5-EXO EQUATORIAL TRANSITION-STATE

MacSPARTAN '04 Quantum Mechanics Program: (PowerPC(Darwin)) build 123

Job type: Transition state search.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
An unrestricted Hartree-Fock SCF calculation will be
performed using Pulay DIIS extrapolation

Correlation model:
A MP2 calculation will be performed

Optimization:

Step	Energy	Max Grad.	Max Dist.	
1	-344.0101269	0.018737	0.070610	1
2	-344.0109538	0.007836	0.095832	1
3	-344.0107433	0.012224	0.108064	1
4	-344.0110048	0.004664	0.061674	1
5	-344.0110511	0.004717	0.010800	2
6	-344.0110549	0.003662	0.053065	1
7	-344.0110607	0.003033	0.087321	1
8	-344.0110494	0.002843	0.042140	1
9	-344.0110812	0.001630	0.024020	1
10	-344.0110855	0.001487	0.016198	1
11	-344.0110790	0.000412	0.013092	1
12	-344.0110847	0.000360	0.017676	1
13	-344.0110856	0.000363	0.008287	1
14	-344.0110813	0.000291	0.004744	1
15	-344.0110851	0.000121	0.002101	1
16	-344.0110901	0.000109	0.000437	1

Program Wall Time: 1:10:57.0
Reason for exit: Sucessful completion
Quantum Mechanics Program CPU Time : 0:55:03.8
Quantum Mechanics Program Wall Time: 1:10:57.4

SPARTAN PROPERTIES PACKAGE: MAC/G5 build 123
All calculations using Post-HF corrected density matrix

Reason for exit: Successful completion
Properties Program CPU Time : 0:00:00.9
Properties Program Wall Time: 0:00:01.0

