

Supporting Information

for

The Mechanism of Metal-Free C-H Activation of Branched Aldehydes and Acylation of Alkenes Using Hypervalent Iodine Compound: A Theoretical Study

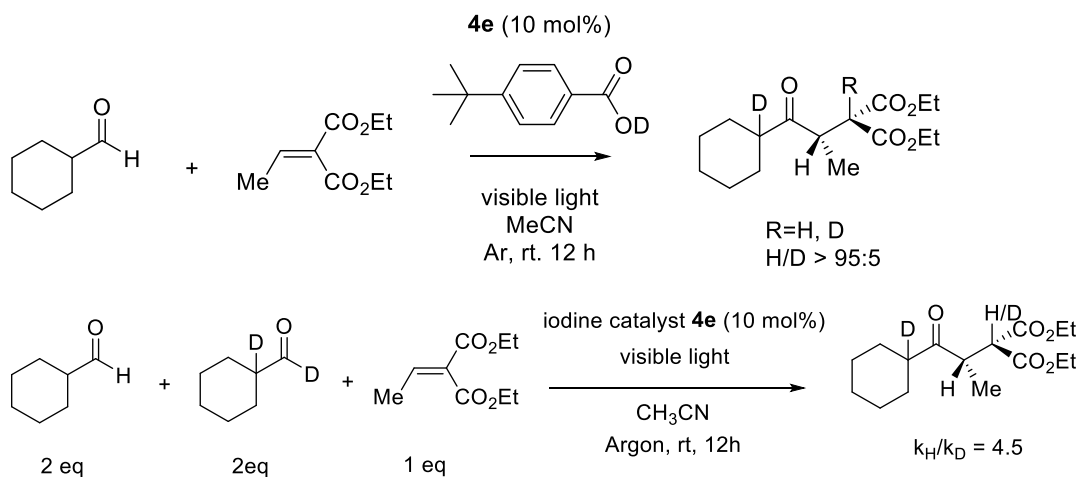
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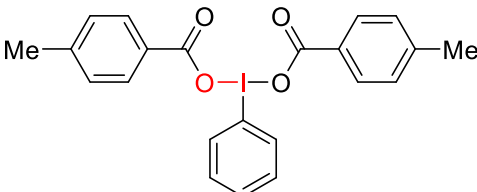
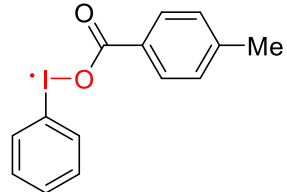
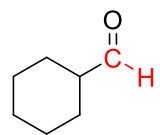
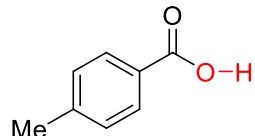
*Email: morokuma@fukui.kyoto-u.ac.jp

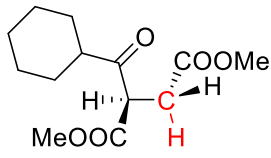
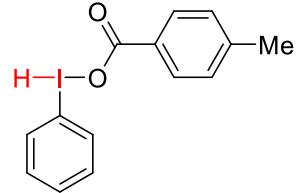
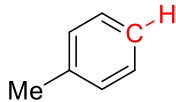
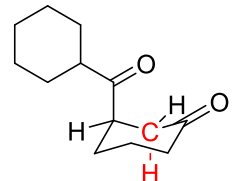
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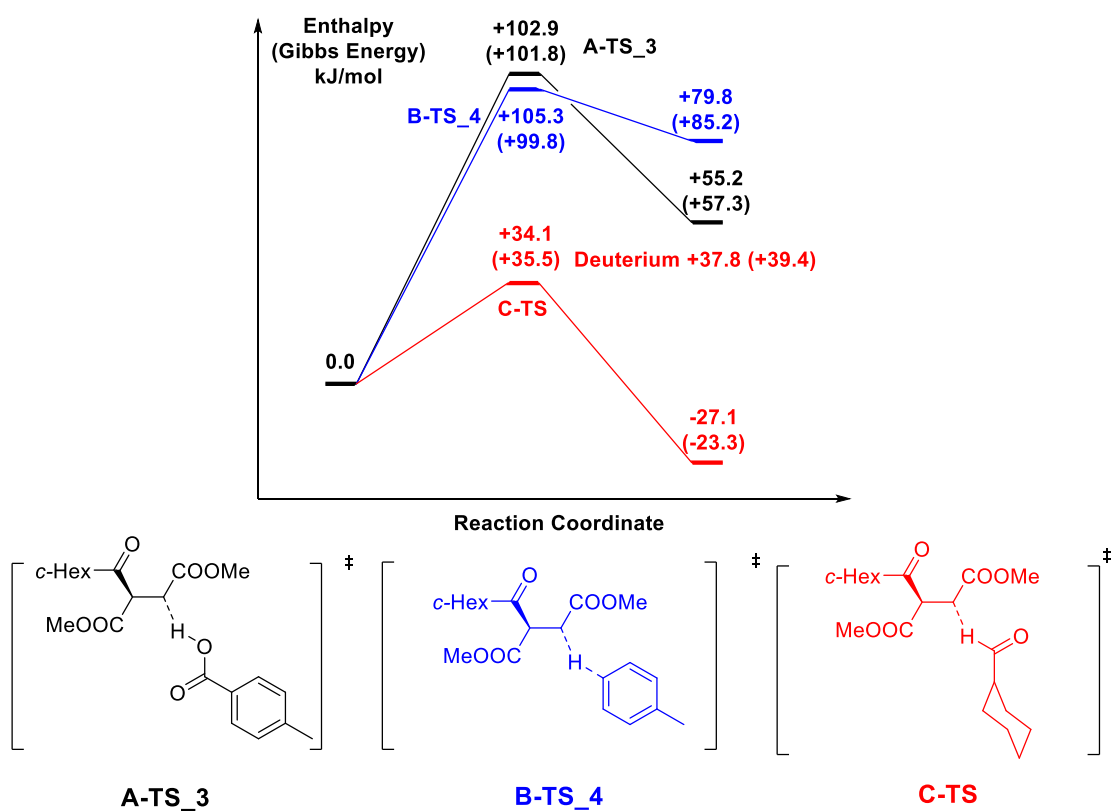


Scheme S1. Experiments involving deuterated species.

Table S1: Bond Enthalpies of various Specific Bonds (in red) involved in the mechanism (BDE, Bond-Dissociation-Energy) in PCM acetonitrile.

Species/Bond	Bond Enthalpy (kJ/mol)
	+155.4
	+15.4
	+368.1
	+436.1

	+383.5
	+200.6
	+465.9
	+368.3



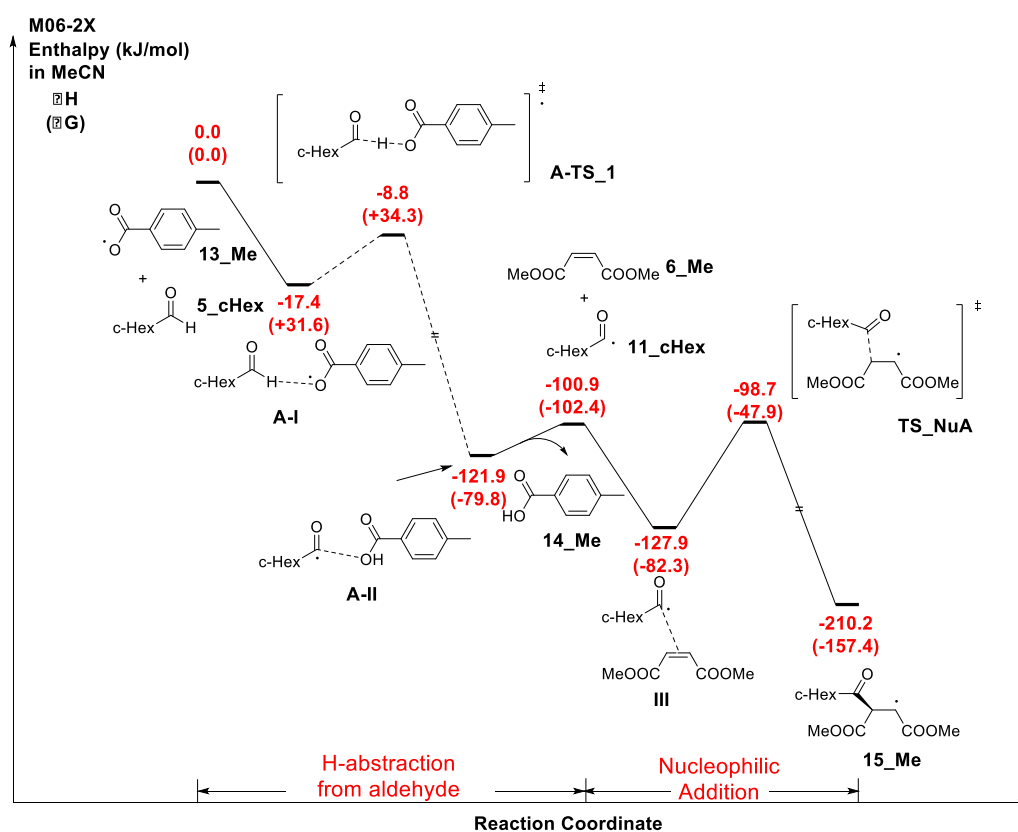
Scheme S2. Energy profiles for the H atom transfer to the carbon-centered radical 15_Me

Detailed calculation of KIE from the Eyring equation:

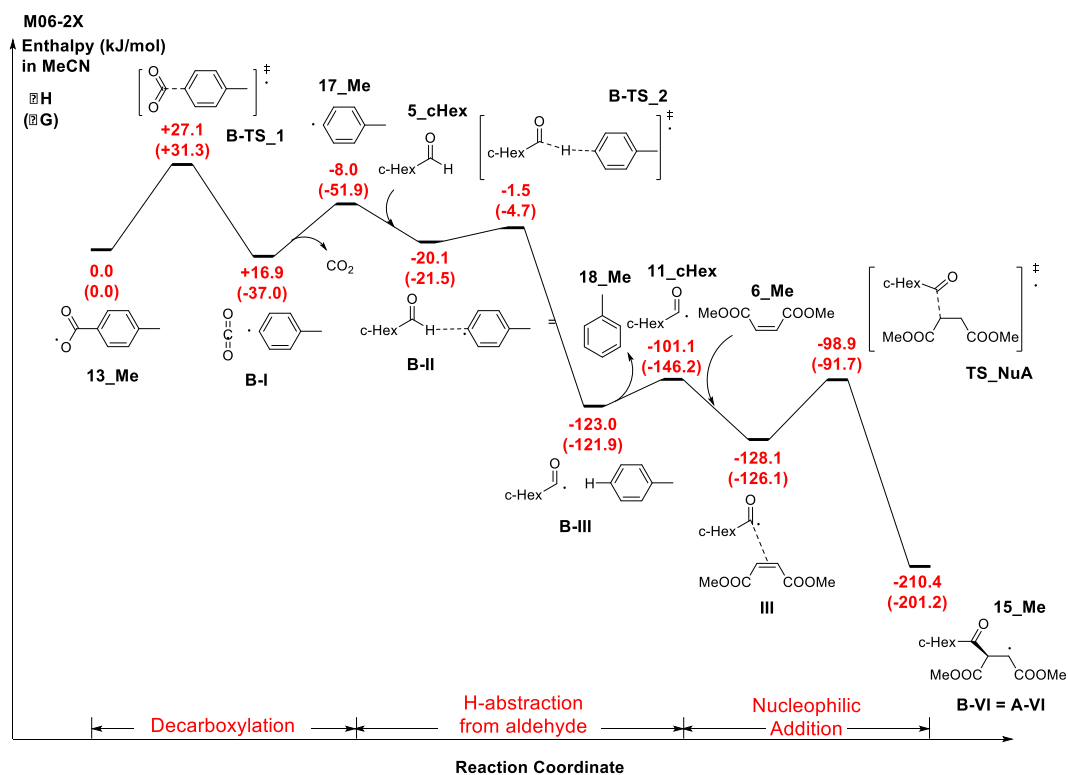
$$k_H = \frac{k_B T}{h} e^{(-\frac{\Delta G_H^\ddagger}{RT})}; k_D = \frac{k_B T}{h} e^{(-\frac{\Delta G_D^\ddagger}{RT})}$$

$$KIE = k_H/k_D = \exp\left\{\frac{(\Delta G_D^\ddagger - \Delta G_H^\ddagger)}{RT}\right\}$$

