

Electronic Supplementary Information

A Molecular Electron Density Theory Study of the Higher-Order Cycloaddition Reactions of Tropone with Electron-rich Ethylene. The Role of the Lewis Acid Catalyst in the Mechanism and *Pseudocyclic* Selectivity

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- S7** Table with the ω B97X-D/6-311G(d,p) total and relative enthalpies, entropies and Gibbs free energies for the stationary points involved in the LA B(C₆F₅)₃ catalyzed cycloaddition reaction of tropone **11** with CKA **27**.
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- S28** ω B97X-D/6-311G(d,p) gas phase computed total energies, unique imaginary frequency, and Cartesian coordinates of the stationary points involved in the non-catalyzed and LA catalyzed cycloaddition reactions of tropone **11** with ketene diethyl acetal **24**.

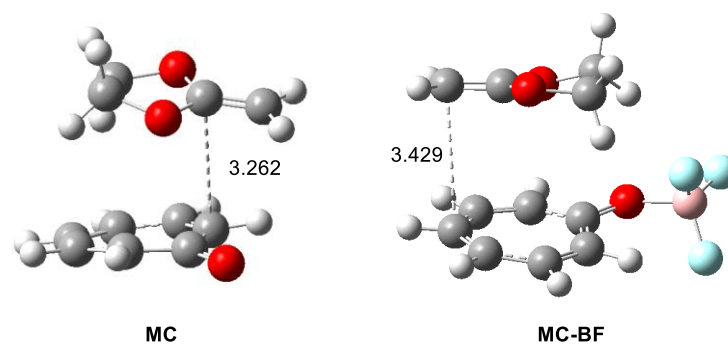


Figure S1. ω B97X-D/6-311G(d,p) gas phase geometries of **MC** and **MC-BF**. Distances are given in Angstroms.

Table S1. ω B97X-D/6-311G(d,p) and B3LYP-D3BJ/6-311G(d,p) total (E, in au) and relative (ΔE , in kcal mol⁻¹) energies, with respect to the separated reagents, in gas phase and DCM, of the stationary points involved in the cycloaddition reaction of tropone **11** with CKA **27**.

	ω B97X-D				B3LYP-D3BJ	
	Gas phase		DCM			
	E	ΔE	E	ΔE	E	ΔE
11	-345.495830		-345.503648		-345.6589668	
27	-306.422249		-306.428322		-306.5461649	
MC	-651.928580	-6.6	-651.941504	-6.0	-652.2149066	-6.1
TS-11	-651.896966	13.2	-651.912728	12.1	-652.1889782	10.1
IN-1	-651.897896	12.7	-651.922289	6.1	-652.1911405	8.8
TS-12	-651.896731	13.4	-651.920578	7.1	-652.1906456	9.1
TS-2	-651.899627	11.6	-651.910768	13.3	-652.1894882	9.8
TS-3	-651.892775	15.9	-651.907238	15.5	-652.1819086	14.6
28	-651.964067	-28.9	-651.973712	-26.2	-652.2330190	-17.5
29	-651.965842	-30.0	-651.973227	-25.9	-652.2341419	-18.2
30	-651.965245	-29.6	-651.974389	-26.6	-652.2334177	-17.7

Table S2. ω B97X-D/6-311G(d,p) gas phase total (E, in au) and relative (ΔE , in kcal mol⁻¹) energies, with respect to the separated reagents of the stationary points involved in the cycloaddition reaction of tropone **11** with ketene diethyl acetal **24**.

	E	ΔE
11	-345.49583	
24	-386.258367	
MC-exp	-731.771015	-10.6
TS-11-exp	-731.734167	12.6
IN-1-exp	-731.739458	9.2
TS-12-exp	-731.738615	9.8
TS-2-exp	-731.736726	11.0
TS-3-exp	-731.731742	14.1
28-exp	-731.802069	-30.0
29-exp	-731.800802	-29.2
30-exp	-731.793099	-24.4

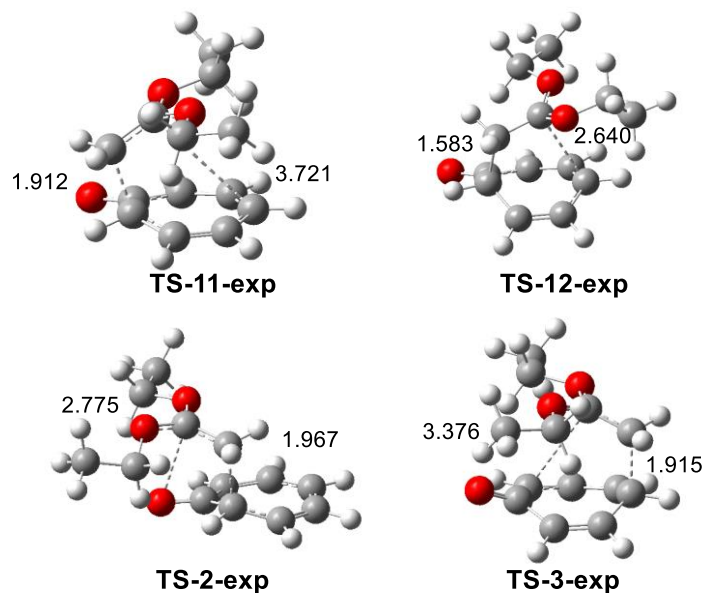


Figure S2. ω B97X-D/6-311G(d,p) Gas phase geometries of the transition state structures involved in the cycloaddition reaction of tropone **11** with ketene diethyl acetal **24**. Distances are given in Angstroms.

Table S3. ω B97X-D/6-311G(d,p) and B3LYP-D3BJ/6-311G(d,p) total (E, in au) and relative (ΔE , in kcal mol⁻¹) energies, with respect to the separated reagents, in gas phase and in DCM, of the stationary points involved in the LA BF₃ catalyzed cycloaddition reaction of tropone **11** with CKA **27**.

	ω B97X-D				B3LYP- D3BJ	
	Gas phase		DCM			
	E	ΔE	E	ΔE	E	ΔE
31	-670.085140		-670.106186		-670.360034	
27	-306.422249		-306.428322		-306.546165	
MC-BF	-976.528918	-13.5	-976.548621	-8.9	-976.921274	-9.5
TS-BF-1	-976.500634	4.2	-976.529446	3.2	-976.904264	1.2
TS-BF-2	-976.514671	-4.6	-976.532615	1.2	-976.909659	-2.2
TS-BF-3	-976.505453	1.2	-976.529513	3.1	-976.904244	1.2
33	-976.547209	-25.0	-976.565555	-19.5	-976.923102	-10.6
34	-976.541275	-21.3	-976.562091	-17.3	-976.924566	-11.5
35	-976.548678	-25.9	-976.566363	-20.0	-976.923477	-10.8

Table S4. ω B97X-D/6-311G(d,p) Total enthalpies (H, in a.u.), entropies (S, in cal/mol.K) and Gibbs free energies (G, in a.u.), and relative enthalpies (Δ H in kcal·mol⁻¹), entropies, (Δ S in cal·mol⁻¹K⁻¹), and Gibbs free energies (Δ G in kcal·mol⁻¹), with respect to the separated reagents, computed at 273.15 K and 1 atm in DCM, for the stationary points involved in the BF₃ LA catalyzed cycloaddition reaction of tropone **11** with CKA **27**.

	H	Δ H	S	Δ S	G	Δ G
31	-669.970659		98.4		-670.013482	
27	-306.324813		70.3		-306.355419	
MC-BF	-976.307607	-7.6	135.9	-32.8	-976.366754	1.3
TS-BF-1	-976.288960	4.1	124.7	-44.0	-976.343249	16.1
TS-BF-2	-976.292040	2.2	123.3	-45.4	-976.345721	14.5
TS-BF-3	-976.289145	4.0	125.0	-43.7	-976.343557	15.9
33	-976.322532	-17.0	121.5	-47.2	-976.375427	-4.1
34	-976.319267	-14.9	121.1	-47.6	-976.371996	-1.9
35	-976.323018	-17.3	120.1	-48.6	-976.375279	-4.0

Table S5. B3LYP-D3BJ/6-311G(d,p) Total enthalpies (H, in a.u.), entropies (S, in cal/mol.K) and Gibbs free energies (G, in a.u.), and relative enthalpies (Δ H in kcal·mol⁻¹), entropies, (Δ S in cal·mol⁻¹K⁻¹), and Gibbs free energies (Δ G in kcal·mol⁻¹), with respect to the separated reagents, computed at 273.15 K and 1 atm in DCM, for the stationary points involved in the BF₃ LA catalyzed cycloaddition reaction of tropone **11** with CKA **27**.

	H	Δ H	S	Δ S	G	Δ G
31	-306.443775		70.5		-306.474459	
27	-670.225601		99.2		-670.268764	
TS-BF-1	-976.665665	2.3	124.6	-45.1	-976.719902	14.6
TS-BF-2	-976.670992	-1.0	123.6	-46.1	-976.724774	11.6
TS-BF-3	-976.665715	2.3	123.2	-46.5	-976.719336	15.0
33	-976.682424	-8.2	121.8	-47.9	-976.735432	4.9
34	-976.684119	-9.3	122.4	-47.2	-976.737418	3.6
35	-976.682543	-8.3	121.2	-48.4	-976.735308	5.0

Table S6. ω B97X-D/6-311G(d,p) total (E, in au) and relative (ΔE , in kcal mol⁻¹) energies, in gas phase and in DCM, with respect to the separated reagents, of the stationary points involved in the B(C₆F₅)₃ LA catalyzed cycloaddition reactions of tropone **11** with CKA **27**.

