Generation and Trapping of Electron-Deficient 1,2-Cyclohexadienes. Unexpected Hetero-Diels-Alder Reactivity

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Electronic Supplementary Information, Part 2 (Computational Results)

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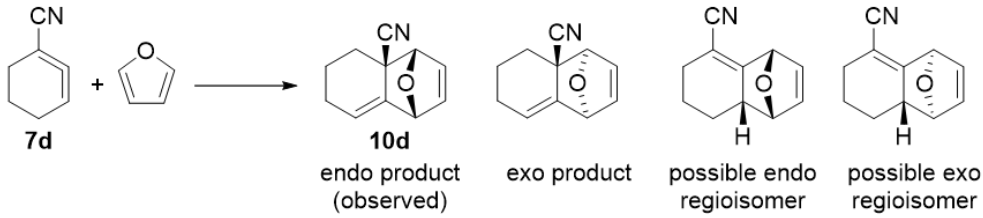
1. Computational Methods

All structures were optimized using M06-2X[1] with the double-ζ split valence 6-31+G(d,p) basis set. Solvation with tetrahydrofuran was performed using the Integration Equation Formalism Polarizable Continuum Model (IEFPCM)[2] model and vibrational analysis verified that each structure was either a minimum or transition state. All optimizations were performed in Gaussian 09.e01.[3] Non-covalent interaction (NCI)[4,5] plots were used to further elucidate the secondary orbital interactions in cycloaddition transition state structures. NCI figures were generated on VMD[6] with isovalue of 0.3 and the remaining figures were created using Vesta.[7]

1.1.Choice of Computational Method

DFT methods were used to study the reactivity of allene **7d** with furan (Figure S1). The results from both, M06-2X/6-31+G(d,p)/IEFPCM(THF) and ωB97XD/6-31+G(d,p)/IEFPCM(THF), were able to explain the observed selectivity.



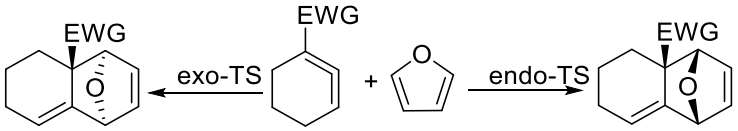
	Diastereoselectivtity		Regioselectivity	
Level of Theory	**$\Delta G^{\ddagger}_{Obs}$**	**$\Delta G^{\ddagger}_{Exo}$**	**$\Delta G^{\ddagger}_{RegioEndo}$**	**$\Delta G^{\ddagger}_{RegioExo}$**
M06-2X/6-31+G(d,p)/IEFPCM(THF)	12.3	14.2	13.7	13.3
ωB97XD/6-31+G(d,p)/IEFPCM(THF)	11.6	13.8	14.2	13.8

Figure S1:DFT methods tested to explain the observed selectivity between allene 7d and furan. All values reported in kcal/mol

2. Computational Results

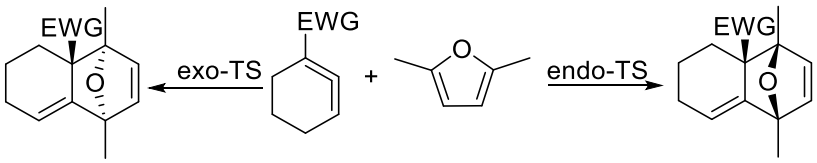
2.1. Computed energies of trapping reactions between allenes and dienes

The results of computations performed on the Diels-Alder reactions of allenes **7a** and **7d** with furan, 2,5-Dimethylfuran, and DPIBF are presented in Table S1, S2, and S3. It was determined that the formation of endo product was favoured for both allenes **7a** and **7d**.



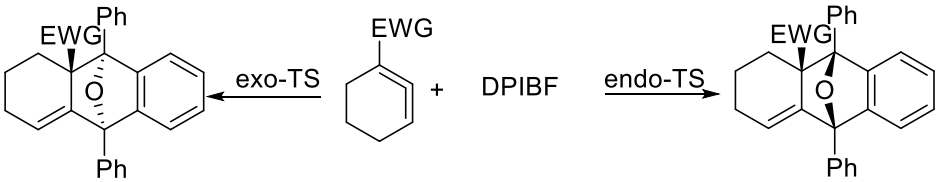
Allene	Exo	Exo-TS	Allene + Furan	Endo-TS	Endo
7a	-24.1	+14.2	0.0	+12.3	-23.7
7d	-29.4	+12.7	0.0	+10.6	-30.4

Table S1: Energies of trapping reactions with Furan. All free energies reported in kcal/mol



EWG	Exo	Exo-TS	Allene + DiMeFuran	Endo-TS	Endo
7a	-21.4	+15.4	0.0	+13.5	-20.5
7d	-30.4	+12.3	0.0	+9.0	-31.5

Table S2:Energies of trapping reactions with 2,5-Dimethylfuran. All free energies reported in kcal/mol



EWG	Exo	Exo-TS	Allene + DPIBF	Endo-TS	Endo
7a	-35.0	+9.7	0.0	+8.6	-35.7
7d	-46.6	+6.0	0.0	+5.9	-45.1

Table S3: Energies of trapping reactions with DPIBF. All free energies reported in kcal/mol

2.2.Discussion of observed exo cycloadduct 13d

The computations show that the barrier for formation of endo cycloadduct is generally favoured (Table S2). However, both *endo* and *exo* cycloadducts were observed with allene **7d** (EWG=CN) when trapping reaction with DPIBF. The DFT calculations performed on substrate 5d shows that the barrier for formation of *endo* cycloadduct is favoured by 2.1 kcal/mol for furan, 3.3 kcal/mol for 2,5-Dimethylfuran, and 0.1 kcal/mol for DPIBF (Table S4). Since the barrier for formation is similar for both endo and exo cycloadducts, the theoretical results are consistent with experimental results such that both cycloadducts are observed.

	Furan	Dimethylfuran	DPIBF	Isobenzofuran	Diphenylfuran
Endo-TS	10.6	9.0	5.9	6.7	11.0
Exo-TS	12.7	12.3	6.0	7.7	12.5

Table S4: Transition state energies of trapping allene 7d with various dienes. All free energies are reported in kcal/mol.

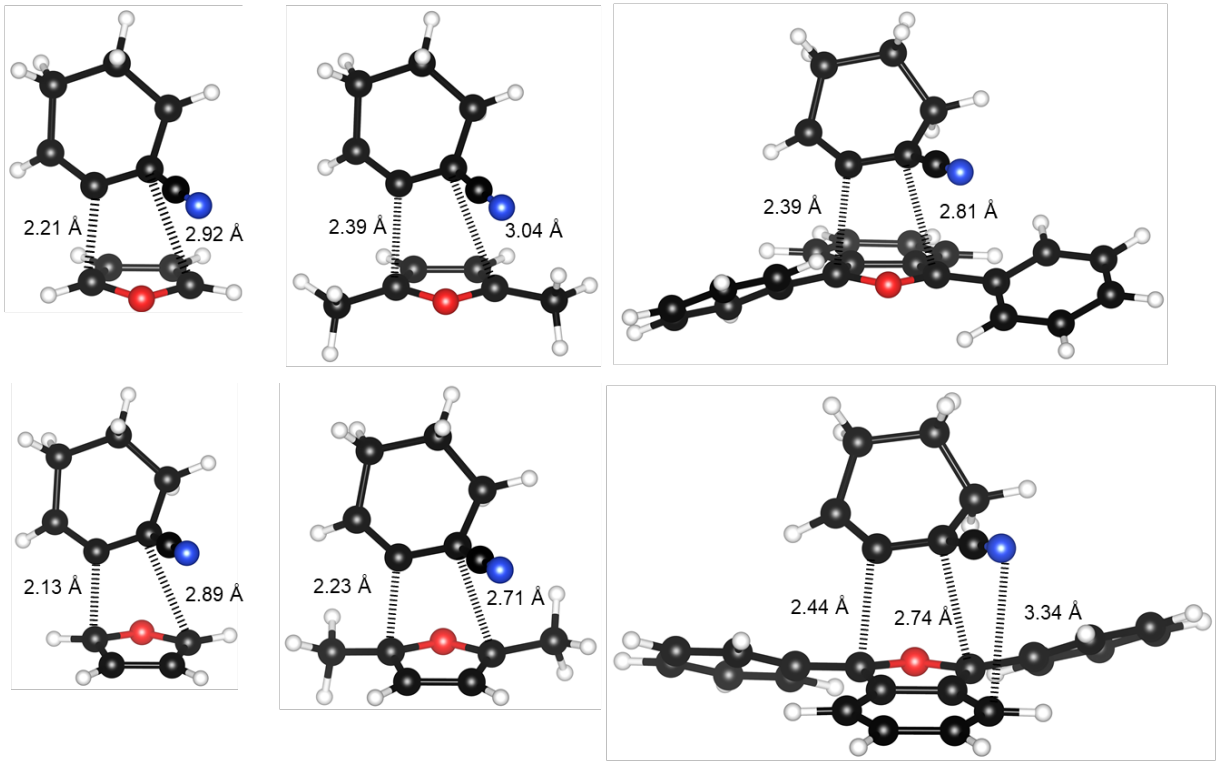


Figure S2: Transition state structures of endo approach (top) and exo approach (bottom) of furan (left), 2,5-Dimethylfuran (center), and DPIBF (right)

In order to understand the observation of both endo and exo product for allene **7d** with DPIBF, the transition state structures were examined. In figure S2, the cyano group is directly on top the pi-system of isobenzofuran moiety of DPIBF, for exo TS, which might result in favourable secondary orbital interactions to lower the barrier. This interaction is absent in the endo TS.

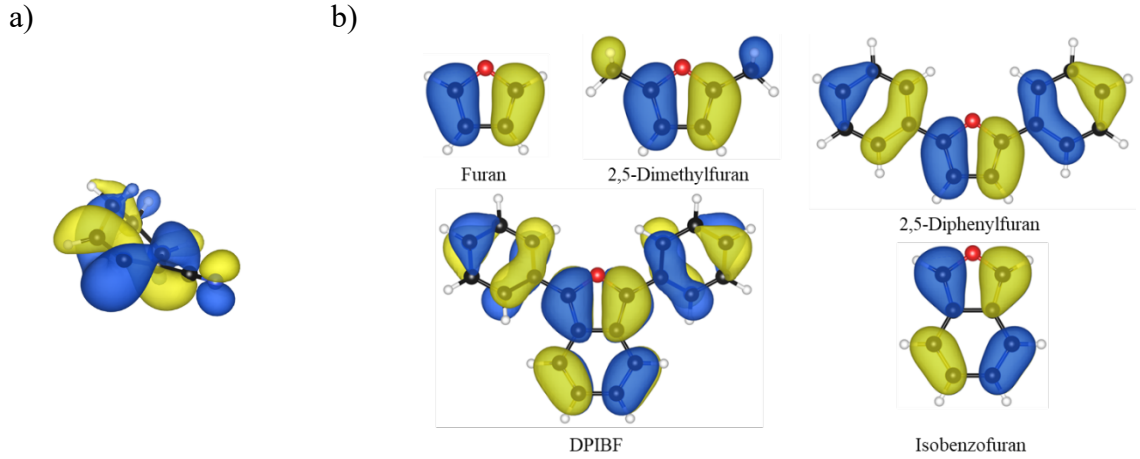


*Figure S3a) LUMO of allene **7d**. b) HOMOs of various Dienes*

In order to gain more insight about this favourable orbital interaction, barriers for formation of endo and exo cycloadducts with 2,5-Diphenylfuran and Isobenzofuran were also calculated. The difference is barriers between formation endo and exo cycloadduct is 1.5 kcal/mol for Diphenylfuran and 1.0 kcal/mol for isobenzofuran, favouring the endo. Similar to DPIBF exo-TS, favourable interaction in the exo approach for isobenzofuran can be observed (Figure S4). This favourable interaction helps explain the presence of exo adduct from **7d** and DPIBF.

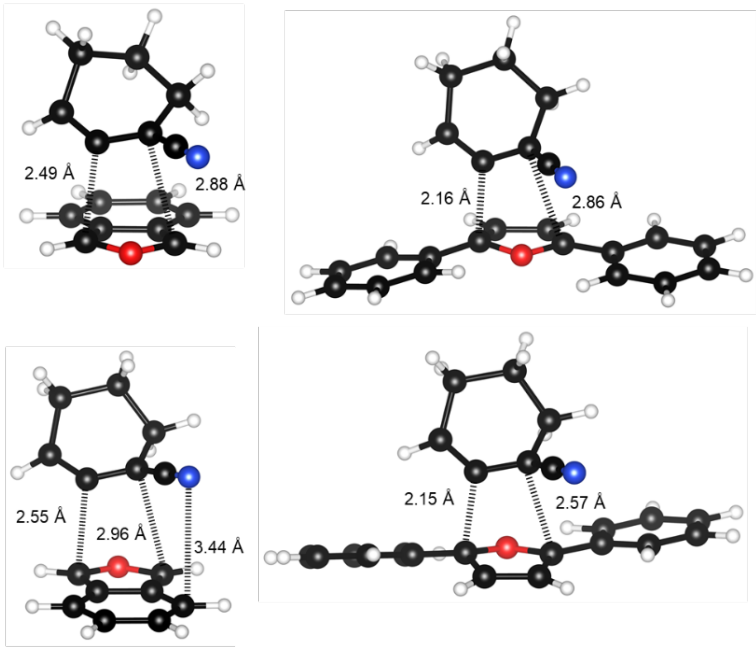


Figure S4: Transition state structures of endo approach (Top) and exo approach (bottom) of isobenzofuran (left) and 2,5-Diphenylfuran (right)

2.3. Lowest Unoccupied Molecular Orbital (LUMO) Coeffecients of Allenes

EWG (allene)	1	2	3
COPh (7a)	11.56	28.07	31.98
CN (7d)	19.24	32.17	12.16

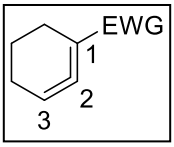
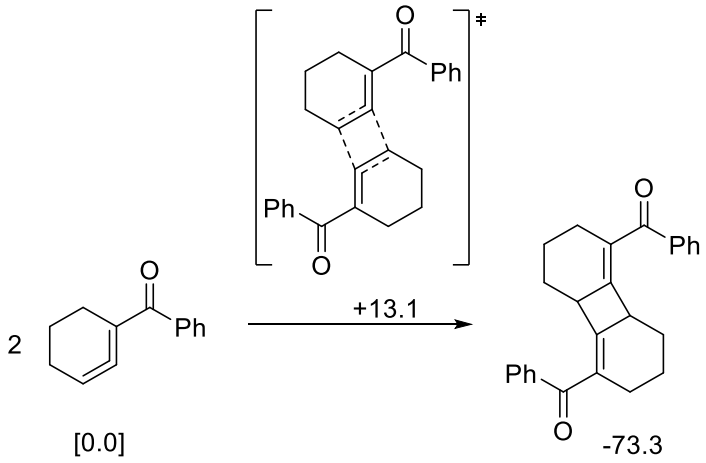


Table S5: LUMO Coeffecients of Allenes

2.4. Discussion of [2+2] dimerization of 7a

The dimerization of **7a** via a [2+2] cycloaddition was also considered and found to be 4.6 kcal/mol lower in energy that the [4+2] pathway. This is consistent with previous studies on allene dimerization however it is not consistent with the observed product distribution and suggests that this system may be more complex than initially expected. Further computational work into the reactivity of this system is ongoing



*Scheme S1: [2+2] Dimerization of Allene **7a***

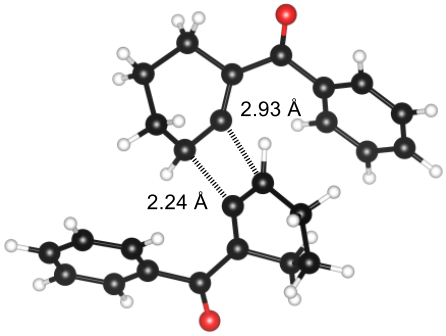


Figure S 5: Transition state strucutre of [2+2]

2.5.Discussion of trapping allene 7a with enamine 15a

The trapping of allene **7a** with enamine **15a** resulted in only one observed cycloadduct. The observed cycloadduct proceeds via an asynchronous Diels-Alder pathway with a barrier of 12.4 kcal/mol and is exergonic by 52.4 kcal/mol. We further examined the reactivity of enamine **15a** with **7a** to determine if a [2+2] product (**16a'**) was plausible. The DFT calculations suggest that the observed product **16a** is thermodynamically favoured by 21.5 kcal/mol compared to **17a**. The calculations also suggest that the formation of **17a**. proceeds via stepwise ionic addition of nucleophilic **15a** to electron deficient **7a**. The first step to form **INT1** has a barrier of 16.2 kcal/mol (3.8 kcal/mol higher than [4+2] barrier) and is exergonic by 20.3 kcal/mol. Additionally, relative to **INT**, the second step proceeds with a barrier of 11.6 kcal/mol, resulting in **17a**. Hence, the formation of **16a** is both kinetically and thermodynamically favoured than **17a**.