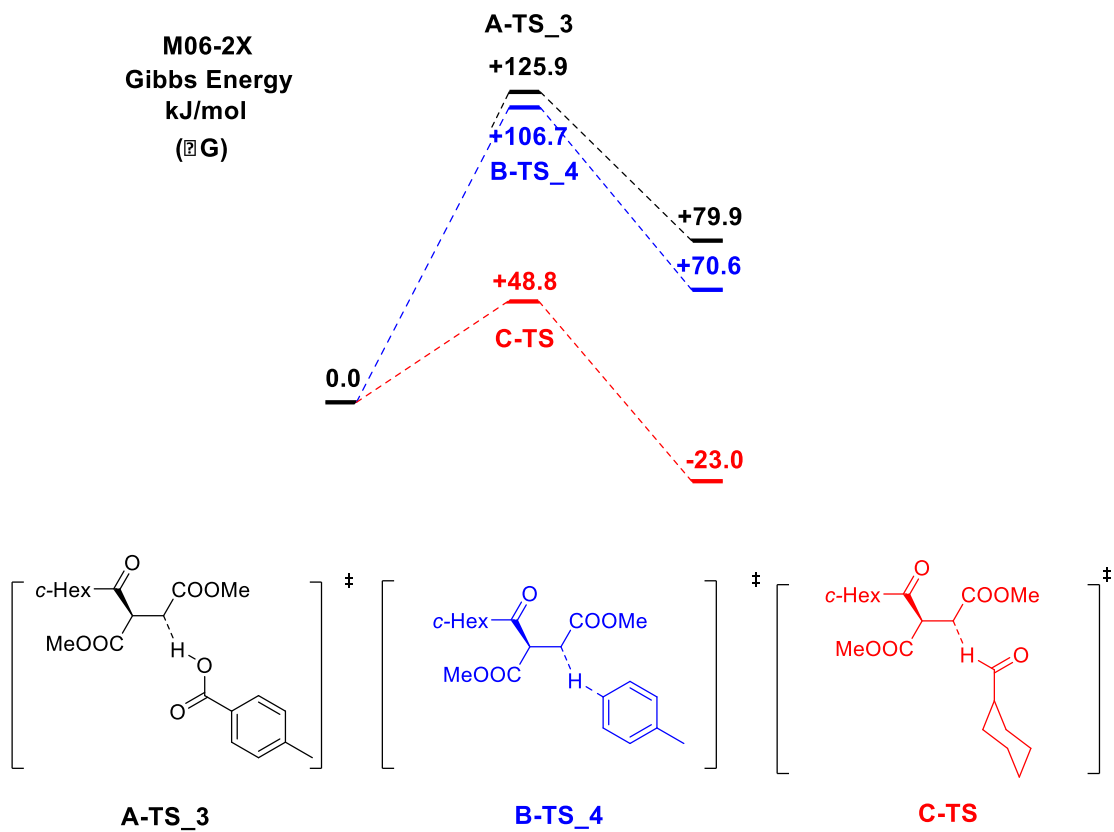
$$= \exp\left\{\frac{(39400 - 35500)}{(8.314 \times 298.15)}\right\} = 4.82$$



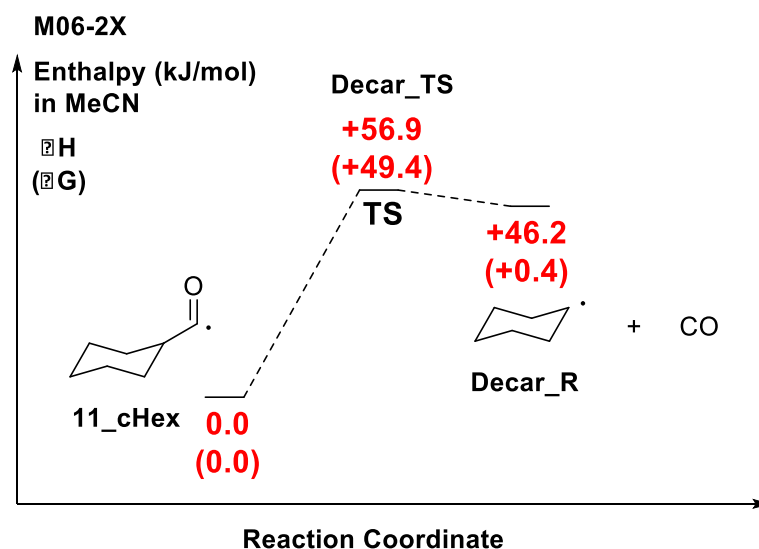
Scheme S3. Enthalpy profile for Pathway A with the M06-2X functional



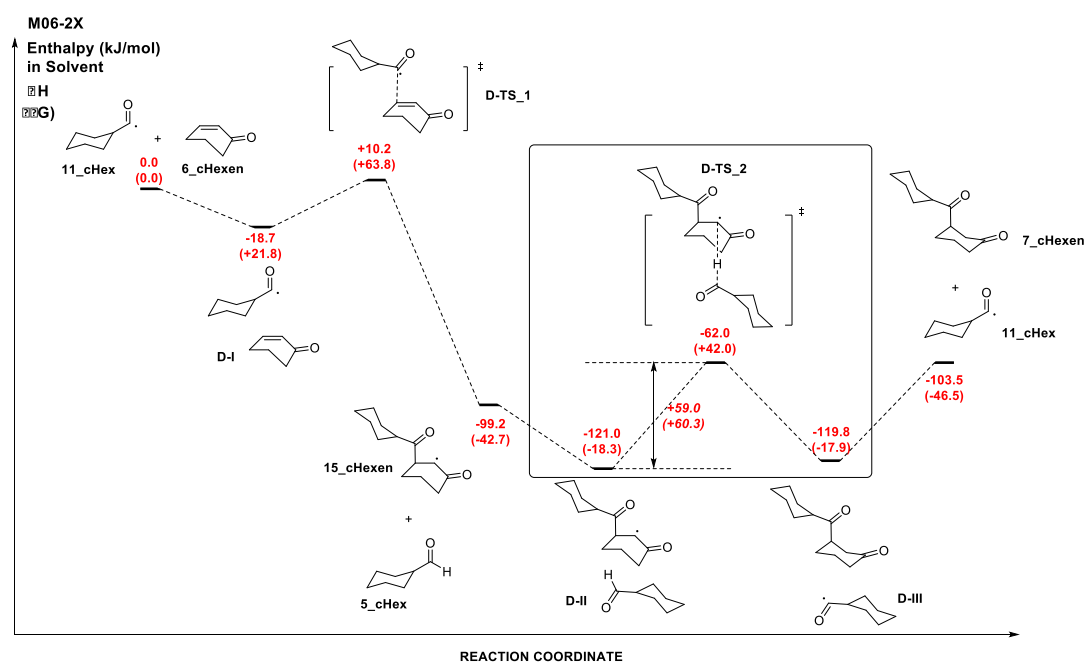
Scheme S4. Energy profile for Pathway B with the M06-2X functional



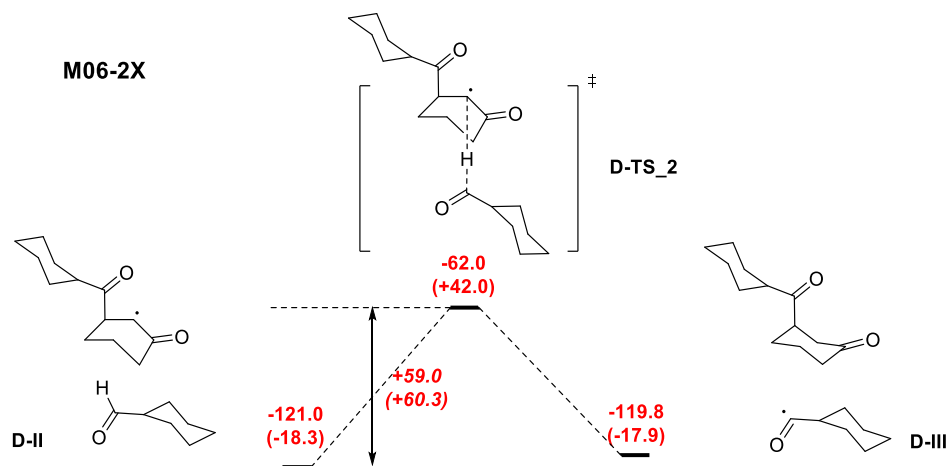
Scheme S5. Energy profile for the H atom transfer at the final stage with the M06-2X functional



Scheme S6. Energy profile for the decarbonylation reaction of the acyl radical 11_cHex with the M06-2X functional

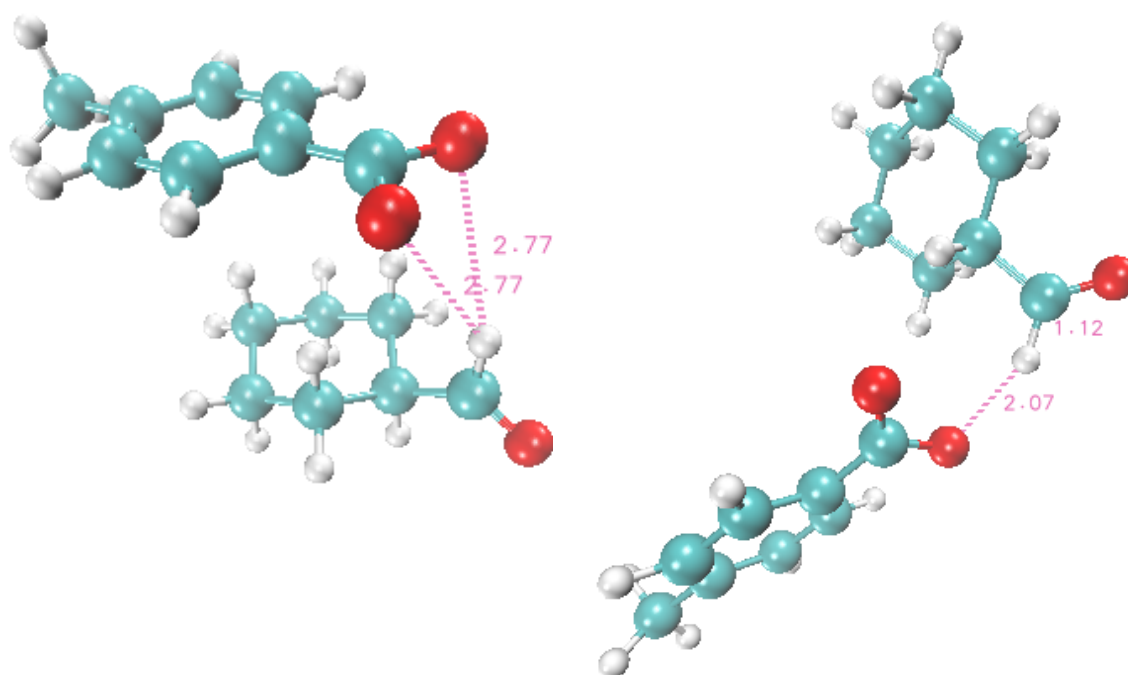


Scheme S7A. Energy profile for the self-propagating reaction involving 2-cyclohexen-1-one with the M06-2X functional

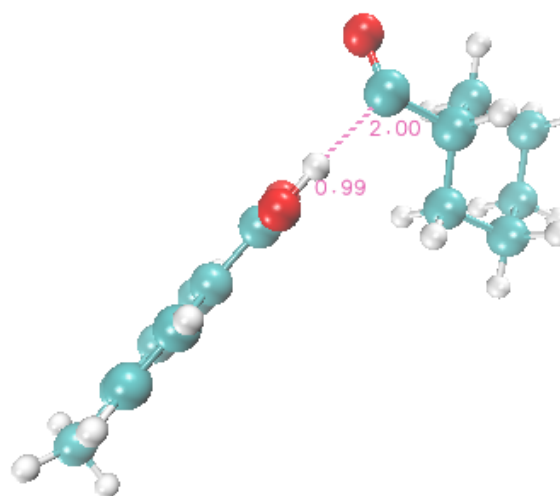


Scheme S7B. H-transfer reaction between aldehyde and the carbon-centered radical with the M06-2X functional

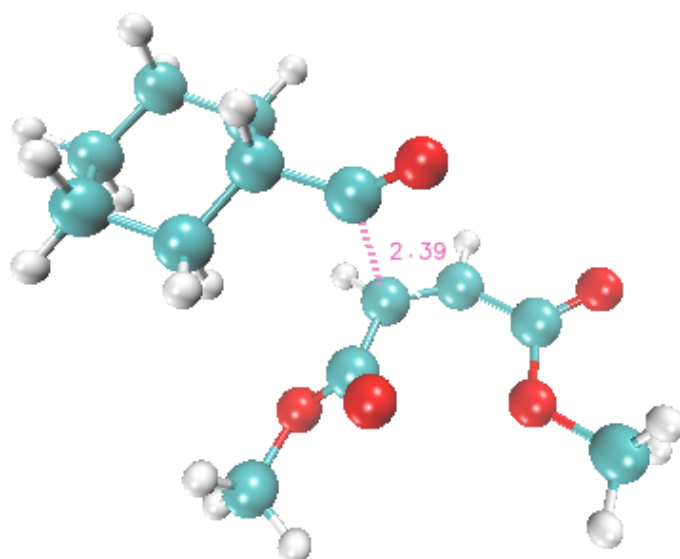
Figure S1: Meaningful intermediates and TS of pathway A
A-I **A-TS-1**



