

Electronic Supplementary Information

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Understanding the Higher-Order Cycloaddition Reactions of Heptafulvene, Tropone and its Nitrogen Derivatives with Electrophilic and Nucleophilic Ethylenes inside the Molecular Electron Density Theory

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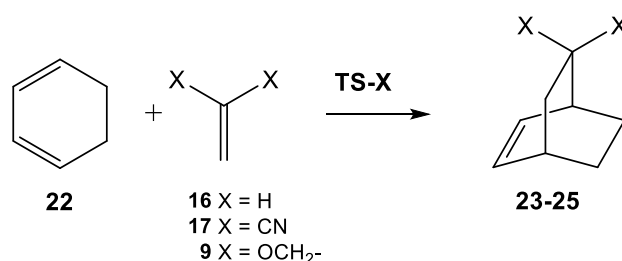
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*Study of the Diels-Alder reactions of cyclohexadiene **22** with ethylene **16**, DCE **17**, and CKA **9**.*

The Diels-Alder (DA) reactions of cyclohexadiene (CHD) **22** with ethylene **16**, DCE **17**, and CKA **9** were also studied as energy references for the [4+2] cycloadditions of the CHT derivatives **1,13-15**. The stationary points involved in these DA reactions are represented in Scheme S1, while the gas phase total and relative energies are given in Table S1.



Scheme S1. DA reactions of CHD **22** with ethylene **16**, DCE **17**, and CKA **9**.

Some appealing conclusions can be obtained from the relative energies given in Table S1: i) the non-polar DA (N-DA) reaction of CHD **22** with ethylene **16** presents a very high activation energy of 20.0 kcal·mol⁻¹ because of the non-polar character of the reaction (see later). This activation energy is closer to that for the N-DA reaction between butadiene **26** and ethylene **16**, 21.3 kcal·mol⁻¹ (see Figure S2); ii) the polar (P-DA) reaction of CHD **22** with DCE **17** presents a very low activation energy of only 7.2 kcal·mol⁻¹. The considerable reduction of this activation energy with respect to that with ethylene **16** is a consequence of the high polar of the reaction, resulting from the strong electrophilic character of DCE **16** and the strong nucleophilic character of CHD **22** (see Table 2); iii) the N-DA reaction of CHD **22** with CKA **9** presents a activation energy even higher than the unfavorable N-DA reaction with ethylene **16**, 24.2 kcal·mol⁻¹, as a consequence of the high nucleophilic character of the two species; iv) the three DA reactions as strongly exothermic by more than -39.2 kcal·mol⁻¹. Consequently, these DA reactions can be considered irreversible; finally, v) the substitution on the ethylene only affects the kinetics of the reactions as the thermodynamics remain unchanged.

Table S1. ω B97X-D/6-311G(d,p) total (E, in au) and relative (ΔE , in kcal·mol⁻¹) energies of the stationary points involved in the cycloaddition reaction of cycloaddition reactions of CHD **22** with ethylene **16**, DCE **17**, and CKA **9**.

	E	ΔE
16	-78.579526	
17	-263.025126	
9	-306.422249	
22	-233.393147	
TS-5	-311.940838	20.0
23	-312.040605	-42.6
TS-6	-496.406828	7.2
24	-496.485587	-42.2
TS-7	-539.776770	24.2
25	-539.877895	-39.2

The geometries of the three TSs are given in Figure S1. **TS-5**, with C–C distances between the four interacting carbons of 2.251 Å, is associated with a synchronous C–C single bond formation process. These distances are very similar to those found in the TS of the N-DA reaction between butadiene **26** and ethylene **16**, 2.243 Å (see Figure S2). The C–C distances between the four interacting carbons at **TS-6**, 1.980, and 2.840 Å, indicate that this TS corresponds with a high asynchronous single bond formation process characterized by the nucleophilic attack of one terminal carbon of the diene system of CHD **22** on the β -conjugated position of DCE **17**, which corresponds with the most electrophilic center of this molecule. Finally, these C–C distances at **TS-7**, 1.918, and 2.747 Å, indicate that this TS also corresponds with a high asynchronous single bond formation process. At these unfavorable TSs, the shorter distance corresponds with the most nucleophilic center of CKA **9**.

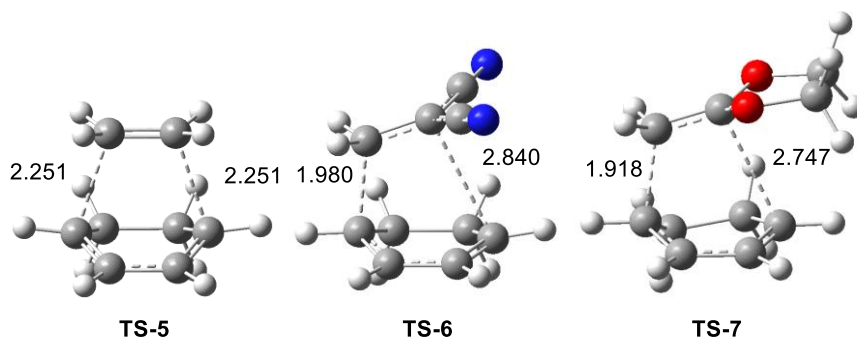


Figure S1. ω B97X-D/6-311G(d,p) geometries of the TSs involved in cycloaddition reactions of CHD22 with ethylene **16**, DCE **17**, and CKA **9**. The distances are given in Angstroms Å.

Analysis of GEDT at TSs associated with these three DA reactions permits assessment of the polar character of these cycloaddition reactions. GEDT values lower than 0.05 e correspond with non-polar processes, while values higher than 0.20 e correspond with polar processes. The GEDT values at the TSs are -0.02 e (**TS-5**), -0.31 e (**TS-6**), and 0.22 e (**TS-7**). These values indicate that while the DA reaction with ethylene **5** is non-polar, those with DCE **17** or CKA **9** have polar nature. The high GEDT found at the most favorable **TS-7** is a consequence of the strong nucleophilic character of CHD **22** and the strong electrophilic character of DCE **17** (see Table 2).

The electronic nature of these ethylene derivatives changes the classification of these DA reactions based on the electron density flux at the TSs: thus, the N-DA reaction with ethylene **16** is classified as the null electron density flux (NEDF), the P-DA reaction with DCE **17** is classified as the forward electron density flux (FEDF), and the P-DA reaction with CKA **9** is classified of the reverse electron density flux (REDF).

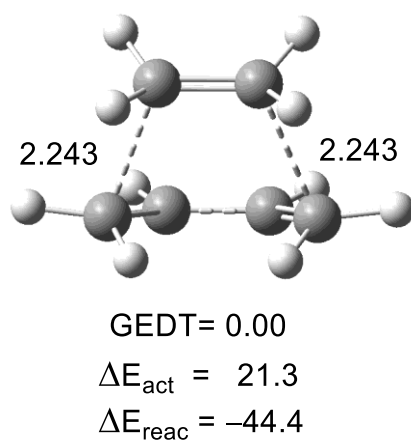


Figure S2. ω B97X-D/6-311G(d,p) geometry of the TS involved in the N-DA reaction between butadiene **26** and ethylene **16**. Relative energies, with respect to the *s-trans* conformation of butadiene **26**, are given in kcal·mol⁻¹, the GEDT is given in e, and the distances are shown in Angstroms Å.

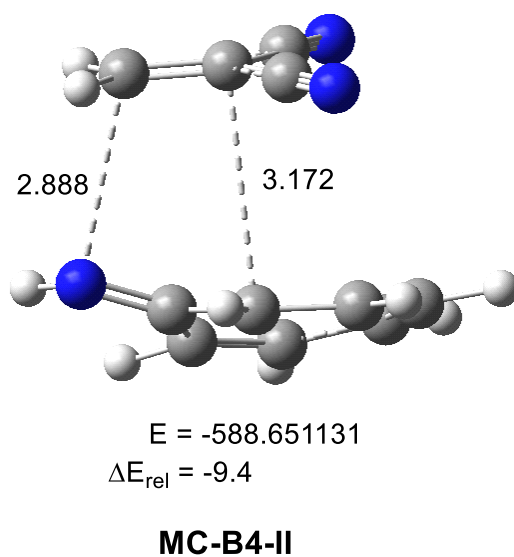


Figure S3. ω B97X-D/6-311G(d,p) geometry of **MC-B4-II** involved in the polar cycloaddition reaction between imine **14** and DCE **17**. The total electronic energy E is given in au, while the relative energy ΔE_{rel} with respect to the separated reagents is given in $\text{kcal}\cdot\text{mol}^{-1}$. The distances are shown in Angstroms Å.

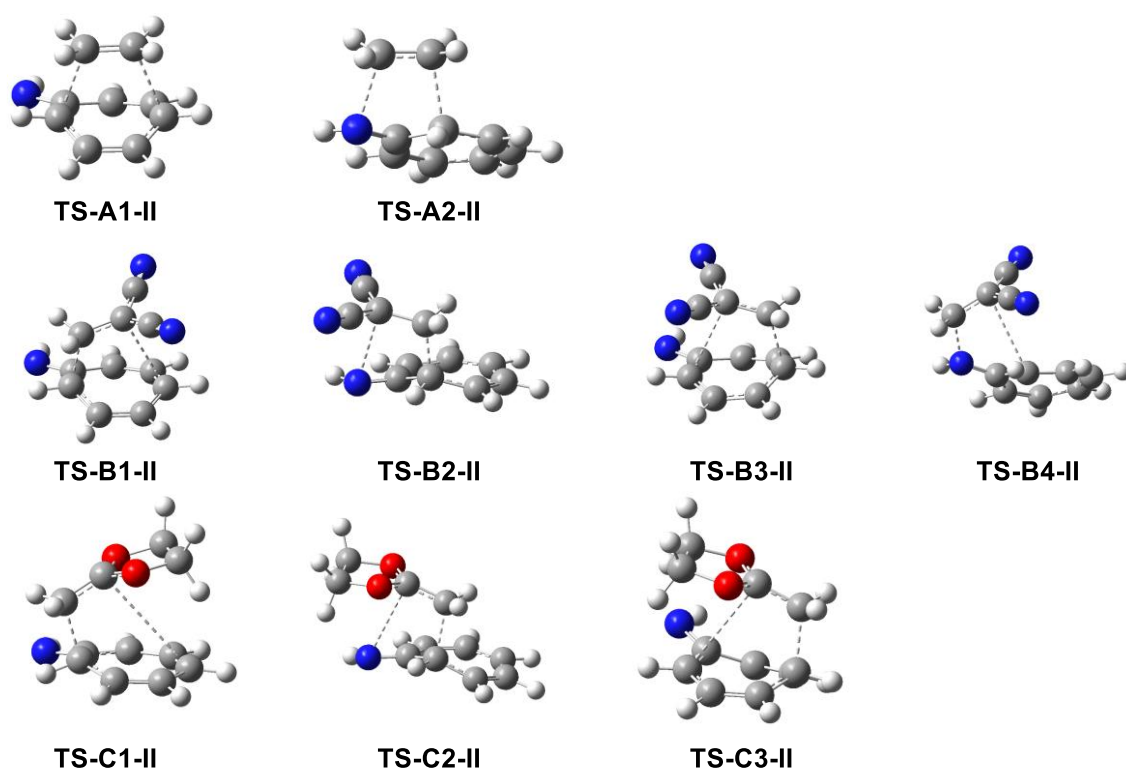


Figure S4. ω B97X-D/6-311G(d,p) geometries of the TSs involved in the competitive A, B and C reaction paths associated with the cycloaddition reactions of imine **14** with ethylene **16**, at the top, DCE **17**, in the middle, and CKA **9**, at the bottom.

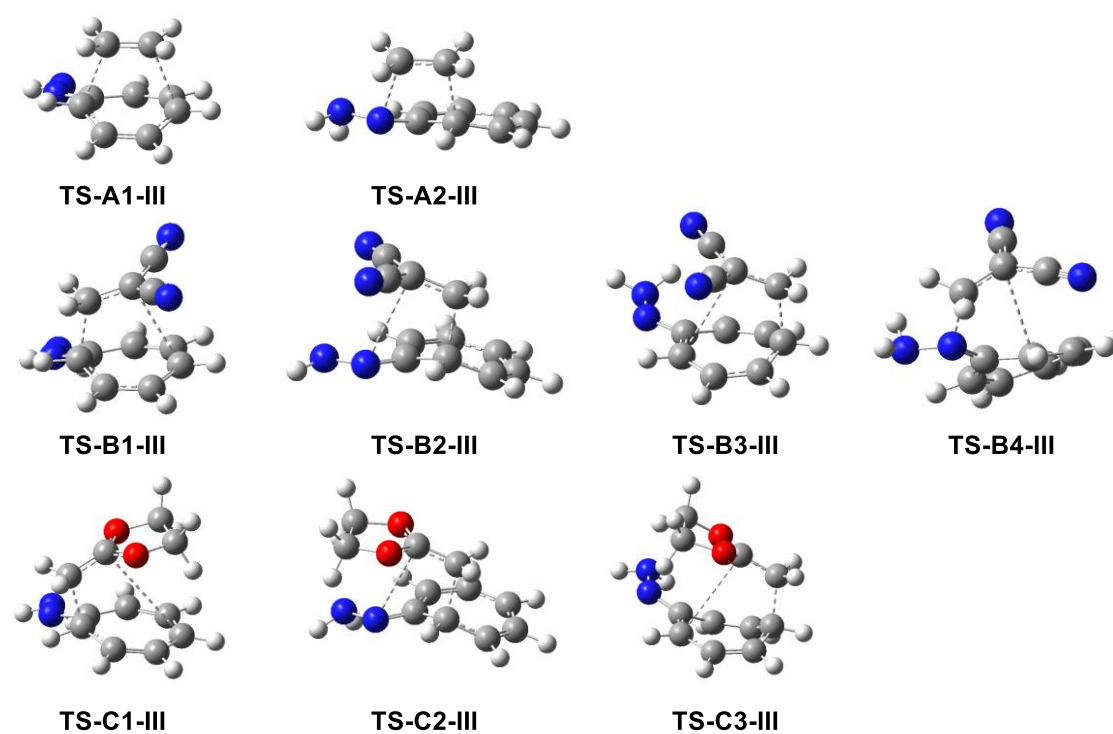


Figure S5. ω B97X-D/6-311G(d,p) geometries of the TSs involved in the competitive A, B and C reaction paths associated with the cycloaddition reactions of ylidenehydrazine **15** with ethylene **16**, at the top, DCE **17**, in the middle, and CKA **9**, at the bottom.