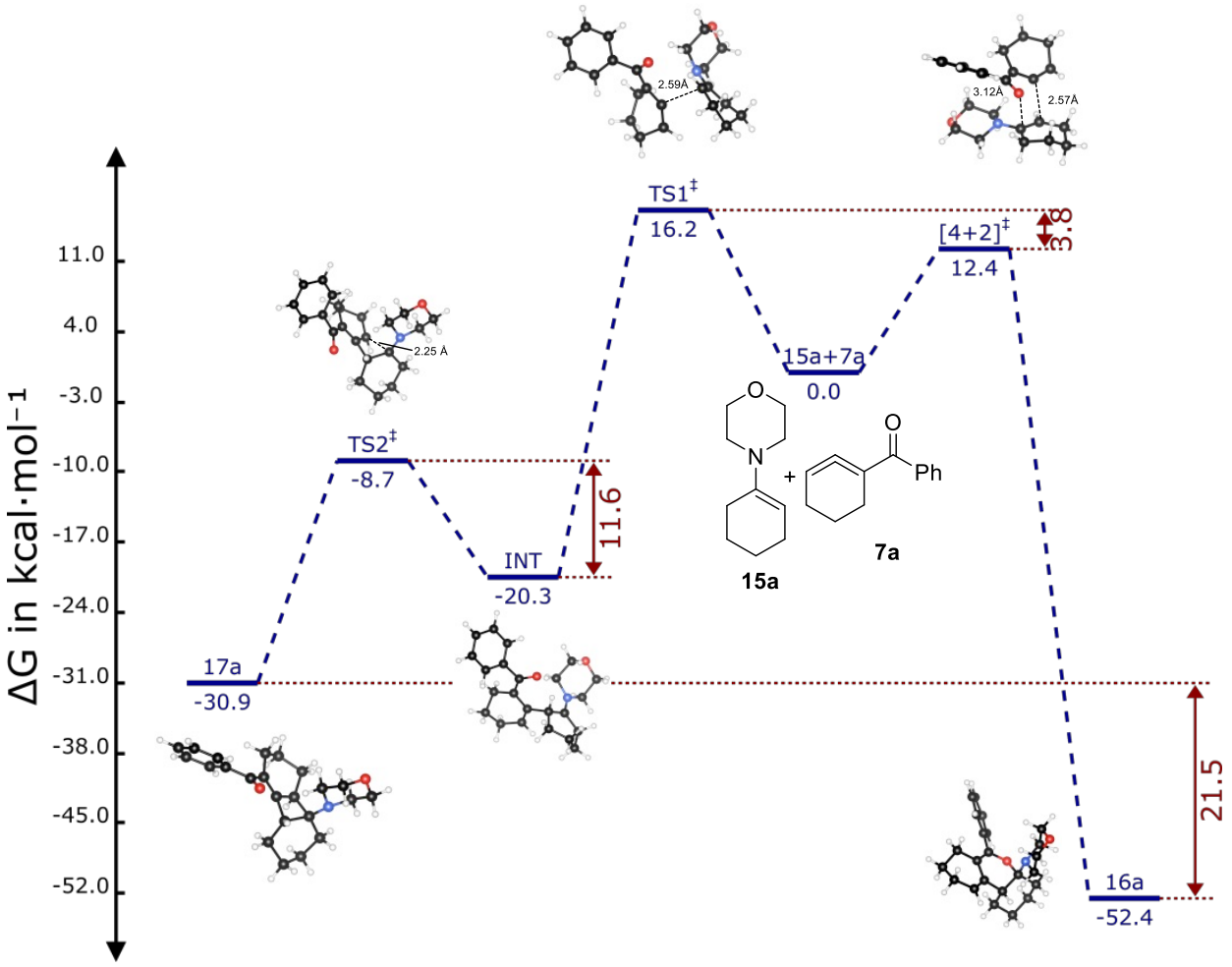
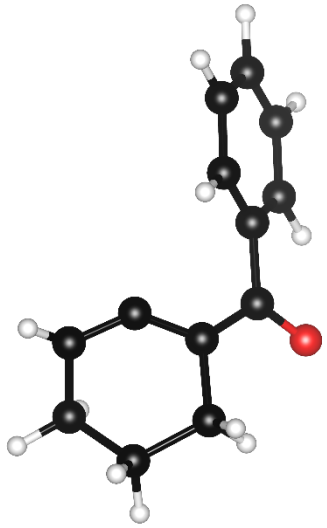


*Figure S5: Potential energy surface of reactivity of enamine **15a** with allene **7a***

3. Energies and Reaction Coordinates

Allene 7a



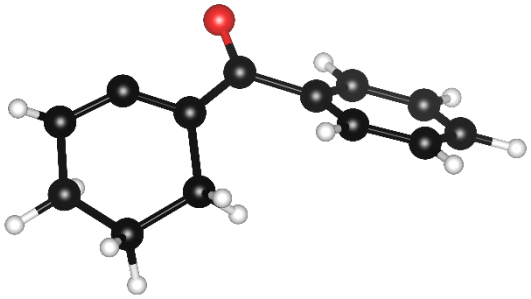
HF (M062X/6-31+G(d,p)) = -577.5243274 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.213763 (Hartree/Particle)
Thermal correction = 0.174502 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.916646	-1.404020	-0.633421
2	6	0	3.873501	-0.791467	0.173188
3	6	0	3.575416	0.409178	0.822053
4	6	0	2.323470	0.992572	0.661637
5	6	0	1.349229	0.370425	-0.129922
6	6	0	1.654259	-0.829833	-0.782724
7	1	0	3.151998	-2.327385	-1.152790
8	1	0	4.853041	-1.244002	0.292950
9	1	0	4.320043	0.887872	1.450093
10	1	0	2.079090	1.929079	1.153127
11	1	0	0.922769	-1.300938	-1.429464
12	6	0	0.022564	1.053057	-0.258690
13	6	0	-1.189574	0.236744	-0.481425
14	8	0	-0.055970	2.272197	-0.154195
15	6	0	-1.330518	-1.045267	-0.162128
16	6	0	-2.300580	-1.778813	0.336761
17	6	0	-2.543229	0.916733	-0.717797
18	6	0	-3.700185	0.197047	0.035767
19	1	0	-4.325692	0.949115	0.527569
20	6	0	-3.248847	-0.851271	1.096606
21	1	0	-4.113581	-1.391904	1.489234
22	1	0	-2.411777	1.937929	-0.345503
23	1	0	-2.778889	0.994108	-1.783124
24	1	0	-4.336817	-0.322989	-0.686831

25	1	0	-2.742120	-0.359827	1.930850
26	1	0	-2.583225	-2.779147	0.028019

Rotated Allene 7a

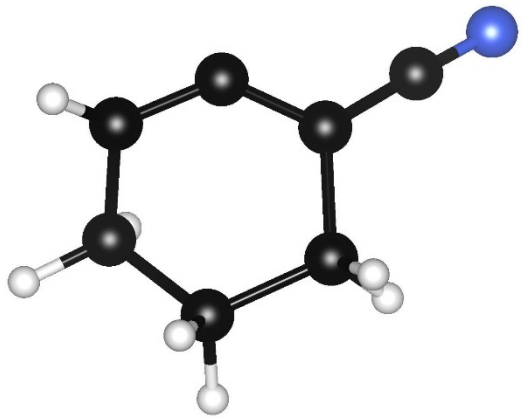


HF (M062X/6-31+G(d,p)) = -577.5186449 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.214001 (Hartree/Particle)
Thermal correction = 0.175151 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.938213	1.355411	0.651715
2	6	0	-3.880396	0.747143	-0.177460
3	6	0	-3.561278	-0.431944	-0.853795
4	6	0	-2.301989	-1.003389	-0.697348
5	6	0	-1.346242	-0.384546	0.115340
6	6	0	-1.668876	0.797259	0.790031
7	1	0	-3.190935	2.262947	1.190325
8	1	0	-4.864970	1.189270	-0.294289
9	1	0	-4.295629	-0.905449	-1.497593
10	1	0	-2.042943	-1.928598	-1.202932
11	1	0	-0.940330	1.267486	1.444023
12	6	0	-0.017994	-1.050290	0.297540
13	6	0	1.198154	-0.213737	0.500854
14	8	0	0.058578	-2.271220	0.280739
15	6	0	2.382468	-0.757504	0.753283
16	6	0	3.624656	-0.522110	0.401282
17	6	0	1.346290	1.242397	0.025515
18	6	0	2.737289	1.504174	-0.633687
19	1	0	2.587263	2.055642	-1.567450
20	6	0	3.590579	0.235112	-0.927253
21	1	0	4.593573	0.521782	-1.252923
22	1	0	0.550726	1.404582	-0.710350
23	1	0	1.183383	1.969286	0.826696
24	1	0	3.328619	2.148480	0.024028
25	1	0	3.131994	-0.366064	-1.716124
26	1	0	4.503925	-0.557457	1.034572

Allene 7d



HF (M062X/6-31+G(d,p)) = -325.4744092 Hartrees
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Thermal correction = 0.089440 Hartrees

Coordinates from last standard orientation:

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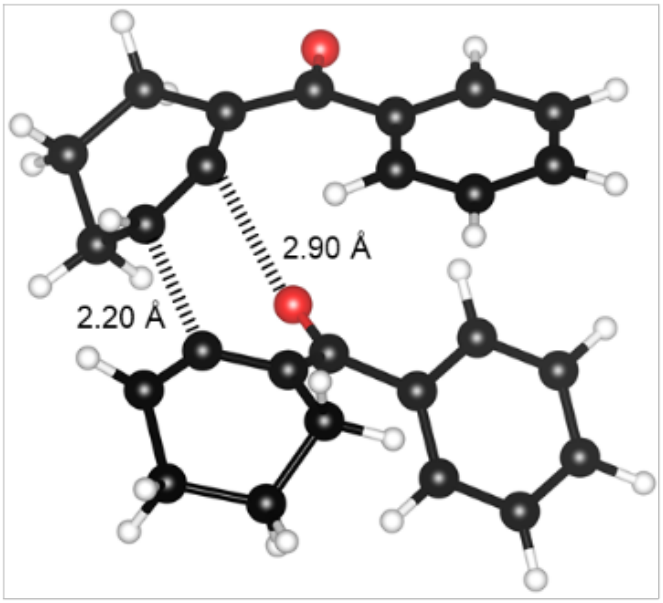
1	6	0	0.712299	-0.079119	-0.337109
2	6	0	-0.074341	-1.143408	-0.430077
3	6	0	-1.365865	-1.317030	-0.242597
4	6	0	-0.044181	1.259150	-0.400868
5	6	0	-1.528338	1.089029	0.033617
6	1	0	-1.793409	1.910360	0.706451
7	6	0	-1.869070	-0.261553	0.735070
8	1	0	-2.945647	-0.339458	0.901710
9	1	0	0.479443	1.934216	0.284517
10	1	0	0.013000	1.707397	-1.396226
11	1	0	-2.173991	1.174397	-0.845162
12	1	0	-1.362069	-0.334022	1.699930
13	1	0	-2.034078	-1.891843	-0.875021
14	6	0	2.079842	-0.113464	0.085427
15	7	0	3.193524	-0.108953	0.409003

Allene 7a: Diels-Alder Dimerization Transition State



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Imaginary Frequencies: 1 (-209.59 cm^{-1})
Zero-point correction = 0.428352 (Hartree/Particle)
Thermal correction = 0.373832 Hartrees

Coordinates from last standard orientation:

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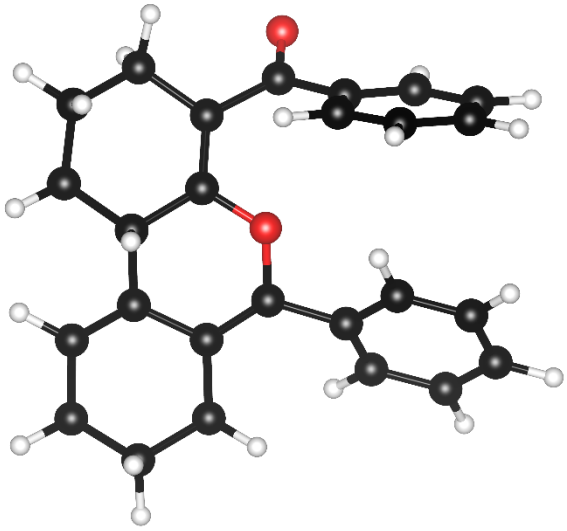
1	6	0	-1.408977	3.989827	0.801956
2	6	0	-1.350720	2.514566	1.276407
3	6	0	-0.380855	1.805938	0.343385
4	6	0	0.827028	2.432776	0.405763
5	6	0	1.138820	3.676340	0.739965
6	6	0	-0.017222	4.671273	0.706910
7	6	0	-0.663590	0.769541	-0.634117
8	6	0	2.713144	1.309476	0.369189
9	6	0	2.522135	0.004473	0.559396
10	6	0	2.831995	-1.142650	0.000710
11	6	0	4.073394	-0.999305	-0.900111
12	6	0	4.389405	0.482529	-1.231826
13	6	0	3.183256	1.448740	-1.087543
14	1	0	-1.885864	4.009145	-0.183754
15	1	0	-0.979627	2.471557	2.306411
16	1	0	2.093673	3.985469	1.153695
17	1	0	0.027117	5.312890	-0.179242
18	1	0	4.950814	-1.493607	-0.472813
19	1	0	5.188612	0.841174	-0.573793
20	1	0	2.365864	1.166876	-1.756013
21	1	0	3.805735	-1.553208	-1.806977
22	1	0	4.773939	0.535877	-2.255792
23	1	0	3.477572	2.482469	-1.294508
24	1	0	3.131983	1.939509	1.149789
25	1	0	0.139845	5.328242	1.570396
26	1	0	-2.048293	4.571190	1.474717

27	1	0	-2.345744	2.063378	1.265540
28	8	0	0.262813	0.220736	-1.243753
29	6	0	-2.066326	0.287071	-0.872097
30	6	0	-2.272776	-1.087193	-1.035545
31	6	0	-3.145532	1.164461	-1.015323
32	6	0	-3.546813	-1.579299	-1.302712
33	1	0	-1.425882	-1.761724	-0.939628
34	6	0	-4.417925	0.673643	-1.306275
35	1	0	-2.990916	2.236047	-0.927113
36	6	0	-4.622076	-0.699375	-1.439675
37	1	0	-3.700992	-2.649053	-1.408208
38	1	0	-5.246568	1.363761	-1.430144
39	1	0	-5.614696	-1.082602	-1.655888
40	6	0	1.984307	-2.353771	-0.100852
41	8	0	2.338353	-3.266999	-0.834382
42	6	0	0.708198	-2.475919	0.687638
43	6	0	0.021946	-3.693218	0.589611
44	6	0	0.161648	-1.451591	1.469345
45	6	0	-1.185668	-3.883389	1.254758
46	1	0	0.447379	-4.480872	-0.023250
47	6	0	-1.049472	-1.639164	2.131405
48	1	0	0.657902	-0.486291	1.555211
49	6	0	-1.724588	-2.854822	2.028042
50	1	0	-1.707435	-4.831120	1.166488
51	1	0	-1.469253	-0.827870	2.718581
52	1	0	-2.670904	-2.996869	2.540949

Allene 7a Dimerization product



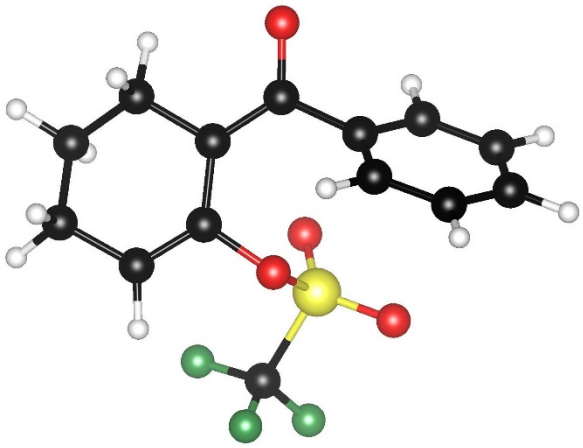
HF (M062X/6-31+G(d,p)) = -1155.2285749 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.437060 (Hartree/Particle)
Thermal correction = 0.384690 Hartrees

Coordinates from last standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.175111	2.333655	-0.529226
2	6	0	-2.785487	2.396019	0.103072
3	6	0	-2.027607	1.095858	-0.081081
4	6	0	-2.818760	-0.135363	-0.234335
5	6	0	-4.159656	-0.118503	-0.125495
6	6	0	-4.954586	1.149002	0.034875
7	6	0	-0.679498	1.025973	-0.079423
8	6	0	-2.062490	-1.402137	-0.604454
9	6	0	-0.649792	-1.361095	-0.085258
10	6	0	0.020556	-2.409029	0.430817
11	6	0	-0.630656	-3.765819	0.579832
12	6	0	-1.832020	-3.903484	-0.351998
13	6	0	-2.763628	-2.704177	-0.204156
14	1	0	-4.705596	3.272443	-0.343847
15	1	0	-2.213062	3.228856	-0.315108
16	1	0	-4.715002	-1.049176	-0.202102
17	1	0	-5.186450	1.324185	1.095541
18	1	0	0.111441	-4.544134	0.370943
19	1	0	-1.483456	-3.970720	-1.390812
20	1	0	-3.094519	-2.621806	0.839402
21	1	0	-0.940398	-3.911248	1.622686
22	1	0	-2.372161	-4.829131	-0.131876
23	1	0	-3.657871	-2.841037	-0.818598
24	1	0	-1.959769	-1.386429	-1.703532
25	1	0	-5.917845	1.040014	-0.474329
26	1	0	-4.079508	2.216542	-1.615691
27	1	0	-2.910591	2.600185	1.176017
28	8	0	0.003766	-0.170583	-0.211705
29	6	0	0.304663	2.122572	0.071041
30	6	0	1.522171	2.044529	-0.623187
31	6	0	0.090600	3.204680	0.934626
32	6	0	2.479570	3.045291	-0.488799
33	1	0	1.719358	1.188469	-1.261161
34	6	0	1.052562	4.204496	1.069019
35	1	0	-0.812725	3.254198	1.531424
36	6	0	2.246250	4.133636	0.352754
37	1	0	3.414432	2.967368	-1.036221
38	1	0	0.872133	5.031791	1.748335
39	1	0	2.995328	4.911652	0.461760
40	6	0	1.401618	-2.272383	0.972356
41	8	0	1.698559	-2.839723	2.016216
42	6	0	2.446177	-1.513521	0.212910
43	6	0	3.467277	-0.870433	0.917150
44	6	0	2.448817	-1.500008	-1.185033
45	6	0	4.472348	-0.196590	0.227493
46	1	0	3.456840	-0.895445	2.002580
47	6	0	3.473962	-0.856321	-1.874413
48	1	0	1.650246	-1.997993	-1.728540
49	6	0	4.480287	-0.195046	-1.168086
50	1	0	5.251674	0.323149	0.775930
51	1	0	3.483089	-0.861304	-2.959868
52	1	0	5.270413	0.321197	-1.705025

5a conjugate base



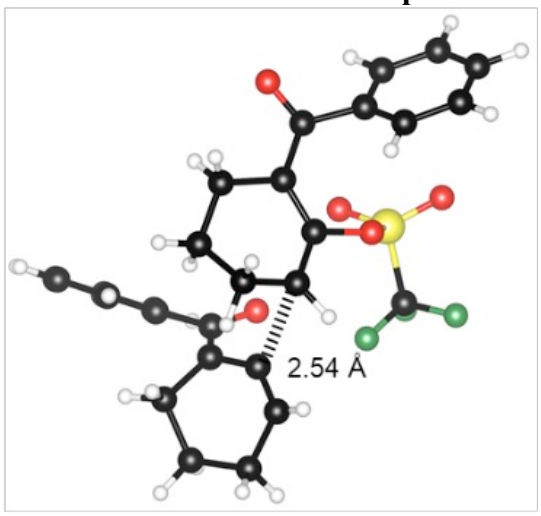
HF (M062X/6-31+G(d,p)) = -1538.9291625 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.244850 (Hartree/Particle)
Thermal correction = 0.196083 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.721131	-1.038976	-0.735731
2	6	0	3.943764	-1.407952	0.591335
3	6	0	3.308345	-0.707934	1.617336
4	6	0	2.447843	0.346513	1.315597
5	6	0	2.216265	0.721731	-0.010856
6	6	0	2.872678	0.026484	-1.031639
7	1	0	4.210122	-1.580899	-1.540357
8	1	0	4.607671	-2.235219	0.824772
9	1	0	3.481890	-0.984985	2.653409
10	1	0	1.942715	0.884661	2.113952
11	1	0	2.707070	0.327025	-2.062814
12	6	0	1.384129	1.934986	-0.358861
13	6	0	0.033744	2.051919	-0.008154
14	8	0	2.023261	2.857142	-0.960432
15	6	0	-0.828503	1.072259	0.581854
16	6	0	-2.097730	1.248253	1.008634
17	6	0	-0.635541	3.391457	-0.268084
18	6	0	-2.158426	3.297294	-0.387623
19	1	0	-2.588947	4.298491	-0.499523
20	6	0	-2.764627	2.584979	0.825942
21	1	0	-3.843685	2.446761	0.692253
22	1	0	-0.385337	4.103075	0.535471
23	1	0	-0.208836	3.813039	-1.183664
24	1	0	-2.415664	2.727307	-1.289754
25	1	0	-2.641931	3.215485	1.719716
26	8	0	-0.311164	-0.259185	0.794165
27	16	0	-0.380386	-1.333955	-0.359980
28	8	0	-0.398021	-0.751250	-1.681160
29	8	0	0.528373	-2.394573	0.006448
30	6	0	-2.078816	-2.050679	-0.100250
31	9	0	-2.340492	-2.166718	1.197418

32	9	0	-3.008517	-1.298717	-0.671789
33	9	0	-2.103076	-3.259824	-0.655005
34	1	0	-2.635257	0.416794	1.451447

