Mechanistic insight for tunable regioselective cyclization of aryl propiolates with radicals: *ipso*-versus *ortho*-cyclization

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1. Computational Methods

Geometry optimizations and harmonic vibrational frequency computations for the structures considered were carried out with DFT, the M062X hibrit functional.[1] For this purpose, a Pople-type polarized triple-ζ split-valence basis sets, 6-311G(d,p), was used.[2-4] Single point energies were computed at the optimized geometries with the coupled-cluster singles and doubles with perturbative triples method employing the domain based local pair natural orbitals approach [DLPNO-CCSD(T)].[5,6] In DLPNO-CCSD(T) computations Dunning's correlation consistent triple-ζ split valence basis set, cc-pVTZ, is employed.[7,8] DFT computations were carried out by using the Gaussian 16 program,[9] while the ORCA package[10,11] (ORCA 4.2.1) is employed for DLPNO-CCSD(T) computations. For the TS between species A and B, the TSA-B notation is used throughout the article.

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2. The Optimized Geometries of The Transition States with Selected Interatomic Distances
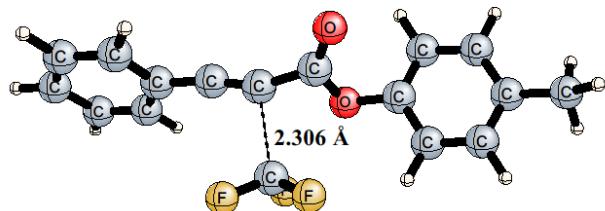
Figure S1. Computed structure of **TS1-3a** at the M062X/6-311G(d,p) level (im. freq.= 397*i*).
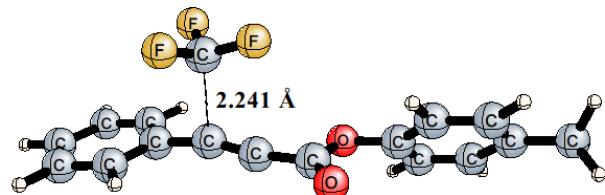
Figure S2. Computed structure of **TS1-4a** at the M062X/6-311G(d,p) level (im. freq.= 463*i*).
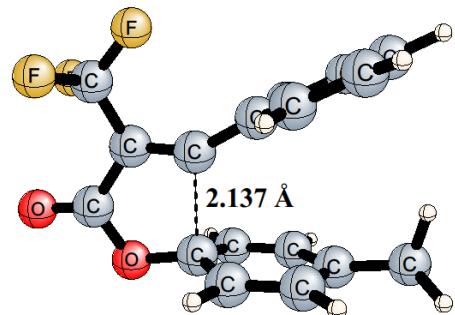
Figure S3. Computed structure of **TS3a-5a** at the M062X/6-311G(d,p) level (im. freq.= 424*i*).
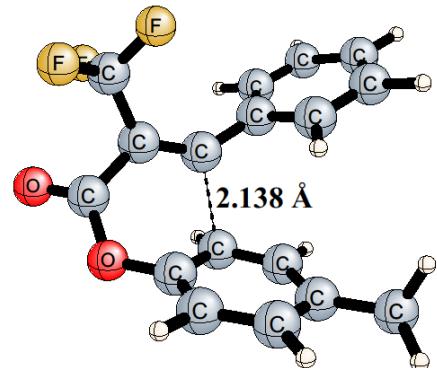
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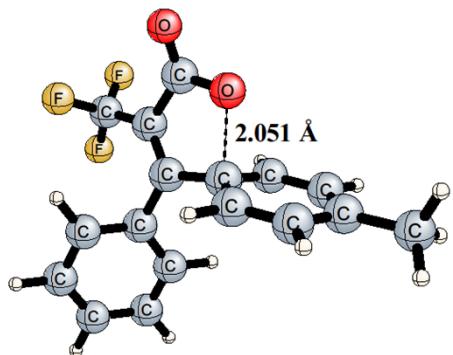
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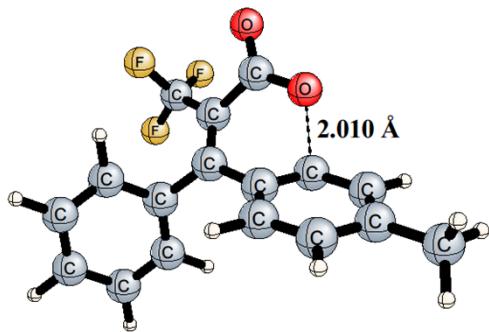
Figure S6. Computed structure of **TS9a-8a** at the M062X/6-311G(d,p) level (im. freq.= 321*i*).
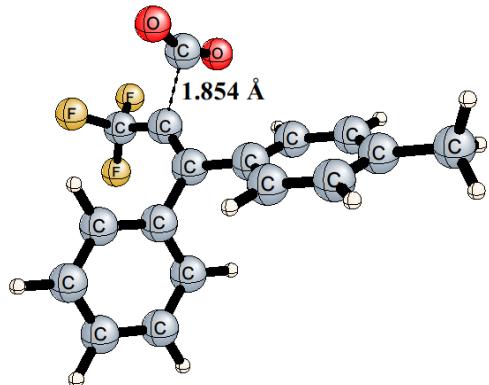
Figure S7. Computed structure of **TS9a-11a** at the M062X/6-311G(d,p) level (im. freq.= 482*i*).
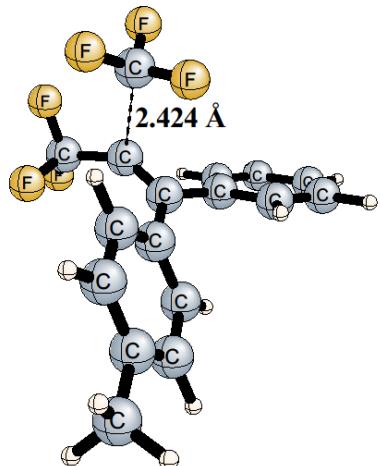
Figure S8. Computed structure of **TS11a-12a** at the M062X/6-311G(d,p) level (im. freq.= 387*i*).
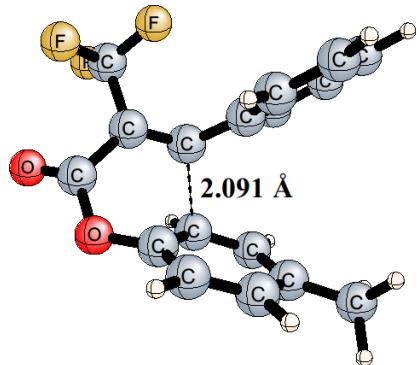
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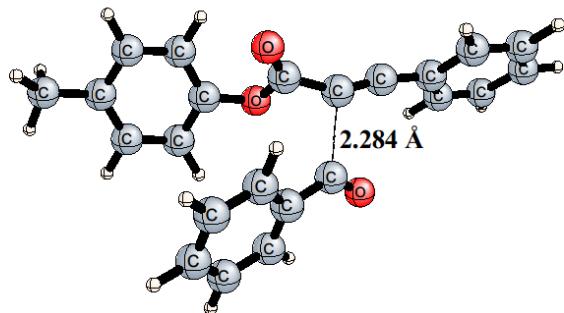
Figure S10. Computed structure of **TS1-3b** at the M062X/6-311G(d,p) level (im. freq.= 333*i*).
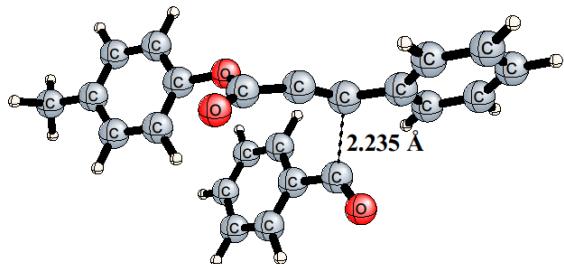
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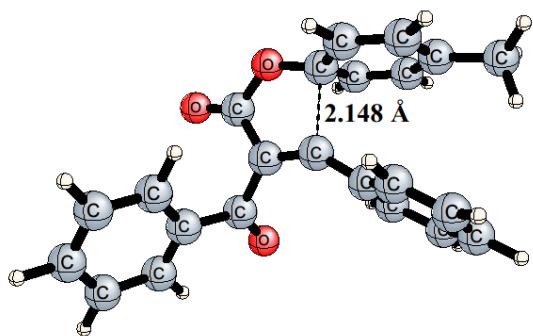
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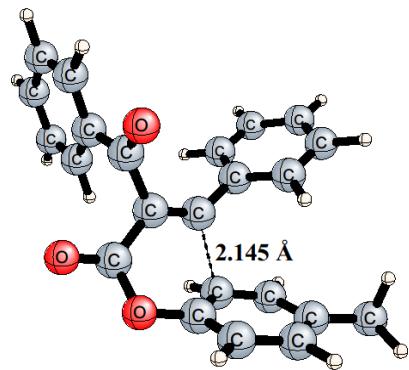
Figure S13. Computed structure of **TS3b-6b** at the M062X/6-311G(d,p) level (im. freq.= 399*i*).
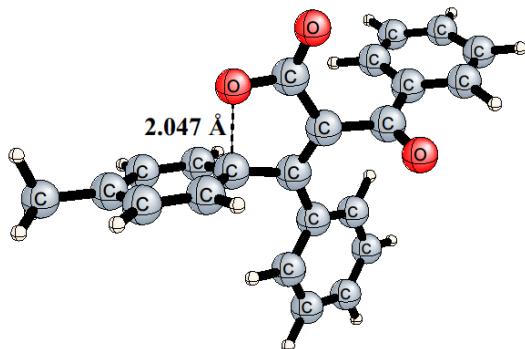
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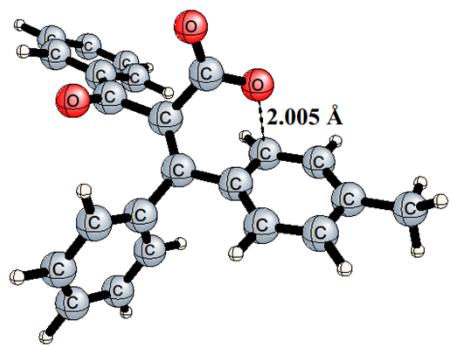
Figure S15. Computed structure of **TS9b-8b** at the M062X/6-311G(d,p) level (im. freq.= 328*i*).
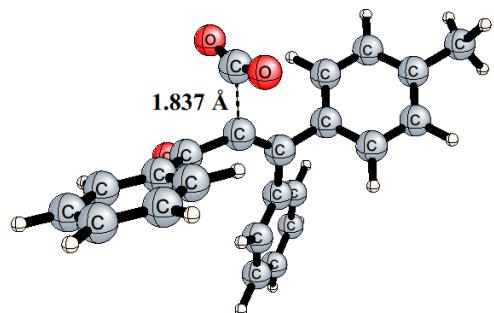
Figure S16. Computed structure of **TS9b-11b** at the M062X/6-311G(d,p) level (im. freq.= 424*i*).
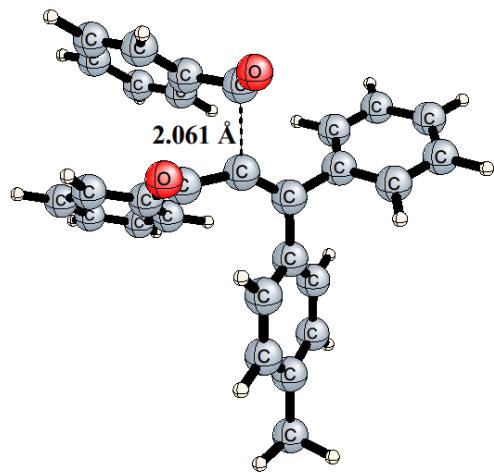
Figure S17. Computed structure of **TS11b-12b** at the M062X/6-311G(d,p) level (im. freq.= 409*i*).
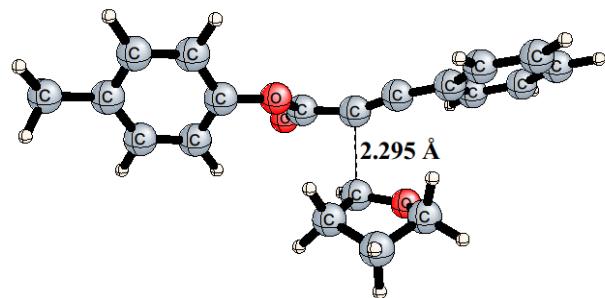
Figure S18. Computed structure of **TS1-3c** at the M062X/6-311G(d,p) level (im. freq.= 429*i*).
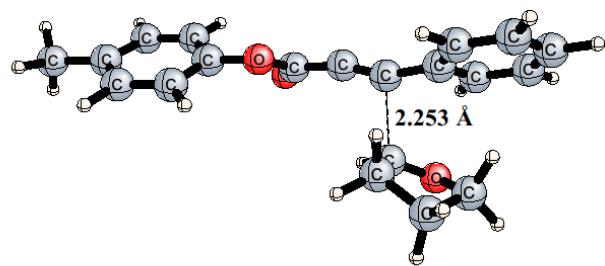
Figure S19. Computed structure of **TS1-4c** at the M062X/6-311G(d,p) level (im. freq.= 398*i*).
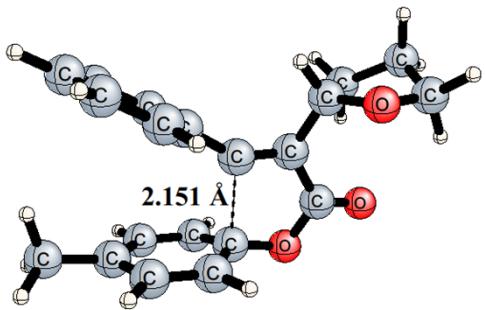
Figure S20. Computed structure of **TS3c-5c** at the M062X/6-311G(d,p) level (im. freq.= 413*i*).
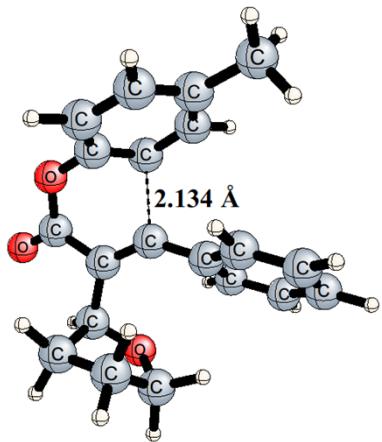
Figure S21. Computed structure of **TS3c-6c** at the M062X/6-311G(d,p) level (im. freq.= 418*i*).
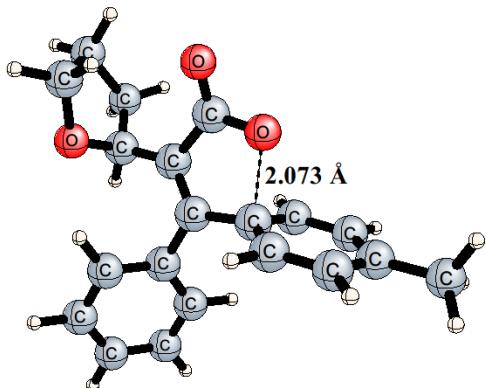
Figure S22. Computed structure of **TS5c-9c** at the M062X/6-311G(d,p) level (im. freq.= 228*i*).
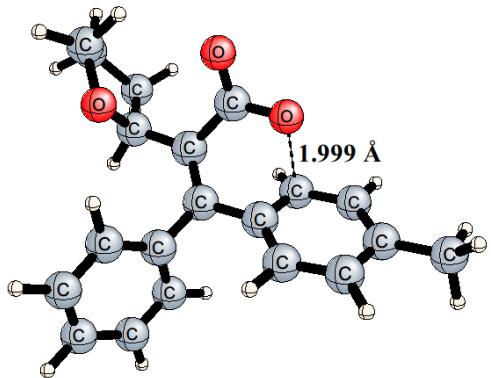
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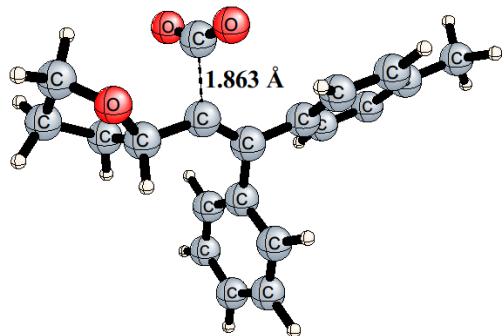
Figure S24. Computed structure of **TS9c-11c** at the M062X/6-311G(d,p) level (im. freq.= 353*i*).
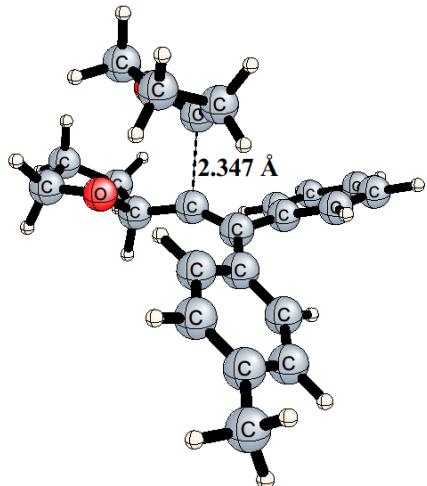
Figure S25. Computed structure of **TS11c-12c** at the M062X/6-311G(d,p) level (im. freq.= 412*i*).
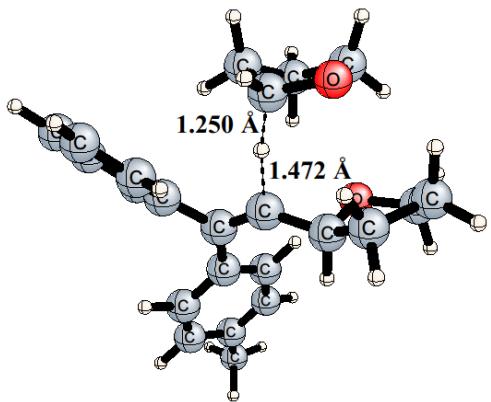
Figure S26. Computed structure of **TS11c-12cH** at the M062X/6-311G(d,p) level (im. freq.= 1415*i*).

3. Single Point Energy Computations

Table S1. Single point energies (**E**) for **a** using the DLPNO-CCSD(T)-cc-pVTZ level in a.u.

Molecule	E	TS	E
1	-765.95425755	**TS1-3a**	-1103.12062435
2a	-337.17035515	**TS1-4a**	-1103.11723243
3a	-1103.18961222	**TS3a-5a**	-1103.18567376
4a	-1103.17662619	**TS3a-6a**	-1103.17447032
5a	-1103.21939893	**TS5a-9a**	-1103.19163888
6a	-1103.21001154	**TS9a-8a**	-1103.19063190
7a	-1102.92605614	**TS9a-11a**	-1103.18194983
8a	-1103.22117209	**TS11a-12a**	-1252.05127891
9a	-1103.19272609		
10a	-1102.68026861		
11a	-914.88472385		
12a	-1252.22263114		
13a	-1102.67956561		
14a	-1102.96821178		
15a	-1102.96010707		
16a	-1102.95092174		
CO2	-188.32453962		

Table S2. Single point energies (**E**) for **b** using the DLPNO-CCSD(T)-cc-pVTZ level in a.u.

Molecule	E	TS	E
2b	-344.30572322	**TS1-3b**	-1110.25699120
3b	-1110.30617366	**TS1-4b**	-1110.25626546
4b	-1110.29730083	**TS3b-5b**	-1110.30081785
5b	-1110.33829763	**TS3b-6b**	-1110.29170638
6b	-1110.32913690	**TS5b-9b**	-1110.31222535
7b	-1110.06034388	**TS9b-8b**	-1110.30894120
8b	-1110.34051651	**TS9b-11b**	-1110.30717132

9b	-1110.31316530	**TS11b-12b**	-1266.31113053
10b	-1109.80207696		
11b	-922.01011261		
12b	-1266.46470640		
13b	-1109.80148844		
14b	-1110.09674965		
15b	-1110.08616011		
16b	-1110.08351776		
CO2	-188.32453962		

Table S3. Single point energies (**E**) for **c** using the DLPNO-CCSD(T)-cc-pVTZ level in a.u.

