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Supporting Informationto "The $[C_6H_{10}]^+$ Hypersurface: The Parent Radical Cation Diels-Alder Reaction."

by Matthias Hofmann and Henry F. Schaefer III

Cartesian coordinates of $[C_6H_{10}]^+$ stationary points optimized at the UMP2(fc)/DZP level unless stated otherwise. Absolute energies at the level of optimization and from CCSD(T)/DZP single point energy calculations are also given.

1

MP2=-78.32171; CCSD(T)=-78.36095

C	0.00000	0.00000	0.00000
C	1.34697	0.00000	0.00000
H	-0.56607	0.92933	0.00000
H	-0.56607	-0.92933	0.00000
H	1.91304	0.92933	0.00000
H	1.91304	-0.92933	0.00000

2

MP2=-155.14653; CCSD(T)=-155.22023

C	0.00000	0.00000	0.00000
C	1.38908	0.00000	0.00000
C	2.20255	1.17018	0.00000
C	1.71862	2.47223	0.00000
H	-0.54531	-0.94155	0.00000
H	2.41122	3.31140	0.00000
H	-0.58970	0.91380	0.00000
H	0.65663	2.70664	0.00000
H	1.89954	-0.96281	0.00000
H	3.28288	1.02711	0.00000

3

MP2=-233.48403; CCSD(T)=-233.59574

C	0.00000	0.00000	0.00000
C	1.37072	0.00000	0.00000
C	2.18289	1.16031	0.00000
C	1.72239	2.47937	0.06598
C	0.89009	3.10531	-2.29433
C	2.19892	3.48671	-2.29546
H	-0.54985	-0.93765	0.00388
H	-0.58473	0.91586	-0.00365
H	1.88263	-0.96175	0.00605
H	3.26200	1.00976	-0.03747
H	2.43217	3.28637	0.23321
H	0.67410	2.72165	0.22564
H	0.59582	2.10347	-2.60394

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H	0.09963	3.82198	-2.07467
H	2.98990	2.79646	-2.58547
H	2.48554	4.50910	-2.05258

TS - 3/4

MP2=-233.47897; CCSD(T)=-233.59614

C	0.00000	0.00000	0.00000
C	1.35562	0.00000	0.00000
C	2.17261	1.16544	0.00000
C	1.72079	2.50122	0.00495
C	1.48067	2.70730	-2.13190
C	1.64531	4.05771	-2.00087
H	-0.55208	-0.93586	0.00863
H	-0.58769	0.91444	-0.00124
H	1.87435	-0.95722	0.01648
H	3.25218	1.01202	-0.02831
H	2.45038	3.26640	0.26294
H	0.68680	2.73096	0.25429
H	2.29703	2.09569	-2.51280
H	0.48393	2.26833	-2.15007
H	2.62333	4.51924	-2.12642
H	0.81648	4.70537	-1.71916

4

MP2=-233.49428; CCSD(T)=-233.59901

C	0.00000	0.00000	0.00000
C	1.37916	0.00000	0.00000
C	2.13067	1.19905	0.00000
C	1.65449	2.57224	-0.14686
C	2.25018	3.13322	-1.50075
C	3.73488	3.31227	-1.46186
H	-0.55338	-0.93815	0.01955
H	-0.57698	0.92251	-0.00905
H	1.91520	-0.94682	0.03078
H	3.21858	1.08644	0.05614
H	2.09437	3.17882	0.65873
H	0.56675	2.66948	-0.13827
H	1.94540	2.48713	-2.33213
H	1.73863	4.09863	-1.63885
H	4.33761	3.08031	-2.33388
H	4.18162	3.91677	-0.67667

TS-4/5

MP2=-233.48644; CCSD(T)=-233.59139

C	0.00000	0.00000	0.00000
C	1.38009	0.00000	0.00000
C	2.15303	1.18107	0.00000
C	1.74731	2.59864	-0.16039
C	0.71637	2.94597	-1.26189
C	1.09504	2.38528	-2.60145
H	-0.55101	-0.93713	0.07537

H	-0.57477	0.92113	-0.03779
H	1.90765	-0.94868	0.08325
H	3.22160	1.01270	0.17478
H	2.66125	3.18345	-0.31036
H	1.35864	2.90162	0.83267
H	0.68439	4.04637	-1.30463
H	-0.29804	2.64051	-0.98553
H	2.13638	2.41073	-2.91555
H	0.34089	2.30746	-3.37917

5

MP2=-233.48738; CCSD(T)=-233.59449

C	0.00000	0.00000	0.00000
C	1.38119	0.00000	0.00000
C	2.17153	1.16940	0.00000
C	1.86177	2.59300	0.21375
C	0.44810	3.12853	0.43328
C	-0.41802	3.10735	-0.79270
H	-0.54155	-0.94568	-0.02021
H	-0.57628	0.92068	-0.03654
H	1.90674	-0.95247	-0.04606
H	3.24282	0.98338	-0.13840
H	2.37256	3.12568	-0.61121
H	2.51594	2.84109	1.07608
H	-0.03428	2.60906	1.27394
H	0.56334	4.17101	0.77171
H	-1.47445	3.34479	-0.69721
H	0.03297	3.22456	-1.77557

TS-5/6

MP2=-233.48451; CCSD(T)=-233.59562

C	-1.26700	-1.17949	-0.42868
C	-1.66011	-0.01631	0.18403
C	-0.83912	1.11191	0.17215
C	0.59950	1.24164	-0.12421
C	1.49440	0.01892	-0.36802
C	1.30861	-1.11619	0.59405
H	-1.91134	-2.06059	-0.39900
H	-0.38230	-1.25057	-1.04843
H	-2.64302	0.04669	0.64493
H	-1.30242	2.04080	0.52244
H	0.97361	1.82665	0.73765
H	0.68092	1.97321	-0.95077
H	1.40564	-0.33119	-1.40596
H	2.53382	0.37747	-0.28534
H	1.78689	-2.06928	0.37947
H	1.04057	-0.91604	1.62909

6

MP2=-233.55967; CCSD(T)=-233.66206

C	0.71605	1.30303	0.04684
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C	0.32210	0.63689	1.29721
C	-0.32210	-0.63689	1.29721
C	-0.71605	-1.30303	0.04684
C	-0.64756	-0.40873	-1.19587
C	0.64756	0.40873	-1.19587
H	1.68860	1.79858	0.18987
H	0.00000	2.15182	-0.03465
H	0.49258	1.13316	2.25577
H	-0.49258	-1.13316	2.25577
H	-1.68860	-1.79858	0.18987
H	0.00000	-2.15182	-0.03465
H	-1.51577	0.26425	-1.20661
H	-0.71060	-1.03283	-2.09347
H	0.71060	1.03283	-2.09347
H	1.51577	-0.26425	-1.20661