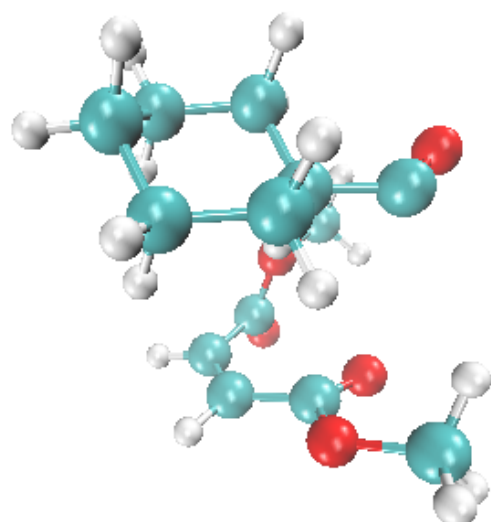
A-II



TS-NuA



III



15_Me

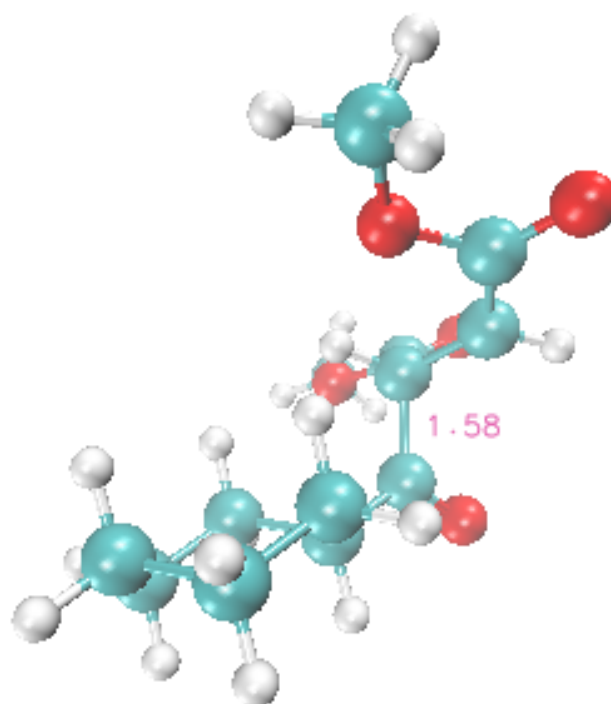


Table S2. Cartesian coordinates (in Å) and absolute energies of all optimized structures at the level: B3LYP-GD3/6-311G(d,p) with SDD(d) on I

4e_Me

E=-1162.41785254 hartree

0 1

C	-1.29817444	0.49695740	0.00000000
C	-2.17068144	-0.15505060	0.85711700
C	-3.04310544	0.49697040	1.71431200
C	-3.03486444	1.89231240	1.70255000
C	-2.17049444	2.58631140	0.85728900
C	-1.30622344	1.89230040	0.01193700
H	-0.62673544	-0.05154160	-0.64571000
H	-3.71462844	-0.05151960	2.35994300
H	-3.70449344	2.42924540	2.36350800
H	-2.17041744	3.66958640	0.85736000
H	-0.63652244	2.42922240	-0.64895700
I	-2.17082044	-2.30826760	0.85700000
O	-4.32249944	-2.21710560	1.18787800
O	-0.01913644	-2.21732060	0.52611700
C	-5.09160044	-1.82936860	0.17295700
C	0.75003956	-1.82971160	1.54102800
C	-6.54686644	-1.79794160	0.51751900
C	-7.02057144	-2.12749860	1.79225600
C	-7.46054044	-1.41555060	-0.47120200
C	-8.38286344	-2.07496860	2.06667100
H	-6.31872544	-2.41893260	2.56249800
C	-8.81972544	-1.36676160	-0.18965300
H	-7.08884644	-1.15666660	-1.45482600
C	-9.30505544	-1.69720460	1.08281000
H	-8.73740144	-2.32842060	3.06015000
H	-9.51656844	-1.06566660	-0.96471100
C	2.20526856	-1.79816560	1.19632400
C	2.67881856	-2.12711560	-0.07862600
C	3.11906156	-1.41625360	2.18512200
C	4.04107956	-2.07445060	-0.35318000
H	1.97687656	-2.41817460	-0.84892100
C	4.47821256	-1.36734460	1.90343800
H	2.74748456	-1.15782960	3.16891000
C	4.96338856	-1.69716960	0.63075400
H	4.39549756	-2.32741260	-1.34682600
H	5.17515056	-1.06663660	2.67856100
O	-4.66525944	-1.51680060	-0.92624700
O	0.32379356	-1.51733760	2.64032300
C	-10.78400144	-1.67279060	1.37473300
H	-11.24189844	-2.63252660	1.11182900
H	-10.97917644	-1.49558060	2.43432700
H	-11.29172544	-0.89942160	0.79416200
C	6.44230456	-1.67262860	0.33868400
H	6.95003956	-0.89930860	0.91931300

H	6.90028656	-2.63237060	0.60142000
H	6.63736556	-1.49526160	-0.72090300

12_Me

E=-702.74700620 hartree

0 2

C	-0.40564475	-1.65314399	0.00531018
C	0.10407725	-2.49612599	0.99037618
C	0.88393225	-2.02825199	2.04604118
C	1.16592125	-0.66387999	2.10582318
C	0.66863325	0.20156201	1.13244918
C	-0.11641875	-0.29222799	0.09038518
H	-1.03659875	-2.04430599	-0.78048782
H	1.26369025	-2.70123499	2.80314618
H	1.77225625	-0.28322199	2.91908518
H	0.88937925	1.26084101	1.18794818
H	-0.51014975	0.38016901	-0.66267382
I	-0.31757775	-4.57628999	0.87387818
O	-2.82745275	-4.04492199	1.42220418
C	-3.47793275	-3.58362399	0.39346318
C	-4.92558775	-3.27052699	0.71701818
C	-5.50066375	-3.56718999	1.95718618
C	-5.70758275	-2.65944099	-0.26776182
C	-6.83510475	-3.25957299	2.20104118
H	-4.90082575	-4.03621699	2.72639218
C	-7.04009775	-2.35356299	-0.01546082
H	-5.25678475	-2.42958199	-1.22486282
C	-7.62798675	-2.65007599	1.22077818
H	-7.26869375	-3.49395799	3.16765418
H	-7.63376975	-1.87609799	-0.78811882
O	-3.02866475	-3.38783799	-0.73211382
C	-9.08280375	-2.34798499	1.47873718
H	-9.42073875	-1.48786899	0.89674718
H	-9.70824575	-3.20154499	1.19558518
H	-9.26663275	-2.14469799	2.53590918

13_Me

E=-459.60778395 hartree

0 2

C	0.18255578	-0.29411764	0.00000000
C	1.57021978	-0.28825564	0.00644800
C	2.26875978	-1.50080664	0.01005800

C	1.56979878	-2.71331164	0.00652400
C	0.18235378	-2.70705064	0.00005500
C	-0.53265622	-1.50039664	-0.00128100
H	-0.35721122	0.64608936	-0.00647100
H	2.11690278	0.64762436	0.00553100
H	2.11637978	-3.64925364	0.00568200
H	-0.35783722	-3.64703564	-0.00640000
C	3.73029078	-1.50103264	0.01340800
O	4.45622278	-2.53725864	0.01517700
C	-2.03845122	-1.50107864	0.02421000
H	-2.44495422	-2.37979064	-0.48019800
H	-2.39906022	-1.51982264	1.05828100
H	-2.44589422	-0.60594264	-0.44933200
O	4.45674078	-0.46499464	0.01537500

5_cHex

E=-349.31304417 hartree

0 1

C	0.20283976	-0.35496957	0.00000000
C	-1.29650924	-0.18631957	-0.28136300
C	-1.79808724	1.18198943	0.19020000
C	-0.97629124	2.33495243	-0.43445500
C	0.52115576	2.15584443	-0.14812100
C	1.02307876	0.78443043	-0.62147700
H	-1.48263424	-0.27514357	-1.35799900
H	-1.87401324	-0.98018157	0.20041700
H	0.36721276	-0.36668257	1.08510600
H	0.54673776	-1.32165757	-0.38052000
H	-1.14120924	2.33877443	-1.51907600
H	-1.32640724	3.29934643	-0.05309600
H	1.08791876	2.95740043	-0.63168800
H	0.69240276	2.25154343	0.93147200
H	0.94229276	0.73072343	-1.71475600
H	2.08324376	0.66617043	-0.37678700
H	-1.67935224	1.26090243	1.28292100
C	-3.26584524	1.40351843	-0.07009200
H	-3.65175124	2.38638443	0.27850000
O	-4.00524024	0.61796243	-0.61942900

16_Me

E=-703.33155294 hartree

0 1

C	-0.00012858	0.37522139	-0.00491023
C	-0.87318558	-0.33400561	0.80399677
C	-1.87236158	0.25793939	1.56258777
C	-1.99607458	1.64718439	1.49851977
C	-1.13701258	2.39593339	0.69670077
C	-0.14437458	1.76255239	-0.04922323
H	0.77962942	-0.12810261	-0.55792923
H	-2.53459658	-0.32177061	2.19149677
H	-2.76543458	2.13495339	2.08489777
H	-1.23968458	3.47356739	0.65517677
H	0.52581242	2.34144139	-0.67335823
I	-0.67668358	-2.48731861	0.87726577
O	1.73799842	-2.02355161	0.52345577
C	2.38137942	-1.49839561	1.51042377
C	3.85259042	-1.23887461	1.25756977
C	4.45543042	-1.55733061	0.03665677
C	4.63644842	-0.65942061	2.26009677
C	5.80809142	-1.30339861	-0.17289523
H	3.85141542	-2.00079261	-0.74487923
C	5.98770842	-0.40639761	2.04807477
H	4.16601442	-0.40849061	3.20290377
C	6.59841242	-0.72646161	0.82871177
H	6.25862242	-1.55362561	-1.12829223
H	6.57900442	0.04804739	2.83687877
O	1.88797742	-1.19433761	2.60484877
C	8.07168442	-0.48242361	0.61199577
H	8.42139442	0.38025439	1.18373377
H	8.65899742	-1.34862961	0.93599877
H	8.29729942	-0.31123261	-0.44295623
H	-2.34258858	-2.56068761	0.95962777

11_cHex

E=-348.66089621 hartree

0 2

C	0.08113590	-0.13184584	0.00000000
C	1.57292590	-0.36167084	0.28045600
C	2.41991090	0.77892116	-0.32253500
C	1.95992190	2.16060516	0.17757500
C	0.46533090	2.37119516	-0.10189000
C	-0.38311110	1.24301316	0.50120300
H	1.73959790	-0.39218384	1.36377800
H	1.90099090	-1.32306784	-0.12351300
H	-0.09441710	-0.20144184	-1.08086400

H	-0.50634710	-0.92714784	0.46830600
H	2.14691090	2.22122516	1.25584800
H	2.55918590	2.94372416	-0.29431700
H	0.14950790	3.34080416	0.29539200
H	0.30292590	2.40621516	-1.18650700
H	-0.29860010	1.27450416	1.59491900
H	-1.43983310	1.39462116	0.26099900
H	2.31927990	0.72803916	-1.41550400
C	3.89636390	0.52811316	-0.06067600
O	4.69544190	1.24932616	0.43448400

HI

E=-12.02337662 hartree

0 1

I	0.56795132	0.35496957	0.00000000
H	0.56795132	0.35496957	-1.62077200

PhI

E=-243.13091282 hartree

0 1

C	-0.36511156	0.17241379	0.00000000
C	1.03023244	0.16296579	0.00000300
C	1.71112144	1.37835779	-0.00000400
C	1.03024044	2.59378679	-0.00000200
C	-0.36507256	2.58436879	0.00000400
C	-1.06397256	1.37838479	-0.00000300
H	-0.90059456	-0.76999421	0.00000500
H	1.56887544	-0.77549421	-0.00000100
H	1.56893544	3.53221779	-0.00000400
H	-0.90057756	3.52676379	0.00001000
H	-2.14744356	1.37841779	-0.00000700
I	3.85115444	1.37837979	0.00000000

A-I

E=-808.93048395 hartree

0 2

C	1.76470588	-1.02434076	0.00000000
C	0.86325588	0.21795924	-0.00524800
C	-0.01225012	0.28359124	1.26718800
C	0.86396988	0.21842424	2.53917400
C	1.76546788	-1.02385676	2.53381000

C	2.62767188	-1.09308176	1.26666000
H	1.48353188	1.11921624	-0.06233700
H	0.22359888	0.21912524	-0.89309800
H	1.13682888	-1.92179376	-0.06197700
H	2.39944688	-1.01914376	-0.89150200
H	1.48423188	1.11972324	2.59566600
H	0.22479288	0.21983224	3.42736700
H	2.40073688	-1.01832976	3.42493400
H	1.13762088	-1.92128376	2.59649600
H	3.33522988	-0.25838176	1.26628100
H	3.22417288	-2.01067176	1.26666400
H	-0.71554812	-0.55624576	1.26759200
C	-0.82650712	1.55094624	1.26724400
H	-0.22856712	2.48777224	1.26603900
O	-2.03699912	1.59806324	1.26851900
C	5.49271588	1.31633824	2.47433600
C	4.37821188	2.14198824	2.48054900
C	3.81447288	2.55291424	1.26712900
C	4.37885688	2.14244624	0.05385700
C	5.49337188	1.31679224	0.06036000
C	6.06642288	0.88996524	1.26741700
H	5.92195288	0.98889224	3.41422300
H	3.93302788	2.45954424	3.41609500
H	3.93418788	2.46035124	-0.88181400
H	5.92313088	0.98973324	-0.87942200
C	2.61174088	3.37763624	1.26692400
O	1.99623288	3.76846824	0.23163900
C	7.28727788	0.00927624	1.26765300
H	7.32126788	-0.62441176	0.37950900
H	8.19473088	0.62263524	1.26986300
H	7.31888588	-0.62711876	2.15396100
O	1.99603788	3.76903824	2.30171900