Molecule	E	TS	E
THF	-232.05603882	**TS1-3c**	-997.35166529
2c	-231.39708069	**TS1-4c**	-997.34774319
3c	-997.40392598	**TS3c-5c**	-997.40137400
4c	-997.38930994	**TS3c-6c**	-997.39423058
5c	-997.43942075	**TS5c-9c**	-997.41113050
6c	-997.42801475	**TS9c-8c**	-997.40968193
7c	-997.16583508	**TS9c-11c**	-997.40254764
8c	-997.44026685	**TS11c-12c**	-1040.49727774
9c	-997.41178655	**TS11c-12cH**	-1041.15613999
10c	-996.89899008		
11c	-809.09799820		
12c	-1040.65280781		
12cH	-809.78142848		
13c	-996.89954540		
14c	-997.20148466		
15c	-997.19264944		
16c	-997.18732570		
CO2	-188.32453962		

4. Cartesian coordinates for optimized structures

THF

E= -232.4023563 a.u., number of negative frequencies = 0

0 1

C	-0.72692500	0.98961000	-0.23878100
C	-1.15889500	-0.42667000	0.13780200
O	-0.00002400	-1.24334000	0.00000100
C	0.72696300	0.98958400	0.23878400
H	-0.76577200	1.12356000	-1.32289100
H	-1.34157400	1.75845200	0.22943700
H	-1.50715800	-0.46314900	1.17692300
H	-1.94612000	-0.82284600	-0.50626500
H	0.76582900	1.12354800	1.32289100
H	1.34163100	1.75840200	-0.22945200
C	1.15887900	-0.42671100	-0.13780200
H	1.94608700	-0.82292600	0.50626200
H	1.50713500	-0.46320300	-1.17692500

1

E= -767.1963133 a.u., number of negative frequencies = 0

0 1

C	-2.28936200	-0.27295600	-0.05680900
C	-1.10608300	-0.48965400	-0.09900900
C	0.30297800	-0.81758700	-0.17434600
O	1.04503600	0.27850400	0.10358800
O	0.73414900	-1.89841500	-0.44405100
C	-3.69418600	-0.01360000	-0.00316800
C	-4.16128100	1.25634300	0.35511300
C	-5.52549800	1.50208600	0.40641700
C	-6.42966100	0.48887400	0.10157400

C	-5.96914600	-0.77494000	-0.25560000
C	-4.60670900	-1.03013600	-0.30881500
C	2.43577500	0.20324100	0.07121100
C	3.08819500	1.25042800	-0.55853800
C	4.47709400	1.28240000	-0.56504200
C	5.22223100	0.27684200	0.04794800
C	4.53478500	-0.76078600	0.67925300
C	3.14740200	-0.80972200	0.69958900
H	-3.44696800	2.03553800	0.58986000
H	-5.88469300	2.48523500	0.68452600
H	-7.49438300	0.68440600	0.14259100
H	-6.67332500	-1.56286000	-0.49273200
H	-4.23477500	-2.00890400	-0.58479000
H	2.49958400	2.02901100	-1.02712500
H	4.98762300	2.10409400	-1.05522900
H	5.09591000	-1.54999200	1.16813900
H	2.62768400	-1.62296100	1.18593500
C	6.72858800	0.29127500	0.01237000
H	7.14761700	-0.06793800	0.95384500
H	7.10262300	-0.35629300	-0.78524700
H	7.10888600	1.29730000	-0.16894600

2a

E= -337.5471385 a.u., number of negative frequencies = 0

0 2

C	0.00000000	0.00000000	0.32844300
F	0.00000000	1.25099500	-0.07298700
F	-1.08339300	-0.62549700	-0.07298700
F	1.08339300	-0.62549700	-0.07298700

3a

E= -1104.8126421 a.u., number of negative frequencies = 0

0 2

C	-1.05214100	1.03104100	-0.04781500
C	0.06379600	0.02120100	-0.02300700
O	-0.09972500	-1.15369700	0.10754600
O	1.24730000	0.64451700	-0.16782400
C	-0.72195000	2.50505200	-0.09589100
C	-2.29391200	0.61811400	-0.01545900
C	2.45344000	-0.04889000	-0.09345700
C	3.47581500	0.61233500	0.57096900
C	4.72992800	0.02439400	0.64286300
C	4.97707700	-1.21794300	0.05666900
C	3.92812000	-1.85380000	-0.60480900
C	2.66312000	-1.28237200	-0.69141200
C	-3.24158200	-0.40453300	0.04054100
C	-3.67291200	-0.90773900	1.28913800
C	-4.63360400	-1.89975500	1.33669600
C	-5.18821800	-2.40386500	0.16022300
C	-4.77307300	-1.90867800	-1.07587600
C	-3.81501100	-0.91516700	-1.14610600
H	3.26880200	1.57640600	1.01855700
H	5.52957600	0.53882200	1.16475800
H	4.09794800	-2.82146600	-1.06420100
H	1.85711600	-1.79283300	-1.19741300
H	-3.23228000	-0.51475300	2.19646800
H	-4.95318900	-2.28873300	2.29564800
H	-5.94088600	-3.18097300	0.20664800
H	-5.20198800	-2.30329500	-1.98876100
H	-3.48785900	-0.52413100	-2.10118800
F	0.04427600	2.87265800	0.93848600
F	-1.83274500	3.24598900	-0.04948300

F	-0.07046900	2.83444900	-1.21494600
C	6.34947700	-1.83748300	0.11453900
H	6.98874100	-1.43582300	-0.67638400
H	6.83457300	-1.62990300	1.06971400
H	6.29907900	-2.91923100	-0.01496500

4a

E= -1104.8020464 a.u., number of negative frequencies = 0

0 2

C	0.75153700	-0.95710600	-0.34666600
C	-0.56633200	-0.42654500	-0.64758600
O	-0.82203100	0.21779400	-1.62770300
O	-1.44400300	-0.79833500	0.30354600
C	-2.77955800	-0.40255600	0.21638000
C	-3.35323000	0.06683000	1.38599300
C	-4.69952200	0.40923500	1.39122400
C	-5.47653200	0.29037600	0.24013900
C	-4.86836300	-0.19272000	-0.91943700
C	-3.52502900	-0.54272000	-0.94567700
C	2.57377000	0.69610800	-0.03635700
C	3.62867400	0.99259900	0.83146600
C	4.12633800	2.28720300	0.90084000
C	3.58232700	3.29219500	0.10891700
C	2.53797700	2.99784600	-0.76093100
C	2.03504600	1.70626500	-0.83828500
H	-2.74192100	0.14868700	2.27578400
H	-5.15148300	0.77333000	2.30721100
H	-5.45732600	-0.29977800	-1.82393000
H	-3.06492700	-0.91086900	-1.85183500
H	4.05600100	0.21996200	1.45721300
H	4.94247600	2.50925500	1.57744400

H	3.97535700	4.30009000	0.16493400
H	2.11739600	3.77326600	-1.38935600
H	1.23630000	1.47186400	-1.53195900
C	-6.92830500	0.69328800	0.23623600
H	-7.52033400	0.02455200	-0.39066200
H	-7.34486000	0.67526800	1.24399500
H	-7.04642700	1.70688500	-0.15625100
C	2.01185300	-0.67956000	-0.11916700
C	2.95420200	-1.84977700	0.07779000
F	2.40056000	-3.00483200	-0.28989800
F	3.31089700	-1.97545400	1.36701100
F	4.07731100	-1.69015300	-0.62584500

5a

E= -1104.8372527 a.u., number of negative frequencies = 0

0 2

C	3.67359800	-0.80592600	-0.01458900
C	2.92540500	-1.13761100	-1.17072200
C	1.57466600	-1.27735500	-1.13979100
C	0.78137200	-1.12959600	0.12649000
C	1.63507700	-0.81673900	1.31604800
C	2.97476900	-0.66349700	1.22035200
O	0.09483000	-2.38488000	0.35220100
C	-1.24965400	-2.23695200	0.24123600
C	-1.51580700	-0.79960300	-0.03796200
C	-0.36568800	-0.11733400	-0.02670900
O	-2.02142700	-3.13114900	0.38003900
C	5.16210900	-0.65328800	-0.05708000
C	-0.12812700	1.33380700	-0.03467500
C	-0.99414400	2.16924100	0.68107900
C	-0.76659300	3.53612100	0.73504900

C	0.32626700	4.08789200	0.07473800
C	1.19812800	3.26417800	-0.62838100
C	0.98268500	1.89335000	-0.67455900
C	-2.91437900	-0.31149000	-0.24540200
F	-3.64367200	-1.20448500	-0.90913100
F	-3.53231100	-0.07579900	0.92415500
F	-2.94785800	0.82878400	-0.94573100
H	3.45200400	-1.28670500	-2.10776100
H	1.00799000	-1.54487000	-2.02453800
H	1.11830600	-0.72391200	2.26449400
H	3.54744100	-0.43628500	2.11388600
H	5.53969100	-0.69935800	-1.07862800
H	5.47075700	0.29974300	0.38194100
H	5.65045600	-1.44493700	0.52052900
H	-1.83649100	1.74160800	1.21125100
H	-1.44236700	4.17009400	1.29553700
H	0.50090400	5.15635700	0.11358000
H	2.05267800	3.68898600	-1.14063600
H	1.66787600	1.25982900	-1.22193000

6a

E= -1104.8298726 a.u., number of negative frequencies = 0

0 2

C	-1.25315500	-0.39183100	-0.79268400
C	-2.30552900	0.65052000	-0.54562800
C	-3.49744800	0.37665000	0.04297400
C	-3.79064400	-0.94526800	0.49408200
C	-2.84691600	-1.97689300	0.33896400
C	-1.65347300	-1.72212200	-0.25477600
O	-0.75336900	-2.74079100	-0.42573800
C	0.58519600	-2.48162800	-0.36407900

C	0.97434900	-1.08315500	-0.02139900
C	0.15077500	-0.05470400	-0.26394300
C	-4.53793900	1.44964400	0.23238200
O	1.36229200	-3.35570200	-0.58415600
C	2.39214200	-0.94424400	0.48081100
C	0.54651300	1.37222200	-0.17911000
C	1.47508800	1.87812700	-1.08865300
C	1.83597000	3.21944900	-1.04060700
C	1.28243800	4.05579300	-0.07853500
C	0.36219300	3.55065500	0.83516800
C	-0.01418100	2.21533700	0.78167900
F	2.70170500	-1.92916400	1.32545600
F	3.27252900	-0.98055600	-0.52801200
F	2.58838500	0.20226400	1.13871500
H	-1.10880400	-0.48815600	-1.88758300
H	-2.09485400	1.65011600	-0.90649500
H	-4.74115000	-1.15009000	0.96983200
H	-3.04305300	-2.98211500	0.69109500
H	-5.45390200	1.19541000	-0.30643200
H	-4.79657100	1.55101500	1.28919000
H	-4.18279700	2.41451800	-0.12937200
H	1.91926600	1.21602600	-1.82346900
H	2.55722500	3.60677100	-1.74969200
H	1.57070400	5.09908600	-0.03637000
H	-0.06243900	4.19800600	1.59272700
H	-0.73084800	1.81714100	1.49040900

7a

E= -1104.5455826 a.u., number of negative frequencies = 0

1 1

C	4.33407900	-1.66468300	0.58903000

C	5.28965600	-0.90762200	-0.08756300
C	4.88856000	0.29346300	-0.67808100
C	3.57270700	0.72394200	-0.60375500
C	2.65639800	-0.06604800	0.06874500
C	3.00721100	-1.25690600	0.67876600
C	6.71576100	-1.37578900	-0.19909700
O	1.35105400	0.47833700	0.14624700
C	0.28007900	-0.27734400	0.06068100
C	-0.95053800	0.64686700	0.07919000
O	0.17158400	-1.45842800	-0.01896900
C	-2.11712900	0.10820700	0.01468700
C	-3.32256700	-0.48812900	-0.05744100
C	-3.99931400	-0.86625800	1.14885700
C	-5.21930300	-1.48553800	1.05824300
C	-5.77356300	-1.73356200	-0.20774000
C	-5.12651100	-1.37189200	-1.40003500
C	-3.90547800	-0.75068000	-1.34104300
C	-0.81668900	2.17014700	0.15657200
F	-0.20995000	2.51637500	1.27526400
F	-2.02805100	2.72742900	0.13604700
F	-0.12914000	2.61613500	-0.87925800
H	4.62807700	-2.59451800	1.06193800
H	5.61737800	0.90317800	-1.19981000
H	3.25058600	1.65718500	-1.04812600
H	2.27864400	-1.85642800	1.20490600
H	7.41108100	-0.54235000	-0.09051700
H	6.94866700	-2.11925100	0.56300700
H	6.89256300	-1.83017600	-1.17731300
H	-3.53250500	-0.65646100	2.10340900
H	-5.75350300	-1.78332200	1.95077800
H	-6.73898500	-2.22471100	-0.26686700

H	-5.59066400	-1.58473500	-2.35392900
H	-3.36832700	-0.45617500	-2.23426900

8a

E= -1104.8410386 a.u., number of negative frequencies = 0

0 2

C	3.08637900	1.83160600	0.22605500
C	4.00793600	0.74561200	0.01883800
C	3.52592200	-0.48102200	-0.27159500
C	2.07272700	-0.73843100	-0.48036100
C	1.17439200	0.39461000	-0.08893700
C	1.71194300	1.63998500	0.19672900
O	1.73288100	-1.94542800	0.22095700
C	0.42705800	-2.29480900	0.27038100
O	0.11484400	-3.37630100	0.67294500
C	-0.56560900	-1.24739300	-0.09253600
C	-0.22787900	0.07644700	-0.07953400
C	-1.97545600	-1.75442300	-0.25139500
F	-2.75421400	-0.87975200	-0.90213900
F	-2.00371000	-2.88544000	-0.95860800
F	-2.56240300	-2.00158200	0.92930000
C	-1.22075100	1.18009700	-0.00129200
C	-2.12587500	1.22574200	1.05967400
C	-3.03753200	2.26922300	1.15310300
C	-3.05877600	3.26652000	0.18423300
C	-2.16071800	3.22281600	-0.87743200
C	-1.23803500	2.18842700	-0.96583800
C	5.47998700	1.01540500	0.17156800
H	3.48370800	2.81084700	0.46738400
H	4.18283000	-1.33457100	-0.39654600
H	1.89996100	-0.94232100	-1.55257700

S23

H	1.04889200	2.46258400	0.43656600
H	-2.11325300	0.43936200	1.80561500
H	-3.73528100	2.29993000	1.98089100
H	-3.77555800	4.07571500	0.25440700
H	-2.17983900	3.99382800	-1.63806600
H	-0.53683600	2.14919400	-1.79206700
H	5.81152600	1.75878700	-0.55776800
H	5.69596100	1.41147800	1.16668700
H	6.06475300	0.10749400	0.02732700

9a

E= -1104.8144501 a.u., number of negative frequencies = 0

0 2

C	-3.38775000	-0.43291800	1.01837500
C	-4.05154700	0.28310200	0.02905900
C	-3.28978600	0.92230000	-0.96028700
C	-1.91052200	0.84565600	-0.96137900
C	-1.24927700	0.08616600	0.01227100
C	-2.00039300	-0.53941500	1.01283200
C	0.23198700	0.00290800	0.02985100
C	0.83662100	-1.20532400	0.02553500
C	-5.55299200	0.37724200	0.00363400
C	0.93742200	1.30700300	0.01415100
C	2.02211800	1.52055500	-0.84149400
C	2.63533000	2.76428200	-0.89352100
C	2.17883700	3.80220200	-0.08742900
C	1.09531700	3.59892000	0.76113200
C	0.46548700	2.36274000	0.79957900
C	2.30242100	-1.43529700	0.31370500
F	2.46816000	-2.54180700	1.04158400
F	3.02959500	-1.57511700	-0.80434300

F	2.84589400	-0.43522200	1.01710600
C	0.13034400	-2.44224400	-0.41933600
O	0.69632600	-3.43919300	-0.79611900
O	-1.18523800	-2.43584100	-0.48083100
H	-3.95673600	-0.91741600	1.80354500
H	-3.79632100	1.49115500	-1.73275400
H	-1.33126200	1.35726700	-1.72156700
H	-1.49067700	-1.08777200	1.79646200
H	-5.99106200	-0.02492100	0.91696700
H	-5.87756900	1.41381700	-0.10808900
H	-5.95479900	-0.18695400	-0.84189500
H	2.37516900	0.71224800	-1.47111700
H	3.47040100	2.92300400	-1.56456900
H	2.66284800	4.77066300	-0.12563800
H	0.73575600	4.40616800	1.38730300
H	-0.38899200	2.20504700	1.44779600

10a

E= -1104.3041824 a.u., number of negative frequencies = 0

0 1

C	3.11657900	1.76710800	-0.00000100
C	3.99290100	0.66858500	-0.00000300
C	3.46205800	-0.61157100	-0.00000200
C	2.08214200	-0.79105300	0.00000000
C	1.20070000	0.29073300	0.00000200
C	1.75041300	1.58453900	0.00000100
O	1.63461400	-2.07150900	0.00000100
C	0.30069500	-2.39466400	0.00000600
O	-0.00358700	-3.54708900	-0.00000400
C	-0.64952200	-1.26499100	0.00000300

C	-0.22991400	0.02093200	0.00000200
C	-2.09093000	-1.71416600	0.00000000
F	-2.95557200	-0.69516800	-0.00000600
F	-2.36100500	-2.45363700	1.07944100
F	-2.36099900	-2.45364600	-1.07943600
C	-1.13508800	1.20619600	0.00000200
C	-1.53154400	1.77767400	-1.20633900
C	-2.33515400	2.91161700	-1.20391200
C	-2.73789600	3.47936900	0.00000000
C	-2.33515600	2.91161700	1.20391200
C	-1.53154600	1.77767400	1.20634200
C	5.48077200	0.89141100	-0.00000500
H	3.52540500	2.77116800	-0.00000200
H	4.09427600	-1.49112800	-0.00000400
H	1.08426600	2.43842300	0.00000200
H	-1.21774000	1.32727300	-2.14119900
H	-2.64944500	3.34910300	-2.14365700
H	-3.36638600	4.36152500	-0.00000100
H	-2.64944900	3.34910400	2.14365700
H	-1.21774400	1.32727300	2.14120200
H	6.02467500	-0.05266100	-0.00001300
H	5.78252600	1.46235400	-0.88111700
H	5.78252900	1.46234000	0.88111600

11a

E= -916.2580567 a.u., number of negative frequencies = 0

0 2

C	2.95230800	-0.70457100	0.80011600
C	3.14805300	-1.76349100	-0.08449300
C	2.09004800	-2.13179500	-0.91901800
C	0.87637500	-1.46333700	-0.87354300

C	0.69330400	-0.39349300	0.00692000
C	1.74268400	-0.02332500	0.84677000
C	-0.60622400	0.33870000	0.03408600
C	-0.64788000	1.65824900	0.04854700
C	4.47014000	-2.48079000	-0.15955600
C	-1.87488300	-0.44061400	0.05292600
C	-1.92865800	-1.69481600	0.66575700
C	-3.12493000	-2.40010300	0.71473800
C	-4.27620100	-1.86583700	0.14698300
C	-4.22842900	-0.61929400	-0.47024300
C	-3.03618100	0.08879300	-0.51756400
C	0.29014600	2.79333600	-0.02924500
F	-0.31951400	3.87481900	-0.53153000
F	1.34917000	2.53677500	-0.80950900
F	0.76815800	3.14268200	1.17854200
H	3.75625400	-0.40950300	1.46561400
H	2.22115300	-2.95580700	-1.61254100
H	0.06361800	-1.76469500	-1.52487300
H	1.60572600	0.79258400	1.54712100
H	5.04404200	-2.34806500	0.75816400
H	4.32924900	-3.55007800	-0.32594600
H	5.06937400	-2.09280300	-0.98781100
H	-1.03322600	-2.11056400	1.11259900
H	-3.15722000	-3.36849900	1.19923000
H	-5.20663700	-2.41963400	0.18168000
H	-5.12044000	-0.20142300	-0.92106200
H	-2.99026500	1.05432300	-1.00877700

12a

E= -1253.9769768 a.u., number of negative frequencies = 0

0 1

C	3.43138700	-0.50176800	-0.90791500
C	4.11818400	0.33672000	-0.03117400
C	3.37470500	1.11849200	0.85632100
C	1.99013500	1.06490200	0.86838700
C	1.31018400	0.19726700	0.00950900
C	2.04546500	-0.57815800	-0.88796100
C	-0.17460900	0.16467700	0.00228800
C	-0.88035100	-0.98304200	-0.00050300
C	5.62280400	0.38968600	-0.02428600
C	-0.82520100	1.50253400	-0.00232900
C	-1.83066200	1.80382200	0.91835600
C	-2.40005300	3.07067000	0.94004900
C	-1.97671900	4.04098800	0.03891200
C	-0.96943800	3.74790500	-0.87577600
C	-0.38353100	2.49006100	-0.88604900
C	-0.28861600	-2.33731700	0.31995700
F	0.79876100	-2.26394300	1.08741700
F	0.04405300	-3.03398200	-0.77880600
F	-1.18274100	-3.07594800	0.99304000
C	-2.35584600	-1.06137700	-0.32325600
F	-2.61495300	-2.19150100	-0.99666500
F	-2.77581800	-0.05588200	-1.09116100
F	-3.12897600	-1.07544000	0.77451300
H	3.98818800	-1.10259100	-1.61856200
H	3.89049100	1.78432300	1.53997700
H	1.42639300	1.69105600	1.55065800
H	1.52840400	-1.23289200	-1.57961800
H	6.03507800	0.03909100	-0.97091700
H	5.98035100	1.40528900	0.15309000
H	6.02255500	-0.24573100	0.77073600
H	-2.15827600	1.04531300	1.61946200

H	-3.17496100	3.29853500	1.66161100
H	-2.42579300	5.02676600	0.05296300
H	-0.63559000	4.50302700	-1.57687800
H	0.41319700	2.26170700	-1.58473700

13a

E= -1104.3029665 a.u., number of negative frequencies = 0

0 1

C	-3.60715300	0.33169100	0.00000300
C	-3.96805500	-1.02527100	0.00000100
C	-3.01658600	-2.02613300	-0.00000200
C	-1.66932600	-1.67748900	-0.00000400
C	-1.26880900	-0.34202800	-0.00000200
C	-2.26126500	0.65336400	0.00000100
O	-0.77023800	-2.69458900	-0.00000600
C	0.58439800	-2.48749500	-0.00000900
O	1.30587800	-3.43643300	-0.00000400
C	1.03443100	-1.08037400	-0.00000600
C	0.15990800	-0.04925100	-0.00000300
C	-4.67090000	1.39834600	0.00000600
C	2.53920800	-0.95031400	-0.00000100
F	2.95422200	0.31978100	-0.00007300
F	3.06817100	-1.53267000	-1.07960300
F	3.06815000	-1.53254200	1.07968000
C	0.55026500	1.39000100	0.00000000
C	0.70187100	2.06883700	1.20637000
C	1.01780500	3.42228000	1.20393800
C	1.17616700	4.10012600	0.00000600
C	1.01780500	3.42228500	-1.20393000
C	0.70187100	2.06884200	-1.20636800
H	-5.01934600	-1.29333700	0.00000200

H	-3.28158000	-3.07545700	-0.00000300
H	-1.95618900	1.69340500	0.00000300
H	-4.22871200	2.39457600	0.00000600
H	-5.31003200	1.31027500	-0.88154700
H	-5.31002800	1.31027300	0.88156300
H	0.58164400	1.53330800	2.14128200
H	1.14383800	3.94595100	2.14371700
H	1.42510600	5.15428500	0.00000800
H	1.14383800	3.94596000	-2.14370700
H	0.58164300	1.53331800	-2.14128200