TS-6/7 //UHF/6-31G*

HF=-232.68737; CCSD(T)=-233.60647

C	-1.50855	0.93278	0.42117
C	-1.54791	-0.20581	-0.34626
C	-0.59105	-1.20754	-0.21379
C	0.67014	-1.05179	0.54703
C	1.58496	-0.02932	-0.22588
C	1.06396	1.37335	-0.23013
H	-2.14902	1.76632	0.19763
H	-0.94384	0.99392	1.32879
H	-2.29374	-0.29747	-1.11490
H	-0.70485	-2.08417	-0.82855
H	0.49327	-0.67973	1.54938
H	1.18198	-1.99990	0.62571
H	1.74380	-0.38451	-1.23616
H	2.54584	-0.06004	0.27693
H	0.90336	1.89098	-1.15737
H	1.19395	1.98455	0.64568

7 //UHF/6-31G*

HF=-232.68975; CCSD(T)=-233.59843

C	0.00000	0.00000	0.00000
C	1.36156	0.00000	0.00000
C	2.10753	1.18369	0.00000
C	1.63569	2.58069	-0.02816
C	1.76462	3.13509	-1.49530
C	0.74857	2.56514	-2.43647
H	-0.54663	-0.92468	-0.03457
H	-0.58094	0.90107	0.03231
H	1.89140	-0.93388	-0.02381
H	3.17834	1.06140	-0.03589
H	2.28699	3.16468	0.61324
H	0.61825	2.69303	0.31650
H	1.63810	4.20847	-1.40255
H	2.77196	2.97010	-1.85914

H	-0.27911	2.87306	-2.36322
H	1.04907	2.02337	-3.31328

TS-3/7 //UHF/6-31G*

HF=-232.68027; CCSD(T)=-233.59690

C	0.00000	0.00000	0.00000
C	1.36555	0.00000	0.00000
C	2.17169	1.16450	0.00000
C	1.72859	2.49841	-0.07221
C	1.76557	2.94820	-1.91846
C	0.59316	2.44426	-2.53073
H	-0.54362	-0.92541	-0.01922
H	-0.58622	0.89860	0.03729
H	1.88104	-0.94288	-0.00219
H	3.23716	1.01126	-0.00798
H	2.44087	3.23976	0.24612
H	0.71468	2.72820	0.19697
H	1.78996	4.01182	-1.75065
H	2.70635	2.54394	-2.24697
H	-0.33033	2.99022	-2.47838
H	0.58281	1.48662	-3.01552

8

MP2=-233.48604; CCSD(T)=-233.59547

C	-2.13632	0.81702	0.06134
C	-1.71350	-0.46401	-0.25813
C	-0.47643	-1.02700	0.02508
C	0.61022	-0.31385	0.72978
C	2.06567	-0.20396	-0.35307
C	1.42146	1.02942	-0.29479
H	-3.13351	1.14814	-0.20876
H	-1.52053	1.52676	0.60767
H	-2.42133	-1.10584	-0.78153
H	-0.27500	-2.05395	-0.27153
H	1.21392	-0.90532	1.42877
H	0.29113	0.56036	1.31459
H	2.97010	-0.37311	0.22752
H	1.82945	-0.91201	-1.14386
H	1.79430	1.81489	0.36016
H	0.62488	1.27434	-0.99423

TS-8/9

MP2=-233.48189; CCSD(T)=-233.59690

C	0.00000	0.00000	0.00000
C	1.36568	0.00000	0.00000
C	2.18737	1.14374	0.00000
C	1.70779	2.51154	-0.01763
C	1.97673	2.90114	-1.74612
C	0.84455	3.72460	-1.67424
H	-0.55028	-0.93585	0.01012
H	-0.59058	0.91197	-0.00363

H	1.87829	-0.96099	0.00784
H	3.26511	1.00654	-0.08817
H	2.34989	3.25076	0.46270
H	0.66711	2.63041	0.29677
H	2.96308	3.36293	-1.73510
H	1.89194	1.98557	-2.32751
H	0.90270	4.71921	-1.23189
H	-0.13925	3.34830	-1.95372

9

MP2=-233.49296; CCSD(T)=-233.59932

C	2.27457	-0.90139	0.00127
C	1.87638	0.34298	-0.33957
C	0.69834	0.89295	0.24031
C	-0.44221	0.17732	0.77524
C	-1.36817	0.05061	-0.54433
C	-2.71706	-0.43122	-0.13686
H	3.21942	-1.30773	-0.36054
H	1.69375	-1.53306	0.67187
H	2.51014	0.97857	-0.95354
H	0.57622	1.97835	0.15507
H	-0.98755	0.76937	1.51443
H	-0.24635	-0.83640	1.13086
H	-1.43789	1.01794	-1.05534
H	-0.85686	-0.65985	-1.20757
H	-3.55844	0.25144	-0.09818
H	-2.84357	-1.44609	0.22662

TS-4/10

MP2=-233.48821; CCSD(T)=-233.59824

C	-2.17980	0.26169	-0.55413
C	-1.48905	-0.66402	0.13569
C	-0.28763	-0.29994	0.80909
C	0.49001	0.95234	0.63288
C	1.41570	0.53876	-0.55671
C	1.79890	-0.90259	-0.35699
H	-1.82097	1.28152	-0.68158
H	-3.14807	0.02618	-0.99624
H	-1.89025	-1.66358	0.28331
H	0.07913	-1.00916	1.55528
H	-0.10870	1.83220	0.38408
H	1.08629	1.14824	1.52943
H	0.85975	0.65662	-1.49236
H	2.29692	1.19753	-0.58366
H	1.79485	-1.60295	-1.18835
H	2.36228	-1.18398	0.53105

10

MP2=-233.51489; CCSD(T)=-233.61693

C	-2.17486	0.35442	-0.48810
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C	-1.37022	-0.37552	0.40384
C	-0.02332	-0.05122	0.76068
C	0.81621	1.09836	0.21068
C	1.81454	0.06087	-0.36722
C	0.76150	-1.07129	-0.36162
H	-3.19740	0.03964	-0.68045
H	-1.81501	1.25862	-0.97110
H	-1.77599	-1.30194	0.81856
H	0.30019	-0.43956	1.73129
H	0.30873	1.65500	-0.58261
H	1.20392	1.78947	0.96264
H	2.60966	-0.16165	0.35079
H	2.23217	0.27856	-1.35490
H	0.97867	-2.04765	0.07939
H	0.21200	-1.16421	-1.30316