Transition State of nucleophilic attack of 7a by 5a conjugate base



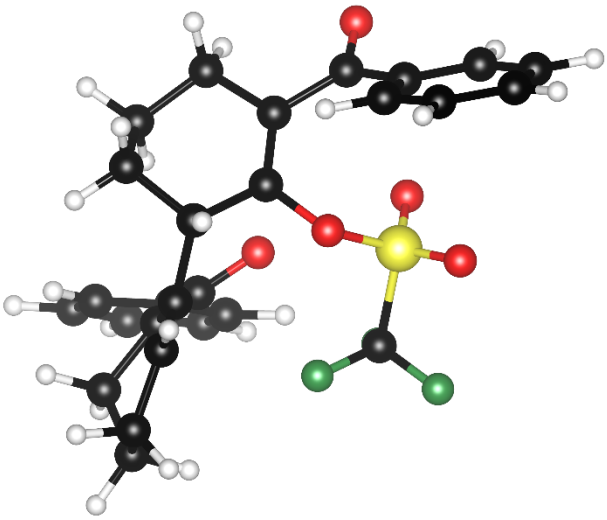
HF (M062X/6-31+G(d,p)) = -2116.44527 Hartrees
Imaginary Frequencies: 1 (-246.41 cm^{-1})
Zero-point correction = 0.459692 (Hartree/Particle)
Thermal correction = 0.394413 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.640359	-0.100417	0.803922
2	6	0	-6.219205	-0.659760	-0.335307
3	6	0	-5.534005	-1.644960	-1.047737
4	6	0	-4.279292	-2.069178	-0.618163
5	6	0	-3.680756	-1.496181	0.508373
6	6	0	-4.375335	-0.512791	1.218847
7	1	0	-6.174263	0.658621	1.368371
8	1	0	-7.201208	-0.332392	-0.664066
9	1	0	-5.980202	-2.084304	-1.935240
10	1	0	-3.746818	-2.850992	-1.152216
11	1	0	-3.921123	-0.074791	2.104054
12	6	0	-2.375523	-2.067755	1.003499
13	6	0	-1.296912	-1.268322	1.468731
14	8	0	-2.332299	-3.324905	1.069345
15	6	0	-1.096146	0.121266	1.316782
16	6	0	-0.178767	0.892440	1.989220
17	6	0	-0.248668	-2.026168	2.266547
18	6	0	0.967440	-1.191729	2.664837
19	1	0	1.527100	-1.706728	3.454068
20	6	0	0.558357	0.213615	3.117731
21	1	0	1.435663	0.795745	3.414969
22	1	0	-0.726021	-2.437322	3.168277

23	1	0	0.071042	-2.899404	1.685624
24	1	0	1.637440	-1.085372	1.804743
25	1	0	-0.089814	0.128897	4.005912
26	8	0	-1.984964	0.873761	0.472576
27	16	0	-1.998516	0.763905	-1.112534
28	8	0	-1.215541	-0.340894	-1.605845
29	8	0	-3.353072	1.000299	-1.555392
30	6	0	-1.108110	2.339191	-1.541273
31	9	0	-0.054687	2.531888	-0.773266
32	9	0	-0.733207	2.272388	-2.815505
33	9	0	-1.945356	3.364396	-1.392129
34	6	0	4.743552	-2.511395	-2.674758
35	6	0	5.210253	-3.367872	-1.675915
36	6	0	4.872417	-3.132570	-0.343155
37	6	0	4.083499	-2.033507	-0.007244
38	6	0	3.613671	-1.171288	-1.003850
39	6	0	3.938693	-1.425495	-2.340288
40	1	0	5.000377	-2.696468	-3.713277
41	1	0	5.829033	-4.220948	-1.937008
42	1	0	5.219795	-3.806358	0.433904
43	1	0	3.814011	-1.857233	1.030988
44	1	0	3.550345	-0.762123	-3.107085
45	6	0	2.699943	-0.020196	-0.685743
46	6	0	2.880790	0.706179	0.569794
47	8	0	1.801949	0.264494	-1.479880
48	6	0	2.016167	1.658912	0.976592
49	6	0	2.176620	2.839513	1.540760
50	6	0	4.195800	0.889204	1.322891
51	6	0	4.643391	2.347617	1.033643
52	1	0	5.566347	2.569502	1.581252
53	6	0	3.579638	3.426958	1.373646
54	1	0	3.608323	4.226586	0.625722
55	1	0	4.061844	0.731603	2.399783
56	1	0	4.971348	0.201881	0.974897
57	1	0	4.886700	2.400746	-0.033198
58	1	0	3.816004	3.895891	2.336570
59	1	0	1.482208	3.301802	2.236470
60	1	0	-0.274125	1.968711	1.924405

Nucleophilic attack of 7a by 5a conjugate base intermediate



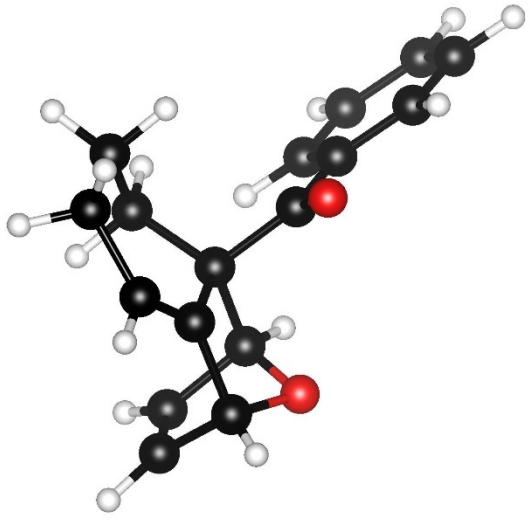
HF (M062X/6-31+G(d,p)) = -2116.542758 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.465089 (Hartree/Particle)
Thermal correction = 0.404368 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.246041	-0.916701	-0.884904
2	6	0	-6.086492	-0.451381	0.125350
3	6	0	-5.775266	0.727893	0.805672
4	6	0	-4.628044	1.440277	0.471754
5	6	0	-3.772001	0.967797	-0.528270
6	6	0	-4.086864	-0.213185	-1.205815
7	1	0	-5.489866	-1.828645	-1.420621
8	1	0	-6.983292	-1.006427	0.383384
9	1	0	-6.427101	1.088134	1.595444
10	1	0	-4.371031	2.360113	0.988126
11	1	0	-3.428593	-0.577890	-1.989128
12	6	0	-2.573871	1.795433	-0.899557
13	6	0	-1.380702	1.149949	-1.505254
14	8	0	-2.648066	3.015618	-0.815829
15	6	0	-0.870348	-0.045797	-1.157693
16	6	0	0.036628	-0.893608	-2.005414
17	6	0	-0.661758	1.988942	-2.540676
18	6	0	0.676347	1.383299	-2.947388
19	1	0	1.070642	1.908979	-3.823523
20	6	0	0.494223	-0.099189	-3.252830
21	1	0	1.422556	-0.544718	-3.622476
22	1	0	-1.307030	2.117891	-3.421973
23	1	0	-0.525746	2.985157	-2.106625
24	1	0	1.395632	1.497183	-2.129774
25	1	0	-0.259580	-0.207598	-4.044336
26	8	0	-1.376261	-0.798916	-0.083962
27	16	0	-1.532904	-0.283533	1.425486
28	8	0	-1.494510	1.152159	1.548931

29	8	0	-2.657591	-1.042471	1.932010
30	6	0	-0.045520	-1.009654	2.338297
31	9	0	0.675735	-1.793338	1.568130
32	9	0	0.683390	-0.049892	2.873611
33	9	0	-0.547193	-1.746291	3.335464
34	6	0	4.457223	2.515595	1.926993
35	6	0	5.521924	2.724339	1.048059
36	6	0	5.507966	2.110882	-0.205029
37	6	0	4.445586	1.282859	-0.566948
38	6	0	3.379222	1.052857	0.311748
39	6	0	3.391988	1.697233	1.554434
40	1	0	4.455127	2.998022	2.900629
41	1	0	6.349318	3.367736	1.332758
42	1	0	6.320776	2.283847	-0.904946
43	1	0	4.430421	0.816517	-1.549260
44	1	0	2.544873	1.547627	2.216706
45	6	0	2.181891	0.214273	-0.071278
46	6	0	2.351280	-0.953693	-0.800026
47	8	0	1.045675	0.677314	0.307938
48	6	0	1.193748	-1.655161	-1.356985
49	6	0	1.218012	-2.992775	-1.566450
50	6	0	3.639267	-1.745652	-0.865117
51	6	0	3.399744	-3.159487	-0.312446
52	1	0	4.332319	-3.736414	-0.285382
53	6	0	2.352591	-3.894312	-1.152766
54	1	0	1.963859	-4.760419	-0.600115
55	1	0	4.005642	-1.840616	-1.902786
56	1	0	4.432118	-1.261780	-0.289105
57	1	0	3.042271	-3.065786	0.720369
58	1	0	2.828355	-4.310318	-2.054107
59	1	0	0.389467	-3.465184	-2.094341
60	1	0	-0.650440	-1.679011	-2.358994

Endo adduct: Allene 7a with furan (Product 10a)



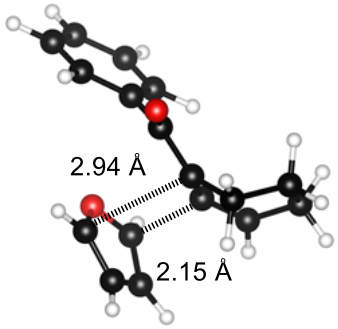
HF (M062X/6-31+G(d,p)) = -807.5321058 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.291267 (Hartree/Particle)

Thermal correction = 0.249445 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.744316	-0.016430	0.193466
2	6	0	2.064448	0.197928	-0.532158
3	6	0	2.796665	1.303582	-0.446941
4	6	0	0.788984	0.792254	1.501125
5	6	0	1.059702	2.265409	1.153428
6	1	0	0.229808	2.637257	0.540903
7	6	0	2.388021	2.477144	0.406490
8	1	0	3.196214	2.645128	1.131599
9	1	0	-0.138844	0.723484	2.073585
10	1	0	1.598710	0.389641	2.122253
11	1	0	1.057743	2.863130	2.069602
12	1	0	2.336174	3.391739	-0.195599
13	1	0	3.770123	1.351221	-0.933789
14	6	0	0.753256	-1.601546	0.204482
15	6	0	1.952361	-2.085323	1.003739
16	6	0	3.014221	-1.849695	0.228316
17	6	0	2.454955	-1.189670	-1.034908
18	8	0	1.178754	-1.832290	-1.144704
19	1	0	-0.201092	-2.091362	0.382166
20	1	0	1.922039	-2.453656	2.021067
21	1	0	4.066410	-1.962889	0.458288
22	1	0	3.026189	-1.258932	-1.958330
23	6	0	-0.437314	0.439319	-0.680974
24	6	0	-1.854107	0.137288	-0.256853
25	6	0	-2.201069	-0.508184	0.937556
26	6	0	-2.876224	0.542182	-1.126336
27	6	0	-3.538575	-0.739654	1.253264
28	1	0	-1.442369	-0.837320	1.638117
29	6	0	-4.210771	0.309362	-0.813334
30	1	0	-2.602815	1.041752	-2.049571
31	6	0	-4.545314	-0.333208	0.379574
32	1	0	-3.791233	-1.240317	2.182261
33	1	0	-4.990119	0.627570	-1.498416
34	1	0	-5.586374	-0.517341	0.626115
35	8	0	-0.250242	1.063085	-1.709028

Endo Transition State of trapping Allene 7a with furan

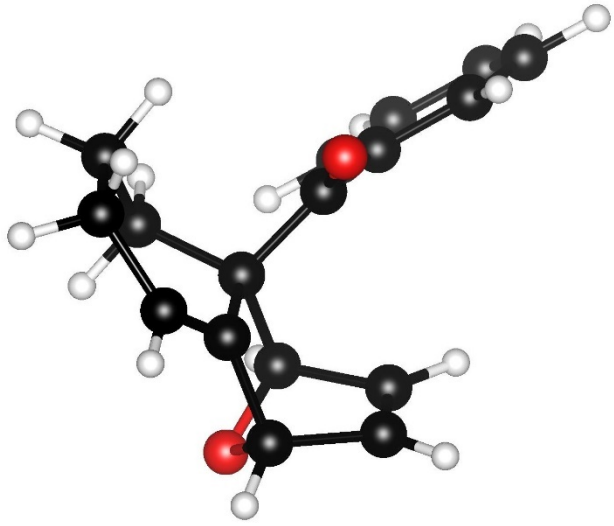


HF (M062X/6-31+G(d,p)) = -807.4666889 Hartrees
Imaginary Frequencies: 1 (-220.31 cm^{-1})
Zero-point correction = 0.285996 (Hartree/Particle)
Thermal correction = 0.241535 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.989966	-0.515253	0.535537
2	6	0	-1.254066	-0.060569	-0.721362
3	6	0	-2.239833	-0.376770	-1.552126
4	6	0	-2.278172	-1.018516	1.164126
5	6	0	-2.800859	-2.131188	0.221186
6	1	0	-2.095428	-2.966739	0.282896
7	6	0	-2.950852	-1.689098	-1.263207
8	1	0	-4.006746	-1.517553	-1.503228
9	1	0	-2.094216	-1.423717	2.161900
10	1	0	-3.009498	-0.205361	1.243877
11	1	0	-3.766021	-2.503961	0.580439
12	1	0	-2.614629	-2.490904	-1.929697
13	1	0	-2.633923	0.296161	-2.308495
14	6	0	-0.219918	2.277963	1.050942
15	6	0	-1.527127	2.644096	0.832123
16	6	0	-1.749188	2.479883	-0.548944
17	6	0	-0.568580	1.949829	-1.069992
18	8	0	0.394285	1.984629	-0.108913
19	1	0	0.397669	2.258588	1.936955
20	1	0	-2.234196	2.957563	1.585561
21	1	0	-2.663882	2.649465	-1.097685
22	1	0	-0.214520	1.860457	-2.086373
23	6	0	0.298114	-0.863824	1.120897
24	6	0	1.568583	-0.672664	0.339328
25	6	0	1.651450	-0.903164	-1.037048
26	6	0	2.715584	-0.288599	1.041313
27	6	0	2.865601	-0.737822	-1.702780
28	1	0	0.773650	-1.226245	-1.587462
29	6	0	3.922948	-0.104084	0.373654
30	1	0	2.643620	-0.131426	2.113499
31	6	0	3.999713	-0.327807	-1.002187
32	1	0	2.925877	-0.931562	-2.769366
33	1	0	4.804710	0.208857	0.924402
34	1	0	4.941813	-0.190112	-1.523956
35	8	0	0.378856	-1.311878	2.269909

Exo adduct: Allene 7a with furan



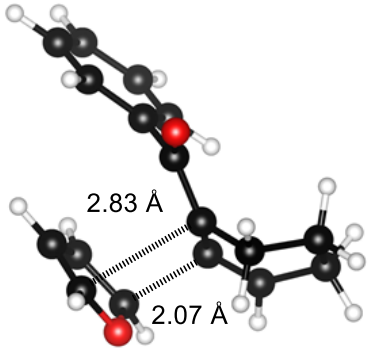
HF (M062X/6-31+G(d,p)) = -807.5325885 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.291333 (Hartree/Particle)
Thermal correction = 0.249242 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.838630	-0.052633	0.355645
2	6	0	-2.151193	0.237645	-0.358007
3	6	0	-3.079196	-0.680728	-0.603491
4	6	0	-1.121712	-1.174373	1.377187
5	6	0	-1.662688	-2.411709	0.644161
6	1	0	-0.865080	-2.819513	0.015680
7	6	0	-2.909313	-2.128357	-0.222991
8	1	0	-3.815335	-2.420872	0.322748
9	1	0	-0.224614	-1.453200	1.939279
10	1	0	-1.857612	-0.788542	2.091871
11	1	0	-1.901065	-3.185925	1.379464
12	1	0	-2.888227	-2.759091	-1.119681
13	1	0	-4.044120	-0.378048	-1.008091
14	6	0	-2.313985	1.748206	-0.269832
15	6	0	-1.166800	2.422208	-1.010687
16	6	0	-0.082443	2.228745	-0.254468
17	6	0	-0.569368	1.399950	0.932745
18	8	0	-1.896048	1.903590	1.103572
19	1	0	-3.321494	2.130580	-0.424093
20	1	0	-1.239228	2.878972	-1.989525
21	1	0	0.947432	2.488633	-0.465774
22	1	0	-0.018400	1.463249	1.869085
23	6	0	0.257465	-0.517575	-0.611457
24	8	0	-0.028861	-1.036189	-1.675606

25	6	0	1.705526	-0.358902	-0.236617
26	6	0	2.144893	-0.153283	1.076292
27	6	0	2.648922	-0.421234	-1.270533
28	6	0	3.504850	-0.015134	1.349390
29	1	0	1.441218	-0.117029	1.899825
30	6	0	4.004244	-0.268656	-0.999919
31	1	0	2.298723	-0.581772	-2.285067
32	6	0	4.434950	-0.066275	0.312864
33	1	0	3.835314	0.132928	2.372383
34	1	0	4.725735	-0.307344	-1.809823
35	1	0	5.492908	0.050395	0.526302

Exo Transition State of trapping Allene 7a with furan



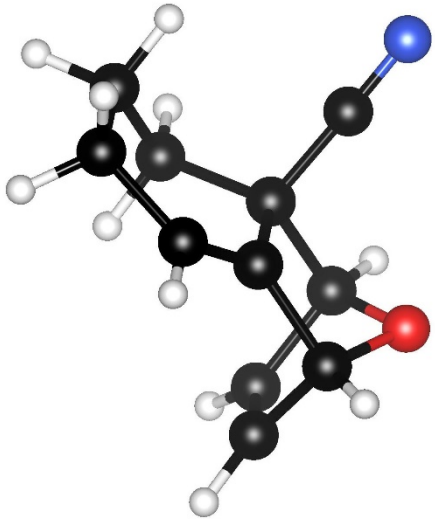
HF (M062X/6-31+G(d,p)) = -807.4635917 Hartrees
Imaginary Frequencies: 1 (-319.25 cm^{-1})
Zero-point correction = 0.286041 (Hartree/Particle)
Thermal correction = 0.241415 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.092323	-0.337278	0.548023
2	6	0	-1.306412	0.042537	-0.752843
3	6	0	-2.243679	-0.363840	-1.599571
4	6	0	-2.410997	-0.764743	1.165323
5	6	0	-2.897282	-1.956451	0.301484
6	1	0	-2.194394	-2.781217	0.462435
7	6	0	-2.985924	-1.637520	-1.217318
8	1	0	-4.030666	-1.474147	-1.507326
9	1	0	-2.279055	-1.076668	2.203834
10	1	0	-3.136761	0.055300	1.130198
11	1	0	-3.875880	-2.301411	0.652747
12	1	0	-2.640009	-2.497999	-1.801054
13	1	0	-2.600397	0.221133	-2.442780
14	6	0	-0.895237	2.044823	-1.096767
15	6	0	0.470341	2.141729	-0.814780
16	6	0	0.568258	2.329408	0.568073
17	6	0	-0.729717	2.425768	1.034294
18	8	0	-1.601763	2.427548	0.018398
19	1	0	-1.416988	2.164738	-2.035589