14a

E= -1104.585284 a.u., number of negative frequencies = 0

1 1

C	3.55331900	0.58432900	-0.02708100
C	3.94424000	-0.76159900	0.30019000
C	3.10281900	-1.84555600	0.25857100
C	1.77264000	-1.63749400	-0.10876600
C	1.29320800	-0.31124100	-0.54919700
C	2.27067300	0.79881100	-0.39551600
O	0.96024200	-2.64835300	-0.10347100
C	-0.46824500	-2.49145400	-0.27456500
O	-1.06636500	-3.45278700	-0.57189000
C	-0.95956400	-1.12843000	-0.00521400
C	-0.16897100	-0.05714200	-0.16669500
C	4.57740600	1.67998600	0.06180700
C	-2.43457000	-1.06109400	0.36843000
F	-3.19008400	-1.05584900	-0.72933600
F	-2.76650100	-2.11611800	1.10275100
F	-2.71065300	0.02834700	1.07468600
C	-0.63985100	1.34353400	-0.12577700

C	-0.16130900	2.22388100	0.84870500
C	-0.63748100	3.52592900	0.89095100
C	-1.56854300	3.95861600	-0.05078400
C	-2.03626800	3.08594500	-1.02609400
C	-1.58274200	1.77310300	-1.06140200
H	4.97424900	-0.92537800	0.60603100
H	3.42101500	-2.84256700	0.53435000
H	1.25468000	-0.43319100	-1.65830700
H	1.92589900	1.78870700	-0.67075600
H	4.99813400	1.72895400	1.06833000
H	5.39835500	1.49271900	-0.63369400
H	4.13884500	2.64749600	-0.17671600
H	0.55200600	1.88129500	1.59160800
H	-0.28881000	4.20194500	1.66140200
H	-1.93379500	4.97749700	-0.01803500
H	-2.76413100	3.42103500	-1.75398500
H	-1.96288000	1.08245400	-1.80563000

15a

E= -1104.5753011 a.u., number of negative frequencies = 0

1 1

C	2.67579700	-1.49785500	0.00000300
C	2.00900900	-1.74104700	-1.23633700
C	0.67067400	-1.95234500	-1.24474400
C	-0.08923700	-1.78443800	0.00000000
C	0.67067200	-1.95233400	1.24474700
C	2.00900600	-1.74103600	1.23634200
O	-1.33871600	-2.39126000	0.00000100
C	-2.36890200	-1.46302200	-0.00000600
C	-1.73738400	-0.11051500	-0.00000100
C	-0.41558600	-0.16749500	0.00000200

O	-3.50473200	-1.76401600	-0.00001400
C	4.06269100	-0.98946900	0.00000300
C	0.63373300	0.85381000	-0.00000100
C	1.13382600	1.34513200	1.21147300
C	2.12699300	2.31464900	1.20829600
C	2.62934700	2.79336400	-0.00000700
C	2.12698000	2.31465000	-1.20830900
C	1.13381500	1.34513600	-1.21148000
C	-2.60783000	1.12081200	0.00000400
F	-3.37997000	1.12686000	-1.07906000
F	-3.37997600	1.12684000	1.07906500
F	-1.86933300	2.22782000	0.00001600
H	2.58426600	-1.73561500	-2.15406200
H	0.10251500	-2.12166400	-2.15392200
H	0.10251000	-2.12164500	2.15392600
H	2.58426100	-1.73559500	2.15407000
H	4.61005400	-1.27332900	-0.89835100
H	3.97834700	0.11166100	0.00002500
H	4.61006200	-1.27336000	0.89834300
H	0.72858600	0.98205000	2.14937800
H	2.49979200	2.70608800	2.14644100
H	3.40073400	3.55381400	-0.00001200
H	2.49977500	2.70609400	-2.14645400
H	0.72856500	0.98205500	-2.14938100

16a

E= -1104.5672373 a.u., number of negative frequencies = 0

1 1

C	3.08431600	1.80101300	0.15944000
C	4.03674000	0.74925800	0.06724400
C	3.54265600	-0.51060300	-0.10553500

C	2.11097800	-0.73728600	-0.36032100
C	1.17080600	0.36188000	-0.07614900
C	1.70204100	1.62896800	0.08658900
O	1.72127300	-2.02757600	-0.00984800
C	0.39774300	-2.34039300	0.16120600
O	0.10212000	-3.42693700	0.51964300
C	-0.59687300	-1.24788400	-0.07519500
C	-0.25586800	0.06335800	-0.08063500
C	-2.03568000	-1.74737500	-0.18510600
F	-2.07718000	-2.84620300	-0.92510000
F	-2.51830900	-2.01750700	1.02452800
F	-2.82204900	-0.84632200	-0.76375100
C	-1.21539800	1.19156300	-0.00931100
C	-2.05870500	1.29696100	1.09775100
C	-2.94983900	2.35865500	1.18390500
C	-3.00890700	3.30333800	0.16524600
C	-2.17196100	3.19456900	-0.94221600
C	-1.26688600	2.14567000	-1.02795000
C	5.50158400	1.04174100	0.22239600
H	3.46046900	2.80678500	0.32941700
H	4.18009200	-1.38873100	-0.14888700
H	2.13308200	-0.64632100	-1.48706800
H	1.04183600	2.47618100	0.22253700
H	-2.01868800	0.55013500	1.88298600
H	-3.60327000	2.44209300	2.04298300
H	-3.71230700	4.12407100	0.23026700
H	-2.23035400	3.92225400	-1.74177200
H	-0.62753600	2.04979500	-1.89953600
H	5.85551400	1.65469700	-0.60944100
H	5.68595300	1.59171600	1.14692100
H	6.08543600	0.12313800	0.24399900

TS1-3a

E= -1104.7447315 a.u., im. freq.= 396.83*i*

0 2

C	-0.94174100	-0.52797600	0.23052900
C	0.45006000	-0.95864800	0.37313700
O	0.79471500	-1.90265300	1.01558600
O	1.25994400	-0.13482400	-0.32167600
C	-0.62925600	1.75227000	0.37832200
C	-2.14491700	-0.67058300	0.09046500
C	2.64528800	-0.27259800	-0.25281700
C	3.29028900	-1.49205800	-0.39615200
C	4.67966800	-1.51244300	-0.38314600
C	5.42793500	-0.34483200	-0.23396900
C	4.74492700	0.86418100	-0.10210300
C	3.35744100	0.90752300	-0.10866500
C	-3.55409500	-0.63629500	-0.09050600
C	-4.40243900	-1.28555300	0.81702800
C	-5.77564900	-1.23380500	0.63422700
C	-6.31199300	-0.54272100	-0.44888700
C	-5.47274700	0.10309300	-1.35291300
C	-4.09834100	0.06137400	-1.17854500
H	2.72118700	-2.40394500	-0.50654400
H	5.19215000	-2.46196800	-0.49364300
H	5.30509900	1.78636800	0.00710800
H	2.81369800	1.83883400	-0.01035300
H	-3.97197000	-1.82182600	1.65332700
H	-6.43043000	-1.73434200	1.33675800
H	-7.38563800	-0.50631000	-0.58804900
H	-5.89174600	0.64323700	-2.19285300
H	-3.43281100	0.56573700	-1.86829100

F	0.28671700	2.08438800	1.27237100
F	-1.81293300	2.20342100	0.74539400
F	-0.30881300	2.23520900	-0.80543100
C	6.93333300	-0.39310700	-0.18958100
H	7.36794200	0.54309200	-0.54258900
H	7.28427900	-0.55876000	0.83265400
H	7.31964200	-1.20440000	-0.80834400

TS1-4a

E= -1104.7400938 a.u., im. freq.= 462.91*i*

0 2

C	0.58580600	-0.43108700	0.62980600
C	-0.81422200	-0.21696800	0.91262300
O	-1.23614700	0.22792300	1.93924200
O	-1.56084500	-0.59462400	-0.15066700
C	-2.94618700	-0.45296600	-0.09795900
C	-3.55419300	0.73965600	0.27063500
C	-4.93820800	0.82403100	0.22401600
C	-5.72362100	-0.25591200	-0.18490600
C	-5.08072400	-1.43460300	-0.55602300
C	-3.69519900	-1.54036700	-0.51283800
C	3.17189500	-0.70048200	0.20955300
C	3.63388100	-1.25236000	-0.98833900
C	4.97775500	-1.56953000	-1.12583900
C	5.86267800	-1.32984400	-0.07892000
C	5.40458800	-0.76981500	1.10968100
C	4.06248300	-0.44929500	1.25683500
H	-2.95464900	1.57957500	0.59356900
H	-5.41970400	1.75255100	0.51185300
H	-5.66859400	-2.28470800	-0.88409700
H	-3.18546500	-2.45032000	-0.80326900

H	2.93470300	-1.42804700	-1.79646800
H	5.33555000	-2.00226600	-2.05188200
H	6.91137700	-1.57719200	-0.19062700
H	6.09427200	-0.58049800	1.92289600
H	3.69204000	-0.00883900	2.17416500
C	-7.22627200	-0.14479700	-0.20346200
H	-7.54454000	0.79638400	-0.65589800
H	-7.67514300	-0.96301700	-0.76753200
H	-7.62923700	-0.17623500	0.81221500
C	1.77453000	-0.36643300	0.36011100
C	1.93408100	1.69907700	-0.49339200
F	0.73508400	2.24121100	-0.45422300
F	2.36227100	1.61011100	-1.73656000
F	2.78163300	2.39160800	0.23933600

TS3a-5a

E= -1104.8063829 a.u., im. freq.= 424.15*i*

0 2

C	2.12341000	-1.68151800	-1.20630200
C	0.77639400	-1.96912500	-1.22199900
C	0.06146700	-1.94832000	-0.00000100
C	0.77638500	-1.96912000	1.22200200
C	2.12340200	-1.68151500	1.20631300
C	2.81148400	-1.47491100	0.00000800
C	-0.48592400	0.11719000	-0.00000300
C	-1.78027500	-0.08727600	-0.00000100
C	-2.26717900	-1.49960100	-0.00000500
O	-1.24659000	-2.40744300	-0.00000500
O	-3.40162400	-1.84857200	-0.00000800
C	-2.83130500	0.99251100	0.00000300
C	0.55423300	1.07928200	-0.00000400

C	1.11442200	1.51784900	1.21465100
C	2.19737400	2.38169200	1.20631500
C	2.74487900	2.81453400	-0.00000600
C	2.19738300	2.38167800	-1.20632600
C	1.11443100	1.51783500	-1.21466100
H	2.66809300	-1.61786200	-2.14215900
H	0.22997700	-2.13980800	-2.14146200
H	0.22996200	-2.13980100	2.14146100
H	2.66807900	-1.61785700	2.14217400
H	0.68617700	1.17507200	2.14870200
H	2.61594900	2.72347700	2.14521900
H	3.59041900	3.49141700	-0.00000700
H	2.61596600	2.72345300	-2.14523100
H	0.68619400	1.17504600	-2.14871000
F	-3.61486500	0.90967200	-1.07792300
F	-3.61486400	0.90966400	1.07792800
F	-2.27034800	2.20533300	0.00000700
C	4.24565500	-1.03084200	0.00001200
H	4.29093700	0.06372600	0.00000400
H	4.77360900	-1.38640700	0.88618200
H	4.77362000	-1.38642000	-0.88614700

TS3a-6a

E= -1104.796205 a.u., im. freq.= 404.39*i*

0 2

C	-0.93584500	-1.29335600	-1.16978500
C	-2.29173300	-0.94072800	-0.99340900
C	-3.03749200	-1.46886000	0.04960600
C	-2.44623700	-2.42243100	0.89048800
C	-1.12802400	-2.83976300	0.69958600
C	-0.39905700	-2.29528700	-0.33338000

O	0.90888000	-2.67279200	-0.52455900
C	1.90867800	-1.74216100	-0.46376700
C	1.52762400	-0.33906800	-0.09038500
C	0.33596600	0.18835800	-0.29837200
C	-4.45290200	-1.01019100	0.28398800
O	3.03059400	-2.07758600	-0.66906100
C	2.67925900	0.45793900	0.48997300
C	-0.32186700	1.45335100	-0.16668800
C	0.02736500	2.52742300	-0.99985600
C	-0.66745500	3.72403100	-0.91362000
C	-1.71135100	3.86668600	-0.00300700
C	-2.06294300	2.80290900	0.82409200
C	-1.38612100	1.59572500	0.73751500
F	3.30462500	-0.21887300	1.45610900
F	3.58226700	0.76057000	-0.44691200
F	2.25668300	1.60914700	1.02062900
H	-0.44342600	-1.08832700	-2.11470400
H	-2.74115400	-0.22276400	-1.67004500
H	-3.02622800	-2.84984000	1.70042100
H	-0.66360400	-3.57685300	1.34207200
H	-4.95333100	-0.78541600	-0.65881300
H	-5.03418700	-1.76741600	0.81105600
H	-4.46139700	-0.09764800	0.88763600
H	0.84988400	2.41348200	-1.69632100
H	-0.38821000	4.55230700	-1.55337000
H	-2.24735500	4.80541800	0.06384900
H	-2.86959300	2.91549000	1.53856700
H	-1.65656200	0.75953100	1.37229100

TS5a-9a

E= -1104.8107684 a.u., im. freq.= 262.35*i*

0 2

C	-3.28014400	-0.26657900	1.17801800
C	-1.90644200	-0.37844100	1.16155400
C	-1.18385500	-0.17289100	-0.04392800
C	-1.89467200	0.27815700	-1.18643900
C	-3.26410900	0.36642200	-1.15597200
C	-3.98403700	0.08599600	0.02077500
C	0.30581900	-0.03031700	0.01606500
C	0.99341000	-1.18011600	0.03045700
C	0.20525300	-2.41391600	-0.30568800
O	-1.08325700	-2.18654000	-0.42244300
O	0.69609500	-3.49539300	-0.50543100
C	2.46917100	-1.34453300	0.26354100
C	0.82766100	1.35439300	0.01062700
C	1.94828000	1.68645500	-0.75757200
C	2.40098900	2.99684800	-0.80379100
C	1.74420900	3.98971200	-0.08349200
C	0.62147200	3.67053200	0.67229800
C	0.15536900	2.36322500	0.70747600
H	-3.82530900	-0.46022600	2.09454300
H	-1.35717000	-0.66448200	2.05115700
H	-1.33936800	0.51342300	-2.08669200
H	-3.80568400	0.66842100	-2.04548600
H	2.45565000	0.91637300	-1.32640400
H	3.26721800	3.24337100	-1.40524500
H	2.10237900	5.01149900	-0.11809300
H	0.10330400	4.44131500	1.22947300
H	-0.72887600	2.12076400	1.28639300
F	3.14384600	-1.46831700	-0.89048300
F	2.99865600	-0.30189600	0.91963100
F	2.72266600	-2.42509800	0.99747400

C	-5.48301800	0.15252500	0.02051300
H	-5.87783300	0.25658500	1.03114400
H	-5.84003400	0.98698300	-0.58547900
H	-5.89562900	-0.76558000	-0.40856500

TS9a-8a

E= -1104.8098112 a.u., im. freq.= 320.95*i*

0 2

C	-1.18219000	0.35321300	0.09120700
C	-2.02360700	-0.47263500	0.88106700
C	-3.42538200	-0.29056100	0.83346000
C	-3.98559600	0.64246600	-0.00903100
C	-3.12856600	1.45436500	-0.78819700
C	-1.75224700	1.32337200	-0.73131900
O	-1.64013200	-2.10259100	-0.23059800
C	-0.35329200	-2.31388100	-0.36858600
O	0.05343900	-3.32226400	-0.89238700
C	0.61738700	-1.24121500	0.05948400
C	2.02927900	-1.73862700	0.25384700
C	0.26086000	0.06138700	0.08922200
C	1.18091900	1.22383200	0.04502900
C	0.94825900	2.32458700	0.87402200
C	1.78224100	3.43304200	0.81772800
C	2.83890700	3.46309500	-0.08644200
C	3.06195800	2.38008600	-0.93065600
C	2.24000300	1.26350900	-0.86537800
H	-1.59050000	-1.00587700	1.71776400
H	-4.05527900	-0.90425100	1.46616800
H	-3.56806800	2.19173000	-1.45164300
H	-1.11262000	1.94561700	-1.34600800
H	0.11901900	2.30174400	1.57223400

H	1.60543700	4.27445900	1.47645500
H	3.48515100	4.33112400	-0.13608600
H	3.87821300	2.40387500	-1.64205300
H	2.41173300	0.41992500	-1.52346800
F	2.03661800	-2.88367400	0.93844600
F	2.66464800	-1.95434200	-0.90612400
F	2.77497800	-0.87290200	0.95538200
C	-5.47446300	0.83198900	-0.10392500
H	-6.00129800	0.17990300	0.59195900
H	-5.74947800	1.86627000	0.11465200
H	-5.82178900	0.60444700	-1.11461300

TS9a-11a

E= -1104.8035218 a.u., im. freq.= 482.14*i*

0 2

C	3.47548600	-0.53479800	-0.90102400
C	4.11225200	0.32319200	-0.00554100
C	3.32165900	1.08683100	0.85702400
C	1.93978600	0.99540200	0.82695200
C	1.31039000	0.10838500	-0.05327600
C	2.09173600	-0.64927000	-0.92670700
C	-0.17184400	0.02994300	-0.06856800
C	-0.84749600	-1.11731400	-0.08045400
C	5.61387200	0.41517500	0.04793400
C	-0.91150700	1.32620600	-0.01072200
C	-1.96119300	1.51508900	0.88890000
C	-2.63008900	2.73250100	0.93000200
C	-2.25932200	3.76179500	0.07282100
C	-1.20702900	3.57877000	-0.82011900
C	-0.52533400	2.37080300	-0.85503000
C	-2.28512900	-1.42831400	-0.35955100

F	-2.39788500	-2.63155200	-0.92892600
F	-3.01560500	-1.45688000	0.76443300
F	-2.84766100	-0.53885700	-1.18010800
C	-0.08233600	-2.65591200	0.61570500
O	-0.33058200	-2.77948400	1.76019500
O	0.41727700	-3.05140300	-0.40494000
H	4.07033000	-1.12158500	-1.59228500
H	3.79789200	1.76662600	1.55534100
H	1.33867800	1.60474300	1.49214800
H	1.61273200	-1.31837900	-1.62915500
H	5.93901400	1.43754600	0.24704500
H	6.00538100	-0.21881700	0.84818800
H	6.06371000	0.08572500	-0.88911300
H	-2.23959400	0.71454500	1.56368200
H	-3.43959000	2.87575000	1.63507900
H	-2.78421000	4.70890100	0.10422100
H	-0.91373000	4.38063300	-1.48664600
H	0.30279100	2.22609600	-1.53920800

TS11a-12a

E= -1253.8072444 a.u., im. freq.= 387.33i

0 3

C	3.25854200	-0.33345300	-0.59444000
C	3.92289000	0.78209100	-0.08750300
C	3.17063400	1.74966100	0.58274200
C	1.80107800	1.60938000	0.73867800
C	1.14188200	0.47916300	0.23995200
C	1.88884000	-0.48986800	-0.43226500
C	-0.32322000	0.33880500	0.43750600
C	-0.90959600	-0.83709200	0.66829700
C	5.41325500	0.93533200	-0.23598900

C	-1.19180000	1.53225400	0.26772900
C	-2.35659800	1.66604000	1.03002000
C	-3.18773000	2.76282300	0.85387100
C	-2.87041400	3.73312600	-0.09236100
C	-1.71796300	3.60247600	-0.86018900
C	-0.87878200	2.51056500	-0.68033900
C	-0.63845200	-2.10451300	1.37452600
F	-1.00435900	-2.00672200	2.66077900
F	0.65673700	-2.45176500	1.35742400
F	-1.32675800	-3.12738300	0.84976900
C	-1.15600400	-1.73533300	-1.56932000
F	-0.38917300	-2.76408300	-1.89396400
F	-0.85108400	-0.69150600	-2.31793500
F	-2.42595700	-2.04586100	-1.70295000
H	3.82000500	-1.09123500	-1.12982200
H	3.66686800	2.62679400	0.98449900
H	1.23327600	2.37267300	1.25817900
H	1.40026200	-1.36526400	-0.84096700
H	5.68508800	1.97546900	-0.42343100
H	5.92286800	0.61956500	0.67848600
H	5.79300800	0.32657100	-1.05709200
H	-2.59351600	0.90859800	1.76934100
H	-4.08251900	2.86251800	1.45611700
H	-3.52061400	4.58849900	-0.23088300
H	-1.47323100	4.35100500	-1.60396600
H	0.01446600	2.40194600	-1.28404200

TS11a-12a (at B3LYP/6311G(d,p) level)

E= -1104.9891214 a.u., im. freq.= 233.44*i*

1 1

C	-0.64410700	-1.56258900	-1.08625900

C	-2.03358900	-1.30313000	-1.21876700
C	-2.89672500	-1.51880100	-0.16719900
C	-2.36150300	-2.04265200	1.05186000
C	-1.03136300	-2.36572500	1.20224100
C	-0.16822800	-2.15490500	0.11570600
O	1.11562500	-2.57053800	0.18499700
C	2.12447300	-1.65743600	-0.13081200
C	1.62499300	-0.23621300	-0.11710400
C	0.34858800	0.06655900	-0.23009500
C	-4.37300100	-1.26385000	-0.27489400
O	3.23457800	-2.01364800	-0.31421200
C	2.71700700	0.82718600	0.05259100
C	-0.53510700	1.17275900	-0.08730200
C	-1.00200100	1.89060300	-1.20957500
C	-1.79148700	3.01186800	-1.02383500
C	-2.14807700	3.41441400	0.26941900
C	-1.70804100	2.69834100	1.38233400
C	-0.90613000	1.57715100	1.21406100
F	2.19439900	2.05440500	0.17765700
F	3.43978300	0.56846800	1.14917700
F	3.52413200	0.82299900	-1.01226600
H	-0.02804500	-1.61708200	-1.97630600
H	-2.40628700	-0.93339300	-2.16610600
H	-3.03851400	-2.21387500	1.88245700
H	-0.64166100	-2.79843400	2.11508500
H	-4.64463300	-0.87681100	-1.25667300
H	-4.93546400	-2.18620600	-0.10232500
H	-4.69787000	-0.54403200	0.48221000
H	-0.71393900	1.58374900	-2.20804200
H	-2.12704000	3.58302400	-1.88082200
H	-2.76675900	4.29370200	0.40552100