TS-10/10

MP2=-233.50697; CCSD(T)=-233.60984

C	-1.94669	1.12068	0.00000
C	-0.59175	1.50105	0.00000
C	0.48972	0.58012	0.00000
C	0.48972	-0.67700	-1.05365
C	1.05730	-1.63036	0.00000
C	0.48972	-0.67700	1.05365
H	-2.73077	1.87448	0.00000
H	-2.25023	0.07604	0.00000
H	-0.37644	2.57225	0.00000
H	1.47120	1.06093	0.00000
H	-0.53609	-0.91161	-1.34855
H	1.10200	-0.38846	-1.91509
H	2.15062	-1.63535	0.00000
H	0.67571	-2.65316	0.00000
H	1.10200	-0.38846	1.91509
H	-0.53609	-0.91161	1.34855

TS-6/10

MP2=-233.48672; CCSD(T)=-233.59346

C	1.66231	-0.04061	0.77703
C	0.95694	0.57823	-0.34708
C	-0.30166	1.23614	-0.22504
C	-1.42181	0.46042	0.39142
C	-0.99037	-1.01165	0.18523
C	0.20595	-0.91405	-0.77762
H	1.15680	-0.25760	1.71523
H	2.60859	-0.53541	0.56834
H	1.62508	0.96056	-1.12408
H	-0.48926	2.14389	-0.80101
H	-1.58287	0.74749	1.44277
H	-2.34959	0.70141	-0.14057
H	-0.70152	-1.49344	1.12283
H	-1.78724	-1.61359	-0.26275

H	0.93150	-1.72971	-0.71887
H	-0.07972	-0.77439	-1.82551

11

MP2=-155.15334; CCSD(T)=-155.22612

C	0.00000	0.00000	0.00000
C	1.39096	0.00000	0.00000
C	2.11464	1.21626	0.00000
C	3.50559	1.21626	0.00000
H	-0.56342	-0.93089	0.00000
H	-0.55765	0.93537	0.00000
H	1.93169	-0.94713	0.00000
H	1.57390	2.16339	0.00000
H	4.06902	2.14715	0.00000
H	4.06324	0.28089	0.00000

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MP2=-233.49057; CCSD(T)=-233.60101

C	-2.83221	-0.47790	0.32675
C	-1.68286	-0.19234	-0.36395
C	-0.71402	0.68650	0.16449
C	0.43298	1.04672	-0.54956
C	2.15491	-0.86643	-0.37004
C	2.35200	-0.15430	0.77647
H	-3.59107	-1.13830	-0.08551
H	-3.01708	-0.04383	1.30719
H	-1.51990	-0.63242	-1.34838
H	-0.87765	1.11242	1.15578
H	0.56547	0.71173	-1.57742
H	1.06639	1.86228	-0.20878
H	1.44440	-1.69099	-0.40627
H	2.75905	-0.68020	-1.25686
H	3.10827	0.62752	0.82951
H	1.79726	-0.38171	1.68568

TS-12/13

MP2=-233.48571; CCSD(T)=-233.60147

C	1.68947	-0.94930	2.14428
C	1.12617	-0.93273	0.91121
C	-0.23399	-0.57430	0.73894
C	-0.87923	-0.57516	-0.51181
C	-0.76492	1.54106	-0.86662
C	-0.81493	1.33011	-2.22043
H	2.72170	-1.25634	2.29196
H	1.12009	-0.66271	3.02606
H	1.70871	-1.23070	0.03938
H	-0.79988	-0.26162	1.61935
H	-0.36125	-1.03889	-1.35096
H	-1.96672	-0.59808	-0.54294
H	0.18315	1.79477	-0.39580
H	-1.67263	1.78368	-0.31568

H	0.09521	1.24955	-2.81175
H	-1.76380	1.18227	-2.73309

13

MP2=-233.49921; CCSD(T)=-233.60533

C	2.86622	-0.35191	-0.19073
C	1.69308	-0.14601	0.46161
C	0.69232	0.59072	-0.21478
C	-0.64822	0.80638	0.27958
C	-1.43426	-0.48797	-0.30544
C	-2.87901	-0.35246	0.02609
H	3.69565	-0.88747	0.27151
H	3.01628	0.01840	-1.20547
H	1.53003	-0.50168	1.47681
H	0.92653	0.93014	-1.23020
H	-0.72296	0.77294	1.36933
H	-1.12140	1.69544	-0.14432
H	-0.99253	-1.37382	0.16638
H	-1.28171	-0.54538	-1.38892
H	-3.22373	-0.54514	1.03690
H	-3.56692	0.08407	-0.68999

TS-13/14

MP2=-233.49377; CCSD(T)=-233.60265

C	0.06952	2.75110	-3.01037
C	0.97099	2.02700	-2.31497
C	0.86269	2.04842	-0.89739
C	1.91482	1.50616	0.00000
C	1.50562	0.00000	0.00000
C	0.00000	0.00000	0.00000
H	0.14937	2.88577	-4.08904
H	-0.76533	3.24278	-2.51013
H	1.81515	1.53997	-2.79830
H	0.01402	2.59240	-0.47197
H	2.92240	1.65555	-0.40338
H	1.83067	1.92803	1.00571
H	1.89028	-0.48735	-0.90058
H	1.92652	-0.50353	0.88283
H	-0.56578	-0.63722	-0.67598
H	-0.52690	0.40566	0.86280

14

MP2=-233.51551; CCSD(T)=-233.61739

C	2.47178	0.06384	-0.05381
C	1.14343	-0.20642	-0.42671
C	0.10882	-0.46770	0.52197
C	-1.25228	-1.00212	0.04351
C	-1.71368	0.39260	-0.44981
C	-0.61189	1.09036	0.35578
H	3.23917	0.22266	-0.80685
H	2.75676	0.10003	0.99560

H	0.88090	-0.17528	-1.48800
H	0.45260	-0.66019	1.54235
H	-1.19718	-1.80174	-0.70153
H	-1.83565	-1.34069	0.90426
H	-1.57358	0.52985	-1.52614
H	-2.72972	0.69006	-0.17392
H	-0.02645	1.89757	-0.09456
H	-0.84393	1.31440	1.40322

TS-14/14

MP2=-233.51119; CCSD(T)=-233.61361

C	2.44084	1.07645	0.00000
C	1.44512	0.09093	0.00000
C	0.06177	0.39375	0.00000
C	-0.90066	-0.43185	-1.04629
C	-1.99217	-0.65357	0.00000
C	-0.90066	-0.43185	1.04629
H	3.49520	0.81011	0.00000
H	2.17543	2.13195	0.00000
H	1.75029	-0.95863	0.00000
H	-0.17806	1.46107	0.00000
H	-1.09230	0.23295	-1.89599
H	-0.38259	-1.34733	-1.34388
H	-2.73438	0.14863	0.00000
H	-2.48411	-1.62755	0.00000
H	-1.09230	0.23295	1.89599
H	-0.38259	-1.34733	1.34388