	E	ΔE	E	ΔE
32	-2553.749157		-2553.766893	
27	-306.4222490			
MC-BPhF	-2860.195151	-14.9	-2860.212066	-10.6
TS-BPhF-1	-2860.175239	-2.4	-2860.196851	-1.0
TS-BPhF-2	-2860.170648	0.5	-2860.18666	5.4
36	-2860.217370	-28.8	-2860.231873	-23.0
37	-2860.200050	-18.0	-2860.209201	-8.8

Table S7. ω B97X-D/6-311G(d,p) Total enthalpies (H, in a.u.), entropies (S, in cal/mol.K) and Gibbs free energies (G, in a.u.), and relative enthalpies (ΔH in kcal·mol⁻¹), entropies, (ΔS in cal·mol⁻¹K⁻¹), and Gibbs free energies (ΔG in kcal·mol⁻¹), with respect to the separated reagents, computed at 273.15 K and 1 atm in DCM, for the stationary points involved in the B(C₆F₅)₃ LA catalyzed cycloaddition reaction of tropone **11** with CKA **27**.

	H	ΔH	S	ΔS	G	ΔG
32	-2553.46565		209.6		-2553.55691	
27	-306.324813		70.3		-306.355419	
MC-BPhF	-2859.80508	-9.2	243.0	-37.0	-2859.91085	0.9
TS-BPhF-1	-2859.79062	-0.1	234.1	-45.9	-2859.89251	12.4
TS-BPhF-2	-2859.78071	6.1	232.0	-47.9	-2859.88172	19.2
36	-2859.82304	-20.4	227.1	-52.9	-2859.9219	-6.0
37	-2859.80090	-6.6	238.3	-41.6	-2859.90464	4.8

ω B97X-D/6-311G(d,p) gas phase computed total energies, unique imaginary frequency, and Cartesian coordinates of the stationary points involved in the non-catalyzed and LA catalyzed cycloaddition reactions of tropone **11** with CKA **27**.

11

E = -345.495830 a.u.

C	1.84228500	0.67659800	-0.00009900
C	1.84301900	-0.67573800	-0.00012100
C	0.71353100	-1.56137500	-0.00002100
C	-0.60792600	-1.28510100	0.00003000
C	0.71220100	1.56146600	0.00005900
C	-0.60928300	1.28511100	0.00011900
C	-1.32591300	-0.00020800	0.00009100
H	2.81181900	1.16503700	-0.00020700
H	2.81303700	-1.16320300	-0.00023700
H	0.97125900	-2.61709800	-0.00000500
H	-1.29774800	-2.12390500	0.00006200
H	-1.29878000	2.12412000	0.00021000
O	-2.54708600	-0.00084500	-0.00003600
H	0.96961300	2.61729600	0.00012600

27

E = -306.422249 a.u.

C	0.00000000	0.00000000	2.11513500
C	0.00000000	0.00000000	0.78898700
H	-0.05314800	0.93544400	2.64982200
H	0.05314800	-0.93544400	2.64982200
O	0.00000000	1.11696500	0.01706200
O	0.00000000	-1.11696500	0.01706200
C	0.24471900	-0.72006400	-1.32705900
H	1.31584600	-0.78856700	-1.54423800
H	-0.31153200	-1.37881700	-1.99209000
C	-0.24471900	0.72006400	-1.32705900
H	-1.31584600	0.78856700	-1.54423800
H	0.31153200	1.37881700	-1.99209000

MC

E = -651.928580 a.u.

C	2.37548400	1.44288300	-0.04573100
C	2.16101400	1.07307100	1.23860300
C	1.49002900	-0.09952100	1.72339200
C	1.00954500	-1.16490100	1.04737700
C	-2.32779900	-1.50237700	0.79727100

C	-2.04439600	-0.31362800	0.28114200
C	1.97716000	0.75333900	-1.24052300
C	1.39755800	-0.45717900	-1.38937700
C	1.04781100	-1.48102500	-0.39022000
H	2.89251000	2.38445400	-0.20409600
H	2.52115900	1.75018500	2.00728000
H	1.36369200	-0.13208700	2.80188100
H	0.54002100	-1.95897300	1.61769200
H	1.18102100	-0.79598800	-2.39789600
O	0.75161000	-2.60227800	-0.76537300
H	2.18769200	1.29108200	-2.16175400
O	-2.03526400	0.85053700	0.97716000
O	-1.70804800	-0.10219300	-1.01658700
C	-1.43050100	1.84602100	0.15719100
C	-1.67262600	1.30153100	-1.24207900
H	-1.91855400	2.80005000	0.35167400
H	-0.36321700	1.91451200	0.38680400
H	-2.63109700	1.63087800	-1.65591800
H	-0.86643300	1.51877100	-1.94165600
H	-2.54036300	-1.58776200	1.85175100
H	-2.33248400	-2.37294100	0.16036400

TS-11

E = -651.896966 a.u.

1 imaginary frequency -351.0184 cm⁻¹

C	0.29321400	2.29507700	-0.08696000
C	0.53893400	1.88553400	1.22676300
C	1.08233500	0.70744700	1.68998800
C	1.38294700	-0.49638700	0.97111800
C	0.01837300	-1.76368700	1.07660500
C	-1.04748700	-1.16931800	0.41063000
C	0.73152900	1.64699600	-1.25021200
C	1.40378300	0.45851700	-1.42962700
C	1.78041100	-0.56202800	-0.48793900
H	-0.15395300	3.27543400	-0.21862100
H	0.29257300	2.61454000	1.99620700
H	1.23389700	0.64363200	2.76393000
H	2.07256100	-1.14098900	1.51387300
H	1.70885200	0.20724400	-2.44064600
O	2.39632400	-1.56681400	-0.83838700
H	0.54247600	2.19742000	-2.17132300
O	-1.88827300	-0.36021900	1.01228000
O	-1.15255500	-1.17541400	-0.89634800
C	-2.50919700	0.47981100	0.02353700
C	-2.12240900	-0.19151700	-1.29841200
H	-3.57880600	0.50194000	0.22037700
H	-2.06027800	1.47170400	0.11677500
H	-2.94234800	-0.71220900	-1.79253900
H	-1.62614700	0.49455100	-1.98312200
H	-0.13163300	-1.88164700	2.14268000

H 0.48423900 -2.59470900 0.55908300

IN-1

E = 651.897896 a.u.

C	0.04693200	2.22498400	-0.12840700
C	0.38690600	1.89411700	1.20449400
C	1.03945000	0.79641100	1.67989800
C	1.38863500	-0.44012500	0.96920400
C	0.21941500	-1.63849400	1.08718000
C	-0.94109400	-1.16007400	0.41640300
C	0.57084800	1.62377500	-1.27186600
C	1.40074600	0.52621400	-1.43798900
C	1.85415500	-0.44556700	-0.49189600
H	-0.50854900	3.14639800	-0.27514600
H	0.12184500	2.64059200	1.95137700
H	1.26747100	0.78630000	2.74224300
H	2.18488400	-0.96004300	1.50527600
H	1.75240000	0.31636600	-2.44314000
O	2.58260200	-1.38781400	-0.80589800
H	0.31583100	2.13095500	-2.20302600
O	-1.84775800	-0.45384300	1.02269000
O	-1.07078600	-1.22987700	-0.87168000
C	-2.60935500	0.27121200	0.03308900
C	-2.12626900	-0.33626600	-1.28972700
H	-3.66513900	0.12020300	0.24576300
H	-2.31438000	1.31861000	0.12374300
H	-2.87079500	-0.92942500	-1.81757800
H	-1.66919500	0.40572400	-1.94263200
H	0.02791000	-1.80414900	2.14376400
H	0.66304000	-2.49637000	0.58615300

TS-12

E = -651.896731 a.u.

1 imaginary frequency -75.5334 cm^{-1}

C	0.12277100	1.59982300	0.98989000
C	-0.43549300	2.13666400	-0.20566200
C	-1.26802800	1.49808800	-1.06041500
C	-1.53236300	0.04247300	-1.03167200
C	-0.26220800	-0.83834700	-1.50349100
C	0.95163600	-0.65376600	-0.74219500
C	-0.46456800	0.59932600	1.77747600
C	-1.50034300	-0.27279200	1.51631500
C	-2.11361400	-0.56546800	0.25369400
H	0.86513400	2.21634000	1.49111500
H	-0.18164600	3.17018400	-0.43354300
H	-1.69790100	2.05292200	-1.88761700
H	-2.26788300	-0.21693700	-1.79434000
H	-1.87013800	-0.88594400	2.33118900

O	-3.04621700	-1.35292000	0.12082500
H	-0.05142900	0.52127600	2.78458400
O	1.91221300	0.12838600	-1.14772700
O	1.25257700	-1.39811700	0.27901200
C	2.89262800	0.21609100	-0.09775600
C	2.43333000	-0.85841000	0.90043500
H	3.87015100	0.03768900	-0.54065300
H	2.82002300	1.21941900	0.32096300
H	3.13477100	-1.67748000	1.04387300
H	2.12307700	-0.43056200	1.85346200
H	-0.05753700	-0.56809300	-2.53825500
H	-0.57769100	-1.87969600	-1.42737400

TS-2

E = -651.899627 a.u.