A-TS_1

E=-808.92612327 hartree

0 2

C	-0.02028398	0.57809330	0.00000000
C	1.27134102	0.09160830	0.14959800
C	1.86888502	0.08286930	1.41664000
C	1.16183502	0.56246630	2.52645200
C	-0.12705598	1.04782430	2.36461500
C	-0.73886698	1.06480630	1.10090500
H	-0.47885598	0.58694330	-0.98238400

H	1.82340102	-0.27400970	-0.70797300
H	1.63035602	0.54523230	3.50310200
H	-0.67383198	1.41513030	3.22599700
C	3.23747002	-0.43078970	1.59964700
O	3.97318902	-0.15470470	2.56028600
C	-2.12717398	1.62243730	0.93095800
H	-2.74771798	1.41547830	1.80550300
H	-2.08601998	2.71046730	0.81063400
H	-2.61887898	1.21084330	0.04778200
O	3.72992602	-1.22607270	0.71085900
C	8.51501502	2.12823930	1.97339200
C	8.43502002	0.63263530	1.63473300
C	6.99120302	0.22487030	1.32962500
C	6.38509602	1.07869030	0.19047900
C	6.46572902	2.57041130	0.54391700
C	7.90757102	2.99301430	0.85943400
H	9.05748002	0.41567430	0.75895800
H	8.82798902	0.02825030	2.45703500
H	7.97314402	2.31361530	2.90944500
H	9.55653902	2.41368930	2.15054900
H	6.94749702	0.89055130	-0.73226600
H	5.35044502	0.78126630	0.00306000
H	6.06486202	3.16689930	-0.28128200
H	5.82852702	2.76269430	1.41602700
H	8.51682802	2.89069030	-0.04770400
H	7.93732002	4.04982930	1.14236400
H	6.35612602	0.38018730	2.21230100
C	6.83381502	-1.23728970	0.99202900
H	5.77183002	-1.54550570	0.83366400
O	7.72988702	-2.03840370	0.88165800

A-II

E=-808.95960967 hartree

0 2

C	-0.83164300	-0.25354969	0.00000000
C	-1.69997000	-1.48372269	0.29564700
C	-0.82051500	-2.71921669	0.55272300
C	0.20972600	-2.47723069	1.67326200
C	1.06145700	-1.23811969	1.36477800
C	0.18713500	-0.00058969	1.12012000
H	-2.31560200	-1.30241269	1.18185600
H	-2.38478500	-1.67942769	-0.53379600
H	-0.29746900	-0.40743569	-0.94616800

H	-1.47268300	0.62206531	-0.13777600
H	-0.32971500	-2.32888169	2.61565700
H	0.83642900	-3.36374969	1.79642700
H	1.75681000	-1.05863669	2.19046000
H	1.67111300	-1.43324869	0.47374100
H	-0.34885300	0.24990031	2.04429300
H	0.81398000	0.86161531	0.87347900
H	-0.29203400	-2.96743469	-0.38057100
C	-1.64358000	-3.96973869	0.81533900
O	-1.39063600	-4.90795769	1.48782400
C	-8.46292800	-2.34875169	-0.07071600
C	-7.13531800	-2.75969869	-0.04232900
C	-6.35006000	-2.51799869	1.09112200
C	-6.91815000	-1.86229169	2.18959100
C	-8.24491400	-1.45543069	2.15286200
C	-9.03957900	-1.68912969	1.02207900
H	-9.06310400	-2.54412269	-0.95285900
H	-6.70509300	-3.26997369	-0.89403500
H	-6.30748200	-1.68148269	3.06549100
H	-8.67448700	-0.95133369	3.01188800
C	-4.92758500	-2.93778369	1.17310200
O	-4.21344500	-2.74319369	2.13965300
C	-10.47011400	-1.21675069	0.97383700
H	-10.92661200	-1.22713969	1.96585900
H	-10.51978200	-0.18785269	0.60131700
H	-11.07309200	-1.83642069	0.30708800
O	-4.48735500	-3.55531969	0.06328800
H	-3.53753200	-3.78981469	0.20555600

14_Me

E=-460.28743904 hartree

0 1

C	1.78498985	-0.88227732	-0.01154964
C	0.39515185	-0.86554732	-0.00562764
C	-0.29108115	0.35466268	-0.00193064
C	0.43735585	1.54992568	-0.00540664
C	1.82530685	1.52368568	-0.01138064
C	2.52312685	0.30812768	-0.01226364
H	2.30680885	-1.83313132	-0.01799064
H	-0.15943215	-1.79465032	-0.00707064
H	-0.09843515	2.49107768	-0.00655164
H	2.37853585	2.45660468	-0.01781664
C	-1.77308315	0.43231868	0.00143236

O	-2.41220715	1.46385368	0.00346136
C	4.02984385	0.28353068	0.01388236
H	4.45121685	1.15448468	-0.49243564
H	4.39353385	0.29714268	1.04701936
H	4.42260685	-0.61832232	-0.46001464
O	-2.36764215	-0.78117032	0.00303636
H	-3.32555215	-0.63507332	0.00571736

6_Me

E=-534.50919136 hartree

0 1

C	-0.81135902	-1.04462473	0.00000000
H	-0.35325502	-0.09907973	0.27058200
C	-2.13650902	-1.18218873	0.04233000
H	-2.76682102	-0.36467073	0.36917600
C	-2.82401502	-2.43341773	-0.36149300
C	0.14943698	-2.09164273	-0.47374800
O	0.71073398	-2.03379473	-1.54252800
O	-2.29583302	-3.38961373	-0.88885900
O	-4.13334202	-2.36711373	-0.07354800
O	0.35607398	-3.03351673	0.44925900
C	1.24859898	-4.10629873	0.06687300
H	2.22961698	-3.71007773	-0.19702400
H	1.31548598	-4.75121073	0.93885600
H	0.83047098	-4.64912273	-0.78176600
C	-4.91926902	-3.52796673	-0.42391200
H	-4.55498202	-4.40598173	0.11112500
H	-5.93664502	-3.29107073	-0.12429900
H	-4.86622102	-3.70933973	-1.49823600

III

E=-883.18320765 hartree

0 2

C	-0.14197566	-0.53750361	-0.00517759
H	-0.10195366	-0.96113561	-1.00282959
C	0.22093834	0.72971239	0.19814941
H	0.59160034	1.33542139	-0.61928159
C	0.14359434	1.38266839	1.52910341
C	-0.68913766	-1.45635361	1.04331441
O	-1.83446666	-1.83973061	1.04886141
O	-0.45709166	0.95107639	2.49008541
O	0.84217634	2.52861539	1.53675941

O	0.24886234	-1.83611561	1.91549141
C	-0.19688866	-2.65346161	3.02354241
H	-0.53399866	-3.62599161	2.66379641
H	0.66943534	-2.75304961	3.67094641
H	-1.00848766	-2.14939561	3.54854541
C	0.86325434	3.24797739	2.79218641
H	1.34826934	2.64051339	3.55837541
H	1.43460134	4.15158539	2.59774741
H	-0.15285166	3.49113839	3.10378341
C	4.37612734	0.56949239	0.60856441
C	3.91534134	0.84882739	2.04607741
C	3.04102734	-0.30331761	2.56157641
C	3.75311534	-1.66591961	2.46647841
C	4.20914134	-1.92611361	1.02403641
C	5.09033234	-0.78498761	0.49659641
H	4.78907234	0.95743239	2.69938641
H	3.35730234	1.78672639	2.09073241
H	3.49947734	0.57104839	-0.05154059
H	5.03117734	1.37593239	0.26589241
H	4.62084034	-1.66359961	3.13635541
H	3.08126034	-2.45631161	2.80836041
H	4.74620734	-2.87836061	0.97286841
H	3.32307234	-2.02634161	0.38485741
H	6.02006334	-0.75058361	1.07874241
H	5.37479834	-0.97713061	-0.54249259
H	2.13301234	-0.35873661	1.94967241
C	2.48098434	-0.04047861	3.94734341
O	2.14587834	-0.82395761	4.77075241

TS_NuA

E=-883.17093995 hartree

0 2

C	0.20283976	0.45638945	0.00000000
H	1.02155776	0.42298245	-0.70929600
C	-0.82874124	-0.41508555	-0.18948000
H	-0.66829724	-1.25597855	-0.85337600
C	-2.13215624	-0.46062055	0.48148300
C	0.16866976	1.70413745	0.82297800
O	-0.12012624	1.79966345	1.99281300
O	-2.79927924	-1.47710355	0.56506400
O	-2.54392024	0.72860545	0.95794800
O	0.58397876	2.74427845	0.07346800
C	0.67426576	4.01677445	0.75264300

H	1.40754476	3.95995345	1.55861300
H	0.99243676	4.72828845	-0.00480000
H	-0.29613824	4.29789845	1.16270200
C	-3.78543024	0.72696845	1.68748000
H	-3.71806324	0.06622845	2.55343500
H	-3.93656424	1.75563545	2.00569600
H	-4.60638824	0.39984345	1.04718800
C	5.19223476	-0.75696755	0.44888100
C	3.68228476	-1.03695955	0.45451500
C	3.01356276	-0.32922455	1.65778000
C	3.29312076	1.18326145	1.63885000
C	4.80475976	1.44654245	1.63758100
C	5.49071876	0.74834445	0.45537100
H	3.23560076	-0.66521055	-0.47396800
H	3.49126376	-2.11217555	0.50026900
H	5.64637576	-1.22231455	1.33193400
H	5.64232276	-1.23304255	-0.42706600
H	2.85345076	1.62055045	0.73716800
H	2.81560776	1.66207845	2.49690700
H	4.98532976	2.52460945	1.60200900
H	5.23763076	1.08328345	2.57759400
H	5.13075576	1.19126045	-0.48171500
H	6.57095076	0.91681245	0.49113900
H	3.40327876	-0.76559355	2.58769800
C	1.53985376	-0.65479755	1.64701100
O	0.90866876	-1.44816955	2.23861200

15_Me

E=-883.21036184 hartree

0 2

C	-0.93306288	-0.67951317	0.00000000
H	-0.36941888	-0.76950317	-0.92583000
C	-1.21333788	-2.01069817	0.58530100
H	-1.85362388	-2.07466217	1.45431900
C	-0.67974788	-3.26198317	0.09211800
C	-2.20737688	0.11564083	-0.27575600
O	-3.31098688	-0.16418817	0.11971000
O	-0.88908888	-4.34231217	0.62131600
O	0.07529212	-3.11846517	-1.02295700
O	-1.91073088	1.19900483	-1.00476500
C	-3.01074588	2.09193183	-1.30252700
H	-3.44233088	2.47481583	-0.37724600
H	-2.57722188	2.89830483	-1.88758800

H	-3.77561388	1.56736983	-1.87570200
C	0.65810612	-4.32594217	-1.55128100
H	-0.12301188	-5.03355117	-1.83313800
H	1.22663412	-4.01662717	-2.42463100
H	1.31344412	-4.78661917	-0.81038500
C	3.63564712	-0.65034917	0.37482800
C	2.14598112	-0.93253217	0.61693000
C	1.36063012	0.38954583	0.76265700
C	1.55629912	1.28793183	-0.48115100
C	3.04855412	1.55661183	-0.72057100
C	3.84196212	0.24950683	-0.85105700
H	1.74863412	-1.50914117	-0.22314000
H	2.01478612	-1.54305117	1.51558200
H	4.06040512	-0.16161017	1.26019200
H	4.16990212	-1.59668317	0.24824100
H	1.13244312	0.79638183	-1.36347600
H	1.01265412	2.22733683	-0.34894900
H	3.16934912	2.16835383	-1.61957200
H	3.44759012	2.14144283	0.11721900
H	3.50924312	-0.28534517	-1.74972400
H	4.90596212	0.46560183	-0.98667200
H	1.73748112	0.92746283	1.63910600
C	-0.10515388	0.15514183	1.04833300
O	-0.66272088	0.56388783	2.03933300

B_TS-1

E=-459.59011111 hartree

0 2

C	-1.33874239	-0.43610547	0.00000000
C	-2.73744939	-0.45638247	0.00480200
C	-3.36472839	0.76840753	0.00921000
C	-2.73746039	1.99319853	0.00478100
C	-1.33874939	1.97293553	-0.00001800
C	-0.62568039	0.76841953	-0.00053900
H	-0.80507339	-1.38070847	-0.00582100
H	-3.29259039	-1.38343247	0.00261300
H	-3.29260839	2.92024553	0.00258500
H	-0.80509239	2.91754453	-0.00583700
C	-5.27989939	0.76839853	0.01463500
O	-5.59273839	1.92350353	0.01530100
C	0.88330761	0.76839753	0.02527200
H	1.24867161	0.76797853	1.05738500
H	1.28914761	-0.11717747	-0.46757200

H	1.28925461	1.65429453	-0.46690600
O	-5.59272739	-0.38670847	0.01525900

B-I

E=-459.60381207 hartree

0 2

C	0.56795132	0.09127789	0.00000000
C	-0.82179068	-0.09907111	-0.00535300
C	-1.37757568	-1.38501311	-0.01109100
C	-0.52115268	-2.49363911	-0.00687900
C	0.87236232	-2.33486911	-0.00152000
C	1.34223532	-1.04361011	0.00015800
H	0.99301332	1.08875489	0.00728500
H	-1.47471468	0.76836389	-0.00239000
H	-0.93949768	-3.49554411	-0.00513200
H	1.53377332	-3.19360411	0.00450800
C	-2.87645768	-1.57312711	-0.05019600
H	-3.23489968	-1.62128111	-1.08390000
H	-3.17430968	-2.50098511	0.44292200
H	-3.39463168	-0.74470111	0.43761100
C	4.41904732	-1.40949111	-0.02974500
O	4.60436232	-0.26402311	-0.04227000
O	4.25031632	-2.55803911	-0.01737200