TS-10/14

MP2=-233.50279; CCSD(T)=-233.60743

C	-0.29774	-2.36744	0.81419
C	-0.71861	-1.01054	0.74555
C	0.00000	0.00000	0.00000
C	1.57657	0.00000	0.00000
C	1.46740	1.54984	0.00000
C	-0.00586	1.47940	0.48726
H	-0.91441	-3.11790	1.30532
H	0.64127	-2.67374	0.35674
H	-1.61930	-0.73232	1.30276
H	-0.33886	-0.04401	-1.05708
H	1.97220	-0.38121	0.94859
H	2.07494	-0.48597	-0.84338
H	2.17127	2.08099	0.64648
H	1.52115	1.93956	-1.02193
H	-0.07739	1.53502	1.57928
H	-0.73255	2.15373	0.02700

TS-10/14* //UHF/6-31G*

HF=-232.65866

C	-1.57822	1.46099	-1.33533
C	-0.42986	0.86051	-1.07910

C	-0.38598	-0.42002	-0.32000
C	-0.38725	-0.44513	1.18869
C	1.15820	-0.45404	1.38582
C	1.52198	-0.93263	0.01099
H	-1.59823	2.38483	-1.88199
H	-2.52875	1.06575	-1.02157
H	0.49990	1.28114	-1.41866
H	-0.69213	-1.31137	-0.84745
H	-0.86291	0.42532	1.61788
H	-0.83796	-1.35123	1.56805
H	1.53985	0.53797	1.57597
H	1.47587	-1.13242	2.16675
H	2.09693	-0.32894	-0.66954
H	1.51424	-1.98905	-0.19590

TS-14/15

MP2=-233.50158; CCSD(T)=-233.60454

C	-2.30752	0.01984	-0.01473
C	-0.88553	0.04346	-0.36128
C	-0.01742	1.07549	0.09192
C	1.44592	0.82160	-0.01970
C	1.49515	-0.70763	-0.19254
C	0.14528	-1.08741	0.42935
H	-3.01129	-0.51324	-0.64256
H	-2.67127	0.52598	0.87361
H	-0.64109	-0.31390	-1.37139
H	-0.40691	1.90544	0.69361
H	1.90183	1.43866	-0.81139
H	1.91436	1.13906	0.92256
H	1.52498	-1.00366	-1.24668
H	2.34118	-1.17313	0.32181
H	-0.31508	-2.03898	0.14556
H	0.10793	-0.95830	1.51673

15 //UHF/6-31G*

HF=-232.69840; CCSD(T)=-233.61238

C	0.00000	0.00000	0.00000
C	1.50044	0.00000	0.00000
C	2.17340	1.30140	0.00000
C	3.41057	1.28623	0.76953
C	3.66394	-0.20061	1.08790
C	2.25233	-0.80516	1.08960
H	-0.52318	0.00659	0.93704
H	-0.55418	-0.02143	-0.91736
H	1.86652	-0.35011	-0.98742
H	1.79290	2.16855	-0.51689
H	4.21448	1.87254	0.33902
H	3.10122	1.83030	1.67852
H	4.27503	-0.64145	0.30857
H	4.18240	-0.32890	2.02680
H	2.23896	-1.86423	0.87739

H	1.76450	-0.65201	2.04656
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16

MP2=-233.55599; CCSD(T)=-233.65795

C	0.00000	0.00000	0.00000
C	1.42357	0.00000	0.00000
C	2.26637	-0.04515	1.21233
C	3.68943	-0.33044	0.69500
C	3.68943	0.33044	-0.69500
C	2.26638	0.04515	-1.21233
H	-0.55362	0.00000	0.93652
H	-0.55362	-0.00000	-0.93652
H	2.21259	0.99989	1.59211
H	1.86852	-0.68159	2.01313
H	4.45677	0.07075	1.36288
H	3.83989	-1.41416	0.61001
H	3.83989	1.41416	-0.61001
H	4.45677	-0.07075	-1.36288
H	1.86852	0.68159	-2.01313
H	2.21259	-0.99989	-1.59211

TS-16/17

MP2=-233.49121; CCSD(T)=-233.59012

C	-1.75916	-0.24395	0.38215
C	-0.63499	-0.69520	-0.48767
C	0.67806	-1.26148	0.00171
C	1.59837	-0.01068	0.04763
C	0.65137	1.19789	0.25870
C	-0.60453	0.77698	-0.51247
H	-2.77073	-0.34370	-0.02304
H	-1.61923	-0.33637	1.46305
H	0.54511	-1.72429	0.98785
H	1.05725	-2.03165	-0.67831
H	2.35509	-0.07528	0.83574
H	2.11478	0.09845	-0.91269
H	1.03617	2.14508	-0.13256
H	0.41811	1.34302	1.32146
H	-1.06278	1.34258	-1.33016
H	-1.64845	1.00076	0.32833

17

MP2=-233.57244; CCSD(T)=-233.67472

C	-1.75916	-0.24395	0.38215
C	-0.63499	-0.69520	-0.48767
C	0.67806	-1.26148	0.00171
C	1.59837	-0.01068	0.04763
C	0.65137	1.19789	0.25870
C	-0.60453	0.77698	-0.51247
H	-2.77073	-0.34370	-0.02304
H	-1.61923	-0.33637	1.46305
H	0.54511	-1.72429	0.98785

H	1.05725	-2.03165	-0.67831
H	2.35509	-0.07528	0.83574
H	2.11478	0.09845	-0.91269
H	1.03617	2.14508	-0.13256
H	0.41811	1.34302	1.32146
H	-1.06278	1.34258	-1.33016
H	-1.64845	1.00076	0.32833

