 3139) 0.0391494 ( 6053) 0.0387147 ( 5911)-0.0380802 ( 2969) 0.0372420
(  5996)-0.0364433 ( 3205)-0.0362722 ( 6081)-0.0362720 ( 1434)-0.0353511 (  430) 0.0342031 ( 1264)-0.0339897 (   33) 0.0337368
(  6049)-0.0337241 ( 5966)-0.0336356 (   16)-0.0323194 (   92)-0.0319201 ( 2973) 0.0304298 (  429) 0.0303257 ( 6058) 0.0298813
(  3200)-0.0284795 ( 3116)-0.0264775 (  706)-0.0257136 ( 3035)-0.0253364 ( 1356)-0.0238923 (   93)-0.0222296 ( 3120)-0.0217386
(  5975) 0.0214652 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195184D+01
     2 -0.129176D-05  0.191292D+01
     3 -0.242593D-06  0.109690D-05  0.188351D+01
     4 -0.919724D-05  0.268047D-04  0.342896D-05  0.999827D+00
     5  0.516822D-07  0.743594D-05 -0.123486D-04 -0.756959D-03  0.999766D+00
     6  0.785632D-05 -0.725137D-05 -0.607407D-05  0.194275D-04  0.863824D-05
     7  0.171273D-05 -0.127229D-05  0.105027D-05  0.529598D-05 -0.334913D-06
     8  0.492387D-05  0.301029D-06  0.349274D-05 -0.799686D-05 -0.168456D-05
     9 -0.562783D-06  0.175543D-05 -0.376603D-05  0.824931D-05  0.510568D-05
                6             7             8             9
     6  0.843762D-01
     7 -0.254436D-06  0.112793D+00
     8  0.170079D-05  0.815113D-06  0.401205D-01
     9 -0.110451D-05 -0.112418D-05 -0.115611D-06  0.148442D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 6

GEOMETRY

C	-3.56780200	0.14720200	-0.53568600
C	-2.99046300	-1.12663600	-0.30518000
C	-1.78548800	-1.25426900	0.35165700
C	-1.08770300	-0.09058400	0.82574200
C	-1.71704200	1.15085900	0.56137500
C	-2.91975000	1.30809900	-0.09533000
H	-3.50805600	-2.00558600	-0.64084200
H	-1.36387200	-2.22631500	0.53386200
C	0.14328500	-0.16945200	1.49311600
H	0.48087800	-1.12687700	1.85374900
H	0.49901800	0.69434000	2.02933700
C	1.83018700	1.73648000	-0.96498900
H	2.61547200	1.99010700	-1.67621000
H	0.88484600	1.77651400	-1.49387400
H	1.83284000	2.49785600	-0.19302300
C	1.82072900	-1.42163300	-1.36752900
H	2.58826100	-1.47611400	-2.13870400
H	1.84764600	-2.35531400	-0.81688800
H	0.86266300	-1.33463800	-1.86743500
C	3.50182100	-0.12482700	1.00701700
H	3.45828400	-1.07881400	1.52046200
H	4.47092800	-0.06614300	0.51259700
H	3.46517400	0.67164800	1.74179800
Si	2.16831800	0.04348400	-0.27774900
H	-4.51068600	0.21893200	-1.04429000
H	-3.34648800	2.28020100	-0.25321800

E_0(CASSCF,vacuo) -676.111481

E_0(CASSCF,CPCM) **-676.179838**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1114805721
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67611148E+03
(     1) 0.9178384 ( 1349)-0.1366779 (  428) 0.1115696 (  506) 0.0933259 ( 2950)-0.0931680 ( 1345) 0.0752800 (    5)-0.0745344
(    10)-0.0673788 ( 2941) 0.0671876 ( 3028)-0.0614974 ( 1271)-0.0582675 (  171)-0.0564883 ( 5970) 0.0549735 ( 1460) 0.0534042
(   617)-0.0486552 ( 4621)-0.0481876 (   23)-0.0465009 (  508) 0.0454414 ( 5892) 0.0443951 ( 2101)-0.0442143 ( 1373)-0.0430223
(  3139) 0.0408448 (  685)-0.0408196 ( 1377) 0.0405699 ( 6053) 0.0401742 ( 1430) 0.0386467 ( 5996)-0.0379894 ( 5911)-0.0379239
(  2969) 0.0365732 ( 6081)-0.0358906 ( 1434)-0.0352062 ( 3205)-0.0348188 ( 6049)-0.0342335 (   33) 0.0341940 (  430) 0.0331657
(  1264)-0.0328957 (   16)-0.0327244 ( 5966)-0.0325691 (   92)-0.0323678 ( 2973) 0.0317948 ( 6058) 0.0311796 (  429) 0.0307076
(  3200)-0.0306144 ( 3116)-0.0269816 ( 3035)-0.0242804 (  706)-0.0235004 (   93)-0.0229968 ( 3120)-0.0225382 ( 1356)-0.0215807
(  2116) 0.0206312 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195170D+01
     2  0.795737D-07  0.190991D+01
     3 -0.177312D-06  0.412595D-06  0.188283D+01
     4 -0.310313D-06  0.958718D-05  0.535556D-05  0.999515D+00
     5  0.768661D-05  0.741951D-05  0.459428D-06 -0.971205D-03  0.999730D+00
     6  0.133572D-05 -0.349279D-05 -0.840675D-07  0.711484D-05 -0.156222D-05
     7  0.202022D-06  0.257224D-05 -0.218359D-05 -0.405644D-05  0.140993D-04
     8 -0.216015D-05  0.241831D-05  0.169351D-05 -0.534916D-05  0.128891D-04
     9 -0.180584D-05  0.340782D-06  0.433779D-06  0.461792D-05 -0.175345D-06
                6             7             8             9
     6  0.874317D-01
     7  0.387395D-06  0.113891D+00
     8 -0.951150D-08  0.194470D-06  0.406829D-01
     9 -0.604545D-06  0.758276D-07 -0.244535D-07  0.143094D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 7

GEOMETRY

C	-3.58796900	0.15672600	-0.55668000
C	-3.01867400	-1.11997900	-0.32843400
C	-1.82205800	-1.25682100	0.34357200
C	-1.12593200	-0.10040900	0.83526900
C	-1.74686500	1.14447800	0.57232900
C	-2.94076000	1.31123200	-0.09884300
H	-3.53470500	-1.99482900	-0.67717200
H	-1.40726600	-2.23227100	0.52403900
C	0.09641600	-0.19005800	1.51791900
H	0.43513600	-1.15152200	1.86551300
H	0.45854700	0.66922400	2.05642400
C	1.86771200	1.75018700	-0.93728800
H	2.64127500	2.02027700	-1.65558200
H	0.91441500	1.79537000	-1.45131300
H	1.87906900	2.49622000	-0.15073200
C	1.85430500	-1.40406300	-1.38746200
H	2.61034400	-1.45241900	-2.17059700
H	1.88586400	-2.34323000	-0.84675700
H	0.88938900	-1.30745300	-1.87224000
C	3.52165200	-0.14616600	1.02358900
H	3.46182600	-1.10782700	1.52062800
H	4.50252000	-0.08433000	0.55273000
H	3.47066800	0.63984300	1.76859000
Si	2.22083100	0.04710700	-0.28828700
H	-4.52398200	0.23639800	-1.07675800
H	-3.36169500	2.28628300	-0.25459000

E_0(CASSCF,vacuo) -676.108723

E_0(CASSCF,CPCM) **-676.177551**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1087232049
Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610872E+03
(     1) 0.9167441 ( 1349)-0.1369270 (  428) 0.1136488 ( 2950)-0.0957910 (  506) 0.0933621 ( 1345) 0.0755391 (    5)-0.0748599
(    10)-0.0687517 ( 2941) 0.0684834 ( 3028)-0.0626933 ( 1271)-0.0591911 (  171)-0.0570371 ( 5970) 0.0563143 ( 1460) 0.0539410
( 4621)-0.0496256 (  617)-0.0492779 (   23)-0.0480401 ( 5892) 0.0454944 (  508) 0.0449096 ( 2101)-0.0432563 ( 3139) 0.0421443
( 1373)-0.0418748 ( 1377) 0.0414463 ( 6053) 0.0410806 (  685)-0.0398672 ( 5996)-0.0389530 ( 5911)-0.0376738 ( 1430) 0.0369580
( 6081)-0.0357011 ( 2969) 0.0355873 ( 1434)-0.0349749 ( 6049)-0.0345997 (   33) 0.0345287 (   16)-0.0330998 (   92)-0.0328239
( 2973) 0.0327701 ( 3205)-0.0327669 ( 6058) 0.0321387 ( 1264)-0.0320166 (  430) 0.0319544 ( 3200)-0.0317858 ( 5966)-0.0314526
(  429) 0.0311261 ( 3116)-0.0270862 ( 3035)-0.0238112 (   93)-0.0235867 ( 3120)-0.0232013 ( 3026)-0.0219613 (  706)-0.0214532
( 2116) 0.0209198 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195165D+01
     2  0.176478D-05  0.190739D+01
     3  0.154657D-06  0.753988D-06  0.188226D+01
     4 -0.293255D-05  0.228681D-04  0.582726D-05  0.999389D+00
     5 -0.305033D-05  0.639239D-05  0.505207D-05 -0.106527D-02  0.999712D+00
     6  0.670475D-06 -0.311929D-05  0.372276D-05  0.115492D-05 -0.505235D-06
     7 -0.853771D-06  0.561319D-05 -0.156104D-05 -0.186510D-05 -0.203832D-05
     8 -0.897176D-06 -0.370597D-06  0.193621D-07  0.337387D-05  0.546422D-06
     9  0.495530D-05 -0.541523D-05 -0.267095D-05 -0.243481D-05 -0.252696D-06
                6             7             8             9
     6  0.900084D-01
     7  0.708977D-06  0.114853D+00
     8 -0.270215D-05  0.677847D-06  0.411284D-01
     9 -0.112070D-05 -0.461420D-06 -0.945713D-07  0.136054D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 8

GEOMETRY

C	-3.60770800	0.17360700	-0.57790000
C	-3.04885300	-1.10877400	-0.36022500
C	-1.86176300	-1.26184600	0.32628100
C	-1.16537000	-0.11741000	0.84355800
C	-1.77594300	1.13398900	0.59089400
C	-2.96021900	1.31705700	-0.09361400
H	-3.56467700	-1.97591500	-0.72819800
H	-1.45558100	-2.24253900	0.49841600
C	0.04790200	-0.22506300	1.53981700
H	0.38547400	-1.19379800	1.86680700
H	0.41729700	0.62408900	2.08880100
C	1.93506100	1.78466300	-0.86984000
H	2.70397000	2.07476300	-1.58566400
H	0.97678100	1.86254600	-1.37093600
H	1.96475700	2.49665300	-0.05291800
C	1.87172000	-1.35092700	-1.44237200
H	2.62480400	-1.39086200	-2.22899700
H	1.88208100	-2.30759600	-0.93259400
H	0.90826200	-1.21494700	-1.92109100
C	3.53263600	-0.21627600	1.03861300
H	3.44082900	-1.19563800	1.49441500
H	4.52770200	-0.15475000	0.59810100
H	3.47418400	0.54097700	1.81224100
Si	2.27276400	0.05282600	-0.29709200
H	-4.53602000	0.26650400	-1.10953300
H	-3.37332700	2.29683900	-0.24082100