H	-1.97972200	3.02027100	2.38021300
H	-0.54071900	1.02824600	2.07319100

2b

E= -344.8587758 a.u., number of negative frequencies = 0

0 2

C	-1.26284600	1.33111100	-0.00001600
C	-2.16387200	0.26695200	0.00003300
C	-1.70744900	-1.04717800	0.00006400
C	-0.34162100	-1.30236900	0.00004700
C	0.55656000	-0.23934000	-0.00000200
C	0.10082400	1.08171100	-0.00003400
C	2.01780000	-0.52102000	-0.00002000
O	2.90100100	0.25738800	-0.00006800
H	-1.62851500	2.35077200	-0.00004000
H	-3.22902800	0.46603100	0.00004700
H	-2.41408200	-1.86774300	0.00010200
H	0.04278000	-2.31571500	0.00007100
H	0.82446200	1.88834900	-0.00007200

3b

E= -1112.1040801 a.u., number of negative frequencies = 0

0 2

C	-5.14130100	-1.29878700	-0.09804400
C	-4.59296600	-0.03109300	-0.29834500
C	-3.22577200	0.14020200	-0.46400900
C	-2.39643700	-0.97265200	-0.43348900
C	-2.90731300	-2.24833700	-0.24615600
C	-4.27989900	-2.39493900	-0.07843600
O	-1.04809600	-0.71869400	-0.65930100
C	-0.09042400	-1.24265500	0.14378100

O	-0.24827100	-2.14995200	0.90372400
C	1.18480700	-0.49453800	-0.08550600
C	2.34337400	-1.03447100	0.22288100
C	-6.62261800	-1.47439100	0.11675800
C	1.12741900	0.90496900	-0.67251400
C	3.75001100	-0.88834200	0.16800700
C	4.39223300	-0.69332300	-1.07075800
C	5.77250500	-0.58649300	-1.11991500
C	6.52746500	-0.66592100	0.04791000
C	5.89835000	-0.85746600	1.27696600
C	4.52138100	-0.98025100	1.34213200
O	1.87393800	1.23283200	-1.56067800
C	0.13281900	1.85791100	-0.08430500
C	-0.41616900	1.65960700	1.18278700
C	-1.34394900	2.56249400	1.68672200
C	-1.73413700	3.65702300	0.92139600
C	-1.18349600	3.85942900	-0.34204200
C	-0.24407500	2.96711400	-0.84048600
H	-5.24474900	0.83552800	-0.32562600
H	-2.78606200	1.11918900	-0.62160300
H	-2.24646700	-3.10256300	-0.22459300
H	-4.68786400	-3.38916700	0.06857700
H	-7.19141200	-0.71707800	-0.42489600
H	-6.95559700	-2.45725900	-0.21958400
H	-6.87337300	-1.38329800	1.17722500
H	3.78843300	-0.60157800	-1.96398300
H	6.26302600	-0.43020400	-2.07288100
H	7.60614700	-0.57847100	0.00133800
H	6.48710800	-0.91891000	2.18397600
H	4.02294200	-1.14656300	2.28925300
H	-0.11815800	0.80476900	1.78108200

H	-1.76733000	2.40759100	2.67134300
H	-2.46618700	4.35472800	1.31051000
H	-1.48588600	4.71403400	-0.93511700
H	0.20401100	3.10522800	-1.81700400

4b

E= -1112.0953697 a.u., number of negative frequencies = 0

0 2

C	5.17864300	0.99947500	-0.08852800
C	4.56457300	2.15737000	-0.56095100
C	3.18071900	2.29052400	-0.55224700
C	2.40468800	1.25164800	-0.06829600
C	2.98284800	0.07965700	0.40315600
C	4.36582900	-0.03181200	0.38727500
O	1.02325400	1.40396800	-0.16725800
C	0.23875900	1.00692300	0.86149700
O	0.62594000	0.68460600	1.94807600
C	-1.16539100	1.02906400	0.47621000
C	-2.16083700	0.18469700	0.32365200
C	6.67949500	0.86691200	-0.06449700
C	-3.55599800	0.58312700	0.02238900
C	-1.83467800	-1.28578600	0.58823000
O	-2.57671700	-1.95157100	1.26190500
C	-4.48573400	-0.34685200	-0.44675700
C	-5.77713600	0.05530300	-0.76704200
C	-6.15546400	1.38388200	-0.61987300
C	-5.23474900	2.31547500	-0.14726700
C	-3.94593000	1.91828300	0.17195800
C	-0.56520700	-1.84091600	0.02241500
C	0.02578700	-2.92449300	0.67566400
C	1.18254000	-3.49509100	0.16477500

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C         1.73916100  -3.00387700  -1.01487500
C         1.14329200  -1.93713000  -1.67797300
C        -0.00412000  -1.34885900  -1.15787800
H         5.17403400   2.96943300  -0.94191500
H         2.69360100   3.18383300  -0.92241100
H         2.36341500  -0.72543300   0.77743400
H         4.82385000  -0.94406700   0.75485200
H         7.14846700   1.56656400  -0.75732700
H         7.06970100   1.07419900   0.93555400
H         6.98964400  -0.14347200  -0.33692700
H        -4.20724800  -1.38732900  -0.55101600
H        -6.48967800  -0.67570300  -1.12928000
H        -7.16408600   1.69301800  -0.86612700
H        -5.52474100   3.35169700  -0.02216800
H        -3.23056900   2.64039200   0.54992400
H        -0.43482400  -3.29805600   1.58214100
H         1.64909700  -4.32525800   0.68101100
H         2.64102200  -3.45186700  -1.41502500
H         1.57593100  -1.55517400  -2.59429200
H        -0.46398200  -0.51392800  -1.67243500
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5b

E= -1112.1282575 a.u., number of negative frequencies = 0

0 2

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C         4.43389000  -1.02220800   0.33948400
C         3.88771700  -1.10070900  -0.96635900
C         2.54808700  -1.10622300  -1.18761400
C         1.54879600  -1.07973200  -0.06663900
C         2.19052100  -1.00144800   1.28333100
C         3.53404200  -0.97693000   1.44336100
O         0.79020600  -2.31472100  -0.15128900
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C	-0.50109100	-2.06732600	-0.48547500
C	-0.67603700	-0.59601400	-0.58172000
C	0.48179300	0.00500200	-0.27816300
O	-1.31368200	-2.92652800	-0.64202400
C	5.91304500	-1.04204400	0.57144400
C	0.75386900	1.43789900	-0.09935800
C	-0.29264800	2.31004000	0.22935700
C	-0.05383500	3.66212400	0.41798600
C	1.23572600	4.16870300	0.28780800
C	2.28505700	3.31056700	-0.01770800
C	2.05102100	1.95389400	-0.20099100
C	-1.96395800	0.00579700	-1.06717000
C	-3.19230900	-0.18656400	-0.24309300
O	-1.97461100	0.63153900	-2.09913100
C	-4.40239200	0.30235100	-0.74094400
C	-5.56370000	0.16686300	0.00300300
C	-5.52150000	-0.45393300	1.24997600
C	-4.31872700	-0.93883600	1.75092400
C	-3.15389900	-0.80859400	1.00453700
H	4.56503400	-1.15467500	-1.81242000
H	2.13488400	-1.16976500	-2.18784900
H	1.51819000	-0.97840800	2.13344500
H	3.94827200	-0.92776100	2.44538100
H	6.46367800	-0.84174900	-0.34814400
H	6.20487700	-0.30016300	1.31899200
H	6.23315700	-2.02028900	0.94658500
H	-1.29722000	1.92699000	0.36281400
H	-0.87510600	4.32059000	0.67264300
H	1.42151500	5.22613200	0.43271800
H	3.29293300	3.69616900	-0.11135500
H	2.87929800	1.29918400	-0.43674700

H	-4.40443600	0.78128700	-1.71250100
H	-6.50307700	0.54153600	-0.38482900
H	-6.42998700	-0.56101300	1.83088000
H	-4.28890100	-1.42415000	2.71852800
H	-2.21923000	-1.19229600	1.39555000

6b

E= -1112.1210459 a.u., number of negative frequencies = 0

0 2

C	4.31757100	-0.16131700	0.35881500
C	4.48191500	-1.46798900	-0.19129300
C	3.37812500	-2.32987600	-0.32260400
C	2.15039200	-1.93433600	0.10092100
C	1.87639400	-0.62205600	0.75300700
C	3.09661900	0.25253300	0.78267400
O	1.09120100	-2.79554500	-0.03037800
C	-0.16660900	-2.31387500	-0.25885500
O	-1.06944000	-3.08555200	-0.38432600
C	-0.31219600	-0.84126200	-0.35664900
C	0.63116400	-0.00886000	0.10005000
C	5.52268400	0.73814700	0.45182500
C	-1.56156100	-0.33769600	-1.05518300
C	0.45083600	1.46353200	0.07135300
C	1.27695300	2.26495200	-0.72050100
C	1.08044700	3.63843600	-0.76136900
C	0.06858500	4.22449300	-0.00601500
C	-0.75404200	3.43148600	0.78428700
C	-0.56787700	2.05381600	0.82046600
C	-2.86539900	-0.40549600	-0.33126000
O	-1.46625500	0.13273900	-2.16020500
C	-3.99568700	0.10996600	-0.96756100

C	-5.22271200	0.09741600	-0.32191300
C	-5.32659900	-0.43022900	0.96298100
C	-4.20322200	-0.94623400	1.60036300
C	-2.97335600	-0.93528500	0.95427900
H	5.45877500	-1.78633100	-0.53228600
H	3.47605200	-3.31052300	-0.77181800
H	1.56817600	-0.81433900	1.80075500
H	2.97600000	1.23981700	1.21314100
H	5.96153400	0.89572100	-0.53643400
H	5.26081000	1.70963400	0.87098600
H	6.29122200	0.28620800	1.08363900
H	2.05649000	1.80312200	-1.31493800
H	1.71428300	4.25273200	-1.38929000
H	-0.08078900	5.29690700	-0.03953500
H	-1.54666200	3.88125900	1.36967200
H	-1.21509100	1.43197300	1.42938100
H	-3.88492900	0.51570300	-1.96566500
H	-6.09949500	0.49711900	-0.81669100
H	-6.28583700	-0.44155300	1.46696400
H	-4.28698200	-1.36317900	2.59641300
H	-2.10215900	-1.34900500	1.44808000

7b

E= -1111.8551735 a.u., number of negative frequencies = 0

1 1

C	-5.13772100	-1.73837500	0.12894000
C	-4.47009000	-2.00460200	-1.06657800
C	-3.15385700	-1.60361600	-1.26007300
C	-2.51502000	-0.92957400	-0.23747100
C	-3.14034800	-0.63402100	0.96108500
C	-4.45490800	-1.04646500	1.13182400

O	-1.20008400	-0.48021300	-0.50382600
C	-0.23214400	-0.75198100	0.35754800
O	-0.27881400	-1.34026100	1.38662700
C	1.05388700	-0.12598700	-0.18737600
C	2.22065900	-0.58831000	-0.00318900
C	-6.55281300	-2.20413300	0.34539300
C	0.88644000	1.15622200	-1.12473600
C	3.49740400	-1.05551500	0.11008400
C	4.01816300	-1.89941400	-0.91338900
C	5.30554400	-2.37056100	-0.79999000
C	6.07305300	-2.01653700	0.31618000
C	5.57389700	-1.18889700	1.33080000
C	4.29142500	-0.70234900	1.23888600
O	1.17441900	1.03768200	-2.26859400
C	0.34953300	2.34645400	-0.44249300
C	0.13840200	2.38366100	0.93781400
C	-0.37195300	3.53503800	1.52025300
C	-0.67012700	4.63930900	0.72710600
C	-0.45837100	4.60127000	-0.64963000
C	0.05188400	3.45688300	-1.23975900
H	-4.98578100	-2.53082200	-1.86151800
H	-2.63037800	-1.79724900	-2.18764900
H	-2.61730600	-0.09885000	1.74284000
H	-4.96086300	-0.82313000	2.06418100
H	-7.07771400	-2.32454600	-0.60238800
H	-6.56200800	-3.16946600	0.85810100
H	-7.11031300	-1.49640800	0.95990900
H	3.39192100	-2.14639000	-1.76184000
H	5.72430900	-3.01031000	-1.56549900
H	7.08586900	-2.39471900	0.39852800
H	6.19611800	-0.93769500	2.17955400

H	3.86939300	-0.06260900	2.00388600
H	0.37410200	1.52996200	1.56445500
H	-0.53669600	3.57280500	2.58936500
H	-1.07084900	5.53560300	1.18466800
H	-0.69373700	5.46390600	-1.25980500
H	0.22213700	3.40125400	-2.30782600

8b

E= -1112.1311793 a.u., number of negative frequencies = 0

0 2

C	-3.97871000	1.46723200	0.27343200
C	-4.70027500	0.24668000	0.52589200
C	-4.02446700	-0.91985800	0.58169400
C	-2.53709700	-0.98189600	0.49724500
C	-1.88841700	0.28559700	0.03046100
C	-2.61774800	1.46504500	0.00439400
O	-2.18324500	-2.11291200	-0.31075800
C	-0.87462000	-2.28541500	-0.63232600
O	-0.49405400	-3.35652800	-1.00130300
C	0.00062100	-1.08688100	-0.55046100
C	-0.50365600	0.16186400	-0.32775900
C	1.44698500	-1.31273900	-0.91861700
C	2.49275400	-1.05510900	0.12184100
O	1.73841300	-1.67579600	-2.03078200
C	0.35148900	1.37069900	-0.46159200
C	1.08155100	1.59688800	-1.62983600
C	1.91393900	2.70563400	-1.72937200
C	2.02853900	3.59146400	-0.66443000
C	1.29973700	3.37388100	0.50117600
C	0.45941200	2.27348700	0.59968800
C	-6.19532000	0.31699700	0.67908400

C	2.17531100	-0.78143000	1.45190300
C	3.18725100	-0.55605100	2.37755800
C	4.51756300	-0.59970400	1.97628400
C	4.83909100	-0.87481800	0.64889700
C	3.83070400	-1.10444300	-0.27410400
H	-4.53205300	2.39820900	0.22770000
H	-4.53204100	-1.86627100	0.73099600
H	-2.14190900	-1.19261200	1.50986000
H	-2.12217600	2.38726400	-0.27581200
H	0.99479800	0.90061500	-2.45598200
H	2.47550500	2.87393600	-2.64012600
H	2.68425400	4.45038700	-0.74098700
H	1.39033900	4.05951600	1.33494400
H	-0.10435600	2.09630400	1.50940600
H	-6.46451000	0.94225100	1.53424200
H	-6.65185000	0.76054500	-0.20903900
H	-6.62372600	-0.67355800	0.82906500
H	1.13828100	-0.74984900	1.76521900
H	2.93828300	-0.34790900	3.41099500
H	5.30588900	-0.42186000	2.69822500
H	5.87629800	-0.91123200	0.33857600
H	4.05224000	-1.32658800	-1.31083300

9b

E= -1112.1064676 a.u., number of negative frequencies = 0

0 2

C	-4.07652600	-1.10945200	0.83279400
C	-4.69061300	-0.89613000	-0.39695200
C	-3.94529400	-0.29518700	-1.41991200
C	-2.62822900	0.07590900	-1.22049800
C	-2.00357400	-0.17808500	0.00593200

C	-2.74612300	-0.75941100	1.03738100
C	-0.59348900	0.23536400	0.23290200
C	0.35376900	-0.66615900	0.55696800
C	-6.11854000	-1.30566900	-0.63923200
C	-0.31212000	1.68498700	0.08675500
C	0.85883700	2.14095600	-0.52616600
C	1.09845400	3.50199000	-0.65795600
C	0.17491200	4.42391700	-0.17726600
C	-0.99875600	3.97942600	0.42267700
C	-1.24845500	2.61936700	0.54129200
C	1.73258700	-0.27831300	1.06400600
C	0.12464900	-2.13421800	0.52489700
O	0.98765600	-2.95371800	0.74381900
O	-1.07111000	-2.58694200	0.19905000
C	2.92994500	-0.60320200	0.23187900
O	1.82710300	0.28676400	2.12422600
C	2.81507400	-1.13358700	-1.05301500
C	3.95529100	-1.38454700	-1.80557900
C	5.21151100	-1.11361700	-1.27323000
C	5.32966500	-0.58604000	0.01031800
C	4.19184900	-0.32848100	0.76011500
H	-4.64148200	-1.55581200	1.64335800
H	-4.41491000	-0.11266200	-2.38073800
H	-2.06730800	0.55828700	-2.01319500
H	-2.27882700	-0.92184500	2.00196600
H	-6.62900600	-1.53421200	0.29644900
H	-6.67180800	-0.51552100	-1.15052300
H	-6.15693300	-2.19725600	-1.27067700
H	1.57487600	1.43019500	-0.92221300
H	2.00665000	3.84161600	-1.14065000
H	0.36561000	5.48570700	-0.27661500

H	-1.72325000	4.69344300	0.79492200
H	-2.16698300	2.27313200	1.00096500
H	1.83687500	-1.34688400	-1.46925200
H	3.86492300	-1.79750000	-2.80266600
H	6.10052300	-1.31524800	-1.85908300
H	6.30927000	-0.37800700	0.42315500
H	4.25364900	0.08483500	1.75935300

10b

E= -1111.5975841 a.u., number of negative frequencies = 0

0 1

C	4.04493100	1.38086000	0.36622400
C	4.73373500	0.16232000	0.47923600
C	4.03333900	-1.01974400	0.29830300
C	2.66979000	-0.98773600	0.01965200
C	1.96844500	0.21697000	-0.07254300
C	2.69325300	1.40872400	0.09306000
O	2.06020100	-2.18821000	-0.16165000
C	0.72866800	-2.30559200	-0.48604300
O	0.26685200	-3.39931100	-0.61246000
C	-0.02391800	-1.05100600	-0.60342900
C	0.54638100	0.15420400	-0.37920800
C	-1.47465200	-1.21425100	-1.00088400
C	-2.52403100	-1.01108600	0.04178100
O	-1.74864300	-1.48991600	-2.14186400
C	-0.26730000	1.39640900	-0.43455400
C	-0.36867200	2.21450800	0.69382900
C	-1.18084600	3.33995800	0.66965100
C	-1.88640200	3.66567300	-0.48511200
C	-1.77963400	2.86143800	-1.61335100
C	-0.97633900	1.72680800	-1.58993000

C	6.20720300	0.15281500	0.78531200
C	-2.20670000	-0.81290000	1.38499100
C	-3.21972300	-0.63475600	2.31958200
C	-4.54909000	-0.65049700	1.91317900
C	-4.86981400	-0.84991800	0.57190500
C	-3.86084100	-1.03259700	-0.36056400
H	4.58852100	2.31100700	0.48825600
H	4.52065600	-1.98527800	0.36049700
H	2.17830600	2.35578500	-0.00929500
H	0.17578800	1.95215600	1.59474200
H	-1.26742900	3.96060300	1.55319500
H	-2.51945400	4.54452200	-0.50313300
H	-2.32570300	3.11251700	-2.51437400
H	-0.89862600	1.09042100	-2.46384200
H	6.60729300	-0.86074500	0.78158900
H	6.75725800	0.74250800	0.04861200
H	6.39764100	0.59239700	1.76738100
H	-1.17013200	-0.80279400	1.70137200
H	-2.97233400	-0.48592300	3.36348300
H	-5.33823800	-0.51004900	2.64243500
H	-5.90665200	-0.86484000	0.25876700
H	-4.08088000	-1.19641700	-1.40841300

11b

E= -923.5576606 a.u., number of negative frequencies = 0

0 2

C	2.11206500	-2.95629500	-0.67714000
C	2.99321900	-3.00534800	0.40393700
C	3.09559000	-1.88078600	1.22349600
C	2.34774000	-0.73863000	0.97108400
C	1.46852600	-0.69924400	-0.11253100

C	1.35784500	-1.82083300	-0.93699500
C	0.62500700	0.50692600	-0.37058800
C	-0.61350400	0.33962500	-0.76419500
C	3.83345100	-4.22914900	0.65904700
C	1.19214100	1.87288300	-0.18049800
C	0.37427700	2.92753400	0.23311600
C	0.89341100	4.20720600	0.37476000
C	2.23721600	4.44891200	0.10761900
C	3.05758000	3.40393600	-0.30334100
C	2.54095400	2.12182500	-0.44462400
C	-1.80364300	-0.28343900	-1.23775000
O	-1.85528500	-0.74439400	-2.37394900
C	-2.98160800	-0.32892800	-0.31477900
C	-4.18397300	-0.83781300	-0.80536900
C	-5.29765400	-0.90218600	0.01955000
C	-5.21451900	-0.46310100	1.33863100
C	-4.01541400	0.04025700	1.83218600
C	-2.89990200	0.10935100	1.00664800
H	2.01781500	-3.81961900	-1.32733000
H	3.76844500	-1.90138500	2.07431200
H	2.43791400	0.12480300	1.62069600
H	0.68087800	-1.79069200	-1.78458400
H	4.10803400	-4.30657200	1.71189000
H	3.30073400	-5.13786600	0.37477300
H	4.75749600	-4.19015300	0.07549900
H	-0.67140800	2.73455300	0.44732000
H	0.24964600	5.01575400	0.69952900
H	2.64313900	5.44683000	0.22121800
H	4.10354200	3.58706000	-0.51817100
H	3.18003400	1.30993900	-0.77138400
H	-4.21998400	-1.17600400	-1.83368300

H	-6.23202600	-1.29474400	-0.36302200
H	-6.08478700	-0.51451400	1.98213400
H	-3.94931300	0.37717200	2.85952000
H	-1.96071500	0.49437600	1.38929500