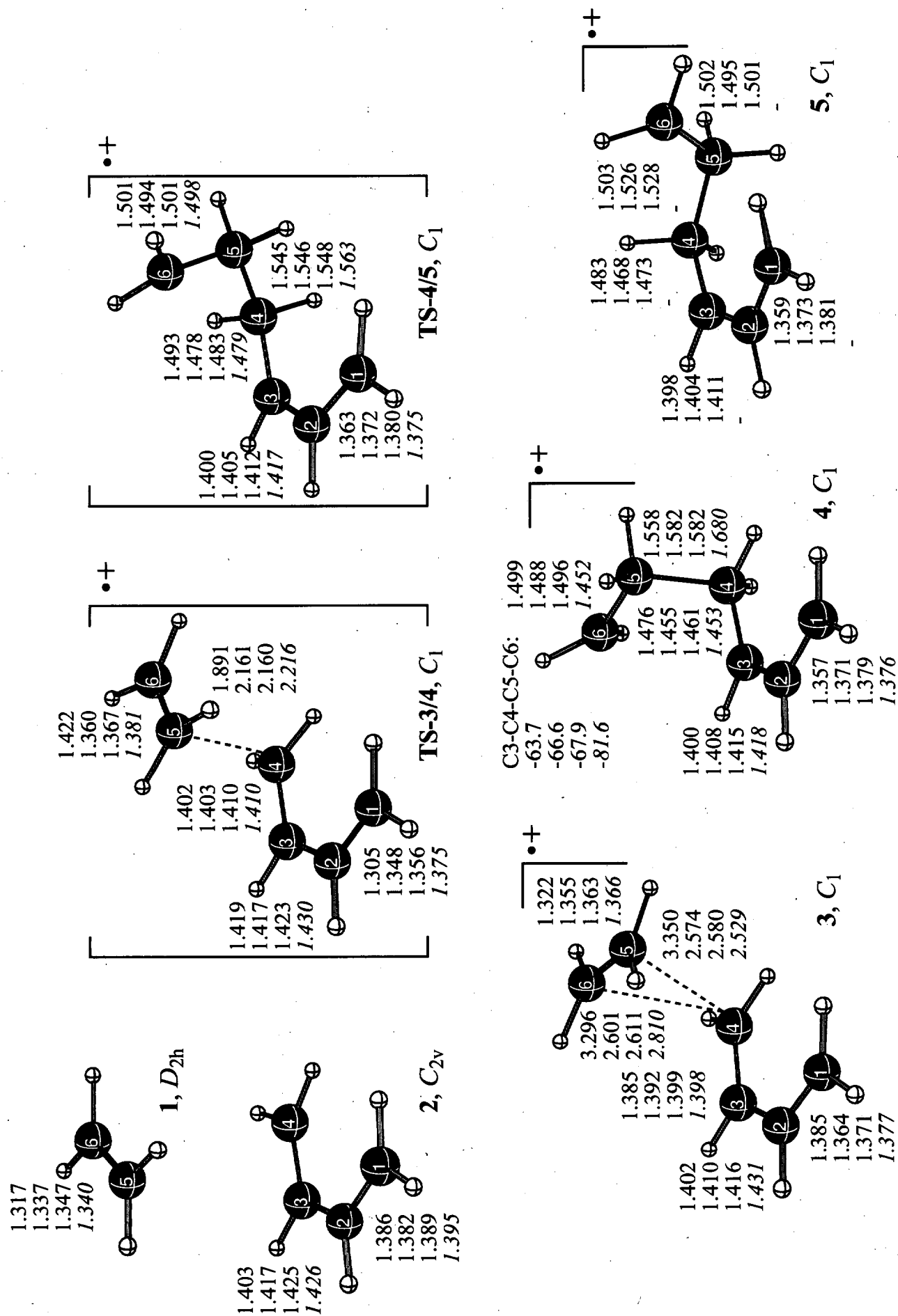


Figure 1

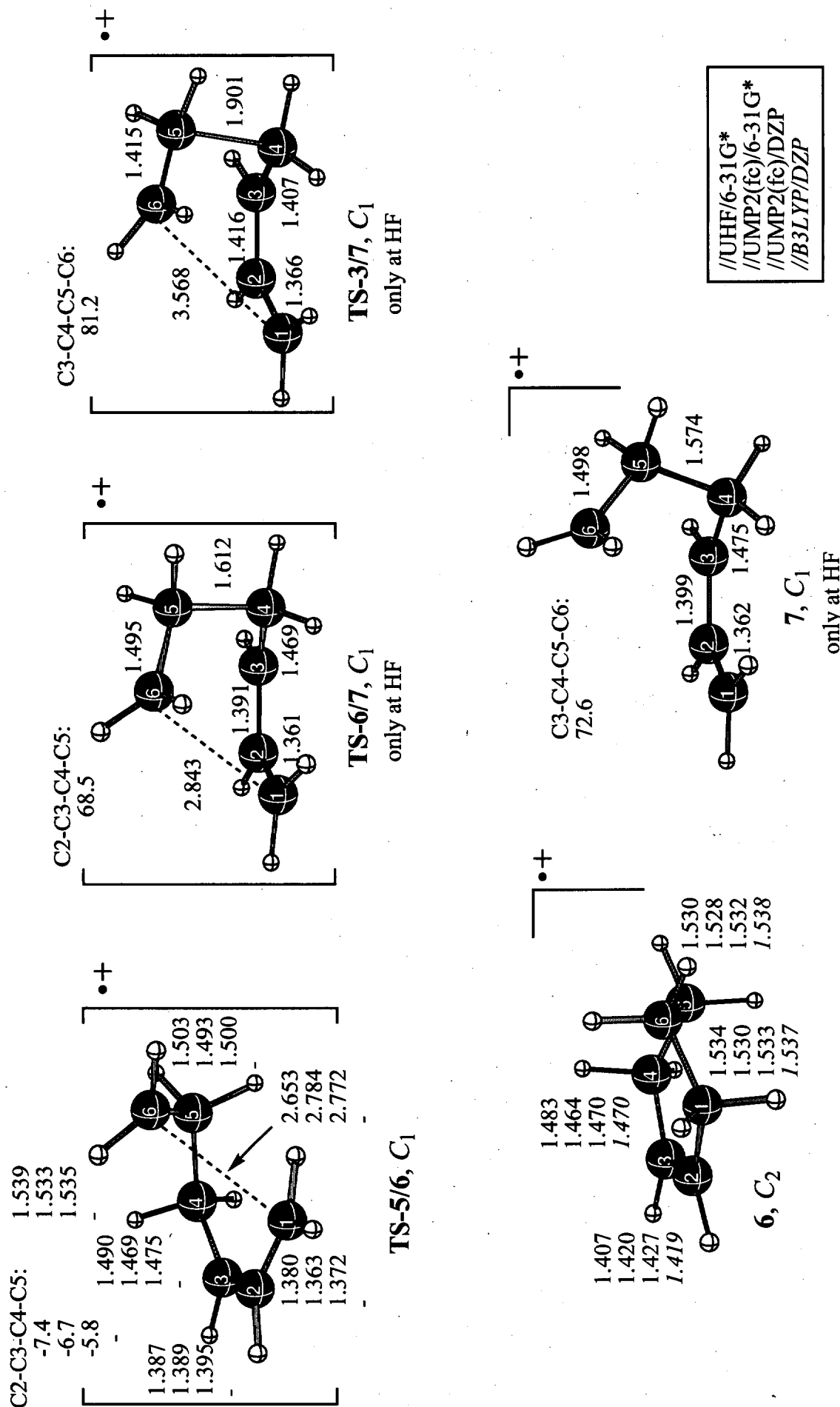