1 imaginary frequency -424.6756 cm⁻¹

C	3.16602300	-0.86078700	0.09924600
C	3.27259400	0.41239700	0.66216000
C	2.41456300	1.48776400	0.44344200
C	2.10716600	-1.40935700	-0.58969900
C	1.25173300	1.58664500	-0.30220600
C	0.78520000	-0.88401900	-0.72602500
C	0.46757500	0.56852600	-0.90659800
H	4.03685400	-1.50252400	0.21395400
H	4.16435200	0.61607900	1.24544700
H	2.73635500	2.42353000	0.89617600
H	2.24121100	-2.42215400	-0.95911600
H	0.81684500	2.57539400	-0.41181600
H	0.16679100	-1.44827400	-1.42068600
O	-0.59296100	0.82058100	-1.50997100
C	-1.40222300	-0.70830400	0.70214400
C	-0.18527300	-1.36174800	0.85654900
H	0.45130700	-0.96966600	1.64053600
H	-0.21723800	-2.43863600	0.75451200
O	-2.39543500	-1.18449400	-0.01871800
O	-1.60240600	0.50934400	1.14848100
C	-3.22934100	-0.07965300	-0.41891500
C	-2.73866600	1.07406800	0.46433000
H	-2.37546800	1.91080400	-0.12709700
H	-3.45426300	1.39318800	1.22136900
H	-3.03089300	0.11078300	-1.47144100
H	-4.26554400	-0.36516900	-0.24674600

TS-3

E = -651.892775 a.u.

1 imaginary frequency -419.1234 cm⁻¹

C	1.86646800	-1.07445400	-0.36906800
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C	2.10173400	-0.76013200	1.01028800
C	1.56628700	0.31915000	1.68165100
C	0.73870900	1.34036100	1.22116900
C	-0.84936800	-1.26642400	-0.26077700
C	0.27105900	-2.03806600	-0.58976500
C	1.83183800	0.01321000	-1.36407100
C	1.21039800	1.19307200	-1.24727100
C	0.39134800	1.69338700	-0.12111800
H	2.49846900	-1.89222000	-0.71102500
H	2.66230300	-1.48750800	1.58748800
H	1.77611100	0.34791400	2.74915100
H	0.30761800	2.00707700	1.96345500
H	1.21858100	1.87222400	-2.09468700
O	-0.54034500	2.47292700	-0.38134300
H	2.33047700	-0.20347000	-2.30589100
H	0.43383100	-2.86636500	0.08927200
H	0.31225200	-2.29729100	-1.64212700
O	-1.36244900	-1.23370200	0.94706400
O	-1.46803000	-0.49746400	-1.12553900
C	-2.54087500	0.20039300	-0.44561700
H	-3.48223900	-0.23114600	-0.79076100
H	-2.45091000	1.25407800	-0.69420600
C	-2.23417600	-0.08697400	1.02207000
H	-1.66165700	0.72201000	1.48136800
H	-3.09876800	-0.36051700	1.62156400

28

E = -651.964067 a.u.

C	-0.22067700	-0.24213400	1.18068800
C	0.51085100	-1.56706900	1.13916300
C	1.34977000	-1.77929100	0.13577600
C	1.52361100	-0.68320700	-0.89051500
C	0.13885900	-0.15699900	-1.34331500
C	-0.88616600	-0.02615500	-0.20884200
C	0.69525600	0.91829600	1.49229300
C	1.82850800	1.20545700	0.84813500
C	2.37009400	0.44952000	-0.30776700
H	-1.01986600	-0.26793400	1.92344500
H	0.31953800	-2.30603100	1.90752000
H	1.91296400	-2.69908500	0.03304500
H	2.07467800	-1.04149100	-1.75981900
H	2.43256800	2.05516400	1.14834100
O	3.43973400	0.74412000	-0.79105600
H	0.38687600	1.57253400	2.30183800
O	-1.91403600	-0.97550400	-0.40166200
O	-1.51503700	1.24954100	-0.21724200
C	-3.11970700	-0.37611600	0.02824500
C	-2.91141500	1.07371800	-0.38063700
H	-3.94806300	-0.86902200	-0.47932000
H	-3.24924100	-0.47560400	1.11417900

H	-3.19606700	1.23724400	-1.42638900
H	-3.43706900	1.78801400	0.25484800
H	-0.27624000	-0.85211800	-2.07297700
H	0.24072600	0.81695700	-1.82438300

29

E = -651.965842 a.u.

C	-3.30799700	0.97382500	0.17178000
C	-3.69727800	-0.37419200	-0.18278500
C	-2.92067000	-1.47768400	-0.06271100
C	-2.06738800	1.47733000	0.11562500
C	-1.54598000	-1.54770300	0.36531700
C	-0.91080300	0.75156500	-0.51784500
C	-0.66774300	-0.54249200	0.22429500
H	-4.09872600	1.61452500	0.55407200
H	-4.74102100	-0.52501300	-0.44181600
H	-3.40151800	-2.43641300	-0.23847400
H	-1.87294500	2.46604300	0.52240900
H	-1.18907200	-2.47444300	0.80046400
H	-1.14489700	0.51845000	-1.56343800
O	0.59718300	-0.60418000	0.70036200
C	1.40098700	0.35832400	-0.00125900
C	0.43937800	1.46442300	-0.39056300
H	0.42771600	2.19006100	0.42470400
H	0.77357900	1.95475400	-1.30249000
O	1.97657500	-0.24128100	-1.11279700
O	2.42773800	0.74816700	0.83079300
C	3.10032000	-0.95097200	-0.61180300
C	3.57142900	-0.05321900	0.53977900
H	3.86018800	-0.62225500	1.42494800
H	4.38846600	0.61010700	0.24720900
H	2.79429000	-1.93943600	-0.25712300
H	3.82645800	-1.05325700	-1.41630400

30

E = -651.965245 a.u.

C	1.78631400	-1.21918100	0.53310400
C	1.87703200	-1.29779900	-0.97902700
C	1.00977700	-0.58283500	-1.68111500
C	0.03231400	0.28682700	-0.93096900
C	-0.65774300	-0.53539700	0.20653500
C	0.31164100	-1.46832000	0.92900800
C	2.26675800	0.12021300	1.04972100
C	1.79772500	1.30919200	0.66495000
C	0.71130200	1.51470500	-0.32210900
H	2.39636800	-2.00271900	0.98478600
H	2.61745700	-1.93907100	-1.44266400
H	0.98917600	-0.58928200	-2.76391900

H	-0.73451100	0.67796900	-1.60040100
H	2.19668000	2.22560500	1.08638700
O	0.35050600	2.62990800	-0.62481900
H	3.04868200	0.09860500	1.80422100
H	0.04157000	-2.49093300	0.66361700
H	0.16520000	-1.33818200	2.00171700
O	-1.71907600	-1.28863100	-0.33624700
O	-1.26373800	0.33586100	1.13385700
C	-2.49144700	0.73765600	0.55238600
H	-3.20755000	0.89968500	1.35745800
H	-2.36397800	1.66855800	-0.01050000
C	-2.86133300	-0.44674600	-0.36809300
H	-3.07305100	-0.11477600	-1.38988500
H	-3.71162000	-1.02244900	0.00050600

31

E = -670.085140 a.u.

C	3.40698400	0.25666400	-0.00001800
C	3.02553600	-1.04978300	-0.00011200
C	1.70576400	-1.57422100	-0.00009700
C	2.56915800	1.40236100	-0.00015800
C	0.49730400	-0.94883600	0.00030700
C	1.21280000	1.49387100	0.00011200
C	0.20804700	0.46284100	0.00058500
H	4.47355400	0.45589700	0.00013500
H	3.81954500	-1.78942800	-0.00009800
H	1.65280200	-2.65892600	-0.00025900
H	3.09484100	2.35259200	-0.00048800
H	-0.38067100	-1.58074800	0.00053000
H	0.77705700	2.48752300	0.00008600
O	-0.98028900	0.88782500	0.00105300
B	-2.30944800	-0.03048100	-0.00015700
F	-3.32273500	0.87163200	0.00006800
F	-2.21586100	-0.79464900	-1.14742600
F	-2.21708600	-0.79637100	1.14610800

MC-BF

E = -976.528918 a.u.

C	-1.71817800	2.46331000	-0.94784500
C	-2.31198000	2.14346000	0.23589800
C	-1.71372700	1.54326100	1.37105100
C	-0.45571800	1.05084100	1.53721600
C	-3.47303100	-1.07074400	0.51391500
C	-2.27921100	-1.44484600	0.05484700
C	-0.36563100	2.26631400	-1.31868500
C	0.65222400	1.63660400	-0.66642500
C	0.62177300	0.96173900	0.59919300
H	-2.34319700	2.94099300	-1.69476500

H	-3.36473400	2.38338800	0.33701300
H	-2.37038000	1.43128400	2.22714200
H	-0.21926800	0.58435200	2.48665200
H	1.61173800	1.60320500	-1.16648000
O	1.60093000	0.24682800	0.98343600
H	-0.09943100	2.66830800	-2.29190400
O	-1.94815400	-1.50889200	-1.25076700
O	-1.23629900	-1.78161200	0.84228000
C	-0.55652600	-1.83536800	-1.35210800
C	-0.24874600	-2.41678500	0.01891500
H	-0.42510500	-2.54507700	-2.16672100
H	0.02491000	-0.93499500	-1.55365000
H	-0.39907900	-3.49930600	0.05757400
H	0.73843900	-2.15690000	0.39100400
H	-4.24727700	-0.78483000	-0.18120800
H	-3.67496900	-1.11857500	1.57289900
B	2.84751600	-0.16289500	0.09749500
F	2.30720400	-0.72588100	-1.06201100
F	3.51428000	-1.06862200	0.86431200
F	3.54423500	0.99509300	-0.17790800

TS-BF-1

E = -976.500634 a.u.