12b

E= -1268.5615378 a.u., number of negative frequencies = 0

0 1

C	3.70716100	0.19804500	-1.32965100
C	4.44462400	0.65193000	-0.23680000
C	3.76382400	1.29670600	0.79873900
C	2.38849500	1.46371400	0.75435400
C	1.64733500	0.96259400	-0.32044400
C	2.32818500	0.34996300	-1.37458200
C	0.16817900	1.06138100	-0.32256000
C	-0.61737900	0.02492000	-0.68684500
C	5.93314400	0.43730300	-0.16573900
C	-0.41028100	2.36044000	0.10944700
C	-1.48392100	2.39953300	1.00271900
C	-2.01306000	3.61497100	1.41529600
C	-1.47640500	4.80599700	0.93796800
C	-0.40153300	4.77646900	0.05513100
C	0.13690300	3.56179000	-0.34753500
C	-2.08380100	0.22408100	-1.01952900
C	-3.08699700	-0.68176700	-0.37265700
O	-2.42312200	1.08133900	-1.79497400
C	-0.12785200	-1.35467700	-1.02808000
O	-0.55893300	-1.89426900	-2.02323700
C	-2.75455800	-1.51288300	0.69638400
C	-3.72758900	-2.30925500	1.28980800
C	-5.03318900	-2.27895300	0.81354500

C	-5.36953300	-1.44812700	-0.25324400
C	-4.40107800	-0.64931200	-0.84143600
C	0.82210900	-2.08564100	-0.12086400
C	1.44980600	-3.22224800	-0.63137400
C	2.33173500	-3.94743100	0.15672100
C	2.58052700	-3.55011100	1.46757500
C	1.94206200	-2.42937500	1.98842000
C	1.06660200	-1.69694700	1.19651700
H	4.21929300	-0.28007000	-2.15769600
H	4.32257100	1.67307500	1.64910600
H	1.87483000	1.96835300	1.56559800
H	1.77117600	0.00091700	-2.23739900
H	6.37673500	0.41502000	-1.16202300
H	6.41955200	1.22521700	0.41103000
H	6.15632700	-0.51727600	0.31916000
H	-1.89872100	1.47056200	1.38101600
H	-2.84353200	3.63193000	2.11059500
H	-1.89177900	5.75462000	1.25626700
H	0.01848500	5.70190000	-0.32001100
H	0.97701900	3.53571300	-1.03200700
H	-1.73813000	-1.54223900	1.07449800
H	-3.46546200	-2.95399000	2.11970500
H	-5.79033300	-2.90360600	1.27267800
H	-6.38734400	-1.42688300	-0.62356300
H	-4.63534600	0.00989300	-1.66826400
H	1.23141300	-3.51669000	-1.65061800
H	2.82410700	-4.82347100	-0.24789700
H	3.26825400	-4.11637800	2.08454200
H	2.12862800	-2.12311300	3.01056900
H	0.57762100	-0.81871900	1.60269500

13b

E= -1111.5965043 a.u., number of negative frequencies = 0

0 1

C	4.24506100	0.72781300	0.43091600
C	4.72501300	-0.58264000	0.57910000
C	3.89643000	-1.67578900	0.41725300
C	2.55432200	-1.47137800	0.10978700
C	2.03345000	-0.18315700	-0.02474100
C	2.90600800	0.90695500	0.12815000
O	1.78744500	-2.58224100	-0.05483500
C	0.46036300	-2.52151300	-0.40255700
O	-0.15083300	-3.54152600	-0.51290600
C	-0.10702000	-1.17700400	-0.56546500
C	0.61989100	-0.05663200	-0.35876800
C	-1.56032400	-1.14723800	-0.98616300
C	-2.58722900	-0.79384600	0.03808600
O	-1.85111300	-1.39363500	-2.12960300
C	-0.01512000	1.28307400	-0.46207300
C	-0.03348400	2.13508400	0.64554300
C	-0.68344800	3.35949100	0.57365200
C	-1.30743000	3.74920400	-0.60800100
C	-1.28230100	2.90990400	-1.71534600
C	-0.64227900	1.67762400	-1.64434800
C	-2.26438600	-0.62535200	1.38410700
C	-3.25693300	-0.30250600	2.30169500
C	-4.57058100	-0.14368100	1.87540500
C	-4.89684300	-0.31273500	0.53124600
C	-3.90905400	-0.63976300	-0.38427100
C	5.17860500	1.89954000	0.59096300
H	5.77177400	-0.74033000	0.81673100
H	4.25621400	-2.69186400	0.51563700

H	2.51679900	1.90918100	-0.00859200
H	0.44703300	1.82385600	1.56703900
H	-0.70754200	4.00805700	1.44091200
H	-1.81391000	4.70519700	-0.66314200
H	-1.76578700	3.20994700	-2.63691500
H	-0.63036500	1.01415900	-2.50129600
H	-1.24047800	-0.75140900	1.71640000
H	-3.00616400	-0.17723700	3.34787500
H	-5.34350400	0.10981500	2.59137700
H	-5.92180100	-0.19125800	0.20259800
H	-4.13467300	-0.78386700	-1.43382600
H	4.65314000	2.84385300	0.44788800
H	5.62667000	1.90755900	1.58734200
H	5.99232600	1.85083000	-0.13630500

14b

E= -1111.886677 a.u., number of negative frequencies = 0

1 1

C	4.15344500	-0.51677300	0.83336700
C	4.14619800	-1.94671300	0.66826500
C	3.12893400	-2.64781500	0.07489200
C	2.01791700	-1.94013400	-0.40039500
C	2.03967000	-0.46487500	-0.47868100
C	3.11942800	0.18371100	0.31835900
O	0.99521100	-2.61615400	-0.81381600
C	-0.31023200	-2.01242000	-1.06174800
O	-1.12866300	-2.74064100	-1.48033400
C	-0.41414400	-0.58912500	-0.74415500
C	0.65843400	0.17115600	-0.47767800
C	5.29119500	0.12271700	1.57766600
C	-1.80354200	0.01114200	-0.99597400

C	-2.89500700	-0.33197200	-0.05825600
O	-1.92818300	0.72287500	-1.95505600
C	0.55851700	1.62604200	-0.24642600
C	1.30804100	2.51647700	-1.02128900
C	1.17732000	3.88378500	-0.82529800
C	0.31455000	4.36745000	0.15458500
C	-0.42636100	3.48379700	0.93104100
C	-0.31243800	2.11412600	0.72960100
C	-4.18573900	0.10886100	-0.36201700
C	-5.23278300	-0.18543400	0.49641500
C	-4.99555100	-0.91563000	1.65939600
C	-3.71121100	-1.35285300	1.96788200
C	-2.66040100	-1.06314600	1.10805000
H	4.98803000	-2.50514000	1.06893100
H	3.11675300	-3.72889100	0.02605800
H	2.41519100	-0.32744500	-1.52442000
H	3.07875800	1.26346300	0.40258700
H	5.37127000	-0.29290200	2.58424700
H	6.23666500	-0.06386700	1.06372100
H	5.15070600	1.19918100	1.65979800
H	1.96147500	2.14755300	-1.80586600
H	1.73977000	4.57231400	-1.44318500
H	0.21634000	5.43495100	0.30730000
H	-1.09916600	3.85953300	1.69146500
H	-0.89283600	1.42357700	1.33212100
H	-4.34309500	0.67334700	-1.27292000
H	-6.23526100	0.14958400	0.26201300
H	-5.81636300	-1.14589400	2.32770800
H	-3.53304900	-1.92010500	2.87257800
H	-1.65954400	-1.40214800	1.35591400

15b

E= -1111.8765008 a.u., number of negative frequencies = 0

1 1

C	3.77111700	-0.82869400	0.35965700
C	3.38889600	-1.18694800	-0.96241500
C	2.17130700	-1.74539900	-1.17886400
C	1.21584200	-1.83756700	-0.07251900
C	1.78446800	-1.83191000	1.27381200
C	3.00546000	-1.27501900	1.47413300
O	0.18110700	-2.73956600	-0.27405400
C	-1.02319800	-2.10322300	-0.55001800
C	-0.78185900	-0.63209500	-0.47815200
C	0.47942400	-0.35329100	-0.18468800
O	-2.00908400	-2.70204500	-0.78652600
C	4.96707600	0.01533300	0.57494400
C	1.20168600	0.90918500	-0.03471100
C	1.64325400	1.59070900	-1.17567500
C	2.33761600	2.78423100	-1.04223000
C	2.59047800	3.30741800	0.22477500
C	2.13462300	2.64520200	1.36191800
C	1.44720000	1.44528100	1.23525700
C	-1.81329000	0.42407600	-0.85392200
C	-3.12643600	0.40775100	-0.18075200
O	-1.48651500	1.22443200	-1.69283800
C	-4.12104800	1.25905600	-0.67330300
C	-5.36144600	1.29476700	-0.05899500
C	-5.61034500	0.49041200	1.05182600
C	-4.62079600	-0.35078900	1.55009200
C	-3.37941000	-0.39713700	0.93175400
H	4.07016800	-0.98968000	-1.78085900
H	1.81248600	-2.01730500	-2.16633300

H	1.15004300	-2.17377700	2.08494200
H	3.40562800	-1.14486200	2.47215100
H	5.71349000	-0.12013600	-0.20755200
H	4.61703200	1.05991500	0.51779100
H	5.40728800	-0.13064300	1.56062000
H	1.41195700	1.19363400	-2.15703000
H	2.66580000	3.31674500	-1.92593000
H	3.12647200	4.24350500	0.32441100
H	2.30563900	3.06756600	2.34414700
H	1.08084100	0.93261000	2.11752800
H	-3.90049900	1.87675300	-1.53506800
H	-6.13682600	1.94607400	-0.44185300
H	-6.58186400	0.51884200	1.53015300
H	-4.82027700	-0.97307800	2.41300400
H	-2.61516200	-1.05684300	1.32568200

16b

E= -1111.8717757 a.u., number of negative frequencies = 0

1 1

C	-4.13619700	1.10353200	0.30957100
C	-4.78721900	-0.16638400	0.35625800
C	-3.99154100	-1.26830000	0.31465700
C	-2.52267800	-1.14566500	0.38109700
C	-1.92659400	0.17386900	0.10105500
C	-2.76525400	1.28063500	0.19784100
O	-1.88200700	-2.28179900	-0.10887100
C	-0.56359400	-2.24817800	-0.48270700
O	-0.01134700	-3.25688200	-0.76454600
C	0.10772800	-0.91613900	-0.50664600
C	-0.51754600	0.24893100	-0.20327300
C	1.53265700	-0.96301900	-1.04605900

C	2.65975900	-0.95665000	-0.09872900
O	1.62676300	-0.99923600	-2.24565900
C	0.17325500	1.56267500	-0.23579300
C	0.77176900	2.01652600	-1.41240600
C	1.43257000	3.23954100	-1.41915700
C	1.50455400	4.00277900	-0.25962800
C	0.90887900	3.55052700	0.91477200
C	0.23752300	2.33592000	0.92725600
C	-6.28699300	-0.23672300	0.39582200
C	3.95441800	-1.04668600	-0.61807600
C	5.03925800	-1.04816200	0.24281300
C	4.83532000	-0.95992000	1.61900600
C	3.54781200	-0.87021800	2.13896800
C	2.45767800	-0.86843900	1.28004500
H	-4.76408900	1.99065200	0.32590100
H	-4.38656600	-2.27927200	0.32969500
H	-2.41041300	-1.12943200	1.50500100
H	-2.34878500	2.27484800	0.09544600
H	0.71897800	1.41684200	-2.31340200
H	1.89373800	3.59268400	-2.33279300
H	2.02685500	4.95137200	-0.26844100
H	0.97328700	4.14066000	1.82026900
H	-0.21465700	1.97590400	1.84632900
H	-6.66365000	0.19812300	1.32421800
H	-6.71744900	0.32434300	-0.43573800
H	-6.63360700	-1.26687300	0.33366200
H	4.08334500	-1.12014400	-1.69104800
H	6.04440100	-1.12173400	-0.15247600
H	5.68578700	-0.96401000	2.28995800
H	3.39795300	-0.80490100	3.20908300
H	1.45420400	-0.79844300	1.68681700

TS1-3b

E= -1112.0548571 a.u., im. freq.= 333.27*i*

0 2

C	-4.79093800	-1.69352100	-0.41944700
C	-4.29629600	-0.44767600	-0.79712400
C	-2.93014100	-0.18711100	-0.79894200
C	-2.05132200	-1.18766200	-0.42063000
C	-2.51050100	-2.44255500	-0.04307500
C	-3.87693800	-2.68194200	-0.04624700
O	-0.69205500	-0.88906000	-0.49978400
C	0.09270200	-1.09986800	0.58370000
O	-0.27149600	-1.61104000	1.60187200
C	1.43570100	-0.58058100	0.34775400
C	2.64850600	-0.72797900	0.26079000
C	-6.27047500	-1.98015900	-0.40585300
C	0.92494900	1.55432400	-0.28262600
C	4.05162700	-0.67795800	0.06705700
C	4.57110500	-0.39269300	-1.20635000
C	5.94251600	-0.34282100	-1.39845600
C	6.80964500	-0.56697500	-0.33185800
C	6.30024400	-0.84392800	0.93431100
C	4.93065100	-0.90414300	1.13792900
O	1.73009800	1.98824600	-1.01966400
C	-0.36967400	2.14711400	0.13883100
C	-0.99011900	1.73422200	1.31578100
C	-2.22946800	2.26190400	1.65565300
C	-2.84883300	3.18038500	0.81366200
C	-2.22523400	3.59265700	-0.36289300
C	-0.97910100	3.08386100	-0.70033100
H	-4.98540000	0.33542300	-1.09426900

H	-2.53880700	0.77990200	-1.09204700
H	-1.80960900	-3.20974200	0.25583500
H	-4.24245000	-3.65986600	0.24901000
H	-6.61922800	-2.18003000	0.61032300
H	-6.83909300	-1.13638700	-0.79789100
H	-6.50409100	-2.85782800	-1.01263700
H	3.88481700	-0.20078600	-2.02143800
H	6.33848800	-0.12118100	-2.38201700
H	7.88089800	-0.52386700	-0.48667700
H	6.97438500	-1.01673900	1.76437200
H	4.52366300	-1.12537600	2.11668700
H	-0.50754400	1.00536500	1.95700900
H	-2.71794300	1.94405700	2.56806300
H	-3.82282900	3.57732300	1.07397400
H	-2.70983900	4.31259600	-1.01142700
H	-0.46942600	3.39059700	-1.60608300

TS1-4b

E= -1112.0541643 a.u., im. freq.= 379.02*i*

0 2

C	-5.17942700	-0.93011800	-0.12412800
C	-4.57056700	-1.94775600	-0.85547900
C	-3.18814900	-2.09675800	-0.86556500
C	-2.40579300	-1.21443400	-0.13991200
C	-2.98083000	-0.18356100	0.59263900
C	-4.36216200	-0.05357900	0.59314000
O	-1.02836600	-1.34712200	-0.26274000
C	-0.25092300	-1.24811500	0.85209400
O	-0.66579200	-1.23936400	1.97498600
C	1.13303500	-1.13980700	0.47665900
C	2.23508300	-0.67676500	0.20157200

C	-6.67950300	-0.79203700	-0.08152100
C	3.65451700	-0.72040400	-0.07503200
C	1.85600800	1.50485600	0.50829500
O	2.53973400	1.98372700	1.33474300
C	4.26143400	0.17361300	-0.95934800
C	5.61893300	0.07232400	-1.22753800
C	6.38192400	-0.91432700	-0.61126000
C	5.78226800	-1.80370100	0.27468000
C	4.42413700	-1.71073200	0.54439200
C	0.50194300	1.92221700	0.05810700
C	-0.17512600	2.90390300	0.78693900
C	-1.41747200	3.34203100	0.35075600
C	-1.97487400	2.80579600	-0.80837200
C	-1.29716700	1.82963400	-1.53246600
C	-0.05491100	1.38389800	-1.10028400
H	-5.18350100	-2.63710600	-1.42590900
H	-2.70553800	-2.88211600	-1.43366600
H	-2.35520400	0.50171900	1.15052800
H	-4.81564300	0.74955700	1.16467600
H	-7.14337700	-1.25770600	-0.95201700
H	-7.08684200	-1.27391100	0.81142800
H	-6.97809900	0.25741000	-0.05548100
H	3.66333300	0.94556800	-1.42860400
H	6.08330700	0.76787500	-1.91572400
H	7.44277000	-0.98731100	-0.81797300
H	6.37385800	-2.57044100	0.75985700
H	3.94545400	-2.39624200	1.23249100
H	0.28495300	3.30737400	1.68119700
H	-1.95121900	4.10023000	0.91082500
H	-2.94877800	3.14267700	-1.14331100
H	-1.74351900	1.40534800	-2.42313300

| H | 0.47916800 | 0.61208700 | -1.64131000 |

TS3b-5b

E= -1112.0953931 a.u., im. freq.= 405.05*i*

0 2

C	3.86615500	-1.00126800	0.30066100
C	3.39423100	-1.22861800	-1.00009700
C	2.14084900	-1.75685300	-1.22529200
C	1.28164500	-1.96959000	-0.12169200
C	1.81712600	-1.95065600	1.18641300
C	3.07605500	-1.42485600	1.38104400
O	0.09250900	-2.64915000	-0.33427200
C	-1.04674900	-1.93583100	-0.59122600
C	-0.84948000	-0.46046200	-0.49506300
C	0.34652400	-0.03605800	-0.15663100
O	-2.06203800	-2.49511700	-0.85984900
C	5.17735700	-0.30753100	0.53541500
C	1.16265000	1.11311200	0.00690800
C	1.58097400	1.52575800	1.28568700
C	2.46120700	2.58744700	1.41874800
C	2.95385000	3.23828300	0.28887400
C	2.54665500	2.83300300	-0.98077500
C	1.65528800	1.78271400	-1.12923600
C	-1.96682700	0.48946700	-0.88054700
C	-3.27122900	0.40316300	-0.16303400
O	-1.75634300	1.31965900	-1.73035600
C	-4.33627000	1.16410800	-0.64926800
C	-5.56068300	1.13954800	-0.00006800
C	-5.72415900	0.36272700	1.14460400
C	-4.66336900	-0.38928800	1.63736300
C	-3.43874200	-0.37399900	0.98207500

H	4.03194600	-0.98738300	-1.84361300
H	1.76336500	-1.94370000	-2.22320200
H	1.19630600	-2.28754600	2.00746500
H	3.46920200	-1.33802900	2.38844700
H	5.65432000	-0.65582800	1.45311000
H	5.86634400	-0.46507200	-0.29571900
H	5.01116200	0.77080600	0.63285400
H	1.20638000	1.00485100	2.15848100
H	2.76865400	2.90875000	2.40672200
H	3.64608100	4.06431600	0.39821000
H	2.91736600	3.34812200	-1.85875000
H	1.31287200	1.47202900	-2.10844500
H	-4.17861800	1.76553500	-1.53606100
H	-6.38845600	1.72453300	-0.38193000
H	-6.68105100	0.34356800	1.65278900
H	-4.79191600	-0.99206300	2.52782500
H	-2.61531300	-0.96193900	1.36846200

TS3b-6b

E= -1112.0856365 a.u., im. freq.= 398.93i

0 2

C	-4.17446500	-0.33925400	-0.25655400
C	-4.08061600	-1.40496500	0.64719000
C	-2.98801900	-2.27484500	0.63047700
C	-1.98593000	-2.07158500	-0.28993700
C	-2.01407700	-0.97979300	-1.18361700
C	-3.16121300	-0.15816900	-1.18769800
O	-0.88388300	-2.89838000	-0.29708900
C	0.35654100	-2.38168100	-0.04600400
O	1.30272000	-3.10820900	-0.05348900
C	0.45471200	-0.92513300	0.26379400

C	-0.41942800	-0.01702200	-0.12005800
C	-5.34515300	0.60799700	-0.21303800
C	1.66367900	-0.51357200	1.10321200
C	-0.54883500	1.40924900	-0.03394600
C	-1.60082400	1.97163700	0.70692400
C	-1.75503000	3.34867400	0.75526800
C	-0.88386400	4.17896700	0.05373300
C	0.15372500	3.62624700	-0.69193300
C	0.32469700	2.25042200	-0.74143300
C	2.95822100	-0.28275100	0.39723700
O	1.53029100	-0.33409700	2.28479900
C	4.02694200	0.22588300	1.13767500
C	5.24371300	0.47196500	0.52059500
C	5.40032200	0.20587500	-0.83788300
C	4.34031000	-0.30765500	-1.57740900
C	3.11890900	-0.55221900	-0.96151900
H	-4.87289200	-1.56176200	1.37013100
H	-2.90515300	-3.09954500	1.32677300
H	-1.35969000	-0.99903100	-2.04841100
H	-3.23121100	0.64525400	-1.91234500
H	-5.64711900	0.90404800	-1.21883700
H	-6.20365600	0.15661000	0.28510800
H	-5.07791100	1.51834200	0.33182700
H	-2.27152200	1.31584300	1.25030000
H	-2.55690700	3.77830000	1.34381000
H	-1.01143300	5.25391400	0.09115100
H	0.83666500	4.27045700	-1.23241000
H	1.13647900	1.81497100	-1.31336900
H	3.87711600	0.42134600	2.19244800
H	6.07185100	0.86936600	1.09466600
H	6.35216200	0.39605900	-1.31964600