CO₂

E=-188.64384800 hartree

0 1

C	-0.52738337	-1.42989772	-0.01871839
O	-0.52738337	-1.42989772	1.14164161
O	-0.52738337	-1.42989772	-1.17907839

17_Me

E=-270.95635393 hartree

0 2

C	0.22312373	0.43610547	0.00000000
C	1.62575173	0.42102547	-0.01142900
C	2.33815973	-0.78494353	-0.01502100
C	1.62627773	-1.99139253	-0.01141800
C	0.22382173	-2.00719953	-0.00001400
C	-0.40737827	-0.78565153	0.00655400
H	-0.32068127	1.37435847	-0.00029300

H	2.16518573	1.36328947	-0.02016200
H	2.16629973	-2.93333553	-0.02019000
H	-0.31958027	-2.94568553	-0.00028600
C	3.84936573	-0.78511753	0.00545300
H	4.22379173	-0.79777453	1.03453700
H	4.25386373	-1.66428553	-0.50098800
H	4.25395873	0.10586547	-0.47966300

B-II

E=-620.27698041 hartree

0 2

C	0.26369168	-1.14604461	0.00000000
C	0.76781868	-2.41939261	-0.30404200
C	1.32401368	-2.69853361	-1.55815100
C	1.38089568	-1.67729261	-2.51568700
C	0.88449368	-0.39536561	-2.24011500
C	0.34604368	-0.19701561	-0.99037400
H	-0.16898532	-0.94021461	0.97263300
H	0.71908468	-3.20033361	0.44821800
H	1.81171668	-1.88006361	-3.49135400
H	0.92866668	0.38811839	-2.98838300
C	1.81645368	-4.08680161	-1.89109800
H	1.03824968	-4.65733261	-2.40887900
H	2.68861768	-4.05319961	-2.54779000
H	2.08594768	-4.64173761	-0.99033000
C	-2.18356932	-4.10683361	-2.88874600
C	-2.29534932	-2.58104661	-2.76749100
C	-3.45576632	-2.17183761	-1.83282900
C	-3.30020732	-2.84403461	-0.44935400
C	-3.19490132	-4.36963561	-0.58254900
C	-2.04407932	-4.77329261	-1.51376900
H	-1.35849632	-2.18183161	-2.36746500
H	-2.43927532	-2.13150761	-3.75496900
H	-3.07748732	-4.49689061	-3.39121000
H	-1.32833932	-4.36018261	-3.52328300
H	-2.39404832	-2.45905061	0.03306100
H	-4.14626232	-2.57496861	0.19044700
H	-3.05854732	-4.81616861	0.40729600
H	-4.13930232	-4.76172261	-0.98021400
H	-1.09441032	-4.46669161	-1.06123200
H	-2.00872532	-5.86167361	-1.62282500
H	-4.41200632	-2.46925361	-2.27720300
C	-3.47695932	-0.67522361	-1.67311600

H	-2.54436432	-0.24572161	-1.24511900
O	-4.40404832	0.04525239	-1.97143200

B-TS_2

E=-620.27109443 hartree

0 2

C	0.24340771	0.17239902	-0.00225683
C	-1.06066329	-0.31503498	0.14244017
C	-1.82473729	-0.00786798	1.27550117
C	-1.25609129	0.79726902	2.27056117
C	0.04655771	1.29342802	2.14106817
C	0.76097871	0.96840002	1.00308617
H	0.82602371	-0.07845398	-0.88323683
H	-1.48520429	-0.94418598	-0.63445083
H	-1.83368829	1.03828102	3.15818717
H	0.47466171	1.91367002	2.92243217
C	-3.24262529	-0.51246398	1.40839117
H	-3.95006229	0.19142602	0.95694517
H	-3.37239829	-1.47329998	0.90513917
H	-3.52612629	-0.63380998	2.45626817
C	5.06902171	-1.59792598	1.23042217
C	4.15203171	-0.51921198	0.63727717
C	4.36588171	0.83356802	1.35722917
C	5.83591671	1.26847002	1.32633317
C	6.74415271	0.17849702	1.91211717
C	6.54157371	-1.16547298	1.19827117
H	4.37946871	-0.39218598	-0.42811383
H	3.10404271	-0.82224798	0.70996717
H	4.76957771	-1.78974698	2.26840817
H	4.93423171	-2.53560198	0.68284717
H	6.12003071	1.46719202	0.28655917
H	5.95699571	2.20924502	1.87038517
H	7.79037171	0.49191302	1.84363717
H	6.52007871	0.05764702	2.97956117
H	6.86505071	-1.07040798	0.15384417
H	7.17053371	-1.93565998	1.65520617
H	4.03685571	0.70052502	2.39927517
C	3.42784171	1.86430502	0.77748717
H	2.26400971	1.52581702	0.84689017
O	3.72843971	2.91351702	0.27804417

B-III

E=-620.31786874 hartree

0 2

C	-0.56795131	0.03042596	0.00000000
C	-0.75746531	1.54465296	-0.16578000
C	-1.68894131	2.09019896	0.93104600
C	-1.18530931	1.74785896	2.34461600
C	-0.98047031	0.23428896	2.49439500
C	-0.05478431	-0.32266504	1.40350700
H	0.21573269	2.04517196	-0.09469300
H	-1.16917331	1.77852796	-1.15145300
H	-1.53001931	-0.46888204	-0.17065800
H	0.12189069	-0.34255604	-0.76294300
H	-0.23719231	2.27005796	2.51906300
H	-1.89890631	2.11762796	3.08484700
H	-0.57568831	0.01297596	3.48704800
H	-1.95451631	-0.26353504	2.43185400
H	0.95045969	0.09810796	1.53384800
H	0.04066569	-1.40789004	1.50806200
H	-2.67717131	1.63846096	0.78263500
C	-1.95360631	3.57259296	0.75243800
O	-2.01975231	4.42249596	1.57654600
C	-5.32512531	1.87171096	-0.05881500
C	-5.04548631	0.50942696	0.02848700
C	-4.74817931	-0.08849804	1.26052700
C	-4.74362731	0.71804596	2.40374300
C	-5.02151731	2.08283796	2.32127600
C	-5.31261331	2.66533396	1.08924900
H	-5.54774231	2.31540296	-1.02278500
H	-5.05273031	-0.09951904	-0.86987000
H	-4.51195831	0.27564596	3.36688000
H	-5.00321431	2.69087696	3.21869600
H	-5.52153031	3.72663296	1.02235000
C	-4.40965431	-1.55712804	1.33704700
H	-3.40448331	-1.74437504	0.94447600
H	-4.43611031	-1.92119704	2.36584400
H	-5.10484631	-2.15569104	0.74279500

18_Me

E=-271.64670550 hartree

0 1

C	0.85185396	0.45652493	0.00079932
C	2.24625296	0.45401493	-0.01043968
C	2.96518396	-0.74717007	-0.01393368

C	2.24669596	-1.94878407	-0.01044068
C	0.85244196	-1.95190607	0.00080232
C	0.14865696	-0.74778607	0.00716032
H	0.31507996	1.39890293	0.00087332
H	2.78450896	1.39652793	-0.01898368
H	2.78544796	-2.89102807	-0.01903468
H	0.31601396	-2.89448107	0.00088232
H	-0.93546304	-0.74805707	0.01296732
C	4.47518196	-0.74739107	0.00788032
H	4.84876496	-0.76003307	1.03767932
H	4.88111396	-1.62710307	-0.49714968
H	4.88127296	0.14400393	-0.47593668

A-TS_3_R

E=-1343.51764504 hartree

0 2

C	-0.26422763	-0.32520325	0.00000000
H	-0.49825563	-0.66270825	1.00246500
C	0.23499137	1.06642575	-0.01159400
H	0.34647137	1.56617675	-0.96379600
C	0.62124637	1.83233075	1.14651500
C	-1.50422263	-0.48762925	-0.87774300
O	-1.72289063	0.12519075	-1.89133100
O	1.10060237	2.95036675	1.09333800
O	0.41879637	1.18767875	2.34074300
O	-2.29518363	-1.44097225	-0.37041700
C	-3.50433063	-1.74031825	-1.10918700
H	-3.24965863	-2.21419425	-2.05762500
H	-4.06747063	-2.41750725	-0.47321400
H	-4.06994463	-0.82715025	-1.28667600
C	0.90469037	1.88259975	3.51503600
H	0.37505937	2.82707775	3.63968500
H	0.70498937	1.21510075	4.34949000
H	1.97403937	2.06879975	3.42013500
C	2.71292637	-2.79808025	2.43905100
C	2.12354837	-1.70636425	1.53478900
C	1.40212237	-2.33627725	0.32098700
C	0.31087337	-3.33246925	0.77848700
C	0.91287037	-4.41214525	1.68816800
C	1.63552637	-3.79251225	2.89169300
H	1.42034437	-1.10075425	2.11399700
H	2.91186037	-1.03211625	1.18669400
H	3.49735137	-3.33613925	1.89289300

H	3.19224137	-2.33286925	3.30554800
H	-0.47581863	-2.80042625	1.32323000
H	-0.16364163	-3.78777625	-0.09535800
H	0.12094537	-5.08816825	2.02399200
H	1.62263937	-5.01659725	1.11031700
H	0.90403337	-3.26937825	3.52075200
H	2.08150137	-4.57738225	3.50988600
H	2.13917637	-2.87905125	-0.28012100
C	0.83897437	-1.28011025	-0.60429100
O	1.18780637	-1.13698125	-1.74976300
C	-5.66814863	-2.09064225	2.36424900
C	-4.45555863	-1.42746125	2.51134800
C	-4.24463163	-0.20322325	1.86772800
C	-5.26760663	0.34643675	1.08744100
C	-6.47868463	-0.31811025	0.95255500
C	-6.69760163	-1.55102025	1.58225400
H	-5.82001263	-3.04204425	2.86236700
H	-3.66728063	-1.85974925	3.11332200
H	-5.09543863	1.29133675	0.58718600
H	-7.26548163	0.11962375	0.34780500
C	-2.94772963	0.50903875	1.93767100
O	-2.66100863	1.47896275	1.26042300
C	-7.99718163	-2.29127125	1.39661200
H	-8.83439163	-1.60093525	1.27378200
H	-7.95427963	-2.91666625	0.49837800
H	-8.20813863	-2.94693425	2.24367200
O	-2.07746963	-0.03601225	2.80907800
H	-1.23210163	0.45267175	2.72992100

A-TS_3_TS

E=-1343.47217030 hartree

0 2

C	-0.18292682	0.14227642	0.00000000
H	0.04595718	0.35321142	-1.04128000
C	-0.60912982	-1.30108358	0.16971000
H	-0.84154682	-1.55896058	1.19902600
C	0.29064418	-2.32259458	-0.46803700
C	-1.29442582	1.07900942	0.46555500
O	-1.99981282	0.87551742	1.42197700
O	0.81812318	-3.22417058	0.14037200
O	0.43961818	-2.10012358	-1.77837800
O	-1.36242582	2.16133442	-0.31582100
C	-2.35285682	3.15240042	0.05678700

H	-2.14460982	3.52897942	1.05835000
H	-2.25853682	3.94365342	-0.68149900
H	-3.34994882	2.71276642	0.02760700
C	1.32274418	-3.00241458	-2.48795900
H	0.98329418	-4.03103258	-2.36719400
H	1.27072218	-2.69685058	-3.52900400
H	2.33980518	-2.90155358	-2.10753200
C	4.16183418	0.59002542	-1.44374100
C	2.88895218	0.01714642	-0.80516700
C	2.29611518	1.01711042	0.21473800
C	2.01123118	2.38267442	-0.44988500
C	3.28839818	2.94164942	-1.09339900
C	3.89310318	1.95168042	-2.09804200
H	2.15693818	-0.18785058	-1.59237400
H	3.10628818	-0.93410858	-0.30979900
H	4.93375418	0.70155742	-0.67284200
H	4.54908218	-0.11954658	-2.18082800
H	1.23750118	2.27116942	-1.21607100
H	1.62058418	3.08258342	0.29427000
H	3.06223318	3.89312842	-1.58358100
H	4.02322718	3.15592942	-0.30786000
H	3.19648018	1.81721042	-2.93521000
H	4.81827218	2.35771942	-2.51771100
H	3.02461218	1.16424042	1.01874400
C	1.07150718	0.44470742	0.89808800
O	1.02224418	0.20632042	2.07904500
C	-6.14802282	1.36936642	-1.71220300
C	-4.99101182	0.66602242	-1.39631400
C	-5.06283482	-0.46658258	-0.57507300
C	-6.30651082	-0.89446158	-0.09503900
C	-7.45515382	-0.18863158	-0.42139100
C	-7.39660882	0.95580142	-1.23323300
H	-6.08152382	2.25171842	-2.33904000
H	-4.03144382	0.99521942	-1.77318500
H	-6.35354782	-1.77131558	0.53870000
H	-8.41454082	-0.52285558	-0.04117600
C	-3.84035082	-1.23651758	-0.17603700
O	-3.77881882	-1.95267758	0.80477600
C	-8.64816782	1.73040942	-1.55311800
H	-8.91934982	2.37977442	-0.71376000
H	-8.51457082	2.36288042	-2.43243400
H	-9.49316582	1.06087342	-1.73021600
O	-2.86111682	-1.05076758	-1.04891500
H	-1.64639382	-1.38295658	-0.42755300