1 imaginary frequency -436.6772 cm⁻¹

C	-2.29930000	1.72302300	-1.23192000
C	-2.67225600	1.87662200	0.11358600
C	-1.92824500	1.67043400	1.24614400
C	-0.63870700	1.08537100	1.40276700
C	-0.89722800	-0.82445500	2.10389200
C	-1.05520200	-1.48329700	0.90267800
C	-1.03571800	1.43288800	-1.69860500
C	0.15112500	1.14192100	-1.01573700
C	0.37791800	0.95989200	0.34710200
H	-3.05973100	1.93949900	-1.97447600
H	-3.67622400	2.25756700	0.28012600
H	-2.41460600	1.92710300	2.18281600
H	-0.15564700	1.30597700	2.34898900
H	1.03515600	1.03688900	-1.63002900
O	1.52098700	0.60937200	0.82429000
H	-0.92459800	1.45626600	-2.78013300
O	-2.20155500	-1.55924700	0.26167100
O	-0.03205900	-1.89947400	0.21085900
C	-1.93799800	-1.89695100	-1.11637200
C	-0.45344200	-2.28354500	-1.10983600
H	-2.60574100	-2.70927600	-1.39551700
H	-2.14621300	-1.00567500	-1.71083100
H	-0.27949700	-3.35405800	-1.21553700
H	0.16386000	-1.72671200	-1.81042400
H	-1.78437700	-0.68264300	2.70460600
H	0.04470000	-0.99488200	2.60763000

B	2.74236600	0.19009700	-0.04426200
F	2.29964300	-0.80637900	-0.93183700
F	3.66133400	-0.28263300	0.85224300
F	3.16418000	1.30932700	-0.74514600

TS-BF-2

E = -976.514671 a.u.

1 imaginary frequency -421.6612 cm⁻¹

C	3.79310900	-0.28482800	-0.38922900
C	3.67656400	0.43303300	0.80837300
C	2.55559200	1.09086400	1.27343800
C	2.79555000	-0.67052700	-1.24979300
C	1.27427300	1.20604200	0.72732200
C	1.39258500	-0.54545000	-1.08951300
C	0.72902800	0.51842400	-0.35004400
H	4.80143900	-0.57328900	-0.67280800
H	4.58312800	0.54937100	1.39246100
H	2.69877400	1.65731800	2.18940800
H	3.10500600	-1.22379700	-2.13107800
H	0.59581500	1.88469000	1.22700400
H	0.80700000	-0.81937600	-1.95967000
O	-0.49543900	0.68551700	-0.75141600
C	-0.52671300	-2.06517900	0.20342100
C	0.79903800	-2.31433700	-0.07206000
H	1.48403800	-2.26342400	0.76260100
H	1.01128000	-3.01359800	-0.86815800
O	-1.50659100	-2.31895100	-0.63684200
O	-0.90704200	-1.44283100	1.29512800
C	-2.66518500	-1.55623400	-0.21950900
C	-2.33432200	-1.21059500	1.23042900
H	-2.50541100	-0.16486200	1.47062300
H	-2.80509300	-1.87450500	1.95682900
H	-2.73212800	-0.66978000	-0.84857000
H	-3.53870000	-2.19381000	-0.33471000
B	-1.43621700	1.82004600	-0.31593200
F	-2.62363900	1.53979500	-0.97516100
F	-1.61844200	1.73003000	1.07828800
F	-0.86776400	3.01991600	-0.66937600

TS-BF-3

E = -976.505453 a.u.

1 imaginary frequency -446.2075 cm⁻¹

C	2.23962300	-1.43354300	-0.86209100
C	2.48152400	-1.85898500	0.47618300
C	1.60470500	-1.78676300	1.52758200
C	0.28216000	-1.32792900	1.57383900
C	1.96198600	1.27689700	-0.40850000
C	2.90406900	0.49797300	-1.05395800

C	0.91476100	-1.47456700	-1.45125400
C	-0.28731300	-1.28575200	-0.86888300
C	-0.58072700	-1.01277600	0.52522200
H	3.01323300	-1.74096800	-1.55843700
H	3.48268700	-2.21806300	0.69002400
H	2.00398000	-2.10419400	2.48717600
H	-0.17581300	-1.23870300	2.55350400
H	-1.16165900	-1.32201800	-1.50676900
O	-1.72986700	-0.51542000	0.85980400
H	0.89915300	-1.63697000	-2.52511900
H	3.85695600	0.39282800	-0.55377100
H	2.91896800	0.59148600	-2.13215000
O	2.01775000	1.56518100	0.87339600
O	0.87962600	1.70685200	-1.00510600
C	0.08163600	2.45472100	-0.05130100
H	0.19762400	3.51277900	-0.29059900
H	-0.94921400	2.12976000	-0.17091200
C	0.72113000	2.06308300	1.27658900
H	0.19465400	1.24509200	1.77218900
H	0.87880800	2.89262200	1.96105300
B	-2.84321600	-0.08744700	-0.10683500
F	-3.81564500	0.46669400	0.68118800
F	-2.27712000	0.86669500	-0.98390800
F	-3.26553300	-1.19933100	-0.82142800

33

E = -976.547209 a.u.

C	1.52941100	0.47869700	1.13579900
C	1.17695300	1.93543400	0.92776000
C	0.38103400	2.24129500	-0.08397300
C	-0.10941600	1.10665900	-0.96230600
C	1.07730600	0.19183900	-1.35849400
C	2.07165800	-0.07442500	-0.22114800
C	0.35860400	-0.36035900	1.56931700
C	-0.84453900	-0.41523100	0.98252300
C	-1.17326700	0.33282500	-0.22388200
H	2.32833600	0.37441500	1.87061500
H	1.60000000	2.68311900	1.58643100
H	0.07533000	3.25460700	-0.31113100
H	-0.58787600	1.48831400	-1.86317000
H	-1.62353100	-1.04595500	1.38700200
O	-2.31197700	0.34884500	-0.71340800
H	0.51549700	-0.99414800	2.43594400
O	3.30349300	0.53467400	-0.52711900
O	2.33089100	-1.45936100	-0.06342200
C	4.32429300	-0.32084500	-0.04545100
C	3.71469100	-1.69408100	-0.27567700
H	5.22893500	-0.13029400	-0.62086800
H	4.52441900	-0.13845200	1.01826900
H	3.88784300	-2.04242300	-1.29971000

H	4.05623300	-2.45140500	0.43041700
H	1.62494600	0.68223400	-2.16240800
H	0.71360200	-0.76681400	-1.72991200
B	-3.66527400	-0.40450100	-0.07352400
F	-3.33379500	-1.73489300	-0.08246600
F	-4.63241400	-0.04071600	-0.94599500
F	-3.77123400	0.12951900	1.18301000

34

E = -976.541275 a.u.

C	3.79886600	-0.51555600	0.71594200
C	4.01486200	0.35029700	-0.42320000
C	3.06270700	1.07533600	-1.05769300
C	2.67989900	-1.20647500	0.97329000
C	1.64666500	1.10179500	-0.78365900
C	1.54667100	-1.31188800	-0.01110700
C	0.98489400	0.06749500	-0.24913600
H	4.61079800	-0.57220500	1.43619300
H	5.04773400	0.53060200	-0.70584100
H	3.40263600	1.78307100	-1.80864600
H	2.57559500	-1.73034800	1.91942100
H	1.09367400	1.99487400	-1.04599800
H	1.91830200	-1.70630600	-0.96404800
O	-0.33712000	0.11294800	0.09506300
C	-0.85954400	-1.25671100	0.06601200
C	0.33031100	-2.09624200	0.48616800
H	0.31535600	-2.15709800	1.57572500
H	0.24664900	-3.09800500	0.06974800
O	-1.28083800	-1.54814600	-1.21395800
O	-1.94305500	-1.32105500	0.90082700
C	-2.60838100	-1.03589100	-1.30033700
C	-3.13546800	-1.28952100	0.11035400
H	-3.78419900	-0.49540400	0.47445100
H	-3.63309700	-2.25802700	0.20059700
H	-2.58444300	0.02931800	-1.54572100
H	-3.13474400	-1.58655700	-2.07711700
B	-1.39665300	2.03638800	0.40119300
F	-2.50748500	1.52887500	0.91889200
F	-0.47102900	2.53679600	1.19763500
F	-1.39612800	2.36081000	-0.88874700

35

E = -976.548678 a.u.

C	-1.80244400	-2.08217900	0.53867800
C	-1.88307200	-2.20848100	-0.97107800
C	-1.39084700	-1.21328400	-1.69126400
C	-0.76224600	-0.05298300	-0.95858500
C	-1.71417900	0.45243800	0.19230100

C	-2.39089500	-0.70147700	0.92477600
C	-0.38221300	-2.21961600	1.02774200
C	0.67044200	-1.48908800	0.63598200
C	0.56154800	-0.40602000	-0.33158000
H	-2.40716600	-2.85489200	1.01349600
H	-2.35370400	-3.07757400	-1.41421000
H	-1.41981100	-1.19602300	-2.77304400
H	-0.56333200	0.77693600	-1.63602900
H	1.65103300	-1.66865700	1.05323300
O	1.52475400	0.30318400	-0.65935800
H	-0.20127000	-2.97990200	1.78239900
H	-3.44800800	-0.68761800	0.65985800
H	-2.29741500	-0.51996600	1.99548500
O	-2.68017900	1.30879100	-0.35509500
O	-0.98081800	1.23412800	1.10007400
C	-0.87769100	2.52769300	0.52357700
H	-0.87276800	3.25444500	1.33427800
H	0.05186100	2.62012000	-0.04723900
C	-2.12710800	2.62018500	-0.37815100
H	-1.87144100	2.91262300	-1.40111100
H	-2.88178000	3.30514300	0.00952300
B	3.07850500	0.20549600	-0.04780400
F	3.70627900	1.19927600	-0.71996200
F	2.91307400	0.41721700	1.29454600
F	3.48103000	-1.06583400	-0.36313700

32

E = -2553.749157 a.u.

