Supplementary Materials

A Mechanism Study on the Photoisomerizations of the Spiro[2,4]hept-1-ene, Vinylidenecyclopentane, and Vinylidenecyclobutane

Ming-Der Su*

Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan

midesu@mail.ncyu.edu.tw

(All geometries were calculated CASSCF(6,6)/6-311G*)

(1) **spiro[2,4]hept-1-ene** (**1**)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.312066
6	1.342667	0.000000	0.655122
6	2.256235	1.238868	0.666567
6	2.256501	-1.238892	0.645435
1	-0.523687	0.000763	2.244448
1	-0.536474	-0.000693	-0.948976
6	3.652227	0.699184	0.336423
6	3.654309	-0.698123	0.967416
1	2.254117	-1.695706	-0.342308
1	1.924047	-1.998737	1.345143
1	4.453199	-1.332571	0.598724
1	3.782880	-0.611419	2.044105
1	3.774348	0.612538	-0.741052
1	4.453121	1.333928	0.700212
1	1.920529	2.001678	-0.028332
1	2.258364	1.691182	1.656420

Hartree Fock Energies = -270.920923
MP2 Energies = -271.991160

(15) **FC-1**

Hartree Fock Energies = -270.646641
MP2 Energies = -271.750982

(2) **Int-1**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.048972	-0.112710	-0.229768
6	0.196443	-0.021607	1.200350
6	1.541342	0.046082	0.670187
6	2.452820	1.246937	0.792060
6	2.392569	-1.178192	0.352144

1	-0.173394	0.828312	1.757809
1	-0.237372	-1.142224	-0.631582
6	3.872867	0.701474	0.539747
6	3.766972	-0.783154	0.907246
1	2.468251	-1.316314	-0.721870
1	1.987355	-2.086254	0.775058
1	4.572905	-1.385679	0.500199
1	3.781327	-0.905833	1.988753
1	4.131353	0.799359	-0.510965
1	4.629791	1.227146	1.109843
1	2.160139	2.023562	0.096577
1	2.365670	1.662123	1.794160

Hartree Fock Energies = -270.76737

MP2 Energies = -271.83594

(3) **TS-1**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.343872
6	1.600954	0.000000	0.693691
6	2.430513	1.252428	0.768016
6	2.482763	-1.225233	0.664694
1	0.089896	-0.728731	2.131158
1	0.117860	-0.741631	-0.772615
6	3.868582	0.754102	0.549184
6	3.853181	-0.680246	1.098082
1	2.536050	-1.619631	-0.348585
1	2.111899	-2.025318	1.294976
1	4.679058	-1.282776	0.738615
1	3.914250	-0.660092	2.182935
1	4.096539	0.737132	-0.513183
1	4.610852	1.381905	1.027622
1	2.105672	1.992627	0.045946
1	2.313670	1.704790	1.751158

One imaginary frequency: -820.8153 cm-1

-1 0.41 -0.13 0.16

-2	-0.41	0.13	0.16
-3	0.00	0.00	-0.33
-4	-0.01	0.00	0.05
-5	0.01	0.00	-0.05
-6	0.48	-0.02	-0.05
-7	-0.41	0.07	-0.11
-8	0.00	0.00	0.01
-9	-0.01	0.00	0.00
-10	0.07	-0.12	-0.01
-11	-0.05	0.07	0.00
-12	0.00	0.00	0.01
-13	-0.02	0.00	0.00
-14	-0.02	0.01	0.01
-15	0.00	0.00	0.01
-16	0.03	0.05	0.08
-17	-0.03	-0.07	0.07

Hartree Fock Energies = -270.73166

MP2 Energies = -271.78483

(4) **CI-1**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.485933	0.286619	0.155092
6	-0.158907	-0.771203	0.732261
6	1.585176	0.153210	-0.753218
6	2.312296	1.314332	-1.389128
6	2.184778	-1.151038	-1.219242
1	-0.983793	-0.701345	1.421706
1	0.162329	1.296922	0.378891
6	3.153944	0.661288	-2.496052
6	3.477792	-0.728977	-1.934957
1	1.503689	-1.641977	-1.911882
1	2.349259	-1.845403	-0.404202
1	3.788864	-1.433228	-2.698039
1	4.289623	-0.653507	-1.215843
1	2.558555	0.562830	-3.400175
1	4.037095	1.235386	-2.752083
1	1.636750	2.078941	-1.759444
1	2.957971	1.795642	-0.655217

Derivative Coupling

-1	0.0016562643	0.0181777313	-0.0193837318
-2	0.0174915628	-0.0281787310	0.0212899243
-3	-0.0129572619	-0.0017777895	0.0115537325
-4	-0.0012593623	0.0008993996	-0.0033951156
-5	-0.0011953982	-0.0000288497	-0.0041176146
-6	-0.0119207631	0.0078414155	-0.0131848172
-7	0.0083415111	0.0030209204	0.0049319260
-8	0.0007121162	0.0000448374	-0.0003710535
-9	0.0000423361	0.0005345205	-0.0001716581
-10	0.0017073798	0.0000552770	0.0001821279
-11	-0.0023356350	0.0009443453	0.0015428825
-12	-0.0000673041	0.0000634402	0.0001274236
-13	0.0000167854	-0.0000392755	-0.0000418375
-14	0.0000180737	0.0000206598	-0.0000322622
-15	-0.0001006267	0.0000529981	-0.0000069392
-16	0.0007258213	-0.0004792334	0.0001675126
-17	-0.0008754995	-0.0011516660	0.0009095005

Unscaled Gradient Difference

-1	-0.0477526645	-0.0692312570	0.0240203068
-2	0.0181994171	0.1074402290	0.0179895995
-3	0.0496607205	0.0014417922	-0.0411211312
-4	-0.0033469282	-0.0011151977	0.0020852541
-5	-0.0086167698	0.0052591239	-0.0036768976
-6	-0.0096902939	-0.0316638764	-0.0154024315
-7	-0.0027566295	-0.0100990942	0.0154943523
-8	-0.0010749783	0.0010083653	0.0014314581
-9	-0.0009048253	-0.0005936495	0.0006525810
-10	0.0019089331	-0.0039652797	-0.0023566419
-11	0.0013889017	-0.0023082978	0.0037392191
-12	0.0002112893	-0.0002029024	-0.0003845013
-13	-0.0003110626	-0.0000268785	0.0002078040
-14	-0.0001965174	-0.0001038866	0.0000114190
-15	0.0006327954	-0.0001494235	-0.0001630850
-16	0.0010530890	0.0016790736	-0.0026256816
-17	0.0015955235	0.0026311593	0.0000983761