20	1	0	1.271498	1.970181	-1.519535
21	1	0	1.461432	2.345675	1.174898
22	1	0	-1.136553	2.593297	2.020794
23	6	0	0.158322	-0.766746	1.159913
24	8	0	0.197884	-1.175243	2.326243
25	6	0	1.444826	-0.718135	0.380996
26	6	0	1.520275	-1.042911	-0.976744
27	6	0	2.615678	-0.381728	1.070218
28	6	0	2.748730	-1.013214	-1.638063
29	1	0	0.624241	-1.329582	-1.517095
30	6	0	3.836799	-0.328415	0.405972
31	1	0	2.550084	-0.152829	2.130083
32	6	0	3.905114	-0.643255	-0.953506
33	1	0	2.800068	-1.278798	-2.689532
34	1	0	4.735973	-0.047777	0.945751
35	1	0	4.857803	-0.608504	-1.473170

Endo adduct: Allene 7d with furan (product 10d)



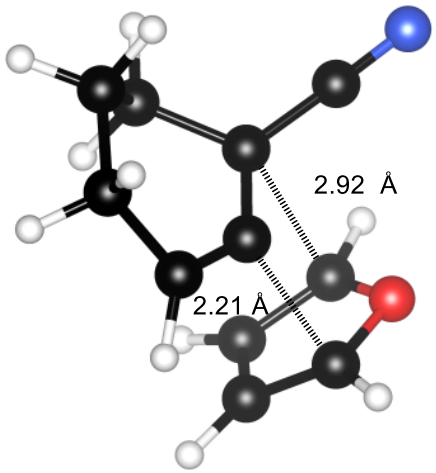
HF (M062X/6-31+G(d,p)) = -555.4920351 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.198464 (Hartree/Particle)
Thermal correction = 0.163567 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.122434	0.543609	0.311199
2	6	0	-0.051780	-0.546725	-0.745279
3	6	0	0.905111	-1.415976	-1.054729
4	6	0	1.113239	0.069920	1.379508
5	6	0	2.428059	-0.312516	0.683655
6	1	0	2.844607	0.586333	0.215062
7	6	0	2.252181	-1.415879	-0.375553
8	1	0	2.366044	-2.402543	0.093131

9	1	0	1.285944	0.847185	2.129983
10	1	0	0.670053	-0.800299	1.877263
11	1	0	3.157423	-0.639378	1.429877
12	1	0	3.054582	-1.348532	-1.118683
13	1	0	0.696183	-2.224677	-1.753464
14	6	0	0.618444	1.783889	-0.311558
15	7	0	1.020682	2.769897	-0.765506
16	6	0	-1.400994	0.789803	0.656298
17	6	0	-1.965114	-0.487714	1.250720
18	6	0	-2.080181	-1.335146	0.224665
19	6	0	-1.559891	-0.573047	-0.995827
20	8	0	-1.936802	0.771482	-0.670223
21	1	0	-1.611569	1.733655	1.156189
22	1	0	-2.138218	-0.666579	2.303752
23	1	0	-2.355350	-2.382410	0.232069
24	1	0	-1.909110	-0.865197	-1.983443

Endo Transition State of trapping Allene 7d with furan



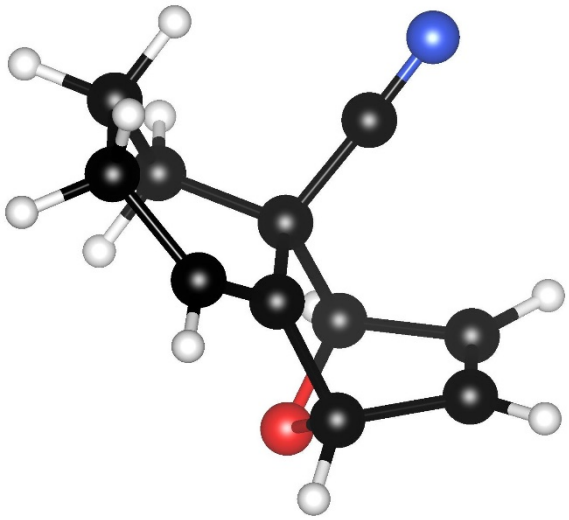
HF (M062X/6-31+G(d,p)) = -555.418494 Hartrees
Imaginary Frequencies: 1 (-169.42 cm^{-1})
Zero-point correction = 0.193221 (Hartree/Particle)
Thermal correction = 0.155483 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.539695	0.697469	0.133582
2	6	0	0.385088	-0.425921	-0.606588
3	6	0	1.188090	-1.468546	-0.757406
4	6	0	1.587837	0.479760	1.219605
5	6	0	2.867385	0.015495	0.480220
6	1	0	3.213239	0.854401	-0.132947
7	6	0	2.653311	-1.231781	-0.416619
8	1	0	2.977961	-2.136305	0.112179
9	1	0	1.784087	1.394911	1.784445
10	1	0	1.240030	-0.289834	1.917472

11	1	0	3.659881	-0.198317	1.205142
12	1	0	3.276085	-1.164027	-1.314694
13	1	0	0.841877	-2.476334	-0.969327
14	6	0	0.231129	2.007043	-0.326714
15	7	0	-0.016169	3.093479	-0.662655
16	6	0	-2.321745	0.448869	0.664644
17	6	0	-2.132070	-0.770165	1.265920
18	6	0	-1.792780	-1.666663	0.229928
19	6	0	-1.743159	-0.909500	-0.933529
20	8	0	-2.199450	0.346113	-0.673580
21	1	0	-2.603632	1.419784	1.043857
22	1	0	-2.200325	-0.974199	2.323979
23	1	0	-1.550517	-2.715999	0.313016
24	1	0	-1.706590	-1.193691	-1.974148

Exo adduct: Allene 7d with furan



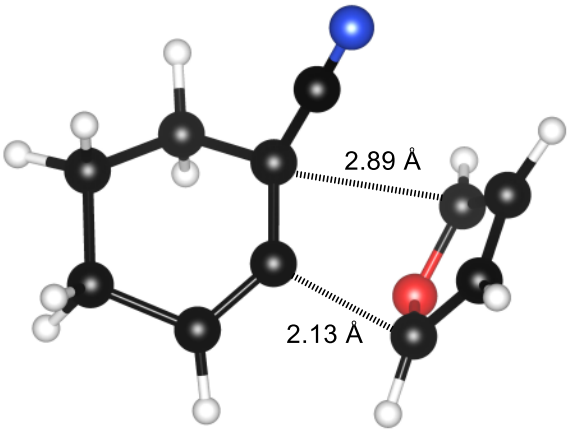
HF (M062X/6-31+G(d,p)) = -555.4903071 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.198513 (Hartree/Particle)
Thermal correction = 0.163509 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.080344	0.458595	0.366062
2	6	0	0.060630	-0.808984	-0.493622
3	6	0	1.167935	-1.435528	-0.878526
4	6	0	1.308637	0.385707	1.286924
5	6	0	2.566616	0.276320	0.413620
6	1	0	2.658542	1.198403	-0.170971
7	6	0	2.549868	-0.942589	-0.532883
8	1	0	3.067198	-1.786982	-0.060077
9	1	0	1.363644	1.270913	1.928349
10	1	0	1.188586	-0.497259	1.923993

11	1	0	3.452808	0.226597	1.052176
12	1	0	3.120344	-0.719123	-1.441439
13	1	0	1.089551	-2.405760	-1.366402
14	6	0	0.156165	1.694122	-0.431053
15	7	0	0.238730	2.683132	-1.027248
16	6	0	-1.350393	-1.358749	-0.316940
17	6	0	-2.350205	-0.366974	-0.893221
18	6	0	-2.363307	0.666332	-0.048239
19	6	0	-1.350138	0.311603	1.034257
20	8	0	-1.476820	-1.105695	1.100069
21	1	0	-1.478202	-2.415537	-0.543266
22	1	0	-2.854190	-0.472222	-1.845226
23	1	0	-2.875701	1.615019	-0.142226
24	1	0	-1.446043	0.770459	2.016995

Exo Transition State of trapping Allene 7d with furan



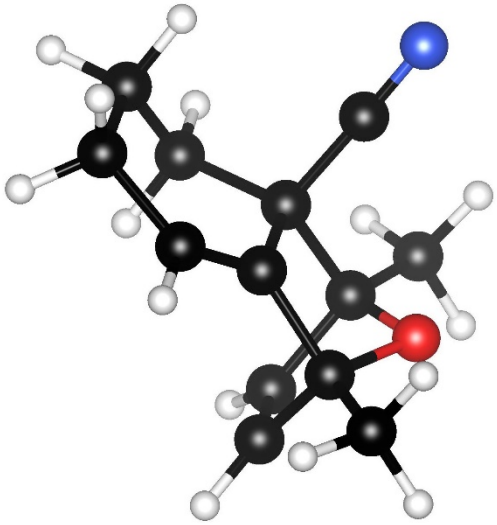
HF (M062X/6-31+G(d,p)) = -555.4154051 Hartrees
Imaginary Frequencies: 1 (-246.36 cm^{-1})
Zero-point correction = 0.193484 (Hartree/Particle)
Thermal correction = 0.155726 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.478373	0.634822	0.197273
2	6	0	0.405666	-0.543898	-0.481896
3	6	0	1.330107	-1.467011	-0.694209
4	6	0	1.636093	0.604811	1.187270
5	6	0	2.895982	0.280338	0.346034
6	1	0	3.061289	1.121995	-0.335525
7	6	0	2.774783	-1.032077	-0.466335
8	1	0	3.244554	-1.857278	0.082756
9	1	0	1.755052	1.560838	1.703879
10	1	0	1.461049	-0.174161	1.936651
11	1	0	3.775234	0.220456	0.996419
12	1	0	3.322165	-0.942123	-1.410664

13	1	0	1.120331	-2.517750	-0.873675
14	6	0	0.063914	1.874413	-0.365107
15	7	0	-0.264594	2.903157	-0.799945
16	6	0	-1.538775	-1.417382	-0.429863
17	6	0	-2.266933	-0.388187	-1.021765
18	6	0	-2.616010	0.487962	0.016885
19	6	0	-2.147157	-0.089415	1.177807
20	8	0	-1.623006	-1.300206	0.929050
21	1	0	-1.273722	-2.397567	-0.798454
22	1	0	-2.421976	-0.257463	-2.082920
23	1	0	-3.102180	1.448784	-0.062147
24	1	0	-2.201854	0.207559	2.214332

Endo adduct: Allene 7d with furan (product 11d)



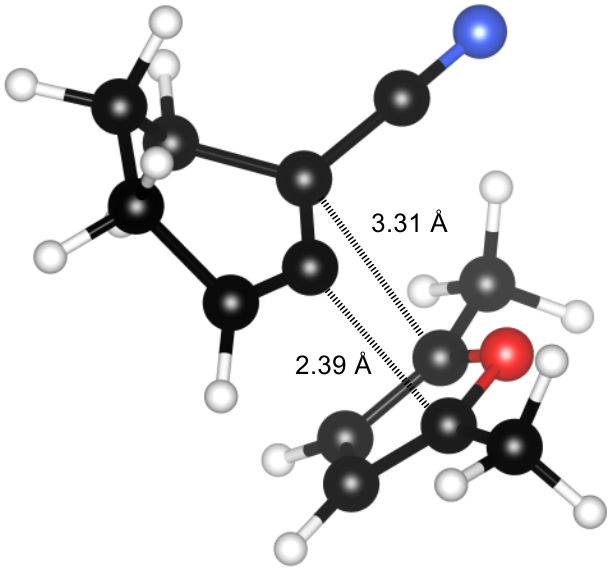
HF (M062X/6-31+G(d,p)) = -634.1012137 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.253023 (Hartree/Particle)
Thermal correction = 0.214982 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.418403	0.592198	-0.046332
2	6	0	-0.195981	-0.884169	0.267427
3	6	0	-1.163404	-1.793812	0.197707
4	6	0	-1.541297	0.738941	-1.078373
5	6	0	-2.796549	0.039542	-0.534916
6	1	0	-3.116469	0.562264	0.373539
7	6	0	-2.571399	-1.451770	-0.223425
8	1	0	-2.785681	-2.053661	-1.116886
9	1	0	-1.749698	1.793025	-1.287888
10	1	0	-1.202032	0.262096	-2.005429
11	1	0	-3.613807	0.139995	-1.254411
12	1	0	-3.288746	-1.785644	0.534652

13	1	0	-0.929984	-2.846941	0.350353
14	6	0	1.074820	1.003356	-0.402862
15	6	0	1.476607	0.195282	-1.630318
16	6	0	1.653566	-1.056277	-1.203771
17	6	0	1.328207	-1.040299	0.294957
18	8	0	1.744979	0.290369	0.646499
19	1	0	1.519339	0.587371	-2.639331
20	1	0	1.860960	-1.953532	-1.775657
21	6	0	1.397329	2.474279	-0.396894
22	1	0	0.812659	2.985485	-1.167384
23	1	0	1.167205	2.919518	0.573933
24	1	0	2.458472	2.620136	-0.611721
25	6	0	1.932069	-2.091193	1.185544
26	1	0	1.572600	-3.080781	0.890502
27	1	0	3.021219	-2.077401	1.098909
28	1	0	1.649509	-1.910956	2.225386
29	6	0	-0.786386	1.311323	1.186749
30	7	0	-1.095778	1.898811	2.135211

Endo Transition State of trapping Allene 7d with 2,5-Dimethylfuran



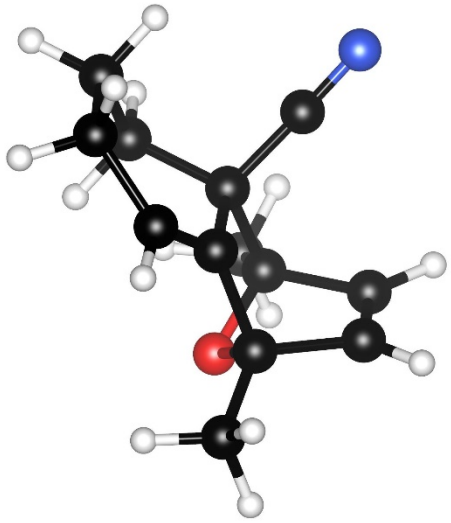
HF (M062X/6-31+G(d,p)) = -634.0288778 Hartrees
Imaginary Frequencies: 1 (-96.31 cm^{-1})
Zero-point correction = 0.248618 (Hartree/Particle)
Thermal correction = 0.207040 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863545	0.779100	-0.104968
2	6	0	0.839061	-0.552644	-0.290249
3	6	0	1.737674	-1.486556	-0.035038
4	6	0	1.932726	1.147064	0.920702

5	6	0	3.252454	0.539265	0.377966
6	1	0	3.513172	1.088345	-0.532607
7	6	0	3.174795	-0.981137	0.064060
8	1	0	3.630025	-1.557754	0.877934
9	1	0	2.031182	2.229727	1.036272
10	1	0	1.674258	0.717525	1.894105
11	1	0	4.060238	0.711643	1.096907
12	1	0	3.754737	-1.209901	-0.835650
13	1	0	1.501093	-2.506439	0.254682
14	6	0	-2.072493	0.492387	0.630898
15	6	0	-1.705128	-0.341782	1.654286
16	6	0	-1.289477	-1.558190	1.054086
17	6	0	-1.398377	-1.383342	-0.311092
18	8	0	-1.945531	-0.157676	-0.554663
19	1	0	-1.713459	-0.089497	2.704858
20	1	0	-0.921650	-2.448726	1.544238
21	6	0	-2.632664	1.867448	0.585634
22	1	0	-2.637010	2.293453	1.590090
23	1	0	-2.037346	2.507286	-0.073233
24	1	0	-3.659277	1.853860	0.206717
25	6	0	-1.329702	-2.328417	-1.460813
26	1	0	-0.661218	-3.156097	-1.214634
27	1	0	-2.319562	-2.738112	-1.685747
28	1	0	-0.948828	-1.825186	-2.351998
29	6	0	0.376618	1.733172	-1.039017
30	7	0	-0.028043	2.547582	-1.764766

Exo adduct: Allene 7d with 2,5-Dimethylfuran



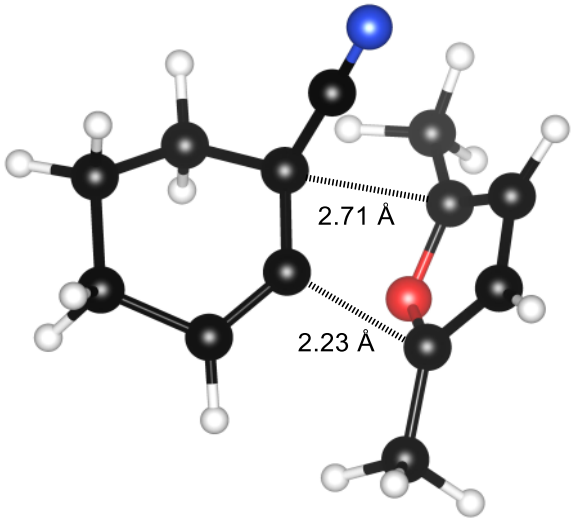
HF (M062X/6-31+G(d,p)) = -634.0999192 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.253326 (Hartree/Particle)
Thermal correction = 0.215371 Hartrees

Coordinates from last standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.418169	-0.574431	-0.044512
2	6	0	0.178000	0.894989	0.302860
3	6	0	1.150467	1.801296	0.304283
4	6	0	1.549954	-0.634885	-1.083603
5	6	0	2.804359	0.008671	-0.474720
6	1	0	3.123510	-0.602943	0.376172
7	6	0	2.584807	1.465701	-0.016204
8	1	0	2.891573	2.155956	-0.812339
9	1	0	1.758734	-1.669619	-1.374350
10	1	0	1.213276	-0.086082	-1.970144
11	1	0	3.620844	-0.023285	-1.201329
12	1	0	3.235052	1.692836	0.836248
13	1	0	0.902565	2.854356	0.429213
14	6	0	0.806128	-1.391792	1.117215
15	7	0	1.133444	-2.062063	2.002943
16	6	0	-1.330452	1.092958	0.135526
17	6	0	-2.034761	0.219486	1.169596
18	6	0	-1.880039	-1.040171	0.761320
19	6	0	-1.052405	-0.962318	-0.521327
20	8	0	-1.487176	0.287534	-1.058701
21	1	0	-2.482710	0.590534	2.083769
22	1	0	-2.164581	-1.959317	1.259572
23	6	0	-1.153839	-2.087112	-1.515418
24	1	0	-0.745150	-3.005486	-1.083123
25	1	0	-2.200573	-2.260511	-1.776276
26	1	0	-0.596108	-1.848628	-2.424499
27	6	0	-1.828650	2.498811	-0.063118
28	1	0	-2.902024	2.488250	-0.266205
29	1	0	-1.651192	3.088036	0.841039
30	1	0	-1.310351	2.972859	-0.900127

Exo adduct: Allene 7d with 2,5-Dimethylfuran



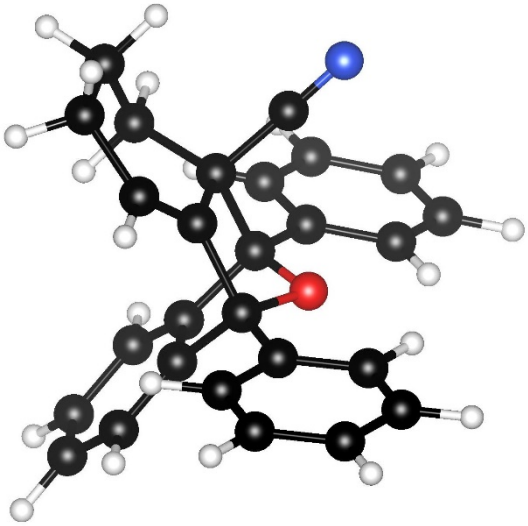
HF (M062X/6-31+G(d,p)) = -634.0238716 Hartrees
Imaginary Frequencies: 1 (-219.99 cm^{-1})
Zero-point correction = 0.248736 (Hartree/Particle)