molecule 5x-6n tstates.2 terminated normally

End- molecule "5x-6n tstates.2" Tue Mar 22 16:22:34 2005

MacSPARTAN '04 Semi-Empirical Program: (PowerPC(Darwin)) build 123
Job run on machine : John-Tamines-Computer.local
Semi-empirical Property Calculation

```
  5X-6N TSTATES.2
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 C  C2          -1.4047315      .2170108      .3181836
  2 C  C1          -1.4669563    -1.1529134     -.2436455
  3 O  O1          -2.3745594    -1.9408888     -.0914052
  4 O  O2           -.3622791    -1.5016110     -.9717621
  5 C  C3            .7175643     -.5513348     -.9097352
  6 H  H1          -1.8893212      .3686179     1.2755446
  7 H  H3          -1.4442272     1.0477090     -.3782021
  8 H  H2           1.6113865    -1.1369208    -1.1418187
  9 C  C4            .8287762      .0794330      .4522491
 10 H  H6            .5944352      .2146843    -1.6852799
 11 C  C5           1.3401974     1.3043180      .6410000
 12 H  H4            .7893004     -.6166067     1.2885864
 13 H  H5           1.5759977     1.6745412     1.6313945
 14 H  H7           1.4844154     1.9939615     -.1851094

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.8
  Properties Program Wall Time:   0:00:01.0

molecule 5x-6n tstates.2 terminated normally

End-   molecule "5x-6n tstates.2" Mon Apr 11 16:07:20 2005

<step 2>
Job type: Frequency calculation.
Method: UMP2(FC)
Basis set: 6-31G(D)

Correlation model:
 A MP2 calculation will be performed

  Program Wall Time:    4:22:-0.0
  Reason for exit: Sucessful completion
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  Quantum Mechanics Program CPU Time :   4:00:02.6
  Quantum Mechanics Program Wall Time:   4:22:00.6

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X-6N TSTATES.2
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
      Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 C  C2          -1.4047315      .2170108      .3181836
  2 C  C1          -1.4669563    -1.1529134     -.2436455
  3 O  O1          -2.3745594    -1.9408888     -.0914052
  4 O  O2           -.3622791    -1.5016110     -.9717621
  5 C  C3            .7175643     -.5513348     -.9097352
  6 H  H1          -1.8893212      .3686179     1.2755446
  7 H  H3          -1.4442272     1.0477090     -.3782021
  8 H  H2           1.6113865    -1.1369208    -1.1418187
  9 C  C4            .8287762      .0794330      .4522491
 10 H  H6            .5944352      .2146843    -1.6852799
 11 C  C5           1.3401974     1.3043180      .6410000
 12 H  H4            .7893004     -.6166067     1.2885864
 13 H  H5           1.5759977     1.6745412     1.6313945
 14 H  H7           1.4844154     1.9939615     -.1851094

  Point Group = C1  Order =  1 Nsymop =  1
   Post HF density not available.  Select the
   density checkbox to generate a density or
   use the "NOPOSTHFDEN" keyword to use the
   HF density.

  Molecule is non-linear

  Normal Modes and Vibrational Frequencies (cm-1)
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	-569.65 A			103.87 A			204.90 A	
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.189	.007	-.029	.017	-.060	.123	.021	.005	-.046
C1	-.016	.001	.000	-.010	-.014	.005	.005	-.019	.004
O1	.001	-.015	.000	-.072	.029	-.129	-.032	.018	-.024
O2	-.003	.017	.022	.018	-.028	.059	.056	-.085	.109
C3	.010	.012	.004	.008	-.016	.028	-.079	.080	-.063
H1	-.136	.004	-.009	.066	-.150	.162	-.015	.046	-.070
H3	.027	.040	.010	-.061	-.004	.193	.032	-.020	-.078
H2	-.020	-.009	-.057	.009	-.014	.024	-.030	.225	-.232
C4	.205	-.010	-.003	.044	.031	.003	.000	.015	-.040
H6	-.014	.019	.015	-.014	-.038	.011	-.326	.089	-.016
C5	.005	-.020	.000	.007	.058	-.082	.039	-.012	.057
H4	.030	.019	.012	.108	.065	.033	.019	-.052	-.095
H5	-.014	-.002	.000	.045	.117	-.113	.071	-.119	.089
H7	-.003	-.009	.004	-.062	.022	-.124	.036	.068	.123

	233.66 A			384.74 A			431.08 A	
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.066	-.014	-.006	-.058	.009	.044	-.069	.045	.046
C1	-.024	-.024	-.007	.010	.019	.010	.053	.062	-.019
O1	.010	-.068	-.021	.006	.021	.005	.078	.047	-.006
O2	-.010	.026	.000	.013	-.019	.026	.061	-.008	.038
C3	-.026	.036	.039	.061	-.058	-.073	-.008	.019	-.007
H1	-.060	-.031	.001	.101	-.121	.145	-.100	-.126	.060
H3	-.126	-.021	-.012	-.280	.050	.106	-.137	.126	.148
H2	-.012	.038	.087	.047	-.144	.085	.029	.105	-.079
C4	-.074	.071	.027	-.028	.051	-.116	-.075	-.079	.018
H6	.003	.021	.019	.146	-.175	-.201	-.090	.071	.056
C5	.173	-.015	-.029	.001	.007	.065	-.043	-.093	-.074
H4	-.189	.118	.059	-.181	.045	-.128	-.149	-.075	.015
H5	.208	.005	-.045	-.211	-.120	.164	-.064	.041	-.121
H7	.370	-.106	-.071	.239	.091	.178	.005	-.219	-.171

	496.65 A			558.52 A			593.39 A	
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.031	-.084	-.020	.017	.049	-.069	-.037	.035	.016
C1	.034	-.034	-.086	-.044	.024	-.059	-.008	.048	-.063
O1	-.053	.102	.095	.016	-.039	.006	.059	-.007	-.001
O2	.038	-.071	-.087	-.010	-.014	.014	-.010	-.037	.010
C3	.006	.022	.021	-.023	.000	.033	-.038	-.044	.016
H1	-.044	-.298	.007	.656	-.066	.268	-.201	-.112	-.041
H3	-.125	.019	.111	-.443	.115	.034	.023	.130	.126
H2	.039	.086	-.003	-.033	.010	-.035	-.009	-.067	.182
C4	.006	.030	.040	.035	-.015	.033	-.035	.024	-.013
H6	-.043	.045	.054	-.054	.035	.073	.059	-.122	-.078
C5	.016	.028	.013	-.003	.003	.006	.029	.015	.012
H4	-.015	.057	.061	.041	-.006	.043	.299	-.048	-.054
H5	.034	.046	.003	.051	.024	-.014	.474	-.223	-.004
H7	.035	.007	-.003	-.091	.000	-.012	-.373	.223	.115

	634.58 A			696.11 A			815.49 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.045	-.019	-.030	-.006	.050	.020	-.080	-.005	-.008
C1	.062	-.055	.110	.101	-.004	.081	.044	-.032	.051
O1	-.049	.042	-.013	.067	.035	-.059	-.001	.024	-.014
O2	.032	.048	-.009	-.063	-.074	-.073	.022	-.030	-.041
C3	.045	.034	-.001	-.092	-.067	.019	-.022	.015	.018
H1	.048	.101	-.004	-.062	.085	-.013	.475	.201	.225
H3	-.433	-.220	-.261	-.216	-.069	-.118	.558	.100	.108
H2	.059	.015	.091	-.077	.000	-.083	.035	.054	.142
C4	-.033	-.021	-.010	.032	.020	.030	-.035	.030	-.014
H6	.116	.019	-.026	-.182	-.030	.072	.023	-.032	-.036
C5	.000	-.037	-.015	.007	.037	.022	-.031	-.020	-.011
H4	.126	-.092	-.060	-.037	.106	.101	-.105	.052	-.001
H5	.269	-.123	-.047	-.070	.041	.040	.153	-.128	-.014
H7	-.259	.039	.005	.084	.034	.033	.006	.002	.014

	860.99 A			953.66 A			957.71 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.018	.139	.076	.029	.039	.026	-.024	.004	-.005
C1	-.064	-.018	.019	-.020	-.009	-.014	.010	-.012	.003
O1	-.055	-.058	.007	-.020	-.016	.010	-.002	.003	.000
O2	.046	-.090	-.076	.039	.006	-.025	.006	.003	-.007
C3	.086	.019	-.043	-.009	.005	.114	-.013	.005	.032
H1	-.096	.225	.032	-.082	.044	-.026	.043	.011	.026
H3	-.057	.099	.019	-.087	.003	-.017	.066	.031	.025
H2	.139	.112	-.077	.045	.121	.037	.004	.030	.043
C4	-.010	-.004	.030	.018	-.013	-.069	-.031	.006	-.014
H6	.013	.062	.011	-.044	.118	.233	-.012	.012	.040
C5	.017	.015	.017	-.047	-.024	-.087	.131	-.049	-.034
H4	.037	-.045	-.001	.060	.164	.074	.060	.011	-.005
H5	.040	.116	-.026	-.093	-.494	.098	-.608	.116	.082
H7	-.070	-.035	-.042	.249	.239	.191	-.476	.246	.107

	1014.10 A			1057.24 A			1085.36 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.054	.043	.014	.031	.077	-.087	.044	.002	.025
C1	.014	-.027	-.008	.065	-.079	.083	-.008	-.003	-.018
O1	-.008	-.009	-.001	-.045	-.026	-.016	-.007	-.007	.005
O2	.007	-.036	-.015	-.030	.028	.006	.017	.012	.001
C3	-.095	.109	.041	.025	.001	-.003	-.005	-.020	-.008
H1	-.080	-.028	-.038	-.101	-.448	-.063	-.052	.017	-.023