Hartree Fock Energies = -270.852681

MP2 Energies = -271.891003

(5) **Int-2**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.528259	0.283097	0.160818
6	-0.084769	-0.893597	0.732287
6	1.564986	0.147771	-0.733988
6	2.284529	1.305653	-1.397504
6	2.175597	-1.150735	-1.219040
1	-0.935059	-0.556842	1.338851
1	0.202549	1.289906	0.390719
6	3.140299	0.654793	-2.495031
6	3.479324	-0.720527	-1.909080
1	1.501371	-1.604972	-1.942862
1	2.302856	-1.868071	-0.419664
1	3.814342	-1.431557	-2.655599
1	4.276755	-0.622363	-1.175201
1	2.552229	0.534767	-3.402807
1	4.015788	1.240898	-2.752624
1	1.600117	2.063842	-1.765028
1	2.922180	1.786429	-0.655781

Hartree Fock Energies = -270.880523

MP2 Energies = -271.916792

(6) **TS-2**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.360597
6	0.281386	0.000000	-1.306446
6	-0.561938	-0.621938	-2.407737
6	1.540421	0.616637	-1.901602
1	-0.626410	0.822382	1.714582
1	-0.878825	-0.682582	0.523568
6	0.403973	-0.679585	-3.600072
6	1.285629	0.560609	-3.416190
1	2.406812	0.016042	-1.638535
1	1.727081	1.622488	-1.544223

1	2.201821	0.521223	-3.994087
1	0.740995	1.446555	-3.732563
1	1.013847	-1.576989	-3.536744
1	-0.107878	-0.701232	-4.555413
1	-0.957839	-1.594436	-2.136789
1	-1.408896	0.017540	-2.643927

One imaginary frequency: -998.4536 cm-1

-1	0.08	0.08	0.00
-2	-0.09	-0.04	-0.08
-3	-0.01	-0.01	-0.01
-4	-0.01	0.00	0.00
-5	0.01	-0.01	0.00
-6	0.04	-0.02	0.04
-7	0.32	-0.27	0.89
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-10	0.01	0.00	0.00
-11	-0.01	-0.01	0.01
-12	0.00	0.00	0.01
-13	0.00	0.00	0.01
-14	0.00	0.00	0.00
-15	0.00	0.00	0.00
-16	0.00	0.00	0.00
-17	-0.02	-0.01	-0.01

Hartree Fock Energies = -270.84152

MP2 Energies = -271.90979

(7) **TS-3**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.282948
6	0.491636	0.000000	-1.339420
6	0.641049	1.233488	-2.197617
6	0.961427	-1.233679	-2.080148
1	-0.799395	-0.087801	1.989416
1	-1.002214	-0.121292	-0.661235
6	0.818830	0.657731	-3.608687

6	1.567980	-0.661360	-3.375472
1	0.137743	-1.908570	-2.298966
1	1.680307	-1.798997	-1.494628
1	1.490917	-1.345953	-4.212202
1	2.624057	-0.456801	-3.223691
1	-0.155548	0.457626	-4.047346
1	1.344968	1.328182	-4.278549
1	-0.194177	1.919213	-2.111778
1	1.530224	1.784020	-1.888652

One imaginary frequency: -1581.4106 cm-1

-1	-0.09	-0.01	-0.07
-2	0.02	0.00	0.02
-3	0.09	0.01	-0.02
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	-0.03	0.00	-0.02
-7	-0.27	0.03	0.95
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-10	-0.02	0.00	0.00
-11	0.00	-0.02	-0.02
-12	0.00	0.00	-0.01
-13	0.00	0.00	0.00
-14	0.00	0.00	0.00
-15	0.00	0.00	-0.01
-16	-0.02	-0.01	0.00
-17	-0.01	0.04	-0.02

Hartree Fock Energies = -270.83143

MP2 Energies = -271.88640

(8) **TS-4**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.345574
6	1.201770	0.000000	-0.860824
6	2.342770	0.630209	-0.645126
6	1.214417	-0.719396	-2.195021

1	−0.788563	0.003413	2.072010
1	−0.957192	−0.016938	−0.503519
6	3.328710	0.445251	−1.771395
6	2.703999	−0.703910	−2.589276
1	0.596328	−0.185239	−2.915656
1	0.814354	−1.726809	−2.129775
1	2.856791	−0.594124	−3.656587
1	3.160964	−1.642492	−2.294238
1	3.414135	1.360457	−2.354936
1	4.329218	0.207960	−1.422657
1	2.541550	1.248788	0.212208
1	3.607872	−1.156052	1.287357

One imaginary frequency: -137.7734 cm-1

-1	0.02	0.00	0.01
-2	0.04	-0.03	0.01
-3	0.00	0.01	-0.01
-4	0.00	0.01	-0.02
-5	0.00	0.00	0.00
-6	0.06	-0.04	0.03
-7	0.01	0.03	0.03
-8	0.00	0.00	-0.02
-9	0.00	0.00	-0.01
-10	-0.01	-0.01	0.00
-11	0.00	0.00	0.00
-12	-0.01	0.00	-0.01
-13	0.00	0.00	-0.01
-14	0.01	0.00	-0.02
-15	0.00	0.00	-0.01
-16	0.01	0.02	-0.02
-17	-0.83	0.09	0.53

Hartree Fock Energies = -270.81411

MP2 Energies = -271.86438

(9) **TS-5**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.414241

6	1.322644	0.000000	0.814591
6	2.125468	1.296707	0.707465
6	2.308110	-1.172461	0.857086
1	-0.589872	0.154914	2.297221
1	-0.474556	-0.986766	0.774036
6	3.490199	0.831400	0.190511
6	3.697267	-0.515314	0.893278
1	2.192854	-1.776890	-0.038867
1	2.139460	-1.826604	1.706992
1	4.465051	-1.124933	0.430241
1	4.001187	-0.343844	1.922990
1	3.445585	0.684129	-0.885341
1	4.284640	1.542167	0.389603
1	1.645225	2.022242	0.058672
1	2.239468	1.764866	1.683389

One imaginary frequency: -1030.8580 cm-1

-1	0.03	0.07	-0.06
-2	-0.04	-0.07	0.00
-3	0.00	-0.01	0.00
-4	-0.01	0.00	0.01
-5	0.00	0.00	-0.01
-6	0.04	0.39	-0.03
-7	0.21	-0.15	0.87
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-10	0.02	-0.01	-0.01
-11	0.00	0.01	0.00
-12	0.00	0.00	0.00
-13	0.00	0.00	0.00
-14	0.00	0.00	0.00
-15	-0.01	0.00	0.00
-16	0.00	0.01	0.00
-17	-0.01	0.00	0.00