Thermal correction = 0.207336 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.776296	-0.688298	0.131309
2	6	0	0.652614	0.633726	0.442204
3	6	0	1.497436	1.630271	0.238847
4	6	0	1.751073	-0.870963	-1.023771
5	6	0	3.081522	-0.236002	-0.543964
6	1	0	3.452941	-0.846998	0.285818
7	6	0	2.937746	1.236755	-0.085843
8	1	0	3.251385	1.911620	-0.891484
9	1	0	1.898203	-1.924460	-1.278017
10	1	0	1.370754	-0.350019	-1.909727
11	1	0	3.830638	-0.292967	-1.340900
12	1	0	3.608371	1.434823	0.756998
13	1	0	1.217695	2.674869	0.145266
14	6	0	0.653639	-1.725072	1.099010
15	7	0	0.567645	-2.598049	1.864392
16	6	0	-1.469629	1.276308	0.259228
17	6	0	-1.942173	0.430436	1.263667
18	6	0	-2.145726	-0.822017	0.672657
19	6	0	-1.818947	-0.683980	-0.665258
20	8	0	-1.557603	0.611902	-0.937038
21	1	0	-2.036002	0.698846	2.306692
22	1	0	-2.415140	-1.749303	1.157141
23	6	0	-1.854763	-1.627648	-1.812420
24	1	0	-1.938231	-2.650313	-1.441498
25	1	0	-2.710946	-1.419496	-2.462095
26	1	0	-0.942558	-1.540883	-2.408867
27	6	0	-1.426187	2.765348	0.190616
28	1	0	-2.436302	3.171083	0.083076
29	1	0	-0.990129	3.166704	1.108171
30	1	0	-0.830791	3.094443	-0.662715

Endo adduct: Allene 7d with furan (product 10d)



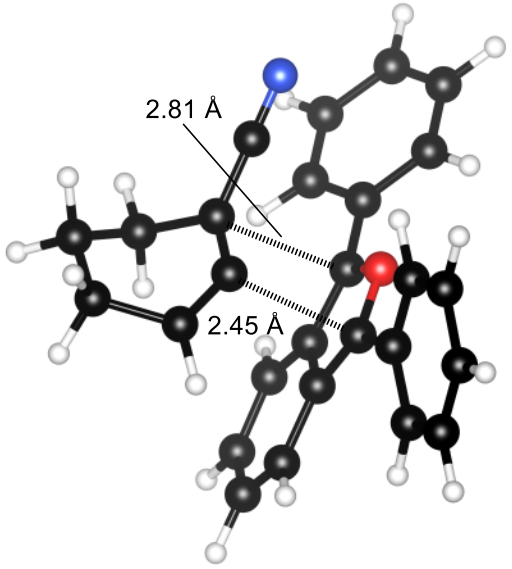
HF (M062X/6-31+G(d,p)) = -1171.047106 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.408415 (Hartree/Particle)
Thermal correction = 0.357823 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.715365	0.721605	1.117374
2	6	0	-0.803002	0.829933	0.998185
3	6	0	-1.506277	1.797889	1.575774
4	6	0	1.323683	2.117200	1.297870
5	6	0	0.659526	2.784551	2.511348
6	1	0	0.905033	2.198582	3.404090
7	6	0	-0.866596	2.905037	2.374210
8	1	0	-1.123301	3.843272	1.863949
9	1	0	2.405271	2.057524	1.450024
10	1	0	1.129529	2.686730	0.381014
11	1	0	1.091787	3.777250	2.662540
12	1	0	-1.327244	2.972580	3.365863
13	1	0	-2.579005	1.867475	1.406702
14	6	0	1.011374	-0.148158	-0.176738
15	6	0	0.574923	0.649201	-1.399622
16	6	0	-0.823548	0.609342	-1.389812
17	6	0	-1.180164	-0.163504	-0.115006
18	8	0	-0.073152	-1.082768	-0.058252
19	6	0	1.063570	-0.121666	2.277688
20	7	0	1.353831	-0.761019	3.197536
21	6	0	2.348274	-0.825566	-0.226780
22	6	0	3.512202	-0.052643	-0.300477
23	6	0	2.446380	-2.217390	-0.192457
24	6	0	4.761486	-0.667213	-0.343081
25	1	0	3.448033	1.031954	-0.323987
26	6	0	3.698566	-2.829703	-0.235019
27	1	0	1.542736	-2.814182	-0.130362
28	6	0	4.857068	-2.058362	-0.311473

29	1	0	5.658697	-0.059002	-0.399058
30	1	0	3.767187	-3.912625	-0.206481
31	1	0	5.830316	-2.537841	-0.344805
32	6	0	-2.505696	-0.857294	-0.026741
33	6	0	-3.690030	-0.126788	-0.174977
34	6	0	-2.572419	-2.230725	0.217800
35	6	0	-4.925429	-0.763382	-0.076672
36	1	0	-3.655582	0.941637	-0.367966
37	6	0	-3.810306	-2.865227	0.313315
38	1	0	-1.653188	-2.795164	0.331322
39	6	0	-4.988747	-2.134977	0.167459
40	1	0	-5.837941	-0.186945	-0.192241
41	1	0	-3.851898	-3.933164	0.503449
42	1	0	-5.951262	-2.630877	0.243792
43	6	0	1.269883	1.306113	-2.400393
44	6	0	0.526152	1.927290	-3.413047
45	1	0	1.042576	2.435756	-4.220763
46	6	0	-0.867326	1.884328	-3.405078
47	1	0	-1.421514	2.359172	-4.208580
48	6	0	-1.565155	1.225568	-2.383184
49	1	0	2.355079	1.326137	-2.422386
50	1	0	-2.649463	1.188239	-2.395651

Endo Transition State of trapping Allene 7d with DPIBF



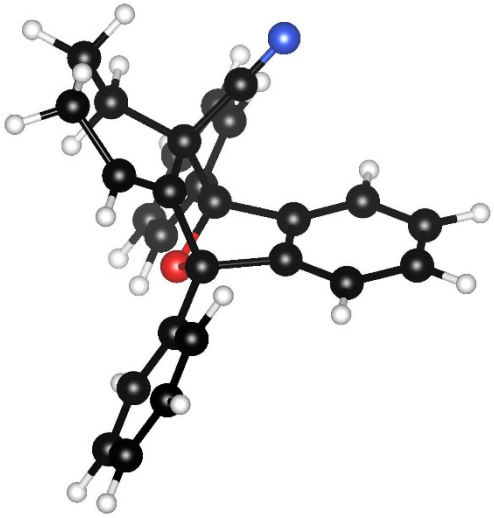
HF (M062X/6-31+G(d,p)) = -1170.957172 Hartrees
Imaginary Frequencies: 1 (-129.44 cm^{-1})
Zero-point correction = 0.403206 (Hartree/Particle)
Thermal correction = 0.349084 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.529426	0.787636	1.632337
2	6	0	-0.788663	0.836032	1.364986
3	6	0	-1.670399	1.805664	1.510404
4	6	0	1.108377	2.195458	1.700199
5	6	0	0.255880	2.934250	2.766958
6	1	0	0.484299	2.481116	3.737123
7	6	0	-1.278695	2.883604	2.518033
8	1	0	-1.620444	3.827839	2.077663
9	1	0	2.163230	2.192053	1.988141
10	1	0	1.015844	2.675119	0.718777
11	1	0	0.569928	3.981577	2.822726
12	1	0	-1.809946	2.776967	3.468911
13	1	0	-2.524037	1.960884	0.854847
14	6	0	1.050894	-0.387296	-0.871837
15	6	0	0.571871	0.759906	-1.509089
16	6	0	-0.856640	0.711427	-1.404959
17	6	0	-1.156905	-0.458050	-0.688042
18	8	0	-0.000196	-1.136997	-0.482280
19	6	0	1.174688	-0.318118	2.257176
20	7	0	1.727283	-1.211846	2.754415
21	6	0	2.380015	-0.947438	-0.666085
22	6	0	3.498562	-0.106261	-0.573005
23	6	0	2.548243	-2.331927	-0.522720
24	6	0	4.764900	-0.644907	-0.367238
25	1	0	3.370682	0.970701	-0.621218
26	6	0	3.816675	-2.863669	-0.311675
27	1	0	1.682404	-2.983886	-0.577589
28	6	0	4.929170	-2.024929	-0.239789
29	1	0	5.622843	0.015609	-0.291205
30	1	0	3.936816	-3.936928	-0.202488
31	1	0	5.917022	-2.443327	-0.075488
32	6	0	-2.397761	-1.171567	-0.383902
33	6	0	-3.566742	-0.931769	-1.116257
34	6	0	-2.419497	-2.116174	0.653599
35	6	0	-4.742768	-1.612184	-0.803255
36	1	0	-3.553257	-0.240793	-1.952416
37	6	0	-3.590856	-2.802216	0.951542
38	1	0	-1.515006	-2.295343	1.228235
39	6	0	-4.759561	-2.547704	0.229264
40	1	0	-5.642428	-1.418264	-1.378826
41	1	0	-3.596694	-3.529901	1.757065
42	1	0	-5.674714	-3.079518	0.469087
43	6	0	-1.644908	1.775531	-1.926116
44	1	0	-2.725002	1.774093	-1.827714
45	6	0	-1.005968	2.816356	-2.546625
46	1	0	-1.588546	3.636635	-2.953816
47	6	0	0.418093	2.849437	-2.678592
48	1	0	0.877813	3.685313	-3.195863
49	6	0	1.205402	1.850041	-2.171604
50	1	0	2.282778	1.882162	-2.290880

Exo adduct: Allene 7d with DPIBF (product 13d)



HF (M062X/6-31+G(d,p)) = -1171.0480176 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.407943 (Hartree/Particle)
Thermal correction = 0.356255 Hartrees

Coordinates from last standard orientation:

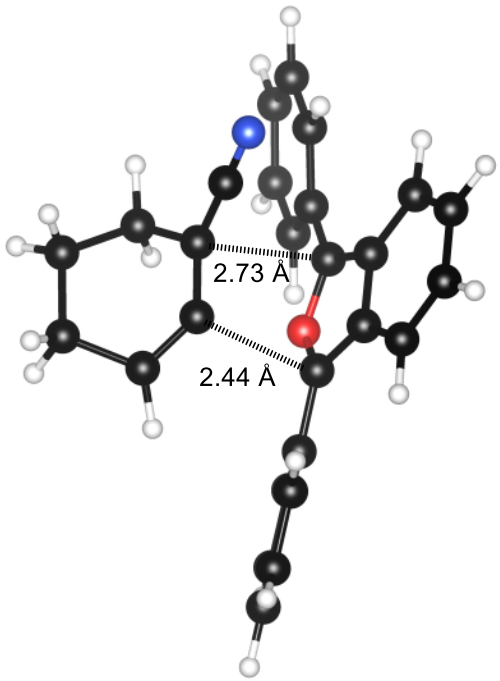
```
HF = -1171.0480176 hartrees
 Zero-point correction=                           0.407943 (Hartree/Particle)
 Thermal correction to Gibbs Free Energy=         0.356255
 Sum of electronic and zero-point Energies=          -1170.640075
 Sum of electronic and thermal Free Energies=        -1170.691762
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.753251	-0.973580	0.876964
2	6	0	0.773733	-1.050854	0.821487
3	6	0	1.445765	-2.156164	1.128279
4	6	0	-1.318091	-2.366469	0.552255
5	6	0	-0.762507	-3.370308	1.570277
6	1	0	-1.139927	-3.098760	2.562413
7	6	0	0.777566	-3.423296	1.593048
8	1	0	1.133274	-4.217978	0.924937
9	1	0	-2.411732	-2.354977	0.582692
10	1	0	-1.006363	-2.615691	-0.468461
11	1	0	-1.156855	-4.366367	1.351824
12	1	0	1.131491	-3.699198	2.592731
13	1	0	2.516588	-2.198883	0.938665
14	6	0	1.195354	0.117611	-0.074960
15	6	0	0.785093	1.433567	0.582699
16	6	0	-0.606712	1.481863	0.473674
17	6	0	-0.990761	0.174842	-0.209298
18	8	0	0.140306	-0.023835	-1.060937
19	6	0	-2.292598	0.117234	-0.948093
20	6	0	-3.492937	0.178838	-0.231065
21	6	0	-2.323608	0.008726	-2.338960

22	6	0	-4.712490	0.137363	-0.901794
23	1	0	-3.477468	0.251857	0.854455
24	6	0	-3.547246	-0.033935	-3.007867
25	1	0	-1.390951	-0.042261	-2.890765
26	6	0	-4.741883	0.031512	-2.293193
27	1	0	-5.638671	0.184490	-0.337916
28	1	0	-3.564711	-0.119236	-4.089897
29	1	0	-5.692397	-0.002284	-2.816234
30	6	0	2.562964	0.046796	-0.681355
31	6	0	3.686039	0.098619	0.151882
32	6	0	2.732361	-0.068463	-2.061398
33	6	0	4.966524	0.038119	-0.393441
34	1	0	3.558755	0.176645	1.229308
35	6	0	4.015934	-0.129766	-2.604438
36	1	0	1.859793	-0.107969	-2.704390
37	6	0	5.134006	-0.076217	-1.774002
38	1	0	5.832437	0.076693	0.259903
39	1	0	4.140596	-0.219295	-3.679145
40	1	0	6.131712	-0.125144	-2.198730
41	6	0	-1.336887	2.544303	0.975325
42	6	0	-0.628571	3.584812	1.590447
43	1	0	-1.168188	4.441670	1.981191
44	6	0	0.761357	3.538379	1.701512
45	1	0	1.286815	4.360455	2.177016
46	6	0	1.491112	2.452563	1.199324
47	1	0	-2.419252	2.581029	0.892108
48	1	0	2.573621	2.429628	1.279623
49	6	0	-1.247819	-0.556872	2.199582
50	7	0	-1.665100	-0.259870	3.237831

Exo Transition State of trapping Allene 7d with DPIBF



HF (M062X/6-31+G(d,p)) = -1170.9584057 Hartrees

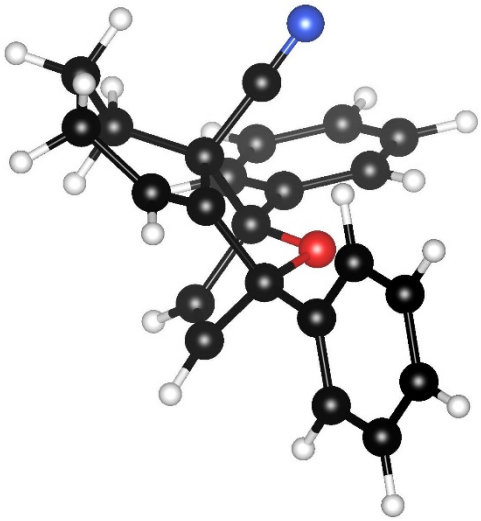
Imaginary Frequencies: 1 (-154.26 cm^{-1})
Zero-point correction = 0.403658 (Hartree/Particle)
Thermal correction = 0.350470 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.677808	0.425308	-1.691976
2	6	0	0.663041	0.509464	-1.558384
3	6	0	1.483151	1.515417	-1.804655
4	6	0	-1.306299	1.812954	-1.684961
5	6	0	-0.608563	2.575861	-2.842342
6	1	0	-0.935761	2.116371	-3.780708
7	6	0	0.943805	2.569359	-2.770472
8	1	0	1.307643	3.529122	-2.385908
9	1	0	-2.387836	1.774711	-1.842798
10	1	0	-1.117067	2.296288	-0.720026
11	1	0	-0.958298	3.613137	-2.857114
12	1	0	1.366782	2.459721	-3.773913
13	1	0	2.405320	1.708275	-1.262416
14	6	0	1.220806	-0.474071	0.606932
15	6	0	0.759275	-1.770643	0.314790
16	6	0	-0.659433	-1.738644	0.488612
17	6	0	-0.973989	-0.434420	0.889989
18	8	0	0.170217	0.250372	1.077489
19	6	0	-2.221238	0.252869	1.199228
20	6	0	-3.421043	-0.162687	0.601913
21	6	0	-2.228105	1.364740	2.054603
22	6	0	-4.607997	0.509593	0.875887
23	1	0	-3.416267	-0.983185	-0.109327
24	6	0	-3.418692	2.035155	2.319821
25	1	0	-1.299811	1.695368	2.510160
26	6	0	-4.612592	1.607690	1.737510
27	1	0	-5.529324	0.183713	0.403503
28	1	0	-3.414329	2.893503	2.984153
29	1	0	-5.539480	2.131893	1.947073
30	6	0	2.556305	0.071944	0.828891
31	6	0	3.643397	-0.389974	0.072735
32	6	0	2.762306	1.085400	1.776401
33	6	0	4.915407	0.136355	0.278928
34	1	0	3.484947	-1.130870	-0.704543
35	6	0	4.035505	1.613291	1.971439
36	1	0	1.923257	1.450686	2.359871
37	6	0	5.117188	1.138814	1.228690
38	1	0	5.748103	-0.226244	-0.315533
39	1	0	4.183483	2.394722	2.710121
40	1	0	6.108725	1.551973	1.383371
41	6	0	-1.436431	-2.909134	0.268401
42	6	0	-0.787467	-4.055197	-0.109248
43	1	0	-1.355662	-4.964323	-0.276976
44	6	0	0.630523	-4.087619	-0.276579
45	1	0	1.102542	-5.022951	-0.560217
46	6	0	1.404814	-2.974560	-0.070548
47	1	0	-2.510971	-2.904415	0.412526
48	1	0	2.482408	-3.024218	-0.179411

49	6	0	-1.369173	-0.673579	-2.276903
50	7	0	-1.978613	-1.552624	-2.733431

Endo adduct: Allene 7d with 2,5-Diphenylfuran



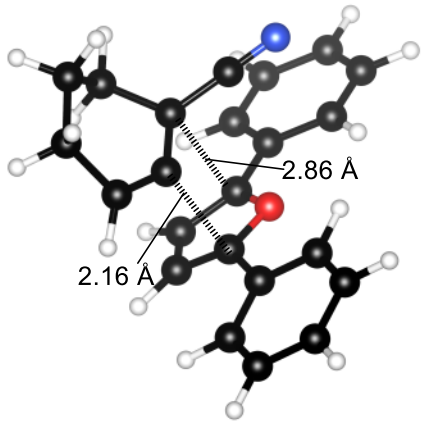
HF (M062X/6-31+G(d,p)) = -1017.4404702 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.359699 (Hartree/Particle)
Thermal correction = 0.311187 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.715747	1.149760	0.102901
2	6	0	-0.791148	1.237832	-0.095646
3	6	0	-1.454790	2.388445	-0.139020
4	6	0	1.391812	2.405716	-0.452145
5	6	0	0.752408	3.635114	0.211758
6	1	0	0.962038	3.594861	1.286681
7	6	0	-0.767101	3.724689	-0.016595
8	1	0	-0.972623	4.268483	-0.948604
9	1	0	2.470113	2.386574	-0.264990
10	1	0	1.225813	2.420519	-1.536103
11	1	0	1.229882	4.544297	-0.163626
12	1	0	-1.228934	4.319087	0.779504
13	1	0	-2.521987	2.386032	-0.358914
14	6	0	1.015372	1.011731	1.539604
15	7	0	1.264887	0.922157	2.666402
16	6	0	0.970876	-0.281081	-0.561586
17	6	0	0.561950	-0.171591	-2.025293
18	6	0	-0.770929	-0.123199	-2.030950
19	6	0	-1.200562	-0.166310	-0.560823
20	8	0	-0.145074	-0.973189	0.004455
21	1	0	1.248349	-0.069454	-2.856227
22	1	0	-1.438816	0.059746	-2.864343

23	6	0	-2.558283	-0.679712	-0.184738
24	6	0	-3.068382	-0.407559	1.088380
25	6	0	-3.297485	-1.470240	-1.066617
26	6	0	-4.306657	-0.915488	1.472262
27	1	0	-2.489750	0.204039	1.775484
28	6	0	-4.540949	-1.974242	-0.685328
29	1	0	-2.899928	-1.699425	-2.051285
30	6	0	-5.046943	-1.696461	0.583349
31	1	0	-4.695374	-0.701296	2.462872
32	1	0	-5.111216	-2.585402	-1.377733
33	1	0	-6.014729	-2.088129	0.880907
34	6	0	2.287502	-0.919747	-0.240075
35	6	0	2.380958	-1.913443	0.736041
36	6	0	3.441222	-0.487657	-0.901456
37	6	0	3.619867	-2.475401	1.041344
38	1	0	1.483119	-2.240065	1.250686
39	6	0	4.678679	-1.046590	-0.590278
40	1	0	3.374967	0.286367	-1.662615
41	6	0	4.769465	-2.043908	0.381034
42	1	0	3.687006	-3.250265	1.798602
43	1	0	5.569851	-0.706641	-1.108454
44	1	0	5.732836	-2.482879	0.620977

Endo Transition State of trapping Allene 7d with 2,5-Diphenylfuran



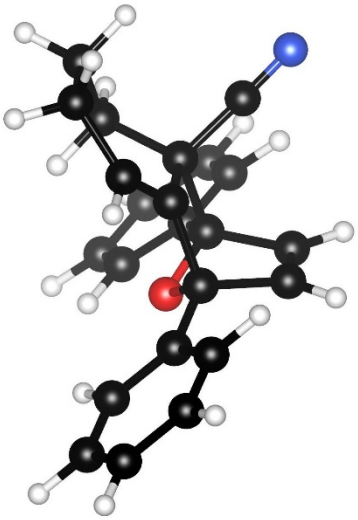
HF (M062X/6-31+G(d,p)) = -1017.3774224 Hartrees
Imaginary Frequencies: 1 (-213.61 cm^{-1})
Zero-point correction = 0.355958 (Hartree/Particle)
Thermal correction = 0.305401 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.279813	1.685929	-0.531600
2	6	0	0.960436	1.363043	-0.078191
3	6	0	1.956851	2.152042	0.297122
4	6	0	-0.656897	3.101764	-0.117906
5	6	0	0.475400	4.012998	-0.653437

6	1	0	0.431596	3.979870	-1.747247
7	6	0	1.890547	3.596408	-0.177215
8	1	0	2.189092	4.200796	0.688380
9	1	0	-1.621584	3.405179	-0.533197
10	1	0	-0.718040	3.160681	0.974868
11	1	0	0.290850	5.051321	-0.357924
12	1	0	2.628687	3.801068	-0.959855
13	1	0	2.727387	1.856692	1.005905
14	6	0	-0.879709	1.067451	-1.659828
15	7	0	-1.398355	0.566546	-2.574185
16	6	0	-1.175472	-0.574206	0.979577
17	6	0	-0.692677	-0.002251	2.147010
18	6	0	0.701597	-0.055272	2.070891
19	6	0	1.016764	-0.605861	0.818743
20	8	0	-0.144383	-1.049072	0.246552
21	1	0	-1.287753	0.422305	2.941892
22	1	0	1.409617	0.319027	2.796068
23	6	0	2.268936	-1.179495	0.303162
24	6	0	2.297460	-1.800898	-0.951051
25	6	0	3.447707	-1.078857	1.049772
26	6	0	3.491268	-2.317041	-1.446453
27	1	0	1.385246	-1.869441	-1.536063
28	6	0	4.642003	-1.587946	0.544427
29	1	0	3.435412	-0.613053	2.030991
30	6	0	4.667853	-2.209740	-0.703203
31	1	0	3.504198	-2.799424	-2.418804
32	1	0	5.551213	-1.506578	1.131728
33	1	0	5.598086	-2.609631	-1.093782
34	6	0	-2.527444	-0.846117	0.505685
35	6	0	-2.741038	-1.646584	-0.623842
36	6	0	-3.628371	-0.303137	1.185271
37	6	0	-4.038379	-1.905829	-1.058610
38	1	0	-1.892122	-2.059345	-1.158247
39	6	0	-4.920103	-0.564999	0.745436
40	1	0	-3.472011	0.331498	2.052673
41	6	0	-5.129575	-1.369434	-0.377472
42	1	0	-4.195638	-2.526014	-1.935405
43	1	0	-5.765474	-0.138230	1.275738
44	1	0	-6.139274	-1.571772	-0.720564

Exo adduct: Allene 7d with 2,5-Diphenylfuran



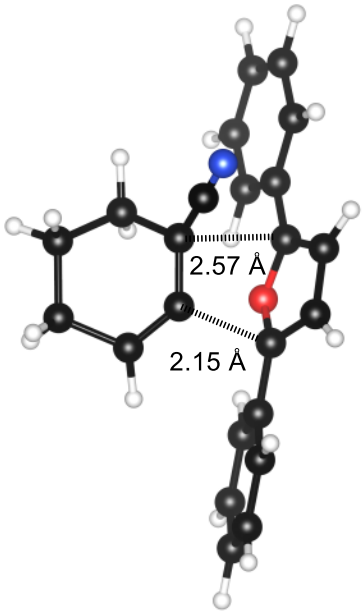
HF (M062X/6-31+G(d,p)) = -1017.4399581 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.360007 (Hartree/Particle)
Thermal correction = 0.311723 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.742474	1.164158	0.090361
2	6	0	-0.782176	1.164728	0.028591
3	6	0	-1.471486	1.973718	-0.769661
4	6	0	1.276191	1.540362	-1.300056
5	6	0	0.726778	2.924729	-1.672011
6	1	0	1.133763	3.656667	-0.965694
7	6	0	-0.814233	2.992676	-1.664119
8	1	0	-1.200257	2.805513	-2.674139
9	1	0	2.370783	1.545596	-1.304587
10	1	0	0.933131	0.771716	-2.001967
11	1	0	1.096926	3.210860	-2.660183
12	1	0	-1.145334	4.004819	-1.405718
13	1	0	-2.545659	1.828778	-0.875921
14	6	0	1.289632	2.106587	1.079533
15	7	0	1.757180	2.850529	1.833537
16	6	0	-1.194447	-0.195090	0.613715
17	6	0	-0.753634	-0.240968	2.075033
18	6	0	0.574200	-0.348853	2.058232
19	6	0	0.968623	-0.344902	0.581402
20	8	0	-0.157639	-0.982149	-0.014382
21	1	0	-1.417307	-0.132997	2.923866
22	1	0	1.268721	-0.344099	2.889119
23	6	0	-2.572550	-0.670805	0.271272
24	6	0	-2.775561	-1.609732	-0.741196
25	6	0	-3.671459	-0.135056	0.948927
26	6	0	-4.069550	-2.016172	-1.066514
27	1	0	-1.919876	-2.022029	-1.265705
28	6	0	-4.963491	-0.538915	0.618948

29	1	0	-3.519195	0.605269	1.730616
30	6	0	-5.164878	-1.482491	-0.389199
31	1	0	-4.220330	-2.752175	-1.850038
32	1	0	-5.811640	-0.117261	1.149223
33	1	0	-6.171145	-1.799769	-0.644073
34	6	0	2.274620	-0.949705	0.170103
35	6	0	2.339185	-1.854713	-0.890544
36	6	0	3.448936	-0.562037	0.823263
37	6	0	3.570605	-2.373121	-1.290688
38	1	0	1.424773	-2.150518	-1.394687
39	6	0	4.677990	-1.077568	0.417906
40	1	0	3.405912	0.146472	1.647394
41	6	0	4.740865	-1.985565	-0.639776
42	1	0	3.614578	-3.079748	-2.113648
43	1	0	5.585085	-0.772053	0.929712
44	1	0	5.698131	-2.389144	-0.954421

Exo Transition State of trapping Allene 7d with 2,5-Diphenylfuran



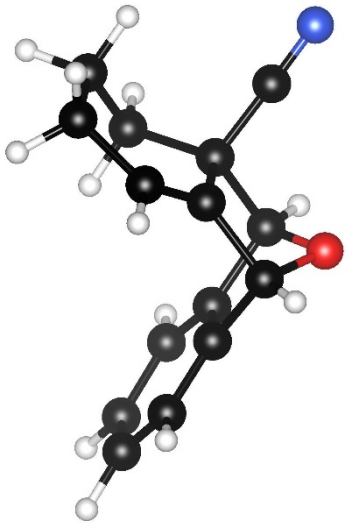
HF (M062X/6-31+G(d,p)) = -1017.3753822 Hartrees
Imaginary Frequencies: 1 (-310.39 cm^{-1})
Zero-point correction = 0.356020 (Hartree/Particle)
Thermal correction = 0.305718 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.657641	1.600001	0.216615
2	6	0	-0.695420	1.399024	0.125836
3	6	0	-1.532380	1.818678	-0.810513
4	6	0	1.258404	1.860457	-1.154596
5	6	0	0.506475	3.097376	-1.706709

6	1	0	0.775820	3.952768	-1.077878
7	6	0	-1.033099	2.928005	-1.730022
8	1	0	-1.362721	2.643405	-2.736676
9	1	0	2.334650	2.049419	-1.104323
10	1	0	1.093153	0.983890	-1.792422
11	1	0	0.857713	3.324276	-2.718781
12	1	0	-1.520528	3.883633	-1.509652
13	1	0	-2.475014	1.330610	-1.045462
14	6	0	1.285074	2.170241	1.360574
15	7	0	1.836413	2.628393	2.277592
16	6	0	-1.167147	-0.574926	0.850264
17	6	0	-0.715287	-0.417105	2.176514
18	6	0	0.659281	-0.588906	2.151732
19	6	0	0.999512	-0.877170	0.825798
20	8	0	-0.125748	-1.072602	0.107455
21	1	0	-1.331289	-0.133644	3.018036
22	1	0	1.353943	-0.451868	2.967304
23	6	0	-2.525001	-0.842619	0.355390
24	6	0	-2.733384	-1.635831	-0.777890
25	6	0	-3.622271	-0.270250	1.009687
26	6	0	-4.027425	-1.860226	-1.242798
27	1	0	-1.883678	-2.076649	-1.289134
28	6	0	-4.912886	-0.499485	0.542200
29	1	0	-3.463715	0.370364	1.872990
30	6	0	-5.120076	-1.295116	-0.585699
31	1	0	-4.181713	-2.479478	-2.120982
32	1	0	-5.757105	-0.049290	1.054673
33	1	0	-6.126678	-1.470012	-0.951838
34	6	0	2.278246	-1.159603	0.182517
35	6	0	2.324399	-1.679589	-1.117819
36	6	0	3.474506	-0.876389	0.857239
37	6	0	3.552352	-1.920109	-1.728820
38	1	0	1.399436	-1.895742	-1.642984
39	6	0	4.697169	-1.117990	0.240119
40	1	0	3.446725	-0.453686	1.857450
41	6	0	4.740722	-1.641799	-1.053454
42	1	0	3.580932	-2.325237	-2.735387
43	1	0	5.618234	-0.892614	0.767948
44	1	0	5.696517	-1.828103	-1.532656

Endo adduct: Allene 7d with Isobenzofuran



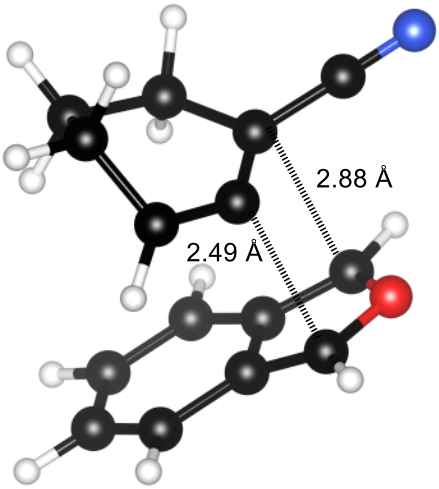
HF (M062X/6-31+G(d,p)) = -709.1003513 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.246431 (Hartree/Particle)
Thermal correction = 0.207962 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.143464	-0.457781	-0.344384
2	6	0	0.806996	0.251222	0.969315
3	6	0	1.206188	1.487608	1.248291
4	6	0	1.317803	0.578730	-1.458936
5	6	0	2.387736	1.588708	-1.018895
6	1	0	3.338431	1.057080	-0.896864
7	6	0	2.026839	2.313428	0.290071
8	1	0	1.435589	3.211834	0.067046
9	1	0	1.603087	0.098311	-2.399837
10	1	0	0.351190	1.074986	-1.603430
11	1	0	2.544158	2.326736	-1.810187
12	1	0	2.938018	2.674038	0.780249
13	1	0	0.851986	1.975975	2.155079
14	6	0	-0.044324	-1.489186	-0.376060
15	6	0	-1.351586	-0.731782	-0.466828
16	6	0	-1.538918	-0.184052	0.808653
17	6	0	-0.298424	-0.604280	1.585972
18	8	0	-0.036951	-1.894165	1.002055
19	6	0	2.382197	-1.244330	-0.197440
20	7	0	3.359539	-1.859050	-0.115752
21	6	0	-2.250026	-0.493682	-1.492509