H3	-.095	.038	.010	.038	.429	.338	-.028	-.041	-.024
H2	-.053	-.022	.540	-.018	-.033	-.078	-.016	-.012	-.070
C4	.065	.002	-.034	-.005	-.001	.001	.047	.015	-.011
H6	.211	-.133	-.238	-.010	.025	.028	-.005	.007	.014
C5	-.019	-.037	.008	-.006	.002	-.004	-.001	-.018	.003
H4	-.098	-.139	-.164	-.035	.024	.021	-.785	.222	.114
H5	-.095	.087	-.024	.036	-.034	-.001	.209	-.073	-.028
H7	.012	-.166	-.092	-.011	.018	.010	-.400	.089	.023

	1117.20 A			1201.52 A			1243.63 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.006	.037	.013	-.001	.014	.010	-.014	.052	.055
C1	-.002	-.042	-.014	.020	-.023	-.021	.109	-.116	-.133
O1	-.042	-.010	.018	-.006	.000	.002	-.017	.004	.016
O2	.140	.095	-.024	.013	-.010	.021	-.050	.022	.036
C3	-.126	-.120	-.018	-.033	.049	-.120	.037	.022	.047
H1	-.005	.051	.014	.015	.062	.012	.005	.294	.033
H3	-.013	.048	.021	-.020	.001	-.006	-.017	.023	.002
H2	-.068	-.044	-.009	-.181	-.235	.027	-.210	-.246	-.201
C4	.002	-.004	.002	-.001	-.027	.129	-.015	.013	-.022
H6	-.102	-.136	-.047	.279	.015	-.214	-.093	-.042	.016
C5	.006	.017	.029	-.006	-.002	-.058	-.004	.001	.007
H4	.098	-.002	.015	.068	.216	.338	.005	-.098	-.117
H5	.001	.121	-.007	-.094	-.216	.046	.026	.012	-.006
H7	.040	-.059	-.032	.088	.192	.126	-.005	-.037	-.024

	1289.45 A			1329.09 A			1423.07 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.014	-.006	-.005	-.016	-.004	-.006	.006	-.003	-.008
C1	-.018	.015	.031	-.003	.005	.010	-.047	.052	.052
O1	.007	.005	-.005	.001	.001	-.001	.004	-.006	-.005
O2	.039	-.037	-.004	.007	.006	-.007	.050	-.016	-.043
C3	-.045	.007	.018	-.002	-.006	.009	.031	.056	.076
H1	-.002	-.036	.005	.016	-.009	.011	-.001	-.152	.009
H3	.033	.001	.005	.017	.004	.004	.036	-.057	-.066
H2	-.321	-.336	-.163	.016	.012	.016	-.345	-.355	-.342
C4	-.015	-.018	-.056	.004	-.072	.076	-.006	.048	.018
H6	.478	.441	.342	-.077	-.097	-.062	-.189	-.322	-.262
C5	.013	.033	.020	.022	.095	-.063	-.006	-.021	-.010
H4	-.043	-.094	-.120	-.301	-.552	-.324	.023	-.033	-.053
H5	.053	.129	-.022	.002	-.042	.003	-.049	-.183	.053
H7	.010	.023	.003	.147	.347	.162	-.069	-.116	-.088

	1492.49 A			1501.29 A			1566.57 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.016	-.099	-.040	-.009	.004	.000	.000	.002	.000
C1	-.025	.013	.033	-.004	.008	.007	-.006	.011	.007
O1	.016	.012	-.005	.000	-.001	-.001	-.002	-.003	.000
O2	.012	-.005	-.013	.007	-.002	-.009	.016	.002	-.007
C3	.004	.011	.009	.016	.051	.041	.044	.007	-.065
H1	-.074	.582	-.185	.004	-.043	.014	.004	-.039	.007
H3	-.251	.345	.492	.023	-.021	-.030	.017	-.022	-.028
H2	-.047	-.063	-.001	-.082	-.082	.008	-.119	-.433	.504
C4	.002	-.007	-.005	-.019	-.103	-.066	.003	.010	.006
H6	-.056	-.040	-.026	-.136	-.159	-.128	-.562	.229	.284
C5	.002	.002	.001	-.007	-.020	.016	-.001	-.003	-.002
H4	-.009	.019	.016	.024	.221	.204	-.011	-.007	-.007
H5	.001	-.001	.003	.176	.514	-.211	-.003	-.026	.006
H7	-.007	-.002	-.003	.146	.333	.319	-.012	-.007	-.008

	1652.78 A			1951.44 A			3102.33 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.026	-.003	.001	.007	.027	.003	.000	.000	.000
C1	-.006	.003	.001	-.156	-.171	.015	.002	.000	-.001
O1	.000	-.002	.000	.106	.098	-.017	.000	.000	.000
O2	.002	-.001	-.002	-.002	.011	.005	-.002	.000	.000
C3	-.002	-.034	-.017	.011	.003	-.003	-.018	-.029	.059
H1	-.013	.013	-.022	-.011	-.054	.022	-.001	.002	.002
H3	-.035	.006	.015	.002	.014	-.020	-.002	.001	.001
H2	.003	-.003	-.072	.011	-.007	-.002	.350	-.239	-.074
C4	.021	.156	.062	.000	.000	.001	.000	.001	-.003
H6	.047	.061	.064	-.016	-.003	-.008	-.122	.604	-.608
C5	-.056	-.149	-.034	.000	.000	-.001	.000	.001	.000
H4	.028	-.142	-.200	.001	.002	.002	-.001	-.021	.023
H5	.046	.228	-.208	.001	-.004	.000	-.002	.001	-.005
H7	.100	.194	.290	.001	.000	.000	.001	-.004	.008

	3174.75 A			3224.74 A			3226.30 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.000	.000	.000	-.002	.007	.001	-.019	.050	.008
C1	-.001	-.001	.000	.000	.000	.000	-.001	-.003	-.002
O1	.000	.000	.000	.000	.000	.000	.000	.000	.000
O2	.000	.001	.000	.000	.000	.000	.000	.000	.000
C3	.063	-.062	.010	.002	-.004	.002	-.002	.003	.000
H1	.000	.001	-.001	.032	-.009	-.067	.235	-.069	-.496
H3	-.002	-.003	.003	-.002	-.071	.059	.006	-.494	.417
H2	-.694	.462	.181	-.024	.016	.007	.023	-.017	-.008
C4	.000	.004	-.005	-.002	-.029	.039	.001	.024	-.027
H6	-.047	.275	-.292	-.007	.029	-.033	.003	-.017	.019
C5	.000	.000	.000	-.016	-.046	-.001	-.004	-.014	.004
H4	-.003	-.053	.060	.025	.365	-.445	-.015	-.265	.321
H5	.001	.001	.002	.104	.158	.455	.020	.030	.085
H7	.001	.000	.001	.076	.367	-.451	.022	.111	-.136

	3227.83 A			3326.58 A			3338.03 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.012	-.027	-.003	.000	.001	-.001	.025	.030	-.086
C1	.000	.002	.001	.000	.000	.000	.001	.001	.000
O1	.000	.000	.000	.000	.000	.000	-.001	.000	.000
O2	.000	.000	.000	.000	.000	.000	.000	.000	.000
C3	-.003	.005	.000	.000	-.001	.000	.000	.000	.000
H1	-.125	.036	.260	-.003	.001	.006	-.319	.106	.638
H3	-.004	.268	-.227	.000	-.008	.006	.017	-.468	.384
H2	.031	-.021	-.011	-.005	.003	.001	.002	-.001	.000
C4	.003	.039	-.040	.000	-.005	.005	.000	.001	.000
H6	.006	-.025	.026	-.001	.003	-.007	.000	-.002	.002
C5	-.013	-.039	.007	.008	-.007	.093	.000	.000	-.001
H4	-.024	-.398	.482	.003	.049	-.057	.001	-.006	.006
H5	.062	.094	.272	-.166	-.260	-.693	.002	.004	.009
H7	.063	.303	-.372	.075	.355	-.417	-.001	-.003	.004

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 1 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	-569.650	0.0000	0.0000	0.0000	0.0000		2.98
					-23842383847515.29		
2	103.873	0.6213	1.9093	14.1431	8.1425	39.42	2.97
3	204.903	1.2256	1.4521	8.7387	7.6689	62.80	4.74
4	233.655	1.3976	1.3386	7.7432	7.4868	67.62	1.67
5	384.738	2.3012	0.8520	4.2696	6.2875	84.38	2.07
6	431.078	2.5784	0.7360	3.5778	5.8682	87.51	1.31
7	496.650	2.9706	0.5949	2.7888	5.2611	90.90	5.24
8	558.518	3.3407	0.4838	2.2041	4.6906	93.25	4.20
9	593.390	3.5493	0.4296	1.9295	4.3758	94.29	2.24
10	634.581	3.7956	0.3725	1.6479	4.0142	95.32	8.26
11	696.109	4.1637	0.2999	1.3001	3.5007	96.52	5.74
12	815.493	4.8777	0.1944	0.8161	2.6172	98.05	10.31
13	860.986	5.1498	0.1642	0.6820	2.3240	98.43	13.05
14	953.657	5.7041	0.1156	0.4715	1.8024	99.00	3.40
15	957.712	5.7284	0.1138	0.4639	1.7818	99.02	50.94
16	1014.104	6.0657	0.0916	0.3697	1.5147	99.25	8.40
17	1057.244	6.3237	0.0774	0.3104	1.3331	99.39	16.87
18	1085.357	6.4919	0.0693	0.2769	1.2248	99.47	33.01
19	1117.203	6.6824	0.0612	0.2431	1.1112	99.54	90.96
20	1201.524	7.1867	0.0437	0.1719	0.8530	99.70	4.75
21	1243.633	7.4386	0.0369	0.1444	0.7449	99.75	141.29
22	1289.445	7.7126	0.0307	0.1194	0.6413	99.80	29.17
23	1329.094	7.9497	0.0261	0.1012	0.5623	99.84	0.20
24	1423.066	8.5118	0.0177	0.0682	0.4091	99.90	34.13
25	1492.487	8.9271	0.0133	0.0508	0.3217	99.93	24.31
26	1501.295	8.9797	0.0128	0.0490	0.3120	99.93	14.86
27	1566.570	9.3702	0.0098	0.0371	0.2478	99.95	3.26
28	1652.782	9.8858	0.0068	0.0257	0.1819	99.97	7.51
29	1951.442	11.6722	0.0019	0.0070	0.0600	99.99	795.42
30	3102.329	18.5560	0.0000	0.0000	0.0006	100.00	25.13
31	3174.751	18.9892	0.0000	0.0000	0.0004	100.00	11.27
32	3224.738	19.2882	0.0000	0.0000	0.0004	100.00	5.03
33	3226.305	19.2976	0.0000	0.0000	0.0003	100.00	0.86
34	3227.828	19.3067	0.0000	0.0000	0.0003	100.00	1.17
35	3326.585	19.8974	0.0000	0.0000	0.0002	100.00	5.46
36	3338.026	19.9658	0.0000	0.0000	0.0002	100.00	0.61
Total Vibrations		295.9031	9.5562	52.7514	75.3418		
Ideal Gas			2.4789				
Translation			3.7184	166.0599	12.4716		
Rotation			3.7184	114.2233	12.4716		
Totals			315.3751	333.0346	100.2851		
Gibb's Free Energy (H - TS)			216.0808				

Reason for exit: Successful completion