E_0(CASSCF,vacuo) -676.106101

E_0(CASSCF,CPCM) **-676.175481**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.1061008731
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67610610E+03
(     1) 0.9157777 ( 1349)-0.1370400 (  428) 0.1158209 ( 2950)-0.0978236 (  506) 0.0938074 ( 1345) 0.0759352 (    5)-0.0753128
(    10)-0.0700415 ( 2941) 0.0697390 ( 3028)-0.0636818 ( 1271)-0.0599053 (  171)-0.0574405 ( 5970) 0.0572287 ( 1460) 0.0542137
( 4621)-0.0505719 (  617)-0.0499338 (   23)-0.0491023 ( 5892) 0.0462565 (  508) 0.0442752 ( 3139) 0.0431263 ( 2101)-0.0424701
( 1377) 0.0419844 ( 6053) 0.0416337 ( 1373)-0.0407190 ( 5996)-0.0395636 (  685)-0.0381793 ( 5911)-0.0373907 ( 6081)-0.0356071
( 1430) 0.0354900 ( 6049)-0.0349382 (   33) 0.0348469 ( 1434)-0.0347096 ( 2969) 0.0345881 (   16)-0.0334778 ( 2973) 0.0334733
(   92)-0.0331958 ( 6058) 0.0328597 ( 3200)-0.0321552 (  429) 0.0314621 ( 1264)-0.0312836 (  430) 0.0305669 ( 3205)-0.0305619
( 5966)-0.0304173 ( 3116)-0.0270846 ( 3026)-0.0242780 (   93)-0.0239595 ( 3120)-0.0237582 ( 3035)-0.0236693 ( 2116) 0.0212366
(  433) 0.0210686 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195162D+01
     2 -0.261124D-06  0.190530D+01
     3  0.886188D-07  0.133395D-06  0.188176D+01
     4  0.258304D-05  0.583982D-05  0.317610D-05  0.999404D+00
     5  0.112322D-06 -0.858481D-05  0.235546D-05 -0.107612D-02  0.999708D+00
     6 -0.192321D-05  0.343776D-05  0.241761D-05  0.571912D-05  0.452773D-06
     7  0.751118D-07 -0.363873D-06  0.198897D-05 -0.232001D-05 -0.165321D-05
     8 -0.100084D-05 -0.139430D-05  0.614138D-07 -0.222481D-05  0.436995D-05
     9 -0.492200D-05  0.752814D-05  0.188990D-05  0.114159D-04  0.435814D-05
                6             7             8             9
     6  0.921813D-01
     7  0.123305D-06  0.115724D+00
     8 -0.175492D-06  0.142033D-07  0.415101D-01
     9 -0.756036D-06  0.297888D-06  0.198717D-06  0.127839D-01
MCSCF converged.
```

$^{3}2^{+}$c STEP 9

GEOMETRY

C	-3.62859200	0.18371800	-0.59812200
C	-3.07784400	-1.10188200	-0.38291800
C	-1.89974800	-1.26486800	0.31790000
C	-1.20485000	-0.12820500	0.85282700
C	-1.80671100	1.12695100	0.60094700
C	-2.98172700	1.32024700	-0.09736300
H	-3.59219300	-1.96439400	-0.76381200
H	-1.50038700	-2.24887100	0.48777500
C	-0.00013800	-0.24671700	1.56332200
H	0.33591300	-1.21880500	1.88125500
H	0.37294200	0.59841500	2.11568800
C	1.95299000	1.78711200	-0.85520600
H	2.69712300	2.09158500	-1.59102000
H	0.97999500	1.85424300	-1.32875900
H	1.99602000	2.49362400	-0.03426200
C	1.91663300	-1.34631800	-1.44504800
H	2.64873000	-1.37083400	-2.25203700
H	1.95375200	-2.30501700	-0.94058600
H	0.93904700	-1.22059000	-1.89700300
C	3.56574300	-0.21274300	1.04798500
H	3.47258800	-1.19533900	1.49639300
H	4.56663700	-0.14328000	0.62157900
H	3.49190100	0.54041000	1.82425000
Si	2.32586200	0.05694900	-0.30448200
H	-4.54984500	0.28480800	-1.14051200
H	-3.38882500	2.30299100	-0.24212600

E_0(CASSCF,vacuo) -676.103663

E_0(CASSCF,CPCM) **-676.173636**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1036631784
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610366E+03
 (     1) 0.9149322 ( 1349)-0.1370434 (  428) 0.1177912 ( 2950)-0.0996683 (  506) 0.0941906 ( 1345) 0.0763055 (    5)-0.0757405
 (    10)-0.0712600 ( 2941) 0.0709423 ( 3028)-0.0646924 ( 1271)-0.0605754 ( 5970) 0.0580070 (  171)-0.0578532 ( 1460) 0.0543899
 ( 4621)-0.0514016 (  617)-0.0504240 (   23)-0.0500393 ( 5892) 0.0468576 ( 3139) 0.0439904 (  508) 0.0436168 ( 1377) 0.0424055
 ( 6053) 0.0420585 ( 2101)-0.0417099 ( 5996)-0.0400172 ( 1373)-0.0395123 ( 5911)-0.0370955 (  685)-0.0358031 ( 6081)-0.0355647
 ( 6049)-0.0352034 (   33) 0.0350986 ( 1434)-0.0344775 ( 1430) 0.0340582 ( 2973) 0.0340396 (   16)-0.0338072 (   92)-0.0337761
 ( 6058) 0.0334558 ( 2969) 0.0334539 (  429) 0.0320231 ( 3200)-0.0318523 ( 1264)-0.0306954 ( 5966)-0.0294118 (  430) 0.0291987
 ( 3205)-0.0280554 ( 3116)-0.0269007 ( 3026)-0.0261528 (   93)-0.0244102 ( 3120)-0.0242519 ( 3035)-0.0237187 (  433) 0.0217295
 ( 2116) 0.0215167 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195163D+01
     2  0.105238D-05  0.190345D+01
     3  0.386690D-07 -0.923504D-06  0.188133D+01
     4  0.251250D-05  0.563555D-05 -0.934663D-05  0.999512D+00
     5 -0.182810D-05 -0.991841D-06  0.789692D-05 -0.103033D-02  0.999711D+00
     6 -0.255483D-05  0.248993D-05 -0.232787D-05  0.106327D-05 -0.538825D-06
     7 -0.585902D-06 -0.177441D-05 -0.529500D-06  0.341256D-05  0.137664D-05
     8  0.104120D-06 -0.731796D-06 -0.505227D-06  0.231154D-05  0.712867D-06
     9 -0.157511D-05  0.502648D-05  0.794845D-06 -0.604420D-05 -0.266169D-05
                6             7             8             9
     6  0.942448D-01
     7 -0.806845D-06  0.116503D+00
     8 -0.146349D-05  0.785412D-08  0.418589D-01
     9 -0.350403D-06 -0.151668D-06 -0.239886D-06  0.117554D-01
 MCSCF converged.
```

$^{3}2^{+}$c STEP 10

GEOMETRY

C	-3.64941000	0.20167500	-0.61764000
C	-3.10935000	-1.08988300	-0.41417300
C	-1.94103600	-1.27041200	0.29945500
C	-1.24547900	-0.14685200	0.86002900
C	-1.83645100	1.11522900	0.61862100
C	-3.00148100	1.32613300	-0.09173100
H	-3.62382000	-1.94376500	-0.81406000
H	-1.55046400	-2.25960900	0.45988000
C	-0.05003500	-0.28411900	1.58287000
H	0.28278900	-1.26274200	1.88300200
H	0.32846900	0.55109300	2.14621400
C	1.99682500	1.80747800	-0.80359000
H	2.72080300	2.13058900	-1.55158200
H	1.01151000	1.88738500	-1.24933500
H	2.06272100	2.49151800	0.03456600
C	1.95034400	-1.30808700	-1.47993300
H	2.66787900	-1.31072200	-2.30041100
H	1.99502300	-2.27989300	-1.00206200
H	0.96517800	-1.16891100	-1.91136900
C	3.58948300	-0.25236500	1.05668000
H	3.48167800	-1.24690800	1.47438200
H	4.59911000	-0.17711500	0.65194300
H	3.50470300	0.47928600	1.85215200
Si	2.37839300	0.06332800	-0.30998500
H	-4.56306400	0.31681000	-1.17006000
H	-3.40047900	2.31361600	-0.22700200

E_0(CASSCF,vacuo) -676.101418

E_0(CASSCF,CPCM) **-676.171999**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =     -676.1014181782
 Full Convergence on CI vector
          ( 1)       EIGENVALUE     -0.67610142E+03
 (     1) 0.9141414 ( 1349)-0.1369683 (  428) 0.1199021 ( 2950)-0.1011113 (  506) 0.0949377 ( 1345) 0.0768109 (    5)-0.0762945
 (    10)-0.0724645 ( 2941) 0.0721576 ( 3028)-0.0655020 ( 1271)-0.0610857 ( 5970) 0.0585620 (  171)-0.0581651 ( 1460) 0.0544568
 ( 4621)-0.0519395 (  617)-0.0510181 (   23)-0.0506755 ( 5892) 0.0472842 ( 3139) 0.0446526 (  508) 0.0429355 ( 1377) 0.0426757
 ( 6053) 0.0423262 ( 2101)-0.0411033 ( 5996)-0.0403159 ( 1373)-0.0384240 ( 5911)-0.0368042 ( 6081)-0.0355592 ( 6049)-0.0355013
 (   33) 0.0353878 ( 2973) 0.0344568 (   92)-0.0342774 ( 1434)-0.0342629 (   16)-0.0341450 ( 6058) 0.0339114 (  685)-0.0332012
 ( 1430) 0.0328527 (  429) 0.0325069 ( 2969) 0.0324328 ( 3200)-0.0310054 ( 1264)-0.0302032 ( 5966)-0.0285313 (  430) 0.0277791
 ( 3026)-0.0275922 ( 3116)-0.0267215 ( 3205)-0.0257458 (   93)-0.0247190 ( 3120)-0.0246672 ( 3035)-0.0238716 (  433) 0.0219339
 ( 2116) 0.0218261 (
 Final one electron symbolic density matrix:
                   1             2             3             4             5
      1  0.195161D+01
      2  0.224359D-05  0.190191D+01
      3  0.111925D-05 -0.329474D-06  0.188092D+01
      4  0.287529D-05  0.120295D-04 -0.330516D-05  0.999681D+00
      5 -0.338700D-05  0.119196D-05  0.115357D-04 -0.946126D-03  0.999720D+00
      6 -0.202890D-06 -0.201147D-05 -0.944893D-06  0.332102D-05 -0.220799D-06
      7  0.124140D-05  0.205838D-06  0.344987D-06  0.214200D-05 -0.273974D-05
      8 -0.638139D-06  0.147912D-05  0.128449D-05  0.183479D-05  0.111058D-05
      9 -0.341656D-07 -0.141110D-05 -0.968510D-06 -0.177198D-05  0.153841D-06
                   6             7             8             9
      6  0.960436D-01
      7 -0.135433D-06  0.117239D+00
      8 -0.314640D-05  0.129555D-05  0.421847D-01
      9 -0.103384D-05 -0.300696D-06 -0.281914D-06  0.106877D-01
 MCSCF converged.
```

$^{3}2^{+}$c STEP 11

GEOMETRY

C	-3.66976500	0.21840200	-0.63749400
C	-3.14058700	-1.07874300	-0.44237000
C	-1.98276800	-1.27524700	0.28422400
C	-1.28705200	-0.16378000	0.86736800
C	-1.86668400	1.10467200	0.63349500
C	-3.02132000	1.33144900	-0.08911800
H	-3.65517900	-1.92458200	-0.85900300
H	-1.60112900	-2.26909600	0.43763900
C	-0.10105000	-0.31820100	1.60194300
H	0.22828800	-1.30224900	1.88734600
H	0.28214900	0.50833900	2.17460500
C	2.00995600	1.80783000	-0.79207500
H	2.72026200	2.15270500	-1.54350400
H	1.01909000	1.86863000	-1.22948200
H	2.06717900	2.48639900	0.05110900
C	2.00898100	-1.30544500	-1.48138700
H	2.71625400	-1.29643600	-2.31083400
H	2.07245000	-2.27739800	-1.00609700
H	1.01672200	-1.17815700	-1.90100200
C	3.62123500	-0.23893900	1.06999800
H	3.51792400	-1.23680800	1.48088100
H	4.63671700	-0.15019000	0.68257500
H	3.51472800	0.48837400	1.86685400
Si	2.43043700	0.06920200	-0.31432400
H	-4.57520000	0.34635400	-1.20036100
H	-3.41205400	2.32328500	-0.21768200

E_0(CASSCF,vacuo) -676.099372

E_0(CASSCF,CPCM) **-676.170575**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0993719487
Full Convergence on CI vector
          ( 1)      EIGENVALUE     -0.67609937E+03
(     1) 0.9134611 ( 1349)-0.1367288 (  428) 0.1221098 ( 2950)-0.1023096 (  506) 0.0959222 ( 1345) 0.0773570 (    5)-0.0768829
(    10)-0.0735649 ( 2941) 0.0732742 ( 3028)-0.0662347 ( 1271)-0.0615136 ( 5970) 0.0590003 (  171)-0.0583178 ( 1460) 0.0544609
( 4621)-0.0523308 (  617)-0.0516498 (   23)-0.0511492 ( 5892) 0.0475836 ( 3139) 0.0451835 ( 1377) 0.0428678 ( 6053) 0.0425140
(  508) 0.0422624 ( 2101)-0.0406096 ( 5996)-0.0405337 ( 1373)-0.0374228 ( 5911)-0.0365156 ( 6049)-0.0357694 (   33) 0.0356521
( 6081)-0.0355716 ( 2973) 0.0347622 (   16)-0.0344859 (   92)-0.0343991 ( 6058) 0.0342556 ( 1434)-0.0340895 (  429) 0.0326166
( 1430) 0.0317943 ( 2969) 0.0314729 (  685)-0.0305447 ( 1264)-0.0298388 ( 3200)-0.0297663 ( 3026)-0.0286997 ( 5966)-0.0277555
(  430) 0.0265108 ( 3116)-0.0264875 ( 3120)-0.0250062 (   93)-0.0247293 ( 3035)-0.0241181 ( 3205)-0.0235968 ( 2116) 0.0221470
(  433) 0.0216863 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195162D+01
     2 -0.448367D-06  0.190062D+01
     3  0.159529D-06  0.536631D-06  0.188060D+01
     4  0.196992D-05  0.482495D-05  0.110831D-04  0.999873D+00
     5 -0.155733D-05 -0.348181D-05  0.457682D-05 -0.845944D-03  0.999735D+00
     6 -0.625845D-06  0.276256D-05  0.475837D-05 -0.374917D-05 -0.276226D-05
     7  0.202190D-06 -0.964520D-06  0.342965D-05 -0.700872D-06 -0.359104D-05
     8  0.473821D-07 -0.982560D-06 -0.131925D-07 -0.557037D-07  0.271386D-05
     9  0.105483D-05 -0.213133D-05 -0.318995D-05 -0.127544D-04 -0.435470D-05
                6             7             8             9
     6  0.976256D-01
     7  0.499731D-06  0.117855D+00
     8  0.228812D-07 -0.385199D-07  0.424658D-01
     9  0.394950D-06  0.945797D-07 -0.172672D-06  0.960371D-02
MCSCF converged.
```