A-TS_3_P

E=-1343.49663069 hartree

0 2

C	-1.32113815	0.83333332	0.00000000
H	-2.35223815	1.17848032	-0.01236400
C	-0.47626015	1.69853532	0.95202700
H	-0.35664115	2.68626832	0.50404200
C	-1.12947915	1.86827432	2.30367500
C	-0.77766415	0.93536332	-1.41654000
O	0.33111885	1.30597532	-1.71267700
O	-0.66845015	1.50157832	3.35905400
O	-2.31900015	2.48803332	2.18842200
O	-1.69866315	0.53023532	-2.30496300
C	-1.29547115	0.53709532	-3.69438100
H	-0.43989815	-0.12267868	-3.84026500
H	-2.15865215	0.17563032	-4.24665200
H	-1.03610515	1.54997232	-4.00352100
C	-3.05630715	2.69605132	3.41200200
H	-2.48084315	3.31778732	4.09797600
H	-3.97357415	3.19746832	3.11718600
H	-3.27981115	1.73837532	3.88359600
C	-4.57489015	-1.47529268	2.28366100
C	-3.29533115	-0.70569268	1.93284500
C	-2.56412015	-1.37193368	0.74360000
C	-3.49813715	-1.46482168	-0.48337200
C	-4.79312915	-2.20996668	-0.13072000
C	-5.50709415	-1.57408868	1.06991600
H	-3.56300915	0.32236132	1.66937800
H	-2.62883415	-0.65416268	2.79887800
H	-4.30980815	-2.48240768	2.62785000
H	-5.08297215	-0.97828168	3.11567400
H	-3.74322015	-0.45921668	-0.83288900
H	-2.98022515	-1.96544268	-1.30593300
H	-5.45443615	-2.22003768	-1.00279300
H	-4.55684815	-3.25598468	0.10031700
H	-5.83949515	-0.56655568	0.79718000
H	-6.40395615	-2.14726068	1.32356700
H	-2.27091115	-2.38455268	1.04016400
C	-1.26682715	-0.65795268	0.42812300
O	-0.18637815	-1.20019468	0.52354200
H	0.50353885	1.24752032	1.09174400
C	-6.55702315	2.63917132	0.42935700

C	-5.40608715	3.41091932	0.49777000
C	-4.37395415	3.20034032	-0.42340800
C	-4.50913515	2.22495832	-1.41774500
C	-5.66767315	1.46372732	-1.48007600
C	-6.70720015	1.65576832	-0.55966700
H	-7.34946415	2.79386832	1.15263500
H	-5.29813215	4.17124832	1.26206600
H	-3.70340015	2.05572832	-2.12118300
H	-5.76584915	0.70137232	-2.24443500
C	-3.14928915	3.99296132	-0.34752100
O	-2.09619115	3.75903732	-1.00838200
C	-7.96690915	0.83540432	-0.64325700
H	-7.77160615	-0.14955868	-1.07122800
H	-8.42213815	0.70438532	0.34020900
H	-8.70187815	1.33478432	-1.28343900
O	-2.98577315	5.00980432	0.38711600

B-TS_4_R

E=-1154.87208866 hartree

0 2

C	0.12195121	-0.18292683	0.00000000
H	0.25828221	-0.82151083	-0.86881700
C	-0.40221579	1.14435617	-0.39467500
H	-0.48521079	1.91921217	0.35516300
C	-0.84810379	1.50118317	-1.72381900
C	1.46735321	-0.08850883	0.71654100
O	2.04992521	0.93173517	0.98916200
O	-1.31557979	2.59175717	-2.01188300
O	-0.69065479	0.50411417	-2.62872000
O	1.90507921	-1.31734083	1.01139000
C	3.16762521	-1.39947083	1.71030200
H	3.08794821	-0.91321483	2.68319300
H	3.36544521	-2.46167083	1.82415200
H	3.95118021	-0.92699283	1.11937300
C	-1.12801479	0.79153417	-3.97061500
H	-0.57467479	1.63913017	-4.37735700
H	-0.92081679	-0.10894283	-4.54350700
H	-2.19564779	1.01577217	-3.98273400
C	-3.33975479	-2.90827583	-1.21034100
C	-2.53580279	-1.68902883	-0.73797300
C	-1.67168579	-2.04792783	0.49226300
C	-0.73942079	-3.24199383	0.18162100
C	-1.55035979	-4.45130483	-0.30293200

C	-2.41987679	-4.09734283	-1.51644600
H	-1.89309579	-1.34579383	-1.55365000
H	-3.20798879	-0.86187083	-0.48996500
H	-4.05704579	-3.19430183	-0.43131300
H	-3.92367079	-2.63898283	-2.09559400
H	-0.01945079	-2.95668183	-0.59124500
H	-0.15873579	-3.49908383	1.07136600
H	-0.86974379	-5.27199783	-0.54775400
H	-2.19321079	-4.80533883	0.51226800
H	-1.77074979	-3.83917983	-2.36253200
H	-3.01110479	-4.96503183	-1.82419000
H	-2.33427179	-2.32783483	1.31815000
C	-0.89396979	-0.85181683	0.99315800
O	-1.02765779	-0.38473183	2.10020900
C	4.21314821	-1.82833183	-1.60211800
C	3.53657321	-3.03096283	-1.78322600
C	2.27545021	-3.06472383	-2.39373200
C	1.71096421	-1.85636083	-2.81200200
C	2.38440021	-0.64697183	-2.62924700
C	3.63767621	-0.62812683	-2.02355000
H	5.18684021	-1.82469183	-1.12482900
H	3.98866621	-3.95828083	-1.44565900
H	0.72815421	-1.85369983	-3.27126400
H	1.91329321	0.27631417	-2.94387700
H	4.15807021	0.31063717	-1.87253200
C	1.55566821	-4.37755783	-2.58485200
H	1.42082121	-4.89407383	-1.63020200
H	0.57063821	-4.23290383	-3.03160200
H	2.12640521	-5.04664983	-3.23585300

B-TS_4_TS

E=-1154.82621021 hartree

0 2

C	1.70717069	-0.08130081	0.02234809
H	1.76203869	-0.04159881	-1.06319191
C	0.89223069	-1.28693681	0.47150609
H	0.75690169	-1.32651581	1.54883709
C	1.30086569	-2.61935881	-0.05225291
C	1.00615769	1.18109419	0.51670509
O	0.75157469	1.40162319	1.67756209
O	0.99970769	-3.67640881	0.45811609
O	2.01051469	-2.51884281	-1.19402891
O	0.67839469	1.99065419	-0.49542491

C	-0.04773331	3.19195819	-0.14222891
H	0.52674969	3.78432519	0.57005309
H	-0.18150831	3.73190319	-1.07552791
H	-1.01311231	2.92511119	0.28904209
C	2.44135269	-3.75957481	-1.79189291
H	1.57806969	-4.36807781	-2.06411891
H	3.00456069	-3.47486981	-2.67684591
H	3.07341069	-4.31382281	-1.09712091
C	5.84030069	0.14246619	-2.14332891
C	4.64401169	-0.43361081	-1.37394791
C	4.26840569	0.48309619	-0.18199791
C	3.97978569	1.91778019	-0.66831691
C	5.18555969	2.48338319	-1.43151191
C	5.57288369	1.57977419	-2.61003191
H	3.78579369	-0.53041581	-2.04700491
H	4.87151669	-1.43838981	-1.00725291
H	6.72408369	0.13114119	-1.49356591
H	6.06827069	-0.50058281	-2.99894691
H	3.10712869	1.91940119	-1.32835391
H	3.73518369	2.55936819	0.18420409
H	4.95618869	3.49329219	-1.78441291
H	6.03781769	2.57241619	-0.74653791
H	4.75511669	1.57432519	-3.34194691
H	6.45305969	1.98092919	-3.12163391
H	5.12152869	0.50719119	0.50473909
C	3.13825969	-0.13994781	0.61207209
O	3.33190469	-0.70884481	1.66468509
C	-1.86598731	-0.91635681	-1.78850191
C	-3.04714731	-0.37398781	-2.30724291
C	-3.87178731	0.44472319	-1.52492691
C	-3.49304731	0.71926319	-0.20441391
C	-2.31743931	0.18586219	0.33508909
C	-1.54806231	-0.62144181	-0.47850591
H	-1.22493231	-1.53887981	-2.40336991
H	-3.32376131	-0.58694781	-3.33518491
H	-4.11713731	1.36051819	0.41018009
H	-2.01864631	0.41575219	1.35181309
H	-0.25906831	-1.10264381	0.04243409
C	-5.15809631	1.00217919	-2.08685991
H	-5.40981031	1.96127119	-1.62900391
H	-5.09207231	1.14433419	-3.16764391
H	-5.99221131	0.31868519	-1.89588691

B-TS_4_P

E=-1154.84246999 hartree

0 2

C	0.42682925	-0.10162601	0.00000000
H	0.60514925	0.45993299	0.91832000
C	-0.36086975	-1.38818001	0.31117300
H	0.23145625	-2.00015801	0.99103100
C	-1.70407975	-1.08736301	0.93511200
C	1.79676725	-0.46145401	-0.56184800
O	2.23130925	-1.58112101	-0.68055300
O	-2.75524775	-1.05695401	0.33582800
O	-1.58973275	-0.81917901	2.24566600
O	2.46666625	0.64510099	-0.90891800
C	3.79769725	0.45339999	-1.43718500
H	3.75923925	-0.14609601	-2.34701500
H	4.17070125	1.45176499	-1.64895600
H	4.42617025	-0.04270701	-0.69703500
C	-2.80696175	-0.46080701	2.93600700
H	-3.54589575	-1.25647901	2.83954100
H	-2.52224375	-0.32609601	3.97632300
H	-3.21185375	0.46608099	2.52809200
C	-2.02022875	3.65692899	0.94916100
C	-1.63196175	2.21835599	0.58352300
C	-0.69914275	2.19124399	-0.64979200
C	0.55003225	3.06884999	-0.40883900
C	0.15309225	4.50178199	-0.03180600
C	-0.78126675	4.53003699	1.18454400
H	-1.12554975	1.75899599	1.43965300
H	-2.52558375	1.62259999	0.38140000
H	-2.61780475	4.08649199	0.13580600
H	-2.65678775	3.64755899	1.83918300
H	1.14899525	2.63286099	0.39406800
H	1.18007425	3.06601699	-1.30139100
H	1.05542625	5.08825899	0.16692700
H	-0.35006875	4.97408699	-0.88459600
H	-0.24174075	4.15694699	2.06385600
H	-1.07905975	5.55839499	1.41032700
H	-1.24787575	2.58992099	-1.50962400
C	-0.32377375	0.77476599	-1.03244400
O	-0.60261575	0.29532099	-2.11171700
H	-0.53184675	-1.93438001	-0.61496100
C	2.98080925	-0.55430701	2.56708600
C	3.37926525	0.74997499	2.24385300
C	2.61597825	1.85931799	2.63052200

C	1.43202725	1.64814199	3.34785000
C	1.00767625	0.35343099	3.68395200
C	1.80991925	-0.68419001	3.27665700
H	3.57160925	-1.40703601	2.25281800
H	4.29344725	0.90040399	1.67866100
H	0.82444025	2.49681599	3.64517500
H	0.07933325	0.19634199	4.21865800
C	3.07908925	3.25534899	2.28691600
H	3.45537625	3.30419999	1.26216900
H	2.27065125	3.98166699	2.38667800
H	3.89185225	3.56921799	2.94942200

C-TS_R

E=-1232.53572187 hartree

0 2

C	-0.89430890	-0.52840999	-0.00691727
H	-0.66581990	-0.16545299	0.99106273
C	-1.43892190	0.55141401	-0.86104727
H	-1.84111590	0.29508301	-1.83129627
C	-1.48869490	1.94985301	-0.49350527
C	-1.85066890	-1.71341299	0.09601273
O	-2.66872290	-2.02046599	-0.73526827
O	-1.98753790	2.81524701	-1.19569027
O	-0.94630690	2.20049701	0.72143673
O	-1.62697290	-2.38568799	1.23138773
C	-2.40346090	-3.59344199	1.43082073
H	-2.26263690	-4.27203899	0.58978873
H	-2.02294390	-4.03014599	2.34979973
H	-3.45983290	-3.34583999	1.53286973
C	-0.98947190	3.57210101	1.17331673
H	-2.02248290	3.86076201	1.36955073
H	-0.40789190	3.58967201	2.09177573
H	-0.54815390	4.23200901	0.42603173
C	3.39112810	0.81261801	0.94407973
C	2.03931310	0.63010201	0.23945073
C	1.72645510	-0.87109199	0.04890673
C	1.75151010	-1.61940299	1.40197573
C	3.10392410	-1.42164199	2.10074373
C	3.42925810	0.06671201	2.28456173
H	1.25368710	1.10127701	0.83664973
H	2.04527010	1.13298401	-0.73233527
H	4.19157710	0.43560001	0.29579273
H	3.58161910	1.87936201	1.09492073