H	4.46723100	-0.52368600	-2.63108900
H	2.29707000	-0.96463900	-1.53434500

TS5b-9b

E= -1112.102747 a.u., im. freq.= 271.80*i*

0 2

C	4.57273500	-1.06326900	0.35640100
C	4.06172500	-0.88783000	-0.93628100
C	2.74406200	-0.53858900	-1.13238600
C	1.86572100	-0.39048900	-0.02393200
C	2.41528600	-0.47639400	1.28240900
C	3.72840700	-0.83801100	1.45895800
O	1.12049400	-2.28624400	-0.22910700
C	-0.12523100	-2.04326100	-0.56514900
C	-0.46604400	-0.58510900	-0.58543100
C	0.52584100	0.24394900	-0.23749400
O	-0.92338600	-2.91773300	-0.80714400
C	5.99242300	-1.50047600	0.56857400
C	0.42485200	1.70668500	-0.04404400
C	-0.76747100	2.29046800	0.39990200
C	-0.85426300	3.66242600	0.58316700
C	0.24749200	4.47427400	0.33105200
C	1.44177100	3.90352700	-0.09275700
C	1.53426500	2.52901400	-0.26888700
C	-1.83181700	-0.18171600	-1.07988100
C	-3.02639200	-0.53436500	-0.25717800
O	-1.92729400	0.42228200	-2.12033100
C	-4.28779100	-0.18989400	-0.74635500
C	-5.42206400	-0.47162400	-0.00099700
C	-5.30112800	-1.09626500	1.23858400
C	-4.04654100	-1.43927800	1.73036200

S73

C	-2.90870400	-1.16200000	0.98271000
H	4.71355200	-1.03449400	-1.78987200
H	2.33941600	-0.40976500	-2.12978800
H	1.76973000	-0.28537400	2.13155100
H	4.13026300	-0.94309700	2.46059500
H	6.42116000	-1.03329600	1.45657300
H	6.02939700	-2.58423400	0.71566000
H	6.61612300	-1.25969300	-0.29256300
H	-1.62497300	1.66746700	0.62652600
H	-1.78316900	4.09805700	0.93028700
H	0.17679900	5.54590900	0.47293100
H	2.30571400	4.52838600	-0.28374300
H	2.47204900	2.09270800	-0.59375600
H	-4.35069500	0.29566800	-1.71258900
H	-6.40108100	-0.20836600	-0.38255000
H	-6.18782600	-1.31813700	1.82071700
H	-3.95517500	-1.93060400	2.69115300
H	-1.93261400	-1.43819900	1.36344300

TS9b-8b

E= -1112.0997213 a.u., im. freq.= 328.14*i*

0 2

C	-4.26430200	-0.10690300	-0.26321400
C	-4.36968600	-1.37640700	0.35345400
C	-3.22680500	-1.97352900	0.83161300
C	-1.96325300	-1.35810900	0.66187700
C	-1.87864300	-0.09029800	0.03100100
C	-3.04558800	0.53130200	-0.40996800
O	-1.06025000	-2.33006000	-0.84092800
C	0.08634500	-1.78250500	-1.16419800
O	0.88880400	-2.37304400	-1.85146200

S74

C	0.39868000	-0.37753800	-0.71501000
C	-0.54243900	0.46760000	-0.24814400
C	1.83779000	0.00001300	-0.98065200
C	2.87887100	-0.60945400	-0.09773300
O	2.13303500	0.76034000	-1.87015800
C	-0.36091800	1.91966200	0.01003700
C	0.18554500	2.78220200	-0.94392900
C	0.30225300	4.14010800	-0.66725100
C	-0.11725500	4.64849800	0.55606500
C	-0.67124000	3.79647400	1.50718500
C	-0.80478700	2.44385500	1.23027800
C	-5.72019200	-2.02423600	0.48978000
C	2.55052900	-1.40030000	1.00231100
C	3.55365400	-1.93297000	1.80264600
C	4.88723400	-1.67713900	1.50443500
C	5.21966700	-0.88747000	0.40602800
C	4.21924900	-0.35463200	-0.39192000
H	-5.16513400	0.36882300	-0.63652000
H	-3.28011600	-2.92867500	1.34026500
H	-1.13805100	-1.68570800	1.28142400
H	-2.98251600	1.49739200	-0.89696600
H	0.51587600	2.38414400	-1.89338200
H	0.72381300	4.80124000	-1.41457900
H	-0.01876800	5.70651200	0.76756300
H	-1.00272100	4.18690300	2.46172100
H	-1.24656300	1.78039700	1.96589200
H	-6.14194500	-2.23287300	-0.49642800
H	-5.65448700	-2.96397600	1.03731500
H	-6.41666500	-1.36594100	1.01398600
H	1.51178700	-1.60105000	1.23814600
H	3.29607300	-2.54873000	2.65560100

S75

H	5.66961700	-2.09488700	2.12698300
H	6.25943900	-0.69163400	0.17393300
H	4.44940500	0.26082900	-1.25272200

TS9b-11b

E= -1112.1017781 a.u., im. freq.= 423.95*i*

0 2

C	3.84367500	-1.60159800	-0.62209100
C	4.54925600	-1.21861100	0.51746100
C	3.94913700	-0.30982700	1.39236300
C	2.68322500	0.19507500	1.14058800
C	1.97027000	-0.21645200	0.01148400
C	2.56899500	-1.11228800	-0.87598500
C	0.61723400	0.33712400	-0.24603400
C	-0.42265400	-0.40990900	-0.61336000
C	5.91472800	-1.78135600	0.81080500
C	0.44335000	1.81140900	-0.11012700
C	-0.66489900	2.34739200	0.54981600
C	-0.80728200	3.72330600	0.67361500
C	0.15154800	4.57471100	0.13594700
C	1.26110000	4.04635700	-0.51771800
C	1.41228500	2.67197000	-0.63398100
C	-1.83089000	-0.06393300	-0.98519100
C	-0.23236600	-2.20401100	-0.95866300
O	-0.31853300	-2.45995000	-2.10992400
O	-0.09167100	-2.57053300	0.18002000
C	-2.94101700	-0.53757500	-0.11384800
O	-2.00632800	0.57488300	-1.99184200
C	-2.70128000	-1.08218100	1.14846700
C	-3.77239200	-1.47567100	1.94210200
C	-5.07408800	-1.32940600	1.47576300

S76

C	-5.31343400	-0.78467400	0.21530600
C	-4.24961100	-0.38548300	-0.57784600
H	4.29959600	-2.28863400	-1.32662900
H	4.48593600	0.00894800	2.27955000
H	2.23553300	0.90933200	1.82264600
H	2.04739100	-1.40446600	-1.78040900
H	5.83670300	-2.64259500	1.48008700
H	6.40934800	-2.11342200	-0.10265100
H	6.55054100	-1.04016400	1.29757500
H	-1.40516400	1.68487000	0.98538300
H	-1.66599100	4.12961200	1.19389000
H	0.03748900	5.64791600	0.22965800
H	2.01017500	4.70701800	-0.93692200
H	2.27681700	2.25517000	-1.13766300
H	-1.68463500	-1.20479500	1.50313900
H	-3.59006900	-1.89970600	2.92168500
H	-5.90665900	-1.64185400	2.09498900
H	-6.32910600	-0.67411000	-0.14415300
H	-4.40500400	0.04548400	-1.55944900

TS11b-12b

E= -1268.410944 a.u., im. freq.= 408.94i

0 3

C	-2.95320300	-2.67307100	1.19232400
C	-3.82583900	-2.87376200	0.12472100
C	-3.87326500	-1.90492600	-0.88160800
C	-3.07574600	-0.77297600	-0.82373800
C	-2.19188100	-0.58565200	0.24481300
C	-2.14304400	-1.54599400	1.25694400
C	-1.30088600	0.61373200	0.27180900
C	-0.04463700	0.43824000	0.64257900

C	-4.71975500	-4.08407600	0.06269100
C	-1.88048300	1.91635400	-0.15501600
C	-1.24443700	2.73259600	-1.09114800
C	-1.81881700	3.93930600	-1.47343900
C	-3.03047100	4.34164500	-0.92401200
C	-3.67481300	3.52726200	0.00238400
C	-3.10846400	2.31666100	0.37731600
C	1.17428100	2.09421100	0.78541000
C	2.48395300	1.55599800	0.30125800
O	0.91797000	2.40666200	1.91832700
C	0.84034800	-0.59616300	1.19020300
O	1.10266100	-0.63315200	2.37548300
C	2.65628800	1.21715300	-1.04012400
C	3.87313200	0.71205600	-1.47385200
C	4.92468600	0.56342800	-0.57235200
C	4.75640900	0.91508500	0.76393000
C	3.53501000	1.40572200	1.20837900
C	1.50815600	-1.49771200	0.19937100
C	2.69897600	-2.11219200	0.58469700
C	3.39465500	-2.90193300	-0.32005400
C	2.89128400	-3.09795300	-1.60314000
C	1.68968800	-2.50570600	-1.98105600
C	1.00125200	-1.69838600	-1.08489000
H	-2.90784000	-3.40683500	1.98966100
H	-4.54744100	-2.04236800	-1.72074900
H	-3.12998300	-0.02609800	-1.60815600
H	-1.48262300	-1.39882200	2.10384500
H	-5.74803700	-3.81715700	0.32119800
H	-4.73282200	-4.51000600	-0.94237900
H	-4.38844900	-4.85567400	0.75808300
H	-0.30370000	2.41491600	-1.52141400

H	-1.31767800	4.56490400	-2.20215200
H	-3.47460000	5.28447900	-1.21988400
H	-4.62002400	3.83522400	0.43277100
H	-3.60969100	1.67644600	1.09456300
H	1.82413000	1.32166900	-1.72742100
H	4.00102000	0.42667600	-2.51089100
H	5.87492000	0.16905700	-0.91218700
H	5.57531200	0.79691800	1.46371600
H	3.37194500	1.65896800	2.24899700
H	3.06888600	-1.93787900	1.58786000
H	4.33037800	-3.36319500	-0.02766100
H	3.43379500	-3.71651900	-2.30852300
H	1.29239800	-2.67025100	-2.97536700
H	0.07078700	-1.22622500	-1.38078500

2c

E= -231.7452977 a.u., number of negative frequencies = 0

0 2

C	0.20004900	1.18521300	-0.22572500
C	-1.08986200	0.48043800	0.18716800
O	-0.86244300	-0.89323200	-0.12877100
C	0.46956100	-1.14539600	0.04724200
C	1.26030000	0.12952800	0.14227000
H	0.19715400	1.35420500	-1.30432800
H	0.34008700	2.14009800	0.28004600
H	-1.26594600	0.57663400	1.26466000
H	-1.97684200	0.80431100	-0.35453000
H	0.80582800	-2.07278700	-0.39338900
H	1.63555700	0.29740600	1.15898300
H	2.12342400	0.14729400	-0.52699800

3c

E= -998.9965689 a.u., number of negative frequencies = 0

0 2

C	5.70899500	-0.45334700	-0.09724000
C	5.11022300	0.71511600	-0.56351000
C	3.73961200	0.91352300	-0.44774500
C	2.95804300	-0.06443900	0.14552900
C	3.52469600	-1.23725200	0.62710300
C	4.89493900	-1.41817800	0.49870400
O	1.60802700	0.23027000	0.29813000
C	0.65999200	-0.69180800	-0.03898300
O	0.90448700	-1.78412800	-0.45279200
C	-0.69761200	-0.10860400	0.18781700
C	-1.75118200	-0.83178200	-0.10183500
C	7.18986700	-0.68636500	-0.25074700
C	-0.79973400	1.31092200	0.74998000
C	-3.14274100	-1.00332800	-0.14418800
C	-3.86833500	-1.27399400	1.03674500
C	-5.23727600	-1.46194400	0.98205900
C	-5.91430200	-1.38930400	-0.23538200
C	-5.20801800	-1.12613000	-1.40796000
C	-3.83688900	-0.94124000	-1.37264400
O	-2.13290200	1.60094100	1.12886000
C	-2.71798500	2.41463500	0.12276900
C	-1.58682700	3.34294300	-0.30399400
C	-0.38289300	2.39047700	-0.28571300
H	5.72185400	1.48297500	-1.02448300
H	3.26650900	1.81972200	-0.80567100
H	2.90335200	-1.99562400	1.08201300
H	5.34209300	-2.33328300	0.87219800
H	7.72167300	0.25179400	-0.41371700

H	7.60660800	-1.16526100	0.63708100
H	7.39245200	-1.33865600	-1.10446200
H	-0.18452200	1.36392800	1.65021700
H	-3.33748100	-1.30937300	1.97928900
H	-5.78630500	-1.66039500	1.89470300
H	-6.98651300	-1.53786300	-0.26959400
H	-5.73165800	-1.07048600	-2.35475100
H	-3.27982300	-0.74934600	-2.28188600
H	-3.57525500	2.92131300	0.56419500
H	-3.06377500	1.79691900	-0.71740700
H	-1.75130400	3.80220400	-1.27891300
H	-1.46310900	4.13257000	0.43967100
H	0.54750400	2.87845300	0.00017800
H	-0.23462700	1.93433800	-1.26683800

4c

E= -998.9845357 a.u., number of negative frequencies = 0

0 2

C	5.92524200	0.13873100	-0.00582000
C	5.33184800	1.00020200	-0.92610600
C	3.96228400	1.23560100	-0.90843200
C	3.17692200	0.60565100	0.04240200
C	3.73799200	-0.25184400	0.97970100
C	5.10713500	-0.47607100	0.94382600
O	1.82712600	0.94544900	0.05227600
C	0.88520500	-0.02043700	0.14076100
O	1.11824200	-1.19811600	0.22199500
C	-0.44888100	0.56055400	0.13407600
C	-1.66364600	0.08232900	-0.09451200
C	7.40509500	-0.14326200	-0.04109200
C	-2.84054800	0.97893600	0.02473200

C	-1.82324400	-1.39387600	-0.44007700
C	-4.10207600	0.50246100	0.39282000
C	-5.16688300	1.37972900	0.55338600
C	-4.99526800	2.74167100	0.33399000
C	-3.74660400	3.22512800	-0.04326300
C	-2.67973200	2.35180000	-0.19484400
C	-1.96827500	-2.29914500	0.79069900
C	-2.70414100	-3.49378700	0.18276100
C	-3.64213200	-2.80746800	-0.81216400
O	-2.97543100	-1.62132000	-1.23977600
H	5.94683000	1.49659600	-1.66869000
H	3.49226600	1.90760700	-1.61535600
H	3.11429000	-0.73871200	1.71616700
H	5.55049200	-1.14537500	1.67345800
H	7.93828300	0.61994500	-0.60903000
H	7.82343100	-0.17336600	0.96664200
H	7.60371500	-1.11028900	-0.51086800
H	-0.93663000	-1.70422900	-1.00002900
H	-4.25559300	-0.55340700	0.56366500
H	-6.13652300	0.99554100	0.84660500
H	-5.83040000	3.42169900	0.45143500
H	-3.60461500	4.28368300	-0.22463800
H	-1.70862100	2.72450800	-0.50020300
H	-0.99295900	-2.53723900	1.21183300
H	-2.57532600	-1.81195100	1.55870700
H	-3.23899500	-4.09485200	0.91797900
H	-1.99640400	-4.13749200	-0.34459400
H	-3.86184000	-3.41755700	-1.68950600
H	-4.59265800	-2.53462000	-0.33660500

5c

E= -999.0260855 a.u., number of negative frequencies = 0

0 2

C	-3.84499500	-1.22104300	-0.09450000
C	-3.10094900	-0.99552800	-1.29006200
C	-1.74917000	-0.98180100	-1.30834100
C	-0.93087700	-1.16275000	-0.06734600
C	-1.76964400	-1.43906400	1.14562800
C	-3.12726800	-1.46558500	1.10181600
O	-0.03840800	-2.29153700	-0.24836700
C	1.25424300	-1.91135100	-0.09719500
C	1.28679000	-0.45533000	0.19816300
C	0.03374600	0.01057600	0.13968500
O	2.16706800	-2.67623700	-0.21882700
C	-5.34169600	-1.23601300	-0.13294000
C	-0.41037800	1.41401000	0.13434100
C	0.33491400	2.35178400	-0.59363200
C	-0.06847600	3.67944500	-0.64622600
C	-1.21901900	4.08796100	0.02006700
C	-1.97182700	3.15987700	0.73154800
C	-1.57761700	1.82910000	0.78325900
C	2.56786200	0.30219500	0.39437800
C	3.59469200	-0.39489100	1.31718900
C	4.90566900	-0.26145200	0.53134500
C	4.39870500	-0.29841600	-0.90413100
O	3.20455200	0.48098500	-0.87438800
H	-3.64628900	-0.84473500	-2.21641900
H	-1.19338200	-0.82666800	-2.22618700
H	-1.22445200	-1.64101600	2.06079400
H	-3.68352600	-1.68557200	2.00741500
H	-5.73253300	-0.28680100	-0.51213200
H	-5.70755300	-2.02213000	-0.80097300

H	-5.76495400	-1.40816200	0.85686900
H	1.21787900	2.02540000	-1.13360300
H	0.51369900	4.39378000	-1.21569400
H	-1.53230400	5.12426900	-0.02182700
H	-2.87217900	3.47217000	1.24685200
H	-2.16924200	1.11220000	1.33800100
H	2.32536500	1.29606500	0.77694000
H	3.63266900	0.08316600	2.29555000
H	3.34592100	-1.44662500	1.44875900
H	5.61391400	-1.05949900	0.75410100
H	5.38160000	0.70131000	0.73175600
H	5.07219100	0.16139700	-1.62712800
H	4.16924000	-1.32459100	-1.20869200

6c

E= -999.017163 a.u., number of negative frequencies = 0

0 2

C	3.52104500	1.02906100	0.23128200
C	4.09393300	-0.19817700	0.68154000
C	3.42021900	-1.41519000	0.47285100
C	2.23963500	-1.43434100	-0.19856000
C	1.60182700	-0.23146200	-0.79945000
C	2.33998600	1.02629400	-0.43694700
O	1.60073400	-2.63122200	-0.38304200
C	0.23597800	-2.69119100	-0.42627900
O	-0.27605100	-3.76550000	-0.53792300
C	-0.51998400	-1.41198100	-0.29659000
C	0.10693600	-0.23835500	-0.44870800
C	4.25054800	2.31480300	0.52303700
C	-1.99519800	-1.59382200	-0.00392800
C	-0.56743100	1.08267000	-0.33911600

C	-0.49631300	1.79253300	0.85977400
C	-1.08612000	3.04881300	0.96850300
C	-1.73789900	3.60755500	-0.12420900
C	-1.79833400	2.90712100	-1.32660900
C	-1.21459200	1.65165000	-1.43607400
C	-2.34938000	-1.40895400	1.48331200
C	-3.77627600	-0.86580000	1.40075800
C	-3.67393300	0.02444300	0.16616200
O	-2.80452300	-0.66771800	-0.72441000
H	5.03521300	-0.18608900	1.21625500
H	3.81134500	-2.35156600	0.85163700
H	1.62922800	-0.33991800	-1.90299700
H	1.90924400	1.95949200	-0.78140400
H	5.23802300	2.31083900	0.05482600
H	3.69715100	3.17691100	0.15083800
H	4.39822700	2.43815800	1.59874000
H	-2.26728000	-2.59992400	-0.32961000
H	0.02829800	1.35880300	1.70441000
H	-1.03196100	3.58899400	1.90608300
H	-2.19759000	4.58506500	-0.04169100
H	-2.30926500	3.33730200	-2.17967000
H	-1.28921300	1.08797900	-2.35779300
H	-2.25716600	-2.34122400	2.04024800
H	-1.68915000	-0.66390900	1.93443100
H	-4.08135400	-0.32073500	2.29422700
H	-4.48467500	-1.67867500	1.22373000
H	-4.62499900	0.17819300	-0.34472500
H	-3.24323200	1.00180200	0.42097100

7c

E= -998.7549234 a.u., number of negative frequencies = 0

1 1

C	5.47934600	-0.85734400	0.00746300
C	4.96068500	-0.23773400	1.14287900
C	3.62856500	0.15684300	1.20107900
C	2.82092300	-0.07848000	0.10574500
C	3.29542200	-0.68641100	-1.04529900
C	4.62733200	-1.07283300	-1.07936600
O	1.49386800	0.40181100	0.19150600
C	0.48153000	-0.40718000	-0.10586500
O	0.52126900	-1.53400600	-0.48399200
C	-0.81842500	0.35500700	0.11791100
C	-1.92588000	-0.29812200	0.07941000
C	6.92235600	-1.28071800	-0.06365000
C	-0.84985300	1.84602300	0.42501300
C	-3.08561700	-1.00236300	0.05811900
C	-3.58447100	-1.57371700	1.26693800
C	-4.75510600	-2.29285400	1.23376800
C	-5.42983900	-2.45247700	0.01620400
C	-4.95466700	-1.89973100	-1.18086500
C	-3.78836700	-1.17335400	-1.17200000
C	-0.33338800	2.72956200	-0.71338500
C	-1.11831500	4.01481600	-0.43652300
C	-2.47443300	3.47017000	0.00275500
O	-2.19534300	2.21312700	0.64793600
H	5.60380600	-0.05880800	1.99660100
H	3.21947100	0.64139800	2.07861400
H	2.64232000	-0.86463200	-1.88888700
H	5.01405400	-1.55335300	-1.97116600
H	7.42759300	-1.12642800	0.88933800
H	7.00409700	-2.33717100	-0.32651800
H	7.45470700	-0.70820300	-0.82661700

H	-0.25259400	1.98667000	1.33399500
H	-3.03107900	-1.42565200	2.18579000
H	-5.15485500	-2.73506200	2.13665400
H	-6.35116900	-3.02421700	-0.00083300
H	-5.50413400	-2.04745700	-2.10109900
H	-3.38410000	-0.73241100	-2.07456600
H	0.74753400	2.84792500	-0.68536800
H	-0.62149800	2.30523200	-1.67935100
H	-1.18892300	4.66234700	-1.30916700
H	-0.64878400	4.57491300	0.37445200
H	-2.99256100	4.10992300	0.71549700
H	-3.12903300	3.28292000	-0.85295900

8c

E= -999.028493 a.u., number of negative frequencies = 0

0 2

C	3.79319300	0.79335100	0.32425700
C	4.26531500	-0.54896800	0.10244200
C	3.38647500	-1.50623300	-0.25893900
C	1.95129700	-1.20844400	-0.53201600
C	1.50511800	0.15950400	-0.11795800
C	2.44663400	1.11449700	0.23860500
O	1.16033200	-2.23422100	0.09056800
C	-0.18337200	-2.07972400	0.09269100
O	-0.87015500	-3.01526600	0.40435500
C	-0.73476100	-0.73356400	-0.21822200
C	0.08184200	0.36302100	-0.15652300
C	-2.23486800	-0.63244700	-0.34525600
C	-0.45562600	1.74906900	-0.08027900
C	-0.02783000	2.72868900	-0.97955700
C	-0.52341700	4.02406200	-0.89694700