Figure 1 continued

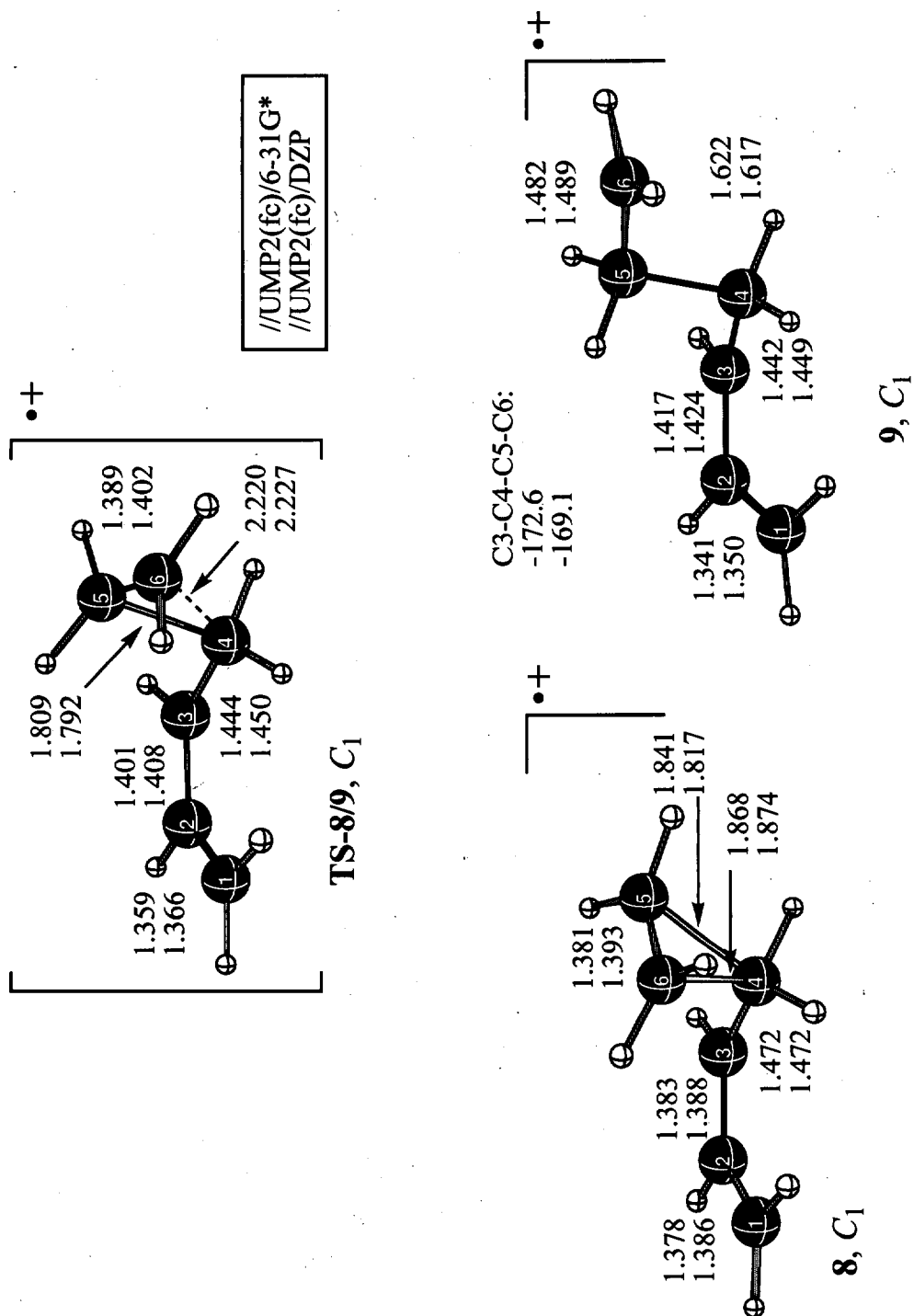


Figure 2

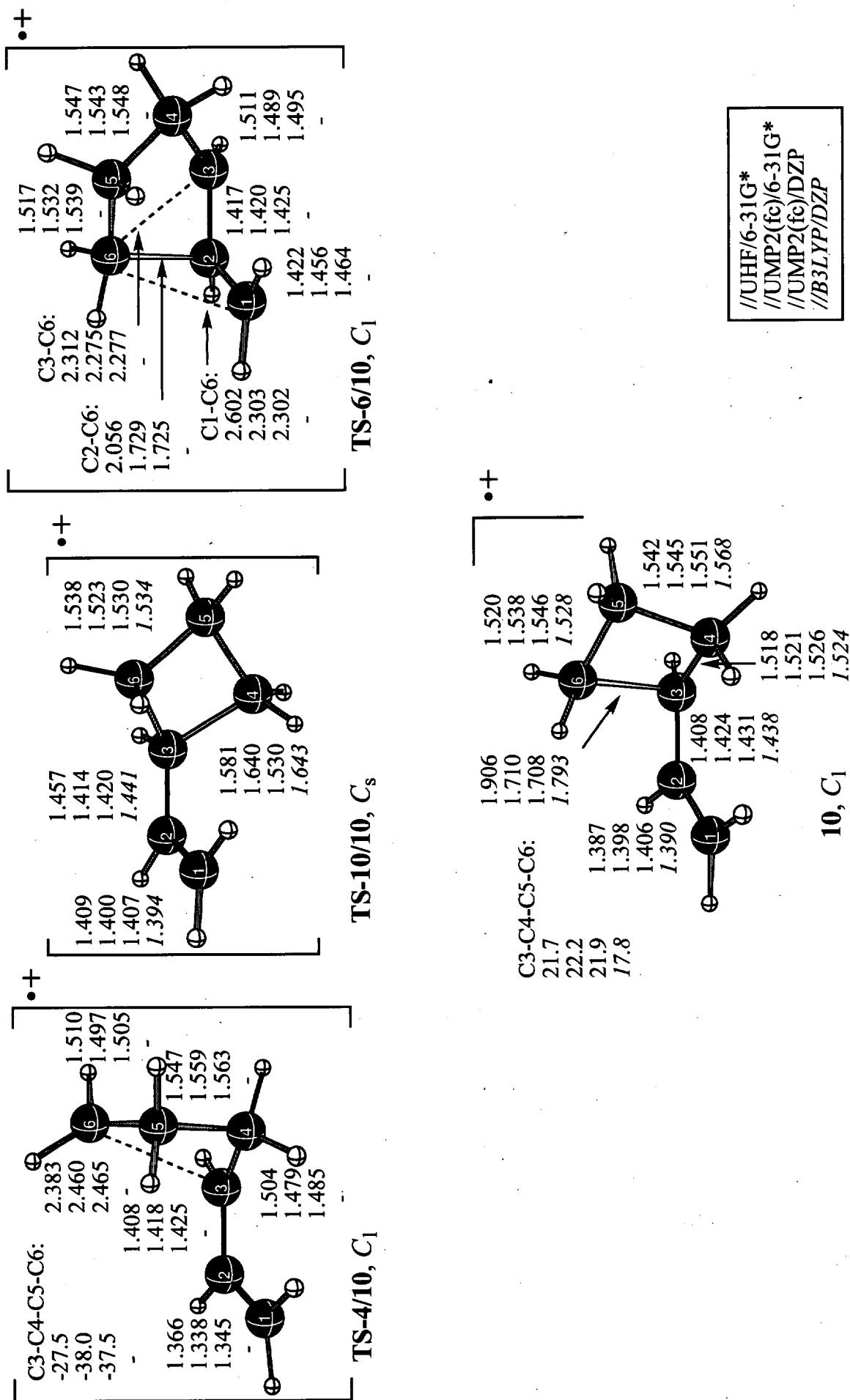