H	0.95241310	-1.24355599	2.04928073
H	1.55484310	-2.68297199	1.24061973
H	3.09249110	-1.93304799	3.06783273
H	3.89143610	-1.89418299	1.50101373
H	2.69493010	0.51416901	2.96641373
H	4.41041410	0.18352901	2.75446373
H	2.49091710	-1.30811799	-0.60229827
C	0.42108910	-1.09044899	-0.68198727
O	0.33766710	-1.65997499	-1.74225427
C	-6.21893390	-0.50993499	-0.39757627
C	-5.15050690	0.52435201	-0.01851227
C	-5.13847090	0.76906101	1.51274573
C	-4.92988690	-0.55335699	2.27437473
C	-5.98374290	-1.59770899	1.87934073
C	-6.01749090	-1.82850999	0.36190773
H	-4.16898790	0.15617801	-0.33774727
H	-5.32422990	1.47076401	-0.53847627
H	-7.21094090	-0.10172899	-0.16750627
H	-6.18948490	-0.68551199	-1.47729827
H	-3.92687990	-0.93867799	2.05254473
H	-4.96317990	-0.37217199	3.35315373
H	-5.78626590	-2.53776399	2.40436273
H	-6.96933090	-1.25254599	2.21528273
H	-5.07286890	-2.27870599	0.03893873
H	-6.81361790	-2.53524499	0.10820373
H	-6.09424190	1.22221801	1.79791273
C	-4.05643190	1.76582701	1.82532073
H	-3.02909590	1.34887601	1.87700873
O	-4.23620490	2.95561701	1.97359573

C-TS_TS

E=-1232.51740956 hartree

0 2

C	1.93089422	-0.08130081	0.00000000
H	1.45195122	-0.39350381	0.92603700
C	3.07400922	-1.00677681	-0.35352300
H	3.52821922	-0.80456381	-1.31785100
C	2.98210022	-2.44321581	-0.07077600
C	2.40828722	1.35757619	0.16724500
O	3.48164922	1.78403219	-0.18608300
O	3.56964822	-3.31043081	-0.69336000
O	2.25307822	-2.70657381	1.03976500
O	1.45307222	2.10471819	0.73404700

C	1.75713322	3.50877519	0.90847300
H	1.95184422	3.97355619	-0.05848400
H	0.87395422	3.93978819	1.37190500
H	2.62788922	3.62547619	1.55424000
C	2.15659822	-4.09265981	1.42262100
H	3.14741122	-4.50197181	1.62374700
H	1.54829622	-4.10437081	2.32369400
H	1.67828222	-4.67263081	0.63181600
C	-2.04354278	-2.45529281	-0.31853300
C	-0.59020078	-2.00592881	-0.52211200
C	-0.52938678	-0.50513481	-0.89034900
C	-1.22373978	0.35067619	0.19205600
C	-2.67401678	-0.10916181	0.39554600
C	-2.74865078	-1.60180181	0.74411600
H	-0.02498178	-2.18035081	0.39722600
H	-0.11360978	-2.60073381	-1.30766400
H	-2.58496378	-2.37249881	-1.26902500
H	-2.06253778	-3.51175881	-0.03398200
H	-0.67989778	0.26314719	1.13836400
H	-1.19035778	1.40581019	-0.09091600
H	-3.14080878	0.49033119	1.18300300
H	-3.24321578	0.07717119	-0.52364300
H	-2.26714278	-1.76845881	1.71617000
H	-3.79202278	-1.91432581	0.84972000
H	-1.05772178	-0.36122481	-1.83912600
C	0.89192922	-0.06200481	-1.16516600
O	1.25933622	0.29161819	-2.26519100
C	8.07348922	-2.05241481	0.07032800
C	6.66003722	-1.86230881	0.63739600
C	6.39655722	-0.37351181	0.95796000
C	6.62000522	0.51043719	-0.28969900
C	8.03316322	0.30437519	-0.85097000
C	8.30460422	-1.17282281	-1.16547800
H	5.92258822	-2.21121381	-0.09388500
H	6.52558922	-2.46544981	1.53996500
H	8.81033122	-1.79630181	0.84144800
H	8.22638722	-3.10725081	-0.17612400
H	5.87784022	0.24799119	-1.05041700
H	6.45200322	1.55945319	-0.03466400
H	8.15877222	0.91626019	-1.74917300
H	8.76836222	0.66068119	-0.11896700
H	7.63378322	-1.49903481	-1.97024800
H	9.32711422	-1.29941381	-1.53357400
H	7.05874922	-0.04385181	1.76766900

C	4.98124422	-0.20650781	1.44877400
H	4.08931622	-0.63170881	0.54069800
O	4.58328722	0.22674219	2.48290100

C-TS_P

E=-1232.54715394 hartree

0 2

C	1.62601618	-0.52845528	0.00000000
H	1.91670818	0.34162372	0.58279600
C	2.84123118	-1.43091228	-0.24925200
H	3.60343118	-0.88792128	-0.81585400
C	3.52567418	-1.94245728	1.00105700
C	1.09557718	-0.04133528	-1.34210900
O	0.57644218	-0.75059328	-2.17044600
O	4.35011118	-2.82485728	1.00112400
O	3.12880118	-1.28795528	2.10288700
O	1.30244018	1.27391372	-1.49703100
C	0.85198918	1.85321772	-2.74399400
H	-0.22943482	1.74653172	-2.83441100
H	1.13177718	2.90178872	-2.69153800
H	1.34222218	1.36345872	-3.58538500
C	3.80058118	-1.62666828	3.33390400
H	4.85624218	-1.36806128	3.25299100
H	3.31657318	-1.02796828	4.10124600
H	3.68936818	-2.68998528	3.54657800
C	-0.78878782	0.79561472	3.74455400
C	0.20837418	0.02727472	2.86773700
C	-0.47326182	-0.48946528	1.57621000
C	-1.12872982	0.67371072	0.80179400
C	-2.12496582	1.43075472	1.69067400
C	-1.45223982	1.94299872	2.97132100
H	1.03945718	0.68801572	2.60475800
H	0.63868718	-0.81316528	3.41795800
H	-1.56174382	0.10428372	4.10200300
H	-0.27356382	1.18000772	4.63025200
H	-0.36113582	1.37469872	0.46077300
H	-1.62985082	0.29014272	-0.09219500
H	-2.55874582	2.26277972	1.12805400
H	-2.95223782	0.76164172	1.95731500
H	-0.69077482	2.68673972	2.70522900
H	-2.18397882	2.45267072	3.60529900
H	-1.25323882	-1.20093428	1.86725000
C	0.51067018	-1.29207228	0.74659900

O	0.45781418	-2.50122428	0.67946800
H	2.54999718	-2.29830028	-0.84070300
C	2.96474518	3.94962372	0.23952200
C	4.01459318	2.86004272	-0.01754100
C	4.75878018	2.50138572	1.29207000
C	3.78600818	2.10190372	2.41692900
C	2.72678918	3.18909472	2.64431000
C	1.98646018	3.53725472	1.34638500
H	3.51401418	1.96899672	-0.40824200
H	4.73231218	3.18533072	-0.77526200
H	3.47078618	4.87933072	0.52739700
H	2.42331218	4.15517372	-0.68844500
H	3.30863318	1.15737072	2.14515300
H	4.34475818	1.91174772	3.33764400
H	2.01906918	2.85669772	3.41053200
H	3.21155618	4.09182272	3.03565700
H	1.41653818	2.66651572	1.00448900
H	1.25935018	4.33454272	1.52745100
H	5.34478918	3.37705472	1.59390800
C	5.75736518	1.40010772	0.97763200
O	5.70666818	0.24967972	1.26067000

Decar_TS

E=-348.63695327 hartree

0 2

C	-0.30557786	1.34055972	0.04468047
C	-1.85219186	1.24047572	0.09972747
C	-2.40807086	2.44014872	0.81087947
C	-2.01216186	3.76976072	0.24108347
C	-0.46566886	3.87098172	0.17812447
C	0.13504714	2.67488772	-0.57378053
H	-2.22755186	1.21535572	-0.93180753
H	-2.16028486	0.31061572	0.58446147
H	0.09628714	1.25896972	1.06146247
H	0.09528014	0.49777372	-0.52744353
H	-2.40552886	3.86202872	-0.77960653
H	-2.42518386	4.59482772	0.82729747
H	-0.18101086	4.81243172	-0.30255453
H	-0.06555286	3.89796872	1.19843447
H	-0.18851086	2.70929772	-1.62191253
H	1.22737614	2.74453572	-0.57770553
H	-2.49556286	2.37168972	1.89171347
C	-4.60579486	2.28710872	0.34198747

O	-4.84153386	2.75014272	-0.67808753
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Decar_R

E=-235.28911662 hartree

0 2

C	-0.79268289	-1.56504063	0.00000000
C	-0.77317589	-0.07552463	0.40457600
C	-2.05939989	0.61025737	0.07197900
C	-3.34568089	-0.07540963	0.40458100
C	-3.32632089	-1.56492463	-0.00000700
C	-2.05953789	-2.26371263	0.51315800
H	-0.60099989	-0.02553963	1.49627500
H	0.07582511	0.43782037	-0.05734500
H	-0.76191789	-1.63849163	-1.09384700
H	0.10307311	-2.06657463	0.37992800
H	-3.51784689	-0.02540563	1.49628200
H	-4.19463689	0.43801637	-0.05733200
H	-4.22212689	-2.06636763	0.37992100
H	-3.35708789	-1.63837763	-1.09385400
H	-2.05954489	-2.25147163	1.61133000
H	-2.05958789	-3.31558863	0.20962000
H	-2.05935289	1.66877037	-0.16573800

CO

E=-113.34694499 hartree

0 1

C	-0.02032520	0.32520325	0.00000000
O	-0.02032520	0.32520325	1.12676200

6_cHexen

E=-308.76588543 hartree

0 1

C	-0.75203249	-0.06097038	-0.00079815
C	-2.09137949	-0.09693738	-0.08139215
C	-2.84849949	-1.36019638	-0.00873215
C	-2.03854349	-2.62111738	0.24526285
C	-0.63563749	-2.54533538	-0.36929715
C	0.10393851	-1.28960338	0.10709085
H	-1.95956749	-2.72696238	1.33596885
H	-2.60861949	-3.47679438	-0.12163215
H	-0.06413049	-3.44285438	-0.12173615

H	-0.72450849	-2.51090638	-1.46059815
H	0.41231351	-1.40342238	1.15649685
H	1.02866851	-1.14287838	-0.45891315
O	-4.06776249	-1.38247938	-0.10407015
H	-2.68169049	0.80856762	-0.17620515
H	-0.24480349	0.90015162	-0.00669415

D-I

E=-657.43495870 hartree

0 2

C	-0.93495931	0.34549884	-0.00452283
C	-0.38088731	1.14282084	0.92213317
C	-0.64185431	2.59291384	0.96469117
C	-1.69123631	3.11773484	0.00217217
C	-1.66953931	2.35557484	-1.32908983
C	-1.82586631	0.84699684	-1.10314483
H	-2.66657831	2.98672284	0.49031217
H	-1.53154331	4.18905284	-0.13054883
H	-2.45541331	2.72629884	-1.99105183
H	-0.71133731	2.54635484	-1.82434483
H	-2.86542531	0.60449584	-0.83897983
H	-1.61774631	0.29171484	-2.02277683
O	-0.05393731	3.32440984	1.75117217
H	0.28198669	0.75170984	1.68675417
H	-0.73760431	-0.72263516	0.02794817
C	3.33747069	0.33290384	-0.53375583
C	2.59505869	1.48306584	-1.22684383
C	2.65383169	2.75788984	-0.36339683
C	4.10182669	3.15856684	-0.02809183
C	4.83523269	1.99684384	0.65718017
C	4.78373469	0.71884084	-0.19206083
H	3.06044969	1.68841284	-2.19825083
H	1.55440169	1.21025484	-1.41512483
H	2.80349869	0.07120684	0.38843417
H	3.32019869	-0.55515416	-1.17262883
H	4.61823069	3.42666584	-0.95705283
H	4.10177269	4.04857784	0.60648417
H	5.87321969	2.28135184	0.85587717
H	4.36852469	1.80284784	1.63111617
H	5.34098869	0.88322584	-1.12313183
H	5.28002369	-0.10339116	0.33247717
H	2.10643569	2.56439784	0.56823117
C	1.86978069	3.88432384	-1.01250983

O	2.17794769	5.01737484	-1.16724183
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D-TS_1

E=-657.42571608 hartree

0 2

C	-1.58522992	-0.08130081	0.02075180
C	-0.43883492	-0.65587481	-0.47069520
C	0.67274008	0.11939019	-0.98848020
C	0.60428408	1.63460619	-0.82854320
C	-0.82767792	2.18026919	-0.77144520
C	-1.66494092	1.41004019	0.25514480
H	1.12748708	1.87049519	0.10806980
H	1.18370108	2.08717619	-1.63643820
H	-0.81695092	3.24609319	-0.52983720
H	-1.29088892	2.07967519	-1.75793320
H	-1.28924992	1.61315219	1.26797580
H	-2.70276092	1.75099919	0.24540080
O	1.66609908	-0.41439281	-1.48846620
H	-0.34452092	-1.73453381	-0.54232320
H	-2.28502692	-0.70820481	0.56193880
C	-6.44817692	-0.43784381	-0.01485420
C	-4.92060192	-0.51301181	-0.14993520
C	-4.48901992	-0.13498581	-1.57169520
C	-5.00530792	1.27039919	-1.97123120
C	-6.53077292	1.34144119	-1.81572020
C	-6.97481192	0.95163819	-0.39952820
H	-4.46445692	0.17877819	0.56558980
H	-4.56440292	-1.51700681	0.09619080
H	-6.90631692	-1.19317581	-0.66531820
H	-6.73769292	-0.68609581	1.01011880
H	-4.53531492	2.02231319	-1.32797820
H	-4.70944292	1.49078419	-2.99967520
H	-6.87122892	2.35218019	-2.05967020
H	-6.99636792	0.66467219	-2.54231520
H	-6.59255092	1.69184019	0.31461680
H	-8.06611192	0.97600919	-0.32758420
H	-4.89903692	-0.86501781	-2.28364720
C	-2.99039292	-0.17284281	-1.81742120
O	-2.42065792	-0.20411581	-2.84808820