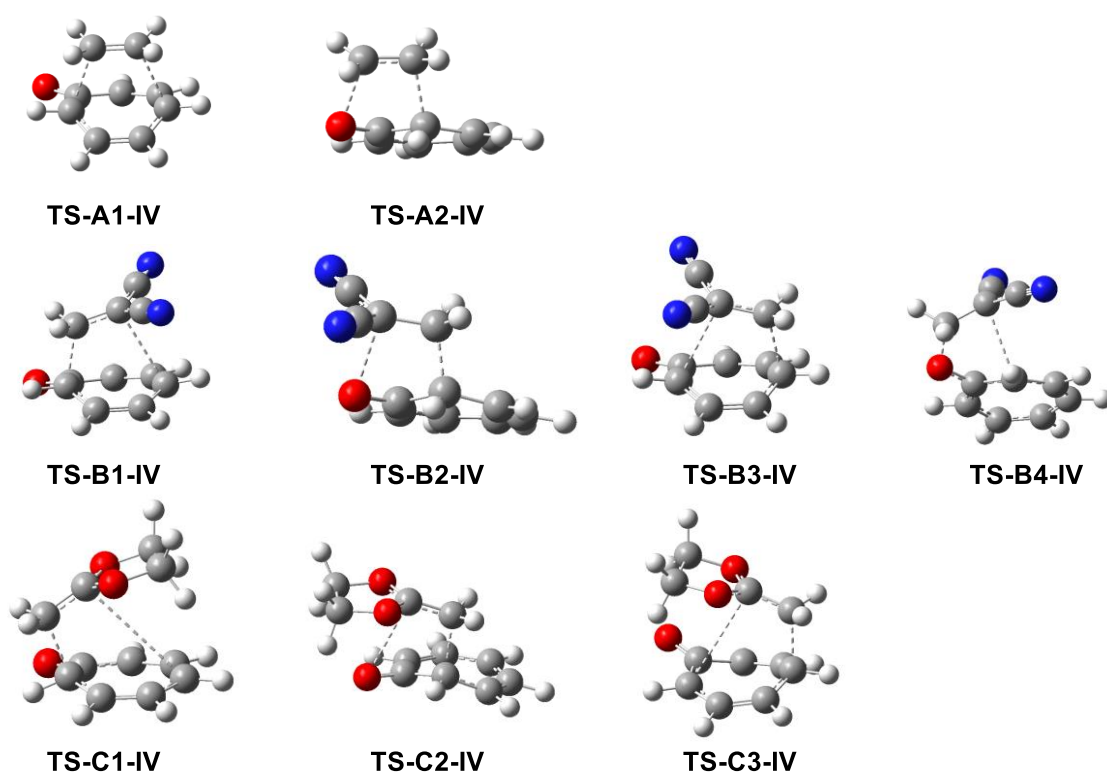


Figure S6. ω B97X-D/6-311G(d,p) geometries of the TSs involved in the competitive A, B and C reaction paths associated with the cycloaddition reactions of tropone **1** with ethylene **16**, at the top, DCE **17**, in the middle, and CKA **9**, at the bottom.

Table S2. ω B97X-D/6-311G(d,p) total (E, in au) energies of the stationary points involved in the cycloaddition reaction of cycloaddition reactions of the CHT derivatives **1**, **13-15** with ethylene **16**, DCE **17**, and CKA **9**.

ethylene 16	-78.579526			
DCE 17	-263.025126			
CKA 9	-306.422249			
	C	O	N	NN
X	-309.561791	-345.495830	-325.611059	-380.937517
TS-A1-X	-388.102853	-424.040919	-404.154739	-459.477615
TS-A2-X	-388.093666	-424.025940	-404.144946	-459.465197
TS-B1-X	-572.565402	-608.496980	-588.614514	-643.938882
TS-B2-X	-572.566543	-608.480629	-588.607480	-643.938382
TS-B3-X	-572.565402	-608.489057	-588.609530	-643.944461
TS-B4-X	-572.585978	-608.501517	-588.637838	-643.960768
TS-C1-X	-615.952762	-651.896966	-632.010446	-687.334781
TS-C2-X	-615.949867	-651.899627	-632.010289	-687.338702
TS-C3-X	-615.944625	-651.892775	-632.003627	-687.323271
CA-A1-X	-388.199617	-424.128922	-404.247635	-459.571798
CA-A2-X	-388.215067	-424.113309	-404.253484	-459.572518
CA-B1-X	-572.641342	-608.566393	-588.687299	-644.013875
CA-B2-X	-572.657009	-608.543226	-588.689572	-644.012004
CA-B3-X	-572.641342	-608.564016	-588.685579	-644.013468
CA-B4-X	-572.655903	-608.547265	-588.690210	-644.009205
CA-C1-X	-616.035355	-651.964067	-632.083243	-687.408356
CA-C2-X	-616.050910	-651.965842	-632.099347	-687.422289
CA-C3-X	-616.034294	-651.965245	-632.084875	-687.409450

ω B97X-D/6-311G(d,p) gas phase Cartesian coordinates of the stationary points involved in the cycloaddition reactions of heptafulvene **13** with ethylene **16**, DCE **17**, and CKA **9**.

Heptafulvene **13**

C	-1.88403600	0.67215300	0.00004400
C	-1.88403600	-0.67215300	0.00004200
C	-0.74139700	-1.56372500	-0.00003800
C	0.57299200	-1.28377200	-0.00005700
C	-0.74139700	1.56372500	-0.00003400
C	0.57299200	1.28377200	-0.00005400
H	-2.85205800	1.16415200	0.00010000
H	-2.85205800	-1.16415100	0.00009700
H	-0.99584400	-2.61995600	-0.00008500
H	1.23890000	-2.14331300	-0.00012000
H	1.23890100	2.14331400	-0.00011500
H	-0.99584400	2.61995600	-0.00007800
C	1.28225300	0.00000000	0.00000500
C	2.62803600	0.00000000	0.00008600
H	3.19277900	-0.92494900	0.00012000
H	3.19277900	0.92494800	0.00012200

TS-A1-I

C	1.53653800	0.91488600	-0.30407500
C	1.50929500	-0.08740800	-1.26964800
C	0.46831800	-0.98917100	-1.39252200
C	-0.64304200	-1.02987900	-0.54872300
C	0.39705200	-1.28602300	1.39692400
C	1.46156000	-0.41238400	1.52913300
C	0.39072700	1.74644900	0.07050900
C	-0.90866100	1.42554500	0.08804500
H	2.49263700	1.41370400	-0.16959100
H	2.43817600	-0.31554800	-1.78372200
H	0.65105900	-1.87505400	-1.99418000
H	-1.21295400	-1.95602100	-0.59923700
H	-1.61322200	2.20301600	0.36965300
H	0.65106600	2.76135900	0.36009600
H	0.59288600	-2.32636000	1.16763400
H	-0.52631700	-1.08974600	1.92763300
H	1.36061700	0.46191200	2.15972900
H	2.47352900	-0.76520600	1.37272100
C	-1.49627400	0.10794500	-0.13753200
C	-2.81177600	-0.08690400	0.05519200
H	-3.27063100	-1.05725000	-0.09527700
H	-3.45926700	0.72685000	0.36071900

TS-A2-I

C	-0.47807200	0.72953400	-0.58481400
C	-0.29626100	-0.72575000	-0.78752100
C	-1.73747400	-1.29106700	0.83168300
C	-2.52791100	-0.14613400	0.82943700
C	2.08265800	-1.11855600	-0.03336900
C	2.47413500	0.12537600	0.44016000
C	1.76122500	1.32075400	0.44290400
C	0.86831700	-1.46429500	-0.62079100
C	0.47226800	1.57355500	-0.01292400
H	2.82004700	-1.91212500	0.03589700
H	3.47875800	0.17902300	0.85107700
H	2.28607500	2.17928400	0.85075800
H	0.80084700	-2.49460400	-0.96340300
H	0.14288100	2.60467200	0.09759700
H	-1.00098000	-1.15360000	-1.49219000
H	-0.96581200	-1.40976200	1.58154800
H	-2.11104500	-2.20815500	0.39113000
H	-2.38529700	0.60282400	1.59908000
H	-3.52932200	-0.18833100	0.41646800
C	-1.79394900	1.15551600	-0.73609400
H	-2.05408600	2.18717300	-0.52076500
H	-2.43167900	0.66000500	-1.45921600

CA-A1-I

C	-1.54150300	0.69223300	0.11686400
C	-1.32005500	-0.17536800	1.33768800
C	-0.32037700	-1.04760400	1.30176700
C	0.53789500	-1.09844900	0.05785400
C	-0.36474400	-1.16072800	-1.20380400
C	-1.59350300	-0.22910900	-1.12658300
C	-0.43928900	1.72284100	-0.02784300
C	0.86668400	1.44622600	-0.07318100
H	-2.49551400	1.21688000	0.20082800
H	-1.96589300	-0.06751300	2.20243700
H	-0.08854700	-1.69762500	2.13845300
H	1.16490100	-1.99270000	0.07535900
H	1.56942600	2.27014600	-0.16619100
H	-0.74755000	2.76177100	-0.10156400
H	-0.69975400	-2.19395000	-1.32387200
H	0.24818800	-0.92394400	-2.07696100
H	-1.66696500	0.38529300	-2.02752600
H	-2.50993400	-0.82242100	-1.06537200
C	1.46396000	0.10539200	-0.00104200
C	2.79149900	-0.04327400	-0.01652000
H	3.25443000	-1.02278500	0.03550300
H	3.45380200	0.81389700	-0.08228900

CA-A2-I

C	0.34426500	0.81951900	0.05678800
C	0.36910700	-0.58498100	0.62418100
C	1.86293500	-0.93890600	0.68922700
C	2.49253200	-0.11311600	-0.44058400
C	-1.74773200	-1.29252300	-0.48486700
C	-2.53669500	-0.20996100	0.06066000
C	-2.10353900	1.05956000	0.26047200
C	-0.42345900	-1.44280400	-0.32356100
C	-0.77559700	1.55506700	-0.01967400
H	-2.28133200	-2.01841100	-1.09284900
H	-3.59784400	-0.40183700	0.19402700
H	-2.84904800	1.80084000	0.53657500
H	0.10114400	-2.22528600	-0.86772500
H	-0.70075400	2.59053700	-0.34401200
H	-0.11139900	-0.60808700	1.60956000
H	2.04506800	-2.01227900	0.59463600
H	2.27423800	-0.61893200	1.65180000
H	2.29645000	-0.59160000	-1.40614900
H	3.57362800	-0.00060100	-0.33893300
C	1.73687700	1.22198700	-0.36498500
H	1.75427400	1.78985500	-1.29723800
H	2.18341000	1.85275000	0.41436200

TS-B1-I

C	-0.32984800	-0.73636300	1.75255000
C	-0.35423700	-1.86802100	0.96294500
C	0.36652400	-2.04911300	-0.20894800
C	1.08115800	-1.04746200	-0.89515300
C	-0.32427200	0.01571700	-1.62987000
C	-1.22120700	0.61032300	-0.71185700
C	0.68765300	0.26888900	1.86904500
C	1.71905000	0.52652300	1.04119000
C	2.00817400	-0.05649300	-0.25989400
H	-1.10528900	-0.68000300	2.51131400
H	-1.09440200	-2.62127600	1.20891200
H	0.15780800	-2.95510000	-0.77077600
H	1.49985300	-1.40093100	-1.83597300
H	2.40983900	1.30510400	1.34990400
H	0.60068500	0.90227200	2.74487700
H	-0.76645300	-0.71075300	-2.30322600
H	0.37016300	0.69909400	-2.11366300
C	-0.93092800	1.88197600	-0.16203600
N	-0.62637600	2.90830600	0.27221100
C	-2.49348200	0.02460200	-0.48066400
N	-3.51404300	-0.49472600	-0.32754900

C	3.09288400	0.34987000	-0.93784200
H	3.75210800	1.10939100	-0.53517300
H	3.34980100	-0.06555300	-1.90563600

TS-B2-I

C	-0.40907300	-1.17605600	0.49078800
C	-0.34431000	0.14199400	1.18950500
C	1.66184600	-0.05500300	-0.75341800
C	0.57357500	-0.90626700	-1.08129200
C	-2.75155800	-1.16473600	-0.44673500
C	-3.00025300	0.19515200	-0.53711900
C	-2.27738600	1.27560900	0.00120300
C	-1.61473900	-1.77763200	0.06208200
C	-1.17243700	1.24816500	0.81129000
H	-3.51089300	-1.82153300	-0.85799300
H	-3.91160900	0.47000300	-1.06079500
H	-2.69761600	2.25740300	-0.18840000
H	-1.58917400	-2.86160100	-0.01989500
H	-0.86507800	2.20230300	1.22814700
H	0.26553600	-1.88972300	0.95915800
H	-0.17356500	-0.46542100	-1.73520400
H	0.83283400	-1.92730300	-1.34183300
C	1.46718400	1.33721600	-0.85154400
N	1.16959900	2.45258700	-0.94451900
C	2.87845600	-0.58312600	-0.25781800
N	3.84753100	-1.06449700	0.14775600
C	0.69942200	0.36437000	2.01680900
H	0.89743000	1.35368900	2.41179400
H	1.36786900	-0.43256700	2.31985400

TS-B3-I

C	-0.09997700	-1.91285900	-0.82983100
C	0.35921800	-2.15705300	0.47471200
C	0.17583800	-1.31036000	1.56457900
C	-0.54554900	-0.13606100	1.59665500
C	1.22036200	0.59501600	-0.71178500
C	1.13044300	-0.57847400	-1.49288000
C	-1.44368900	-1.34085700	-1.09449000
C	-2.08924400	-0.39644400	-0.41237400
C	-1.61292100	0.35497100	0.75607400
H	0.15006000	-2.70591000	-1.53087700
H	1.07749000	-2.96191500	0.60205100
H	0.78639800	-1.51426800	2.43748700
H	-0.36476500	0.48472300	2.47110400
H	-3.06526400	-0.09515500	-0.78026500
H	-1.93702600	-1.75058500	-1.97098800

H	2.02933400	-1.18323700	-1.53832800
H	0.62737400	-0.46783300	-2.44854300
C	0.41807200	1.72865000	-0.96331500
N	-0.26664400	2.64212900	-1.14825900
C	2.25506600	0.69974700	0.25779800
N	3.11234300	0.72442100	1.03148900
C	-2.17188600	1.54331400	1.05816200
H	-2.97518300	1.95545500	0.46057800
H	-1.82271300	2.13532900	1.89533700