```
  Properties Program CPU Time :   0:00:00.1
  Properties Program Wall Time:   0:00:00.2

molecule 5x-6n tstates.2 terminated normally

End-   molecule "5x-6n tstates.2" Sat Apr  2 02:05:55 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1465440 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2191580 hartrees

  Program Wall Time:    0:11:55.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:08:54.4
  Quantum Mechanics Program Wall Time:   0:11:56.8

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X-6N TSTATES.2
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.5

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
Task "SPARTAN Properties" returned [1]

End-   molecule "5x-6n tstates.2" Wed Mar 23 20:02:14 2005
```

5-EXO AXIAL TRANSITION-STATE

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Transition state search.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:
         Step      Energy          Max Grad.      Max Dist.
            1    -344.0042483       0.043027       0.123489   1
            2    -344.0086809       0.008869       0.080554   1
            3    -344.0084383       0.002625       0.010800   2
            4    -344.0084480       0.002275       0.074259   1
            5    -344.0084985       0.001191       0.012722   1
            6    -344.0085126       0.000751       0.014382   1
            7    -344.0085202       0.000645       0.014271   1
            8    -344.0085282       0.000219       0.010942   1
            9    -344.0085277       0.000122       0.001702   1

  Program Wall Time:    0:33:17.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:27:47.0
  Quantum Mechanics Program Wall Time:   0:33:17.8

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

<step 2>
Job type: Frequency calculation.
Method: UMP2(FC)
Basis set: 6-31G(D)

Correlation model:
 A MP2 calculation will be performed

  Program Wall Time:    4:58:37.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   4:09:56.8
  Quantum Mechanics Program Wall Time:   4:58:37.6

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53
```

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C2	-1.3932552	-.0511360	.5373846
2	C	C1	-1.3445484	.2685623	-.9088351
3	O	O1	-2.1245403	.9748709	-1.5092250
4	O	O2	-.2809514	-.2982192	-1.5617931
5	C	C3	.6436856	-.9619419	-.6776893
6	H	H1	-1.8189086	.7108782	1.1787910
7	C	C4	.8463542	-.1638058	.5933889
8	H	H4	-1.5678827	-1.0831785	.8275915
9	H	H5	1.5680782	-1.0480800	-1.2528034
10	H	H6	.2834889	-1.9720908	-.4523582
11	C	C5	1.3329632	1.0872991	.5713219
12	H	H2	.8538711	-.7203776	1.5276554
13	H	H3	1.4292187	1.6389947	-.3583606
14	H	H7	1.5724268	1.6182248	1.4849314

Point Group = C1 Order = 1 Nsymop = 1
Post HF density not available. Select the density checkbox to generate a density or use the "NOPOSTHFDEN" keyword to use the HF density.

Molecule is non-linear

Normal Modes and Vibrational Frequencies (cm-1)

	-581.21 A			97.40 A			196.55 A	
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.190	.008	.018	.014	.087	.001	.015	-.012	.007
C1	.015	.000	-.001	-.028	.006	-.021	.024	.016	.007
O1	-.003	-.007	.010	-.106	-.106	-.053	-.025	-.042	.002
O2	.005	-.007	-.023	.008	.062	-.004	.102	.136	.021
C3	-.008	-.006	-.011	-.003	.034	-.014	-.060	-.054	.041
H1	.131	-.003	.004	.049	.133	-.030	.002	-.014	.002
C4	-.205	-.002	.015	.014	-.020	.017	.011	-.040	.012
H4	-.036	.021	-.046	-.030	.109	.054	-.026	-.009	-.008
H5	.028	.047	.039	-.003	.038	-.014	-.056	-.240	.076
H6	.015	-.022	-.043	-.018	.032	-.047	-.263	.018	.039
C5	-.007	.017	.001	.111	-.058	.079	-.057	-.013	-.086
H2	-.002	-.042	-.010	-.051	-.053	-.003	.113	-.016	.026
H3	-.008	.005	-.003	.184	-.030	.103	-.188	-.053	-.122
H7	.016	.002	.001	.124	-.111	.107	.005	.042	-.135

	240.43 A			365.52 A			465.63 A	
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.049	.109	.033	-.060	.046	.041	.057	-.032	.009
C1	.018	.015	.009	.009	.008	.038	-.048	.076	.019
O1	.008	-.017	-.016	.013	-.017	.003	-.006	.011	-.124
O2	-.014	-.031	-.007	.018	.025	.042	-.059	.002	.081
C3	.017	-.028	-.048	.102	.030	-.040	.008	.028	.017
H1	.166	.201	.000	.019	.118	.010	-.032	-.235	.191
C4	.072	-.063	-.034	-.048	-.052	.022	.031	-.039	.050
H4	-.052	.147	.110	-.185	.073	.063	.233	-.118	-.183
H5	-.001	-.027	-.078	.128	.278	-.036	-.008	.148	-.028
H6	.025	-.030	-.042	.260	-.062	-.201	.109	-.022	-.042
C5	-.136	.011	.058	-.042	-.065	-.084	.000	-.021	-.023
H2	.194	-.135	-.076	-.181	-.003	.049	.193	-.077	.026
H3	-.322	.145	.119	.092	-.241	-.175	-.201	-.041	-.055
H7	-.144	-.062	.103	-.166	.107	-.152	.148	.011	-.081

	524.99 A			530.21 A			568.01 A	
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.026	.085	-.030	.039	-.002	-.104	-.044	.026	-.004
C1	.024	.025	-.010	.004	.038	-.072	-.014	-.077	-.027
O1	-.035	.000	.045	-.107	.047	.061	.025	.011	.033
O2	.014	-.018	-.015	.006	-.048	-.034	.012	-.003	-.037
C3	.016	-.025	-.001	.043	.000	.068	-.004	.057	.006
H1	-.509	-.133	-.122	.224	.042	-.037	-.213	.097	-.196
C4	-.005	-.019	.008	.059	-.028	.092	-.036	-.008	.059
H4	.654	.000	.025	-.187	.013	-.183	.029	.063	.170
H5	.028	-.016	.019	.043	.038	.062	.048	.164	.075
H6	.015	-.030	-.020	.068	-.011	.045	.071	.015	-.067
C5	-.031	-.025	.000	-.016	-.013	-.006	.022	-.022	-.016
H2	-.116	.017	.030	.020	-.008	.104	.304	-.120	-.008
H3	.056	-.076	-.021	-.074	-.130	-.082	-.415	.037	-.027
H7	-.164	.036	-.001	-.026	.125	-.084	.492	-.096	-.098

	635.39 A			718.83 A			799.91 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.047	.023	.000	-.015	.010	-.042	.085	.004	.021
C1	.111	.121	.044	-.089	-.028	-.029	-.054	-.067	-.011
O1	-.027	-.054	.024	-.055	.064	.001	.014	.024	-.012
O2	.005	-.043	.007	.062	.005	.110	-.029	.025	.026
C3	.016	-.026	-.013	.085	-.099	.012	.001	-.009	-.015
H1	-.320	-.130	.006	.008	.034	-.053	-.521	-.029	-.319
C4	-.034	.014	-.039	-.044	.010	-.081	.050	-.025	.024
H4	-.336	-.041	-.370	.018	.026	.032	-.432	.035	-.119
H5	.033	-.012	.011	.080	-.026	-.012	-.054	-.038	-.106
H6	.036	-.029	.005	.140	-.122	.006	-.029	.005	-.004
C5	.016	.014	-.006	.020	.017	-.015	.029	.028	.010
H2	.105	-.017	-.058	.114	.041	-.064	.105	-.052	.008
H3	-.093	.131	.052	-.006	.214	.101	.076	-.045	-.028
H7	.178	-.116	.027	.066	-.187	.093	-.227	.170	-.005

	859.90 A			956.12 A			967.76 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.027	.012	-.157	.031	-.005	.052	.040	.003	.016
C1	.059	-.035	.007	-.014	-.003	-.021	-.018	-.010	-.001
O1	.046	-.046	.046	-.015	.019	-.008	-.002	.009	-.005
O2	-.048	.018	.122	.032	-.030	-.014	.005	.000	-.002
C3	-.069	.064	.004	-.003	.138	.106	.006	.003	.001
H1	.112	.088	-.205	-.097	-.039	.014	-.082	-.016	-.039
C4	.005	-.004	-.032	.009	-.025	-.088	.041	-.006	-.005
H4	.042	.033	-.097	-.080	-.008	-.004	-.065	.003	-.033
H5	-.112	.132	-.071	.045	.049	.200	.000	-.013	-.008
H6	.003	.033	-.017	.000	.169	.228	.008	.007	.023
C5	-.018	-.020	-.015	-.020	-.084	-.059	-.142	.029	.006
H2	-.070	.000	-.033	.004	-.055	-.115	-.111	.052	.029
H3	.011	.028	.017	.031	.103	.061	.492	-.163	-.038
H7	-.006	-.086	.019	-.215	-.277	.099	.577	-.236	-.032

	1001.78 A			1049.13 A			1063.48 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.022	-.023	.019	-.021	-.086	.004	-.043	.079	-.019
C1	.029	.011	-.012	.070	.083	-.019	-.042	-.057	.005
O1	.004	-.006	-.007	-.037	.007	-.020	.026	-.010	.027
O2	-.032	.037	-.045	-.010	-.019	.025	.037	-.009	-.017
C3	-.059	-.072	.057	-.010	.009	.002	-.058	.006	-.001
H1	-.031	.028	-.075	-.009	.159	-.274	.087	-.120	.294
C4	.039	-.004	.036	-.028	-.009	.005	-.012	-.011	.019
H4	-.030	.004	.087	.057	.026	.433	.052	-.025	-.335
H5	.018	.377	.121	-.023	.020	-.024	.012	.128	.088
H6	.173	-.228	-.292	-.007	.005	-.011	.024	-.052	-.122
C5	.001	.005	-.056	-.009	.019	.002	-.005	.024	-.009
H2	-.011	.292	.212	.479	-.171	-.092	.532	-.124	-.046
H3	.064	.297	.127	.326	-.088	-.027	.361	-.032	-.004
H7	-.108	-.263	.131	-.104	.062	.002	-.160	.030	.030

	1099.88 A			1179.69 A			1237.54 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.015	-.014	.050	.004	.000	-.012	.017	-.023	-.074
C1	.004	.012	-.046	-.003	.003	.022	-.108	.059	.163
O1	-.036	.026	-.003	.014	-.012	.000	.015	-.012	-.013
O2	.116	-.073	.055	-.031	.051	-.039	.038	-.032	-.030
C3	-.143	.025	-.062	-.018	-.065	.109	-.020	.014	-.045
H1	-.037	-.022	.030	-.003	.012	-.033	.026	.140	-.272
C4	.034	.004	-.025	.010	.005	-.115	.017	-.007	.003
H4	-.047	-.009	.050	.003	.003	-.008	.006	.010	-.004
H5	-.056	.249	.043	.052	.250	.182	.250	-.055	.390
H6	.077	-.090	-.192	.271	-.166	.112	-.049	.018	-.054
C5	.010	.021	.030	.005	.015	.065	.005	.001	-.001
H2	-.217	-.029	-.044	-.058	-.232	-.260	.004	.061	.047
H3	-.091	-.063	-.034	-.059	-.241	-.098	.003	.010	.003
H7	.044	.156	-.056	.081	.253	-.096	-.022	.005	.005