Hartree Fock Energies = -270.81810

MP2 Energies = -271.89457

(10) **TS-6**

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.346006
6	1.451597	0.000000	1.233410
6	2.304874	1.232422	1.513080
6	2.297480	-1.247955	1.519252
1	-0.717595	-0.014647	2.136472
1	1.288401	0.015663	-0.092361
6	3.735440	0.720200	1.331627
6	3.685182	-0.700920	1.912133
1	2.346826	-1.883744	0.641468
1	1.854844	-1.845108	2.308802
1	4.495548	-1.328440	1.560344
1	3.768640	-0.650953	2.993975
1	3.981231	0.684073	0.272998
1	4.478279	1.344809	1.814112
1	2.043526	2.065151	0.871398
1	2.143680	1.553922	2.540512

One imaginary frequency: -1062.4739 cm-1

-1	-0.09	0.00	0.01
-2	-0.02	0.00	-0.02
-3	0.04	0.00	-0.11
-4	0.00	0.01	0.02
-5	0.00	-0.01	0.02
-6	0.06	0.00	0.06
-7	0.67	0.00	0.72
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-10	0.00	-0.02	0.03
-11	0.00	0.02	0.03
-12	0.00	0.00	0.00
-13	0.01	0.00	0.00
-14	-0.01	0.00	0.00
-15	0.00	0.00	0.00
-16	0.01	0.01	0.02
-17	0.01	-0.01	0.02

Hartree Fock Energies = -270.85692

MP2 Energies = -271.4584

(11) **6**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	−0.012449	−0.013496	0.006517
6	−0.048136	0.030636	1.337609
6	0.023500	−0.054888	−1.305247
6	−1.189940	−0.195322	−2.218075
6	1.284248	0.038208	−2.156972
1	−0.160926	0.964109	1.861240
1	0.034713	−0.864888	1.928656
6	−0.581062	−0.475570	−3.600048
6	0.749991	0.283851	−3.575304
1	1.825756	−0.903576	−2.117702
1	1.960537	0.811838	−1.813968
1	1.439608	−0.038217	−4.347626
1	0.569382	1.345790	−3.724181
1	−0.393005	−1.540492	−3.713397
1	−1.229519	−0.173736	−4.414945
1	−1.870671	−0.970239	−1.886703
1	−1.747961	0.737188	−2.234570

Hartree Fock Energies = -270.96877

MP2 Energies = -272.08815

(12) **5**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.206971
6	0.015924	0.000000	-1.498379
6	-1.293518	0.485891	-2.137703
6	1.111209	0.909164	-2.113237
1	-0.013681	0.017686	2.261206
1	0.188030	-1.023602	-1.816158
6	-0.868387	0.805578	-3.570141
6	0.484712	1.513092	-3.396404
1	2.007579	0.337788	-2.324396
1	1.395455	1.688054	-1.416963

1	1.124793	1.401343	-4.263949
1	0.323573	2.578073	-3.262661
1	-0.743627	-0.118661	-4.129586
1	-1.592396	1.408428	-4.106713
1	-2.087150	-0.249451	-2.069572
1	-1.637373	1.386831	-1.637069

Hartree Fock Energies = -270.97007

MP2 Energies = -272.01663

(13) **7**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.340741
6	1.199218	0.000000	-0.857826
6	2.379559	-0.591492	-0.615044
6	1.242336	0.764023	-2.168075
1	-0.917238	-0.018766	1.902251
1	-0.948363	0.013951	-0.514279
6	3.394769	-0.304076	-1.695406
6	2.525449	0.245819	-2.844774
1	0.357813	0.598641	-2.776493
1	1.290247	1.834030	-1.974381
1	2.271626	-0.565507	-3.519457
1	3.030321	1.004867	-3.430954
1	3.961216	-1.182137	-1.988964
1	4.118653	0.432671	-1.351259
1	2.603224	-1.179096	0.257481
1	0.936317	0.020549	1.914708

Hartree Fock Energies = -270.98160

MP2 Energies = -270.99662

(14) **CI-3**

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	0.077703	0.171501	-0.035580
6	-0.087473	0.166028	1.330835
6	1.303974	0.103178	-0.726395
6	1.427636	0.109201	-2.232811
6	2.677966	0.003828	-0.102790
1	-0.831564	0.231636	-0.659691
1	0.737086	0.100701	2.025463
6	2.876059	-0.329480	-2.490797
6	3.641020	0.219824	-1.281187
1	2.818869	-0.985460	0.329621
1	2.827625	0.718676	0.698696
1	4.603040	-0.256707	-1.132416
1	3.824639	1.282608	-1.415726
1	2.935401	-1.414743	-2.502323
1	3.264890	0.025555	-3.438183
1	0.693145	-0.529753	-2.711953
1	1.262296	1.116689	-2.613354

Derivative Coupling

-1	0.0270528182	-0.0198395760	-0.0283135615
-2	-0.0162885491	0.0326224607	0.0269904625
-3	-0.0209191356	0.0018840362	0.0090308691
-4	0.0013101211	0.0074240237	-0.0009147021
-5	0.0024937315	0.0023506386	0.0014264863
-6	-0.0000823222	-0.0059957161	-0.0009369672
-7	0.0064337939	-0.0168006578	-0.0066245154
-8	0.0005670640	-0.0003472651	0.0004766774
-9	0.0004221330	0.0000171277	-0.0002808933
-10	-0.0014100897	0.0000055745	-0.0003753129
-11	0.0006218300	-0.0009625843	-0.0014981525
-12	-0.0000976750	0.0000635213	0.0000377575
-13	0.0000260642	-0.0000336649	-0.0000536667
-14	0.0000919756	0.0000131402	-0.0000801970
-15	-0.0002628140	-0.0001136067	0.0001398842
-16	-0.0005803089	0.0002846435	0.0016341773
-17	0.0006213628	-0.0005720955	-0.0006583457

Unscaled Gradient Difference

-1	-0.0882972424	-0.0190126618	0.0879008790
-2	0.0594633972	0.0376194241	-0.0824500573
-3	0.0643410079	-0.0031614342	-0.0321346483

-4	-0.0038995405	0.0121374519	0.0047550013
-5	-0.0061749374	0.0010078677	0.0000089233
-6	-0.0014196773	-0.0073668531	0.0024422893
-7	-0.0254270496	-0.0197788712	0.0192223007
-8	-0.0013821247	0.0001050219	0.0023220450
-9	-0.0004078955	-0.0002293442	0.0009903429
-10	0.0007329419	-0.0021447323	0.0026953101
-11	0.0029935172	0.0016144307	0.0004705555
-12	0.0004398112	-0.0002208304	-0.0001168504
-13	-0.0002032832	0.0000311686	0.0000549685
-14	-0.0001098082	-0.0000277028	0.0001228172
-15	-0.0001159783	0.0002962218	-0.0001735118
-16	-0.0008173347	-0.0014084610	-0.0008710423
-17	0.0002841963	0.0005393042	-0.0052393226