C	-1.44184900	4.35598700	0.09381700
C	-1.86981000	3.38614600	0.99447200
C	-1.38373900	2.08707400	0.90856300
C	5.72520700	-0.84002700	0.32112000
O	-2.83949400	-0.81116100	0.94050900
C	-3.73754300	-1.91738000	0.90050500
C	-4.19519800	-1.99253100	-0.55153300
C	-2.90058800	-1.64782800	-1.29726300
H	4.50682000	1.55225200	0.62403500
H	3.69421000	-2.53666500	-0.39804800
H	1.77022800	-1.30006500	-1.61873800
H	2.11627600	2.11419600	0.49430400
H	-2.47842900	0.37854100	-0.67863600
H	0.68957400	2.46724200	-1.74991700
H	-0.19329200	4.77375300	-1.60599800
H	-1.82467400	5.36726500	0.16164400
H	-2.58694300	3.63947400	1.76588800
H	-1.73061800	1.31974900	1.59254500
H	6.34169600	-0.24387000	-0.35659000
H	6.01849700	-0.58445300	1.34228000
H	5.94775600	-1.89321800	0.15183400
H	-4.54550900	-1.71240200	1.60385100
H	-3.21048000	-2.82909100	1.19375500
H	-4.59334700	-2.97064100	-0.82221700
H	-4.96035800	-1.23566000	-0.74199500
H	-3.07676500	-1.20656200	-2.27834300
H	-2.28897600	-2.54018000	-1.41500200

9c

E= -999.0020252 a.u., number of negative frequencies = 0

0 2

C	3.70245700	-0.10982400	-1.03662100
C	4.22200500	-0.89402200	0.00302900
C	3.36769000	-1.28552600	1.02707300
C	2.02225700	-0.92903900	1.01081600
C	1.50619000	-0.16380700	-0.03952400
C	2.37228900	0.26561500	-1.05225800
C	0.07942400	0.25534200	-0.03024800
C	-0.92926600	-0.63923500	-0.05377900
C	5.67203800	-1.29791600	-0.00674600
C	-0.14444800	1.72273300	0.02648100
C	-1.08038000	2.34093000	-0.80731900
C	-1.27108500	3.71670800	-0.75837800
C	-0.52959100	4.49103300	0.12656100
C	0.41541300	3.88691000	0.95078600
C	0.61773100	2.51515900	0.89138300
C	-2.38015800	-0.32243200	0.24637900
C	-0.67005600	-2.07453200	-0.37690200
O	-1.52765100	-2.86933100	-0.69809400
O	0.56927600	-2.51914400	-0.38871300
C	-3.37502800	-0.48623200	-0.92148300
C	-4.60438000	-1.07287800	-0.22049600
O	-2.81355800	-1.20408700	1.28200000
C	-3.95913700	-1.93786400	0.85654200
H	4.36058900	0.21047600	-1.83764900
H	3.75277200	-1.87841600	1.84909400
H	1.36530000	-1.23153700	1.81823000
H	1.98610800	0.88581300	-1.85349000
H	5.86340200	-2.01555900	-0.80870400
H	6.31759900	-0.43376100	-0.17734400
H	5.96029500	-1.76156500	0.93674600
H	-1.63825600	1.73733800	-1.51392700

H	-1.99386300	4.18383800	-1.41641000
H	-0.67947100	5.56316800	0.16730600
H	1.00026000	4.48759900	1.63679100
H	1.36283600	2.04557200	1.52371100
H	-2.43299600	0.69404000	0.64417400
H	-3.58151000	0.46805000	-1.40741000
H	-2.98888100	-1.18594900	-1.66162100
H	-5.24631900	-1.64160100	-0.89335200
H	-5.19543600	-0.27769200	0.24097300
H	-4.59480700	-2.09265600	1.72919600
H	-3.64594800	-2.90340500	0.45035700

10c

E= -998.4913494 a.u., number of negative frequencies = 0

0 1

C	-3.85809600	0.63851800	-0.04812000
C	-4.23495700	-0.71314800	0.00115100
C	-3.24423100	-1.68224100	0.01572400
C	-1.90367900	-1.30824200	-0.01227400
C	-1.51522400	0.03123200	-0.04457300
C	-2.52781400	1.00400800	-0.07133100
O	-0.98945800	-2.31110800	-0.02057100
C	0.36461900	-2.08291400	-0.09468400
O	1.07930700	-3.03575000	-0.20598700
C	0.81256400	-0.67893500	-0.04471200
C	-0.08978800	0.32920300	-0.04247500
C	2.30376800	-0.47858000	0.04151100
C	0.32836100	1.75910500	-0.03431500
C	0.17642900	2.52655400	1.12084300
C	0.56487900	3.86093100	1.12892800
C	1.09621000	4.44087800	-0.01870100

S90

C	1.24211000	3.68168400	-1.17440100
C	0.86072600	2.34442700	-1.18261600
C	-5.69160200	-1.09108700	0.03542200
O	2.75674900	-1.10674400	1.23430700
C	4.05378900	-1.62471800	0.99314500
C	4.01694900	-2.13440100	-0.44454300
C	3.12107200	-1.09139500	-1.12998600
H	-4.62678900	1.40296200	-0.07019500
H	-3.48169500	-2.73891100	0.04352800
H	-2.25037400	2.05022600	-0.11322400
H	2.50743400	0.59366100	0.10954400
H	-0.23624300	2.06855200	2.01293600
H	0.45450800	4.44755100	2.03296300
H	1.39680900	5.48156700	-0.01134400
H	1.65514000	4.12907400	-2.07043400
H	0.97437300	1.74561600	-2.07982400
H	-5.82168900	-2.17290200	0.01643700
H	-6.16692800	-0.70551100	0.94061900
H	-6.22077100	-0.66618400	-0.82049600
H	4.24242800	-2.40060700	1.73427200
H	4.80481700	-0.82982800	1.10907100
H	5.00932100	-2.19994100	-0.89195400
H	3.53632700	-3.11039300	-0.47528500
H	3.71445000	-0.30860300	-1.60658400
H	2.47958800	-1.54278000	-1.88597200

11c

E= -810.4402899 a.u., number of negative frequencies = 0

0 2

| C | -3.39910100 | -1.62385900 | 0.26560600 |
| C | -4.27937000 | -0.55950500 | 0.04746700 |

S91

C	-3.73706100	0.67815400	-0.28538300
C	-2.36150100	0.85586300	-0.39590000
C	-1.48615100	-0.20789200	-0.17650800
C	-2.02938500	-1.45383800	0.15946600
C	-0.01462900	-0.03913700	-0.32691300
C	0.76761200	-1.06718500	-0.60681200
C	-5.76655000	-0.75715100	0.18376100
C	0.58395300	1.31932700	-0.14118800
C	0.27962900	2.07800200	0.99328500
C	0.88738600	3.30947000	1.20016800
C	1.79924700	3.80582500	0.27245800
C	2.09678200	3.06472400	-0.86527200
C	1.49188800	1.82935000	-1.07014300
C	2.18723200	-1.43107800	-0.81780400
O	2.36085100	-2.84068200	-0.66257500
C	2.83092100	-3.06411600	0.65518700
C	3.85279600	-1.95384400	0.86986600
C	3.14646900	-0.75767800	0.21527800
H	-3.79872600	-2.59813300	0.52893800
H	-4.39875300	1.51868200	-0.46636500
H	-1.96646500	1.82851700	-0.66597900
H	-1.35909300	-2.28776800	0.33800900
H	-6.03599600	-0.98165000	1.21907200
H	-6.31287800	0.13619700	-0.12049400
H	-6.10794400	-1.59182100	-0.43271100
H	-0.43208500	1.69041900	1.71397600
H	0.65033900	3.88375400	2.08799300
H	2.27028900	4.76791500	0.43415300
H	2.79623500	3.45028600	-1.59762200
H	1.71351600	1.25402800	-1.96267500
H	2.47729800	-1.20419700	-1.84743300

S92

H	3.24167500	-4.07208700	0.69599600
H	2.00684000	-2.98081000	1.37770500
H	4.08956900	-1.77952600	1.91972900
H	4.77272300	-2.20089600	0.33673600
H	3.83358500	-0.06549800	-0.27006700
H	2.57207000	-0.19456400	0.95192200

12c

E= -1042.3422448 a.u., number of negative frequencies = 0

0 1

C	-3.34487400	-1.70350700	0.79284200
C	-4.31572400	-1.21095800	-0.07647800
C	-3.96623600	-0.15672300	-0.92377200
C	-2.69285900	0.39090500	-0.89607300
C	-1.71456400	-0.11672500	-0.03439800
C	-2.06210300	-1.16707300	0.81839800
C	-0.35348600	0.49216000	0.00661400
C	0.78094300	-0.24109600	0.00218600
C	-5.71345900	-1.77331200	-0.08973200
C	-0.35238400	1.98421600	0.05362900
C	0.45563800	2.72873300	-0.81179600
C	0.42362100	4.11855100	-0.78449400
C	-0.41432000	4.78309600	0.10407500
C	-1.22771400	4.05046800	0.96346000
C	-1.20534100	2.66240600	0.93003400
C	0.73820900	-1.72277300	-0.28776900
C	2.11619900	0.40483100	0.28716600
O	2.86573100	0.56092800	-0.93056600
C	4.26115100	0.43812100	-0.65890000
C	1.78998600	-2.28529800	-1.24967600
C	1.74804800	-3.76783600	-0.87312400

C	4.39814500	0.32019900	0.86197600
C	3.06434300	-0.32505900	1.24442200
C	1.58805500	-3.69712400	0.64851900
O	0.90609600	-2.47501400	0.92678200
H	-3.59489500	-2.51822400	1.46442800
H	-4.70635900	0.24188900	-1.61030200
H	-2.44432900	1.21886400	-1.55119100
H	-1.31430200	-1.56868800	1.49395600
H	-5.75839300	-2.73159000	0.42898500
H	-6.41004400	-1.09095000	0.40496600
H	-6.06752800	-1.92018800	-1.11209400
H	1.11541400	2.20666400	-1.49645200
H	1.05275000	4.68247400	-1.46308600
H	-0.43886200	5.86621700	0.12333900
H	-1.88508000	4.56159900	1.65685700
H	-1.85058200	2.09078600	1.58810600
H	-0.24336600	-1.96526600	-0.70548100
H	1.93780700	1.39931100	0.70670000
H	4.78253400	1.30535000	-1.06922400
H	4.63991600	-0.46074400	-1.16033400
H	1.52893100	-2.08345800	-2.28825600
H	2.77664900	-1.86369100	-1.06263200
H	2.63863900	-4.31942800	-1.17492900
H	0.87586300	-4.24639900	-1.32513300
H	5.26738800	-0.26664900	1.15946800
H	4.47978600	1.31161500	1.31412100
H	2.77810100	-0.16968100	2.28435000
H	3.08245300	-1.39782800	1.05696800
H	1.01082400	-4.52926400	1.05681500
H	2.56441800	-3.67723100	1.14766600

12cH

E= -811.1196046 a.u., number of negative frequencies = 0

0 1

C	-3.46427200	-1.64521400	0.44365400
C	-4.33132000	-0.61691100	0.06671900
C	-3.77215100	0.56408700	-0.41500100
C	-2.39462000	0.71631000	-0.52195600
C	-1.52871800	-0.31861700	-0.16168500
C	-2.09006400	-1.49983400	0.33750000
C	-0.05810300	-0.16067500	-0.31106900
C	-5.82233500	-0.78394800	0.20322400
C	0.49882200	1.21108600	-0.12912600
C	0.30947800	1.89517400	1.07431800
C	0.86993800	3.15100600	1.26817100
C	1.60901400	3.75121300	0.25234000
C	1.77687300	3.09171200	-0.96001000
C	1.22433800	1.82895900	-1.14846000
C	2.24318600	-1.19370300	-0.69637200
O	2.70460100	-2.54676100	-0.78406400
C	3.43036300	-2.86960900	0.39115600
C	4.09655500	-1.56253300	0.79828300
C	2.96940900	-0.56461000	0.51972300
H	-3.87542200	-2.56919300	0.83799500
H	-4.42348400	1.37918600	-0.71246700
H	-1.98445200	1.64617400	-0.89993900
H	-1.43824500	-2.30215300	0.66364200
H	-6.11190400	-0.84960400	1.25524300
H	-6.35572300	0.05710200	-0.24085300
H	-6.15974000	-1.69923800	-0.28819100
H	-0.27317700	1.42755500	1.86086300
H	0.72913800	3.66444000	2.21196500

H	2.04310200	4.73237500	0.40289600
H	2.33562700	3.56093800	-1.76121100
H	1.34688100	1.31492500	-2.09551400
H	2.56147200	-0.70415900	-1.62232000
H	4.12619900	-3.67155900	0.14468800
H	2.75078700	-3.21896300	1.18102700
H	4.42936000	-1.55101500	1.83655600
H	4.95466200	-1.36933600	0.15029000
H	3.31904800	0.44634400	0.31254500
H	2.28647200	-0.51388600	1.37098600
C	0.73523100	-1.19947900	-0.60134200
H	0.29285400	-2.17233900	-0.79609600

13c

E= -998.4927589 a.u., number of negative frequencies = 0

0 1

C	3.73647500	0.96704400	0.06086600
C	4.37472200	-0.28256000	0.07498000
C	3.65216100	-1.45954400	0.03366900
C	2.26336100	-1.39919700	-0.02341900
C	1.59032300	-0.17850900	-0.03971600
C	2.35316200	1.00011600	0.00419500
O	1.59328000	-2.58232300	-0.05417800
C	0.22782300	-2.64950400	-0.10669500
O	-0.28487200	-3.73230700	-0.05912600
C	-0.51603000	-1.37963400	-0.19970200
C	0.13372000	-0.19658500	-0.11973600
C	-2.01202500	-1.56505700	-0.30452300
C	-0.57081200	1.11752800	-0.06492600
C	-0.93812800	1.79347800	-1.22793000
C	-1.55914500	3.03241900	-1.14550200

C	-1.81207700	3.61148900	0.09649600
C	-1.43809800	2.94654400	1.25722800
C	-0.81478000	1.70347400	1.17608900
C	4.55108700	2.23397100	0.10464600
C	-2.72565900	-1.54520500	1.06058500
C	-4.09299000	-0.97030700	0.68863000
C	-3.69908800	0.04954800	-0.37581100
O	-2.62726300	-0.55316600	-1.09434100
H	5.45790700	-0.32485900	0.11909400
H	4.12988800	-2.43079600	0.04476600
H	1.83793000	1.95396300	-0.01132800
H	-2.18474000	-2.52769200	-0.79180400
H	-0.76263000	1.32646200	-2.18898400
H	-1.85186400	3.54703500	-2.05287500
H	-2.29815000	4.57786500	0.15590500
H	-1.62803800	3.39133000	2.22669300
H	-0.51105300	1.18458800	2.07926600
H	3.90921600	3.11483500	0.08464300
H	5.15763500	2.27647000	1.01238800
H	5.23062600	2.28985900	-0.74901600
H	-2.75819500	-2.53753500	1.50877000
H	-2.20657700	-0.86726900	1.74321700
H	-4.61564500	-0.52229900	1.53396100
H	-4.72693600	-1.74620100	0.25273900
H	-4.49569000	0.27326800	-1.08609900
H	-3.35683500	0.98629900	0.08328700

14c

E= -998.7886545 a.u., number of negative frequencies = 0

1 1

C	3.82913700	-0.67908800	0.00066300

C	3.67175000	-2.07430400	0.32150100
C	2.48417900	-2.75485200	0.25090300
C	1.33875200	-2.05446700	-0.14414200
C	1.41381800	-0.64910000	-0.59049800
C	2.73476500	0.00500700	-0.39859900
O	0.20439400	-2.67533600	-0.15374300
C	-1.06304700	-1.97807800	-0.35580900
O	-1.96673200	-2.66340600	-0.65341800
C	-1.01098500	-0.52454000	-0.11989900
C	0.14930200	0.13656200	-0.23550000
C	5.18915100	-0.05368200	0.13092000
C	-2.33418800	0.08265300	0.29697800
C	0.24745700	1.60963800	-0.11074500
C	0.96705800	2.18185500	0.94264500
C	1.02124700	3.56240700	1.07514000
C	0.37573200	4.37817900	0.14885700
C	-0.33309200	3.81309600	-0.90455600
C	-0.40402300	2.43007100	-1.03301000
O	-2.87710700	-0.74419600	1.31130300
C	-4.21658700	-1.12869700	0.96941000
C	-4.67963000	-0.08934100	-0.04384800
C	-3.38748400	0.17525000	-0.82274800
H	4.55451000	-2.61699300	0.64910200
H	2.39072900	-3.79682500	0.52764500
H	1.37153800	-0.75970900	-1.70042100
H	2.79862900	1.05331300	-0.66730300
H	5.56650100	-0.16667700	1.14944900
H	5.89929200	-0.53812900	-0.54272900
H	5.15720900	1.00780100	-0.10930500
H	-2.13289600	1.07218400	0.71700000
H	1.45817700	1.54594000	1.67253600

H	1.56096600	4.00292500	1.90405600
H	0.42402500	5.45501800	0.25229300
H	-0.83514300	4.44678900	-1.62482500
H	-0.95813300	1.98342900	-1.85138900
H	-4.80050400	-1.13952100	1.88839100
H	-4.20256900	-2.13176600	0.53309000
H	-5.48960100	-0.44761600	-0.67774000
H	-5.00813700	0.81806800	0.46723800
H	-3.36668200	1.14759500	-1.31459400
H	-3.23222900	-0.60375200	-1.57160300

15c

E= -998.7793158 a.u., number of negative frequencies = 0

1 1

C	-3.18049300	-0.61718500	-0.07657700
C	-2.67777500	-1.09854900	1.16116300
C	-1.52082900	-1.81085100	1.18207800
C	-0.73494000	-1.94030200	-0.04548800
C	-1.46478100	-1.77830900	-1.30021200
C	-2.62414800	-1.07449300	-1.30583400
O	0.19889600	-2.96899500	-0.03707300
C	1.48951600	-2.48688200	0.11703000
C	1.42618000	-1.00220300	0.19157700
C	0.18270700	-0.56089000	0.06649700
O	2.43154700	-3.19582500	0.16379500
C	-4.28390900	0.36972600	-0.09146000
C	-0.39220300	0.78438900	0.04044000
C	-0.64642000	1.46547300	1.23704800
C	-1.18069800	2.74511600	1.20768800
C	-1.46865700	3.35499900	-0.01297800
C	-1.20719600	2.68942100	-1.20744000

C	-0.67436300	1.40602400	-1.18178000
C	2.68071300	-0.19600200	0.37638100
C	3.35832500	0.17451700	-0.95903200
C	3.93375400	1.55466500	-0.63255400
C	2.84188700	2.12660900	0.26222700
O	2.38567100	1.01596700	1.04145500
H	-3.21524700	-0.87308100	2.07384000
H	-1.07399600	-2.18555800	2.09726400
H	-0.98519400	-2.13628700	-2.20523500
H	-3.13005200	-0.83357000	-2.23272400
H	-4.91389100	0.29903500	0.79463200
H	-3.80611500	1.36358400	-0.08020600
H	-4.88366900	0.30563700	-0.99894100
H	-0.39001300	0.99712100	2.17994100
H	-1.36122400	3.27430700	2.13499000
H	-1.88330600	4.35562300	-0.03180600
H	-1.41047000	3.17066100	-2.15597900
H	-0.46225100	0.88755100	-2.11061100
H	3.35697200	-0.79383200	0.99787700
H	4.10076200	-0.56328300	-1.25908100
H	2.60766100	0.25859000	-1.75006400
H	4.11917600	2.15744600	-1.52068100
H	4.86601300	1.45659500	-0.07298000
H	3.18914400	2.89465300	0.95140900
H	2.00677500	2.52399700	-0.32969900

16c

E= -998.7744831 a.u., number of negative frequencies = 0

1 1

C	3.75794700	0.74123500	0.27058500
C	4.25579600	-0.59813500	0.19464700

C	3.35568600	-1.57201400	-0.09258200
C	1.96690400	-1.23615000	-0.47100900
C	1.47250500	0.11886700	-0.15956900
C	2.43209900	1.09872900	0.09546000
O	1.09990800	-2.30313000	-0.23122900
C	-0.24953100	-2.11516000	-0.11940600
O	-0.93206900	-3.06455500	0.08416100
C	-0.77950600	-0.71750200	-0.25330000
C	0.05514000	0.36298600	-0.20936400
C	-2.28198600	-0.57920100	-0.24735200
C	-0.43304700	1.76483000	-0.11131400
C	-1.20632900	2.14556800	0.98798800
C	-1.64259400	3.45992800	1.10086900
C	-1.31605800	4.39174300	0.12064000
C	-0.55208400	4.01188100	-0.97851800
C	-0.10459800	2.70136800	-1.09334300
C	5.70403100	-0.87164600	0.48314600
O	-2.68738300	-0.91183900	1.07381300
C	-3.66141900	-1.96711900	1.02906700
C	-4.28085000	-1.86244900	-0.35704600
C	-3.07244200	-1.47447400	-1.22310400
H	4.46705600	1.52585400	0.52165000
H	3.62421800	-2.62208600	-0.14888400
H	2.09978800	-1.12213700	-1.58271800
H	2.12150200	2.12564100	0.23840000
H	-2.53215000	0.46588900	-0.43267900
H	-1.47639000	1.40657300	1.73568300
H	-2.24141800	3.75435600	1.95356400
H	-1.66164400	5.41413400	0.21018500
H	-0.30900100	4.73375900	-1.74811500
H	0.48254700	2.40237500	-1.95590200