Figure 3

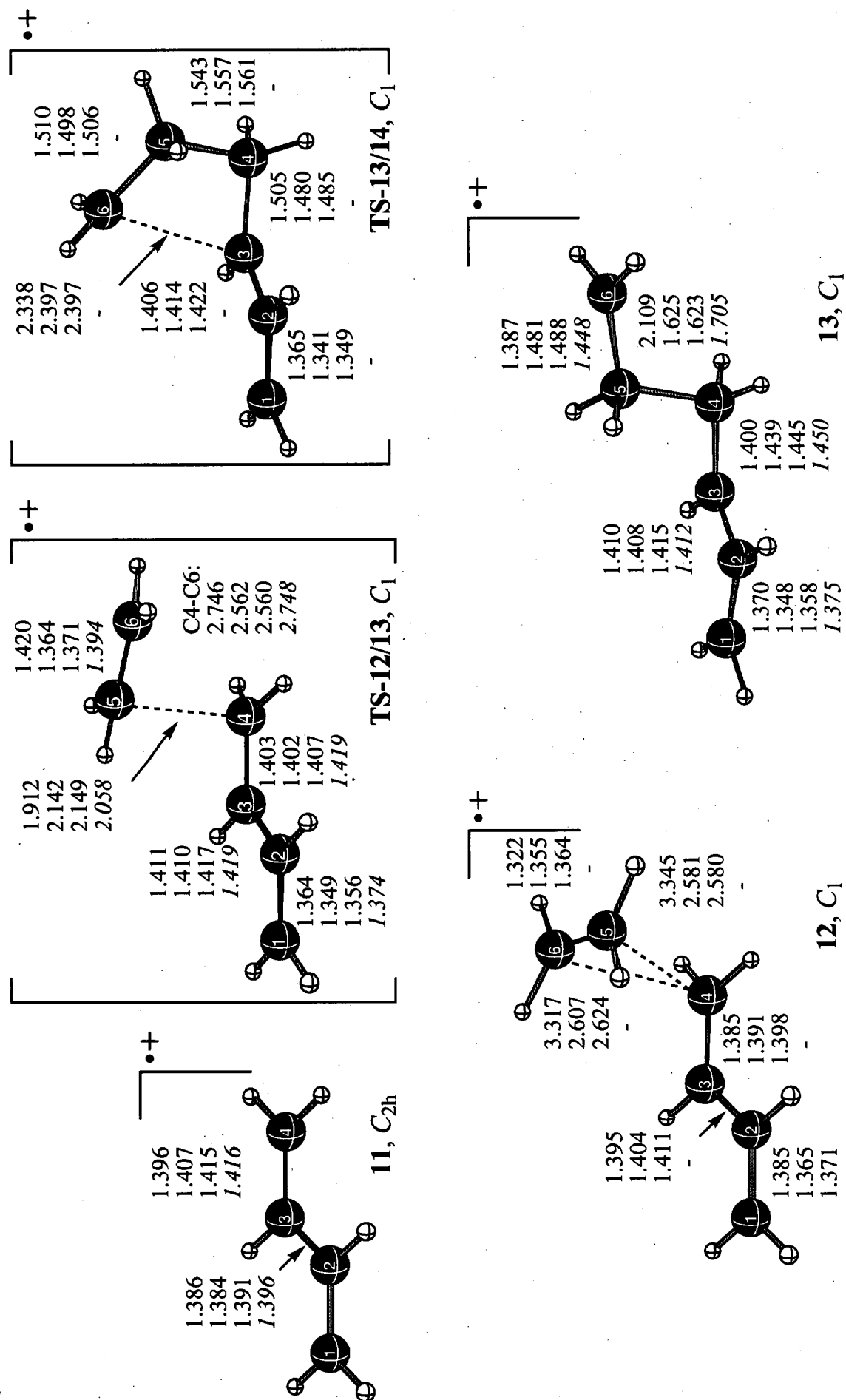
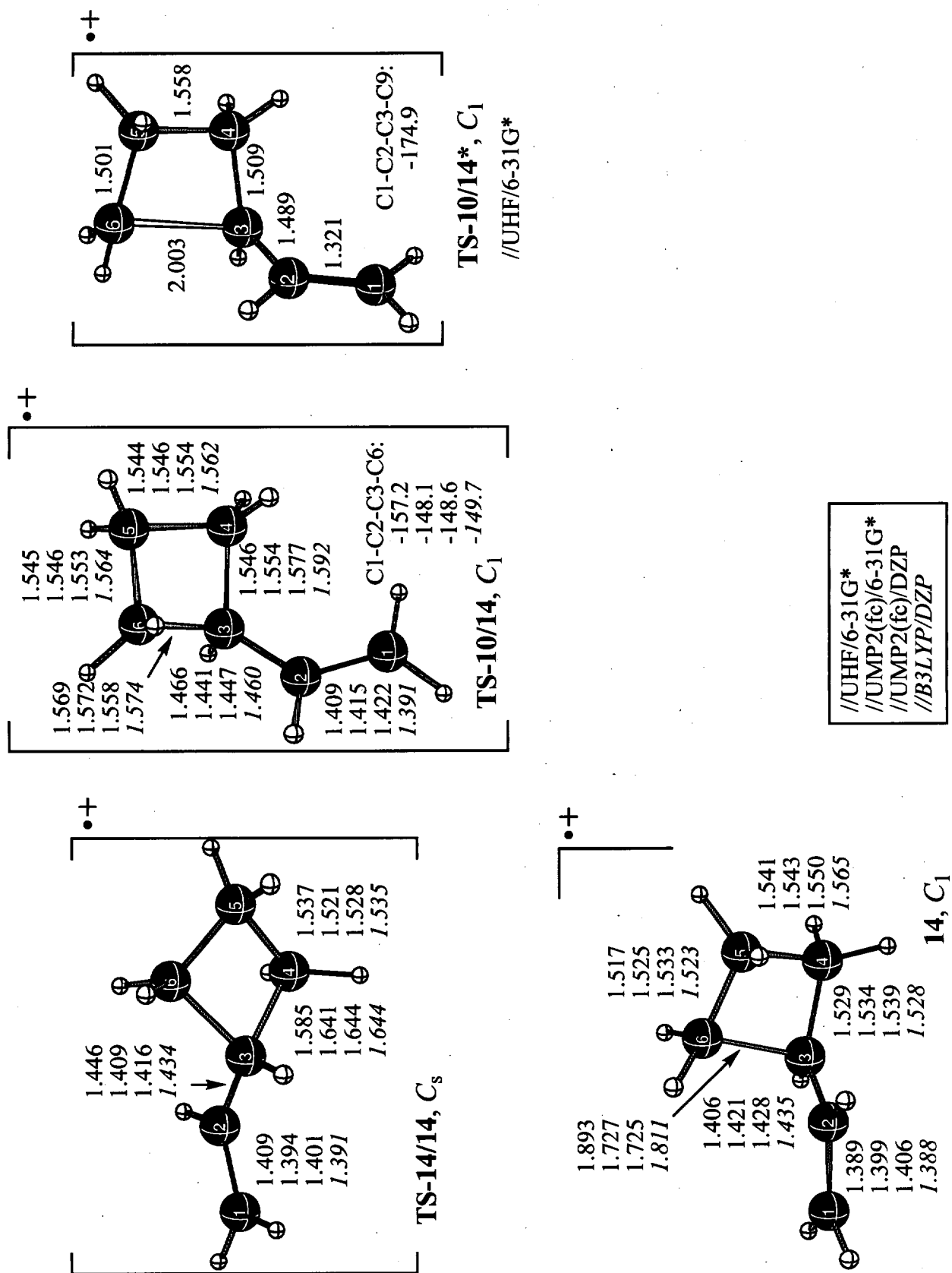