Hartree Fock Energies = -270.8458698

MP2 Energies = -271.891103

(15) **Int-3**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.444483
6	1.111486	0.000000	-0.813498
6	1.042882	-0.029810	-2.327981
6	2.572396	0.015707	-0.396645
1	1.067941	0.051828	1.777493
1	-0.958822	-0.028500	-0.495828
6	2.469946	-0.365875	-2.778131
6	3.340888	0.285104	-1.699077
1	2.839272	-0.960733	-0.000798
1	2.782322	0.739839	0.379103
1	4.353231	-0.100156	-1.673969
1	3.406866	1.355502	-1.876000
1	2.618003	-1.442679	-2.773584
1	2.692183	-0.013435	-3.778279
1	0.292546	-0.721749	-2.691023
1	0.760464	0.959688	-2.681649

Hartree Fock Energies = -270.875470

MP2 Energies = -271.918625

(16) **TS-7**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.347846
6	1.406640	0.000000	-0.266568
6	2.019587	-0.867547	-1.349297
6	2.469687	0.922672	0.286358
1	-0.675670	-0.654843	1.884534
1	-0.745803	-0.309586	-0.720405
6	3.466404	-0.357215	-1.493718
6	3.429012	1.059764	-0.904462
1	2.995428	0.466373	1.117852
1	2.047102	1.851556	0.644711
1	4.409003	1.423781	-0.617360
1	3.022740	1.757081	-1.633385
1	4.138298	-0.977244	-0.907348
1	3.819058	-0.384510	-2.518081
1	1.971175	-1.923929	-1.108988
1	1.450226	-0.733502	-2.268073

One imaginary frequency: -453.7871 cm-1

-1	0.12	-0.13	0.03
-2	-0.11	0.22	0.16
-3	-0.02	0.01	-0.10
-4	0.00	0.05	-0.09
-5	-0.01	-0.06	0.02
-6	-0.25	-0.15	-0.39
-7	0.25	-0.70	0.14
-8	0.01	0.01	-0.02
-9	0.00	-0.01	0.02
-10	-0.03	-0.12	0.00
-11	-0.01	-0.09	0.07
-12	-0.01	0.00	0.04
-13	-0.01	0.01	0.04
-14	-0.01	-0.01	-0.01
-15	0.05	0.04	-0.01

-16	-0.03	0.06	-0.03
-17	0.05	0.01	-0.12

Hartree Fock Energies = -270.8645231

MP2 Energies = -271.9083545

(17) **TS-8**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.347846
6	1.406640	0.000000	-0.266568
6	2.019587	-0.867547	-1.349297
6	2.469687	0.922672	0.286358
1	-0.675670	-0.654843	1.884534
1	-0.745803	-0.309586	-0.720405
6	3.466404	-0.357215	-1.493718
6	3.429012	1.059764	-0.904462
1	2.995428	0.466373	1.117852
1	2.047102	1.851556	0.644711
1	4.409003	1.423781	-0.617360
1	3.022740	1.757081	-1.633385
1	4.138298	-0.977244	-0.907348
1	3.819058	-0.384510	-2.518081
1	1.971175	-1.923929	-1.108988
1	1.450226	-0.733502	-2.268073

One imaginary frequency: -761.7340 cm-1

-1	0.06	-0.12	-0.01
-2	-0.08	0.07	-0.08
-3	-0.01	0.01	0.00
-4	-0.01	0.00	0.00
-5	0.01	0.01	0.00
-6	0.01	0.03	0.02
-7	0.38	0.22	0.88
-8	0.00	0.00	0.00
-9	0.00	0.00	0.00
-10	0.00	0.01	0.01
-11	0.01	0.01	0.01
-12	0.00	0.00	0.01

-13	0.00	0.00	0.00
-14	0.00	0.00	0.00
-15	0.00	0.00	0.01
-16	-0.01	0.00	-0.01
-17	-0.01	0.00	0.01

Hartree Fock Energies = -270.84399

MP2 Energies = -271.89665

(18) **TS-9**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.00768	-0.11362	-0.00209
6	0.01542	0.06199	1.35829
6	1.27657	-0.08097	-0.63381
6	1.71856	0.45456	-1.9702
6	2.37025	-0.24267	0.28156
1	-0.79134	-0.31338	1.97961
1	-0.91545	-0.19101	-0.55637
6	3.25876	0.4214	-1.8575
6	3.56994	0.46858	-0.34523
1	2.54947	-1.22856	0.68449
1	1.6989	0.19999	1.30572
1	4.52306	0.01064	-0.10826
1	3.61344	1.49741	0.00013
1	3.62738	-0.51385	-2.26813
1	3.73443	1.22382	-2.40938
1	1.35453	-0.13958	-2.80258
1	1.34389	1.46612	-2.11933

One imaginary frequency: -1822.0036 cm-1

-1	0.01	0.00	-0.01
-2	-0.05	0.00	0.02
-3	-0.03	0.00	-0.02
-4	0.00	-0.01	-0.01
-5	0.00	0.01	0.06
-6	-0.08	-0.06	-0.05
-7	0.00	0.07	0.00
-8	0.00	0.00	0.00
-9	0.00	0.01	0.00

-10	0.07	-0.10	-0.21
-11	0.87	-0.01	-0.40
-12	0.00	0.00	0.00
-13	0.01	0.01	-0.01
-14	0.00	0.00	0.00
-15	0.00	0.00	0.00
-16	0.01	0.01	-0.02
-17	0.00	-0.01	0.02

Hartree Fock Energies = -270.8341669

MP2 Energies = -271.8856465

(19) **CI-4**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.031002	0.506953	-0.204986
6	0.091760	0.301930	1.201001
6	1.255413	0.207957	-0.710030
6	1.414886	0.008526	-2.198859
6	2.643566	0.021921	-0.096638
1	-0.802241	0.190576	1.796859
1	1.004769	0.199417	1.774100
6	2.872905	-0.384162	-2.454152
6	3.610264	0.242663	-1.266966
1	2.733589	-1.006413	0.245996
1	2.833517	0.664679	0.751343
1	4.587644	-0.188475	-1.085621
1	3.751692	1.307221	-1.435554
1	2.985628	-1.464883	-2.430113
1	3.243105	-0.044152	-3.413726
1	0.675088	-0.688899	-2.568507
1	1.168302	0.969602	-2.647448

Derivative Coupling

-1	-0.0321484075	0.0124976341	-0.0284726941
-2	0.0229660438	-0.0056870702	-0.0059278948
-3	0.0015794115	-0.0020001200	0.0289423987
-4	0.0023749498	-0.0087447148	0.0025671358
-5	0.0068690471	0.0098375910	-0.0048813993
-6	-0.0002433788	0.0036890756	-0.0000090985