C	-1.92008300	0.69500200	3.34879800
C	-3.53402300	2.18058300	1.14556900
C	-4.40549700	2.24665400	2.26005300
C	-4.18659400	1.77690400	3.52144300
C	-3.04068200	1.10083200	4.00757000
C	-2.31513900	1.58621100	1.00817600
C	-1.56930200	0.82509800	1.96676500
O	-0.49515100	0.22791900	1.64978300
B	0.09450400	-0.04983400	0.23036700
C	0.71268100	1.31154500	-0.43783300
C	1.32373500	1.20209100	-1.68325600
C	0.82320100	2.55876500	0.15737700
C	1.98006000	2.24341200	-2.31201700
C	1.47093400	3.63353700	-0.43705800
C	2.05359400	3.47546900	-1.68009500
C	1.36599900	-1.02881600	0.53342600
C	1.67713300	-2.18794500	-0.16493900
C	2.28074500	-0.66795800	1.51720000
C	2.80045300	-2.95617500	0.10471200
C	3.41045600	-1.40939400	1.82017200

C	3.67110200	-2.56716200	1.10688600
C	-1.14107100	-0.76581100	-0.57600900
C	-1.66337100	-1.95776300	-0.08076800
C	-1.78574200	-0.27454300	-1.70215700
C	-2.70967800	-2.64269000	-0.67256500
C	-2.83891500	-0.92582400	-2.32828000
C	-3.29971000	-2.12354500	-1.81369700
F	1.53303000	4.81120300	0.18186700
F	2.67613000	4.49255300	-2.26451800
F	2.53718500	2.07841200	-3.50797600
F	1.28284500	0.03191600	-2.33129500
F	0.28530800	2.80432600	1.36731200
F	2.10356900	0.46061200	2.22028300
F	4.24731300	-1.01739600	2.77973500
F	4.74979700	-3.29356500	1.37902700
F	3.04644600	-4.06388300	-0.59127200
F	0.89231300	-2.63008000	-1.15446800
F	-1.45080000	0.91782300	-2.22349200
F	-3.42165300	-0.39597000	-3.40146500
F	-4.31007400	-2.75943200	-2.39409300
F	-3.15664900	-3.78487600	-0.15722800
F	-1.14690700	-2.50237400	1.02835500
H	-1.83754700	1.70010200	0.04375800
H	-3.89565700	2.68496500	0.25455600
H	-5.34777700	2.75534200	2.08582200
H	-4.97258500	1.94891300	4.24927200
H	-3.06783000	0.85457700	5.06458900
H	-1.16227700	0.16764000	3.91811300

MC-BPhF

E = -2860.195151 a.u.

C	-2.01973000	-0.81708000	-2.47729700
C	-2.43655300	-2.89840300	-0.20944200
C	-5.69438200	0.12320100	-1.42651200
C	-6.60556400	-0.43284400	-2.22086900
C	-3.59321800	-3.07960800	-0.99996100
C	-3.92284200	-2.43546000	-2.15764400
C	-3.19468300	-1.41844800	-2.81867300
C	-1.39171600	-2.02949100	-0.34758600
C	-1.17985900	-1.02301000	-1.34040900
O	-0.18746900	-0.22356900	-1.27862100
O	-5.50929100	-0.20469500	-0.12794300
O	-4.81040700	1.06487500	-1.82291200
C	-4.34688300	0.47267200	0.34957600
C	-4.18134400	1.60250900	-0.65776500
H	-4.53617600	0.81853000	1.36434100
H	-3.49547300	-0.21526200	0.34925800
H	-4.70364300	2.51060700	-0.34747000
H	-3.14704400	1.83725300	-0.89880000
H	-7.25700700	-1.19986700	-1.83106300

H	-6.73304800	-0.06386600	-3.22694100
B	0.78692000	0.03395000	-0.09478000
C	1.79631300	-1.22962800	0.16336500
C	2.71966600	-1.12651700	1.19881800
C	1.93864200	-2.35419800	-0.63562800
C	3.70114600	-2.06679400	1.45043000
C	2.90788100	-3.32478500	-0.41968200
C	3.79525400	-3.18077200	0.63020100
C	1.72934200	1.26070100	-0.61873000
C	2.07853700	2.38405900	0.11885300
C	2.31818100	1.17289300	-1.87592500
C	2.92901400	3.37049200	-0.35855200
C	3.16790400	2.13765300	-2.39103200
C	3.47439800	3.24904100	-1.62413700
C	-0.22209400	0.43022300	1.14153500
C	-1.02707100	1.55798500	1.01213000
C	-0.44015800	-0.30178000	2.29948700
C	-1.95058600	1.95694600	1.96005000
C	-1.36359800	0.05427700	3.27428800
C	-2.12455300	1.19518400	3.10376500
F	2.98633400	-4.38978500	-1.21498300
F	4.72769100	-4.09957700	0.85260100
F	4.54975600	-1.91598500	2.46286600
F	2.67344200	-0.06490700	2.01322500
F	1.11771900	-2.57564500	-1.67801100
F	2.09034800	0.10426700	-2.65244300
F	3.69641600	2.00288700	-3.60600600
F	4.28820800	4.18632600	-2.09735000
F	3.22208500	4.43227600	0.38887500
F	1.59748700	2.57595600	1.35395700
F	0.20651700	-1.45779200	2.51560100
F	-1.53969300	-0.70652100	4.35039700
F	-3.04022600	1.53919700	4.00171700
F	-2.71108900	3.03558100	1.76158100
F	-0.94797700	2.31807700	-0.09073500
H	-0.60962700	-2.11539200	0.39494000
H	-2.36351000	-3.55891200	0.64952500
H	-4.28991500	-3.83141100	-0.64575100
H	-4.85820200	-2.71503500	-2.62718100
H	-3.65903000	-1.04378300	-3.72467500
H	-1.64639700	-0.03881600	-3.13400000

TS-BPhF-1

E = -2860.175239 a.u.

1 imaginary frequency -422.2905 cm⁻¹

C	1.94889600	0.79746100	-2.68791400
C	2.76886600	2.73188200	-0.37252300
C	3.81834000	-0.67481500	-1.44917200
C	2.89707900	-1.02431800	-2.40545000
C	3.64712600	3.10657900	-1.36808800

C	3.62719300	2.68389300	-2.70862600
C	2.85049800	1.71738400	-3.29197100
C	1.69166900	1.84053200	-0.39392600
C	1.26273400	0.99491700	-1.41255900
O	0.22351600	0.23297400	-1.31680400
O	5.02124200	-0.21506100	-1.72857000
O	3.51054700	-0.59996500	-0.17457900
C	5.57331100	0.39552300	-0.54830800
C	4.61117500	-0.04380900	0.55985200
H	6.59064100	0.03213500	-0.42323000
H	5.56220300	1.47626800	-0.70150600
H	5.00495500	-0.82266200	1.21327500
H	4.22711300	0.78565700	1.15245500
H	3.27961000	-1.20152900	-3.40107500
H	2.04287200	-1.60137200	-2.07508600
B	-0.65035200	-0.06391200	-0.08993400
C	-1.41675800	1.26311700	0.50076600
C	-2.12998300	1.14950000	1.68960100
C	-1.56454000	2.47932300	-0.15274100
C	-2.90552900	2.16236300	2.22344300
C	-2.33144300	3.52344400	0.34792500
C	-3.00556200	3.36590500	1.54403000
C	-1.85123500	-1.02967300	-0.64929900
C	-2.35421900	-2.14426600	0.01025800
C	-2.51222900	-0.69827500	-1.82758300
C	-3.41594100	-2.89778800	-0.46837800
C	-3.57196600	-1.42787300	-2.34224600
C	-4.02787600	-2.53982100	-1.65599700
C	0.40104100	-0.82009500	0.93040000
C	0.91709900	-2.05994800	0.56870700
C	0.96744000	-0.27866100	2.07401400
C	1.88955100	-2.73491900	1.28260100
C	1.96418200	-0.90528800	2.80932800
C	2.42344900	-2.14731000	2.41548500
F	-2.42253800	4.67446300	-0.31765300
F	-3.74343500	4.35598900	2.03649600
F	-3.55466100	1.99421300	3.37345500
F	-2.08336500	0.00182900	2.37822800
F	-0.95502200	2.72198600	-1.32299600
F	-2.15191400	0.38790100	-2.52524700
F	-4.15981300	-1.06443200	-3.48219800
F	-5.04491200	-3.25273800	-2.13107000
F	-3.84750800	-3.96468400	0.20256500
F	-1.81870000	-2.56435800	1.16382300
F	0.61396700	0.94179800	2.51409500
F	2.50820500	-0.30342600	3.86927200
F	3.40711400	-2.74566600	3.08704700
F	2.35828500	-3.90867400	0.86073900
F	0.51127000	-2.65738500	-0.56476300
H	1.08604400	1.83371100	0.50147200
H	2.89647000	3.24541500	0.57717100
H	4.36802700	3.87710000	-1.11493600

H	4.29845200	3.21381100	-3.37835600
H	2.97575200	1.58542600	-4.36193200
H	1.29022700	0.29087300	-3.38487900

TS-BPhF-2

E = -2860.1706481 a.u.