$^{3}2^{+}$c STEP 12

GEOMETRY

C	-3.69225600	0.24906600	-0.65225800
C	-3.17692100	-1.05728200	-0.48639500
C	-2.02903000	-1.28420500	0.24798500
C	-1.32927000	-0.19601600	0.86941800
C	-1.89517100	1.08337700	0.66277900
C	-3.03945200	1.34062700	-0.06661400
H	-3.69394500	-1.88699100	-0.93163600
H	-1.65837200	-2.28554500	0.37841100
C	-0.15299200	-0.38166600	1.61246800
H	0.16989800	-1.37573800	1.86825500
H	0.23729900	0.42632000	2.20620200
C	2.08220100	1.84869200	-0.68163800
H	2.75003500	2.21248000	-1.46244500
H	1.06756100	1.95184600	-1.05189000
H	2.20893400	2.48466200	0.18657000
C	2.02837800	-1.21395800	-1.55835300
H	2.71773400	-1.15682300	-2.40083900
H	2.09172000	-2.21475500	-1.14745500
H	1.02908100	-1.05125300	-1.94800200
C	3.64053500	-0.33818400	1.06740300
H	3.51140400	-1.35834500	1.41068200
H	4.66529000	-0.24329200	0.70650200
H	3.52988900	0.33882200	1.90695800
Si	2.48337900	0.07970300	-0.31548000
H	-4.59029800	0.40083200	-1.22129700
H	-3.41966400	2.33923300	-0.17209000

E_0(CASSCF,vacuo) -676.097529

E_0(CASSCF,CPCM) **-676.169334**

DATA from the CASSCF calculation in vacuo:

```
 Energy state  1 =    -676.0975292384
 Full Convergence on CI vector     -0.67609753E+03
          ( 1)        EIGENVALUE
 (     1) 0.9127633 ( 1349)-0.1366678 (  428) 0.1242468 ( 2950)-0.1033328 (  506) 0.0969326 ( 1345) 0.0779287 (    5)-0.0774946
 (    10)-0.0746967 ( 2941) 0.0744289 ( 3028)-0.0668590 ( 1271)-0.0618934 ( 5970) 0.0593605 (  171)-0.0584868 ( 1460) 0.0544725
 ( 4621)-0.0526559 (  617)-0.0522771 (   23)-0.0515402 ( 5892) 0.0478594 ( 3139) 0.0456474 ( 1377) 0.0430257 ( 6053) 0.0426632
 (  508) 0.0416919 ( 5996)-0.0406825 ( 2101)-0.0402100 ( 1373)-0.0365627 ( 5911)-0.0362733 ( 6049)-0.0360671 (   33) 0.0359461
 ( 6081)-0.0356082 ( 2973) 0.0350361 (   16)-0.0348195 (   92)-0.0347333 ( 6058) 0.0345657 ( 1434)-0.0339391 (  429) 0.0329230
 ( 1430) 0.0309148 ( 2969) 0.0306010 ( 3026)-0.0297084 ( 1264)-0.0294999 ( 3200)-0.0281848 (  685)-0.0278936 ( 5966)-0.0270850
 ( 3116)-0.0262774 ( 3120)-0.0253261 (  430) 0.0252396 (   93)-0.0248778 ( 3035)-0.0243208 ( 2116) 0.0224729 ( 3205)-0.0217120
 (  536) 0.0216355 (
 Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195157D+01
     2  0.182994D-05  0.189943D+01
     3  0.584126D-06 -0.344034D-06  0.188020D+01
     4  0.434471D-05 -0.651294D-05 -0.323122D-05  0.100009D+01
     5 -0.128679D-05 -0.433186D-05  0.148031D-04 -0.744146D-03  0.999747D+00
     6  0.158216D-06  0.191640D-05 -0.488332D-06  0.404946D-05  0.113245D-05
     7 -0.111063D-05 -0.335577D-05  0.351679D-06 -0.269062D-05  0.395187D-06
     8 -0.627206D-07 -0.115648D-05 -0.164502D-05  0.204738D-05  0.589251D-06
     9 -0.508081D-06  0.567894D-05 -0.134378D-05 -0.789615D-05 -0.226164D-05
                6             7             8             9
     6  0.991330D-01
     7 -0.102544D-06  0.118553D+00
     8 -0.217826D-05  0.436545D-06  0.427699D-01
     9 -0.145012D-06  0.264796D-06 -0.467518D-06  0.850772D-02
 MCSCF converged.
```

$^{3}2^{+}$c STEP 13

GEOMETRY

C	-3.71380000	0.28021600	-0.66597000
C	-3.21272900	-1.03476600	-0.52862600
C	-2.07543300	-1.29210100	0.21258500
C	-1.37204300	-0.22810000	0.87074300
C	-1.92362600	1.06160600	0.69117700
C	-3.05710100	1.34914000	-0.04408300
H	-3.73229200	-1.84757300	-1.00137600
H	-1.71602900	-2.30026200	0.32044500
C	-0.20556300	-0.44506600	1.62038500
H	0.11082400	-1.44811700	1.84695400
H	0.19148400	0.34392600	2.23464600
C	2.11890600	1.86701900	-0.61650900
H	2.74326400	2.25168400	-1.42265800
H	1.08597800	1.97522600	-0.93212200
H	2.28734900	2.48174900	0.25971700
C	2.07594700	-1.16132500	-1.59797600
H	2.73989700	-1.05552600	-2.45592900
H	2.16808600	-2.17652400	-1.23039000
H	1.06346700	-1.00184700	-1.95441200
C	3.66755000	-0.37740900	1.07144900
H	3.53118400	-1.40889700	1.37600200
H	4.69893800	-0.27140500	0.73295400
H	3.54207000	0.27032300	1.93182700
Si	2.53596300	0.09015500	-0.31548000
H	-4.60383300	0.45583600	-1.24075700
H	-3.42652400	2.35395000	-0.12722500

E_0(CASSCF,vacuo) -676.095873

E_0(CASSCF,CPCM) **-676.168263**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0958725083
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609587E+03
(     1) 0.9121643 ( 1349)-0.1364604 (  428) 0.1261460 ( 2950)-0.1041912 (  506) 0.0979859 ( 1345) 0.0785086 (    5)-0.0781069
(    10)-0.0757134 ( 2941) 0.0754720 ( 3028)-0.0674212 ( 1271)-0.0622166 ( 5970) 0.0596482 (  171)-0.0586304 ( 1460) 0.0544456
( 4621)-0.0528915 (  617)-0.0528371 (   23)-0.0518220 ( 5892) 0.0480584 ( 3139) 0.0460252 ( 1377) 0.0431395 ( 6053) 0.0427699
(  508) 0.0410718 ( 5996)-0.0407968 ( 2101)-0.0398349 ( 6049)-0.0363349 (   33) 0.0362125 ( 5911)-0.0360382 ( 1373)-0.0357341
( 6081)-0.0356479 ( 2973) 0.0352421 (   16)-0.0351165 (   92)-0.0351133 ( 6058) 0.0348029 ( 1434)-0.0338229 (  429) 0.0332840
( 3026)-0.0304668 ( 1430) 0.0301066 ( 2969) 0.0297520 ( 1264)-0.0292576 ( 5966)-0.0264643 ( 3200)-0.0263047 ( 3116)-0.0260043
( 3120)-0.0255927 (  685)-0.0253200 (   93)-0.0250397 ( 3035)-0.0245741 (  430) 0.0240965 ( 2116) 0.0227542 (  536) 0.0217838
( 4643) 0.0210227 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195155D+01
     2  0.252022D-06  0.189843D+01
     3 -0.357617D-06  0.392200D-06  0.187989D+01
     4  0.475071D-05 -0.420447D-05 -0.109025D-04  0.100030D+01
     5 -0.108227D-05 -0.355496D-05 -0.158550D-05 -0.637132D-03  0.999759D+00
     6 -0.147578D-05  0.206753D-05  0.156439D-05  0.164112D-05  0.844350D-06
     7 -0.280937D-05 -0.480460D-06  0.191464D-05 -0.264517D-06 -0.894774D-06
     8  0.401638D-06 -0.385457D-07  0.228474D-05  0.270127D-05 -0.230299D-06
     9 -0.206233D-05  0.811414D-06  0.319727D-05 -0.458114D-05 -0.312962D-05
                6             7             8             9
     6  0.100458D+00
     7  0.631326D-06  0.119129D+00
     8 -0.156632D-06 -0.160199D-06  0.430323D-01
     9  0.428924D-06 -0.164466D-06 -0.465433D-06  0.745077D-02
MCSCF converged.
```

$^{3}2^{+}$c STEP 14

GEOMETRY

C	-3.73313500	0.32660300	-0.67247600
C	-3.25191400	-0.99971700	-0.58188000
C	-2.12618000	-1.30248500	0.16003300
C	-1.41458200	-0.27571300	0.86689800
C	-1.94625900	1.02792000	0.73222400
C	-3.06787200	1.36060900	-0.00252800
H	-3.77761300	-1.78581100	-1.09167800
H	-1.78197400	-2.31920400	0.23115700
C	-0.25803300	-0.53792800	1.61619500
H	0.04947900	-1.55259000	1.79840900
H	0.14931800	0.22120600	2.26053600
C	2.14131500	1.88493000	-0.54778200
H	2.65321600	2.27680100	-1.42577400
H	1.07512200	1.98947500	-0.72969400
H	2.41332900	2.49421600	0.30566400
C	2.13333800	-1.10322900	-1.63685300
H	2.78714500	-0.95875400	-2.49694700
H	2.23891400	-2.13007700	-1.30744600
H	1.11555600	-0.94083900	-1.97822700
C	3.69562000	-0.40728700	1.07609100
H	3.56299500	-1.45140800	1.33595000
H	4.73296800	-0.27784100	0.76473300
H	3.54535500	0.20473400	1.95849700
Si	2.58850400	0.10550900	-0.31329100
H	-4.61448400	0.53753900	-1.24886000
H	-3.42218200	2.37320400	-0.04977700

E_0(CASSCF,vacuo) -676.094397

E_0(CASSCF,CPCM) **-676.167304**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0943967347
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609440E+03
(     1) 0.9115884 ( 1349)-0.1362413 (  428) 0.1292333 ( 2950)-0.1049115 (  506) 0.0996610 ( 1345) 0.0791333 (    5)-0.0787605
(    10)-0.0767223 ( 2941) 0.0765132 ( 3028)-0.0678867 ( 1271)-0.0624765 ( 5970) 0.0598712 (  171)-0.0582328 ( 1460) 0.0543994
(   617)-0.0538381 ( 4621)-0.0530451 (   23)-0.0520024 ( 5892) 0.0482211 ( 3139) 0.0463405 ( 1377) 0.0432184 ( 6053) 0.0428456
(  5996)-0.0408794 (  508) 0.0406690 ( 2101)-0.0397181 ( 6049)-0.0366270 (   33) 0.0365036 ( 5911)-0.0358192 ( 6081)-0.0356883
(    16)-0.0356156 ( 2973) 0.0354176 ( 1373)-0.0351510 ( 6058) 0.0350038 ( 1434)-0.0337249 (   92)-0.0336865 (  429) 0.0318034
(  3026)-0.0312849 ( 1430) 0.0295619 ( 2969) 0.0291069 ( 1264)-0.0290397 ( 5966)-0.0260386 ( 3116)-0.0258794 ( 3120)-0.0258449
(  3035)-0.0248375 ( 3200)-0.0241811 (   93)-0.0240022 ( 2116) 0.0232266 (  430) 0.0230891 (  685)-0.0228614 (  536) 0.0220668
(   593)-0.0211872 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195151D+01
     2 -0.359502D-06  0.189755D+01
     3  0.432005D-06 -0.108973D-05  0.187959D+01
     4 -0.238400D-05  0.187608D-05  0.177542D-05  0.100053D+01
     5  0.277815D-05  0.591871D-05 -0.966820D-05 -0.568567D-03  0.999775D+00
     6  0.658096D-06 -0.182824D-05 -0.111651D-05  0.423351D-05  0.167334D-05
     7 -0.168350D-05  0.218266D-05  0.241447D-07 -0.293057D-05  0.327119D-05
     8  0.157295D-05 -0.122093D-05 -0.794197D-06 -0.166803D-05 -0.224656D-06
     9  0.828295D-06 -0.122262D-05  0.290581D-05  0.151987D-04  0.218711D-05
                6             7             8             9
     6  0.101676D+00
     7 -0.876036D-06  0.119686D+00
     8  0.834752D-06  0.518533D-06  0.432915D-01
     9 -0.826273D-07  0.751998D-06  0.357467D-06  0.639528D-02
MCSCF converged.
```