-7	0.0011541414	-0.0098394828	0.0041972761
-8	0.0003273989	-0.0003925445	-0.0001278084
-9	0.0024874908	-0.0005929560	0.0005740504
-10	-0.0027930993	0.0003593400	-0.0019389137
-11	0.0000883451	-0.0009855022	-0.0002564953
-12	0.0000961369	0.0002959702	-0.0004535138
-13	0.0001157475	0.0000116940	0.0000315750
-14	0.0000921541	0.0000346130	-0.0001350475
-15	-0.0001335084	0.0000231047	0.0001659045
-16	-0.0017508555	0.0015928730	0.0013056986
-17	-0.0010816175	-0.0000995049	0.0044188264

Unscaled Gradient Difference

-1	-0.0467550876	0.0074372810	-0.0007146077
-2	0.0333139388	0.0061048398	-0.0207352170
-3	0.0142018635	-0.0025392669	0.0086451554
-4	0.0030474231	0.0123209260	-0.0004286691
-5	-0.0070874138	-0.0455438643	0.0048435386
-6	-0.0008848873	-0.0243856099	-0.0060802388
-7	0.0019722508	0.0373926719	0.0124138486
-8	0.0010603479	0.0010178387	-0.0002133450
-9	-0.0033785740	0.0010107079	-0.0031463879
-10	0.0107380528	0.0002428071	0.0016909946
-11	-0.0052204226	0.0011844709	0.0003918953
-12	-0.0007900360	0.0004160915	0.0011267540
-13	0.0001644621	0.0000306914	-0.0003555367
-14	0.0000262830	-0.0000437407	-0.0000449433
-15	0.0001218944	-0.0000286818	0.0001562161
-16	0.0028894902	0.0021898857	0.0036063909
-17	-0.0034195853	0.0031929517	-0.0011558479

Hartree Fock Energies = -270.8370902

MP2 Energies = -271.8929112

(20) **Int-4**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.591039	0.252577	0.371658
6	-0.392113	0.452207	1.248072
6	1.567664	0.088891	-0.490492
6	1.426792	0.154654	-2.007695

6	3.024158	-0.182559	-0.133163
1	-0.983305	-0.365346	1.622496
1	-0.623044	1.439529	1.608319
6	2.781571	-0.350120	-2.527507
6	3.776055	0.083639	-1.444949
1	3.143641	-1.222058	0.162478
1	3.370192	0.428103	0.692174
1	4.724319	-0.439339	-1.502145
1	3.985053	1.146474	-1.542482
1	2.770313	-1.435055	-2.600115
1	3.025542	0.036366	-3.510776
1	0.588220	-0.426908	-2.371534
1	1.262788	1.183406	-2.317639

Hartree Fock Energies = -270.9687425

MP2 Energies = -272.0882443

(21) **TS-10**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.008733	0.055399	0.024251
6	-0.013789	-0.058733	1.344230
6	0.258012	0.029037	-1.273883
6	-1.576966	0.150114	-0.922686
6	0.600395	1.324355	-1.997852
1	0.882730	-0.345157	1.860892
1	-0.904869	0.107688	1.917116
6	-1.819113	1.101601	-2.096157
6	-0.697156	2.137526	-2.077902
1	0.972006	1.091294	-3.013424
1	1.388644	1.870185	-1.485380
1	-0.728877	2.793916	-2.940487
1	-0.796816	2.761269	-1.193828
1	-1.792543	0.543128	-3.024399
1	-2.801547	1.555931	-2.007492
1	-1.951658	-0.848711	-1.051122
1	-2.030830	0.596657	-0.017717

One imaginary frequency: -532.2906 cm-1

-1	0.33	-0.03	0.15
-2	0.05	-0.03	0.11
-3	-0.33	0.07	0.11
-4	0.06	-0.05	-0.25
-5	-0.05	-0.03	0.02
-6	-0.13	-0.43	0.19
-7	0.07	0.43	0.00
-8	-0.05	0.04	-0.08
-9	-0.01	0.02	-0.03
-10	-0.04	-0.11	0.04
-11	-0.02	-0.05	0.00
-12	0.01	0.04	-0.01
-13	-0.02	0.00	-0.02
-14	-0.07	0.11	-0.13
-15	-0.04	0.06	-0.02
-16	-0.06	-0.01	-0.15
-17	0.34	-0.03	-0.11

Hartree Fock Energies = -270.8244029

MP2 Energies = -271.9009165

(22) **Int-5**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.	0.	0.
6	0.	0.	1.35471
6	1.35251	0.	-0.60748
6	-1.27531	0.08377	-0.81822
6	1.39225	0.66117	-1.95752
1	-0.89859	0.14913	1.93009
1	0.92074	-0.11784	1.8938
6	-1.11096	1.0337	-2.00525
6	0.1222	0.65109	-2.81881
1	1.64882	1.69266	-1.69105
1	2.24713	0.29923	-2.51956
1	-0.0203	-0.3424	-3.23987
1	0.24926	1.32215	-3.66322
1	-2.00024	1.01138	-2.6279
1	-1.00895	2.05531	-1.64377
1	-1.52176	-0.90885	-1.19062

1	-2.10611	0.38607	-0.18867

Hartree Fock Energies = -270.8849585

MP2 Energies = -271.9187225

(23) **TS-11**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.	0.	0.
6	0.	0.	1.34252
6	1.35484	0.	-0.69227
6	-1.2723	0.0811	-0.81797
6	1.27569	0.23748	-2.06725
1	-0.90927	0.07419	1.91555
1	0.92354	-0.06982	1.88674
6	-1.10451	1.08749	-1.95814
6	0.05882	0.68382	-2.86266
1	2.20762	0.24567	-2.61398
1	1.40316	-0.94762	-1.59719
1	-0.23797	-0.11848	-3.53411
1	0.35746	1.50963	-3.50186
1	-2.01711	1.17018	-2.53955
1	-0.91044	2.07026	-1.5364
1	-1.49823	-0.89911	-1.23859
1	-2.11627	0.3483	-0.19123

One imaginary frequency: -1439.4296 cm-1

-1	0.00	0.00	0.01
-2	0.00	0.00	0.00
-3	-0.02	-0.06	-0.07
-4	0.00	0.00	0.00
-5	-0.02	0.06	-0.01
-6	0.00	-0.01	0.00
-7	0.00	0.00	0.01
-8	0.00	0.00	0.00
-9	0.00	0.01	0.00
-10	-0.04	-0.19	-0.05
-11	0.45	-0.09	0.85
-12	0.03	-0.02	0.02