TS-B4-I

C	0.48946700	2.26501600	0.31148000
C	-0.55072100	1.36457900	0.52928100
C	-0.27016600	0.26147900	1.41140000
C	1.77392000	-0.14337100	-0.74031800
C	1.61223100	1.21073300	-1.04894000
C	-1.91732000	-1.50330000	0.70862200
C	-2.74015300	-0.83560200	-0.14552700
C	-2.69852400	0.53519600	-0.51485600
C	-0.84519900	-0.96813200	1.47478300
C	-1.75114500	1.47449100	-0.23825800
H	-2.11422800	-2.55984800	0.85139900
H	-3.52999900	-1.41754100	-0.60904400
H	-3.50980500	0.86214700	-1.15802800
H	-0.39005500	-1.65952300	2.17746000
H	-1.89962300	2.44570600	-0.70356500
H	0.57430200	0.41891700	2.07605900
H	2.46621600	1.86125300	-0.89963300
H	0.99740600	1.44644500	-1.90994400
C	2.74965000	-0.55472000	0.20446900
N	3.53344500	-0.84507000	1.00245800
C	0.87364600	-1.10534900	-1.25668200
N	0.10809300	-1.85799300	-1.68997900
H	0.29229700	3.17498200	-0.24666100
H	1.26859200	2.34278800	1.06188000

CA-B1-I

C	-0.50048300	-0.03617800	1.22351400
C	0.03107300	-1.45069000	1.28568200
C	0.81850200	-1.85954500	0.30041200
C	1.15792100	-0.87889500	-0.79812700
C	-0.12062100	-0.18459100	-1.32970600
C	-1.15129700	0.15463700	-0.19899400
C	0.58479300	0.99694100	1.45072600
C	1.74268800	1.04889300	0.78841500
C	2.15733300	0.15023500	-0.29607800

H	-1.28769500	0.10825000	1.96410500
H	-0.24819600	-2.08534400	2.11746600
H	1.24170600	-2.85670400	0.27534200
H	1.61460200	-1.40455100	-1.63847800
H	2.45498400	1.82283200	1.05915400
H	0.38771000	1.73830500	2.21691000
H	-0.60902700	-0.83626300	-2.05429100
H	0.15581600	0.73316600	-1.84948300
C	-1.62994800	1.53761800	-0.34166200
N	-1.98116100	2.62669800	-0.44523300
C	-2.31647300	-0.74121400	-0.29367900
N	-3.21095000	-1.45933000	-0.36120100
C	3.37055200	0.26095700	-0.84117500
H	4.07479700	1.01106000	-0.49756200
H	3.69583500	-0.39132700	-1.64409500

CA-B2-I

C	0.57502900	-0.01766500	-0.98483300
C	0.57407800	0.91925500	0.20338400
C	-1.66997600	0.06433400	-0.01112900
C	-0.90644300	-0.18259400	-1.34662400
C	2.57231800	-1.30522600	-0.25089700
C	3.42117100	-0.14031700	-0.11716400
C	3.03099300	1.07930400	0.32401900
C	1.26835000	-1.28654500	-0.56156400
C	1.69024700	1.44375300	0.72581700
H	3.04090000	-2.26581800	-0.05706800
H	4.48602700	-0.29992400	-0.26048800
H	3.80719900	1.81635200	0.50889300
H	0.69156600	-2.20637100	-0.52784500
H	1.60199900	2.17940100	1.52133100
H	1.13052900	0.43004700	-1.81744800
H	-1.15153200	-1.15125400	-1.78358400
H	-1.21561900	0.59550800	-2.04762000
C	-1.65075200	-1.14546600	0.82671000
N	-1.61375100	-2.09409900	1.47382500
C	-3.06217000	0.46202700	-0.24260300
N	-4.13810500	0.80736200	-0.45039700
C	-0.83826000	1.19808300	0.65452000
H	-0.96730300	1.22392900	1.73663300
H	-1.18827600	2.15163600	0.24539400

CA-B3-I

C	-0.50048200	-0.03617600	1.22351100
C	0.03108800	-1.45068900	1.28568000
C	0.81851600	-1.85953900	0.30040800

C	1.15791800	-0.87888500	-0.79813600
C	-0.12062700	-0.18458300	-1.32970600
C	-1.15130500	0.15463900	-0.19898900
C	0.58479200	0.99694200	1.45072400
C	1.74268500	1.04889700	0.78841200
C	2.15733300	0.15023900	-0.29608200
H	-1.28768900	0.10823700	1.96411300
H	-0.24817200	-2.08533800	2.11747100
H	1.24174000	-2.85669000	0.27533700
H	1.61459500	-1.40454100	-1.63849000
H	2.45497800	1.82283900	1.05914700
H	0.38771400	1.73830800	2.21690700
H	-0.60903300	-0.83624700	-2.05429800
H	0.15581000	0.73317900	-1.84947600
C	-1.62996300	1.53761200	-0.34166400
N	-1.98117500	2.62669200	-0.44523100
C	-2.31647700	-0.74121800	-0.29367400
N	-3.21093900	-1.45935400	-0.36119300
C	3.37055800	0.26095700	-0.84116900
H	3.69584300	-0.39132800	-1.64408800
H	4.07480600	1.01105000	-0.49754100

CA-B4-I

C	-0.29820300	2.09930300	0.36884900
C	0.76885700	1.09586000	0.02220500
C	0.13778500	-0.24184000	-0.30384200
C	-1.40404300	0.02535900	-0.17589600
C	-1.52021900	1.56509700	-0.38233500
C	1.98703700	-1.66695700	0.53608300
C	3.01954600	-0.99125700	-0.22464500
C	3.06303400	0.33051900	-0.50622300
C	0.69507500	-1.32092600	0.58242900
C	2.07689200	1.32776400	-0.14403300
H	2.30949300	-2.51346000	1.13548500
H	3.89101100	-1.58495200	-0.48473200
H	3.96702300	0.70862000	-0.97511000
H	0.02631100	-1.83216600	1.26730400
H	2.43936300	2.34442200	-0.01726900
H	0.34722200	-0.49052700	-1.35261000
H	-1.43260400	1.76887700	-1.45227500
H	-2.47679100	1.94975800	-0.02951100
C	-2.17089300	-0.73052600	-1.17001800
N	-2.75210600	-1.30135800	-1.98024500
C	-1.90502400	-0.30192000	1.16824300
N	-2.28319600	-0.51500800	2.23222400
H	-0.49252400	2.10696400	1.44742600
H	-0.03045200	3.11418100	0.07254000

TS-C1-I

C	-0.18353600	1.94615200	-0.50778500
C	0.28600500	2.03356400	0.81882800
C	1.11839600	1.17642300	1.47942600
C	1.49155200	-0.17253900	1.02579000
C	0.27945500	-1.27051300	1.28422800
C	-0.92340200	-0.96367500	0.56908000
C	0.41157600	1.19055700	-1.54875600
C	1.38020500	0.22821500	-1.52226100
C	2.03276800	-0.37801200	-0.38007900
H	-0.86784700	2.72738300	-0.82826000
H	-0.04962300	2.90401900	1.38137200
H	1.41797500	1.43313600	2.49042800
H	2.24089700	-0.57369200	1.71131500
H	1.72106400	-0.14496600	-2.48398800
H	0.05498800	1.44630700	-2.54741400
O	-1.91886700	-0.32602200	1.11979900
O	-1.12467800	-1.33339900	-0.66074600
C	-2.80486300	0.10969700	0.07408400
C	-2.28836700	-0.64572600	-1.15980800
H	-3.82176800	-0.13821800	0.37034200
H	-2.65442500	1.18577800	-0.02963200
H	-2.97070300	-1.39544800	-1.55608200
H	-1.94308100	0.03369000	-1.93841100
H	0.07725600	-1.27047100	2.35306200
H	0.68190100	-2.22364100	0.94361300
C	3.09393900	-1.19652300	-0.52642400
H	3.53231600	-1.37920200	-1.50140000
H	3.56704700	-1.67502700	0.32470400

TS-C2-I

C	-1.78837000	-1.19527600	-0.35288800
C	-1.84670300	-1.09843400	1.09084900
C	-1.22981300	-0.09763400	1.81119000
C	-0.56003800	1.04545200	1.37845100
C	0.85264200	-1.11262700	-0.51079100
C	-0.28850200	-1.85463600	-0.91473000
C	-2.03117100	0.04454900	-1.15309000
C	-1.50997400	1.25721000	-0.95968600
H	-2.45340700	-1.98293300	-0.71044700
H	-2.27116500	-1.93791500	1.62973100
H	-1.21941000	-0.24279700	2.89072100
H	-0.07629300	1.62674500	2.16134900
H	-1.77361500	2.02334200	-1.68457500
H	-2.68569500	-0.08341200	-2.01242500
H	-0.26544600	-2.85433400	-0.49049400
H	-0.37948400	-1.86617700	-1.99820000

O	1.50491600	-1.39298800	0.59412500
O	1.39154200	-0.15109000	-1.22527400
C	2.52070000	0.37747300	-0.49415200
H	3.42670300	0.07171200	-1.02145500
H	2.41430500	1.45831900	-0.47173800
C	2.36214500	-0.27592700	0.87819000
H	1.81462800	0.36625000	1.57356000
H	3.28525800	-0.65474100	1.30987100
C	-0.59621000	1.71587900	0.10029900
C	0.14279800	2.82872600	-0.14903700
H	0.79455600	3.25148500	0.60982400
H	0.05238000	3.36855700	-1.08415700

TS-C3-I

C	-0.82845500	-0.88959700	0.80724600
C	-0.51735600	0.55355100	1.07488800
C	1.28359400	-0.70511500	-0.68738400
C	0.03477700	-1.32635500	-0.74356500
C	-3.12441400	-0.78130600	-0.19699700
C	-3.05692200	0.42853200	-0.87561700
C	-2.14326700	1.47728100	-0.63796800
C	-2.18044700	-1.34041400	0.64730100
C	-1.10208700	1.57407800	0.24789100
H	-4.01924100	-1.37582200	-0.36976200
H	-3.85669600	0.64379000	-1.57678400
H	-2.34071200	2.38428100	-1.20614900
H	-2.39795800	-2.32527300	1.04996600
H	-0.62492500	2.54801800	0.32442900
H	-0.27450800	-1.51680500	1.50499900
H	-0.62786100	-0.91093600	-1.49845500
H	0.07206900	-2.40821000	-0.70171400
O	2.32809700	-1.21852600	-0.05452800
O	1.48523700	0.51618000	-1.12927800
C	3.34082200	-0.20666600	0.06013600
C	2.64680100	1.04853900	-0.47516800
H	2.29658000	1.69597100	0.32974700
H	3.22683700	1.60158400	-1.21062100
H	3.61300900	-0.11998600	1.11103600
H	4.20192600	-0.51965900	-0.53168700
C	0.42692700	0.83509800	2.00768500
H	0.66711000	1.86198600	2.26479600
H	0.87785200	0.05408100	2.60995400

CA-C1-I

C	0.26329500	0.28893500	1.17213600
C	-0.45836100	1.61712400	1.10260000

C	-1.31705100	1.80149400	0.10959500
C	-1.51405100	0.67218300	-0.87855800
C	-0.13753500	0.13637800	-1.34025700
C	0.90128000	0.01741000	-0.21492500
C	-0.67496800	-0.83856800	1.54834700
C	-1.81859300	-1.12652500	0.92272100
C	-2.35290600	-0.42987900	-0.25483200
H	1.07407500	0.33027200	1.90222200
H	-0.26407000	2.37349700	1.85390000
H	-1.88785400	2.71642700	-0.00206100
H	-2.04691600	1.03603900	-1.75937300
H	-2.41780500	-1.95371200	1.29354600
H	-0.37755500	-1.45759800	2.38797500
O	1.94720700	0.93969200	-0.45775600
O	1.50821000	-1.27064300	-0.19931300
C	3.14333100	0.33430500	-0.01471000
C	2.90558700	-1.12555600	-0.37006800
H	3.97809100	0.79253300	-0.54439800
H	3.28313400	0.46918600	1.06635500
H	3.18638400	-1.33168800	-1.40977800
H	3.42169800	-1.82536500	0.28965600
H	0.27713400	0.81631100	-2.08549300
H	-0.25485500	-0.84596700	-1.80019300
C	-3.53199400	-0.78178800	-0.77383200
H	-4.12249200	-1.58143600	-0.33850200
H	-3.94050900	-0.28396300	-1.64660700

CA-C2-I

C	0.85453700	-0.24051000	-0.92554900
C	0.93551300	0.95030700	0.00994400
C	-1.37515300	0.34177700	-0.16781100
C	-0.61898700	-0.29779200	-1.34011000
C	2.62345500	-1.54469900	0.23359600
C	3.62217400	-0.50453200	0.11459800
C	3.38937600	0.82771000	0.21662700
C	1.34037100	-1.42859500	-0.14177300
C	2.10353000	1.44842300	0.44203600
H	2.94651600	-2.47202400	0.69922200
H	4.65912200	-0.82743000	0.07778500
H	4.25625400	1.48213100	0.25688200
H	0.62305500	-2.20317800	0.11265900
H	2.09973800	2.36435400	1.02815900
H	1.51972300	-0.08875600	-1.78378000
H	-0.97760800	-1.30791500	-1.55235100
H	-0.79314800	0.31649000	-2.22675200
O	-2.65609800	0.80515500	-0.55578200
O	-1.58509500	-0.57915800	0.88551800
C	-3.64278900	0.08378200	0.16190600

C	-2.87259100	-1.12266900	0.68079800
H	-3.23825400	-1.51266400	1.62996400
H	-2.84831400	-1.93207200	-0.06160100
H	-4.03254200	0.69199700	0.98611700
H	-4.45898700	-0.17828600	-0.51369200
C	-0.44850000	1.45760900	0.31744900
H	-0.61948400	1.68141400	1.37097000
H	-0.67213700	2.35310000	-0.27174900

CA-C3-I

C	0.85453700	-0.24051000	-0.92554900
C	0.93551300	0.95030700	0.00994400
C	-1.37515300	0.34177700	-0.16781100
C	-0.61898700	-0.29779200	-1.34011000
C	2.62345500	-1.54469900	0.23359600
C	3.62217400	-0.50453200	0.11459800
C	3.38937600	0.82771000	0.21662700
C	1.34037100	-1.42859500	-0.14177300
C	2.10353000	1.44842300	0.44203600
H	2.94651600	-2.47202400	0.69922200
H	4.65912200	-0.82743000	0.07778500
H	4.25625400	1.48213100	0.25688200
H	0.62305500	-2.20317800	0.11265900
H	2.09973800	2.36435400	1.02815900
H	1.51972300	-0.08875600	-1.78378000
H	-0.97760800	-1.30791500	-1.55235100
H	-0.79314800	0.31649000	-2.22675200
O	-2.65609800	0.80515500	-0.55578200
O	-1.58509500	-0.57915800	0.88551800
C	-3.64278900	0.08378200	0.16190600
C	-2.87259100	-1.12266900	0.68079800
H	-3.23825400	-1.51266400	1.62996400
H	-2.84831400	-1.93207200	-0.06160100
H	-4.03254200	0.69199700	0.98611700
H	-4.45898700	-0.17828600	-0.51369200
C	-0.44850000	1.45760900	0.31744900
H	-0.61948400	1.68141400	1.37097000
H	-0.67213700	2.35310000	-0.27174900

ω B97X-D/6-311G(d,p) gas phase Cartesian coordinates of the stationary points involved in the cycloaddition reactions of imine **14** with ethylene **16**, DCE **17**, and CKA **9**.