$^{3}2^{+}$c STEP 15

GEOMETRY

C	-3.75491400	0.36429900	-0.67960800
C	-3.28925700	-0.96926700	-0.62489900
C	-2.17342200	-1.30710500	0.11729800
C	-1.45564500	-0.31100500	0.86169200
C	-1.97268600	1.00193500	0.76197200
C	-3.08381300	1.36923800	0.02787100
H	-3.81860900	-1.73390200	-1.16286600
H	-1.84197100	-2.32970500	0.15988900
C	-0.30866800	-0.61000400	1.61099400
H	-0.00774300	-1.63209700	1.75644800
H	0.10825200	0.12592200	2.27543000
C	2.08191700	1.84325900	-0.67293800
H	2.37643500	2.13708300	-1.67788200
H	0.99455600	1.88770100	-0.63781500
H	2.47892500	2.56265200	0.03337200
C	2.29686400	-1.20360500	-1.55730700
H	2.96243000	-1.07945400	-2.41167400
H	2.45444500	-2.19697600	-1.15432900
H	1.28168500	-1.12632400	-1.93263100
C	3.69984200	-0.23756200	1.15981600
H	3.62090400	-1.27120600	1.47655400
H	4.74312900	-0.05518800	0.89810900
H	3.46029700	0.41436500	1.99283800
Si	2.64293900	0.11901000	-0.31409500
H	-4.62883500	0.60303200	-1.25642800
H	-3.42634800	2.38686000	0.00897400

E_0(CASSCF,vacuo) -676.093107

E_0(CASSCF,CPCM) **-676.165684**

DATA from the CASSCF calculation in vacuo:

```
Energy state  1 =     -676.0931071183
Full Convergence on CI vector
         ( 1)       EIGENVALUE     -0.67609311E+03
(     1) 0.9109834 ( 1349)-0.1360447 (  428) 0.1120720 ( 2950)-0.1055469 (  506) 0.0932714 ( 1345) 0.0797988 (    5)-0.0794481
(    10)-0.0778108 ( 2941) 0.0776341 ( 3028)-0.0682091 (  171)-0.0659755 ( 1271)-0.0626399 ( 5970) 0.0600376 ( 1460) 0.0543332
(    92)-0.0538108 ( 4621)-0.0531384 (   23)-0.0520949 (  429) 0.0518595 ( 5892) 0.0483616 (  617)-0.0481190 ( 3139) 0.0466082
(    93)-0.0433728 ( 1377) 0.0432788 ( 6053) 0.0429017 ( 5996)-0.0409392 ( 6049)-0.0369701 (   33) 0.0368428 (  508) 0.0365979
( 2101)-0.0359641 ( 6081)-0.0357166 ( 5911)-0.0356146 ( 2973) 0.0355766 ( 6058) 0.0351824 ( 1434)-0.0336479 (   16)-0.0329620
( 1373)-0.0315259 ( 3026)-0.0291365 ( 1264)-0.0288254 ( 1430) 0.0265120 ( 3120)-0.0260983 ( 2969) 0.0258436 (  282) 0.0256939
( 3035)-0.0250767 ( 5966)-0.0233971 ( 3116)-0.0233969 (  170)-0.0219442 ( 4643) 0.0212622 ( 2116) 0.0204773 (  507) 0.0204064
(  536) 0.0202262 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.195144D+01
     2  0.301942D-06  0.189668D+01
     3  0.456455D-06 -0.547229D-06  0.187930D+01
     4 -0.109982D-04 -0.173075D-05  0.292709D-04  0.100084D+01
     5  0.211420D-04 -0.342112D-05 -0.521642D-04  0.103989D-05  0.999727D+00
     6 -0.987377D-06  0.186194D-05  0.177025D-05  0.144676D-05  0.170383D-05
     7  0.157778D-06  0.948380D-06 -0.409870D-06 -0.163526D-04  0.257990D-04
     8  0.849030D-06 -0.164765D-05 -0.686651D-06 -0.592583D-05  0.884900D-05
     9  0.331438D-05 -0.288018D-05  0.197424D-05  0.178877D-04  0.120934D-04
                6             7             8             9
     6  0.102882D+00
     7 -0.535137D-06  0.120233D+00
     8 -0.258233D-06  0.523823D-06  0.435680D-01
     9  0.405372D-07  0.401887D-06  0.508270D-07  0.533758D-02
MCSCF converged.
```

7. Relaxed PES scans - TMS detachment from radical cation $4^{\cdot+}$

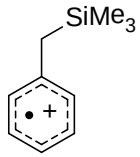
The level of theory chosen for performing the analysis of the detachment of the TMS group from benzyltrimethylsilane radical cation was the CASSCF(7,8)/6-31G(d), where the orbitals included in the active space were the 3 π and the 3 π^* orbitals of the aromatic ring and the σ/σ^* couple of the C-Si bond.
The same approach adopted for describing the detachment of the TMS group from phenyl cations was adopted (see previous section for details). Solvent effect was again evaluated by single point calculations at the CPCM-CASSCF/6-31G(d) level of theory (methanol bulk) on the optimized geometries obtained in vacuo.

As in the case of phenyl cations, the occupancy of the σ^* orbital of the C_α-Si (becoming the *p* orbital of the Si atom upon stretching of the bond) showed quite low values (< 0.01) for some of the structures reported below. Nevertheless, this orbital was kept in the active space for comparison purposes.

In the following, the optimized geometries for the relaxed PES scans are reported along with the most relevant data. The data reported in Table S8 have been reported in blue color for all of the structures reported below. Further notice that “step 0” refers to the equilibrium geometry of benzyltrimethylsilane radical cation.

Table S8. Total electronic energy (E_0(CASSCF,CPCM)) calculated at the CPCM-CASSCF(7,8)/6-31G(d) level of theory (MeOH bulk).

STEP	Benzyltrimethylsilane radical cation ($4^{\bullet+}$)	
	C_α-Si length [Å]	$E_{0(CASSCF,CPCM)}$ [H]
0	2.06005	-676.843877
1	2.16005	-676.841807
2	2.26005	-676.839282
3	2.36005	-676.835690
4	2.46005	-676.833038
5	2.56005	-676.830361
6	2.66005	-676.827724
7	2.76005	-676.825223
8	2.86005	-676.822902
9	2.96005	-676.820870
10	3.06005	-676.819045
11	3.16005	-676.817410
12	3.26005	-676.816006
13	3.36005	-676.814794
14	3.46005	-676.813721
15	3.56005	-676.812776



$4^{\bullet+}$ STEP 0 (equilibrium geometry)

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41702089
C	1.18822197	0.00000000	2.10200848
C	2.44215136	-0.00924839	1.39515964
C	2.41420031	-0.00096936	-0.04400907
C	1.22065794	-0.00098479	-0.71968249
H	-0.93203380	-0.00210340	-0.53245191
H	-0.93283232	-0.00669736	1.94785412
H	1.20241893	-0.00717307	3.17538412
H	3.34604366	-0.00888574	-0.57692430
H	1.20415815	-0.00844309	-1.79284435
C	3.68655179	0.00742798	2.10603591
H	3.62652207	-0.41179692	3.10285932
H	4.51460691	-0.41226552	1.54819366
Si	4.33391289	1.92792920	2.47536448
C	5.94169447	1.62641345	3.39350047
H	6.40047085	2.57667318	3.65528791
H	5.78783532	1.07700704	4.31734563
H	6.65904770	1.07671589	2.79163159
C	3.03668067	2.77937407	3.53429241
H	2.09920817	2.93179483	3.00782466
H	2.82848264	2.23188943	4.44912326
H	3.39915232	3.76133462	3.82839115
C	4.58671465	2.77895200	0.81979155
H	5.26869469	2.23123090	0.17566096
H	3.65687527	2.93138068	0.27995655
H	5.02434828	3.76089057	0.98228013

E_0(CASSCF,vacuo) -676.774108

E_0(CASSCF,CPCM) **-676.843877**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67677411E+03
(    1) 0.9424018 (   22) 0.1261101 (   36) 0.1116794 (   40)-0.0919487 (    5) 0.0820527 (  118) 0.0778963 (  269)-0.0700091
(  312) 0.0694084 (   48) 0.0638833 (  334) 0.0626480 (   52) 0.0600516 (  176) 0.0567332 (   25) 0.0552146 (   64) 0.0484218
(   79) 0.0467549 (    7) 0.0466083 (   20)-0.0465465 (   47)-0.0439597 (  298) 0.0405355 (  109) 0.0388507 (  201)-0.0372965
(  102) 0.0330416 (  154)-0.0328976 (  134)-0.0300425 (  530) 0.0282342 (  424) 0.0267353 (  345) 0.0254060 (   60)-0.0242720
(  304) 0.0228923 (  241) 0.0221372 (  414)-0.0215970 (   18)-0.0206562 (  208)-0.0202931 (  175) 0.0202529 (  129) 0.0202017
(  832) 0.0197654 (  198) 0.0192412 (   21) 0.0182730 (  160) 0.0174503 (  186) 0.0173798 (  156) 0.0170855 (   91)-0.0170319
(  943) 0.0170208 (   83) 0.0168349 (  108) 0.0155523 (   16)-0.0148397 (  288) 0.0146169 (  601) 0.0143769 (   54)-0.0136217
(  242)-0.0133075 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.193330D+01
     2 -0.946960D-06  0.197374D+01
     3 -0.572413D-06 -0.663814D-06  0.190318D+01
     4  0.430189D-05 -0.126485D-04 -0.177627D-06  0.100461D+01
     5 -0.298967D-05  0.904389D-05  0.235789D-05 -0.217756D-05  0.871765D-01
     6  0.142866D-05 -0.162566D-05  0.907052D-06 -0.652482D-05  0.302602D-06
     7 -0.261002D-07 -0.278818D-05  0.712154D-06  0.155260D-05 -0.217074D-06
     8  0.180726D-05 -0.154197D-05  0.142638D-06 -0.173732D-05 -0.224368D-06
                6             7             8
     6  0.548473D-01
     7  0.293541D-06  0.160565D-01
     8  0.317792D-06  0.179263D-06  0.270930D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 1

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41487612
C	1.18865681	0.00000000	2.10276668
C	2.44328621	-0.00993273	1.39786478
C	2.41513045	-0.00138200	-0.04095922
C	1.21972043	-0.00137307	-0.71704647
H	-0.93163670	-0.00281769	-0.53300845
H	-0.93245246	-0.00748272	1.94650721
H	1.20018316	-0.00889870	3.17639851
H	3.34651154	-0.01131696	-0.57511955
H	1.20545969	-0.00988983	-1.79030271
C	3.67474985	0.00268876	2.10240441
H	3.63147202	-0.37218421	3.11618093
H	4.52655362	-0.37319438	1.55168652
Si	4.35840938	2.01426755	2.49224747
C	5.95337168	1.65350388	3.40496419
H	6.43309891	2.59042986	3.67881579
H	5.78464019	1.09738082	4.32170354
H	6.65782821	1.09639871	2.79543191
C	3.04788444	2.83586277	3.55051824
H	2.11332389	2.97937085	3.01755051
H	2.84285618	2.27701118	4.45858870
H	3.39806780	3.81974634	3.85437300
C	4.60695879	2.83414120	0.82537477
H	5.28555331	2.27431488	0.18894090
H	3.67394311	2.97764615	0.28970611
H	5.04691033	3.81792527	0.97232197

E_0(CASSCF,vacuo) -676.773209

E_0(CASSCF,CPCM) **-676.841807**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67677321E+03
(    1) 0.9383485 (   22) 0.1285505 (   36) 0.1148348 (    5) 0.0938957 (   40)-0.0778529 (  118) 0.0773508 (  334) 0.0667499
(  269)-0.0662761 (   48) 0.0656501 (  312) 0.0587715 (   52) 0.0578425 (   25) 0.0545672 (    7) 0.0535033 (  176) 0.0518406
(   20)-0.0455075 (   64) 0.0448312 (   79) 0.0443450 (   47)-0.0438524 (  109) 0.0418017 (  424) 0.0389239 (  530) 0.0384011
(  154)-0.0381642 (  298) 0.0380745 (   21) 0.0362124 (  102) 0.0347041 (  201)-0.0346424 (  345) 0.0344928 (  186) 0.0323820
(   60)-0.0311205 (  134)-0.0301773 (  129) 0.0286414 (  160) 0.0247809 (  304) 0.0241285 (   53) 0.0236841 (  241) 0.0231437
(  198) 0.0224474 (  156) 0.0218898 (  114)-0.0212347 (  175) 0.0203919 (  108) 0.0203593 (  136) 0.0200814 (  208)-0.0199290
(   91)-0.0191464 (  288) 0.0187136 (   83) 0.0187102 (  199)-0.0186842 (  943) 0.0173243 (  128) 0.0159219 (  229)-0.0158439
(   18)-0.0153149 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.193209D+01
     2  0.130228D-05  0.196572D+01
     3 -0.281475D-07 -0.180423D-07  0.190092D+01
     4 -0.187008D-04  0.792251D-05 -0.172789D-06  0.100370D+01
     5  0.110277D-07 -0.117636D-06  0.952779D-06 -0.711086D-07  0.914198D-01
     6  0.692338D-06 -0.132424D-05 -0.593260D-07 -0.197427D-04  0.130669D-07
     7  0.197153D-05 -0.301954D-05  0.192985D-06  0.366198D-05 -0.510732D-09
     8 -0.132085D-05 -0.760151D-07  0.132367D-07 -0.953536D-05 -0.189302D-07
                6             7             8
     6  0.599564D-01
     7 -0.105011D-05  0.167852D-01
     8  0.131680D-05 -0.696736D-06  0.294060D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 2