-13	-0.02	0.00	-0.03
-14	0.00	0.00	0.00
-15	0.00	0.00	0.00
-16	0.01	0.00	0.00
-17	0.00	0.00	0.00

Hartree Fock Energies = -270.8558508

MP2 Energies = -271.9233562

(24) **5**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.343090
6	1.252963	0.000000	-0.772934
6	-1.273924	-0.036465	-0.817339
6	1.280997	0.129875	-2.110525
1	-0.912583	0.000813	1.913398
1	0.940764	-0.004169	1.911119
6	-1.140795	0.799945	-2.091756
6	0.036951	0.321658	-2.943098
1	2.226417	0.094366	-2.625554
1	2.174837	-0.110198	-0.226947
1	-0.215904	-0.615189	-3.437982
1	0.236322	1.033994	-3.738719
1	-2.060833	0.757206	-2.666696
1	-0.986687	1.841308	-1.820313
1	-1.483557	-1.069126	-1.092224
1	-2.113225	0.304767	-0.221173

Hartree Fock Energies = -270.9918179

MP2 Energies = -272.03562287

(25) **6**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.585526	0.009161	0.412325
6	-0.114783	-0.097444	1.521181

6	1.289165	0.140958	-0.703282
6	1.802255	1.342774	-1.485856
6	1.848338	-0.844674	-1.720777
1	-1.190834	-0.107942	1.505917
1	0.365696	-0.176652	2.480676
6	2.246052	0.366082	-2.609559
1	1.129694	-1.532108	-2.150606
1	2.691593	-1.417487	-1.351132
1	1.651850	0.450550	-3.510815
1	3.291611	0.417849	-2.885012
1	1.054202	2.075975	-1.762684
1	2.622699	1.857867	-0.998603

Hartree Fock Energies = -231.8919587

MP2 Energies = -232.7588235

(26) **FC-3**

Hartree Fock Energies = -231,662400

MP2 Energies = -232.508612

(27) **CI-5**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.411010	-0.329846	0.049613
6	0.380450	0.676592	1.013180
6	0.447576	-0.170004	-1.317968
6	0.371093	1.036194	-2.228091
6	0.622121	-1.138429	-2.470102
1	-0.408274	1.151524	1.562077
1	0.564884	-1.357350	0.439721
6	0.520476	0.073658	-3.439427
1	-0.164084	-1.879306	-2.577691
1	1.576314	-1.656297	-2.489587
1	-0.340823	0.046630	-4.094981
1	1.403152	0.242147	-4.043175
1	-0.564025	1.586877	-2.189325
1	1.182791	1.746822	-2.105003

Derivative Coupling

-1	0.0084552022	-0.0106237858	0.0199419162
-2	-0.0082283980	0.0298318144	-0.0366927664
-3	0.0115794048	0.0047591517	-0.0021161303
-4	-0.0007399211	-0.0001864214	-0.0000704122
-5	-0.0043236754	-0.0006380275	-0.0002058780
-6	0.0037797189	-0.0184674319	0.0202740372
-7	-0.0116014540	-0.0043480421	-0.0018920083
-8	0.0000530530	0.0000427866	0.0000915154
-9	0.0002883793	-0.0001120468	-0.0009040668
-10	0.0001415603	0.0001322348	0.0011859934
-11	-0.0000006550	-0.0000776653	0.0000128436
-12	0.0000207355	-0.0000536495	-0.0000251449
-13	0.0005260654	-0.0002726050	-0.0005917624
-14	0.0000499840	0.0000136878	0.0009918635

Unscaled Gradient Difference

-1	-0.0184738001	-0.0344155575	-0.1024050202
-2	0.0574277244	0.0587944612	0.0444295459
-3	-0.0021396644	-0.0087877032	0.0658996443
-4	-0.0014596337	0.0025762415	-0.0006004827
-5	0.0007759989	-0.0039143509	-0.0002908024
-6	-0.0312890118	-0.0209587352	-0.0084004227
-7	-0.0051845219	0.0045649033	0.0044010342
-8	-0.0000357645	0.0002114529	0.0002959008
-9	0.0001711813	0.0008043710	-0.0008504117
-10	-0.0002585892	0.0005232772	-0.0007376405
-11	-0.0001101682	0.0000434902	-0.0000419880
-12	0.0000578021	0.0001282815	-0.0000614172
-13	-0.0000428277	0.0002709875	-0.0015911549
-14	0.0005612747	0.0001588806	-0.0000467848

Hartree Fock Energies = -231.7507685

MP2 Energies = -232.6131229

(28) **Int-6**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.450294	-0.230850	0.014439
6	0.317531	0.964861	0.811628
6	0.348013	-0.133605	-1.330274
6	0.218124	1.028312	-2.289737

6	0.462059	-1.126326	-2.467193
1	0.230800	0.653983	1.858993
1	0.606357	-1.241892	0.436917
6	0.711462	0.078612	-3.414044
1	-0.482552	-1.622162	-2.668013
1	1.235626	-1.880330	-2.382170
1	0.157977	0.089908	-4.342643
1	1.762310	0.214530	-3.633345
1	-0.816070	1.325237	-2.423498
1	0.800731	1.908935	-2.061820

Hartree Fock Energies = -231.7968761

MP2 Energies = -232.6618458

(29) **TS-12**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.126594	-0.278721	0.120638
6	0.017633	-0.165345	1.464259
6	1.375347	0.115810	1.774433
6	2.000500	1.039784	2.798998
6	2.699483	-0.557086	1.486961
1	-0.816213	0.072805	2.109749
1	-0.624620	0.201511	-0.496763
6	3.232724	0.094066	2.793934
1	3.197325	-0.172364	0.607391
1	2.670697	-1.637695	1.422877
1	4.204939	0.566706	2.739900
1	3.223716	-0.591782	3.632138
1	2.228769	2.021956	2.398193
1	1.455183	1.165511	3.728852

One imaginary frequency: -501.4033 cm-1

-1	0.06	0.23	0.15
-2	-0.10	-0.14	0.03
-3	0.04	-0.01	-0.12
-4	0.00	0.05	-0.10
-5	0.01	-0.07	0.04
-6	-0.13	-0.69	0.19

-7	0.32	-0.13	-0.37
-8	-0.02	0.01	0.00
-9	0.05	-0.11	0.05
-10	0.03	-0.08	0.09
-11	-0.01	0.00	0.00
-12	-0.05	0.07	0.05
-13	0.05	0.08	0.00
-14	-0.08	-0.01	-0.13