Imine **14**

C	1.87276700	-0.64552500	-0.00044900
C	1.85048500	0.70198500	-0.00044900
C	0.69654500	1.56763900	0.00031100
C	0.75147900	-1.55402600	0.00027900
C	-0.61594600	1.26793000	0.00058700
C	-0.56991600	-1.29974400	0.00052600
C	-1.30800000	-0.02982600	0.00002600
H	2.84987600	-1.11911200	-0.00095000
H	2.80926800	1.21100600	-0.00095000
H	0.93294400	2.62835500	0.00069400
H	1.02547000	-2.60528200	0.00062700
H	-1.29800200	2.11593300	0.00119400
H	-1.24494700	-2.14986100	0.00102200
N	-2.58843700	-0.13194300	-0.00079000
H	-3.02004100	0.79196600	-0.00109600

TS-A1-II

C	1.52651400	0.93799300	-0.23722500
C	1.53121000	-0.02870700	-1.24176700
C	0.50128700	-0.92700000	-1.43023100
C	-0.62573500	-1.01733800	-0.60838600
C	0.33126800	-1.35010100	1.34181400
C	1.37372500	-0.46992700	1.56454000
C	0.36893300	1.74116400	0.12995400
C	-0.93183800	1.41561700	0.09827300
C	-1.49945400	0.09135300	-0.15750500
H	2.47519700	1.43431700	-0.05292400
H	2.47019900	-0.21732900	-1.75301900
H	0.69146600	-1.77219500	-2.08496500
H	-1.21809200	-1.92282000	-0.71170700
H	-1.65092700	2.17837400	0.38634800
H	0.61201800	2.74598100	0.46743000
H	0.55522300	-2.37141800	1.05955200
H	-0.61394300	-1.20740100	1.85133200
H	1.23355900	0.37293300	2.22949400
H	2.39720000	-0.79336700	1.42221000
N	-2.73623900	-0.20355300	0.01517000
H	-3.25368300	0.61946500	0.32325200

TS-A2-II

N	-1.68353800	1.22021000	-0.68981900
C	-0.47074700	0.78138100	-0.45796500
C	-0.38935300	-0.68887300	-0.66628700
C	-1.77718300	-1.19991900	0.77767100
C	-2.69737000	-0.17295700	0.61482800
C	2.01003800	-1.20941400	-0.04632100
C	2.51315000	0.00808700	0.39552800
C	1.87647200	1.24538100	0.38949700
C	0.76080800	-1.48790300	-0.57776300
C	0.58236600	1.58018700	0.02685500
H	2.70621500	-2.04341900	-0.02470700
H	3.53771000	0.00240800	0.75428400
H	2.48097400	2.07869500	0.73749000
H	0.63395900	-2.49934200	-0.95634700
H	0.32701700	2.63276900	0.13199700
H	-1.08891300	-1.00184900	-1.43459200
H	-1.13993700	-1.20023800	1.65475900
H	-2.00677600	-2.17834900	0.37248000
H	-2.78165900	0.61818400	1.34817200
H	-3.54134900	-0.28689700	-0.05155300
H	-1.79156900	2.20073700	-0.43950500

CA-A1-II

C	1.50881900	0.72041200	-0.13225800
C	1.30810400	-0.17361900	-1.33819900
C	0.33065800	-1.06935500	-1.28597900
C	-0.52758300	-1.11985900	-0.04335200
C	0.37079000	-1.13153700	1.22382800
C	1.58338500	-0.18316200	1.12618900
C	0.38515800	1.72418600	0.00988000
C	-0.91455200	1.42400300	0.06287700
C	-1.48378400	0.06091000	-0.00329500
H	2.44913000	1.26715700	-0.22504300
H	1.96027300	-0.07144700	-2.19849400
H	0.12125500	-1.74719300	-2.10573200
H	-1.16088800	-2.00682000	-0.04487200
H	-1.63761000	2.23090900	0.15983000
H	0.67127300	2.76995000	0.08340400
H	0.72016500	-2.15569700	1.37135000
H	-0.24839800	-0.88487900	2.08983300
H	1.65605300	0.44346500	2.01868200
H	2.50899500	-0.76075300	1.06221300
N	-2.73453100	-0.18360100	0.00252000
H	-3.26449500	0.68863500	0.05304000

CA-A2-II

N	-1.68494900	-1.02637100	-0.51323500
C	-0.40641000	-0.73678300	-0.10654000
C	-0.38571400	0.67840800	0.42894300
C	-1.84679100	1.14684000	0.27784300
C	-2.64974300	-0.15090200	0.13649900
C	1.93270800	1.23437400	-0.33470300
C	2.56019500	0.04832500	0.20535200
C	1.99396400	-1.18335600	0.26911800
C	0.61912300	1.50165800	-0.33109500
C	0.65777600	-1.57361700	-0.09189800
H	2.59424300	1.94512200	-0.82457200
H	3.61499200	0.12519200	0.45175500
H	2.64793200	-2.00037400	0.56519000
H	0.24618100	2.36320200	-0.87883100
H	0.49707800	-2.61945600	-0.33845900
H	-0.09134500	0.63392700	1.48581600
H	-1.95005800	1.73728300	-0.63639500
H	-2.18470800	1.75784000	1.11529400
H	-3.54457800	-0.02967000	-0.47737000
H	-2.95577700	-0.53532000	1.12012600
H	-1.92996600	-1.98283100	-0.71102300

TS-B1-II

C	-0.35877900	-0.72790900	1.68975600
C	-0.34636100	-1.88481800	0.93310900
C	0.39913000	-2.06902000	-0.21819700
C	1.09780400	-1.05304100	-0.90368900
C	-0.29895700	0.02239200	-1.61460600
C	-1.18604600	0.59970300	-0.67556200
C	0.68649300	0.24722400	1.84371700
C	1.73916400	0.50518100	1.04606800
C	2.00992800	-0.03699000	-0.28442700
H	-1.15883200	-0.64860800	2.41982500
H	-1.07789000	-2.64540800	1.18258200
H	0.23305000	-2.98981900	-0.76915600
H	1.54676600	-1.37702600	-1.83969300
H	2.44195300	1.26364800	1.37892700
H	0.59718200	0.86074800	2.73438500
H	-0.74466400	-0.70292400	-2.28595200
H	0.38947500	0.70796900	-2.10312600
C	-0.91262900	1.88619600	-0.14498400
N	-0.62442400	2.92381000	0.27139600
C	-2.46453600	0.01881000	-0.45581900
N	-3.48753800	-0.49589400	-0.30829000
N	2.97681200	0.34603100	-1.02694800
H	3.52774400	1.06742400	-0.56308900

TS-B2-II

C	-0.40034400	-1.13883700	0.41945500
C	-0.35478200	0.20764700	1.08091400
N	0.75324300	0.36401900	1.73748500
C	1.70895700	-0.07267700	-0.57770600
C	0.59002000	-0.91949000	-0.95202400
C	-2.79208500	-1.19591200	-0.41747300
C	-3.09269900	0.17333100	-0.50405500
C	-2.40844200	1.25662100	0.03242600
C	-1.64387000	-1.77505600	0.04935300
C	-1.23874400	1.27431800	0.77378500
H	-3.56664400	-1.87053100	-0.76897700
H	-4.02435500	0.41498600	-1.00688900
H	-2.87489500	2.22483800	-0.11844400
H	-1.61932400	-2.86165500	0.04148700
H	-0.94356100	2.23651300	1.18241000
H	0.21700900	-1.80699000	1.01918500
H	-0.04895800	-0.45996000	-1.70391300
H	0.88950900	-1.92231500	-1.24758800
C	1.57282100	1.31085700	-0.79647200
N	1.29626800	2.42215000	-0.97114200
C	2.93502500	-0.62147800	-0.13572600
N	3.92286400	-1.11370900	0.20273600
H	0.90944700	1.34194900	1.98431400

TS-B3-II

C	-0.38565800	-1.83451100	-0.93163800
C	0.08606900	-2.25368500	0.32797600
C	0.11149900	-1.45583300	1.46195400
C	-0.37751500	-0.17053200	1.56806700
C	1.18299000	0.49415500	-0.66455700
C	0.98955500	-0.62091400	-1.51267400
C	-1.63032300	-1.05453700	-1.09460600
C	-2.10536900	-0.07870000	-0.31937900
C	-1.46915500	0.50985800	0.86890700
H	-0.27678200	-2.58956800	-1.70665100
H	0.65969300	-3.17508300	0.35854900
H	0.72563200	-1.80161500	2.28655800
H	-0.05188600	0.40636100	2.42904800
H	-3.03596300	0.39528700	-0.61818100
H	-2.20179600	-1.30893400	-1.98264800
H	1.81965500	-1.31475600	-1.57806100
H	0.52553700	-0.40327000	-2.46935200
C	0.52309100	1.72225900	-0.92799800
N	-0.04695300	2.69908900	-1.15895100
C	2.27699000	0.48732400	0.24754300
N	3.17970800	0.42175800	0.96357200

N	-1.81822800	1.63192200	1.37997800
H	-2.57882300	2.05288500	0.84696200

TS-B4-II

C	0.68178200	0.95130000	-0.73054100
C	0.38710300	-0.43020300	-1.05657600
C	-2.17698300	0.23820100	0.32157500
C	-2.05025300	1.44424600	-0.37567800
C	2.17834400	-1.71805300	0.15773000
C	3.05813700	-0.75556800	0.53143100
C	2.99427700	0.64183000	0.24974900
C	1.00715300	-1.55999700	-0.64191300
C	1.98799600	1.37733500	-0.28302400
H	2.40941500	-2.73641100	0.45189000
H	3.92788600	-1.07605100	1.09530000
H	3.86923100	1.20797800	0.55533100
H	0.53147800	-2.48380600	-0.95721600
H	2.15754600	2.44948600	-0.34569400
H	-0.47877000	-0.56402000	-1.69301400
H	-2.53170700	1.51196200	-1.34281700
H	-2.08250900	2.35687900	0.20978500
C	-2.56832100	-0.94443300	-0.35231700
N	-2.85955300	-1.89306500	-0.94669300
C	-1.68812700	0.14546800	1.64917200
N	-1.24062700	0.11105600	2.71438000
H	-0.02104300	2.76747800	-0.68715400
N	-0.27813000	1.81425700	-0.92540900

CA-B1-II

C	-0.47386800	-0.04309600	1.22249900
C	0.05531100	-1.45991900	1.27213100
C	0.82850500	-1.86561900	0.27478400
C	1.15632700	-0.88207100	-0.82304300
C	-0.12501400	-0.18005700	-1.33681900
C	-1.14159100	0.15476500	-0.19344600
C	0.60932500	0.99375000	1.43490000
C	1.75726400	1.05675100	0.75912300
C	2.16465000	0.14563200	-0.33174000
H	-1.25141300	0.10045000	1.97314800
H	-0.22624600	-2.09949400	2.09908100
H	1.24129400	-2.86615400	0.23302800
H	1.63292100	-1.38349500	-1.66451000
H	2.46884800	1.83853400	1.01194000
H	0.41601700	1.73749900	2.20055300
H	-0.61981200	-0.82874400	-2.05910700
H	0.14495800	0.73858700	-1.85875100

N	3.29845900	0.18505000	-0.90614800
C	-2.30795400	-0.73997100	-0.27376100
N	-3.20469700	-1.45609200	-0.32948200
C	-1.62012900	1.53920700	-0.32218600
N	-1.96557500	2.63143700	-0.41070900
H	3.87915500	0.92382300	-0.50565900

CA-B2-II

C	0.60291500	0.48044000	0.66310500
C	0.52132700	-0.43128500	-0.53741900
N	-0.76781600	-0.36378600	-1.05847500
C	-1.69040300	0.05011900	-0.01765900
C	-0.81942300	1.04915000	0.79369300
C	2.95715800	1.20944400	0.27810300
C	3.49487100	-0.12714400	0.13383500
C	2.86298800	-1.17778200	-0.44234000
C	1.66435800	1.52319600	0.43333300
C	1.52011200	-1.22269800	-0.96702600
H	3.67453000	2.02349300	0.21632800
H	4.54064300	-0.25821100	0.39425800
H	3.45217300	-2.07690600	-0.60009900
H	1.35540200	2.56443100	0.41246200
H	1.31176900	-1.95588000	-1.74034700
H	0.86619100	-0.12712100	1.53768600
H	-0.89357000	2.02098900	0.30258600
H	-1.16883000	1.14502200	1.82019600
C	-2.88550200	0.69247700	-0.58854200
N	-3.80984800	1.20859400	-1.03320800
C	-2.11414600	-1.08527400	0.83992600
N	-2.38674500	-1.98975100	1.49431600
H	-1.07297100	-1.08508100	-1.69555300

CA-B3-II

C	-0.76119800	-1.59817100	-0.94276900
C	-0.69379400	-2.11692200	0.47835900
C	-0.30395800	-1.27636300	1.42651900
C	0.00156400	0.14933000	1.03485700
C	0.99146300	0.13651900	-0.19765900
C	0.58828200	-0.92707000	-1.28013800
C	-1.90255700	-0.62236900	-1.14353500
C	-2.11254300	0.47322500	-0.41266200
C	-1.27725700	0.91503000	0.72143000
H	-0.89258000	-2.43004000	-1.63617800
H	-0.94237500	-3.15099000	0.68551500
H	-0.21464500	-1.56255800	2.46673700
H	0.48036000	0.69307700	1.84775300