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41260509
C	1.18981825	0.00000000	2.10275022
C	2.44356457	-0.00948353	1.39945222
C	2.41573752	-0.00151718	-0.03782217
C	1.21839143	-0.00150824	-0.71482264
H	-0.93140202	-0.00310925	-0.53341706
H	-0.93209777	-0.00794655	1.94503026
H	1.19878104	-0.01042500	3.17666151
H	3.34653162	-0.01308337	-0.57351335
H	1.20593928	-0.01059171	-1.78818491
C	3.66740452	0.00052562	2.10034626
H	3.63766016	-0.33503466	3.12709289
H	4.53773058	-0.33614813	1.55548374
Si	4.38587908	2.10374451	2.51033195
C	5.96828613	1.69126624	3.41687889
H	6.46757789	2.61491824	3.70217247
H	5.78577192	1.12875328	4.32666369
H	6.66028381	1.12766597	2.79968051
C	3.05804911	2.89161869	3.56564454
H	2.12530054	3.01988759	3.02663716
H	2.85996127	2.32278080	4.46853381
H	3.39035464	3.87995741	3.87642333
C	4.62465275	2.88968395	0.83019851
H	5.30282086	2.31976557	0.20305907
H	3.68782701	3.01795636	0.29830932
H	5.06146238	3.87789462	0.95849973

E_0(CASSCF,vacuo) -676.771207

E_0(CASSCF,CPCM) **-676.839282**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.67677121E+03
(    1) 0.9340936 (   22) 0.1308362 (   36) 0.1200819 (    5) 0.1008696 (  334) 0.0721582 (  118) 0.0717209 (   48) 0.0687226
(  269)-0.0609557 (    7) 0.0575988 (   40)-0.0571284 (   25) 0.0563431 (   52) 0.0554527 (   21) 0.0532446 (  186) 0.0505694
(  424) 0.0453430 (   47)-0.0444057 (   20)-0.0436078 (  109) 0.0429728 (  176) 0.0428192 (  312) 0.0419278 (   64) 0.0409244
(  530) 0.0404540 (   79) 0.0398280 (  129) 0.0393876 (   53) 0.0389023 (  154)-0.0385058 (  298) 0.0372727 (  345) 0.0358959
(  102) 0.0349012 (  160) 0.0317305 (   60)-0.0307060 (  201)-0.0300875 (  114)-0.0300394 (  136) 0.0298781 (  466) 0.0288123
(  199)-0.0278721 (  108) 0.0271375 (  229)-0.0269620 (  558) 0.0250329 (  241) 0.0238286 (  198) 0.0227155 (  304) 0.0226839
(   85) 0.0226558 (  100)-0.0223655 (  156) 0.0217358 (  208)-0.0211332 (  175) 0.0202859 (  128) 0.0202747 (  134)-0.0188364
(  143)-0.0184663 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192846D+01
     2 -0.706611D-05  0.195965D+01
     3 -0.789425D-08  0.148718D-07  0.189885D+01
     4  0.694778D-04 -0.676824D-04  0.441485D-07  0.100248D+01
     5 -0.689800D-10 -0.213482D-07  0.397837D-05  0.677286D-08  0.950901D-01
     6 -0.639468D-05  0.124805D-04 -0.290023D-07  0.130154D-04  0.415168D-08
     7  0.452133D-05 -0.645650D-05  0.146192D-06  0.704497D-05  0.124116D-08
     8 -0.129456D-06  0.419759D-05 -0.811542D-07  0.304509D-06  0.128095D-07
                6             7             8
     6  0.662549D-01
     7 -0.432179D-06  0.168156D-01
     8 -0.455097D-05 -0.847434D-06  0.324022D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 3

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.41052278
C	1.19129453	0.00000000	2.10224229
C	2.44327627	-0.00834614	1.40030596
C	2.41606941	-0.00217459	-0.03477846
C	1.21704165	-0.00216145	-0.71300583
H	-0.93127948	-0.00376995	-0.53373360
H	-0.93179893	-0.00839374	1.94364589
H	1.19815544	-0.01184613	3.17642974
H	3.34636866	-0.01565989	-0.57183213
H	1.20601352	-0.01218959	-1.78646687
C	3.66386653	-0.00051224	2.09984548
H	3.64391963	-0.30459105	3.13563870
H	4.54723135	-0.30619484	1.55951532
Si	4.41720126	2.19444488	2.52936540
C	5.98855786	1.74177172	3.43040542
H	6.50314246	2.65468623	3.72439659
H	5.79488840	1.17477835	4.33476014
H	6.67046561	1.17322193	2.80702683
C	3.07035451	2.94910308	3.57904540
H	2.13744909	3.05327456	3.03583686
H	2.88485716	2.37645568	4.48178133
H	3.37950984	3.94584718	3.88821789
C	4.64273814	2.94631130	0.83550509
H	5.32737563	2.37212018	0.22000349
H	3.70255610	3.05049561	0.30499304
H	5.06665226	3.94285208	0.94444256

E_0(CASSCF,vacuo) -676.768641

E_0(CASSCF,CPCM) **-676.835690**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67676864E+03
(   1) 0.9307354 (   22) 0.1327160 (   36) 0.1248620 (    5) 0.1032318 (  334) 0.0781029 (   48) 0.0716628 (  118) 0.0664549
(  186) 0.0648184 (   21) 0.0617312 (    7) 0.0590136 (   25) 0.0585146 (  269)-0.0534881 (   52) 0.0526140 (  129) 0.0490518
(   53) 0.0477686 (   47)-0.0450030 (  466) 0.0447515 (  424) 0.0429030 (  109) 0.0426977 (   20)-0.0410432 (  530) 0.0384958
(   64) 0.0378542 (  298) 0.0372925 (  136) 0.0369138 (   40)-0.0368432 (  229)-0.0360987 (   79) 0.0358333 (  154)-0.0358268
(  160) 0.0357143 (  102) 0.0349603 (  100)-0.0345899 (  176) 0.0344866 (  558) 0.0339427 (  108) 0.0333995 (  114)-0.0319319
(  345) 0.0304227 (  312) 0.0279696 (   85) 0.0276829 (   70) 0.0265383 (  201)-0.0248418 (  199)-0.0243812 (  241) 0.0242567
(   60)-0.0237465 (  128) 0.0228859 (  393) 0.0227338 (  198) 0.0219442 (  208)-0.0216344 (  143)-0.0212481 (  175) 0.0212096
(  212)-0.0207150 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.192358D+01
     2  0.215964D-05  0.195659D+01
     3  0.377843D-10  0.397427D-09  0.189731D+01
     4 -0.256096D-04  0.149281D-04  0.870770D-08  0.100110D+01
     5  0.189867D-07 -0.139227D-08 -0.184956D-05  0.260112D-07  0.977273D-01
     6  0.256992D-05 -0.189438D-05 -0.729338D-07 -0.528742D-05 -0.521414D-10
     7 -0.323618D-05  0.133387D-05  0.976174D-09 -0.462784D-05  0.830243D-09
     8  0.339526D-06 -0.461607D-06 -0.336370D-09 -0.405859D-06  0.399097D-08
                6             7             8
     6  0.723509D-01
     7  0.129501D-06  0.166705D-01
     8  0.132172D-05  0.219191D-06  0.346759D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 4

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40877825
C	1.19270698	0.00000000	2.10170818
C	2.44279512	-0.00710639	1.40106064
C	2.41634298	-0.00248651	-0.03175375
C	1.21598876	-0.00247054	-0.71135111
H	-0.93117014	-0.00417970	-0.53406249
H	-0.93150261	-0.00870898	1.94259758
H	1.19765890	-0.01296252	3.17613748
H	3.34622540	-0.01732852	-0.56998136
H	1.20638997	-0.01305222	-1.78491165
C	3.66239508	0.00002797	2.10054672
H	3.64980454	-0.27830391	3.14288389
H	4.55545236	-0.28014342	1.56384785
Si	4.44863502	2.28754193	2.54882513
C	6.01036167	1.80314927	3.44510858
H	6.53716770	2.70721966	3.74620186
H	5.80762296	1.23290389	4.34515225
H	6.68428931	1.23112203	2.81664476
C	3.08226135	3.00969435	3.59129367
H	2.15232802	3.09622475	3.04036488
H	2.90301424	2.43025190	4.49060325
H	3.36993924	4.01181250	3.90504600
C	4.65922713	3.00648974	0.84178508
H	5.34437498	2.42529140	0.23398450
H	3.71421445	3.09305103	0.31714649
H	5.07631273	4.00834552	0.92990955

E_0(CASSCF,vacuo) -676.765782

E_0(CASSCF,CPCM) **-676.833038**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67676578E+03
(    1) 0.9283349 (   22) 0.1342674 (   36) 0.1283982 (    5) 0.1031887 (  334) 0.0837279 (   48) 0.0739164 (  186) 0.0737081
(  118) 0.0639253 (   21) 0.0638663 (   25) 0.0599749 (    7) 0.0590306 (  129) 0.0564823 (  466) 0.0546242 (   53) 0.0520181
(   52) 0.0495164 (  269)-0.0464250 (   47)-0.0455823 (  109) 0.0421506 (  229)-0.0419295 (  136) 0.0411114 (  100)-0.0392511
(   20)-0.0384555 (  108) 0.0380427 (  558) 0.0377792 (  160) 0.0373661 (  424) 0.0372844 (  298) 0.0372286 (  530) 0.0368134
(   64) 0.0357210 (  102) 0.0355035 (   79) 0.0329145 (  154)-0.0326624 (   70) 0.0322143 (  114)-0.0301673 (   85) 0.0300549
(  176) 0.0292802 (  393) 0.0271612 (  212)-0.0269971 (  241) 0.0246002 (  128) 0.0240445 (  345) 0.0240244 (  284)-0.0233000
(  175) 0.0221110 (  143)-0.0217715 (  198) 0.0214257 (  208)-0.0213213 (   24) 0.0212343 (   40)-0.0209912 (  201)-0.0204190
(  312) 0.0193221 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191878D+01
     2 -0.100958D-04  0.195529D+01
     3 -0.325487D-08 -0.481388D-08  0.189623D+01
     4  0.127183D-03 -0.624978D-04  0.138059D-07  0.999907D+00
     5 -0.798473D-08  0.149336D-07  0.231371D-05  0.477998D-08  0.996297D-01
     6 -0.573925D-05  0.187859D-04 -0.523509D-08  0.385724D-04  0.149559D-08
     7  0.101735D-04 -0.760137D-05 -0.152617D-07  0.184942D-04  0.110640D-08
     8  0.289640D-05  0.489296D-05  0.691061D-07  0.225112D-05 -0.597795D-08
                6             7             8
     6  0.775922D-01
     7 -0.504594D-06  0.164366D-01
     8 -0.848650D-05 -0.950134D-06  0.361248D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 5

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40742808
C	1.19386338	0.00000000	2.10128395
C	2.44232249	-0.00611274	1.40183815
C	2.41657947	-0.00291329	-0.02898012
C	1.21528191	-0.00289462	-0.70988440
H	-0.93105203	-0.00459537	-0.53439292
H	-0.93135217	-0.00893135	1.94168292
H	1.19736411	-0.01379494	3.17592450
H	3.34625618	-0.01891298	-0.56795967
H	1.20682686	-0.01402154	-1.78353571
C	3.66198993	0.00084059	2.10188570
H	3.65468397	-0.25704231	3.14890834
H	4.56208036	-0.25920931	1.56800816
Si	4.48051861	2.38121900	2.56843323
C	6.03411905	1.87215500	3.46085766
H	6.57147810	2.76819573	3.76805807
H	5.82308172	1.29868635	4.35677154
H	6.70059643	1.29658937	2.82793107
C	3.09530867	3.07185538	3.60331875
H	2.16503623	3.12907059	3.04939097
H	2.93119197	2.49277639	4.50551655
H	3.35572935	4.08366524	3.91059545
C	4.67626165	3.06807339	0.84893068
H	5.37182644	2.48693853	0.25336385
H	3.72881053	3.12532977	0.32493234
H	5.07414079	4.07955485	0.91672389