Hartree Fock Energies = -231.788917

MP2 Energies = -232.659122

(30) **7**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.317445
6	1.348829	0.000000	0.715145
6	2.424875	1.096136	0.690205
6	2.424450	-1.096538	0.690014
1	-0.548749	-0.000346	2.235422
1	-0.538279	-0.000049	-0.923918
6	3.473008	-0.000354	0.371075
1	2.301468	-1.881342	-0.048756
1	2.576947	-1.561793	1.659748
1	3.770583	-0.000435	-0.671152
1	4.368281	-0.000568	0.980679
1	2.302337	1.881204	-0.048347
1	2.577559	1.561046	1.660078

Hartree Fock Energies = -231.8529365

MP2 Energies = -232.7397158

(31) **TS-13**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.	0.	0.
6	0.	0.	1.28159

6	0.34845	0.	-1.38237
6	0.53585	1.10408	-2.39955
6	0.71168	-1.10227	-2.35271
1	-0.8014	-0.06242	1.98866
1	-0.994	-0.08792	-0.61108
6	0.92817	0.00292	-3.42653
1	-0.07279	-1.81626	-2.58002
1	1.60164	-1.65843	-2.07399
1	0.263	-0.06808	-4.27755
1	1.94438	0.07624	-3.79045
1	-0.35144	1.67396	-2.65407
1	1.32536	1.806	-2.14861

One imaginary frequency: -1588.4204 cm-1

-1	-0.08	-0.01	-0.06
-2	0.02	0.00	0.02
-3	0.09	0.01	-0.03
-4	0.00	0.00	0.00
-5	0.00	0.00	0.00
-6	-0.03	0.00	-0.02
-7	-0.30	0.00	0.94
-8	0.00	0.00	0.00
-9	-0.01	0.00	0.00
-10	0.00	-0.02	-0.02
-11	0.00	0.00	-0.01
-12	0.00	0.00	0.00
-13	-0.01	-0.01	0.00
-14	0.00	0.02	-0.02

Hartree Fock Energies = -231.745766

MP2 Energies = -232.631622

(32) **8**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.00697	0.00779	-0.03601
6	-0.06327	0.01503	1.1815
6	0.07483	-0.00911	-1.50103
6	-0.25007	-1.32462	-2.25353
6	-1.0539	0.67373	-2.31474

1	-0.1224	0.01962	2.23517
1	1.04042	0.36967	-1.81807
6	-0.95718	-0.48044	-3.33609
1	-0.8718	1.68325	-2.66247
1	-1.99274	0.65549	-1.77409
1	-0.29285	-0.23845	-4.1585
1	-1.88294	-0.86536	-3.74508
1	0.58713	-1.944	-2.5513
1	-0.95175	-1.93242	-1.69465

Hartree Fock Energies = -231.9132143

MP2 Energies = -232.8190032

(33) **CI-6**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.151093	-0.834113	0.149521
6	-0.061576	0.172944	1.095471
6	1.125880	-0.261061	-0.736550
6	1.758372	1.091345	-1.080165
6	1.879119	-0.926278	-1.856883
1	-0.611637	-0.036461	2.001770
1	0.301289	1.194330	1.042293
6	2.198459	0.475808	-2.433727
1	1.302478	-1.627821	-2.445609
1	2.759776	-1.435714	-1.476750
1	1.535543	0.749298	-3.244790
1	3.218960	0.661628	-2.739797
1	1.109056	1.956620	-1.095240
1	2.606251	1.304385	-0.437771

Derivative Coupling

-1	-0.0151051972	-0.0230639428	0.0094066757
-2	0.0110894541	0.0052855507	-0.0186670764
-3	0.0045882446	0.0104114460	0.0016705860
-4	0.0182874362	-0.0025872021	0.0112228024
-5	-0.0095076733	0.0037043773	-0.0042270588
-6	0.0087425575	-0.0035607633	0.0046417285
-7	-0.0149896568	0.0083381106	-0.0058872015

-8	-0.0008897140	0.0002790971	0.0001713748
-9	-0.0003850284	-0.0016954622	0.0005168526
-10	-0.0015513916	0.0013781910	0.0018638198
-11	0.0001898351	-0.0000823973	-0.0000575267
-12	-0.0002906610	0.0001937882	0.0004122056
-13	-0.0021250540	-0.0021723974	0.0019681958
-14	0.0019468487	0.0035716043	-0.0030353777

Unscaled Gradient Difference

-1	0.0341027975	0.0711856183	0.0096690225
-2	-0.0331021297	-0.0177956858	0.0264682233
-3	0.0061655110	-0.0469063281	-0.0349695574
-4	0.0174846268	-0.0068203012	0.0241406640
-5	-0.0141691146	0.0021487885	-0.0078755517
-6	0.0095950158	-0.0020378848	0.0051901920
-7	-0.0199232771	-0.0021400953	-0.0178129388
-8	-0.0022933266	-0.0028005843	0.0028358762
-9	0.0021651960	-0.0021394280	-0.0061591591
-10	0.0003794125	0.0009456627	-0.0006126009
-11	-0.0004753246	0.0001319763	0.0001569993
-12	0.0004916639	0.0008569233	0.0004883550
-13	-0.0034535182	-0.0013206082	0.0009478447
-14	0.0030324674	0.0066919466	-0.0024673691

Hartree Fock Energies = -231.7658312

MP2 Energies = -232.6133849

(34) **Int-7**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.006209	-0.006537	0.017184
6	0.016677	-0.012035	1.315267
6	-0.015723	-0.000768	-1.289542
6	0.047186	1.113137	-2.369757
6	-0.196232	-1.078528	-2.351019
1	-0.891514	0.089908	1.884867
1	0.934290	-0.118530	1.868557
6	-0.372106	0.042298	-3.410307
1	-1.037843	-1.745251	-2.210017
1	0.696417	-1.676703	-2.497584
1	-1.400478	0.154722	-3.731330

1	0.253792	-0.034164	-4.290265
1	-0.621145	1.953003	-2.230001
1	1.075324	1.498288	-2.517970

Hartree Fock Energies = -231.8749794

MP2 Energies = -232.7510034

(35) **TS-14**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.340994
6	0.268803	0.000000	-1.298047
6	-1.096402	1.168171	-0.988147
6	-0.676539	-0.742937	-2.231638
1	-0.765117	0.498717	1.904356
1	0.773217	-0.523362	1.870966
6	-1.612364	0.476369	-2.269769
1	-1.143775	-1.633439	-1.815767
1	-0.239159	-0.990947	-3.188181
1	-2.671723	0.251741	-2.238610
1	-1.411656	1.096704	-3.132325
1	-1.811015	1.095731	-0.178098
1	-0.725032	2.174165	-1.063630