H	-2.96330900	1.10840500	-0.64358400
H	-2.58724700	-0.83651700	-1.95852200
H	1.36234300	-1.69368000	-1.32006400
H	0.54231400	-0.44762100	-2.25827800
N	-1.54968700	1.89970100	1.47705500
C	2.32789000	-0.19325700	0.32162200
N	3.35831700	-0.48562200	0.73732000
C	1.05370500	1.47586300	-0.80284300
N	1.07263600	2.51187300	-1.29889600
H	-2.42330700	2.34337700	1.18919400

CA-B4-II

C	0.76119600	1.08489100	0.06376900
C	0.11920900	-0.22035700	-0.35481900
C	-1.41143500	0.05368500	-0.13541400
C	-1.48396100	1.60671500	-0.18158400
C	1.97650800	-1.72602600	0.34512300
C	3.03588900	-0.97070700	-0.28725800
C	3.08005600	0.37657500	-0.41620200
C	0.68309000	-1.38619100	0.40964900
C	2.07966300	1.34357000	-0.04038900
H	2.27711600	-2.64194800	0.84663300
H	3.92530900	-1.52709000	-0.56550500
H	4.00768200	0.79935500	-0.79243300
H	0.00424400	-1.97797700	1.01417300
H	2.41699200	2.36085700	0.13446000
H	0.28521300	-0.36395500	-1.42974500
H	-1.54198600	1.92688300	-1.23037100
H	-2.34682000	1.99165400	0.36127400
C	-2.23344100	-0.56475500	-1.17819800
N	-2.86209600	-1.02487000	-2.02229400
C	-1.87471300	-0.40137300	1.18370100
N	-2.24590000	-0.73618400	2.21782400
H	-0.01317200	2.92270900	0.60814200
N	-0.23585200	1.95153200	0.46205500

TS-C1-II

C	-0.21137800	2.30723100	0.14696800
C	-0.46383400	1.94354600	-1.17559500
C	-1.03887400	0.79434400	-1.67965700
C	-1.38165800	-0.42330900	-1.00333300
C	-0.06834400	-1.70830000	-1.14557200
C	1.01392300	-1.18149900	-0.44476100
C	-0.66451600	1.62627900	1.29299900
C	-1.36022200	0.45233200	1.43075800
C	-1.79893200	-0.50846800	0.44289800

H	0.25455000	3.27364300	0.31180400
H	-0.18864800	2.68529600	-1.92319800
H	-1.17341400	0.76256900	-2.75714100
H	-2.09164700	-1.02018600	-1.57290900
H	-1.64887400	0.18710000	2.44566100
H	-0.45965600	2.13828400	2.23280800
O	1.88550900	-0.37919600	-1.00857200
O	1.11067400	-1.24344100	0.86186800
C	2.51856400	0.40760000	0.01545700
C	2.11632900	-0.31390600	1.30544000
H	3.58882700	0.41981800	-0.17840900
H	2.08320100	1.40927500	-0.03582600
H	2.92062200	-0.88637500	1.76766300
H	1.64699700	0.35450300	2.02533100
H	0.09830400	-1.78818600	-2.21309800
H	-0.56207600	-2.54905200	-0.67111100
N	-2.51798600	-1.54709500	0.70532500
H	-2.77810900	-1.55102900	1.69118000

TS-C2-II

C	-0.76662200	-0.82946600	0.76834400
C	-0.50804100	0.63390600	0.92634600
N	0.53051000	0.91232100	1.66057700
C	1.37859800	-0.71312200	-0.69855600
C	0.13435200	-1.31776400	-0.82323700
C	-3.14222800	-0.89815500	-0.06693400
C	-3.25678500	0.32402700	-0.71977300
C	-2.41044300	1.43029600	-0.56278600
C	-2.08006900	-1.38091700	0.67457600
C	-1.27581000	1.59840800	0.19824200
H	-3.99668200	-1.56581300	-0.15551200
H	-4.14084900	0.47644900	-1.32972800
H	-2.73418500	2.32603800	-1.08934100
H	-2.19193600	-2.37653700	1.09405300
H	-0.86250100	2.60450800	0.22218000
H	-0.12758200	-1.36380800	1.46742900
H	-0.50768400	-0.90721400	-1.59420200
H	0.13657100	-2.39526500	-0.72384700
O	2.36629200	-1.22894300	0.00602900
O	1.62704200	0.49787800	-1.14964900
C	3.21487300	-0.14532100	0.42832200
C	2.84208000	0.97572900	-0.54534000
H	2.61489700	1.90975500	-0.03574700
H	3.56957900	1.13554500	-1.34176900
H	2.92745300	0.10438900	1.44945400
H	4.24814800	-0.47754300	0.35507500
H	0.62510500	1.92604400	1.73165000

TS-C3-II

C	-1.71998400	-1.30002900	-0.28549800
C	-1.57371200	-1.29266300	1.13922100
C	-1.00700700	-0.24900200	1.85214400
C	-0.52659100	0.97651500	1.41214000
C	0.94751100	-0.98335200	-0.68204400
C	-0.14045000	-1.73200100	-1.15544000
C	-2.21872000	-0.07141700	-0.94698800
C	-1.80693600	1.18323800	-0.74482800
C	-0.73381900	1.64864900	0.15369800
H	-2.27761100	-2.16809300	-0.63339200
H	-1.80000700	-2.21064000	1.66946300
H	-0.85400400	-0.44287500	2.91247700
H	0.00056600	1.59233200	2.13568400
H	-2.27320600	1.96790200	-1.33668500
H	-2.99578000	-0.23071300	-1.69100000
H	-0.05882000	-2.78055500	-0.89164000
H	-0.36091500	-1.55153500	-2.20206200
O	1.59601600	-1.34452800	0.40241200
O	1.41952500	0.09581400	-1.25928900
C	2.38105000	0.71631200	-0.37103200
H	3.31798800	0.80240400	-0.92008700
H	1.97249800	1.69171700	-0.09928900
C	2.44205500	-0.25788600	0.81297700
H	2.00121000	0.17119900	1.71298400
H	3.43220100	-0.66398800	1.01260800
N	-0.02277300	2.69799900	-0.12924300
H	-0.32942100	3.09637200	-1.01543700

CA-C1-II

C	0.23605400	0.28819600	1.17371200
C	-0.49136200	1.61370000	1.10020900
C	-1.33830600	1.79724800	0.09745600
C	-1.51699000	0.67287400	-0.89822900
C	-0.13282100	0.14561300	-1.34596000
C	0.89262800	0.02481200	-0.20948800
C	-0.69200500	-0.85235500	1.52682400
C	-1.82482000	-1.15081600	0.88832600
C	-2.35647400	-0.43969600	-0.29270700
H	1.03827500	0.32964900	1.91272900
H	-0.29966900	2.37079600	1.85102900
H	-1.90508100	2.71284000	-0.02448500
H	-2.06780200	1.01305800	-1.77459200
H	-2.41811100	-1.99284100	1.23733400
H	-0.39416500	-1.47921900	2.36105300
O	1.93809100	0.95026200	-0.43073000

O	1.50077900	-1.26231900	-0.18531300
C	3.13387600	0.34054900	0.00983500
C	2.89783100	-1.11470200	-0.36269000
H	3.96953500	0.80583400	-0.51190000
H	3.26929300	0.46337400	1.09284600
H	3.17303400	-1.30728100	-1.40629900
H	3.41629900	-1.82271800	0.28586900
H	0.28345600	0.83445900	-2.08130700
H	-0.23696700	-0.83251200	-1.81799800
N	-3.46608600	-0.72259500	-0.85151200
H	-3.92212900	-1.49336700	-0.35907600

CA-C2-II

C	-3.30260200	-1.10471900	-0.12002000
C	-3.78473300	0.20814300	0.24769900
C	-3.09645200	1.36868600	0.10682900
C	-2.02370400	-1.50667200	-0.10846200
C	-1.74522100	1.55364600	-0.35061300
C	-0.90962100	-0.69120400	0.49084300
C	-0.77513700	0.61752800	-0.25909800
H	-4.05199600	-1.80758400	-0.47632800
H	-4.82997800	0.28007500	0.53319100
H	-3.65027300	2.28587500	0.29255000
H	-1.76380800	-2.47662700	-0.52395200
H	-1.48993900	2.52406400	-0.76625100
H	-1.14699300	-0.45853300	1.53594500
C	1.40713400	-0.19018500	-0.07322000
C	0.48438200	-1.32690300	0.36604700
H	0.49909100	-2.07756600	-0.42656900
H	0.84525100	-1.77590900	1.28949800
O	2.04142800	0.38539900	1.05614800
O	2.43879600	-0.56464500	-0.95570700
C	3.32377600	0.81375700	0.64584200
C	3.69204400	-0.25704500	-0.36762000
H	4.37134500	0.08579100	-1.14878100
H	4.11173000	-1.14294400	0.12228500
H	3.28065500	1.80976000	0.18379500
H	3.97565000	0.84896000	1.51778700
N	0.50507500	0.70033300	-0.74341500
H	0.85274100	1.52608300	-1.20215700

CA-C3-II

C	-1.77523300	-1.24827800	-0.52033400
C	-1.86234100	-1.31115900	0.99212400
C	-1.00068800	-0.57826100	1.68299300
C	-0.03341400	0.29313200	0.91891800

C	0.66141100	-0.53966400	-0.20696300
C	-0.30171100	-1.48815900	-0.91930600
C	-2.27094100	0.08481300	-1.04312200
C	-1.80729400	1.27794500	-0.66620400
C	-0.72362600	1.50126700	0.31197600
H	-2.38161300	-2.03976900	-0.96347600
H	-2.59978600	-1.94908700	1.46568100
H	-0.98053600	-0.56779800	2.76602700
H	0.73227700	0.69069700	1.58509700
H	-2.23604700	2.17519000	-1.10594100
H	-3.05933000	0.05452000	-1.78992200
H	-0.02063500	-2.50629500	-0.64725300
H	-0.15973700	-1.36481500	-1.99369300
O	1.72569100	-1.28121100	0.35266400
O	1.26935600	0.31419000	-1.14765800
C	2.48141900	0.74298400	-0.55454000
H	3.20305200	0.91857800	-1.35204600
H	2.32499400	1.67059600	0.00710400
C	2.86456700	-0.43430000	0.36961700
H	3.08399100	-0.09512400	1.38744200
H	3.71460300	-1.00770600	-0.00409900
N	-0.30631500	2.65323200	0.66263500
H	-0.83028900	3.38263500	0.17563100

ω B97X-D/6-311G(d,p) gas phase Cartesian coordinates of the stationary points involved in the cycloaddition reactions of ylidenhydrazine **15** with ethylene **16**, DCE **17**, and CKA **9**.

Ylidenhydrazine **15**

E = a.u.

C	-2.32779500	-0.32438000	0.29731000
C	-2.04684500	0.99264300	0.25316600
C	-0.82278500	1.60777100	-0.21403400
C	-1.47452100	-1.43288100	-0.07566800
C	0.38748100	1.04791100	-0.38096800
C	-0.14268800	-1.44353600	-0.26033500
C	0.80254900	-0.33650500	-0.11733000
H	-3.32934500	-0.60111300	0.61421900
H	-2.83895900	1.67997000	0.53450400
H	-0.90587700	2.66268300	-0.46288400
H	-1.98319200	-2.38648600	-0.18238400
H	1.17752300	1.67920400	-0.78120200
H	0.33559500	-2.38952500	-0.49618200
N	2.02266400	-0.67539200	0.11883000
N	2.95623700	0.33328600	0.22021200
H	3.79512500	-0.05215600	0.62721100
H	2.64444600	1.13603400	0.76057800

TS-A1-III

C	1.73983100	1.10738500	-0.38297300
C	1.87604100	0.05168800	-1.28144300
C	1.01435700	-1.02599900	-1.32538500
C	-0.07675600	-1.18967500	-0.46608900
C	0.94496600	-1.17227300	1.45700300
C	1.85972500	-0.13940700	1.55931000
C	0.48741800	1.73336700	0.02140700
C	-0.75255800	1.22093800	0.05176100
C	-1.11290000	-0.17450800	-0.17896200
H	2.59826700	1.76823100	-0.29887900
H	2.82166300	-0.03476700	-1.80809500
H	1.34255400	-1.90652100	-1.86974600
H	-0.52034900	-2.18162100	-0.44595800
H	-1.54683600	1.86412400	0.41316100
H	0.59440300	2.76299600	0.35451800
H	1.30779600	-2.17859800	1.28756400
H	0.00243800	-1.10320200	1.98678800
H	1.62019300	0.73702300	2.14778800
H	2.91410500	-0.32776600	1.40017200
N	-2.30763100	-0.64503000	-0.09704600

N	-3.33455500	0.25913900	0.17295500
H	-3.31615500	1.06515500	-0.44760000
H	-4.20353000	-0.23290700	0.02114500

TS-A2-III

N	1.75870900	-0.38448000	-0.60093000
C	0.46563800	-0.41356900	-0.38939300
C	-0.10524400	0.93809400	-0.66982600
C	0.79420100	1.92272500	0.79894300
C	2.05073200	1.32461200	0.77597500
C	-2.57086300	0.58109100	-0.21240700
C	-2.62278300	-0.68104800	0.36554400
C	-1.58097400	-1.59327600	0.51843000
C	-1.47485400	1.25649500	-0.72519700
C	-0.24252200	-1.48692100	0.18066800
H	-3.52345600	1.09549300	-0.30775100
H	-3.59853200	-1.01332900	0.70621300
H	-1.86068100	-2.54077100	0.97143000
H	-1.69426500	2.21465800	-1.18994800
H	0.35511500	-2.35940800	0.42343800
H	0.48489600	1.43866700	-1.43199900
H	0.12739200	1.68366900	1.62016000
H	0.69355400	2.93020900	0.40987400
H	2.33635600	0.57027200	1.49746000
H	2.85531000	1.74987300	0.19023700
N	2.52766300	-1.48811700	-0.19344300
H	2.11898100	-2.35839600	-0.52488400
H	3.42073400	-1.39197100	-0.66004500