22	6	0	-3.370599	0.298950	-1.205789
23	1	0	-4.106275	0.486412	-1.981409
24	6	0	-3.556496	0.844176	0.065246
25	1	0	-4.435878	1.449142	0.263248
26	6	0	-2.629066	0.619740	1.092662
27	1	0	-2.103224	-0.910630	-2.484508
28	1	0	-2.772187	1.057766	2.075831

29	1	0	-0.357359	-0.658599	2.670986
30	1	0	0.100600	-2.341201	-1.038603

Endo Transition State of trapping Allene 7d with Isobenzofuran



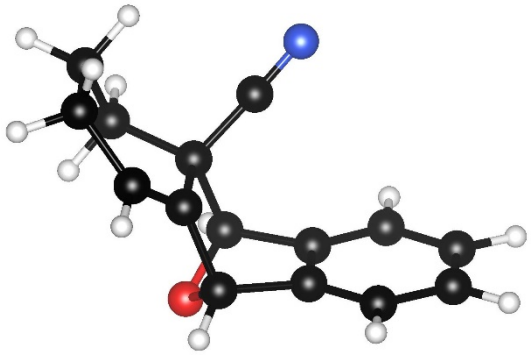
HF (M062X/6-31+G(d,p)) = -708.9967282 Hartrees
Imaginary Frequencies: 1 (-134.21 cm^{-1})
Zero-point correction = 0.240331 (Hartree/Particle)
Thermal correction = 0.198535 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.672902	-0.047281	0.212826
2	6	0	-1.167536	0.313551	-0.977104
3	6	0	-0.880766	1.508063	-1.461924
4	6	0	-1.425346	0.964531	1.339518
5	6	0	-1.172740	2.390369	0.777595
6	1	0	-1.681112	3.120877	1.415128
7	6	0	-1.624545	2.591084	-0.698480
8	1	0	-1.356959	3.592436	-1.044051
9	1	0	-2.321436	0.957880	1.969635
10	1	0	-0.582600	0.657858	1.969761
11	1	0	-0.101149	2.612747	0.825254
12	1	0	-2.708199	2.473441	-0.785192
13	1	0	-0.033255	1.735026	-2.102671
14	6	0	0.346629	-2.084050	0.462873
15	6	0	1.295887	-1.081845	0.529037
16	6	0	1.474174	-0.618715	-0.819851
17	6	0	0.580906	-1.351821	-1.592007
18	8	0	-0.012780	-2.285730	-0.817164
19	6	0	-2.629779	-1.091439	0.388866
20	7	0	-3.404586	-1.939801	0.563103
21	6	0	2.008922	-0.464747	1.601432
22	6	0	2.869312	0.553856	1.299191

23	1	0	3.426977	1.041234	2.092647
24	6	0	3.068083	0.996338	-0.053082
25	1	0	3.777355	1.797048	-0.237541
26	6	0	2.392603	0.434443	-1.101092
27	1	0	1.868840	-0.802164	2.623676
28	1	0	2.547708	0.776449	-2.119773
29	1	0	0.414338	-1.430688	-2.654861
30	1	0	-0.093584	-2.741720	1.196789

Exo adduct: Allene 7d with Isobenzofuran



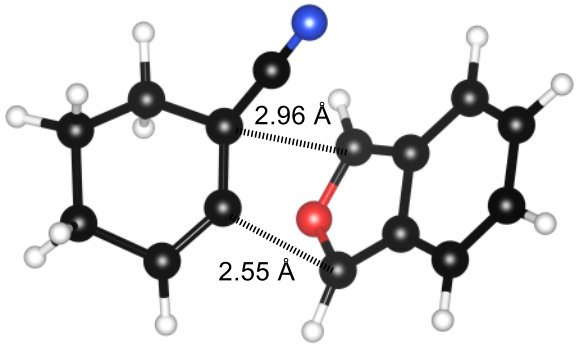
HF (M062X/6-31+G(d,p)) = -709.0983945 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.246431 (Hartree/Particle)
Thermal correction = 0.207807 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.972105	0.475035	0.403169
2	6	0	0.992564	-0.892501	-0.287044
3	6	0	2.071910	-1.373450	-0.896279
4	6	0	2.381571	0.754961	0.949932
5	6	0	3.376504	0.723632	-0.217557
6	1	0	3.134055	1.548365	-0.896604
7	6	0	3.367778	-0.610096	-0.993361
8	1	0	4.145163	-1.275922	-0.597472
9	1	0	2.412674	1.726582	1.452863
10	1	0	2.605926	-0.024153	1.686459
11	1	0	4.385426	0.917679	0.156464
12	1	0	3.635629	-0.435943	-2.041588
13	1	0	2.070788	-2.403699	-1.248164
14	6	0	-0.184369	-1.640887	0.315972
15	6	0	-1.485728	-0.947442	-0.040472
16	6	0	-1.487185	0.229607	0.717352
17	6	0	-0.167993	0.198776	1.464668
18	8	0	-0.006927	-1.205569	1.688937
19	6	0	-2.518033	1.147681	0.622162
20	6	0	-3.576887	0.848507	-0.245852
21	1	0	-4.410610	1.538319	-0.330090
22	6	0	-3.575136	-0.323175	-1.003767

23	1	0	-4.408441	-0.531375	-1.667511
24	6	0	-2.516396	-1.237741	-0.917735
25	1	0	-2.513235	2.068963	1.196724
26	1	0	-2.515752	-2.144169	-1.515444
27	6	0	0.591442	1.564975	-0.510704
28	7	0	0.326057	2.444934	-1.214434
29	1	0	-0.077107	0.764084	2.391376
30	1	0	-0.144390	-2.726011	0.239616

Exo Transition State of trapping Allene 7d with Isobenzofuran



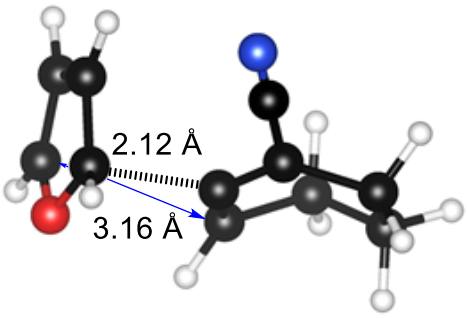
HF (M062X/6-31+G(d,p)) = -708.9950869 Hartrees
Imaginary Frequencies: 1 (-99.53 cm^{-1})
Zero-point correction = 0.240509 (Hartree/Particle)
Thermal correction = 0.198520 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.291734	0.681588	0.110565
2	6	0	1.307730	-0.461019	-0.589766
3	6	0	2.292561	-1.258827	-0.953388
4	6	0	2.568983	0.802418	0.938651
5	6	0	3.725559	0.684747	-0.091219
6	1	0	3.698624	1.583655	-0.715355
7	6	0	3.662258	-0.579042	-0.995741
8	1	0	4.371165	-1.334782	-0.638707
9	1	0	2.624574	1.756879	1.468455
10	1	0	2.613091	-0.007059	1.673222
11	1	0	4.684240	0.693085	0.437522
12	1	0	3.966426	-0.326260	-2.016010
13	1	0	2.222983	-2.338294	-1.046675
14	6	0	-0.579746	-1.923585	0.295290
15	6	0	-1.604442	-1.092813	-0.129443
16	6	0	-1.755662	-0.097515	0.897213
17	6	0	-0.826906	-0.415357	1.870333
18	8	0	-0.181750	-1.545307	1.529998
19	6	0	-2.716684	0.948100	0.747417
20	6	0	-3.482990	0.959120	-0.383076
21	1	0	-4.222876	1.740401	-0.524427
22	6	0	-3.332161	-0.038032	-1.407309

23	1	0	-3.966789	0.020585	-2.286023
24	6	0	-2.414692	-1.045323	-1.301614
25	1	0	-2.826703	1.710371	1.511804
26	1	0	-2.300510	-1.790407	-2.082296
27	6	0	0.524852	1.832508	-0.235980
28	7	0	-0.088886	2.787017	-0.485982
29	1	0	-0.577146	0.013168	2.828715
30	1	0	-0.173232	-2.849824	-0.079940

1,3 addition: Endo transition state of Allene 7d and furan



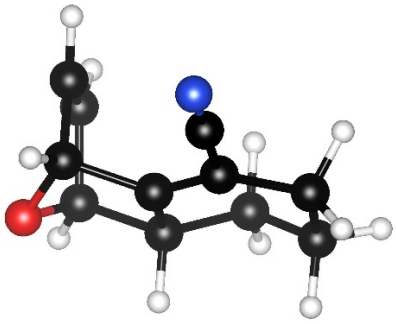
HF (M062X/6-31+G(d,p)) = -555.4133096 Hartrees
Imaginary Frequencies: 1 (-287.77 cm^{-1})
Zero-point correction = 0.193182 (Hartree/Particle)
Thermal correction = 0.155138 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.252693	-1.501688	-0.228217
2	6	0	-0.256261	-0.173743	-0.397531
3	6	0	-1.252024	0.713540	-0.228409
4	6	0	-1.397008	-1.922492	0.678749
5	6	0	-2.692139	-1.376411	0.024647
6	1	0	-2.810936	-1.875486	-0.942641
7	6	0	-2.676171	0.156083	-0.186813
8	1	0	-3.176439	0.657238	0.650195
9	1	0	-1.453370	-3.009675	0.777659
10	1	0	-1.277824	-1.497127	1.682041
11	1	0	-3.563826	-1.642480	0.632199
12	1	0	-3.235870	0.421527	-1.089792
13	6	0	2.616775	-1.084692	0.093254
14	6	0	2.515205	-0.167191	1.116572
15	6	0	1.926917	0.978321	0.557557
16	6	0	1.620222	0.646643	-0.766492
17	8	0	2.213878	-0.548085	-1.071782
18	1	0	3.031083	-2.080533	0.044325
19	1	0	2.811150	-0.328337	2.142463
20	1	0	1.662810	1.902157	1.051411
21	1	0	1.400341	1.284546	-1.611143
22	6	0	-1.028096	2.091832	0.064685
23	7	0	-0.868795	3.228213	0.251756

24	1	0	0.235057	-2.205850	-0.892760

1,3 addition: Endo adduct of Allene 7d and furan

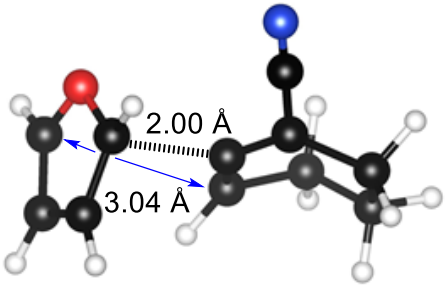


HF (M062X/6-31+G(d,p)) = -555.4996432 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.198973 (Hartree/Particle)
Thermal correction = 0.163673 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.749709	1.021418	-0.506615
2	6	0	0.101714	-0.223728	-0.433996
3	6	0	1.412129	-0.202219	-0.162566
4	6	0	-0.175717	2.104682	0.394383
5	6	0	1.282789	2.334602	-0.031677
6	1	0	1.288250	2.644839	-1.083194
7	6	0	2.161478	1.084198	0.133541
8	1	0	2.527471	1.015165	1.165929
9	1	0	-0.744923	3.035100	0.306131
10	1	0	-0.219796	1.778234	1.441749
11	1	0	1.725366	3.153707	0.542029
12	1	0	3.049181	1.158308	-0.503061
13	6	0	-2.145427	0.368308	-0.253331
14	6	0	-2.149771	-0.259237	1.133765
15	6	0	-1.378483	-1.345715	1.040100
16	6	0	-0.899929	-1.374415	-0.415729
17	8	0	-2.013438	-0.788877	-1.096709
18	1	0	-3.005974	0.966489	-0.546599
19	1	0	-2.616347	0.162948	2.014531
20	1	0	-1.040226	-2.019788	1.816852
21	1	0	-0.602363	-2.326409	-0.850758
22	6	0	2.124744	-1.442191	-0.016722
23	7	0	2.715580	-2.433104	0.103928
24	1	0	-0.765113	1.379933	-1.544354

1,3 addition: Exo transition state of Allene 7d and furan

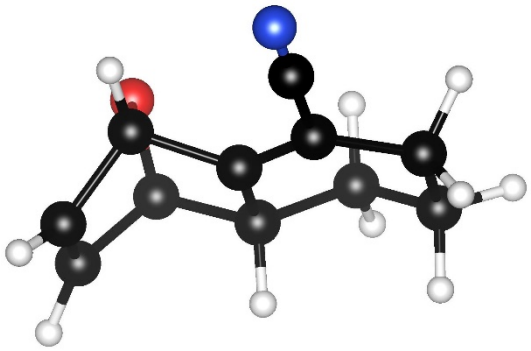


HF (M062X/6-31+G(d,p)) = -555.4138819 Hartrees
Imaginary Frequencies: 1 (-225.76 cm^{-1})
Zero-point correction = 0.193276 (Hartree/Particle)
Thermal correction = 0.155072 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.114799	-1.409351	0.149848
2	6	0	-0.253793	-0.102731	-0.089655
3	6	0	-1.376340	0.633688	-0.206526
4	6	0	-1.372410	-1.971516	0.785767
5	6	0	-2.521199	-1.647369	-0.206180
6	1	0	-2.313603	-2.180197	-1.139873
7	6	0	-2.671581	-0.135682	-0.494486
8	1	0	-3.436702	0.294987	0.161563
9	1	0	-1.296115	-3.050268	0.942628
10	1	0	-1.570943	-1.497901	1.753256
11	1	0	-3.469199	-2.035839	0.180599
12	1	0	-3.013362	0.019826	-1.523266
13	6	0	1.563178	0.969816	-0.294198
14	6	0	2.111002	0.139138	-1.266670
15	6	0	2.904249	-0.802512	-0.575347
16	6	0	2.845404	-0.449744	0.749581
17	8	0	2.122652	0.672546	0.915729
18	1	0	1.120577	1.953205	-0.370810
19	1	0	1.898541	0.183588	-2.324884
20	1	0	3.435665	-1.648533	-0.985537
21	1	0	3.292042	-0.867001	1.639461
22	6	0	-1.434266	2.014284	0.129983
23	7	0	-1.475997	3.153124	0.365114
24	1	0	0.627191	-2.052225	-0.307464

1,3 addition: Exo adduct of Allene 7d and furan

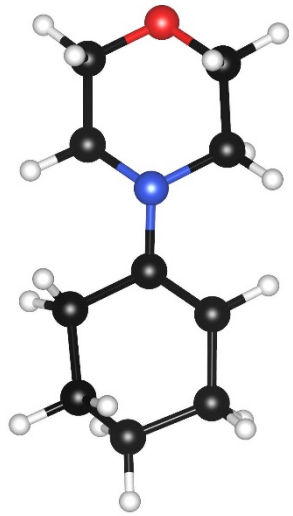


HF (M062X/6-31+G(d,p)) = -555.4969357 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.199055 (Hartree/Particle)
Thermal correction = 0.163698 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.652721	1.073635	-0.253837
2	6	0	0.075687	-0.252939	-0.188583
3	6	0	1.410535	-0.346491	-0.185837
4	6	0	0.194269	2.130471	0.447984
5	6	0	1.541094	2.195124	-0.286602
6	1	0	1.345572	2.466393	-1.330656
7	6	0	2.319545	0.867254	-0.241861
8	1	0	2.948800	0.831552	0.656042
9	1	0	-0.298636	3.107148	0.413569
10	1	0	0.335557	1.857974	1.501304
11	1	0	2.170529	2.985172	0.132285
12	1	0	3.000199	0.794965	-1.096471
13	6	0	-0.970819	-1.260292	0.278820
14	6	0	-2.055197	-1.337941	-0.788647
15	6	0	-2.713625	-0.178873	-0.711033
16	6	0	-2.009503	0.619895	0.378774
17	8	0	-1.591618	-0.425925	1.272096
18	1	0	-0.594516	-2.186554	0.709699
19	1	0	-2.174802	-2.145896	-1.498456
20	1	0	-3.502906	0.194225	-1.351494
21	1	0	-2.573489	1.384933	0.909991
22	6	0	2.031628	-1.627941	0.020130
23	7	0	2.552182	-2.651926	0.178977
24	1	0	-0.814002	1.389559	-1.291260

Enamine 15a



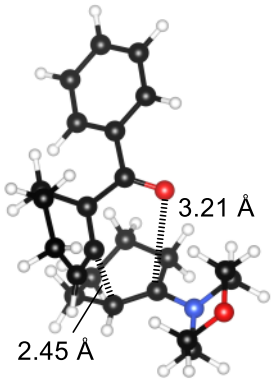
HF (M062X/6-31+G(d,p)) = -521.0482236 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.264311 (Hartree/Particle)
Thermal correction = 0.228208 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.373528	1.195389	-0.168792
2	6	0	0.703961	0.052494	0.073064
3	6	0	1.429893	-1.265284	0.261604
4	6	0	2.906014	-1.063046	0.603056
5	6	0	3.542697	-0.082104	-0.378507
6	6	0	2.878026	1.287681	-0.249811
7	1	0	0.927733	-1.832693	1.053842
8	1	0	2.995415	-0.664559	1.622361
9	1	0	3.423334	-2.027713	0.585661
10	1	0	4.620524	0.001920	-0.205241
11	1	0	3.406561	-0.461911	-1.399980
12	1	0	3.262201	1.798787	0.645591
13	1	0	3.155773	1.923590	-1.098593
14	1	0	1.355250	-1.867684	-0.654164
15	1	0	0.831684	2.127886	-0.292270
16	6	0	-1.430088	1.238341	0.122560
17	6	0	-1.357260	-1.066078	-0.549202
18	6	0	-2.887641	1.035026	0.506039
19	1	0	-1.371066	1.642594	-0.904565
20	1	0	-0.987949	1.971871	0.803256
21	6	0	-2.815244	-1.195596	-0.141806
22	1	0	-1.297567	-0.832885	-1.627729
23	1	0	-0.861475	-2.024046	-0.379713
24	1	0	-3.451001	1.957397	0.348516
25	1	0	-2.954414	0.750713	1.567428
26	1	0	-3.324189	-1.922831	-0.778359
27	1	0	-2.877957	-1.528070	0.905955
28	7	0	-0.700549	-0.016775	0.237259

29	8	0	-3.501541	0.035514	-0.290253

Transition state of trapping Allene 7a with Enamine 15a



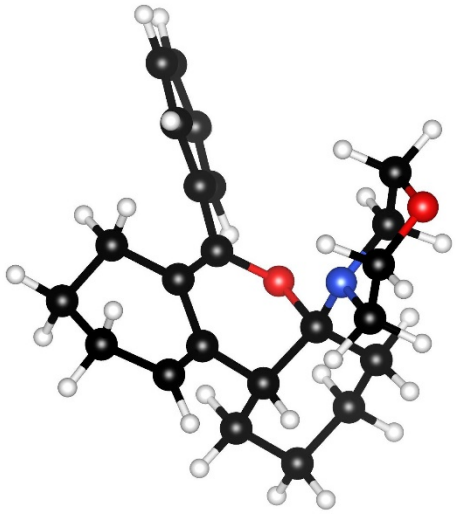
HF (M062X/6-31+G(d,p)) = -1098.5687231 Hartrees
Imaginary Frequencies: 1 (-164.98 cm^{-1})
Zero-point correction = 0.479750 (Hartree/Particle)
Thermal correction = 0.427048 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.897851	-0.652235	0.327124
2	6	0	-5.462079	-0.769448	-0.943559
3	6	0	-4.679306	-0.549080	-2.078020
4	6	0	-3.334431	-0.215679	-1.940785
5	6	0	-2.768345	-0.074846	-0.669826
6	6	0	-3.557252	-0.297220	0.464197
7	1	0	-5.500715	-0.839497	1.210226
8	1	0	-6.508726	-1.037829	-1.049487
9	1	0	-5.116620	-0.644120	-3.067013
10	1	0	-2.707247	-0.058358	-2.813147
11	1	0	-3.115226	-0.211828	1.454054
12	6	0	-1.303797	0.237227	-0.559508
13	6	0	-0.829323	1.054236	0.550856
14	8	0	-0.527853	-0.240429	-1.393858
15	6	0	0.488582	1.273245	0.745730
16	6	0	1.193787	2.333905	1.086441
17	6	0	-1.615120	2.159332	1.255181
18	6	0	-1.063105	3.493345	0.686618
19	1	0	-1.329633	3.524984	-0.375545
20	6	0	0.470953	3.660793	0.839224
21	1	0	0.695861	4.276855	1.718059
22	1	0	-2.686688	2.095648	1.049153
23	1	0	-1.474687	2.116268	2.341265
24	1	0	-1.564399	4.341440	1.165986
25	1	0	0.878607	4.194116	-0.026104
26	1	0	2.112204	2.326677	1.664007
27	6	0	-0.252485	-2.524496	1.356713
28	6	0	0.826404	-2.463421	0.274493

29	6	0	1.830424	-1.346548	0.490428
30	6	0	1.808029	-0.595127	1.636011
31	6	0	0.959808	-0.937574	2.839843
32	6	0	0.358215	-2.339045	2.742053
33	1	0	-0.992783	-1.732590	1.186176
34	1	0	1.399282	-3.401902	0.264708
35	1	0	1.567570	-0.844194	3.747612
36	1	0	-0.394882	-2.482251	3.523840
37	1	0	2.584935	0.147027	1.788183
38	1	0	0.139804	-0.209962	2.937850
39	1	0	1.140687	-3.093445	2.899523
40	1	0	-0.781991	-3.479579	1.279157
41	1	0	0.348989	-2.370032	-0.701221
42	6	0	4.083185	-0.556540	-0.202480
43	6	0	2.537684	-1.280925	-1.892454
44	6	0	4.084033	0.843166	-0.805402
45	1	0	4.881598	-1.135080	-0.687232
46	1	0	4.287115	-0.532603	0.869408
47	6	0	2.557880	0.143127	-2.443158
48	1	0	3.303899	-1.882819	-2.398476
49	1	0	1.560430	-1.723153	-2.077429
50	1	0	5.066451	1.310600	-0.699149
51	1	0	3.326055	1.470876	-0.315119
52	1	0	2.417886	0.138298	-3.527436
53	1	0	1.748739	0.717294	-1.970769
54	8	0	3.812946	0.769878	-2.198722
55	7	0	2.831057	-1.256225	-0.458394

Product 16a

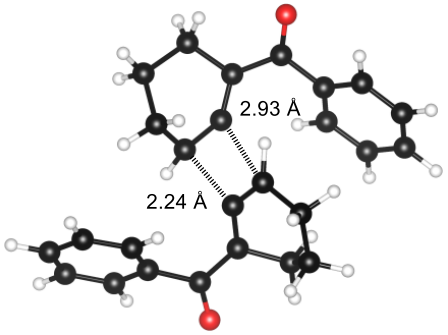


HF (M062X/6-31+G(d,p)) = -1098.689286 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.485730 (Hartree/Particle)