One imaginary frequency: -753.5184 cm-1

-1	-0.16	0.23	-0.12
-2	-0.04	0.03	-0.08
-3	0.22	-0.17	-0.11
-4	-0.07	-0.08	0.23
-5	0.01	-0.01	0.00
-6	0.28	0.38	0.05
-7	-0.27	-0.43	-0.19
-8	0.05	0.00	0.06
-9	-0.05	0.03	0.03
-10	-0.06	-0.05	-0.02
-11	0.06	-0.01	0.03
-12	0.05	0.07	0.11
-13	-0.31	0.13	0.02

-14 0.12 -0.15 0.20

Hartree Fock Energies = -231.7736957

MP2 Energies = -232.6508322

(36) **Int-8**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.347826
6	1.300986	0.000000	-0.742112
6	-1.204595	-0.056343	-0.924504
6	0.851547	-0.090209	-2.178603
1	-0.906556	-0.038106	1.928362
1	0.930005	0.038384	1.883742
6	-0.599642	-0.601655	-2.225037
1	1.548266	-0.634135	-2.805739
1	0.901060	0.951916	-2.512992
1	-0.605676	-1.688125	-2.210640
1	-1.137053	-0.289295	-3.113204
1	-2.014644	-0.663307	-0.536740
1	-1.599203	0.945433	-1.079490

Hartree Fock Energies = -231.8424098

MP2 Energies = -232.7024510

(37) **TS-15**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.339831
6	1.270889	0.000000	-0.793777
6	-1.230699	-0.096424	-0.895990
6	0.811925	-0.246245	-2.123007
1	-0.906696	-0.093104	1.913696
1	0.922982	0.079506	1.884084
6	-0.667893	-0.559517	-2.250866
1	1.496002	-0.379954	-2.944650

	1	1.145238	0.913544	-1.740511
	1	-0.776837	-1.631985	-2.389264
	1	-1.133462	-0.079410	-3.103506
	1	-1.987947	-0.763858	-0.502977
	1	-1.690479	0.883332	-0.997415

One imaginary frequency: -1114.1084 cm-1

-1	0.00	0.00	0.01
-2	0.00	0.00	0.00
-3	-0.03	0.05	-0.08
-4	0.00	0.00	0.00
-5	-0.02	-0.06	0.02
-6	0.00	0.01	0.00
-7	-0.01	0.00	0.01
-8	0.00	-0.01	0.00
-9	-0.04	0.22	-0.05
-10	0.67	0.09	0.69
-11	-0.03	-0.01	-0.02
-12	0.03	0.01	-0.01
-13	0.00	0.00	0.00
-14	0.01	0.00	0.00

Hartree Fock Energies = -231.8165547

MP2 Energies = -232.6836250

(38) **9**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.	0.	0.
6	0.	0.	1.31932
6	1.19838	0.	-0.90135
6	-1.22933	-0.00953	-0.94123
6	0.83115	-0.16954	-2.17844
1	-0.91474	-0.01899	1.88609
1	0.91728	0.02032	1.88185
6	-0.66212	-0.33447	-2.34035
1	1.51154	-0.23029	-3.0087
1	2.20663	0.10104	-0.54389
1	-0.89903	-1.35135	-2.64281
1	-1.0648	0.31826	-3.10808

1	-1.97977	-0.71734	-0.61268
1	-1.68266	0.97596	-0.93393

Hartree Fock Energies = -231.9325696

MP2 Energies = -232.8053510

(39) **CI-7**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.259711	-0.045634	-0.520944
6	-0.238161	-0.404998	0.634248
6	0.895110	0.496971	-1.555922
6	0.198992	0.955281	-2.816178
6	-0.471240	-1.294230	-2.350501
1	-0.457794	-1.431335	0.862948
1	-0.432447	0.333070	1.392277
6	-0.972474	-0.017112	-2.986282
1	-1.150969	-1.944211	-1.829102
1	0.368280	-1.785631	-2.810404
1	-1.834135	0.341397	-2.435512
1	-1.281907	-0.153762	-4.019785
1	-0.102480	1.995222	-2.739078
1	0.898946	0.890856	-3.671043

Derivative Coupling

-1	0.0095783972	0.0076177850	-0.0163944305
-2	0.0007207479	0.0021572011	0.0023347179
-3	-0.0065179220	0.0247271570	0.0186226198
-4	0.0047283880	-0.0092208183	0.0044525368
-5	-0.0098880770	-0.0146915048	-0.0148675265
-6	-0.0109194830	0.0011875764	-0.0047420639
-7	0.0102509710	-0.0020970318	0.0050665154
-8	-0.0002315517	-0.0084280250	0.0055092602
-9	0.0004435766	-0.0000773240	0.0000608717
-10	-0.0010190135	-0.0011731781	-0.0015922365
-11	-0.0007349993	-0.0001843330	-0.0001875658
-12	0.0020835305	0.0002029263	0.0005033017
-13	0.0020436688	0.0005646931	0.0015862171
-14	-0.0005382335	-0.0005851239	-0.0003522174

Unscaled Gradient Difference

-1	-0.0732348256	-0.0493961577	-0.0341020125
-2	-0.0066305663	-0.0027727204	0.0157292400
-3	0.0556094396	0.0089320649	-0.0435531591
-4	-0.0227891586	-0.0130229417	0.0120288476
-5	0.0501968822	0.0481930672	0.0569943195
-6	-0.0082754816	0.0035620209	-0.0044518527
-7	0.0131292620	-0.0011193457	0.0042392501
-8	-0.0054795172	0.0092570336	-0.0094491416
-9	0.0016790350	0.0008316257	0.0013365839
-10	-0.0030735966	-0.0010632670	-0.0018171959
-11	0.0003250545	-0.0017946531	0.0004555625
-12	-0.0024156865	-0.0042219583	-0.0002041390
-13	0.0005980707	0.0026214870	0.0004193194
-14	0.0003610884	-0.0000062555	0.0023743779

Hartree Fock Energies = -231.7165321

MP2 Energies = -232.5788361

(40) **10**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.593091	-1.345506	-2.473005
6	-1.184891	-0.270112	-3.002021
1	-0.891019	-1.743052	-1.518089
1	0.203925	-1.860092	-2.980675
1	-1.987284	0.240024	-2.498074
1	-0.890911	0.123764	-3.960058

Hartree Fock Energies = -78.0752205

MP2 Energies = -78.3747002

(41) **11**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.031672	0.057520	-0.483984
6	-0.207086	-0.446972	0.691935
6	0.262152	0.561268	-1.634259

6	0.461915	1.150134	-2.799386
1	-0.031067	-1.487869	0.899306
1	-0.588218	0.160833	1.493689
1	0.257099	2.196587	-2.937295
1	0.836237	0.599360	-3.643363

Hartree Fock Energies = -153.7715384

MP2 Energies = -154.3213392