Figure 4



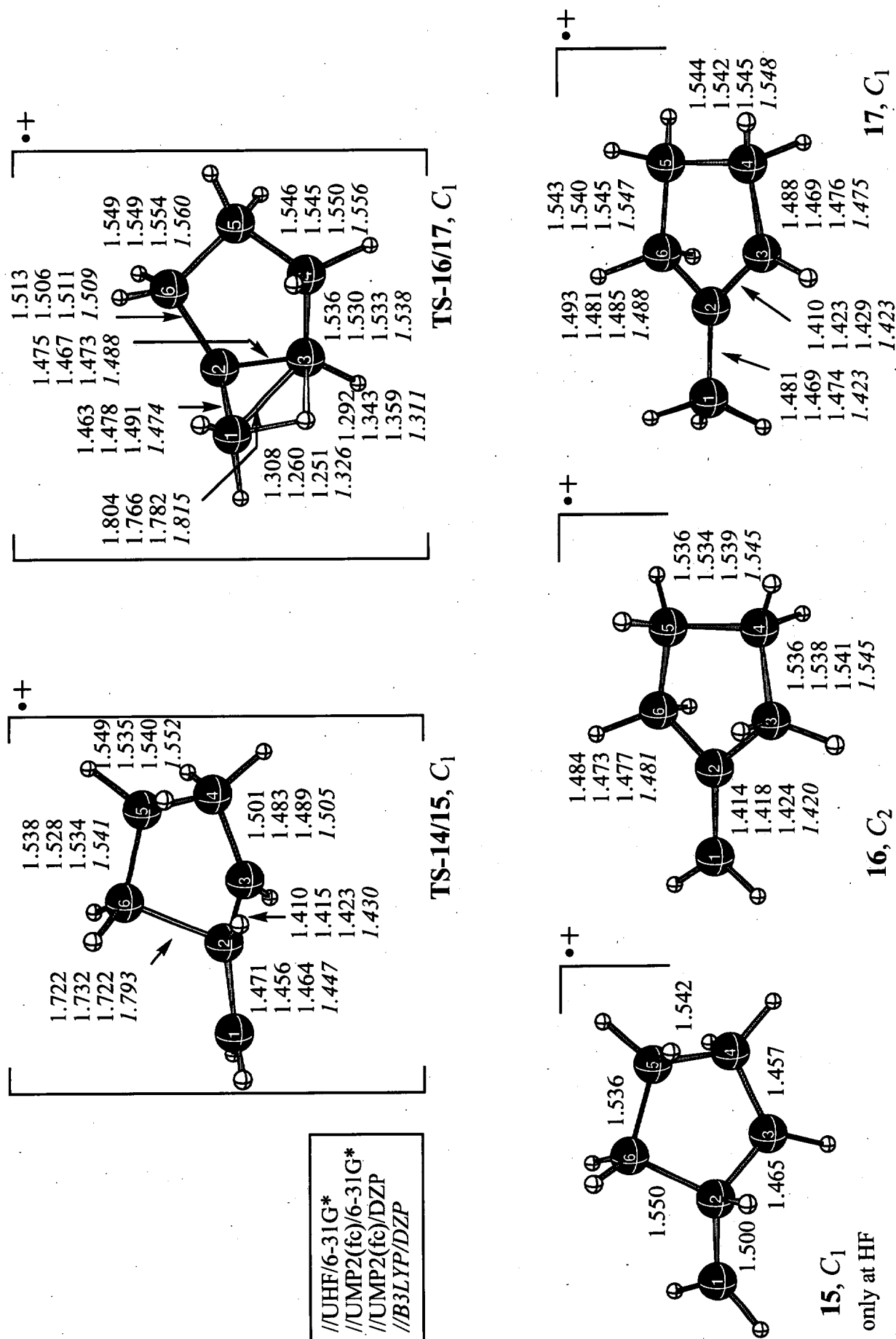


Figure 5