E_0(CASSCF,vacuo) -676.762795

E_0(CASSCF,CPCM) **-676.830361**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67676280E+03
(    1) 0.9266866 (   22) 0.1354946 (   36) 0.1307931 (    5) 0.1021226 (  334) 0.0884446 (  186) 0.0789166 (   48) 0.0754822
(  118) 0.0633843 (   21) 0.0630838 (  129) 0.0619203 (   25) 0.0606212 (  466) 0.0605915 (    7) 0.0584507 (   53) 0.0538106
(   52) 0.0465752 (   47)-0.0461069 (  229)-0.0450817 (  136) 0.0435324 (  109) 0.0416254 (  108) 0.0412049 (  269)-0.0408491
(  100)-0.0399151 (  558) 0.0383555 (  160) 0.0379089 (  298) 0.0369809 (  102) 0.0363106 (   20)-0.0362428 (  530) 0.0359232
(   70) 0.0354776 (   64) 0.0342390 (  424) 0.0319183 (  212)-0.0316453 (   85) 0.0310418 (   79) 0.0309128 (  393) 0.0300134
(  154)-0.0298621 (  114)-0.0276817 (  176) 0.0265056 (  284)-0.0255529 (  241) 0.0248515 (  128) 0.0243258 (  175) 0.0225432
(   24) 0.0213786 (  143)-0.0213776 (  198) 0.0212611 (  208)-0.0207464 (  832) 0.0202975 (  172)-0.0196348 (  345) 0.0189430
(  141) 0.0185677 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191469D+01
     2  0.109070D-05  0.195481D+01
     3 -0.742266D-08 -0.599058D-09  0.189552D+01
     4  0.597445D-05 -0.180607D-05  0.125076D-06  0.999064D+00
     5  0.385152D-07  0.879125D-07  0.111428D-05  0.187242D-07  0.100996D+00
     6 -0.264480D-05  0.115884D-05  0.205828D-07  0.788884D-06 -0.731099D-08
     7 -0.878235D-06 -0.154897D-05 -0.512972D-07 -0.214844D-05  0.191846D-07
     8  0.152614D-05 -0.926181D-06  0.120299D-07  0.925994D-06  0.981220D-08
                6             7             8
     6  0.817779D-01
     7  0.922788D-06  0.161263D-01
     8  0.993898D-06  0.142374D-06  0.370175D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 6

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40642640
C	1.19472469	0.00000000	2.10107089
C	2.44207125	-0.00530489	1.40282452
C	2.41685701	-0.00329259	-0.02643977
C	1.21491849	-0.00326899	-0.70852661
H	-0.93091573	-0.00480315	-0.53474541
H	-0.93126300	-0.00903839	1.94099966
H	1.19696393	-0.01436593	3.17588280
H	3.34642364	-0.02014982	-0.56593637
H	1.20753510	-0.01477048	-1.78226448
C	3.66211492	0.00257893	2.10366103
H	3.65909174	-0.23780355	3.15436729
H	4.56790620	-0.24028701	1.57230220
Si	4.51128042	2.47658166	2.58749103
C	6.05761719	1.94827450	3.47728347
H	6.60259587	2.83852755	3.78899604
H	5.84016778	1.37319224	4.37045899
H	6.71911979	1.37051645	2.84137720
C	3.10751292	3.13756458	3.61327303
H	2.17673364	3.15826404	3.05766047
H	2.96162802	2.56506855	4.52257715
H	3.33641673	4.16132222	3.90640660
C	4.69218128	3.13260348	0.85642409
H	5.40362896	2.55744647	0.27427241
H	3.74364669	3.15334327	0.33170029
H	5.06225498	4.15593103	0.90393421

E_0(CASSCF,vacuo) -676.759790

E_0(CASSCF,CPCM) **-676.827724**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67675979E+03
(    1) 0.9254997 (   22) 0.1364602 (   36) 0.1325861 (    5) 0.1009059 (  334) 0.0922035 (  186) 0.0820369 (   48) 0.0766401
(  129) 0.0658411 (  466) 0.0644726 (  118) 0.0637577 (   21) 0.0613245 (   25) 0.0606858 (    7) 0.0577788 (   53) 0.0545682
(   47)-0.0465840 (  229)-0.0463572 (  136) 0.0449673 (   52) 0.0439825 (  108) 0.0433090 (  109) 0.0409336 (  100)-0.0391075
(  160) 0.0380210 (   70) 0.0373916 (  558) 0.0373504 (  102) 0.0371220 (  269)-0.0366264 (  298) 0.0366179 (  530) 0.0354888
(  212)-0.0349065 (   20)-0.0344947 (   64) 0.0331038 (  393) 0.0320550 (   85) 0.0314474 (   79) 0.0295315 (  424) 0.0274993
(  154)-0.0274196 (  284)-0.0263303 (  114)-0.0254343 (  176) 0.0250571 (  241) 0.0250416 (  128) 0.0241767 (  175) 0.0225554
(  172)-0.0224073 (  832) 0.0214152 (   24) 0.0213730 (  198) 0.0212788 (  143)-0.0206166 (  208)-0.0202347 (  123)-0.0197151
(  141) 0.0196784 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.191134D+01
     2 -0.177533D-05  0.195465D+01
     3 -0.357452D-08 -0.621479D-07  0.189502D+01
     4  0.260606D-04 -0.846319D-05 -0.127070D-05  0.998557D+00
     5  0.787998D-06 -0.371113D-06  0.219430D-05  0.113389D-05  0.102038D+00
     6 -0.291707D-05  0.478982D-06  0.817555D-06  0.502177D-05  0.514687D-07
     7  0.327841D-05  0.690819D-08 -0.561236D-06  0.145548D-05  0.998087D-07
     8 -0.101581D-05  0.581715D-06  0.267995D-06 -0.490216D-07 -0.105483D-06
                6             7             8
     6  0.850652D-01
     7  0.540426D-06  0.157288D-01
     8 -0.795085D-06 -0.196617D-06  0.376033D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 7

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40562438
C	1.19539467	0.00000000	2.10101938
C	2.44198644	-0.00469791	1.40404590
C	2.41716044	-0.00363620	-0.02395038
C	1.21477221	-0.00358953	-0.70717816
H	-0.93075169	-0.00506166	-0.53513492
H	-0.93121571	-0.00917865	1.94044853
H	1.19639849	-0.01492544	3.17598559
H	3.34665222	-0.02133216	-0.56386517
H	1.20846011	-0.01548279	-1.78100397
C	3.66250026	0.00421547	2.10578502
H	3.66262208	-0.22134462	3.15935788
H	4.57274382	-0.22422022	1.57647405
Si	4.54207186	2.57196797	2.60665533
C	6.08109836	2.02504788	3.49412385
H	6.63434105	2.90881783	3.81054795
H	5.85663261	1.44824086	4.38432938
H	6.73711244	1.44456036	2.85519000
C	3.12125854	3.20446551	3.62352567
H	2.19249596	3.19743100	3.06423479
H	2.98771931	2.63475013	4.53628167
H	3.32339734	4.23616293	3.90927552
C	4.70960763	3.19797527	0.86514859
H	5.43083212	2.62476424	0.29348727
H	3.75965422	3.19106691	0.34265724
H	5.06033642	4.22905948	0.89290171

E_0(CASSCF,vacuo) -676.756846

E_0(CASSCF,CPCM) **-676.825223**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67675685E+03
(    1) 0.9245621 (   22) 0.1372577 (   36) 0.1342467 (    5) 0.0999426 (  334) 0.0952000 (  186) 0.0839913 (   48) 0.0776724
(  129) 0.0687093 (  466) 0.0671829 (  118) 0.0644709 (   25) 0.0603899 (   21) 0.0593403 (    7) 0.0572472 (   53) 0.0549989
(   47)-0.0470371 (  229)-0.0462118 (  136) 0.0458377 (  108) 0.0447037 (   52) 0.0417396 (  109) 0.0399675 (   70) 0.0385748
(  160) 0.0379506 (  100)-0.0378636 (  102) 0.0378368 (  212)-0.0369975 (  298) 0.0361913 (  558) 0.0355206 (  530) 0.0352667
(  393) 0.0336301 (  269)-0.0334024 (   20)-0.0331544 (   64) 0.0321468 (   85) 0.0316786 (   79) 0.0285338 (  284)-0.0266020
(  241) 0.0252220 (  154)-0.0251800 (  172)-0.0250310 (  176) 0.0243076 (  424) 0.0238810 (  128) 0.0238460 (  114)-0.0235543
(  832) 0.0223187 (  175) 0.0222832 (  198) 0.0213796 (   24) 0.0213793 (  123)-0.0210978 (  141) 0.0202466 (  208)-0.0198916
(  143)-0.0196657 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190860D+01
     2  0.403740D-06  0.195461D+01
     3  0.316961D-06 -0.448115D-07  0.189461D+01
     4  0.159433D-04 -0.498837D-05 -0.338204D-06  0.998318D+00
     5 -0.101769D-05  0.735146D-06  0.492336D-06 -0.100881D-05  0.102920D+00
     6 -0.115265D-05 -0.167025D-05  0.152484D-05  0.211133D-05 -0.193894D-06
     7  0.505877D-05 -0.151693D-05  0.188657D-05  0.652667D-05 -0.135952D-06
     8 -0.153749D-05 -0.363358D-06  0.235077D-06  0.113522D-05  0.491560D-07
                6             7             8
     6  0.877274D-01
     7  0.387103D-06  0.151810D-01
     8  0.965814D-06 -0.156616D-06  0.380313D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 8

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40503505
C	1.19584972	0.00000000	2.10111114
C	2.44209741	-0.00427001	1.40542245
C	2.41748466	-0.00376688	-0.02165135
C	1.21483360	-0.00376054	-0.70590205
H	-0.93057639	-0.00525985	-0.53553158
H	-0.93122724	-0.00929121	1.94000158
H	1.19575431	-0.01538464	3.17620812
H	3.34697071	-0.02202673	-0.56182871
H	1.20950519	-0.01592395	-1.77981267
C	3.66302518	0.00622434	2.10803745
H	3.66562728	-0.20693468	3.16388797
H	4.57692147	-0.20975274	1.58038862
Si	4.57190552	2.66819359	2.62546939
C	6.10652010	2.10803560	3.50880208
H	6.66551324	2.98726900	3.82855347
H	5.87824825	1.52940321	4.39676718
H	6.75812145	1.52652985	2.86641061
C	3.13560450	3.27100947	3.63560933
H	2.20812213	3.23180133	3.07542728
H	3.01819518	2.70683094	4.55386452
H	3.30820449	4.31125618	3.91013609
C	4.72302463	3.26528584	0.87408585
H	5.45558721	2.69732131	0.31191138
H	3.77187838	3.22727795	0.35501682
H	5.05016160	4.30461426	0.88186019

E_0(CASSCF,vacuo) -676.754025

E_0(CASSCF,CPCM) **-676.822902**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.67675403E+03
(    1) 0.9237580 (   22) 0.1378891 (   36) 0.1361072 (    5) 0.0993248 (  334) 0.0976118 (  186) 0.0852716 (   48) 0.0787824
(  129) 0.0707936 (  466) 0.0691555 (  118) 0.0652178 (   25) 0.0599032 (   21) 0.0574391 (    7) 0.0569121 (   53) 0.0553956
(   47)-0.0474813 (  136) 0.0463674 (  108) 0.0456128 (  229)-0.0449776 (   52) 0.0398279 (   70) 0.0393520 (  109) 0.0387240
(  102) 0.0384159 (  212)-0.0381198 (  160) 0.0377984 (  100)-0.0365708 (  298) 0.0357590 (  530) 0.0351415 (  393) 0.0348795
(  558) 0.0332926 (   20)-0.0321562 (   85) 0.0318984 (   64) 0.0312931 (  269)-0.0309305 (   79) 0.0277760 (  172)-0.0272949
(  284)-0.0267346 (  241) 0.0254298 (  176) 0.0239249 (  128) 0.0234689 (  832) 0.0230763 (  154)-0.0230469 (  123)-0.0221664
(  114)-0.0220149 (  175) 0.0218490 (  198) 0.0214985 (   24) 0.0214432 (  424) 0.0208928 (  141) 0.0204774 (  943) 0.0199052
(    4)-0.0197770 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190632D+01
     2 -0.502242D-06  0.195462D+01
     3  0.238072D-06 -0.666095D-06  0.189427D+01
     4  0.120938D-05  0.474002D-05  0.192385D-05  0.998282D+00
     5 -0.483023D-05  0.257729D-05 -0.220388D-05 -0.118573D-05  0.103678D+00
     6  0.986437D-06 -0.882295D-06 -0.515560D-05 -0.657803D-05 -0.312568D-07
     7 -0.306285D-05  0.826856D-05  0.172321D-04  0.118477D-04 -0.805044D-06
     8 -0.339840D-07 -0.166419D-05 -0.307345D-05 -0.306159D-05 -0.618899D-07
                6             7             8
     6  0.899833D-01
     7 -0.716468D-06  0.144699D-01
     8 -0.483890D-06 -0.908880D-07  0.383835D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 9