1 imaginary frequency -432.4066 cm⁻¹

C	-0.82120200	-2.72036600	-0.75925800
O	0.07873200	-0.59008600	-1.10950600
C	1.69765400	-2.89211700	-1.94527200
C	0.77388200	-3.83960800	-1.55826300
C	-2.80590500	-3.89277000	-1.75881000
C	-2.84268100	-3.33097300	-3.05168400
C	-2.19922400	-2.19571100	-3.48037000
C	-1.94363800	-3.60205600	-0.74036400
C	-1.35388000	-1.32281200	-2.77468100
C	-0.76572300	-1.50229000	-1.54147200
H	-3.54644300	-4.66074100	-1.55575000
H	-3.51811100	-3.80095200	-3.75866500
H	-2.42778800	-1.88146400	-4.49449700
H	-2.06794700	-4.16185600	0.18117600
H	-1.09984100	-0.38580800	-3.25506400
H	-0.32861300	-2.60481300	0.19451200
H	0.18916100	-4.26978700	-2.35989200
H	1.04087300	-4.46897000	-0.72091400
O	2.70673300	-2.48667500	-1.20428000
O	1.57362300	-2.22992600	-3.07469500
C	3.38491100	-1.41184700	-1.88500700
C	2.42214100	-1.05948000	-3.01493700
H	1.78576100	-0.20838000	-2.77761100
H	2.89938800	-0.94452600	-3.98502900
H	3.52697800	-0.59997100	-1.17562000
H	4.34745500	-1.79140400	-2.22969300
B	0.02698400	0.35246400	0.10698300
C	-1.14741400	-0.15578200	1.14893600
C	-2.45888900	-0.24997800	0.69234000
C	-0.98646500	-0.46753400	2.49452300
C	-3.52018200	-0.69969600	1.46050600
C	-2.02062000	-0.91605200	3.30310900
C	-3.29598300	-1.04351000	2.78130600
C	-0.38681200	1.85215900	-0.42250500
C	-0.33477900	2.28762500	-1.73772800
C	-0.82952300	2.80869300	0.48399600
C	-0.73602900	3.55124900	-2.14456200
C	-1.23614600	4.08256800	0.12600400
C	-1.19715900	4.45607700	-1.20656700
C	1.56578400	0.29532600	0.69534800
C	2.47905200	1.34447000	0.66132900
C	2.08514000	-0.89118400	1.20408300
C	3.79532600	1.23000500	1.09811100

C	3.38332800	-1.05294800	1.64969500
C	4.25266400	0.02422500	1.59586800
F	-2.76044700	0.11151600	-0.56610300
F	-4.74439000	-0.79453700	0.94463600
F	-4.29452900	-1.47739300	3.54294300
F	-1.79979400	-1.21380100	4.58165100
F	0.19441800	-0.32137200	3.10481100
F	-0.84372800	2.53039300	1.79637800
F	-1.65321600	4.94997400	1.04522000
F	-1.58305200	5.67286700	-1.57740800
F	-0.67052500	3.90186600	-3.42958900
F	0.14694500	1.50270400	-2.72691200
F	1.31064300	-1.98736900	1.29156400
F	3.80551800	-2.22630600	2.11478700
F	5.50731900	-0.10194800	2.01328100
F	4.61878500	2.27424100	1.03833300
F	2.14891400	2.55202500	0.18951400

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E = -2860.21737 a.u.

C	1.96449300	0.47292500	-2.66568600
C	2.78211400	2.26613200	-0.43428100
C	4.13872000	0.33724700	-1.28625200
C	3.11040200	-0.43501900	-2.12382600
C	3.90678300	1.88124300	-1.35355700
C	3.57202500	2.29580200	-2.77119800
C	2.60079900	1.63801100	-3.38513600
C	1.52098400	1.81439400	-0.50837500
C	1.10549600	0.83348900	-1.48568500
O	0.06581400	0.15362400	-1.36434100
O	5.42916300	0.01911400	-1.75358700
O	4.09857000	-0.02129500	0.08385600
C	6.24948400	-0.25007300	-0.62542600
C	5.24525000	-0.81328500	0.36231800
H	7.02532800	-0.95136100	-0.92875200
H	6.71088100	0.67070800	-0.24758400
H	5.03826300	-1.87201700	0.17347400
H	5.50968700	-0.67335200	1.40942500
H	3.62472500	-0.84776100	-2.99039200
H	2.70794300	-1.25992500	-1.53516100
B	-0.81886700	-0.06972400	-0.05086400
C	-1.71068500	1.25196900	0.28506200
C	-2.53749000	1.20072500	1.40242800
C	-1.84684500	2.39045900	-0.49479300
C	-3.42055700	2.20564200	1.74968000
C	-2.71942900	3.42461600	-0.18315600
C	-3.51078900	3.33232600	0.94644100
C	-1.85057800	-1.24633700	-0.49434500
C	-2.16052000	-2.36457300	0.26802100
C	-2.55752900	-1.12350500	-1.68525900

C	-3.09023000	-3.31453700	-0.12873900
C	-3.48860000	-2.05193600	-2.11938500
C	-3.75543400	-3.15961400	-1.33217200
C	0.31899500	-0.50891000	1.03852800
C	1.09780000	-1.63172700	0.77546100
C	0.70848000	0.21572500	2.15534400
C	2.17583500	-2.01810500	1.54644500
C	1.78458800	-0.13631100	2.95823500
C	2.52389600	-1.26162200	2.65023100
F	-2.79834500	4.49994600	-0.96394500
F	-4.35005000	4.31227700	1.25988300
F	-4.17919100	2.10454600	2.83676300
F	-2.48922800	0.12814100	2.20119300
F	-1.11783200	2.56033000	-1.61228200
F	-2.36304700	-0.05560400	-2.47251300
F	-4.13051200	-1.88715800	-3.27439600
F	-4.64596200	-4.06256700	-1.72710100
F	-3.34582700	-4.37334400	0.63606100
F	-1.56384600	-2.58204500	1.44512200
F	0.09651500	1.36402300	2.48073900
F	2.13119800	0.62122100	3.99622600
F	3.59073400	-1.58843400	3.37471800
F	2.91618200	-3.07338600	1.20409300
F	0.85172100	-2.37956000	-0.31284200
H	0.79141600	2.13555800	0.22208400
H	3.01845300	2.95046400	0.37423300
H	4.82807600	2.35196900	-1.01110600
H	4.10930400	3.11616800	-3.22928600
H	2.28022500	1.86919600	-4.39308300
H	1.33430400	-0.11894900	-3.32794700

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E = -2860.20005 a.u.

C	2.98716100	-2.01896300	-1.41689100
O	1.66674500	-0.05362100	-1.47846200
C	3.01964900	0.38947600	-1.29352400
C	3.79424100	-0.84551800	-0.85844500
C	2.87865900	-3.64895600	-3.29267500
C	1.58161300	-4.17972500	-2.92288400
C	0.54935300	-3.45352800	-2.42959300
C	3.49980400	-2.62002000	-2.69936400
C	0.55632100	-2.04370400	-2.11993100
C	1.65320300	-1.38983600	-1.71331100
H	3.35733400	-4.11049800	-4.15242900
H	1.38151000	-5.21160600	-3.19560500
H	-0.41412500	-3.95080600	-2.34729200
H	4.40917800	-2.20878500	-3.12765500
H	-0.36287600	-1.48538000	-2.23968700
H	4.81578800	-0.79349200	-1.23193300
H	3.82195900	-0.86681300	0.22920500

O	3.00926900	1.42128400	-0.36738700
O	3.50002300	0.91290800	-2.48134500
C	3.10683500	2.66601700	-1.06096400
C	3.01531000	2.25012100	-2.52746500
H	1.98326600	2.26708200	-2.88783900
H	3.65733200	2.82330600	-3.19312500
H	2.29229300	3.31911600	-0.74892500
H	4.06877000	3.12489300	-0.81847800
B	-1.02888700	0.35427300	0.80841900
C	0.30391000	0.76283600	1.51651900
C	1.33557000	-0.14603400	1.76587600
C	0.54718600	2.06940200	1.94382400
C	2.50717900	0.20170600	2.40629300
C	1.71892900	2.45493300	2.56986400
C	2.70654400	1.51340200	2.79968500
C	-1.57628400	-1.11353400	0.91579900
C	-2.18386100	-1.75047700	-0.16478800
C	-1.45651800	-1.87637500	2.07654200
C	-2.57469200	-3.07658900	-0.13260700
C	-1.86717600	-3.19405100	2.15646100
C	-2.41594000	-3.80137000	1.03707000
C	-1.85822000	1.40018700	-0.02155900
C	-3.24839400	1.45059200	0.05662200
C	-1.26673900	2.30526900	-0.89787200
C	-4.01091600	2.33457500	-0.68638500
C	-1.99706300	3.18728800	-1.67284100
C	-3.37861300	3.20294800	-1.56283100
F	3.46736800	-0.69915400	2.60168800
F	3.83737000	1.86603500	3.38510200
F	1.90349100	3.71572900	2.94720000
F	-0.37432700	3.02059700	1.78340700
F	-0.93647400	-1.33889300	3.18071500
F	-1.73591600	-3.88180400	3.28387200
F	-2.79410900	-5.06703700	1.08873400
F	-3.09296200	-3.65817100	-1.20874800
F	-2.38540700	-1.09921700	-1.31374500
F	0.05877500	2.34616000	-1.03175300
F	-1.38668500	4.01987400	-2.50978500
F	-4.09166900	4.04857700	-2.28790600
F	-5.33299500	2.35731800	-0.57120900
F	-3.90253300	0.63832000	0.88905600
F	1.24490500	-1.41179600	1.35658100
H	2.85392200	-2.81221700	-0.67342500

ω B97X-D/6-311G(d,p) gas phase computed total energies, unique imaginary frequency, and Cartesian coordinates of the stationary points involved in the non-catalyzed and LA catalyzed cycloaddition reactions of tropone **11** with ketene diethyl acetal **24**.