15_cHexen

E=-657.46232788 hartree

0 2

C	0.22357723	-0.97560974	0.00000000
C	-0.27677477	0.42833726	0.03472000
C	-1.56192677	0.84639126	-0.45083200
C	-2.51865377	-0.20720574	-0.98323400
C	-1.81577177	-1.49706274	-1.42164100
C	-0.87251977	-2.00145874	-0.32409600
H	-3.22802677	-0.42479074	-0.17429100
H	-3.09641977	0.24412426	-1.79328300
H	-2.55934677	-2.26183374	-1.66003800
H	-1.23803177	-1.31575974	-2.33189100
H	-1.44536877	-2.19692374	0.58826000
H	-0.40479077	-2.94091874	-0.62440600
O	-1.88841877	2.04300026	-0.40545800
H	0.36405923	1.21663126	0.41549300
C	5.03326823	-0.82028174	0.29566600
C	3.68844023	-1.43838874	-0.10822300
C	2.69968923	-0.34726674	-0.58985200
C	3.30940123	0.47390426	-1.74007300
C	4.65820423	1.08169826	-1.33419200
C	5.63718923	0.00355926	-0.84960400
H	3.83894423	-2.15158474	-0.92637300
H	3.25696323	-1.99410374	0.73041100
H	4.88478423	-0.17380174	1.16956300
H	5.72318323	-1.61263874	0.60187600
H	3.44084023	-0.18658774	-2.60316500
H	2.61101823	1.26083026	-2.04210900
H	5.08419823	1.63133426	-2.17913300
H	4.49862523	1.81221026	-0.53098600
H	5.87761223	-0.66580074	-1.68536900
H	6.57806823	0.46191926	-0.52992800
H	2.49703123	0.31672826	0.25730800
C	1.40914223	-1.02751274	-1.00984600
O	1.30902023	-1.62065574	-2.06003500
H	0.68794323	-1.19775874	0.97188100

D-II

E=-1006.78704748 hartree

0 2

C	1.44308936	0.46747967	0.00000000
C	2.26530736	-0.38209133	-0.90485700
C	3.13335436	0.13134367	-1.92574800
C	3.30396136	1.63293767	-2.05566800

C	2.16801536	2.43725667	-1.41199800
C	1.88914936	1.93551267	0.00941700
H	4.25140536	1.86765267	-1.55548200
H	3.43296736	1.86847667	-3.11469800
H	2.43244236	3.49760167	-1.39288700
H	1.25701336	2.34704767	-2.01121500
H	2.80004136	2.01311567	0.60891700
H	1.11569536	2.54059367	0.48487400
O	3.77100736	-0.64986433	-2.65262100
H	2.20486036	-1.46260533	-0.83260000
C	-2.60251964	-2.56629333	0.25678600
C	-1.99247864	-1.16116733	0.34157200
C	-0.63704464	-1.09926833	-0.38768500
C	-0.78913364	-1.55776633	-1.85919700
C	-1.39929964	-2.96319333	-1.93628700
C	-2.74348564	-3.03087833	-1.19913400
H	-2.66663464	-0.43217233	-0.11897300
H	-1.86396164	-0.86350433	1.38696300
H	-1.96224964	-3.27190433	0.80119100
H	-3.57640064	-2.57562333	0.75571800
H	-1.43818964	-0.84104733	-2.37483200
H	0.18009436	-1.53512533	-2.36676400
H	-1.52282164	-3.25149333	-2.98466400
H	-0.70222064	-3.68317933	-1.48969800
H	-3.46747664	-2.38642933	-1.71370800
H	-3.14348464	-4.04884033	-1.23521700
H	0.06473136	-1.77518133	0.11323300
C	-0.06701864	0.30827367	-0.36798400
O	-0.74445164	1.27514367	-0.63055800
H	1.49684936	0.03886067	1.01241300
C	7.55311836	-1.41025133	-2.04510900
C	6.76883936	-0.42839633	-1.16470500
C	5.90057136	-1.17569333	-0.14820600
C	6.73288036	-2.15890333	0.70757700
C	7.51158836	-3.13340333	-0.18697900
C	8.38692236	-2.38505733	-1.20214500
H	7.46366936	0.22601467	-0.62535700
H	6.13759436	0.21253667	-1.78332400
H	6.84505636	-1.97885033	-2.66108800
H	8.19799336	-0.85800733	-2.73574100
H	7.43880236	-1.58643633	1.32206900
H	6.08096036	-2.70784433	1.39465500
H	8.12531636	-3.79444933	0.43270600
H	6.79883836	-3.77141833	-0.72455700

H	9.16077436	-1.82353233	-0.66295900
H	8.90709336	-3.09838633	-1.84911500
H	5.14947036	-1.76922033	-0.69204600
C	5.10446036	-0.26357033	0.74573600
H	4.47269136	-0.78600433	1.49556300
O	5.11383536	0.94828967	0.69899400

D-TS_2

E=-1006.76411295 hartree

0 2

C	-0.28455283	0.75203251	0.00000000
C	0.91416917	1.18854951	-0.82806800
C	1.36981817	2.58242451	-0.75979100
C	1.20563717	3.29986651	0.56974800
C	-0.06778683	2.92408051	1.34031100
C	-0.25283383	1.40486051	1.40535200
H	2.08680217	3.01853951	1.16488800
H	1.27745617	4.37427851	0.38908700
H	-0.01904083	3.33146651	2.35404500
H	-0.93158583	3.37905551	0.85097900
H	0.57949917	0.95234051	1.95407300
H	-1.16527683	1.15751751	1.95329800
O	1.97695217	3.10878551	-1.69226300
H	0.95769317	0.78186051	-1.83806500
C	-4.19871583	-1.55492249	0.34069000
C	-3.15110183	-0.44329349	0.49423700
C	-2.63409183	0.02867051	-0.88809700
C	-3.79677683	0.46069851	-1.79008500
C	-4.83894783	-0.65567949	-1.93604300
C	-5.35592083	-1.12131049	-0.56828400
H	-3.60002083	0.41303351	1.01218000
H	-2.32454283	-0.79679849	1.11564300
H	-3.71573383	-2.44275349	-0.08663300
H	-4.57443683	-1.84295049	1.32739300
H	-4.26573783	1.34998551	-1.35454900
H	-3.41206183	0.76117051	-2.76845200
H	-5.66946583	-0.30942149	-2.55902800
H	-4.38621183	-1.50762849	-2.45949100
H	-5.89951383	-0.29676149	-0.08942700
H	-6.06927283	-1.94243749	-0.68961400
H	-2.11911383	-0.82805549	-1.34861000
C	-1.58135683	1.11496251	-0.73977000
O	-1.74197183	2.23626451	-1.18493900

H	-0.25413283	-0.33475949	0.12257400
C	5.93819517	0.67255451	-1.73368700
C	4.69482517	0.85611251	-0.85208800
C	4.09430517	-0.51914149	-0.47435600
C	5.12892517	-1.43780549	0.19279400
C	6.36730417	-1.60019349	-0.69944900
C	6.97662017	-0.24037149	-1.06761300
H	4.97394117	1.38342151	0.06793000
H	3.94957517	1.47006351	-1.36327700
H	5.63374817	0.23632151	-2.69326600
H	6.37462317	1.65104651	-1.95466500
H	5.41955817	-0.99678449	1.15305100
H	4.67696517	-2.40863149	0.41251200
H	7.10722317	-2.22526949	-0.19047700
H	6.08337817	-2.13018549	-1.61727600
H	7.35099717	0.24481951	-0.15729300
H	7.83688217	-0.37833849	-1.72952500
H	3.72435917	-0.98160549	-1.40134300
C	2.86224217	-0.32062549	0.37256300
H	1.94888617	0.49573351	-0.23146300
O	2.60889417	-0.76434049	1.44806000

D-III

E=-1006.78772140 hartree

0 2

C	0.10162601	-0.77235771	0.00000000
C	-0.57961099	0.16064829	-1.02482800
C	-2.04119499	-0.16739471	-1.26502600
C	-2.87524199	-0.37657871	-0.01558900
C	-2.19585899	-1.29748571	1.01451600
C	-0.74991799	-0.87005771	1.28896300
H	-3.01127199	0.61849229	0.42978900
H	-3.85940699	-0.74470171	-0.31060500
H	-2.76614099	-1.28476371	1.94721900
H	-2.21285899	-2.32319771	0.63990500
H	-0.73678299	0.12003229	1.75710500
H	-0.28288099	-1.56023271	1.99626200
O	-2.52126799	-0.18970871	-2.38189500
H	-0.53723499	1.17636829	-0.61439000
C	3.56787001	-3.51237371	1.06006200
C	2.13491201	-2.97034771	0.96309800
C	1.73286701	-2.73307171	-0.51380300
C	1.90628601	-4.01144971	-1.34078200

C	3.34107901	-4.54601571	-1.24000300
C	3.74951901	-4.78332071	0.22020200
H	1.43819501	-3.69331571	1.40388400
H	2.04568701	-2.04922371	1.54465700
H	4.26511901	-2.74271971	0.70642200
H	3.81668601	-3.70641771	2.10782700
H	1.20151001	-4.76625971	-0.97471500
H	1.63860601	-3.81546271	-2.38259400
H	3.43534701	-5.47147271	-1.81631300
H	4.02888101	-3.82047571	-1.69319300
H	3.12852301	-5.58398571	0.64182700
H	4.78751001	-5.12589271	0.27457800
H	2.40818601	-1.96107971	-0.91109600
C	0.33634901	-2.14622871	-0.61949600
O	-0.57200899	-2.72905371	-1.18508300
H	1.06543501	-0.33814271	0.26508900
H	-0.05837699	0.16529929	-1.98389000
C	5.28158001	0.17057129	-0.28297100
C	4.13877101	0.48848729	0.69102000
C	3.46691501	1.83234829	0.32184100
C	2.98554501	1.84851129	-1.14103600
C	4.14114601	1.52298029	-2.09726700
C	4.80552101	0.18587829	-1.74179100
H	3.39093601	-0.30957171	0.64269500
H	4.50306701	0.52159729	1.72081400
H	6.07885301	0.91245729	-0.15335000
H	5.71151201	-0.80372071	-0.03194800
H	2.18897701	1.10813929	-1.26206400
H	2.54919901	2.82280729	-1.37663500
H	3.77054801	1.50325029	-3.12661000
H	4.88925301	2.32373929	-2.04578600
H	4.08546601	-0.62749771	-1.89623600
H	5.64688001	-0.00908671	-2.41330000
H	4.20683301	2.62649729	0.47846700
C	2.34701401	2.10868829	1.31089500
O	1.17582001	2.12260929	1.12517300

7_cHexen

E=-658.11587673 hartree

0 1

C	-0.99593491	0.42682926	0.00000000
C	-2.20176091	1.26564626	0.48018600
C	-3.17924591	1.61847326	-0.62800200

C	-3.58001691	0.47020126	-1.53500700
C	-2.38628791	-0.38206174	-2.00179200
C	-1.48531791	-0.78773674	-0.82989200
H	-4.25818891	-0.15957374	-0.94266700
H	-4.15173091	0.87184226	-2.37338900
H	-2.75406691	-1.27858274	-2.50804700
H	-1.80805691	0.18572326	-2.73376000
H	-2.03983391	-1.44530374	-0.15115100
H	-0.63163891	-1.36260274	-1.19654800
O	-3.66675691	2.72758926	-0.72654100
H	-2.75936291	0.66430126	1.20880800
C	3.49504209	-0.24359274	-0.41755500
C	1.99584509	-0.18534574	-0.74331500
C	1.43269309	1.24087126	-0.52099900
C	2.23330809	2.27826926	-1.31769900
C	3.72951309	2.21035826	-0.98564500
C	4.28950909	0.79998726	-1.21307000
H	1.83839009	-0.46591574	-1.79187500
H	1.45622809	-0.91258174	-0.13167700
H	3.63320309	-0.06229974	0.65582800
H	3.87479509	-1.24980274	-0.62010900
H	2.08325509	2.08980026	-2.38662600
H	1.83839609	3.27871826	-1.12152400
H	4.27746209	2.93963226	-1.59031100
H	3.88111809	2.49368526	0.06387800
H	4.23167709	0.55786926	-2.28204800
H	5.34767409	0.76050026	-0.93637600
H	1.52698509	1.45930026	0.55366300
C	-0.05454391	1.30217226	-0.82469800
O	-0.50643491	2.02473726	-1.69583500
H	-0.45744391	0.05581126	0.87526900
H	-1.88771791	2.18504326	0.97703300