CA-A1-III

C	-1.77863500	0.89098200	-0.03157400
C	-1.84559500	0.03579400	1.21839200
C	-0.98487500	-0.96985000	1.31907300
C	-0.02418100	-1.20402200	0.17713600
C	-0.82098800	-1.21458400	-1.15282900
C	-1.80610200	-0.03194500	-1.27713400
C	-0.52398700	1.73853000	-0.00049700
C	0.72485600	1.26484200	0.06446400
C	1.07878700	-0.15988300	0.11901600
H	-2.64171900	1.55813700	-0.07609700
H	-2.56458200	0.27001600	1.99581100
H	-0.95247800	-1.61797400	2.18788700
H	0.48581300	-2.16103200	0.29067400
H	1.53535400	1.98125100	0.14631400
H	-0.66181100	2.81634700	-0.00297000
H	-1.37358700	-2.15629500	-1.19706400

H	-0.11233700	-1.22308900	-1.98486400
H	-1.58396400	0.56636900	-2.16441500
H	-2.82615500	-0.40746700	-1.39236100
N	2.27560100	-0.61857500	0.09082300
N	3.33111700	0.26380000	-0.01464100
H	4.15186000	-0.26122700	-0.27619500
H	3.18090100	1.01920100	-0.67628000

CA-A2-III

C	-2.45381700	0.79665500	0.47229400
C	-2.75676400	-0.46508100	-0.16998500
C	-1.87855200	-1.47942500	-0.37084500
C	-1.26828100	1.42111400	0.45619600
C	-0.46970100	-1.51464200	-0.07572000
C	-0.12291500	0.97166800	-0.41041100
C	0.31295300	-0.41709400	-0.01174200
H	-3.25830400	1.24538300	1.05030800
H	-3.80348100	-0.66214700	-0.38233400
H	-2.29723800	-2.41596900	-0.73205700
H	-1.11558600	2.30250600	1.07367800
H	-0.00270300	-2.47847900	0.08991400
H	-0.45808700	0.93140800	-1.45547100
C	2.28621800	0.78478100	-0.30135800
C	1.16068700	1.81676700	-0.27779500
H	1.16444500	2.33561300	0.68426500
H	1.25847300	2.56361900	-1.06596500
H	3.16873900	1.09113400	0.26570700
H	2.60339600	0.55017000	-1.33176800
N	1.65529300	-0.37280900	0.32278000
N	2.34867500	-1.57735600	0.42853000
H	2.79070300	-1.81293800	-0.45878200
H	3.06289000	-1.48760000	1.13953100

TS-B1-III

C	-0.72469600	-0.54743900	1.77121900
C	-0.80114600	-1.75906500	1.11304900
C	-0.10749500	-2.09064900	-0.04217500
C	0.70514600	-1.20615300	-0.77872900
C	-0.57269900	-0.05259600	-1.59480900
C	-1.49769800	0.60310900	-0.74492800
C	0.32903500	0.43463900	1.78017300
C	1.41897000	0.51380500	0.99456500
C	1.73527900	-0.32038000	-0.15675800
H	-1.50255800	-0.36886700	2.50805700
H	-1.58556700	-2.43707900	1.43025400
H	-0.40086600	-3.00932900	-0.54166800

H	1.12215100	-1.63329600	-1.68741100
H	2.09154600	1.34742500	1.16935600
H	0.20164000	1.22351800	2.51329200
H	-1.00919200	-0.77062800	-2.28015500
H	0.17541400	0.58701000	-2.05546700
C	-1.24187000	1.91758100	-0.28112500
N	-0.98054900	2.98141900	0.08444900
C	-2.78625200	0.04025000	-0.54844700
N	-3.81253800	-0.47355600	-0.41735900
N	2.85845700	-0.30206000	-0.78070300
N	3.85812000	0.52077600	-0.31995600
H	3.98513000	0.51068400	0.68711700
H	4.71843200	0.26590500	-0.78059900

TS-B2-III

C	0.50638300	-0.94926400	-0.84070500
C	0.35380100	0.53945800	-0.81775900
N	-0.70074500	0.93988000	-1.46515000
C	-1.51673700	-0.74019400	0.82038900
C	-0.34439700	-1.53435700	0.71620400
C	2.92736700	-1.21127800	-0.18175100
C	3.14150800	-0.05158100	0.53855700
C	2.31743800	1.08567500	0.67487600
C	1.75773500	-1.59751500	-0.83217400
C	1.13930700	1.37350800	0.04053300
H	3.74469800	-1.92483000	-0.19867000
H	4.09421600	0.00983900	1.05696500
H	2.70297100	1.86128700	1.32818200
H	1.76841300	-2.59419800	-1.26654400
H	0.72957100	2.35537800	0.25459900
H	-0.19892600	-1.36772000	-1.55397100
H	0.41341600	-1.34807400	1.47201700
H	-0.50203200	-2.58717900	0.50684100
N	-1.12417300	2.20130300	-1.39973400
H	-1.82450800	2.41283300	-2.08852800
H	-0.48679500	2.95210900	-1.17453900
C	-1.43632800	0.50611500	1.46577500
N	-1.24942600	1.52830400	1.97875800
C	-2.71432500	-1.11781100	0.16530900
N	-3.67301800	-1.46748600	-0.37556900

TS-B3-III

C	1.09396400	-1.72749200	-0.86964700
C	1.53737800	-1.81416800	0.46425900
C	0.93218200	-1.23054400	1.57335300
C	-0.26221300	-0.54203300	1.61168600

C	1.16755900	1.07895600	-0.66116000
C	1.66861600	-0.00397100	-1.42324100
C	-0.34979700	-1.79788600	-1.21105400
C	-1.38304300	-1.26081100	-0.56213400
C	-1.34441400	-0.46884700	0.67306200
H	1.69773100	-2.31708700	-1.55591200
H	2.53306700	-2.22070700	0.61875900
H	1.51577000	-1.21453400	2.48684100
H	-0.47987000	0.00434300	2.52496800
H	-2.37429700	-1.44080800	-0.96648700
H	-0.56828700	-2.36662900	-2.11045400
H	2.74346600	-0.14549700	-1.38137700
H	1.26546700	-0.08971100	-2.42856200
C	-0.06291300	1.68848700	-0.99189600
N	-1.09032000	2.13812000	-1.27298100
C	1.94899800	1.61766400	0.39178700
N	2.63312600	2.01609800	1.23403200
N	-2.30595200	0.31739800	1.06365100
N	-3.36938300	0.48848800	0.25972700
H	-3.16165700	0.56577700	-0.73137100
H	-3.92159700	1.26800000	0.58250900

TS-B4-III

C	0.70931700	0.78251600	-0.61816700
C	0.32022500	-0.51782100	-1.12214200
C	-2.12162300	-0.01931300	0.37403100
C	-1.97523600	1.25821900	-0.18648900
C	1.94939100	-2.04779800	0.02760300
C	2.91194400	-1.19958000	0.47057900
C	3.00361500	0.20483300	0.23737900
C	0.83663800	-1.72846200	-0.80577100
C	2.06331300	1.06970800	-0.21870200
H	2.06730700	-3.09860400	0.27003500
H	3.73175600	-1.63464200	1.03276400
H	3.95142900	0.65513900	0.51780500
H	0.30841500	-2.57712400	-1.22997800
H	2.32026700	2.12271900	-0.25976800
H	-0.51902300	-0.51317700	-1.80696000
H	-2.46060900	1.43271800	-1.14010700
H	-2.02348200	2.10117800	0.49710500
C	-2.56299600	-1.11115700	-0.41007200
N	-2.89765500	-1.98238800	-1.09365400
C	-1.59096300	-0.25709000	1.66547100
N	-1.09495500	-0.39182400	2.70137000
N	-0.21619100	1.71125600	-0.64341300
N	0.16661700	2.98422900	-0.20048400
H	-0.52689800	3.64510300	-0.52708700
H	0.18438500	3.01343900	0.81713300

CA-B1-III

C	-0.84100800	-0.01126000	1.22149700
C	-0.42727100	-1.46469800	1.29256600
C	0.31155900	-1.94742400	0.30299300
C	0.74531700	-0.99667600	-0.78977200
C	-0.45502900	-0.17912000	-1.32481700
C	-1.47714000	0.21473400	-0.20415700
C	0.30786800	0.95835900	1.41482100
C	1.48117100	0.89823500	0.77897700
C	1.83638800	-0.09654400	-0.24214600
H	-1.61176100	0.20156400	1.96305900
H	-0.76526000	-2.06851600	2.12545300
H	0.63977000	-2.97964400	0.27576800
H	1.18957300	-1.54137100	-1.62243700
H	2.20888800	1.67698500	0.98312600
H	0.12960000	1.77842100	2.10196900
H	-0.98180000	-0.76082000	-2.08118200
H	-0.08936100	0.72743100	-1.80782400
C	-1.87822700	1.62196400	-0.34953800
N	-2.16438800	2.73030400	-0.44941900
C	-2.68934200	-0.61520500	-0.30431000
N	-3.62455700	-1.27875000	-0.37732300
N	3.00779800	-0.26173800	-0.73409100
N	4.04196600	0.50966100	-0.27530900
H	4.05591600	0.66517700	0.72676300
H	4.91297900	0.11024800	-0.58837200

CA-B2-III

C	-3.11203300	-1.23519100	-0.17982100
C	-3.59207200	0.08698300	0.17115100
C	-2.89783600	1.24151100	0.04630500
C	-1.84159700	-1.65225600	-0.11852900
C	-1.53116800	1.40823300	-0.39184100
C	-0.74518900	-0.82595200	0.50037400
C	-0.58091200	0.46720000	-0.25410300
H	-3.85813800	-1.93015100	-0.55588100
H	-4.64138100	0.16385000	0.43888500
H	-3.44330700	2.16420000	0.22373700
H	-1.57686900	-2.63119800	-0.50802600
H	-1.26927000	2.35819600	-0.84593600
H	-1.00744100	-0.58350500	1.53791500
C	1.58952200	-0.29118100	0.11493500
C	0.64718700	-1.47683700	0.42742600
H	0.70354900	-2.17195500	-0.41202300
H	0.93939500	-1.99817300	1.33708500

N	0.73679400	0.56096500	-0.70676600
N	1.30214000	1.76490800	-1.11113200
H	1.05757200	1.94628900	-2.07555800
H	0.98556000	2.53076100	-0.52029600
C	2.78734500	-0.70790400	-0.62815700
N	3.70583600	-1.07707800	-1.20945800
C	1.99307100	0.40775100	1.35978400
N	2.22843300	0.98228300	2.32663400

CA-B3-III

C	0.72567200	1.87887700	0.80160100
C	0.98474300	2.12220900	-0.67093900
C	0.66526000	1.15319500	-1.51842900
C	0.07564100	-0.11879900	-0.96129200
C	1.02054400	-0.61939700	0.20401200
C	1.35279000	0.53139600	1.22020800
C	-0.76520400	1.91277700	1.07591200
C	-1.66203400	1.09362000	0.51895400
C	-1.34576500	0.04260900	-0.45246700
H	1.20393500	2.65651100	1.39897000
H	1.40417800	3.06643900	-0.99759300
H	0.80659600	1.24030600	-2.58841900
H	0.03631800	-0.90253000	-1.71688200
H	-2.70901400	1.25289800	0.75288400
H	-1.11942700	2.68229500	1.75468700
H	2.43602300	0.64314300	1.27459900
H	0.99837700	0.24893600	2.21187200
N	-2.18130200	-0.80510500	-0.93054100
N	-3.47762600	-0.78974200	-0.51457400
H	-3.91950800	-1.65637800	-0.77916700
H	-3.61966500	-0.59388600	0.47052700
C	2.26676400	-1.10299600	-0.41084300
N	3.24500300	-1.45197400	-0.90236200
C	0.38959300	-1.74614200	0.90753300
N	-0.12405000	-2.59915300	1.48076600

CA-B4-III

C	0.76509100	0.80818600	-0.07098900
C	0.12082300	-0.53041400	-0.33362900
C	-1.41222100	-0.23132700	-0.16233300
C	-1.47708400	1.29855300	-0.39821600
C	1.97053800	-1.94560000	0.53803000
C	3.02663700	-1.27352900	-0.18953200
C	3.07322600	0.04860800	-0.47812300
C	0.67774000	-1.59950100	0.56546500
C	2.07905700	1.05763600	-0.20657800

H	2.27435700	-2.79300700	1.14663500
H	3.91234800	-1.86267400	-0.40571300
H	3.99938000	0.42054600	-0.90803000
H	-0.00180800	-2.11094800	1.23876000
H	2.40057300	2.08951700	-0.12727200
H	0.29168900	-0.80206800	-1.38295300
H	-1.50756400	1.50415100	-1.47933700
H	-2.34209000	1.75777700	0.08118200
C	-2.22551300	-0.97335500	-1.12824900
N	-2.84708800	-1.53341100	-1.91533200
C	-1.88816700	-0.51851900	1.19881600
N	-2.26949400	-0.72022500	2.26332200
N	-0.23502500	1.72927000	0.21791100
N	0.09739800	3.07986200	0.23022000
H	-0.05983300	3.50739000	-0.67972300
H	-0.44834300	3.55642000	0.93562200

TS-C1-III

C	-0.58205600	2.21224500	-0.82940000
C	-0.58564400	2.32928100	0.55874000
C	0.06467100	1.57796200	1.52131500
C	0.84943400	0.38851400	1.36478200
C	-0.11433300	-1.14634500	1.72292800
C	-1.07225900	-1.20096200	0.71343900
C	0.22479000	1.34091300	-1.59264300
C	1.17536700	0.43307800	-1.20801300
C	1.62611800	0.07629900	0.12120200
H	-1.18693600	2.92219200	-1.38476800
H	-1.18808200	3.14640000	0.95196600
H	-0.08823000	1.88648600	2.55147300
H	1.50924700	0.21921900	2.21390000
H	1.66520200	-0.11662900	-2.00513200
H	0.08609500	1.42134700	-2.67076200
O	-2.21175900	-0.55827300	0.80070400
O	-0.81844900	-1.68314900	-0.47822200
C	-2.71702500	-0.33734600	-0.52866100
C	-1.86739600	-1.28449600	-1.38060100
H	-3.78078400	-0.56431500	-0.52956200
H	-2.52246700	0.71086800	-0.77302100
H	-2.38970600	-2.18530200	-1.70398000
H	-1.39757500	-0.77996900	-2.22265200
H	-0.52458500	-0.96056600	2.70824000
H	0.65743600	-1.90502400	1.66362700
N	2.69542200	-0.60604800	0.36974600
N	3.49737900	-0.94020000	-0.72248200
H	3.65182500	-0.14254900	-1.33786000
H	4.39062200	-1.23190400	-0.35070600