	1295.55 A			1343.83 A			1436.84 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.003	-.004	-.014	.017	.000	.014	-.002	-.005	-.006
C1	-.038	.026	.055	.018	-.012	-.029	-.038	.017	.059
O1	.007	-.008	-.002	-.004	.004	.001	.004	-.002	-.006
O2	.056	.002	-.038	-.016	.002	.018	.037	-.033	-.029
C3	-.042	-.004	-.016	.006	-.001	-.019	.038	.026	.119
H1	.004	.049	-.078	-.011	-.018	.018	.014	.081	-.100
C4	-.012	.019	.018	-.004	.070	-.076	-.011	-.001	-.042
H4	.007	-.001	-.016	-.040	-.002	-.020	.036	-.024	-.069
H5	-.304	.075	-.444	.102	.006	.136	-.303	.020	-.430
H6	.414	-.071	.494	-.104	.031	-.091	-.257	-.006	-.527
C5	-.007	-.039	.003	-.019	-.085	.072	.004	.006	.016
H2	.121	.188	.119	.316	.567	.209	.006	.036	-.026
H3	-.030	-.066	-.011	-.127	-.368	-.100	-.041	-.069	-.032
H7	-.043	-.068	.027	-.021	.016	.002	.022	.009	.007

	1483.03 A			1492.30 A			1581.93 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.000	-.012	.048	.026	.017	-.092	.001	.001	-.003
C1	.007	-.010	-.007	-.021	.020	.025	.006	.000	-.012
O1	-.007	.008	-.006	.012	-.011	.006	.002	-.002	.003
O2	-.003	.005	.007	.010	-.007	-.007	-.012	.009	.001
C3	-.006	-.028	-.020	.001	-.013	.001	-.032	.068	.025
H1	.067	.219	-.189	-.125	-.416	.333	-.010	-.031	.032
C4	.019	.118	.052	.013	.055	.021	-.004	-.009	-.007
H4	.099	-.112	-.262	-.235	.214	.481	-.021	.017	.039
H5	.025	-.044	.025	-.017	.034	-.039	-.037	-.662	.087
H6	.035	-.060	-.067	-.040	-.012	-.065	.548	-.240	-.311
C5	.001	.002	-.021	.002	.008	-.009	.002	.005	.003
H2	-.047	-.269	-.181	-.021	-.115	-.081	.009	.040	.019
H3	-.121	-.327	-.214	-.074	-.198	-.131	-.005	-.011	-.006
H7	-.145	-.430	.253	-.076	-.243	.148	.004	.008	.002

	1641.48 A			1957.63 A			3113.09 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.026	-.001	-.004	-.005	.013	-.025	.000	-.001	.000
C1	-.008	.000	.011	.130	-.131	.139	.002	-.001	-.001
O1	.000	.002	-.003	-.091	.085	-.076	.000	.000	.000
O2	.004	.000	-.001	.003	.001	-.012	-.002	.000	-.001
C3	.001	-.025	-.004	-.010	.006	-.001	-.002	.069	.005
H1	-.013	-.025	-.004	.005	-.049	.034	.000	-.002	.001
C4	.019	.158	.035	-.001	-.003	.000	.000	-.003	.001
H4	-.045	.014	.010	-.001	.025	-.002	.000	.008	-.001
H5	-.012	-.030	-.028	-.012	.001	.006	.341	-.011	-.208
H6	.006	-.055	-.109	.016	.001	.008	-.312	-.801	.182
C5	-.051	-.153	-.008	.001	.002	.001	.000	.000	.000
H2	.017	-.167	-.174	.002	.006	.005	.000	.023	-.031
H3	.108	.265	.267	.000	-.003	-.003	-.001	.000	.000
H7	.029	.224	-.256	.000	.001	.001	.000	.001	.001

	3187.88 A			3218.37 A			3229.42 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.000	-.001	.001	.025	.030	-.049	-.002	-.001	.000
C1	-.001	.001	-.001	.001	-.001	.004	.000	.000	.000
O1	.000	.000	.000	.000	.000	.000	.000	.000	.000
O2	.000	.000	.000	.000	.000	.000	.000	.000	.000
C3	.073	.024	-.045	.001	.001	-.001	.003	.002	-.002
H1	.004	-.008	-.005	-.205	.405	.329	.001	.000	.000
C4	.000	-.003	.005	.001	-.004	.006	.000	.007	-.020
H4	.001	.020	-.005	-.108	-.753	.209	.003	.013	-.003
H5	-.733	.059	.460	-.012	.000	.008	-.031	.004	.021
H6	-.124	-.345	.068	-.003	-.009	.002	-.010	-.025	.006
C5	-.001	-.001	.000	.000	.002	-.001	.018	.057	-.007
H2	.002	.035	-.060	.000	.043	-.072	-.002	-.135	.231
H3	.002	.008	-.017	-.003	-.016	.027	-.061	-.349	.605
H7	.004	.010	.020	-.004	-.009	-.016	-.134	-.290	-.524

	3236.88 A			3330.68 A			3335.59 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.004	-.002	.004	.000	.002	.000	.018	-.088	-.027
C1	.000	.000	.000	.000	.000	.000	.001	-.001	.001
O1	.000	.000	.000	.000	.000	.000	-.001	.000	.000
O2	.000	.000	.000	.000	.000	.000	.000	.000	.000
C3	-.005	-.005	.001	.000	.001	.000	-.001	.000	.000
H1	.023	-.042	-.034	.004	-.009	-.007	-.299	.543	.463
C4	.000	-.043	.067	.000	.004	-.006	.001	.000	.001
H4	.011	.067	-.018	-.002	-.010	.003	.084	.510	-.149
H5	.035	-.003	-.021	.000	.001	.001	.002	.001	-.001
H6	.019	.054	-.007	-.001	-.002	.000	.001	.006	-.001
C5	.006	.020	-.010	-.009	-.005	-.094	.000	-.001	-.002
H2	-.003	.463	-.777	.000	-.043	.069	-.001	.004	-.007
H3	-.022	-.128	.220	-.056	-.308	.508	-.001	-.004	.006
H7	-.025	-.054	-.096	.161	.355	.609	.004	.008	.013

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 1 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	-581.207	0.0000	0.0000	0.0000	0.0000		2.24
					-23842383847515.29		
2	97.404	0.5826	1.9418	14.6673	8.1630	37.50	1.55
3	196.547	1.1756	1.4864	9.0590	7.7182	61.27	3.28
4	240.430	1.4381	1.3129	7.5298	7.4413	68.66	0.44
5	365.521	2.1863	0.9043	4.5962	6.4567	82.86	0.18
6	465.631	2.7851	0.6585	3.1375	5.5492	89.43	6.13
7	524.990	3.1401	0.5415	2.5041	4.9985	92.06	11.02
8	530.206	3.1713	0.5322	2.4549	4.9503	92.26	2.62
9	568.014	3.3975	0.4685	2.1257	4.6042	93.55	2.35
10	635.386	3.8005	0.3715	1.6428	4.0073	95.34	5.78
11	718.831	4.2996	0.2765	1.1905	3.3204	96.88	6.66
12	799.908	4.7845	0.2059	0.8677	2.7233	97.89	9.64
13	859.896	5.1433	0.1648	0.6850	2.3308	98.42	11.91
14	956.120	5.7189	0.1145	0.4669	1.7898	99.01	13.49
15	967.761	5.7885	0.1095	0.4456	1.7316	99.06	34.61
16	1001.783	5.9920	0.0961	0.3886	1.5701	99.20	2.71
17	1049.125	6.2752	0.0799	0.3208	1.3658	99.37	34.08
18	1063.484	6.3610	0.0756	0.3027	1.3084	99.41	0.84
19	1099.880	6.5787	0.0655	0.2610	1.1718	99.50	94.15
20	1179.688	7.0561	0.0477	0.1881	0.9142	99.66	9.89
21	1237.541	7.4021	0.0378	0.1481	0.7598	99.75	117.26
22	1295.545	7.7491	0.0299	0.1164	0.6286	99.81	51.89
23	1343.833	8.0379	0.0246	0.0951	0.5353	99.85	7.47
24	1436.837	8.5942	0.0168	0.0643	0.3902	99.90	20.04
25	1483.032	8.8705	0.0138	0.0529	0.3325	99.92	10.63
26	1492.298	8.9259	0.0133	0.0509	0.3219	99.93	18.35
27	1581.926	9.4620	0.0092	0.0347	0.2346	99.95	1.52
28	1641.477	9.8182	0.0071	0.0269	0.1895	99.96	3.54
29	1957.632	11.7092	0.0018	0.0069	0.0586	99.99	723.20
30	3113.090	18.6204	0.0000	0.0000	0.0006	100.00	36.57
31	3187.875	19.0677	0.0000	0.0000	0.0004	100.00	10.20
32	3218.372	19.2501	0.0000	0.0000	0.0004	100.00	0.39
33	3229.419	19.3162	0.0000	0.0000	0.0003	100.00	2.07
34	3236.883	19.3609	0.0000	0.0000	0.0003	100.00	4.59
35	3330.679	19.9219	0.0000	0.0000	0.0002	100.00	4.10
36	3335.585	19.9512	0.0000	0.0000	0.0002	100.00	0.28
Total Vibrations		295.7325	9.6082	53.4305	75.5682		
Ideal Gas			2.4789				
Translation			3.7184	166.0599	12.4716		
Rotation			3.7184	113.7965	12.4716		
Totals			315.2565	333.2870	100.5115		
Gibb's Free Energy (H - TS)			215.8869				

Reason for exit: Successful completion
Properties Program CPU Time : 0:00:00.1

```
  Properties Program Wall Time:   0:00:00.2

molecule E-ax2-ts-mp2tsgeom terminated normally

End-   molecule "E-ax2-ts-mp2tsgeom" Mon Mar 28 06:36:44 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:25.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:19.2
  Quantum Mechanics Program Wall Time:   0:01:26.9

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1486394 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2136383 hartrees

  Program Wall Time:    0:07:51.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:06:38.2
  Quantum Mechanics Program Wall Time:   0:07:53.4

 SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.1
  Properties Program Wall Time:   0:00:00.2

molecule E-ax2-ts-mp2tsgeom terminated normally

End-   molecule "E-ax2-ts-mp2tsgeom" Mon Mar 28 00:28:54 2005
```

6-ENDO TRANSITION-STATE

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Transition state search.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:
         Step      Energy          Max Grad.      Max Dist.
            1    -343.9979880       0.019164       0.063120   1
            2    -343.9990557       0.008563       0.427652   2
            3    -343.9892813       0.082725       0.150924   1
            4    -343.9973297       0.017396       0.293796   1
            5    -343.9981482       0.039736       0.119471   1
            6    -343.9985002       0.013181       0.054810   1
            7    -343.9991849       0.004015       0.010800   2
            8    -343.9992206       0.003521       0.041494   1
            9    -343.9993693       0.001594       0.020177   1
           10    -343.9993847       0.000947       0.011683   1
           11    -343.9993849       0.000509       0.002632   1
           12    -343.9993832       0.000317       0.005965   1
           13    -343.9993797       0.000138       0.000284   1

  Program Wall Time:    0:59:38.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:46:41.3
  Quantum Mechanics Program Wall Time:   0:59:38.3

 SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.7
  Properties Program Wall Time:   0:00:00.8

molecule 5x-6n tstates.3 terminated normally

End-   molecule "5x-6n tstates.3" Tue Mar 22 17:22:19 2005

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53
```

```
Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------ ------------ ------------

  1 C  C2          -1.1291065      .8341840      .3853172
  2 C  C1          -1.2978446      .1128468     -.8966683
  3 O  O1          -2.0498574      .4629063    -1.7796853
  4 O  O2           -.4793708     -.9668835    -1.1338611
  5 C  C3            .4411365    -1.4293756     -.1315063
  6 H  H1          -1.1862656      .2757189     1.3132205
  7 H  H3          -1.5844978     1.8189706      .3929631
  8 H  H2           -.1110807    -1.9826805      .6412369
  9 C  C4           1.2204338     -.3257681      .5179184
 10 H  H6           1.0733788    -2.1514832     -.6576397
 11 H  H4           1.6648249     -.5483151     1.4843891
 12 C  C5           1.0859293      .9472679      .1041999
 13 H  H7            .8316998     1.1943353     -.9199758
 14 H  H8           1.5205904     1.7582762      .6800911

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.6
  Properties Program Wall Time:   0:00:00.7

molecule 5x-6n tstates.3 terminated normally

End-   molecule "5x-6n tstates.3" Mon Apr 11 16:07:21 2005

<step 2>
Job type: Frequency calculation.
Method: UMP2(FC)
Basis set: 6-31G(D)

Correlation model:
 A MP2 calculation will be performed

  Program Wall Time:    4:27:14.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   4:04:39.1
  Quantum Mechanics Program Wall Time:   4:27:13.9

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X-6N TSTATES.3
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.2
```

SPARTAN PROPERTIES PACKAGE: MAC/G5 build 123

Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 2
Electrons: 53

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C2	-1.1291065	.8341840	.3853172
2	C	C1	-1.2978446	.1128468	-.8966683
3	O	O1	-2.0498574	.4629063	-1.7796853
4	O	O2	-.4793708	-.9668835	-1.1338611
5	C	C3	.4411365	-1.4293756	-.1315063
6	H	H1	-1.1862656	.2757189	1.3132205
7	H	H3	-1.5844978	1.8189706	.3929631
8	H	H2	-.1110807	-1.9826805	.6412369
9	C	C4	1.2204338	-.3257681	.5179184
10	H	H6	1.0733788	-2.1514832	-.6576397
11	H	H4	1.6648249	-.5483151	1.4843891
12	C	C5	1.0859293	.9472679	.1041999
13	H	H7	.8316998	1.1943353	-.9199758
14	H	H8	1.5205904	1.7582762	.6800911

Point Group = C1 Order = 1 Nsymop = 1
Post HF density not available. Select the density checkbox to generate a density or use the "NOPOSTHFDEN" keyword to use the HF density.

Molecule is non-linear

Normal Modes and Vibrational Frequencies (cm-1)

	-672.73 A			113.07 A			208.66 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.174	-.035	.021	.039	.081	-.061	.009	-.066	.025
C1	-.014	-.004	-.001	-.009	.008	-.021	.009	-.007	-.012
O1	.002	.001	-.008	-.122	-.093	.036	-.021	-.008	.016
O2	.000	.007	.002	.050	.061	-.050	.096	.066	-.066
C3	.000	.018	.002	.001	.007	-.027	-.100	.023	.084
H1	-.026	-.007	.037	-.022	.133	-.033	.044	-.116	-.002
H3	-.058	.011	.010	.071	.097	-.123	-.044	-.092	.090
H2	.006	.020	.007	-.046	-.024	-.084	-.283	.268	.133
C4	-.019	.042	.001	-.014	-.035	.061	.033	-.007	-.027
H6	.018	.025	.014	.016	.025	-.033	-.198	-.198	.272
H4	.022	.003	-.023	-.088	-.073	.086	.109	.001	-.060
C5	.201	-.036	-.023	.069	-.027	.069	-.017	-.007	-.032
H7	-.118	.026	.074	.133	-.010	.058	-.060	-.025	-.024
H8	.204	-.035	-.031	.063	-.049	.105	.030	.000	-.075

	288.72 A			364.71 A			450.72 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.011	-.018	.027	-.106	.092	.022	.030	-.065	.000
C1	.021	-.001	.023	-.009	.028	.041	-.065	.064	-.048
O1	.010	.025	.045	.031	-.027	-.013	-.058	-.008	-.092
O2	.053	.028	-.029	.061	.080	.040	-.034	.059	.068
C3	.018	-.015	-.007	.040	-.043	-.011	.037	.034	.024
H1	.084	-.025	.026	-.159	.165	.063	.091	-.269	-.118
H3	-.047	-.045	.052	-.056	.116	-.090	.040	-.063	.271
H2	.009	-.136	-.103	.036	-.062	-.026	.080	-.030	.007
C4	-.112	.020	.089	.055	-.063	-.025	.083	-.019	.068
H6	.112	.093	-.044	-.004	-.040	-.070	.005	.078	-.075
H4	-.310	.141	.206	.186	-.051	-.083	.055	.000	.085
C5	-.010	-.044	-.130	-.084	-.079	-.035	.012	-.047	-.012
H7	.077	-.221	-.194	-.156	-.143	-.030	.045	-.195	-.055
H8	-.075	.050	-.217	-.070	-.032	-.113	-.029	.042	-.107

	523.21 A			618.30 A			674.32 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.042	.026	.084	-.038	.058	-.051	.044	.005	-.014
C1	.017	.047	.045	.063	.048	-.040	.039	.021	-.027
O1	.064	-.128	-.056	-.033	.020	.033	-.014	-.001	.008
O2	-.017	.059	.030	.008	-.022	.027	.008	-.016	-.009
C3	-.063	-.003	-.047	.020	-.048	.017	-.019	.007	.027
H1	.168	-.081	.029	.325	-.102	-.126	.009	-.068	-.060
H3	-.079	-.029	.240	-.683	-.236	.118	-.056	-.040	.035
H2	-.038	-.042	-.053	.021	-.016	.042	.017	-.207	-.101
C4	-.081	-.003	-.056	.011	-.022	-.022	-.086	.016	.050
H6	-.050	.024	-.071	-.008	-.076	.019	.171	.201	-.017
H4	-.102	-.015	-.049	-.032	.004	.006	.519	-.119	-.263
C5	.020	.030	-.008	.000	.003	.006	-.028	-.004	.011
H7	.053	.147	.012	.114	.046	-.012	-.316	-.017	.084
H8	.079	-.061	.077	-.022	-.035	.075	.355	-.038	-.228

	688.66 A			729.13 A			818.34 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.018	.032	.004	-.025	.026	.049	-.013	.087	.117
C1	-.094	-.098	.057	.124	.068	-.016	-.047	.052	-.024
O1	.055	.001	-.022	.018	-.059	.035	-.038	.005	-.056
O2	-.032	.003	-.055	-.075	-.051	-.056	.021	-.087	-.092
C3	-.026	.075	-.033	-.021	.081	-.048	.053	-.071	.028
H1	.407	.219	.134	-.307	-.102	-.037	.193	.052	.107
H3	-.290	-.105	-.080	-.093	-.004	.031	.124	.151	.287
H2	-.043	.065	-.054	-.055	.164	-.014	-.001	.013	.050
C4	.049	-.004	.060	.058	.004	.045	.005	.017	.017
H6	-.021	.074	-.024	-.058	.003	.019	.084	-.125	.138
H4	.110	-.110	.008	-.022	-.071	.065	.027	.064	.020
C5	.007	-.012	.027	-.008	-.022	.010	-.003	.010	.008
H7	.008	-.191	-.016	-.016	-.242	-.042	-.055	-.004	.019
H8	.021	.079	-.113	-.078	.127	-.152	-.017	.027	-.006

	864.36 A			956.27 A			1016.37 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.061	.035	.057	-.025	-.029	-.021	-.009	-.027	.065
C1	-.080	-.034	.025	.032	.008	.002	.059	-.002	-.054
O1	-.002	.017	-.034	.011	-.017	.013	-.022	-.006	-.018
O2	.011	.001	-.022	-.037	.043	-.026	-.034	.014	-.033
C3	.001	-.041	.021	-.069	-.155	.004	-.023	.043	.088
H1	-.634	-.106	-.043	.086	.039	.020	.083	.223	.219
H3	-.385	-.154	-.066	.071	.012	-.063	-.046	-.039	-.179
H2	.009	-.091	-.011	-.107	-.284	-.118	.039	-.215	-.063
C4	.022	-.005	.004	.077	.044	.056	.073	-.026	-.019
H6	.023	.001	-.014	-.125	-.059	-.193	.080	.276	-.101
H4	-.010	.046	.031	.133	.158	.064	-.161	.228	.147
C5	.035	.046	-.014	.022	.092	.011	-.044	-.036	-.024
H7	.184	.027	-.060	-.010	-.030	-.013	.001	.232	.032
H8	.217	-.018	-.057	-.080	.236	-.105	.229	-.256	.082

	1040.72 A			1057.85 A			1060.32 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.053	-.014	.006	-.072	.016	-.026	-.016	.055	-.090
C1	.008	-.003	-.022	-.018	.003	.030	-.042	-.025	.060
O1	-.014	.011	.000	.024	-.007	.026	.051	-.012	.041
O2	.039	-.020	.041	.010	-.024	-.034	-.016	.003	-.047
C3	-.019	-.003	-.032	-.049	.038	.045	.001	.003	.016
H1	.097	.040	.044	.003	-.129	-.109	.003	-.301	-.306
H3	.120	.061	.032	.138	.105	.183	.086	.093	.298
H2	.011	.004	.000	.018	-.177	-.061	-.017	-.032	-.025
C4	.012	-.012	-.048	.014	-.016	.004	.054	.001	-.005
H6	-.002	-.019	.005	.132	.222	.006	.017	.036	-.004
H4	-.253	-.152	.044	.284	-.078	-.135	-.227	.220	.177
C5	-.048	.068	.068	-.012	.011	-.032	-.030	-.023	.010
H7	.270	-.270	-.100	.611	.022	-.195	-.279	.121	.113
H8	.546	.053	-.352	-.103	-.092	.187	.266	-.133	-.056

	1088.72 A			1174.33 A			1244.64 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.017	-.039	-.017	.008	-.034	-.031	-.006	.064	.036
C1	.009	.020	.022	-.011	.054	.045	.067	-.163	-.080
O1	.015	-.017	.005	.022	-.024	.007	-.007	.017	.004
O2	-.077	.047	-.030	-.061	.055	-.077	-.039	.057	-.010
C3	.116	-.033	-.019	.061	-.029	.119	.048	.004	.062
H1	.038	.045	.033	.018	.011	-.009	-.043	-.052	-.021
H3	.025	-.023	-.096	-.018	-.049	-.132	.048	.091	.303
H2	-.073	.264	.056	.201	-.067	.190	.080	.012	.085
C4	-.037	.019	.066	-.037	-.016	-.087	-.036	-.001	-.010
H6	-.114	-.301	.078	.196	.091	.118	-.275	-.026	-.270
H4	.208	.136	-.021	-.144	-.191	-.079	-.001	-.161	-.066
C5	-.045	-.006	-.021	.019	.009	.046	.006	.009	.000
H7	.270	.113	-.073	-.016	-.248	-.005	.025	-.050	-.018
H8	.325	-.245	.042	-.082	.148	-.080	-.039	.042	-.015

	1297.27 A			1332.57 A			1442.86 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.008	-.011	-.006	.016	.015	.010	.001	.010	.001
C1	-.021	.048	.018	.014	-.042	-.020	.029	-.056	-.034
O1	.004	-.006	.004	-.004	.007	-.003	-.004	.006	.003
O2	.046	-.033	-.030	-.014	.015	.019	-.022	.051	.005
C3	-.048	.014	-.005	.000	-.002	-.012	-.082	-.063	-.081
H1	.014	.002	-.003	-.023	-.009	-.001	-.041	.066	.039
H3	-.013	-.020	-.072	-.014	.002	.046	-.001	.010	.141
H2	.494	.011	.400	-.190	.016	-.149	.369	.155	.402
C4	-.026	.028	.002	-.031	.034	-.083	.027	.019	.034
H6	-.389	-.003	-.381	.143	.040	.106	.423	.092	.314
H4	.104	.269	-.005	.160	.633	-.044	.029	.011	.037
C5	-.004	-.032	.028	.015	-.054	.083	-.010	-.017	-.009
H7	.035	-.135	-.003	.095	-.420	-.016	.025	.071	.003
H8	.049	-.069	.031	-.052	-.019	.061	.011	-.030	-.003

	1488.75 A			1502.23 A			1557.35 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	-.009	-.023	-.037	.019	-.047	-.082	.001	-.002	-.004
C1	-.005	.011	-.001	-.009	.035	.004	.006	-.011	-.010
O1	.006	-.003	.008	.010	-.007	.012	.001	.000	.003
O2	-.001	-.005	-.005	.006	-.012	.000	-.011	.015	-.003
C3	.020	.037	.004	.001	-.014	.009	-.007	.071	-.017
H1	-.088	.229	.115	-.225	.503	.246	-.021	.048	.025
H3	-.020	-.027	.260	-.077	-.089	.545	-.005	-.004	.059
H2	.039	.045	.021	-.090	.008	-.045	.345	-.550	-.174
C4	-.035	-.129	-.003	.014	.054	-.004	.002	.002	.001
H6	-.014	.005	.010	-.026	.031	-.085	-.190	-.463	.450
H4	.102	.306	.033	-.050	-.128	-.016	.001	.023	.003
C5	.018	.004	.023	-.003	.000	-.009	.002	.007	-.003
H7	.122	.382	.072	-.079	-.184	-.027	-.030	-.054	-.007
H8	-.080	.375	-.396	.038	-.167	.181	.003	-.030	.044

	1668.34 A			2018.70 A			3079.46 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.019	.002	-.001	.008	.004	.029	.000	.000	.000
C1	-.004	.003	.008	-.124	.040	-.189	.001	-.002	.000
O1	-.001	.000	-.004	.089	-.039	.110	.000	.000	.000
O2	.003	.000	.000	-.004	.010	.012	-.002	.001	-.001
C3	-.006	-.021	.007	.006	-.006	.002	.024	.054	-.039
H1	-.020	.005	-.001	.004	-.012	.027	-.001	.002	.000
H3	-.026	-.018	.003	-.010	.012	-.063	.001	-.002	.002
H2	-.042	-.094	-.067	-.015	.001	-.003	-.474	-.442	.637
C4	.015	.160	-.030	-.001	.004	-.001	.001	-.001	.002
H6	-.051	-.048	-.011	.010	-.007	-.003	.197	-.197	-.168
H4	-.077	-.166	-.077	-.001	-.008	-.003	-.012	.011	-.021
C5	-.024	-.154	.051	.000	-.002	-.001	.000	.000	.000
H7	.255	.311	.096	.003	.005	.005	.000	-.001	.002
H8	-.067	.110	-.306	-.006	.001	-.001	-.001	-.002	-.001

	3155.06 A			3218.86 A			3227.85 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.000	.000	.000	.022	-.024	-.053	.001	.000	-.001
C1	.001	-.001	.001	.002	.002	.004	.000	.000	-.001
O1	.000	.000	.000	-.001	.000	-.001	.000	.000	.000
O2	.000	.000	-.001	.000	.000	.000	.000	.000	.000
C3	-.057	.037	.055	.000	.000	.000	.000	.000	.001
H1	.000	-.003	.002	-.014	-.364	.595	.000	-.004	.006
H3	.000	.001	.000	-.270	.621	-.005	-.005	.007	.000
H2	.152	.162	-.205	-.001	-.002	.002	.002	.001	-.003
C4	.000	.000	-.001	.000	.000	.000	.006	.002	.011
H6	.516	-.590	-.443	-.001	.001	.002	.003	-.006	-.003
H4	.005	.000	.011	-.002	.001	-.005	-.073	.035	-.153
C5	.000	.000	.000	.001	.001	.000	-.010	-.059	.023
H7	.001	.000	.005	-.001	-.002	.009	-.168	.137	-.626
H8	-.002	-.003	-.002	-.002	-.007	-.005	.274	.506	.375

	3247.49 A			3318.62 A			3327.35 A		
	X	Y	Z	X	Y	Z	X	Y	Z
C2	.002	.000	-.001	.000	.001	.000	.021	-.080	.046
C1	.000	.000	.000	.000	.000	.001	.001	-.001	.001
O1	.000	.000	.000	.000	.000	.000	-.001	.000	.000
O2	.000	.000	.000	.000	.000	.000	.000	.000	.000
C3	.002	.002	-.001	.000	.001	.000	.000	.000	.000
H1	-.002	-.004	.006	-.001	-.004	.006	.024	.334	-.563
H3	-.002	.002	.000	.002	-.005	.000	-.280	.615	.010
H2	-.015	-.016	.016	-.001	-.001	.002	-.001	.001	.000
C4	-.034	.019	-.071	-.004	.003	-.008	.000	.000	.000
H6	-.003	.000	-.001	.000	.001	.000	.001	-.001	-.001
H4	.384	-.188	.828	.043	-.023	.091	.001	-.001	.003
C5	.001	-.011	.014	-.035	-.030	-.082	.000	.000	-.001
H7	-.045	.041	-.183	.164	-.153	.622	.003	-.002	.004
H8	.018	.036	.027	.262	.496	.351	.003	.004	.003

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 1 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	-672.728	0.0000	0.0000	0.0000	0.0000		4.37
					-23842383847515.29		
2	113.070	0.6763	1.8638	13.4536	8.1112	42.05	0.94
3	208.656	1.2480	1.4369	8.5997	7.6462	63.47	4.06
4	288.722	1.7269	1.1406	6.1983	7.0905	75.17	0.33
5	364.712	2.1815	0.9066	4.6105	6.4638	82.80	4.36
6	450.719	2.6959	0.6910	3.3204	5.6873	88.64	2.12
7	523.206	3.1295	0.5448	2.5211	5.0149	91.99	3.96
8	618.303	3.6983	0.3942	1.7540	4.1556	94.94	3.82
9	674.321	4.0333	0.3240	1.4142	3.6785	96.14	29.06
10	688.657	4.1191	0.3080	1.3380	3.5609	96.40	6.87
11	729.132	4.3612	0.2664	1.1438	3.2404	97.04	10.18
12	818.340	4.8948	0.1924	0.8070	2.5982	98.07	24.51
13	864.358	5.1700	0.1621	0.6730	2.3033	98.46	11.41
14	956.267	5.7197	0.1144	0.4666	1.7891	99.01	1.73
15	1016.375	6.0793	0.0908	0.3663	1.5046	99.26	1.11
16	1040.719	6.2249	0.0826	0.3320	1.4004	99.34	8.49
17	1057.852	6.3274	0.0772	0.3097	1.3307	99.39	10.22
18	1060.320	6.3421	0.0765	0.3066	1.3209	99.40	23.66
19	1088.722	6.5120	0.0684	0.2731	1.2123	99.48	70.45
20	1174.329	7.0240	0.0488	0.1923	0.9298	99.65	34.84
21	1244.645	7.4446	0.0368	0.1438	0.7425	99.75	100.93
22	1297.274	7.7594	0.0297	0.1155	0.6250	99.81	25.88
23	1332.575	7.9706	0.0257	0.0997	0.5558	99.84	14.43
24	1442.855	8.6302	0.0164	0.0627	0.3822	99.91	23.39
25	1488.752	8.9047	0.0135	0.0516	0.3260	99.92	12.57
26	1502.235	8.9854	0.0128	0.0488	0.3110	99.93	12.29
27	1557.349	9.3150	0.0102	0.0386	0.2561	99.95	5.20
28	1668.343	9.9789	0.0064	0.0240	0.1719	99.97	1.35
29	2018.697	12.0745	0.0014	0.0053	0.0464	99.99	1218.07
30	3079.460	18.4193	0.0000	0.0000	0.0006	100.00	31.52
31	3155.061	18.8715	0.0000	0.0000	0.0005	100.00	11.25
32	3218.863	19.2531	0.0000	0.0000	0.0004	100.00	0.72
33	3227.848	19.3068	0.0000	0.0000	0.0003	100.00	1.62
34	3247.491	19.4243	0.0000	0.0000	0.0003	100.00	5.24
35	3318.616	19.8497	0.0000	0.0000	0.0002	100.00	1.43
36	3327.348	19.9020	0.0000	0.0000	0.0002	100.00	1.21
Total Vibrations		298.2540	8.9425	48.6705	72.4579		
Ideal Gas			2.4789				
Translation			3.7184	166.0599	12.4716		
Rotation			3.7184	113.4231	12.4716		
Totals			317.1123	328.1535	97.4011		
Gibb's Free Energy (H - TS)			219.2733				

Reason for exit: Successful completion
Properties Program CPU Time : 0:00:00.1