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H	6.33836600	-0.38922100	-0.26371800
H	5.97998400	-0.47586100	1.46240900
H	5.91168400	-1.94028400	0.47133600
H	-4.36325200	-1.78915100	1.84280900
H	-3.16018500	-2.92632900	1.17586700
H	-4.74490100	-2.79198000	-0.68405000
H	-5.03108000	-1.06945100	-0.37613400
H	-3.35143800	-0.92271400	-2.11962200
H	-2.51531900	-2.36287200	-1.51301800

TS1-3c

E= -998.944915 a.u., im. freq.= 429.03*i*

0 2

C	-5.56033700	-0.58008400	0.23987800
C	-4.82384300	-1.62950100	0.78565600
C	-3.43510900	-1.63685100	0.73023100
C	-2.77460600	-0.57995800	0.12689600
C	-3.47849100	0.48445400	-0.42045400
C	-4.86499500	0.47241600	-0.35831900
O	-1.38366900	-0.60079100	0.17935100
C	-0.66778900	-0.34744100	-0.95065200
O	-1.14969800	-0.12693000	-2.02344200
C	0.74822600	-0.31721700	-0.63813100
C	1.86995400	-0.75385000	-0.41866800
C	-7.06700300	-0.58798700	0.26777600
C	0.81723800	1.97462400	-0.74451300
C	3.23474700	-1.02290000	-0.15688500
C	4.19353300	-0.89495900	-1.17684900
C	5.52982500	-1.14296500	-0.90916700
C	5.93597300	-1.51591900	0.37055300
C	4.99265200	-1.64227000	1.38706200

C	3.65146700	-1.40275300	1.13104200
O	2.13307900	2.18242000	-0.52726700
C	2.31820800	2.36278900	0.88171600
C	1.05579200	3.09454000	1.33191300
C	-0.01662200	2.48406100	0.40662000
H	-5.34115000	-2.45539400	1.26155800
H	-2.85337100	-2.44531600	1.15479000
H	-2.94925700	1.29889100	-0.89659100
H	-5.41972000	1.30086700	-0.78585700
H	-7.44312300	-1.24428600	1.05351400
H	-7.46262600	0.41424600	0.44140800
H	-7.46944200	-0.94249100	-0.68500500
H	0.52464300	2.01369600	-1.78599000
H	3.87048200	-0.59189300	-2.16467400
H	6.26194800	-1.04086600	-1.70118600
H	6.98239700	-1.70758400	0.57394100
H	5.30438700	-1.93394400	2.38284400
H	2.91025800	-1.50964200	1.91397600
H	3.24364500	2.91698600	1.02300200
H	2.40360200	1.37757000	1.35225200
H	0.84159000	2.94832100	2.38966100
H	1.15839100	4.16361100	1.13883600
H	-0.75858000	3.21820600	0.08357200
H	-0.55469100	1.67204700	0.90660500

TS1-4c

E= -998.9422842 a.u., im. freq.= 398.37i

0 2

C	-6.00195600	0.14336400	0.29596000
C	-5.45055500	-0.96908400	-0.34082600
C	-4.08031900	-1.19253500	-0.36684300

C	-3.24056000	-0.27821600	0.25821000
C	-3.76106800	0.83334200	0.90400300
C	-5.13498500	1.03679800	0.92231000
O	-1.86733200	-0.44950100	0.35404400
C	-1.14697200	-0.85519600	-0.73419700
O	-1.61714400	-1.08949400	-1.81434900
C	0.23700600	-0.95560100	-0.39059300
C	1.44564000	-0.76365100	-0.27931800
C	-7.49026600	0.37990300	0.28286100
C	2.79621000	-1.04154700	0.14337800
C	1.85237700	1.33104900	-1.00186100
C	3.79695000	-1.31702600	-0.79509000
C	5.10338500	-1.52001100	-0.37461100
C	5.42701900	-1.44117500	0.97818200
C	4.43370000	-1.17563900	1.91584000
C	3.12172400	-0.97768300	1.50398300
C	1.68623800	2.13979100	0.26226000
C	3.00672800	2.92954200	0.32035500
C	3.94910300	2.02918100	-0.47388700
O	3.10816500	1.44731600	-1.48578700
H	-6.10774200	-1.68125700	-0.82866700
H	-3.66896400	-2.05505000	-0.87065500
H	-3.08017400	1.51853500	1.39344000
H	-5.53777800	1.90493000	1.43285500
H	-8.03859500	-0.55979500	0.36900300
H	-7.79353800	1.02840500	1.10591600
H	-7.79871300	0.85871600	-0.65055700
H	1.09982700	1.25767100	-1.77648500
H	3.53961300	-1.35244900	-1.84587300
H	5.87426200	-1.73562300	-1.10453900
H	6.44966900	-1.59543200	1.30066500

H	4.67939000	-1.12837200	2.96992500
H	2.33694900	-0.78338600	2.22546400
H	0.80269900	2.77849200	0.22517500
H	1.58206800	1.48615300	1.13385800
H	3.35645800	3.10306200	1.33727900
H	2.89713300	3.89150400	-0.18336700
H	4.75155600	2.55433400	-0.98819400
H	4.36996500	1.22936000	0.14279600

TS3c-5c

E= -998.9916989 a.u., im. freq.= 412.65*i*

0 2

C	-3.25580100	-1.28994400	-0.03623700
C	-2.54641000	-1.51066400	-1.22626200
C	-1.21437700	-1.86552700	-1.21176200
C	-0.53345000	-1.90612700	0.02650400
C	-1.27905300	-1.90109000	1.22778100
C	-2.61014400	-1.54571800	1.18295200
O	0.75033600	-2.42691600	0.05416400
C	1.81491400	-1.56892000	0.07276200
C	1.42929600	-0.12611200	0.05124400
C	0.14357100	0.13543800	0.06090800
O	2.92507500	-2.00135700	0.11974000
C	-4.66721000	-0.77656400	-0.06628700
C	-0.84933500	1.14558400	0.03353900
C	-1.34942000	1.61723700	-1.19726800
C	-2.39216900	2.52910100	-1.22264500
C	-2.96211300	2.98321400	-0.03437800
C	-2.47704600	2.52058900	1.18805600
C	-1.43564100	1.60802000	1.22894700
C	2.54283800	0.89985100	-0.02017600

C	3.50357000	0.87675700	1.18475800
C	4.85578700	1.15775300	0.52340900
C	4.68819900	0.43312900	-0.80770200
O	3.33063800	0.66225000	-1.18069400
H	-3.06056500	-1.40193800	-2.17531300
H	-0.65220700	-2.04383000	-2.12020100
H	-0.76628400	-2.10938500	2.15879100
H	-3.17391600	-1.46527500	2.10629500
H	-4.66164500	0.31866600	-0.05158700
H	-5.18832200	-1.09510700	-0.97060000
H	-5.23499400	-1.11905100	0.80040700
H	-0.90520400	1.25633700	-2.11715000
H	-2.76273300	2.89150800	-2.17415700
H	-3.77686000	3.69651600	-0.06052700
H	-2.91500300	2.87515800	2.11355000
H	-1.06253100	1.23640600	2.17587000
H	2.07529700	1.88397300	-0.12291000
H	3.22037400	1.61456500	1.93525500
H	3.51343400	-0.11138300	1.64592800
H	5.70006000	0.78843200	1.10569400
H	4.98525300	2.22976500	0.35457200
H	5.32003500	0.82748400	-1.60410000
H	4.86136900	-0.64068900	-0.69434900

TS3c-6c

E= -998.9859561 a.u., im. freq.= 417.73*i*

0 2

C	3.40702500	-0.12153900	0.31589100
C	3.16893500	-1.20735300	1.16728600
C	2.20413700	-2.16994800	0.85739600
C	1.47539700	-2.03794700	-0.30193000

C	1.64320400	-0.93080100	-1.16060700
C	2.67214900	-0.01308500	-0.85679700
O	0.50046400	-2.96033000	-0.60382800
C	-0.80562900	-2.56638000	-0.71107400
O	-1.63354700	-3.40144300	-0.92028600
C	-1.14549300	-1.12260300	-0.49824600
C	-0.26144100	-0.14832700	-0.60096300
C	4.43141400	0.92607400	0.66661000
C	-2.62362200	-0.91729500	-0.15171000
C	-0.21099700	1.27975900	-0.48014500
C	0.50910700	1.85513100	0.57972800
C	0.59551900	3.23600000	0.69740500
C	-0.00622300	4.05886200	-0.25028700
C	-0.70153100	3.49301100	-1.31802500
C	-0.80440800	2.11612000	-1.43924300
C	-2.89529200	-1.25021700	1.32121100
C	-2.54997200	0.08375700	1.98785800
C	-3.07511100	1.08845800	0.96052200
O	-3.01820200	0.42918700	-0.30856600
H	3.74833700	-1.30848900	2.07780500
H	2.01353600	-3.01561300	1.50600100
H	1.25857900	-0.99557800	-2.17275700
H	2.86246400	0.80879100	-1.53802000
H	5.01677800	1.20978300	-0.20967400
H	3.93837100	1.82916600	1.03859300
H	5.11647400	0.57120200	1.43709300
H	-3.20922000	-1.53561100	-0.83279600
H	0.98462300	1.20597400	1.30760300
H	1.13564700	3.67114300	1.53005600
H	0.06560900	5.13580300	-0.15900300
H	-1.17526200	4.13133000	-2.05426000

H	-1.37243700	1.67027000	-2.24554200
H	-3.95544300	-1.48152700	1.44881000
H	-2.30944900	-2.09513100	1.68266800
H	-1.46700100	0.18254500	2.09808000
H	-3.01088500	0.20894600	2.96731000
H	-4.11722000	1.35609400	1.16030600
H	-2.47623000	2.00153500	0.90988700

TS5c-9c

E= -999.0002217 a.u., im. freq.= 228.09*i*

0 2

C	-4.07084200	-1.04079800	-0.11935500
C	-3.38727900	-0.61810500	-1.27334400
C	-2.06478100	-0.24933400	-1.21814800
C	-1.34268800	-0.35218900	-0.00201400
C	-2.05617000	-0.71087300	1.17132300
C	-3.38760200	-1.06218800	1.10191000
O	-0.56197300	-2.26338000	-0.19186700
C	0.71622200	-2.02932900	-0.02201500
C	1.06361600	-0.58758700	0.21056100
C	0.01969400	0.25325000	0.11278200
O	1.53209900	-2.92554600	-0.08682700
C	-5.50467000	-1.47660600	-0.20753700
C	0.08154200	1.73367600	0.09303800
C	1.11664300	2.39734300	-0.57878600
C	1.15138400	3.78599200	-0.61102700
C	0.15983500	4.53006400	0.01886400
C	-0.88071800	3.87904400	0.67360600
C	-0.92661400	2.49203500	0.70063700
C	2.49307100	-0.16207200	0.47442900
C	3.32639100	-1.15632200	1.31285600

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C	4.27713600	-1.82376600	0.29564900
C	3.87244400	-1.20823000	-1.04950100
O	3.22246500	0.02137900	-0.73392700
H	-3.92143500	-0.57434400	-2.21609100
H	-1.54307300	0.09308200	-2.10408500
H	-1.51960800	-0.73862300	2.11283700
H	-3.91321600	-1.36505600	2.00033000
H	-6.05739800	-0.87034100	-0.92709400
H	-5.55839500	-2.51669100	-0.54310100
H	-6.00081300	-1.41224500	0.76110500
H	1.88079500	1.81955200	-1.08635100
H	1.95459300	4.28684400	-1.13792400
H	0.19151100	5.61270100	-0.00843000
H	-1.66119600	4.45238100	1.15915800
H	-1.74752100	1.99194700	1.20264500
H	2.45508400	0.81406700	0.95983300
H	3.88863800	-0.60106700	2.06391300
H	2.70072600	-1.88536300	1.82325100
H	4.14982400	-2.90457900	0.28152300
H	5.31608900	-1.58978600	0.53148700
H	4.71861800	-0.96583500	-1.69220800
H	3.18636400	-1.87027800	-1.58339300

TS9c-8c

E= -998.9980128 a.u., im. freq.= 329.36*i*

0 2

C	-3.67903000	0.40055700	-0.86943700
C	-4.21962400	-0.65607800	-0.09747700
C	-3.40066800	-1.30701100	0.79469200
C	-2.03125100	-0.96430000	0.90235400
C	-1.50726900	0.09654800	0.11889700

C	-2.35437700	0.77906400	-0.75555100
O	-1.01768600	-2.35439300	-0.11584800
C	0.26499200	-2.09276800	-0.18394000
O	1.02832100	-2.94173200	-0.59635600
C	0.77635700	-0.72436800	0.19579600
C	-0.05870000	0.34143900	0.17402900
C	2.27050800	-0.58589400	0.37782400
C	0.38654200	1.75821800	0.12902300
C	-0.26884700	2.72032100	0.90462800
C	0.11860700	4.05261800	0.85204900
C	1.15268900	4.44342700	0.00727200
C	1.79794400	3.49627600	-0.78089000
C	1.42060000	2.16002400	-0.72399700
C	-5.66996400	-1.02188600	-0.25624100
O	2.93082900	-0.64105000	-0.88976100
C	3.83618800	-1.74172500	-0.91279200
C	4.25236600	-1.92673300	0.54171200
C	2.93397300	-1.65219900	1.27621800
H	-4.32442600	0.91628400	-1.57285600
H	-3.79436000	-2.09793600	1.42191400
H	-1.48010700	-1.28025700	1.77876600
H	-1.95503000	1.58093500	-1.36536900
H	2.46558400	0.40320400	0.79876600
H	-1.07978000	2.41593100	1.55737200
H	-0.38807800	4.78618900	1.46753200
H	1.45097600	5.48395600	-0.03987100
H	2.59711100	3.79759700	-1.44733500
H	1.92275200	1.41910200	-1.33682600
H	-6.31148300	-0.15428900	-0.08560500
H	-5.86229300	-1.37982100	-1.27065400
H	-5.95843400	-1.80716400	0.44194900

H	4.66136300	-1.47459800	-1.57392100
H	3.32432000	-2.62957200	-1.29145400
H	4.65209700	-2.92004800	0.74658300
H	5.00430200	-1.18135400	0.81291100
H	3.08122200	-1.27354700	2.28778500
H	2.33634800	-2.56037100	1.32102300

TS9c-11c

E= -998.9936092 a.u., im. freq.= 352.93*i*

0 2

C	3.74314300	0.03262600	-1.03939500
C	4.31238900	-0.86462800	-0.13379500
C	3.49597700	-1.40744500	0.85710500
C	2.14670900	-1.08598300	0.93595200
C	1.58086900	-0.20304800	0.01615800
C	2.40094600	0.37088100	-0.95932900
C	0.15337200	0.21089600	0.09472400
C	-0.90883300	-0.58022700	0.14907600
C	5.76496500	-1.24869400	-0.23863100
C	-0.09534000	1.69079700	0.09923400
C	-0.85672100	2.29966300	-0.89731100
C	-1.07632100	3.67424900	-0.87214600
C	-0.53829200	4.44582600	0.15002200
C	0.23396300	3.84363800	1.14060000
C	0.46390200	2.47523900	1.11156600
C	-2.36469300	-0.34148300	0.45493800
C	-0.80068200	-2.38009100	-0.32102300
O	-1.40882900	-2.54180800	-1.32872200
O	-0.15505000	-2.82176200	0.58154100
C	-3.25822500	-0.09250500	-0.77777000
C	-4.56198300	-0.78799500	-0.37647500

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O	-2.90112500	-1.47387000	1.12685700
C	-4.03656700	-1.97511100	0.41888700
H	4.36266400	0.47725400	-1.81107600
H	3.92221700	-2.09195100	1.58273700
H	1.52696800	-1.51744800	1.71023500
H	1.97843700	1.08505200	-1.65777100
H	6.16397800	-1.55064400	0.73062100
H	5.88994900	-2.08951400	-0.92658200
H	6.36613100	-0.41987200	-0.61574300
H	-1.25303200	1.69431700	-1.70438900
H	-1.66203500	4.14028400	-1.65553000
H	-0.71036800	5.51513000	0.17181700
H	0.66199800	4.44387900	1.93448600
H	1.07677900	2.00282400	1.87113400
H	-2.40209900	0.51531400	1.13959400
H	-3.37895100	0.97333700	-0.96580800
H	-2.82289000	-0.56886200	-1.65727200
H	-5.16418800	-1.08573900	-1.23469800
H	-5.16044200	-0.13803300	0.26628500
H	-4.73983900	-2.35903300	1.15752100
H	-3.72670100	-2.78640800	-0.24729400

TS11c-12c

E= -1042.192092 a.u., im. freq.= 412.43*i*

0 3

C	-1.74675900	-3.02478300	0.19892400
C	-3.11888200	-2.98549100	-0.04403900
C	-3.67095400	-1.76916200	-0.44976300
C	-2.88826000	-0.63360600	-0.59335500
C	-1.50930800	-0.66833600	-0.33383000
C	-0.95366900	-1.89351000	0.05873600

C	-0.66553500	0.53109600	-0.55216500
C	0.64452500	0.43646700	-0.83719900
C	-3.98320700	-4.20476200	0.14454500
C	-1.23035800	1.89107600	-0.35447800
C	-0.76925900	2.97279400	-1.11759300
C	-1.23677700	4.25947300	-0.89017900
C	-2.17558500	4.49943600	0.10940100
C	-2.63872400	3.43716200	0.87847200
C	-2.17229400	2.14821800	0.65107200
C	1.66470800	-0.42731700	-1.45482200
C	1.74401500	1.01601100	1.15426800
O	3.06786000	0.72119800	1.15995100
C	3.31771800	-0.38483700	2.04367400
C	2.93388600	0.33303500	-1.93091600
C	4.09547600	-0.61258600	-1.56566100
C	1.94795000	-0.90351300	2.48882100
C	1.03651800	0.31435200	2.26718300
C	3.36801200	-1.89509000	-1.15363700
O	2.15145400	-1.45135200	-0.57932100
H	-1.28787800	-3.95946800	0.50572100
H	-4.73340100	-1.71307600	-0.66542500
H	-3.34408900	0.29101000	-0.92787300
H	0.11284700	-1.95884400	0.23908900
H	-3.39718900	-5.12076200	0.05539700
H	-4.44894600	-4.20297700	1.13432200
H	-4.78435900	-4.23812100	-0.59615700
H	-0.04188400	2.78584500	-1.90010200
H	-0.87182100	5.07849000	-1.49913500
H	-2.54185400	5.50345000	0.28633300
H	-3.36314200	3.61268800	1.66534500
H	-2.53178800	1.32870200	1.26327000

H	1.19137000	-0.92440900	-2.31684700
H	1.52553400	2.03378900	0.84758300
H	3.91018900	-0.00262500	2.87929300
H	3.90254500	-1.12596700	1.49814200
H	2.87291000	0.53200900	-3.00099800
H	3.02236200	1.28310700	-1.40616800
H	4.64813300	-0.20703900	-0.71809100
H	4.78924700	-0.77840900	-2.39005200
H	1.63692700	-1.72333100	1.84398300
H	1.95614700	-1.24304000	3.52403800
H	0.99858300	0.94741700	3.16401000
H	0.01104100	0.04682900	2.00304000
H	3.15998000	-2.52662100	-2.02846300
H	3.89460800	-2.49417200	-0.41004600

TS11c-12cH

E= -1042.8479806 a.u., im. freq.= 1415.18*i*

0 2

C	-3.27635200	-1.83165400	0.86707700
C	-4.42681200	-1.27034500	0.31922900
C	-4.28819000	-0.12687900	-0.47258700
C	-3.04274900	0.43300600	-0.70830000
C	-1.88637300	-0.14180400	-0.16692800
C	-2.02106600	-1.27871300	0.63226100
C	-0.54835500	0.45313500	-0.44889200
C	0.52556700	-0.28552300	-0.72837300
C	-5.78868500	-1.86439400	0.56936700
C	-0.41826100	1.93633500	-0.38772200
C	0.40535300	2.61893400	-1.28789200
C	0.60596000	3.98871900	-1.16699400
C	-0.02085200	4.69936100	-0.14853600

C	-0.86075100	4.03328000	0.73910200
C	-1.06467000	2.66441000	0.61638200
C	0.70913400	-1.75300100	-0.85936900
O	3.72354300	-0.39988400	0.02248500
C	3.68362800	-0.76112600	1.41007200
C	1.80976200	-2.18007800	-1.86516800
C	2.62109800	-3.24665000	-1.10255200
C	2.64977100	0.15847100	2.05838200
C	2.73085200	1.40064700	1.16450900
C	1.73505400	-3.53629300	0.10963900
O	1.11130900	-2.29710100	0.40224500
H	-3.36106100	-2.71228900	1.49523600
H	-5.17202800	0.32855000	-0.90822300
H	-2.95547900	1.32349200	-1.32143300
H	-1.13648300	-1.72258300	1.07667100
H	-6.45097400	-1.13679300	1.04465300
H	-6.25776000	-2.17123500	-0.36872800
H	-5.72489300	-2.73879200	1.21771800
H	0.88195200	2.06092300	-2.08596100
H	1.24636200	4.50364200	-1.87358000
H	0.13518800	5.76723800	-0.05319200
H	-1.35671100	4.58161300	1.53135900
H	-1.71421000	2.14508800	1.31231800
H	-0.24930600	-2.21526400	-1.14529600
H	4.68392500	-0.60743300	1.82812200
H	3.41727900	-1.81595600	1.48675400
H	1.35620100	-2.57337400	-2.77532000
H	2.43873700	-1.33117500	-2.13173000
H	3.56941900	-2.81879500	-0.77733600
H	2.81914400	-4.14032000	-1.69482800
H	1.65879000	-0.29295600	1.97802700

H	2.87092300	0.36170500	3.10600600
H	3.59240000	2.02042700	1.43516300
H	1.83237400	2.01837100	1.18958400
H	0.97220400	-4.29014000	-0.13093300
H	2.27851600	-3.85866300	0.99840300
C	2.95492500	0.74941400	-0.18579300
H	3.38595600	1.35875000	-0.98151400
H	1.83277600	0.37634200	-0.59126400