TS-C2-III

C	0.86252900	-0.62172600	-1.02367500
C	0.47361000	0.74373700	-0.57530400
N	-0.55249400	1.21420100	-1.21795300
C	-1.18098300	-1.26406200	0.44454300
C	0.08037900	-1.81134000	0.25491000
C	3.26002900	-0.74669100	-0.27492400
C	3.26255200	0.09057900	0.83394600
C	2.26593800	1.01373200	1.19213100
C	2.22458200	-1.02157400	-1.15207500
C	1.09232700	1.35971400	0.56543900
H	4.18985800	-1.27783300	-0.46791000
H	4.15485400	0.08498100	1.45105100
H	2.48142800	1.58573400	2.09263200
H	2.42276100	-1.75180000	-1.93094000
H	0.51378400	2.14648100	1.03839200
H	0.24412900	-0.90087300	-1.87348600
H	0.75922800	-1.71352700	1.09408000
H	0.10839900	-2.74803300	-0.28572700
O	-2.19865100	-1.48941500	-0.36465700
O	-1.41032900	-0.33040200	1.33767200
C	-3.11154000	-0.38124000	-0.25675400
C	-2.64752400	0.33910500	1.01358500
H	-2.41054500	1.38666500	0.82737300
H	-3.31968900	0.21717300	1.86275000
H	-2.97240900	0.23798100	-1.14231300
H	-4.12164100	-0.78266900	-0.20015400
N	-1.00740500	2.48438500	-0.80683700
H	-1.52143000	2.86677300	-1.59042600
H	-0.22897900	3.11597900	-0.61683500

TS-C3-III

C	-2.22904200	-0.00704200	-0.70486900
C	-2.56450700	-0.01495900	0.70248100
C	-1.69372100	0.37036700	1.70604300
C	-0.41079100	0.89406800	1.62852200
C	-0.00534100	-1.48305200	-0.59887900
C	-1.28787900	-1.38786400	-1.19865100
C	-1.56676700	1.23214800	-1.20836300
C	-0.47934300	1.81995900	-0.70359100
C	0.29564800	1.40774000	0.48085400
H	-3.11416600	-0.20846800	-1.30949000
H	-3.51127200	-0.46115100	0.98535900
H	-2.04730000	0.19077900	2.71975900
H	0.13997600	1.00108800	2.55871100
H	-0.14853900	2.73371200	-1.19415600

H	-2.04056600	1.69968500	-2.06807600
H	-1.91339600	-2.22882200	-0.91530100
H	-1.19741700	-1.28087700	-2.27694800
O	0.21410800	-2.14781400	0.50950200
O	1.06777800	-0.94884500	-1.12424000
C	2.19993200	-1.26480700	-0.27678600
H	2.77229900	-2.04786700	-0.78021600
H	2.77654100	-0.35087800	-0.16066200
C	1.51238600	-1.74220700	0.99677000
H	1.34545300	-0.92469000	1.70295700
H	1.97722300	-2.60297900	1.47045100
N	1.57861500	1.58158400	0.60060600
N	2.31580400	2.01361300	-0.51158600
H	3.04711500	2.62275400	-0.16932400
H	1.77457600	2.51849700	-1.20948600

CA-C1-III

C	0.60870800	0.25383000	1.17941500
C	0.03367100	1.65342600	1.16723800
C	-0.77746400	1.98066200	0.17117600
C	-1.09451300	0.91832100	-0.86047200
C	0.21030600	0.23814500	-1.33551800
C	1.23462600	-0.01045100	-0.21849900
C	-0.42561800	-0.81361400	1.46291200
C	-1.60251800	-0.93551400	0.84206400
C	-2.07023000	-0.06673100	-0.24774400
H	1.40782100	0.17340700	1.91903600
H	0.30732300	2.34923300	1.95153000
H	-1.23489600	2.96020500	0.09103000
H	-1.60363400	1.35381800	-1.72017700
H	-2.23510200	-1.77722400	1.10481600
H	-0.15438400	-1.56398400	2.19813700
O	2.35379600	0.82959900	-0.41760800
O	1.73169200	-1.34440900	-0.25524400
C	3.49165800	0.11136500	0.01055700
C	3.13931500	-1.31008500	-0.40222100
H	4.36643200	0.51888400	-0.49528400
H	3.63092900	0.19428900	1.09691200
H	3.41727100	-1.50166200	-1.44518600
H	3.58572400	-2.07357700	0.23745900
H	0.69510000	0.87492200	-2.07633100
H	-0.01703700	-0.71903100	-1.80672700
N	-3.25278200	-0.07936800	-0.74054300
N	-4.18440200	-0.94211300	-0.19851500
H	-4.18039300	-0.97164600	0.81620300
H	-5.09640600	-0.66491700	-0.52865200

CA-C2-III

C	-3.41516800	-1.11117300	-0.31207200
C	-3.86393300	0.12520600	0.29439700
C	-3.13921500	1.26614200	0.38782100
C	-2.15151500	-1.55366600	-0.35513000
C	-1.77266000	1.48834400	-0.01339800
C	-1.02459900	-0.89998900	0.39991800
C	-0.83381800	0.51852000	-0.07738900
H	-4.17940400	-1.70631100	-0.80618000
H	-4.91081000	0.17447000	0.57876100
H	-3.66644000	2.14911400	0.74103700
H	-1.91419800	-2.44119800	-0.93550200
H	-1.49122100	2.50773800	-0.25761400
H	-1.27600000	-0.86096400	1.46697700
C	1.32952200	-0.39236800	-0.01247500
C	0.35178200	-1.54747000	0.18223600
H	0.36223300	-2.13571200	-0.73706100
H	0.67338100	-2.17684300	1.00983000
O	1.97377800	-0.05826500	1.19547400
O	2.33503900	-0.65740600	-0.94866100
C	3.28642000	0.38027800	0.88167200
C	3.60741100	-0.43050600	-0.36707400
H	4.23234000	0.10964700	-1.07947800
H	4.07738500	-1.38918200	-0.12055100
H	3.29410000	1.45382600	0.67560500
H	3.93475400	0.15291400	1.72797600
N	0.46802000	0.66687900	-0.49640800
N	1.05201600	1.90629200	-0.73634500
H	0.74859200	2.24905400	-1.64007200
H	0.75914300	2.56670900	-0.01999300

CA-C3-III

C	0.74744400	2.17125400	-0.53795200
C	0.70434900	2.30688100	0.97251600
C	0.32406700	1.24237300	1.66571900
C	-0.01656900	-0.01755600	0.90784000
C	-1.01294500	0.33213100	-0.24402100
C	-0.59978800	1.58721800	-1.01343300
C	1.92172900	1.29964700	-0.93725300
C	2.10925200	0.03446200	-0.54795700
C	1.19947800	-0.71230100	0.32898500
H	0.87381700	3.15183300	-0.99987800
H	0.98324700	3.24329500	1.44223600
H	0.26382900	1.24414500	2.74750700
H	-0.49078800	-0.74411000	1.56838200
H	3.02403500	-0.46248600	-0.85206200
H	2.68049600	1.75901700	-1.56444800

H	-1.38402800	2.33087000	-0.86554000
H	-0.56076900	1.33355400	-2.07369100
O	-2.30675300	0.51363300	0.29871700
O	-1.14744600	-0.74664900	-1.13969500
C	-2.02518200	-1.66382000	-0.51630200
H	-2.58338800	-2.18105000	-1.29680500
H	-1.46027800	-2.39436800	0.07364400
C	-2.91126300	-0.76619700	0.37689600
H	-2.93731500	-1.12532200	1.41143900
H	-3.93445000	-0.67819200	0.00732800
N	1.32027400	-1.95203100	0.63171200
N	2.36738000	-2.67040800	0.09163800
H	2.17730200	-3.65128600	0.23094700
H	2.52486300	-2.48924800	-0.89491100

ω B97X-D/6-311G(d,p) gas phase Cartesian coordinates of the stationary points involved in the cycloaddition reactions of tropone **1** with ethylene **16**, DCE **17**, and CKA **9**.

Tropone **1**

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

TS-A1-IV

C	1.52769300	0.90746700	-0.23396900
C	1.51012800	-0.05301200	-1.25072400
C	0.46716100	-0.92928000	-1.44163500
C	-0.65709200	-1.00566900	-0.60964500
C	0.28484300	-1.33670300	1.35497900
C	1.36510100	-0.49747800	1.55274200
C	0.39359200	1.73280200	0.13539400
C	-0.91691700	1.43628400	0.10172000
C	-1.50803500	0.11984900	-0.14411400
H	2.48856400	1.37975400	-0.04948700
H	2.43900900	-0.24075600	-1.77999200
H	0.62657200	-1.75799400	-2.12483800
H	-1.27019500	-1.89763500	-0.71595800
H	-1.63900500	2.19032900	0.39632200
H	0.66053900	2.72716200	0.48612900
H	0.46047900	-2.36641000	1.06950500
H	-0.64191500	-1.15604800	1.88626800
H	1.27477200	0.34356900	2.22853200
H	2.37089700	-0.86013800	1.38201000
O	-2.69607000	-0.07592500	0.05412800

TS-A2-IV

O	-1.62291000	1.29266500	-0.61611900
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C	-0.48473900	0.79758800	-0.42617700
C	-0.44083000	-0.68082500	-0.61195700
C	-1.73393100	-1.14220900	0.75492800
C	-2.69669700	-0.15142600	0.57859300
C	1.96976200	-1.23165800	-0.04817100
C	2.50100800	-0.00979900	0.38171000
C	1.88910500	1.23068400	0.35747400
C	0.71905300	-1.50286900	-0.55024700
C	0.58930500	1.58813000	0.00849100
H	2.66377500	-2.06821700	-0.04581800
H	3.53088100	-0.03042100	0.72322800
H	2.51316200	2.06060500	0.67864500
H	0.57721500	-2.50999300	-0.93485200
H	0.33299000	2.64042200	0.08237300
H	-1.11285000	-0.96035600	-1.42016700
H	-1.13772400	-1.11948600	1.66121200
H	-1.96005000	-2.13877100	0.39072500
H	-2.80577900	0.66886500	1.27296600
H	-3.49056100	-0.26966300	-0.14722200

CA-A1-IV

C	1.50500500	0.70132600	-0.14895100
C	1.28626000	-0.20764200	-1.34093400
C	0.30141900	-1.09357800	-1.27117100
C	-0.55477500	-1.11554500	-0.02778800
C	0.34138300	-1.10759600	1.24394500
C	1.57450500	-0.19247600	1.11933100
C	0.39974400	1.72226800	-0.00398100
C	-0.90576100	1.44731600	0.05784500
C	-1.49818900	0.08734000	-0.00400000
H	2.45339700	1.23125900	-0.25339700
H	1.94001500	-0.13005000	-2.20220400
H	0.08490300	-1.78447800	-2.07767700
H	-1.20386200	-1.99129000	-0.01287000
H	-1.63412900	2.24582000	0.15444600
H	0.70615900	2.76284900	0.06748100
H	0.66516400	-2.13487100	1.42264700
H	-0.27088300	-0.82070400	2.10248800
H	1.67614000	0.43958200	2.00475600
H	2.48389900	-0.79345500	1.04545800
O	-2.69979400	-0.05914200	0.00038700

CA-A2-IV

C	1.91296100	1.23896800	-0.32330300
C	2.54417500	0.04586600	0.19819200
C	1.98126300	-1.18557100	0.25145400

C	0.60118000	1.51240200	-0.30293300
C	0.63988500	-1.56293200	-0.11498200
C	-0.40519700	0.68701400	0.45358500
C	-0.40935500	-0.72308700	-0.08850300
H	2.57182600	1.95310300	-0.81117300
H	3.59974800	0.12236500	0.44121700
H	2.63145400	-2.00793100	0.53854900
H	0.22936200	2.38312200	-0.83648200
H	0.45436600	-2.59283400	-0.39880600
H	-0.13241500	0.65598800	1.51642800
O	-1.64401000	-1.08990600	-0.49716000
C	-2.59991900	-0.20744200	0.09882300
C	-1.86735000	1.12208900	0.25896000
H	-1.96241300	1.71299700	-0.65564100
H	-2.25263000	1.71330100	1.09009100
H	-3.46542400	-0.16456100	-0.56108700
H	-2.90764700	-0.62014600	1.06643400

TS-B1-IV

C	-0.29384300	-0.46866600	1.71343300
C	-0.18827800	-1.72959600	1.14432000
C	0.55136900	-2.02170800	0.01707500
C	1.18079200	-1.05709900	-0.80162700
C	-0.25370600	-0.05526300	-1.58324200
C	-1.23094700	0.44905900	-0.69506900
C	0.68334200	0.58432700	1.72328300
C	1.74467600	0.77948300	0.91589700
C	2.07968500	0.04210600	-0.30291200
H	-1.10014400	-0.33937300	2.42932300
H	-0.85030500	-2.49951900	1.52444100
H	0.45958800	-3.02289600	-0.39226500
H	1.62650500	-1.46151100	-1.70805300
H	2.41344500	1.60899900	1.11677300
H	0.53305300	1.32257100	2.50472600
H	-0.59310700	-0.84668800	-2.24146300
H	0.36991800	0.68416400	-2.07682500
C	-1.18957500	1.80645400	-0.27584300
N	-1.11275900	2.91067200	0.04980000
C	-2.41874700	-0.29992000	-0.46565400
N	-3.35399100	-0.95623400	-0.30242700
O	3.05246000	0.33726400	-0.96578000

TS-B2-IV

C	-0.44619900	-1.07471600	0.24813300
C	-0.38917100	0.26610500	0.91631800
C	1.77488900	-0.07589600	-0.46621000

C	0.66005900	-0.82472500	-1.01715000
C	-2.88008600	-1.12692500	-0.50507500
C	-3.29838200	0.21079900	-0.33130100
C	-2.63434400	1.25070700	0.28494300
C	-1.67914400	-1.69459900	-0.20196300
C	-1.35249600	1.28374900	0.83527500
H	-3.63606500	-1.79928800	-0.89996400
H	-4.29908400	0.43475100	-0.68722500
H	-3.18247900	2.18586900	0.34580400
H	-1.61126000	-2.76921600	-0.35276200
H	-1.02825300	2.21065100	1.29672900
H	0.12492000	-1.77048300	0.86633900
H	0.13344700	-0.28427300	-1.79972500
H	0.93541400	-1.82587000	-1.34081900
C	1.91565100	1.29263500	-0.80144000
N	1.93990200	2.40382500	-1.11365200
C	2.85595500	-0.76314400	0.14398500
N	3.70515400	-1.37392800	0.62894700
O	0.73594700	0.49308000	1.41643200