```
  Properties Program Wall Time:   0:00:00.2

molecule 5x-6n tstates.3 terminated normally

End-   molecule "5x-6n tstates.3" Sat Apr  2 06:36:09 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1334076 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2072506 hartrees

  Program Wall Time:    0:12:21.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:09:09.4
  Quantum Mechanics Program Wall Time:   0:12:22.6

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X-6N TSTATES.3
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.3

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
Task "SPARTAN Properties" returned [1]

End-   molecule "5x-6n tstates.3" Wed Mar 23 20:14:43 2005
```

5-EXO EDUCT RADICAL 2 (EQUATORIAL CH2•)

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Geometry optimization.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:
         Step      Energy          Max Grad.      Max Dist.
            1    -344.0706578       0.046764       0.082969
            2    -344.0743758       0.004218       0.083300
            3    -344.0745227       0.000990       0.075180
            4    -344.0745341       0.001290       0.062491
            5    -344.0745357       0.001483       0.023488
            6    -344.0745413       0.000267       0.019524
            7    -344.0745422       0.000166       0.007783

  Program Wall Time:    0:23:22.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:19:36.7
  Quantum Mechanics Program Wall Time:   0:23:22.6

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.1
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.3

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53
```

```
                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------ ------------ ------------

  1 C  C2           1.0934702     -.3188282     -.1472027
  2 C  C1           1.1348175     -.5618421     1.3517921
  3 O  O1           2.0722344     -.8964097     2.0404916
  4 O  O2           -.1173224     -.3420724     1.8707179
  5 C  C3          -1.0317802     -.0057633      .8056713
  6 H  H1           2.0247578      .1338627     -.4918938
  7 C  C4           -.1597267      .5495031     -.3302081
  8 H  H4            .9767848    -1.2857496     -.6532086
  9 H  H5          -1.7515095      .7129416     1.2008222
 10 H  H6          -1.5615865     -.9133356      .4908765
 11 H  H3            .0994915     1.5862328     -.0863411
 12 C  C5           -.8049485      .4829122    -1.6671341
 13 H  H2           -.7847394     1.3208252    -2.3509163
 14 H  H7          -1.1899430     -.4622766    -2.0334667

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.8
  Properties Program Wall Time:   0:00:00.8

molecule 5x6n local mins.631.1 terminated normally

End-   molecule "5x6n local mins.631.1" Tue Mar 22 13:05:04 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:26.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:20.6
  Quantum Mechanics Program Wall Time:   0:01:27.5

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1957459 hartrees

Correlation model:
 A MP2 calculation will be performed
```

```
 MP2 total energy:    -344.2811052 hartrees

  Program Wall Time:    0:06:44.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:05:39.2
  Quantum Mechanics Program Wall Time:   0:06:46.0

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.1
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.4

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 C  C2           1.0934702     -.3188282     -.1472027
  2 C  C1           1.1348175     -.5618421     1.3517921
  3 O  O1           2.0722344     -.8964097     2.0404916
  4 O  O2           -.1173224     -.3420724     1.8707179
  5 C  C3          -1.0317802     -.0057633      .8056713
  6 H  H1           2.0247578      .1338627     -.4918938
  7 C  C4           -.1597267      .5495031     -.3302081
  8 H  H4            .9767848    -1.2857496     -.6532086
  9 H  H5          -1.7515095      .7129416     1.2008222
 10 H  H6          -1.5615865     -.9133356      .4908765
 11 H  H3            .0994915     1.5862328     -.0863411
 12 C  C5           -.8049485      .4829122    -1.6671341
 13 H  H2           -.7847394     1.3208252    -2.3509163
 14 H  H7          -1.1899430     -.4622766    -2.0334667

  Point Group = C1  Order =  1 Nsymop =  1
Task "SPARTAN Properties" returned [1]

End-   molecule "5x6n local mins.631.1" Sun Mar 27 20:09:56 2005
```

5-EXO EDUCT RADICAL 2 (AXIAL CH2•)

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Geometry optimization.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:
         Step      Energy          Max Grad.      Max Dist.
            1    -344.0694936       0.046743       0.063310
            2    -344.0731655       0.005098       0.120186
            3    -344.0734877       0.001754       0.065424
            4    -344.0735303       0.001345       0.014096
            5    -344.0735351       0.000178       0.004390
            6    -344.0735354       0.000067       0.000889

  Program Wall Time:    0:20:12.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:16:59.8
  Quantum Mechanics Program Wall Time:   0:20:12.8

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.2
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53
```

```
                Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------ ------------ ------------

  1 C  C2            .8625399     -.6441390     -.5136249
  2 C  C1            .9281903     -.9149894      .9799581
  3 O  O1           1.8715289    -1.2802668     1.6446514
  4 O  O2           -.3106676     -.6830490     1.5257563
  5 C  C3          -1.2396100     -.3224088      .4784870
  6 H  H1           1.7979667     -.2054309     -.8647461
  7 C  C4           -.3743458      .2616777     -.6457719
  8 H  H4            .7143702    -1.6011203    -1.0305396
  9 H  H5          -1.9493417      .3889771      .9038505
 10 H  H6          -1.7746011    -1.2230894      .1547399
 11 C  C5           -.0492049     1.6981182     -.4030247
 12 H  H2           -.8615424      .1397290    -1.6190288
 13 H  H3            .1182665     2.0501882      .6085249
 14 H  H7            .2664512     2.3358035    -1.2192321

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.8
  Properties Program Wall Time:   0:00:00.9

molecule 5x6n local mins.631.2 terminated normally

End-   molecule "5x6n local mins.631.2" Tue Mar 22 13:25:20 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:29.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:22.5
  Quantum Mechanics Program Wall Time:   0:01:30.5

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1937799 hartrees

Correlation model:
 A MP2 calculation will be performed
```

```
 MP2 total energy:    -344.2799271 hartrees

  Program Wall Time:    0:06:52.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:05:48.8
  Quantum Mechanics Program Wall Time:   0:06:53.8

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.2
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 C  C2            .8625399     -.6441390     -.5136249
  2 C  C1            .9281903     -.9149894      .9799581
  3 O  O1           1.8715289    -1.2802668     1.6446514
  4 O  O2            -.3106676     -.6830490     1.5257563
  5 C  C3           -1.2396100     -.3224088      .4784870
  6 H  H1            1.7979667     -.2054309     -.8647461
  7 C  C4            -.3743458      .2616777     -.6457719
  8 H  H4             .7143702    -1.6011203    -1.0305396
  9 H  H5           -1.9493417      .3889771      .9038505
 10 H  H6           -1.7746011    -1.2230894      .1547399
 11 C  C5            -.0492049     1.6981182     -.4030247
 12 H  H2            -.8615424      .1397290    -1.6190288
 13 H  H3             .1182665     2.0501882      .6085249
 14 H  H7             .2664512     2.3358035    -1.2192321

  Point Group = C1  Order =  1 Nsymop =  1
Task "SPARTAN Properties" returned [1]

End-   molecule "5x6n local mins.631.2" Sun Mar 27 20:18:25 2005
```

6-ENDO EDUCT RADICAL 3

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Geometry optimization.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:
         Step      Energy          Max Grad.      Max Dist.
            1    -344.0695697       0.049692       0.072247
            2    -344.0734006       0.002550       0.117928
            3    -344.0736080       0.002793       0.051884
            4    -344.0736224       0.001617       0.040178
            5    -344.0736443       0.000909       0.026621
            6    -344.0736522       0.000819       0.011292
            7    -344.0736551       0.000275       0.008279
            8    -344.0736563       0.000070       0.011457
            9    -344.0736564       0.000079       0.001314

  Program Wall Time:    0:30:52.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:25:50.3
  Quantum Mechanics Program Wall Time:   0:30:52.5

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.3
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:-0.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53
```

```
                    Cartesian Coordinates (Angstroms)
      Atom            X             Y             Z
    ---------    ------------ ------------ ------------

  1 C  C3           1.0822717     .3999513     -.4847752
  2 C  C1           1.0886864     .4593292     1.0275018
  3 O  O1           2.0866838     .5569189     1.7141289
  4 O  O2           -.1363414     .3708880     1.6273675
  5 C  C2          -1.2973250     .3290547      .7547003
  6 H  H3          -1.4665240    1.3449937      .3648108
  7 H  H4          -2.1313669     .0870445     1.4156768
  8 H  H1           2.1193863     .3149842     -.8130693
  9 H  H5            .6853178    1.3475300     -.8702816
 10 C  C4            .2109071    -.7622699     -.9790986
 11 H  H6            .7019178   -1.7153732     -.7318349
 12 H  H7            .1328372    -.7401881    -2.0742892
 13 C  C5          -1.1281345    -.6737251     -.3300067
 14 H  H9          -1.9483165   -1.3191381     -.6208306

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.7
  Properties Program Wall Time:   0:00:00.9

molecule 5x6n local mins.631.3 terminated normally

End-   molecule "5x6n local mins.631.3" Tue Mar 22 13:56:16 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:29.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:22.6
  Quantum Mechanics Program Wall Time:   0:01:29.6

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1940559 hartrees

Correlation model:
 A MP2 calculation will be performed
```

```
 MP2 total energy:    -344.2787717 hartrees

  Program Wall Time:    0:06:50.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:05:47.6
  Quantum Mechanics Program Wall Time:   0:06:51.5

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.3
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 C  C3           1.0822717      .3999513     -.4847752
  2 C  C1           1.0886864      .4593292     1.0275018
  3 O  O1           2.0866838      .5569189     1.7141289
  4 O  O2           -.1363414      .3708880     1.6273675
  5 C  C2          -1.2973250      .3290547      .7547003
  6 H  H3          -1.4665240     1.3449937      .3648108
  7 H  H4          -2.1313669      .0870445     1.4156768
  8 H  H1           2.1193863      .3149842     -.8130693
  9 H  H5            .6853178     1.3475300     -.8702816
 10 C  C4            .2109071     -.7622699     -.9790986
 11 H  H6            .7019178    -1.7153732     -.7318349
 12 H  H7            .1328372     -.7401881    -2.0742892
 13 C  C5          -1.1281345     -.6737251     -.3300067
 14 H  H9          -1.9483165    -1.3191381     -.6208306

  Point Group = C1  Order =  1 Nsymop =  1
Task "SPARTAN Properties" returned [1]

End-   molecule "5x6n local mins.631.3" Sun Mar 27 20:26:49 2005
```

Z-1 GLOBAL MINIMUM

MacSPARTAN '04 Quantum Mechanics Program: (PowerPC(Darwin)) build 123

Job type: Geometry optimization.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:

Step	Energy	Max Grad.	Max Dist.	
1	-344.0453853	0.001796	0.027437	
2	-344.0453240	0.000783	0.049104	
3	-344.0451750	0.001549	0.048114	
4	-344.0453627	0.008973	0.207685	
5	-344.0443821	0.012629	0.171788	
6	-344.0453776	0.003750	0.154181	
7	-344.0453926	0.003325	0.113499	
8	-344.0454204	0.001246	0.090519	
9	-344.0453966	0.001913	0.063682	
10	-344.0454040	0.001860	0.018122	
11	-344.0453772	0.001884	0.008990	
12	-344.0453153	0.001514	0.008931	
13	-344.0453203	0.010119	0.012914	
14	-344.0454136	0.006254	0.021895	
15	-344.0454727	0.000572	0.018912	
16	-344.0454627	0.000718	0.009686	
17	-344.0454621	0.000464	0.005876	
18	-344.0454516	0.000123	0.001636	
19	-344.0454479	0.000485	0.001132	
20	-344.0454419	0.000693	0.068293	1
21	-344.0357339	0.079406	0.067039	
22	-344.0454492	0.004259	0.008327	
23	-344.0454779	0.001752	0.005460	
24	-344.0454746	0.000158	0.004802	
25	-344.0454716	0.000094	0.002635	
26	-344.0454709	0.000240	0.001371	

  Program Wall Time: 1:27:36.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   1:13:04.3
  Quantum Mechanics Program Wall Time: 1:27:36.5

MacSPARTAN '04 Semi-Empirical Program: (PowerPC(Darwin))   build 123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

```
  XFER
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:          579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:-0.0
  Semi-Empirical Program Wall Time:   0:00:00.2

SPARTAN PROPERTIES PACKAGE: MAC/G5              build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
      Atom            X             Y             Z
    ---------    ------------- ------------- -------------

  1 C  C2            .6726237    -2.5422007     1.4403228
  2 C  C1            .6541167    -1.0749557     1.3662525
  3 O  O1           1.1775981     -.3212035     2.1629088
  4 O  O2           -.0335554     -.6697531      .2736607
  5 C  C3           -.1042293      .7750852      .1237078
  6 H  H1           1.1894037    -3.0046990     2.2685077
  7 H  H3            .1849506    -3.1419901      .6855508
  8 H  H2            .9072589     1.1764611      .0130434
  9 H  H4           -.5351091     1.1945264     1.0384563
 10 C  C4           -.9464599     1.0422521    -1.0768869
 11 C  C5           -.5244640     1.7714314    -2.1168612
 12 H  H6          -1.9530974      .6293089    -1.0642532
 13 H  H5            .4785143     2.1874192    -2.1489086
 14 H  H7          -1.1675510     1.9783178    -2.9655009

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.8
  Properties Program Wall Time:   0:00:01.0

molecule xfer terminated normally

End-   molecule "xfer" Sun Mar 27 18:43:25 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:15.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:07.6
  Quantum Mechanics Program Wall Time:   0:01:16.0
```