24

E = -386.258366752 a.u.

C	0.33758300	2.13629200	0.13445500
C	-0.01349000	0.86693000	-0.08438400
H	-0.44191900	2.87941400	0.20613100
H	1.36807700	2.44790700	0.20013900
O	-1.29883200	0.52695400	-0.28469500
O	0.80421800	-0.20063500	-0.16930200
C	2.18879100	0.00635400	0.06654800
H	2.32217000	0.47408300	1.04928100
C	-1.73689500	-0.73693200	0.22043100
H	-1.48537400	-0.81016100	1.28501700
H	-1.22643000	-1.54601400	-0.30718600
H	2.58771700	0.68991900	-0.69216300
C	2.87457100	-1.33957000	-0.00007000
H	3.94693100	-1.22119000	0.17158100
H	2.47392200	-2.01308900	0.76020900
H	2.72870900	-1.79654300	-0.98080000
C	-3.23249300	-0.80599800	0.00894100
H	-3.61825700	-1.76192700	0.37156500
H	-3.73602100	0.00052900	0.54550400
H	-3.47102600	-0.71594000	-1.05282400

MC-exp

E = -731.771014964 a.u.

C	3.14391600	-0.25622900	-0.18218300
C	2.65089400	0.33286900	0.93221300
C	1.44887800	0.01360100	1.64359500
C	0.53211300	-0.95049500	1.41224700
C	-2.09555600	1.49538000	1.67806300
C	-1.49980900	1.31110900	0.49430100
C	2.58274000	-1.34674300	-0.92447600
C	1.45466200	-2.05898900	-0.70850800
C	0.44220000	-1.95769900	0.35050100
H	4.07503000	0.14067200	-0.57452100
H	3.22568700	1.15689700	1.34359900
H	1.24152800	0.65590700	2.49417400
H	-0.31363100	-0.99979300	2.09060100
H	1.22069200	-2.85392000	-1.41057300
O	-0.51001700	-2.72865700	0.33675800

H	3.16050300	-1.63969600	-1.79717200
O	-0.48026900	2.10257200	0.11189100
O	-1.78595000	0.37608000	-0.42290100
C	0.15705000	1.85583200	-1.14252300
C	-2.85052900	-0.53341400	-0.14763600
H	0.56923100	0.84299100	-1.15819500
H	-2.59382800	-1.12169000	0.73885900
H	-1.75600200	2.30403800	2.30750600
H	-2.91405500	0.87631700	2.00766000
H	-0.57297100	1.93428300	-1.95279700
H	-3.76250000	0.04027900	0.05272100
C	1.24907400	2.89069100	-1.28979200
H	1.77715600	2.74203600	-2.23509000
H	0.83034500	3.89907600	-1.27883900
H	1.96976500	2.80485300	-0.47400800
C	-3.01146700	-1.42971500	-1.35258000
H	-2.10888400	-2.02294800	-1.50279200
H	-3.84510900	-2.11639100	-1.18778200
H	-3.21806900	-0.84006100	-2.24866500

TS-11-exp

E = -731.734166690 a.u.

1 imaginary frequency -429.4510 cm⁻¹

C	0.39772700	-0.67326500	2.25981300
C	-0.35956700	-1.66187200	1.63465900
C	-0.21946700	-2.20018200	0.36962800
C	0.58478500	-1.73589200	-0.71730600
C	-0.30447600	-0.51474900	-1.89005900
C	-0.64140100	0.57680000	-1.08699200
C	1.61249700	-0.15048700	1.79760100
C	2.30320100	-0.35982800	0.62573600
C	1.93419100	-1.07090100	-0.56801400
H	0.08870000	-0.37355000	3.25572300
H	-1.14968000	-2.10083100	2.24196500
H	-0.87606800	-3.03328300	0.12966000
H	0.67887600	-2.47077700	-1.51414200
H	3.28110200	0.10318200	0.53384700
O	2.68424300	-1.13321300	-1.54058000
H	2.11300900	0.51495100	2.49990300
O	-1.74161200	0.70117300	-0.38259800
O	0.25823800	1.49210100	-0.87146600
C	-2.83728800	-0.21917500	-0.57131900
C	0.10722800	2.39912700	0.24458700
H	-3.26189400	-0.03882000	-1.56413000
H	-0.79193300	2.99836200	0.08752000
H	-1.12307600	-1.09595300	-2.29424600
H	0.52097400	-0.33905200	-2.57012900
H	-2.45841400	-1.23812400	-0.51308500
H	-0.01737700	1.79417900	1.14807400

C	1.35776600	3.24049800	0.29593100
H	1.48320100	3.81364100	-0.62453200
H	1.29004900	3.93855400	1.13351200
H	2.23189500	2.60334200	0.43674900
C	-3.83076700	0.05310900	0.53095900
H	-4.18596500	1.08445400	0.49224900
H	-4.68843500	-0.61431500	0.42347800
H	-3.36850000	-0.12553700	1.50339200

IN-1-exp

E = -731.739458 a.u.

C	-0.16762400	-0.65021700	1.86178200
C	-0.30517700	-1.95379700	1.30306300
C	0.32949000	-2.42625800	0.20426300
C	1.06888000	-1.57858400	-0.76792100
C	0.12972300	-0.64031400	-1.65496000
C	-0.56322100	0.46084300	-0.97532700
C	0.98594000	0.13069300	1.76944700
C	2.10402700	0.01378500	0.96131800
C	2.26198800	-0.76809400	-0.22709900
H	-0.87032300	-0.37702900	2.64419500
H	-0.95916600	-2.64101900	1.83930100
H	0.23559900	-3.47861600	-0.04491400
H	1.52346100	-2.21769200	-1.52641800
H	2.94935500	0.66363600	1.16519900
O	3.28868400	-0.78195700	-0.90288500
H	1.02736500	0.95549800	2.48300900
O	-1.82737700	0.52917400	-0.70311400
O	0.11597700	1.53413900	-0.79480500
H	-0.58802100	-1.26806700	-2.18220200
H	0.80399600	-0.17508200	-2.37764300
C	-0.39791500	2.58120900	0.07099600
H	-0.73503300	2.09123200	0.98793100
H	-1.24925600	3.04749700	-0.42790100
C	0.73998600	3.53885100	0.31556900
H	1.08081500	3.99022900	-0.61769000
H	0.40366800	4.33427100	0.98424500
H	1.57572900	3.01284600	0.77855600
C	-2.66901600	-0.65936200	-0.69139900
H	-3.14512300	-0.71185800	-1.67308200
H	-2.04173300	-1.53201600	-0.52066500
C	-3.66530100	-0.48199000	0.42651000
H	-4.32992300	-1.34814600	0.45642700
H	-3.14063600	-0.41221100	1.38058400
H	-4.26974700	0.41508500	0.28004600

TS-12-exp

E = -731.738615460 a.u.

1 imaginary frequency -201.0834 cm⁻¹

C	-0.26023700	-1.04989800	1.51674900
C	-0.08892900	-2.29777500	0.83146000
C	0.75308900	-2.48055600	-0.20101300
C	1.37781900	-1.33188500	-0.91133500
C	0.27963800	-0.39768200	-1.56513600
C	-0.72790600	0.27838600	-0.71655600
C	0.78547400	-0.15406600	1.78333000
C	2.01684000	-0.01104300	1.17831200
C	2.39884700	-0.51589500	-0.10809000
H	-1.10904300	-0.98832500	2.19281500
H	-0.66876000	-3.14441900	1.19233000
H	0.90427700	-3.47057800	-0.61689400
H	1.94639900	-1.68864100	-1.77140500
H	2.72971600	0.68286900	1.61305800
O	3.46234200	-0.23267600	-0.65656000
H	0.59213100	0.53433500	2.60675500
O	-1.93772000	-0.20764900	-0.76873300
O	-0.64417200	1.51462300	-0.31190400
H	-0.28795000	-1.02607100	-2.24997900
H	0.81115300	0.35862900	-2.14729500
C	0.53088900	2.34524600	-0.53908900
H	0.37324500	2.83221600	-1.50573100
H	1.42518600	1.72909600	-0.57068600
C	-2.95455200	0.37330500	0.07134200
H	-3.18418700	1.37463500	-0.29841600
H	-2.53713900	0.45483700	1.07856800
C	-4.14797800	-0.54887300	0.02474700
H	-3.87882700	-1.53867300	0.39713600
H	-4.94561800	-0.14474200	0.65177900
H	-4.52584600	-0.64834700	-0.99444800
C	0.60483500	3.34250800	0.58849000
H	1.44209400	4.02047100	0.40966500
H	-0.31184700	3.93133100	0.65699700
H	0.77445600	2.82636400	1.53406800

TS-2-exp

E = -731.736726155 a.u.