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40459242
C	1.19615307	0.00000000	2.10130462
C	2.44234835	-0.00399769	1.40690495
C	2.41782224	-0.00406712	-0.01949203
C	1.21502883	-0.00404262	-0.70467545
H	-0.93039029	-0.00547375	-0.53593389
H	-0.93127073	-0.00940190	1.93964501
H	1.19501906	-0.01573047	3.17651612
H	3.34732875	-0.02289077	-0.55985536
H	1.21063745	-0.01652542	-1.77866808
C	3.66358181	0.00812951	2.11036476
H	3.66809003	-0.19401181	3.16813665
H	4.58052343	-0.19705961	1.58417324
Si	4.60099384	2.76443447	2.64508995
C	6.12986016	2.19165129	3.52705795
H	6.69425468	3.06627654	3.85060383
H	5.89634042	1.61157665	4.41265740
H	6.77796551	1.60869732	2.88252136
C	3.14927683	3.33963099	3.64651546
H	2.22523234	3.27409546	3.08299395
H	3.04277987	2.77901348	4.56815909
H	3.29568295	4.38595930	3.91366140
C	4.74020872	3.33433828	0.88525678
H	5.48313548	2.77083077	0.33246593
H	3.78911028	3.26900277	0.36867901
H	5.04659851	4.38010262	0.87493153

E_0(CASSCF,vacuo) -676.751372

E_0(CASSCF,CPCM) **-676.820870**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67675137E+03
(    1) 0.9230220 (   22) 0.1384034 (   36) 0.1382566 (  334) 0.0995809 (    5) 0.0990831 (  186) 0.0861477 (   48) 0.0800308
(  129) 0.0723214 (  466) 0.0706256 (  118) 0.0659051 (   25) 0.0593369 (    7) 0.0567950 (   53) 0.0558636 (   21) 0.0557191
(   47)-0.0479297 (  136) 0.0466865 (  108) 0.0461987 (  229)-0.0429525 (   70) 0.0398863 (  102) 0.0388678 (  212)-0.0384031
(   52) 0.0382049 (  160) 0.0375984 (  109) 0.0372739 (  393) 0.0358830 (  298) 0.0353498 (  100)-0.0353382 (  530) 0.0350669
(   85) 0.0321632 (   20)-0.0314257 (  558) 0.0308953 (   64) 0.0305144 (  172)-0.0290249 (  269)-0.0290121 (   79) 0.0271921
(  284)-0.0268398 (  241) 0.0256817 (  176) 0.0237435 (  832) 0.0237221 (  128) 0.0231063 (  123)-0.0230001 (  198) 0.0216171
(   24) 0.0215731 (  175) 0.0213416 (  154)-0.0210202 (  114)-0.0207431 (  141) 0.0205037 (  943) 0.0202615 (  208)-0.0197850
(   57) 0.0197618 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190439D+01
     2 -0.414042D-06  0.195463D+01
     3 -0.558196D-07  0.730921D-07  0.189395D+01
     4 -0.104344D-04 -0.160513D-05 -0.564316D-07  0.998381D+00
     5  0.448398D-07  0.477749D-07  0.645541D-06 -0.806973D-07  0.104369D+00
     6 -0.250255D-05  0.409617D-06  0.196894D-07 -0.791048D-05  0.274584D-07
     7  0.587021D-05 -0.290299D-05 -0.223886D-06  0.465937D-07  0.199386D-07
     8 -0.256714D-05  0.104563D-05  0.323781D-07 -0.173564D-05  0.629498D-07
                6             7             8
     6  0.919730D-01
     7 -0.111177D-05  0.136047D-01
     8 -0.359925D-06 -0.141870D-06  0.387004D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 10

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40425832
C	1.19633985	0.00000000	2.10157414
C	2.44270574	-0.00377926	1.40844776
C	2.41816436	-0.00424950	-0.01747663
C	1.21531820	-0.00422877	-0.70350892
H	-0.93020305	-0.00557305	-0.53633451
H	-0.93134239	-0.00944257	1.93934578
H	1.19424145	-0.01598417	3.17688754
H	3.34771844	-0.02347651	-0.55795771
H	1.21180277	-0.01690175	-1.77758241
C	3.66411195	0.01022716	2.11267127
H	3.67018909	-0.18200198	3.17209249
H	4.58370157	-0.18517478	1.58775608
Si	4.62975536	2.86114743	2.66375154
C	6.15383908	2.27718814	3.54369180
H	6.72336362	3.14753414	3.87034100
H	5.91598533	1.69590057	4.42731232
H	6.79840757	1.69284937	2.89690435
C	3.16449237	3.41037934	3.65751728
H	2.24361034	3.31617227	3.09267594
H	3.07062271	2.85642986	4.58444909
H	3.28402033	4.46299214	3.91360218
C	4.75669793	3.40485417	0.89613085
H	5.51089051	2.84792122	0.35216829
H	3.80633135	3.31080842	0.38241523
H	5.04009430	4.45688260	0.86812429

E_0(CASSCF,vacuo) -676.748912

E_0(CASSCF,CPCM) **-676.819045**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67674891E+03
(    1) 0.9223318 (   36) 0.1406700 (   22) 0.1388248 (  334) 0.1012232 (    5) 0.0991528 (  186) 0.0867811 (   48) 0.0814175
(  129) 0.0734575 (  466) 0.0717423 (  118) 0.0665046 (   25) 0.0587633 (    7) 0.0568536 (   53) 0.0564084 (   21) 0.0541979
(   47)-0.0483892 (  136) 0.0468796 (  108) 0.0465774 (  229)-0.0403765 (   70) 0.0402692 (  102) 0.0392114 (  212)-0.0379812
(  160) 0.0373733 (   52) 0.0368264 (  393) 0.0366954 (  109) 0.0357036 (  530) 0.0350233 (  298) 0.0349849 (  100)-0.0341845
(   85) 0.0324772 (   20)-0.0308923 (  172)-0.0301029 (   64) 0.0298023 (  558) 0.0284620 (  269)-0.0275048 (  284)-0.0269282
(   79) 0.0267366 (  241) 0.0259756 (  832) 0.0242756 (  176) 0.0236751 (  123)-0.0236624 (  128) 0.0227823 (   24) 0.0217544
(  198) 0.0217270 (   57) 0.0217074 (  175) 0.0208224 (  943) 0.0205583 (  141) 0.0204141 (  208)-0.0199553 (  114)-0.0196779
(    4)-0.0195938 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190274D+01
     2 -0.178881D-05  0.195464D+01
     3  0.537760D-06 -0.595244D-06  0.189366D+01
     4 -0.375095D-06 -0.930030D-06  0.847610D-07  0.998572D+00
     5  0.329607D-06 -0.482978D-06 -0.797514D-06  0.540906D-06  0.105009D+00
     6 -0.302119D-05  0.198613D-06  0.330319D-06 -0.287248D-05 -0.231649D-06
     7  0.643075D-05  0.193370D-05  0.942824D-06 -0.448925D-06 -0.574507D-07
     8 -0.619048D-06  0.112192D-07 -0.140745D-07  0.301054D-06 -0.588730D-06
                6             7             8
     6  0.937860D-01
     7 -0.101546D-05  0.126019D-01
     8 -0.214418D-05  0.168519D-06  0.389999D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 11

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40400461
C	1.19644883	0.00000000	2.10188968
C	2.44313006	-0.00363259	1.40999402
C	2.41850454	-0.00437433	-0.01560669
C	1.21566032	-0.00435471	-0.70240929
H	-0.93001913	-0.00571425	-0.53672314
H	-0.93142833	-0.00953507	1.93909760
H	1.19345617	-0.01625997	3.17729266
H	3.34811871	-0.02397437	-0.55616186
H	1.21296316	-0.01721747	-1.77656098
C	3.66458021	0.01246840	2.11488739
H	3.67198553	-0.17056486	3.17577190
H	4.58652593	-0.17383416	1.59111258
Si	4.65782007	2.95826619	2.68203976
C	6.17790843	2.36589051	3.56052734
H	6.75141037	3.23285329	3.88972054
H	5.93651368	1.78372613	4.44260774
H	6.81984963	1.78057986	2.91200904
C	3.17939687	3.48239519	3.66762189
H	2.26181173	3.34994968	3.10474336
H	3.10250504	2.94326131	4.60469195
H	3.26663210	4.54311053	3.90277721
C	4.77245549	3.47671360	0.90724664
H	5.54437491	2.93454280	0.37351532
H	3.82577533	3.34438893	0.39477755
H	5.02161397	4.53684815	0.86185717

E_0(CASSCF,vacuo) -676.746658

E_0(CASSCF,CPCM) **-676.817410**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67674666E+03
(    1) 0.9216897 (   36) 0.1432337 (   22) 0.1391728 (  334) 0.1026225 (    5) 0.0994338 (  186) 0.0872639 (   48) 0.0828840
(  129) 0.0743302 (  466) 0.0726043 (  118) 0.0670274 (   25) 0.0582202 (    7) 0.0570339 (   53) 0.0569909 (   21) 0.0528588
(   47)-0.0488545 (  136) 0.0470022 (  108) 0.0468329 (   70) 0.0405508 (  102) 0.0394736 (  229)-0.0374723 (  393) 0.0373549
(  160) 0.0371368 (  212)-0.0369914 (   52) 0.0356509 (  530) 0.0350045 (  298) 0.0346758 (  109) 0.0341127 (  100)-0.0330860
(   85) 0.0328148 (   20)-0.0304947 (  172)-0.0304909 (   64) 0.0291604 (  284)-0.0269728 (   79) 0.0263823 (  269)-0.0263047
(  241) 0.0262957 (  558) 0.0260840 (  832) 0.0247483 (  123)-0.0242064 (  176) 0.0236767 (   57) 0.0230537 (  128) 0.0225029
(   24) 0.0219646 (  198) 0.0218275 (  943) 0.0208113 (  175) 0.0203288 (  141) 0.0202639 (  208)-0.0202123 (    4)-0.0194064
(  514)-0.0189760 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190131D+01
     2  0.820274D-07  0.195464D+01
     3  0.119929D-05 -0.117860D-05  0.189338D+01
     4 -0.887763D-05  0.522775D-06 -0.669958D-07  0.998818D+00
     5  0.752033D-06 -0.110720D-05 -0.381524D-06  0.114437D-05  0.105599D+00
     6  0.736084D-06 -0.337713D-06  0.837552D-06 -0.257944D-05 -0.486434D-06
     7 -0.115973D-05 -0.138192D-05  0.216085D-05 -0.460155D-05 -0.669102D-07
     8 -0.418441D-06  0.196334D-06  0.932690D-07 -0.104094D-06 -0.113909D-05
                6             7             8
     6  0.954625D-01
     7 -0.344068D-06  0.114994D-01
     8  0.931563D-07 -0.198269D-07  0.392845D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 12

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40381266
C	1.19650063	0.00000000	2.10222174
C	2.44358370	-0.00357471	1.41148986
C	2.41883026	-0.00448875	-0.01389655
C	1.21602539	-0.00446194	-0.70139208
H	-0.92984412	-0.00586605	-0.53709189
H	-0.93152227	-0.00961802	1.93888996
H	1.19268517	-0.01649805	3.17770542
H	3.34851028	-0.02441428	-0.55449733
H	1.21408196	-0.01748992	-1.77561776
C	3.66497536	0.01435665	2.11696263
H	3.67347866	-0.16013208	3.17914431
H	4.58899806	-0.16350023	1.59418688
Si	4.68607454	3.05491356	2.70030870
C	6.20268321	2.45556965	3.57766647
H	6.77961903	3.31956202	3.90909026
H	5.95817050	1.87268976	4.45843597
H	6.84241388	1.86942171	2.92769340
C	3.19542184	3.55528659	3.67784068
H	2.28208102	3.38130417	3.11892540
H	3.13633586	3.03504650	4.62670617
H	3.24850382	4.62355035	3.88779791
C	4.78905205	3.54939504	0.91905363
H	5.58052481	3.02600824	0.39548547
H	3.84825979	3.37551316	0.40766169
H	4.99942476	4.61707652	0.85671895