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1810598 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2524115 hartrees

  Program Wall Time:    0:06:24.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:05:26.6
  Quantum Mechanics Program Wall Time:   0:06:25.1


MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  XFER
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:          579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1


SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

End-   molecule "xfer" Sun Mar 27 20:52:02 2005
```

Z-1 TO E-1 ROTATIONAL BARRIER (O=C-O-C TORSIONAL ANGLE=90˚)

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:14.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:08.4
  Quantum Mechanics Program Wall Time:   0:01:14.4

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1639492 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2280439 hartrees

  Program Wall Time:    0:06:49.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:05:48.1
  Quantum Mechanics Program Wall Time:   0:06:50.1

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  XFER
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53
```

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C2	1.7758763	-1.5261860	1.1227425
2	C	C1	.3547982	-1.3511757	1.4522012
3	O	O1	-.1449867	-1.5380722	2.5440436
4	O	O2	-.3328737	-.9459732	.3596100
5	C	C3	-.4035474	.4988644	.2096571
6	H	H1	2.4450660	-1.8501945	1.9063616
7	H	H3	2.1418013	-1.3334322	.1246458
8	H	H2	.6079403	.9002401	.0989928
9	H	H4	-.8344270	.9183054	1.1244051
10	C	C4	-1.2457776	.7660312	-.9909370
11	C	C5	-.8237819	1.4952102	-2.0309109
12	H	H6	-2.2524147	.3530882	-.9783034
13	H	H5	.1791959	1.9111978	-2.0629582
14	H	H7	-1.4668686	1.7020965	-2.8795502

Point Group = C1 Order = 1 Nsymop = 1

Post HF density not available. Select the density checkbox to generate a density or use the "NOPOSTHFDEN" keyword to use the HF density.

Reason for exit: Successful completion
Properties Program CPU Time : 0:00:00.1
Properties Program Wall Time: 0:00:00.2

molecule xfer terminated normally

End- molecule "xfer" Mon Mar 28 00:38:38 2005

E-1 LOCAL MINIMUM (LEADS TO AX-5-EXO AND 6-ENDO T-STATES)

MacSPARTAN '04 Quantum Mechanics Program: (PowerPC(Darwin)) build 123

Job type: Geometry optimization.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
An unrestricted Hartree-Fock SCF calculation will be
performed using Pulay DIIS extrapolation

Correlation model:
A MP2 calculation will be performed

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-344.0272379	0.016996	0.097409
2	-344.0303263	0.004574	0.072985
3	-344.0305201	0.004202	0.156382
4	-344.0304837	0.008696	0.151806
5	-344.0305910	0.005527	0.034728
6	-344.0306585	0.005229	0.074370
7	-344.0307443	0.005073	0.068576
8	-344.0308123	0.004944	0.104360
9	-344.0309122	0.002962	0.061948
10	-344.0309559	0.002970	0.017371
11	-344.0309841	0.002044	0.023511
12	-344.0309807	0.000950	0.049188
13	-344.0309887	0.000910	0.010390
14	-344.0309976	0.000417	0.018415
15	-344.0309958	0.000654	0.009901
16	-344.0309962	0.000316	0.007268
17	-344.0309921	0.000138	0.003990
18	-344.0309899	0.000142	0.003069
19	-344.0309926	0.000066	0.001157

Program Wall Time: 1:28:14.0
Reason for exit: Sucessful completion
Quantum Mechanics Program CPU Time : 1:08:43.5
Quantum Mechanics Program Wall Time: 1:28:15.1

MacSPARTAN '04 Semi-Empirical Program: (PowerPC(Darwin)) build 123
Job run on machine : John-Tamines-Computer.local
Semi-empirical Property Calculation

5X6N LOCAL MINS.631.5
Solvation implemented only for closed shell systems
Energy Due to Solvation
Memory Used: 579.55 Kb
Reason for exit: Successful completion
Semi-Empirical Program CPU Time : 0:00:-0.0
Semi-Empirical Program Wall Time: 0:00:00.2

```
SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------ ------------ ------------

  1 C  C2          -1.2945147    -1.3744867     -.3033858
  2 C  C1           -.1612003    -1.2055130    -1.2433914
  3 O  O1           -.2038479    -1.5865456    -2.3845216
  4 O  O2            .9595535     -.5811249     -.7850171
  5 C  C3           1.0766868     -.2310584      .6033147
  6 H  H1          -2.0188278    -2.1334851     -.5621899
  7 H  H3          -1.5235777     -.6524838      .4670637
  8 H  H2           2.1556839     -.2097674      .7856754
  9 H  H4            .6568531    -1.0242157     1.2330797
 10 C  C4            .4639417     1.1006469      .9253841
 11 C  C5           -.0575676     1.9346664      .0160692
 12 H  H6            .4894603     1.3808439     1.9779596
 13 H  H5           -.0702195     1.6902340    -1.0404815
 14 H  H7           -.4724241     2.8922895      .3104411

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.8
  Properties Program Wall Time:   0:00:00.9

molecule 5x6n local mins.631.5 terminated normally

End-   molecule "5x6n local mins.631.5" Tue Mar 22 16:34:28 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:21.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:16.1
  Quantum Mechanics Program Wall Time:   0:01:22.5

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
```

```
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1648924 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2381858 hartrees

  Program Wall Time:    0:07:28.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:06:23.1
  Quantum Mechanics Program Wall Time:   0:07:29.2

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.5
  Solvation implemented only for closed shell systems

  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

End-   molecule "5x6n local mins.631.5" Sun Mar 27 20:35:43 2005
```

E-1 LOCAL MINIMUM (LEADS TO EQ-5-EXO T-STATE)

```
MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Geometry optimization.
Method: UMP2(FC)
Basis set: 6-31G(D)
Number of shells: 42
Number of basis functions: 119

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
 performed using Pulay DIIS extrapolation

Correlation model:
 A MP2 calculation will be performed

Optimization:
         Step      Energy          Max Grad.      Max Dist.
            1    -344.0268416       0.014111       0.088046
            2    -344.0297192       0.063793       0.097028
            3    -344.0268549       0.038302       0.058378
            4    -344.0293933       0.022341       0.153470
            5    -344.0300009       0.013442       0.117658
            6    -344.0300903       0.002616       0.153977
            7    -344.0299864       0.007293       0.088939
            8    -344.0302260       0.003080       0.040461
            9    -344.0302621       0.005010       0.133328
           10    -344.0302457       0.005789       0.036282
           11    -344.0303096       0.001689       0.044002
           12    -344.0303545       0.001308       0.056169
           13    -344.0303773       0.001470       0.013291
           14    -344.0303733       0.000881       0.018868
           15    -344.0303946       0.000682       0.013711
           16    -344.0303904       0.000359       0.005118
           17    -344.0304028       0.000449       0.007841
           18    -344.0304126       0.000142       0.000853

  Program Wall Time:    1:14:01.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   1:00:16.4
  Quantum Mechanics Program Wall Time:   1:14:01.2

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.6
  Solvation implemented only for closed shell systems
  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1
```

```
SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------ ------------ ------------

  1 C  C2           1.4961786     .2700530    -1.1510461
  2 C  C1            .4856127    -.5766006    -1.8279738
  3 O  O1            .5114267    -.7946457    -3.0119374
  4 O  O2           -.5094280   -1.1100995    -1.0678903
  5 C  C3           -.4938500    -.9792801     .3717797
  6 H  H1           2.4390522     .3925520    -1.6648016
  7 H  H3           1.2443021     .9180699     -.3242077
  8 H  H2            .5232888   -1.0852412     .7635902
  9 H  H4          -1.0805890   -1.8378987     .7098063
 10 C  C4          -1.1282354     .3021856     .8139607
 11 C  C5           -.6153303    1.0951811    1.7453412
 12 H  H6          -2.0788985     .5408661     .3410985
 13 H  H5           .3310170     .8692689    2.2304724
 14 H  H7          -1.1245469    1.9955891    2.0718081

  Point Group = C1  Order =  1 Nsymop =  1
   All calculations using Post-HF corrected density matrix

  Reason for exit: Successful completion
  Properties Program CPU Time :   0:00:00.8
  Properties Program Wall Time:   0:00:00.8

molecule 5x6n local mins.631.6 terminated normally

End-   molecule "5x6n local mins.631.6" Tue Mar 22 17:48:33 2005

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Reading previous wavefunction

  Program Wall Time:    0:01:18.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:01:12.5
  Quantum Mechanics Program Wall Time:   0:01:19.0

MacSPARTAN '04 Quantum Mechanics Program:  (PowerPC(Darwin))  build  123

Job type: Single point.
Method: UMP2(FC)
Basis set: 6-311+G**
Number of shells: 70
Number of basis functions: 196

SCF model:
 An unrestricted Hartree-Fock SCF calculation will be
```

```
 performed using Pulay DIIS extrapolation

 SCF total energy:    -343.1652703 hartrees

Correlation model:
 A MP2 calculation will be performed
 MP2 total energy:    -344.2373659 hartrees

  Program Wall Time:    0:07:12.0
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time :   0:06:10.3
  Quantum Mechanics Program Wall Time:   0:07:13.8

MacSPARTAN '04 Semi-Empirical Program:  (PowerPC(Darwin))     build  123
   Job run on machine : John-Tamines-Computer.local
    Semi-empirical Property Calculation

  5X6N LOCAL MINS.631.6
  Solvation implemented only for closed shell systems
  Energy Due to Solvation
  Memory Used:         579.55 Kb
  Reason for exit: Successful completion
  Semi-Empirical Program CPU Time :   0:00:00.0
  Semi-Empirical Program Wall Time:   0:00:00.1

SPARTAN PROPERTIES PACKAGE: MAC/G5             build 123
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2
  Electrons:          53

                    Cartesian Coordinates (Angstroms)
       Atom            X             Y             Z
    ---------    ------------ ------------ -------------

  1 C  C2          1.4961786     .2700530    -1.1510461
  2 C  C1           .4856127    -.5766006    -1.8279738
  3 O  O1           .5114267    -.7946457    -3.0119374
  4 O  O2          -.5094280   -1.1100995    -1.0678903
  5 C  C3          -.4938500    -.9792801     .3717797
  6 H  H1          2.4390522     .3925520    -1.6648016
  7 H  H3          1.2443021     .9180699     -.3242077
  8 H  H2           .5232888   -1.0852412     .7635902
  9 H  H4         -1.0805890   -1.8378987     .7098063
 10 C  C4         -1.1282354     .3021856     .8139607
 11 C  C5          -.6153303    1.0951811    1.7453412
 12 H  H6         -2.0788985     .5408661     .3410985
 13 H  H5           .3310170     .8692689    2.2304724
 14 H  H7         -1.1245469    1.9955891    2.0718081

  Point Group = C1  Order =  1 Nsymop =  1
Task "SPARTAN Properties" returned [1]

End-   molecule "5x6n local mins.631.6" Sun Mar 27 20:44:18 2005
```