TS-B3-IV

C	0.68619600	-1.76424100	-0.93620800
C	0.25880900	-2.24605800	0.31818500
C	0.05948400	-1.44361900	1.42459500
C	0.29930600	-0.08035200	1.47330700
C	-1.21159100	0.33571600	-0.62585600
C	-0.88089600	-0.71043300	-1.51139200
C	1.77856800	-0.79826900	-1.10941000
C	2.11121000	0.23489800	-0.32842200
C	1.40422000	0.70457800	0.87230100
H	0.67530800	-2.51611800	-1.72136000
H	-0.14796900	-3.25188400	0.34876500
H	-0.51053800	-1.86654400	2.24517900
H	-0.16003500	0.47162700	2.28912400
H	2.94237400	0.87035600	-0.61320700
H	2.36097400	-0.94475300	-2.01492600
H	-1.59050900	-1.52564400	-1.57983300
H	-0.44526900	-0.41285800	-2.45845000
C	-0.77452400	1.66535800	-0.89834100
N	-0.40461500	2.72821400	-1.14814500
C	-2.32260800	0.16303900	0.25538400
N	-3.22325800	-0.03308400	0.94812000
O	1.72771600	1.74327600	1.41250400

TS-B4-IV

O	0.38192800	-1.80769100	-0.91657400
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C	-0.53519200	-0.88674100	-0.72785600
C	-0.16386200	0.46427200	-0.99211100
C	1.85513000	-0.23275600	0.32549000
C	1.80483100	-1.42441800	-0.53759500
C	-2.05224500	1.75247800	0.04254100
C	-2.99278300	0.76644400	0.32181700
C	-2.87584300	-0.60237000	0.12910500
C	-0.82901200	1.61756500	-0.59979900
C	-1.77250600	-1.34065600	-0.28052200
H	-2.34252400	2.76850900	0.28970900
H	-3.93039500	1.10777400	0.74739700
H	-3.74088500	-1.19225700	0.41507900
H	-0.30804300	2.54026900	-0.83658400
H	-1.84774100	-2.42114100	-0.22009800
H	0.66752200	0.60371900	-1.66964200
H	2.35171000	-1.27785800	-1.46849300
H	2.12448600	-2.34828300	-0.05833300
C	2.55184200	0.92041300	-0.07822500
N	3.07569100	1.87424300	-0.47649400
C	1.27471300	-0.30468400	1.60555000
N	0.69288300	-0.40231200	2.60266400

CA-B1-IV

C	-0.45169900	-0.01961200	1.22397800
C	0.09767100	-1.42886500	1.28598800
C	0.85871400	-1.84184600	0.28265000
C	1.16706600	-0.87003100	-0.82988600
C	-0.11849400	-0.16532900	-1.33499400
C	-1.13733200	0.14290500	-0.18973200
C	0.61133100	1.04266100	1.40526000
C	1.75572000	1.11469000	0.72389800
C	2.17941400	0.17265700	-0.34496200
H	-1.22451700	0.12126800	1.97982700
H	-0.17187600	-2.06267000	2.12103200
H	1.27731900	-2.83989500	0.24637300
H	1.64339100	-1.37309700	-1.67084300
H	2.47174400	1.90099100	0.93689100
H	0.40455800	1.80061600	2.15396300
H	-0.60612400	-0.80391000	-2.07088000
H	0.14364600	0.76499700	-1.84030500
C	-1.66436900	1.50850000	-0.32745700
N	-2.04752000	2.58746500	-0.42221400
C	-2.27179700	-0.79308100	-0.25335000
N	-3.14370100	-1.53990900	-0.29736800
O	3.28038300	0.24786400	-0.83341700

CA-B2-IV

C	-0.58928300	-0.46369000	0.72385100
C	-0.49501500	0.42334900	-0.49046700
C	1.65857400	-0.05111600	-0.01333600
C	0.82713200	-1.04438700	0.83404900
C	-2.94488200	-1.17876900	0.28789900
C	-3.47258500	0.15349800	0.07689400
C	-2.82167600	1.18168000	-0.51480900
C	-1.66158100	-1.49787500	0.49897600
C	-1.46049400	1.19716700	-0.99633400
H	-3.66551100	-1.99031600	0.23426800
H	-4.52541600	0.29503400	0.30050000
H	-3.39766400	2.07893300	-0.72083200
H	-1.36679400	-2.54283900	0.53045500
H	-1.19876900	1.88592600	-1.79126900
H	-0.83717600	0.15181300	1.59720900
H	0.88482400	-2.02417700	0.35665600
H	1.20217000	-1.12295800	1.85285900
C	2.81567900	-0.68743500	-0.65817000
N	3.71141300	-1.22199800	-1.13695500
C	2.11288300	1.08991500	0.81491200
N	2.41855600	1.97372400	1.48140300
O	0.77275400	0.40906000	-1.01897200

CA-B3-IV

C	0.81705300	-1.53964700	-0.97597700
C	0.76916700	-2.09149900	0.43429800
C	0.34293300	-1.29153300	1.40159700
C	-0.01449800	0.12985800	1.04223300
C	-0.99477800	0.11620200	-0.19696800
C	-0.56310400	-0.91831500	-1.29378400
C	1.91055400	-0.51110200	-1.16815200
C	2.09302000	0.57291000	-0.41230000
C	1.26265600	0.93878000	0.75860500
H	0.97857500	-2.35171500	-1.68601900
H	1.04938800	-3.12209200	0.61554100
H	0.25879300	-1.60720100	2.43346700
H	-0.50920400	0.64295500	1.86585400
H	2.90731100	1.25982700	-0.61381400
H	2.58524500	-0.67416600	-2.00363900
H	-1.30463200	-1.71618900	-1.33194000
H	-0.54795000	-0.42872100	-2.26767000
C	-1.08373000	1.46558100	-0.77663600
N	-1.12293900	2.51295300	-1.24701200
C	-2.32569000	-0.25254300	0.30986800
N	-3.35044200	-0.57507100	0.71710800
O	1.57683100	1.83999800	1.49510600

CA-B4-IV

C	0.74882000	1.05664700	0.09680900
C	0.10366300	-0.21958300	-0.39388300
C	-1.41172600	0.05811300	-0.11745200
C	-1.41910500	1.61349800	-0.05184300
C	1.98415400	-1.73322900	0.23314400
C	3.04030400	-0.92832700	-0.34399500
C	3.07331700	0.42263700	-0.39337600
C	0.68451400	-1.42082900	0.30132300
C	2.05378500	1.34808000	0.04088300
H	2.29422800	-2.67248200	0.68256800
H	3.93586800	-1.45963600	-0.65021200
H	3.99445800	0.88091800	-0.74113600
H	0.01057400	-2.06176900	0.85954100
H	2.35215500	2.35621200	0.30510700
H	0.24445400	-0.30599400	-1.47839900
H	-1.47964800	2.01644100	-1.06837400
H	-2.22493500	2.01147200	0.56046000
C	-2.27529400	-0.44635400	-1.18581400
N	-2.93955400	-0.81136900	-2.04889200
C	-1.85611500	-0.48409600	1.17353200
N	-2.20537200	-0.88483100	2.19170000
O	-0.18382000	1.93861400	0.54685300

TS-C1-IV

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

TS-C2-IV

C	-0.78531900	-0.88429700	0.72592800
C	-0.46741900	0.56816100	0.90667200
C	1.40218100	-0.70835400	-0.70213900
C	0.18537300	-1.36201300	-0.85661500
C	-3.16612400	-0.86047200	-0.09940800
C	-3.27255500	0.41287400	-0.66196200
C	-2.41427100	1.48802100	-0.44316000
C	-2.10732900	-1.40940700	0.58935300
C	-1.25132300	1.58652100	0.30234600
H	-4.03704300	-1.50206100	-0.21427600
H	-4.16435700	0.61685700	-1.24507600
H	-2.73592100	2.42393500	-0.89568900
H	-2.24151200	-2.42232000	0.95840300
H	-0.81619600	2.57515500	0.41204700
H	-0.16704100	-1.44873900	1.42055100
H	-0.45120900	-0.97003300	-1.64064500
H	0.21747500	-2.43889000	-0.75451400
O	2.39543300	-1.18432300	0.01879800
O	1.60210300	0.50934800	-1.14845800
C	3.22931600	-0.07938800	0.41875500
C	2.73829300	1.07428300	-0.46437400
H	2.37492900	1.91088400	0.12714600
H	3.45375900	1.39361900	-1.22144300
H	3.03118300	0.11099900	1.47134500
H	4.26550000	-0.36479900	0.24628000
O	0.59315200	0.81995200	1.51009600

TS-C3-IV

C	1.86646800	-1.07445400	-0.36906800
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

CA-C1-IV

C	0.22066700	0.24205200	1.18073400
C	-0.51057800	1.56706700	1.13914300
C	-1.34949800	1.77937200	0.13575900
C	-1.52359900	0.68328500	-0.89046500
C	-0.13890200	0.15672500	-1.34330500
C	0.88611200	0.02593200	-0.20887200
C	-0.69541100	-0.91822600	1.49236700
C	-1.82866700	-1.20533700	0.84817400
C	-2.37015200	-0.44940200	-0.30775000
H	1.01997500	0.26766600	1.92337000
H	-0.31908800	2.30611900	1.90737200
H	-1.91241500	2.69932300	0.03292600
H	-2.07462500	1.04159900	-1.75978000
H	-2.43281700	-2.05496100	1.14843600
O	-3.43976400	-0.74398100	-0.79111700
H	-0.38719600	-1.57239100	2.30203600
O	1.91395000	0.97549000	-0.40168300
O	1.51503500	-1.24958800	-0.21730500
C	3.11968100	0.37620800	0.02808800
C	2.91144600	-1.07376600	-0.38047600
H	3.94792700	0.86899000	-0.47978500
H	3.24947700	0.47595600	1.11396800
H	3.19625900	-1.23760500	-1.42613400
H	3.43697800	-1.78788200	0.25531000
H	0.27622300	0.85165700	-2.07312200
H	-0.24105800	-0.81731100	-1.82413600

CA-C2-IV

C	3.30787300	0.97437600	-0.17165600
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C	3.69749300	-0.37350600	0.18300400
C	2.92121500	-1.47723600	0.06274100
C	2.06709300	1.47749100	-0.11553800
C	1.54664300	-1.54760100	-0.36553900
C	0.91085300	0.75128200	0.51802900
C	0.66815500	-0.54260600	-0.22446300
H	4.09839500	1.61528000	-0.55403100
H	4.74123300	-0.52406700	0.44219800
H	3.40233700	-2.43582200	0.23853500
H	1.87224700	2.46604800	-0.52251000
H	1.19000600	-2.47432100	-0.80094900
H	1.14533500	0.51793200	1.56348400
C	-1.40085600	0.35751300	0.00103300
C	-0.43959800	1.46370000	0.39125800
H	-0.42820400	2.19000500	-0.42341000
H	-0.77403400	1.95316300	1.30357300
O	-1.97659600	-0.24272600	1.11215500
O	-2.42748400	0.74745100	-0.83129100
C	-3.10068000	-0.95152700	0.61054100
C	-3.57282300	-0.05072800	-0.53786300
H	-3.86630200	-0.61719800	-1.42310400
H	-4.38686300	0.61454800	-0.24124200
H	-2.79457600	-1.93888300	0.25280700
H	-3.82597900	-1.05624800	1.41547000
O	-0.59664600	-0.60439900	-0.70087700

CA-C3-IV

C	1.78640000	-1.21883200	-0.53356100
C	1.87765000	-1.29766300	0.97854400
C	1.01034700	-0.58307800	1.68091300
C	0.03247600	0.28655600	0.93122200
C	-0.65766600	-0.53536300	-0.20636900
C	0.31171600	-1.46818300	-0.92894100
C	2.26676000	0.12075200	-1.04985100
C	1.79758000	1.30954400	-0.66468600
C	0.71102600	1.51457700	0.32233000
H	2.39635800	-2.00222900	-0.98562200
H	2.61873600	-1.93836500	1.44190700
H	0.99005500	-0.58957100	2.76372500
H	-0.73404500	0.67752300	1.60107900
H	2.19637000	2.22618600	-1.08576000
O	0.34970500	2.62967700	0.62489000
H	3.04880000	0.09939600	-1.80423800
H	0.04190000	-2.49075500	-0.66314300
H	0.16488300	-1.33839100	-2.00164900
O	-1.71908000	-1.28876900	0.33628900
O	-1.26366500	0.33603600	-1.13350900
C	-2.49190000	0.73719500	-0.55271700

H	-3.20785400	0.89792900	-1.35821500
H	-2.36536500	1.66858800	0.00955500
C	-2.86128600	-0.44695100	0.36823200
H	-3.07238200	-0.11441900	1.39001600
H	-3.71175700	-1.02276600	0.00028600

Ethylene **16**

C	-0.66214800	0.00000000	0.00000400
C	0.66214800	0.00000000	-0.00000300
H	-1.23144700	-0.92379300	-0.00001100
H	-1.23144700	0.92379300	0.00002200
H	1.23144700	0.92379300	0.00001000
H	1.23144700	-0.92379300	-0.00002400

Cyclic ketene acetal **9**

C	0.00000000	0.00000000	2.11537300
C	0.00000000	0.00000000	0.78894000
H	-0.05322900	0.93574600	2.64961800
H	0.05322900	-0.93574600	2.64961800
O	0.00000000	1.11688100	0.01718800
O	0.00000000	-1.11688100	0.01718800
C	0.24469500	-0.72008400	-1.32724100
H	1.31583700	-0.78855400	-1.54450700
H	-0.31160900	-1.37902900	-1.99210800
C	-0.24469500	0.72008400	-1.32724100
H	-1.31583700	0.78855400	-1.54450700
H	0.31160900	1.37902900	-1.99210800

Dicyanoethylene **17**

C	0.00000000	0.00000000	1.73662700
C	0.00000000	0.00000000	0.40058500
H	0.00000100	-0.93153100	2.28791100
H	-0.00000100	0.93153100	2.28791100
C	0.00000000	1.22423300	-0.35083000
N	-0.00000100	2.21053100	-0.94208100
C	0.00000000	-1.22423300	-0.35083000
N	0.00000100	-2.21053100	-0.94208100