E_0(CASSCF,vacuo) -676.744610

E_0(CASSCF,CPCM) **-676.816006**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.67674461E+03
(    1) 0.9210975 (   36) 0.1458273 (   22) 0.1394617 (  334) 0.1038146 (    5) 0.0998707 (  186) 0.0876447 (   48) 0.0843614
(  129) 0.0750041 (  466) 0.0732742 (  118) 0.0674778 (   25) 0.0577283 (   53) 0.0575841 (    7) 0.0573030 (   21) 0.0516951
(   47)-0.0493170 (  136) 0.0470846 (  108) 0.0470099 (   70) 0.0407625 (  102) 0.0396699 (  393) 0.0378874 (  160) 0.0369025
(  212)-0.0355596 (  530) 0.0350049 (   52) 0.0346575 (  229)-0.0344701 (  298) 0.0344233 (   85) 0.0331600 (  109) 0.0325732
(  100)-0.0320586 (  172)-0.0302371 (   20)-0.0302015 (   64) 0.0285899 (  284)-0.0269695 (  241) 0.0266262 (   79) 0.0261193
(  269)-0.0253391 (  832) 0.0251479 (  123)-0.0246573 (  558) 0.0238713 (   57) 0.0238235 (  176) 0.0237160 (  128) 0.0222683
(   24) 0.0221933 (  198) 0.0219175 (  943) 0.0210266 (  208)-0.0205159 (  141) 0.0200893 (  175) 0.0198834 (   40) 0.0193739
(    4)-0.0192091 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.190009D+01
     2  0.225591D-07  0.195464D+01
     3  0.107335D-05 -0.926035D-06  0.189312D+01
     4  0.250349D-06  0.710860D-06 -0.490887D-06  0.999089D+00
     5  0.102055D-05 -0.108611D-05  0.952803D-06  0.778786D-06  0.106143D+00
     6  0.596446D-06  0.129144D-05  0.485284D-06  0.236014D-05 -0.401737D-06
     7 -0.308204D-05  0.130700D-06  0.225559D-05 -0.332587D-05 -0.739374D-07
     8  0.761083D-06  0.678137D-07  0.154137D-06  0.546408D-06 -0.870756D-06
                6             7             8
     6  0.970029D-01
     7  0.363461D-06  0.103572D-01
     8 -0.545250D-07  0.683026D-07  0.395528D-01
MCSCF converged.
```

$4^{\bullet+}$ STEP 13

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40367350
C	1.19650556	0.00000000	2.10254884
C	2.44403949	-0.00344458	1.41288867
C	2.41912523	-0.00457739	-0.01237042
C	1.21639299	-0.00455405	-0.70047689
H	-0.92968430	-0.00594538	-0.53743112
H	-0.93161746	-0.00965259	1.93872398
H	1.19194800	-0.01662622	3.17810056
H	3.34886891	-0.02470157	-0.55299848
H	1.21512744	-0.01768939	-1.77477152
C	3.66529137	0.01620879	2.11884318
H	3.67472511	-0.15041607	3.18215585
H	4.59113077	-0.15384708	1.59693396
Si	4.71419540	3.15153035	2.71841754
C	6.22823381	2.54755515	3.59498036
H	6.80750559	3.40951496	3.92798668
H	5.98153291	1.96424789	4.47489298
H	6.86653736	1.96092964	2.94398667
C	3.21322978	3.63055409	3.68916638
H	2.30475674	3.42348141	3.13318627
H	3.16753056	3.12509484	4.64664178
H	3.23780578	4.70347576	3.87988063
C	4.80729800	3.62457785	0.93172505
H	5.61327219	3.11592306	0.41596045
H	3.87174995	3.41761062	0.42258068
H	4.98685160	4.69691825	0.85436525

E_0(CASSCF,vacuo) -676.742760

E_0(CASSCF,CPCM) **-676.814794**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67674276E+03
(    1) 0.9205575 (   36) 0.1483123 (   22) 0.1396990 (  334) 0.1048135 (    5) 0.1004251 (  186) 0.0879486 (   48) 0.0857711
(  129) 0.0755165 (  466) 0.0737923 (  118) 0.0678555 (   53) 0.0581607 (    7) 0.0576375 (   25) 0.0572917 (   21) 0.0507049
(   47)-0.0497560 (  136) 0.0471441 (  108) 0.0471349 (   70) 0.0409244 (  102) 0.0398117 (  393) 0.0383093 (  160) 0.0366828
(  530) 0.0350200 (  298) 0.0342245 (  212)-0.0338510 (   52) 0.0338369 (   85) 0.0334961 (  229)-0.0316060 (  109) 0.0311528
(  100)-0.0311334 (   20)-0.0299957 (  172)-0.0294757 (   64) 0.0280963 (  241) 0.0269488 (  284)-0.0269239 (   79) 0.0259408
(  832) 0.0254802 (  123)-0.0250239 (  269)-0.0245564 (   57) 0.0240871 (  176) 0.0237700 (   24) 0.0224337 (  128) 0.0220771
(  198) 0.0219946 (  558) 0.0219394 (  943) 0.0212067 (   40) 0.0208995 (  208)-0.0208277 (  141) 0.0199124 (  175) 0.0194975
(  514)-0.0191612 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189904D+01
     2  0.141340D-06  0.195464D+01
     3  0.231172D-05 -0.177455D-05  0.189288D+01
     4 -0.705270D-06 -0.288252D-05 -0.232897D-06  0.999356D+00
     5  0.176886D-05 -0.238957D-05  0.865346D-06  0.216748D-05  0.106642D+00
     6 -0.515088D-05 -0.123435D-05  0.171409D-05 -0.465118D-05 -0.872873D-06
     7  0.103831D-04 -0.256097D-05  0.467845D-05 -0.796669D-06 -0.743474D-07
     8 -0.235907D-05  0.840573D-07  0.558196D-06 -0.112178D-05 -0.166776D-05
                6             7             8
     6  0.983844D-01
     7 -0.753175D-06  0.925460D-02
     8  0.114403D-06 -0.144589D-06  0.398009D-01
 MCSCF converged.
```

$4^{\bullet+}$ STEP 14

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40356958
C	1.19648757	0.00000000	2.10286638
C	2.44449602	-0.00337229	1.41419395
C	2.41939967	-0.00462952	-0.01100059
C	1.21675368	-0.00460819	-0.69964637
H	-0.92953808	-0.00607767	-0.53774120
H	-0.93171552	-0.00972362	1.93858225
H	1.19126392	-0.01678785	3.17847850
H	3.34920881	-0.02495947	-0.55164019
H	1.21609171	-0.01785869	-1.77400670
C	3.66554030	0.01774075	2.12054156
H	3.67580399	-0.14136088	3.18488324
H	4.59302685	-0.14483503	1.59940678
Si	4.74255706	3.24768381	2.73653112
C	6.25408195	2.63892458	3.61233389
H	6.83584386	3.49866950	3.94701201
H	6.00511242	2.05510868	4.49132054
H	6.89086376	2.05174224	2.96028495
C	3.23198383	3.70723803	3.70037491
H	2.32931747	3.45736618	3.15197962
H	3.20340626	3.22601736	4.67081738
H	3.22253796	4.78525446	3.86107378
C	4.82602566	3.70118068	0.94505454
H	5.65214613	3.21671024	0.43813942
H	3.90019239	3.45139707	0.43670279
H	4.96268416	4.77864128	0.85321250

E_0(CASSCF,vacuo) -676.741097

E_0(CASSCF,CPCM) **-676.813721**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)     EIGENVALUE     -0.67674110E+03
(    1) 0.9200686 (   36) 0.1506754 (   22) 0.1398953 (  334) 0.1056719 (    5) 0.1010493 (  186) 0.0881956 (   48) 0.0871150
(  129) 0.0759193 (  466) 0.0742084 (  118) 0.0681806 (   53) 0.0587150 (    7) 0.0580099 (   25) 0.0569021 (   47)-0.0501832
(   21) 0.0498471 (  108) 0.0472315 (  136) 0.0471887 (   70) 0.0410500 (  102) 0.0399162 (  393) 0.0386522 (  160) 0.0364776
(  530) 0.0350451 (  298) 0.0340656 (   85) 0.0338198 (   52) 0.0331437 (  212)-0.0318894 (  100)-0.0302763 (  109) 0.0298453
(   20)-0.0298444 (  229)-0.0288785 (  172)-0.0282533 (   64) 0.0276639 (  241) 0.0272594 (  284)-0.0268430 (   79) 0.0258179
(  832) 0.0257653 (  123)-0.0253342 (   57) 0.0239194 (  269)-0.0239149 (  176) 0.0238370 (   24) 0.0226742 (   40) 0.0221784
(  198) 0.0220618 (  128) 0.0219184 (  943) 0.0213615 (  208)-0.0211384 (  558) 0.0202489 (  141) 0.0197389 (  514)-0.0192340
(   67)-0.0191632 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189815D+01
     2 -0.695189D-07  0.195463D+01
     3 -0.175990D-04  0.800181D-05  0.189266D+01
     4  0.406411D-06 -0.474995D-07 -0.175647D-05  0.999620D+00
     5 -0.245933D-05  0.385579D-05  0.330618D-06 -0.215484D-04  0.107098D+00
     6  0.274820D-06 -0.698986D-07 -0.233786D-04 -0.962459D-06  0.524970D-05
     7 -0.574190D-07  0.110105D-06 -0.198820D-04 -0.817152D-06 -0.361731D-05
     8 -0.362038D-07 -0.121874D-06 -0.265505D-05 -0.165668D-06  0.533457D-05
                6             7             8
     6  0.996384D-01
     7 -0.107133D-06  0.818163D-02
     8  0.184161D-08 -0.276738D-07  0.400300D-01
 MCSCF converged.
```

$4^{\bullet+}$ STEP 15

GEOMETRY

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40356958
C	1.19648757	0.00000000	2.10286638
C	2.44449602	-0.00337229	1.41419395
C	2.41939967	-0.00462952	-0.01100059
C	1.21675368	-0.00460819	-0.69964637
H	-0.92953808	-0.00607767	-0.53774120
H	-0.93171552	-0.00972362	1.93858225
H	1.19126392	-0.01678785	3.17847850
H	3.34920881	-0.02495947	-0.55164019
H	1.21609171	-0.01785869	-1.77400670
C	3.66554030	0.01774075	2.12054156
H	3.67580399	-0.14136088	3.18488324
H	4.59302685	-0.14483503	1.59940678
Si	4.74255706	3.24768381	2.73653112
C	6.25408195	2.63892458	3.61233389
H	6.83584386	3.49866950	3.94701201
H	6.00511242	2.05510868	4.49132054
H	6.89086376	2.05174224	2.96028495
C	3.23198383	3.70723803	3.70037491
H	2.32931747	3.45736618	3.15197962
H	3.20340626	3.22601736	4.67081738
H	3.22253796	4.78525446	3.86107378
C	4.82602566	3.70118068	0.94505454
H	5.65214613	3.21671024	0.43813942
H	3.90019239	3.45139707	0.43670279
H	4.96268416	4.77864128	0.85321250

E_0(CASSCF,vacuo) -676.739609

E_0(CASSCF,CPCM) **-676.812776**

DATA from the CASSCF calculation in vacuo:

```
      ( 1)      EIGENVALUE     -0.67673961E+03
(    1) 0.9196251 (   36) 0.1529570 (   22) 0.1400529 (  334) 0.1064405 (    5) 0.1017196 (   48) 0.0884086 (  186) 0.0883979
(  129) 0.0762495 (  466) 0.0745611 (  118) 0.0684681 (   53) 0.0592520 (    7) 0.0584073 (   25) 0.0565411 (   47)-0.0506173
(   21) 0.0490795 (  108) 0.0473154 (  136) 0.0472220 (   70) 0.0411496 (  102) 0.0399944 (  393) 0.0389413 (  160) 0.0362823
(  530) 0.0350771 (   85) 0.0341334 (  298) 0.0339350 (   52) 0.0325379 (   20)-0.0297213 (  212)-0.0296194 (  100)-0.0294436
(  109) 0.0286182 (  241) 0.0275601 (   64) 0.0272740 (  284)-0.0267281 (  172)-0.0265519 (  229)-0.0262219 (  832) 0.0260229
(   79) 0.0257275 (  123)-0.0256151 (  176) 0.0239226 (  269)-0.0233856 (   57) 0.0233269 (   40) 0.0232822 (   24) 0.0229085
(  198) 0.0221206 (  128) 0.0217812 (  943) 0.0214998 (  208)-0.0214501 (   67)-0.0196302 (  141) 0.0195657 (  514)-0.0192982
(  175) 0.0188569 (
Final one electron symbolic density matrix:
                1             2             3             4             5
     1  0.189736D+01
     2 -0.328789D-06  0.195462D+01
     3  0.306917D-04 -0.143997D-04  0.189246D+01
     4  0.119280D-04 -0.173076D-05 -0.414107D-06  0.999886D+00
     5  0.814902D-05 -0.100116D-04  0.822917D-06  0.366778D-04  0.107512D+00
     6 -0.330265D-06  0.128890D-05  0.382192D-04  0.690062D-05 -0.858640D-05
     7  0.165833D-05 -0.561486D-06  0.362857D-04 -0.509511D-05  0.564549D-05
     8  0.102885D-05 -0.290829D-07  0.413931D-05  0.100238D-05 -0.100086D-04
                6             7             8
     6  0.100806D+00
     7  0.419142D-06  0.711127D-02
     8 -0.256381D-06  0.817045D-07  0.402440D-01
MCSCF converged.
```

8. References

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