1 imaginary frequency -479.7894 cm⁻¹

C	-0.95021900	-1.42531300	0.28738300
C	-0.80109800	-0.19036100	1.11354500
O	0.27279600	-0.08138300	1.73337100
C	0.10994600	-0.95787600	-1.30166800
C	-3.33844800	-1.32134600	-0.51473700
C	1.07713800	-0.02152700	-0.92217600
C	-3.65444200	0.02836900	-0.36262900
C	-2.94548300	0.96737800	0.38399500

C	-2.18509900	-1.98327100	-0.14997200
C	-1.75993400	0.85957400	1.08893000
H	-4.11155500	-1.93832700	-0.96741200
H	-4.59674500	0.36006600	-0.78572900
H	-3.42354000	1.94209300	0.45857100
H	-2.16688600	-3.05371300	-0.33521400
H	-1.45537100	1.71718600	1.68171400
H	-0.25918100	-2.17367100	0.66308100
H	-0.68817100	-0.52502700	-1.89125900
H	0.45767800	-1.93026300	-1.62662900
O	2.29255000	-0.26057500	-0.48271100
O	0.74360600	1.24102700	-0.96148600
C	2.60648400	-1.55434900	0.06382000
C	1.47947800	2.19103100	-0.14833500
H	1.50822200	1.78992900	0.86620300
H	2.43909300	-2.32116500	-0.69858900
H	1.93363800	-1.70563200	0.90979500
H	2.49410500	2.27601500	-0.54206800
C	4.05209400	-1.51838200	0.49647100
H	4.32708400	-2.48343900	0.92759100
H	4.71028600	-1.31684300	-0.35107900
H	4.20322100	-0.74704300	1.25326000
C	0.72967700	3.49830000	-0.22683000
H	-0.28580300	3.37495100	0.15241100
H	1.24247900	4.24769800	0.38056200
H	0.67925500	3.86126700	-1.25538700

TS-3-exp

E = -731.731742134 a.u.

1 imaginary frequency -460.9115 cm⁻¹

C	0.28648800	1.99512400	-1.23052100
C	1.56719000	1.99184000	-0.59792700
C	1.83486500	1.49381100	0.66602800
C	0.98713700	0.90213300	1.59299000
C	0.04050200	-0.75215200	-1.19315600
C	-0.06935200	0.32299000	-2.09373800
C	-0.90087200	2.31623700	-0.41891900
C	-1.20392700	1.82530300	0.78952500
C	-0.44490100	0.83871000	1.59459100
H	0.28757000	2.55653900	-2.16237100
H	2.41053100	2.31838300	-1.19668200
H	2.88576800	1.50746900	0.94994900
H	1.44053600	0.42684700	2.45839400
H	-2.14496900	2.11351400	1.25047200
O	-1.07638100	0.05850500	2.31947500
H	-1.61049100	2.99809700	-0.88260400
H	0.74879500	0.34635400	-2.80325600
H	-1.04559700	0.46778300	-2.54271600
O	1.23839300	-1.20714900	-0.94011800

O	-0.92420400	-1.35599400	-0.54891100
C	1.43648900	-2.02933400	0.23441700
H	0.98248600	-3.00578500	0.05408100
H	0.92527600	-1.54616700	1.07148600
C	-2.30784500	-1.00213000	-0.76940700
H	-2.58835200	-1.37476100	-1.76004200
H	-2.40110500	0.08298800	-0.74494600
C	2.92482000	-2.11575900	0.45990000
H	3.33534900	-1.12019000	0.63694900
H	3.12245300	-2.73538900	1.33736200
H	3.43022600	-2.55932200	-0.40030300
C	-3.10892300	-1.63457800	0.34176900
H	-4.16717500	-1.40286500	0.19884500
H	-2.98862600	-2.71984700	0.33954100
H	-2.77517700	-1.22971500	1.29896200

28-exp

E = -731.802069371 a.u.

C	0.37075700	0.05872400	1.29839200
C	1.11397300	-1.23043500	1.58184600
C	1.87416300	-1.73063800	0.61949900
C	1.93428500	-0.98581900	-0.69395500
C	0.50275000	-0.61947400	-1.15935900
C	-0.42420000	-0.13064900	-0.02856500
C	1.30188000	1.24215400	1.19103000
C	2.36115500	1.32646000	0.38438200
C	2.79656700	0.26994900	-0.56145400
H	-0.36177600	0.24455000	2.08416400
H	0.99698200	-1.70877500	2.54623000
H	2.44439300	-2.64365900	0.74206100
H	2.41785600	-1.58642600	-1.46448200
H	2.98440000	2.21443200	0.38083000
O	3.79757500	0.41368000	-1.22629100
H	1.07503000	2.09457700	1.82574500
O	-1.42655800	-1.05472300	0.32409800
O	-0.99639700	1.06549400	-0.49616900
C	-2.31409700	-1.46311900	-0.70688000
C	-1.87569900	1.74287900	0.38892700
H	-2.44785900	-0.65123800	-1.42919200
H	-2.50239500	1.01993300	0.92136300
H	0.06945100	-1.51052100	-1.61342700
H	0.54102700	0.15316600	-1.92802900
H	-1.29490400	2.30395300	1.13370400
H	-1.89567200	-2.32788100	-1.23726700
C	-3.63606300	-1.83415600	-0.06745600
H	-4.33039000	-2.21298800	-0.82164700
H	-3.48882400	-2.60837300	0.68845900
H	-4.08897500	-0.96467600	0.41475000
C	-2.72315400	2.68870200	-0.43458600

H	-3.38962200	3.26407400	0.21272300
H	-2.08928600	3.38464000	-0.98787200
H	-3.33029800	2.13213500	-1.15214400

29-exp

E = -731.800801942 a.u.

C	3.75562200	-0.00827200	0.94616900
C	4.11042400	-0.27827100	-0.43079600
C	3.32603600	-0.04390000	-1.50967300
C	2.52136600	-0.04144100	1.46690900
C	1.97003900	0.44535600	-1.52720300
C	1.31922200	-0.55769800	0.72269000
C	1.10065800	0.27170600	-0.52072400
H	4.57291300	0.28580600	1.60007100
H	5.13925400	-0.57168500	-0.61697100
H	3.78536500	-0.17133600	-2.48636000
H	2.36504700	0.29782100	2.48736300
H	1.61637700	0.95101700	-2.41860000
H	1.48106500	-1.60084500	0.42509900
O	-0.14742700	0.80025200	-0.53766300
C	-0.96387700	0.06578100	0.36581400
C	-0.00858300	-0.38405900	1.46744000
H	0.05360600	0.42400800	2.19810100
H	-0.35156400	-1.28452100	1.97434300
O	-1.46245000	-0.98355100	-0.41369000
O	-1.95152900	0.86488300	0.87742300
C	-2.32626700	-1.89997400	0.24615000
C	-2.82196700	1.48775400	-0.07834100
H	-3.83285100	1.37512800	0.32135200
H	-2.76835400	0.94876100	-1.02689700
H	-2.98274700	-1.36090700	0.93743900
H	-1.73334600	-2.61712400	0.82810700
C	-3.13195600	-2.62108200	-0.81294600
H	-2.46834300	-3.12427200	-1.51895700
H	-3.78144200	-3.36886500	-0.35134100
H	-3.75267600	-1.91466900	-1.36811100
C	-2.46791000	2.95178200	-0.25268500
H	-2.49893200	3.46852100	0.70905600
H	-1.46633800	3.05215200	-0.67218400
H	-3.18262200	3.43225400	-0.92688900

30-exp

E = -731.793099029 a.u.

C	-1.28921600	-1.70620500	-1.13517800
C	-0.81316900	-2.54742400	0.03461200
C	-0.28208500	-1.91046000	1.06769100

C	-0.16483300	-0.40783300	0.99141900
C	0.54679700	-0.05683000	-0.36401000
C	-0.17029300	-0.71631100	-1.55888000
C	-2.54965100	-0.96079500	-0.75632900
C	-2.64112900	-0.09295700	0.25379800
C	-1.51670300	0.28713200	1.14468300
H	-1.51154600	-2.34641900	-1.99005400
H	-0.91627400	-3.62542100	-0.00036500
H	0.09310400	-2.42824800	1.94226700
H	0.44367000	-0.00426700	1.79929500
H	-3.57461000	0.41532900	0.47186300
O	-1.66960000	1.15229600	1.97968700
H	-3.43383200	-1.14509500	-1.36100500
H	0.59654300	-1.25591000	-2.11327600
H	-0.59078800	0.03747200	-2.22477400
O	1.82986400	-0.61538900	-0.37226100
O	0.72726600	1.33776300	-0.45549800
C	-0.26689600	2.18590400	-1.00674300
H	-0.07179100	2.32275200	-2.07864900
C	2.73727000	-0.20336300	0.64172900
H	2.54444400	-0.76631100	1.56490400
H	-1.26692500	1.75356000	-0.90744600
H	2.60941900	0.86188800	0.84913500
C	4.13652700	-0.48926100	0.13993900
H	4.33919800	0.08969600	-0.76317300
H	4.87456900	-0.22330900	0.90087900
H	4.24834200	-1.54961900	-0.09720200
C	-0.20935700	3.50992700	-0.27474500
H	0.79337900	3.93766800	-0.33981500
H	-0.91851400	4.21711200	-0.71292300
H	-0.46219100	3.36260400	0.77699900