Thermal correction = 0.435890 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.469847	-0.388207	3.459037
2	6	0	1.729244	-1.147253	2.156119
3	6	0	1.167251	-0.429996	0.925926
4	6	0	1.631782	1.032852	0.847076
5	6	0	1.323576	1.760478	2.169319
6	6	0	1.964921	1.053959	3.362469
7	6	0	0.929355	1.704347	-0.306577
8	6	0	-0.479757	1.332235	-0.508605
9	6	0	-0.997477	0.310868	0.209995
10	6	0	-1.256689	2.108557	-1.551514
11	1	0	-2.319332	2.142540	-1.293536
12	6	0	-0.703970	3.524944	-1.723915
13	6	0	0.786460	3.483127	-2.062740
14	6	0	1.526608	2.655079	-1.046456
15	1	0	0.392599	-0.388347	3.665547
16	1	0	2.810657	-1.265824	2.003463
17	1	0	1.686338	2.790207	2.082594
18	1	0	1.742150	1.597358	4.286878
19	1	0	-1.262519	4.047857	-2.506385
20	1	0	0.928821	3.070045	-3.072241
21	1	0	2.580290	2.871224	-0.870611
22	6	0	-2.397597	-0.176191	0.188518
23	6	0	-3.106221	-0.359670	-1.004920
24	6	0	-3.020526	-0.505554	1.401639
25	6	0	-4.416362	-0.836884	-0.984193
26	1	0	-2.624434	-0.153002	-1.955081
27	6	0	-4.330098	-0.975605	1.421532
28	1	0	-2.468339	-0.386404	2.329079
29	6	0	-5.034651	-1.140325	0.227604
30	1	0	-4.949654	-0.979500	-1.919051
31	1	0	-4.802165	-1.214976	2.369582
32	1	0	-6.055462	-1.509214	0.242602
33	8	0	-0.254744	-0.417362	1.113164
34	1	0	-1.181113	1.594010	-2.521084
35	1	0	-0.841174	4.084165	-0.789879
36	1	0	1.203079	4.495939	-2.086138
37	1	0	2.717782	1.072357	0.705085
38	1	0	0.235736	1.810647	2.308752
39	1	0	3.057702	1.059084	3.242709
40	1	0	1.957632	-0.910115	4.289064
41	1	0	1.294744	-2.150448	2.210029
42	6	0	2.770836	-1.063568	-0.878127
43	6	0	0.927398	-2.501301	-0.387981
44	6	0	2.759807	-1.593755	-2.305929
45	1	0	3.485934	-1.656084	-0.277604
46	1	0	3.120910	-0.029963	-0.914636
47	6	0	0.941686	-2.979198	-1.830804
48	1	0	1.554506	-3.185760	0.211238
49	1	0	-0.094174	-2.533865	0.001374
50	1	0	3.773540	-1.624915	-2.712021
51	1	0	2.139500	-0.930930	-2.929342
52	1	0	0.624469	-4.022518	-1.896902
53	1	0	0.263671	-2.355045	-2.433255
54	8	0	2.253589	-2.916691	-2.370680
55	7	0	1.417858	-1.125674	-0.339277

Transition state of Allene 7a [2+2] dimerization



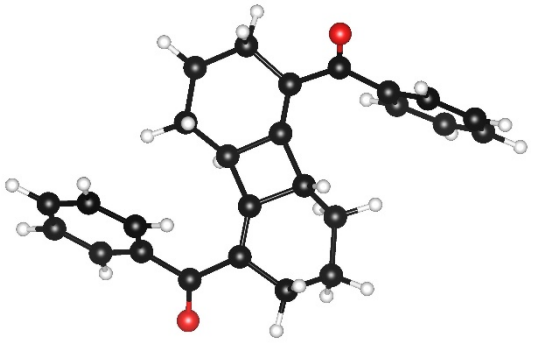
HF (M062X/6-31+G(d,p)) = -1155.0522239 Hartrees
Imaginary Frequencies: 1 (-171.76 cm^{-1})
Zero-point correction = 0.429073 (Hartree/Particle)
Thermal correction = 0.373502 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.395960	-1.660030	-1.571462
2	6	0	4.296028	-2.185334	-0.645148
3	6	0	4.794946	-1.378091	0.379390
4	6	0	4.390702	-0.050691	0.476337
5	6	0	3.463642	0.473396	-0.433949
6	6	0	2.970267	-0.336782	-1.462750
7	1	0	3.021904	-2.281007	-2.379388
8	1	0	4.615391	-3.219846	-0.725530
9	1	0	5.498426	-1.783981	1.099329
10	1	0	4.773062	0.591577	1.263759
11	1	0	2.274086	0.065955	-2.190778
12	6	0	3.034760	1.893473	-0.233514
13	6	0	1.630403	2.263509	-0.533379
14	8	0	3.807596	2.719836	0.233256
15	6	0	0.630537	1.414817	-0.700599
16	6	0	-0.658648	1.345044	-0.369832
17	6	0	1.135684	3.692335	-0.271210
18	6	0	-0.348177	3.721193	0.179462
19	1	0	-0.471550	4.502029	0.936899
20	6	0	-0.880173	2.378069	0.746189
21	1	0	-1.940281	2.456604	1.000168
22	1	0	1.793281	4.066475	0.521822
23	1	0	1.284396	4.342238	-1.138379
24	1	0	-0.983191	3.998918	-0.668128
25	1	0	-0.327579	2.088470	1.645453
26	1	0	-1.461042	1.098888	-1.058658
27	6	0	-4.410695	0.992655	1.149636
28	6	0	-5.361700	1.253238	0.163357
29	6	0	-5.364146	0.506517	-1.016192
30	6	0	-4.419864	-0.499030	-1.203016

31	6	0	-3.449399	-0.749854	-0.226464
32	6	0	-3.449152	0.001471	0.953089
33	1	0	-4.415964	1.562091	2.074184
34	1	0	-6.103258	2.031277	0.315773
35	1	0	-6.105360	0.703196	-1.784415
36	1	0	-4.420798	-1.100695	-2.106659
37	1	0	-2.711122	-0.196637	1.725050
38	6	0	-2.478130	-1.868627	-0.477475
39	6	0	-1.081608	-1.729342	-0.082695
40	8	0	-2.874857	-2.876761	-1.066503
41	6	0	-0.494018	-0.692371	0.554867
42	6	0	0.553183	-0.663300	1.374233
43	6	0	-0.124099	-2.908765	-0.151105
44	6	0	0.293975	-3.203693	1.309478
45	1	0	-0.597494	-3.548683	1.844197
46	6	0	0.898511	-1.979961	2.046586
47	1	0	1.995645	-2.023292	2.014750
48	1	0	-0.619721	-3.776735	-0.592101
49	1	0	0.755327	-2.662889	-0.756557
50	1	0	1.018911	-4.024547	1.332480
51	1	0	0.622211	-1.994596	3.106353
52	1	0	1.230088	0.181535	1.463351

Transition state of Allene 7a [2+2] cycloadduct



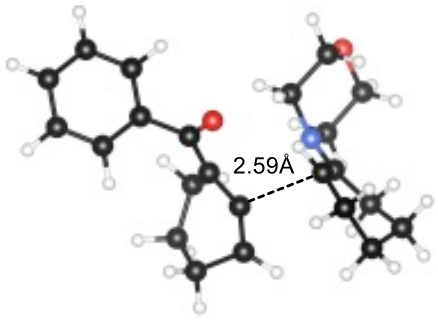
HF (M062X/6-31+G(d,p)) = -1155.1972599 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.435416 (Hartree/Particle)
Thermal correction = 0.380774 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.793701	-0.978148	1.316908
2	6	0	-5.639195	-1.370019	0.280524
3	6	0	-5.552292	-0.748819	-0.968292
4	6	0	-4.630983	0.273084	-1.172251
5	6	0	-3.763067	0.652616	-0.141620
6	6	0	-3.843417	0.020032	1.102665
7	1	0	-4.866812	-1.454387	2.289612

8	1	0	-6.369518	-2.156395	0.444138
9	1	0	-6.209874	-1.055502	-1.775455
10	1	0	-4.568010	0.783907	-2.128384
11	1	0	-3.174521	0.317592	1.904942
12	6	0	-2.831228	1.800656	-0.373856
13	6	0	-1.481710	1.795772	0.249547
14	8	0	-3.187283	2.743638	-1.070334
15	6	0	-0.762071	0.671563	0.368608
16	6	0	0.735409	0.622845	0.634563
17	6	0	-0.835499	3.142959	0.495670
18	6	0	0.615963	3.046650	0.986026
19	1	0	1.103764	4.015901	0.846123
20	6	0	1.407205	1.943642	0.269510
21	1	0	2.458334	1.955232	0.571705
22	1	0	-0.876973	3.691271	-0.453660
23	1	0	-1.437285	3.726137	1.202558
24	1	0	0.628933	2.838974	2.063615
25	1	0	1.369809	2.093507	-0.817300
26	1	0	0.965975	0.378513	1.682472
27	6	0	4.567847	1.289143	-1.337119
28	6	0	5.529628	1.505256	-0.350979
29	6	0	5.623954	0.636469	0.739193
30	6	0	4.764841	-0.453649	0.834346
31	6	0	3.781328	-0.658431	-0.140128
32	6	0	3.682412	0.218438	-1.224555
33	1	0	4.499558	1.959754	-2.187884
34	1	0	6.208683	2.348484	-0.431435
35	1	0	6.372529	0.805741	1.506554
36	1	0	4.840320	-1.150932	1.663272
37	1	0	2.921566	0.056828	-1.982663
38	6	0	2.903522	-1.864968	-0.035164
39	6	0	1.476781	-1.755834	-0.419404
40	8	0	3.356881	-2.924072	0.381166
41	6	0	0.726236	-0.672751	-0.175405
42	6	0	-0.789636	-0.727839	-0.241149
43	6	0	0.703859	-2.973951	-0.867190
44	6	0	-0.533143	-3.239992	0.035666
45	1	0	-1.248179	-3.837129	-0.538016
46	6	0	-1.226738	-1.962863	0.571933
47	1	0	-0.947219	-1.790666	1.618151
48	1	0	0.362739	-2.810606	-1.896536
49	1	0	1.354277	-3.851149	-0.876648
50	1	0	-0.219183	-3.854169	0.884526
51	1	0	-2.312985	-2.073690	0.541844
52	1	0	-1.230535	-0.764922	-1.246476

Transition state: Nucleophilic attack of Enamine 15a on Allene 7a



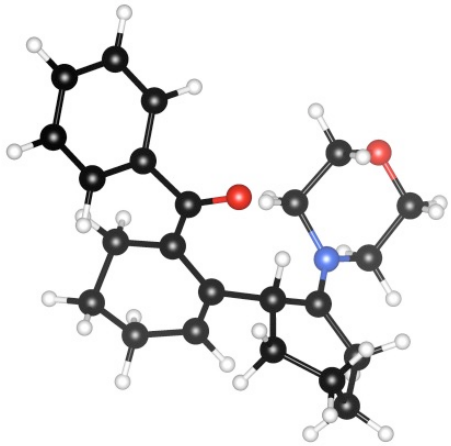
HF (M062X/6-31+G(d,p)) = -1098.5691451 Hartrees
Imaginary Frequencies: 1 (-125.20 cm^{-1})
Zero-point correction = 0.479276 (Hartree/Particle)
Thermal correction = 0.425119 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.358757	0.412520	-0.420967
2	6	0	5.918507	-0.744193	0.122561
3	6	0	5.134417	-1.605488	0.891853
4	6	0	3.793732	-1.306953	1.120827
5	6	0	3.222445	-0.160474	0.560480
6	6	0	4.011434	0.699050	-0.210636
7	1	0	5.971200	1.090243	-1.007189
8	1	0	6.966034	-0.971322	-0.049626
9	1	0	5.569971	-2.504016	1.317391
10	1	0	3.175673	-1.955700	1.734246
11	1	0	3.577910	1.606380	-0.624385
12	6	0	1.791735	0.163619	0.876867
13	6	0	0.945058	0.775928	-0.144432
14	8	0	1.352004	-0.097564	1.998585
15	6	0	-0.064934	1.610395	0.148073
16	6	0	-0.490076	2.716387	-0.426826
17	6	0	1.173862	0.781516	-1.657176
18	6	0	1.244381	2.246437	-2.200290
19	1	0	2.287583	2.513188	-2.400705
20	6	0	0.635320	3.334294	-1.256497
21	1	0	0.260775	4.176845	-1.844052
22	1	0	2.078410	0.227521	-1.922194
23	1	0	0.332316	0.263080	-2.126865
24	1	0	0.723374	2.284547	-3.161308
25	1	0	1.415948	3.720117	-0.594553
26	1	0	-1.516332	3.058328	-0.489891
27	6	0	-4.608994	1.249075	0.517696
28	6	0	-3.705385	0.495497	-0.459674
29	6	0	-2.444753	-0.034766	0.199749
30	6	0	-2.031868	0.467708	1.396086
31	6	0	-2.754856	1.549868	2.159034
32	6	0	-3.813942	2.267444	1.324695
33	1	0	-5.420142	1.730527	-0.037928
34	1	0	-4.275789	-0.335074	-0.887138
35	1	0	-3.230740	1.115764	3.051192

36	1	0	-3.336617	2.975645	0.636138
37	1	0	-1.170661	0.044317	1.901395
38	1	0	-2.018147	2.271676	2.533982
39	1	0	-4.474361	2.853342	1.972282
40	1	0	-5.071498	0.528477	1.205083
41	1	0	-3.432060	1.148445	-1.301561
42	6	0	-2.218956	-1.605534	-1.730014
43	6	0	-0.827186	-1.917847	0.180016
44	6	0	-2.943505	-2.910577	-1.408972
45	1	0	-1.354717	-1.834824	-2.367826
46	1	0	-2.860789	-0.924155	-2.288159
47	6	0	-1.580953	-3.208194	0.485895
48	1	0	0.020336	-2.141255	-0.482782
49	1	0	-0.421014	-1.479112	1.089559
50	1	0	-3.250791	-3.428246	-2.321261
51	1	0	-3.836104	-2.702496	-0.796423
52	1	0	-0.923636	-3.950590	0.945114
53	1	0	-2.415970	-2.993999	1.171861
54	8	0	-2.083997	-3.797261	-0.708092
55	7	0	-1.711381	-0.983331	-0.512632

Intermediate: Nucleophilic attack of Enamine 15a on Allene 7a



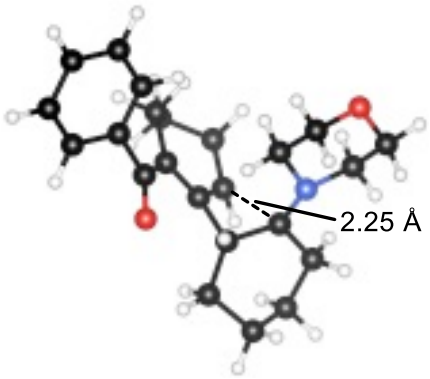
HF (M062X/6-31+G(d,p)) = -1098.630231 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.483149 (Hartree/Particle)
Thermal correction = 0.428032 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.517758	0.294225	0.605198
2	6	0	5.905596	-1.043915	0.533057
3	6	0	4.931264	-2.040201	0.451926
4	6	0	3.580373	-1.696682	0.445834
5	6	0	3.180328	-0.357322	0.495337
6	6	0	4.164506	0.633053	0.581820
7	1	0	6.269255	1.074763	0.682430

8	1	0	6.958565	-1.308982	0.546414
9	1	0	5.225341	-3.084665	0.399878
10	1	0	2.817469	-2.469992	0.405777
11	1	0	3.862382	1.676782	0.633489
12	6	0	1.702594	-0.033677	0.562210
13	6	0	1.135321	0.777140	-0.423636
14	8	0	1.098496	-0.593290	1.549995
15	6	0	-0.256469	1.207600	-0.423369
16	6	0	-0.793160	1.972115	-1.409584
17	6	0	1.874510	1.123094	-1.704952
18	6	0	1.498996	2.512744	-2.226450
19	1	0	1.729574	3.257759	-1.453591
20	6	0	0.004515	2.559904	-2.544869
21	1	0	-0.189636	2.018588	-3.482996
22	1	0	2.955250	1.048027	-1.575908
23	1	0	1.607995	0.393686	-2.490837
24	1	0	2.086889	2.766569	-3.115334
25	1	0	-0.316459	3.594112	-2.723413
26	1	0	-1.843958	2.260570	-1.339932
27	6	0	-3.742172	2.198269	1.409674
28	6	0	-3.814209	0.922853	0.566985
29	6	0	-2.479174	0.282749	0.266401
30	6	0	-1.179490	0.857749	0.757162
31	6	0	-1.305983	2.050395	1.728888
32	6	0	-2.642401	2.088630	2.459933
33	1	0	-3.532559	3.061184	0.766758
34	1	0	-4.411305	0.174971	1.104417
35	1	0	-0.463738	1.990878	2.425471
36	1	0	-2.673576	2.944614	3.140127
37	1	0	-0.687481	0.051377	1.318394
38	1	0	-1.195132	2.985447	1.168687
39	1	0	-2.785664	1.184431	3.067830
40	1	0	-4.724549	2.363766	1.859718
41	1	0	-4.332919	1.113846	-0.379851
42	6	0	-3.660005	-1.503456	-0.953201
43	6	0	-1.247712	-1.631120	-0.677214
44	6	0	-3.754747	-2.926640	-0.410500
45	1	0	-3.527493	-1.525947	-2.039663
46	1	0	-4.563307	-0.948071	-0.719685
47	6	0	-1.445791	-3.051428	-0.160599
48	1	0	-1.107391	-1.623636	-1.763488
49	1	0	-0.375089	-1.192892	-0.198737
50	1	0	-4.599901	-3.436358	-0.875656
51	1	0	-3.906911	-2.898871	0.679041
52	1	0	-0.582820	-3.657416	-0.440475
53	1	0	-1.527468	-3.033932	0.936282
54	8	0	-2.591868	-3.663407	-0.722488
55	7	0	-2.466441	-0.843356	-0.390788

Transition state: Formation of [2+2] adduct with Enamine 15a and Allene 7a



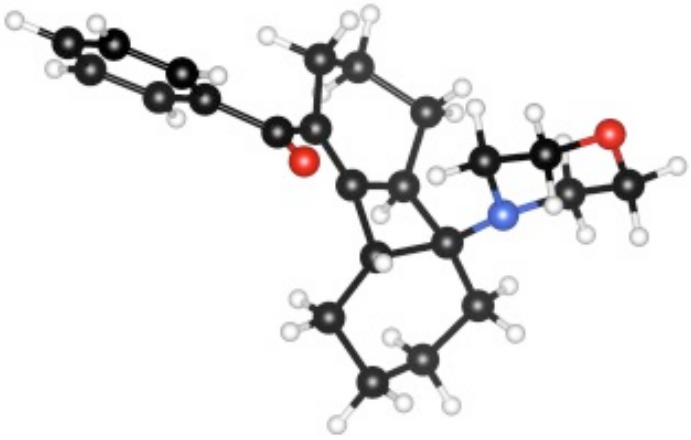
HF (M062X/6-31+G(d,p)) = -1098.6150561 Hartrees
Imaginary Frequencies: 1 (-353.13 cm^{-1})
Zero-point correction = 0.482486 (Hartree/Particle)
Thermal correction = 0.431290 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.507076	0.539199	-0.969695
2	6	0	-5.732996	-0.722098	-0.415551
3	6	0	-4.669169	-1.439406	0.131259
4	6	0	-3.388032	-0.888788	0.140597
5	6	0	-3.153725	0.374378	-0.411893
6	6	0	-4.222001	1.076606	-0.979340
7	1	0	-6.332013	1.098945	-1.400257
8	1	0	-6.732790	-1.145595	-0.414684
9	1	0	-4.835840	-2.427046	0.550605
10	1	0	-2.561602	-1.453334	0.564671
11	1	0	-4.032526	2.047165	-1.428593
12	6	0	-1.764297	0.957671	-0.502341
13	6	0	-0.908741	0.923530	0.646875
14	8	0	-1.433787	1.444312	-1.608350
15	6	0	0.451569	1.200265	0.506383
16	6	0	1.390253	1.156925	1.552333
17	6	0	-1.397553	0.563718	2.037306
18	6	0	-0.541291	1.225587	3.123837
19	1	0	-0.643953	2.315396	3.048852
20	6	0	0.938472	0.850386	2.962686
21	1	0	1.060658	-0.218367	3.187468
22	1	0	-2.446658	0.850341	2.165439
23	1	0	-1.357092	-0.526906	2.199950
24	1	0	-0.901244	0.928619	4.114625
25	1	0	1.552295	1.391176	3.690663
26	1	0	2.291635	1.752437	1.438228
27	6	0	4.059234	2.030151	-0.575140
28	6	0	3.755199	0.568557	-0.239056
29	6	0	2.280350	0.188137	-0.268859
30	6	0	1.235447	1.164424	-0.793543
31	6	0	1.740681	2.538571	-1.274991
32	6	0	3.193668	2.508480	-1.736224
33	1	0	3.881448	2.676433	0.293689

34	1	0	4.234939	-0.054465	-1.007396
35	1	0	1.067433	2.881623	-2.064801
36	1	0	3.502313	3.506414	-2.062064
37	1	0	0.657000	0.712835	-1.602031
38	1	0	1.660640	3.260445	-0.453437
39	1	0	3.314775	1.834530	-2.595752
40	1	0	5.125231	2.106736	-0.809185
41	1	0	4.204339	0.292146	0.718768
42	6	0	2.930270	-2.078827	0.352815
43	6	0	0.661683	-1.668228	-0.357427
44	6	0	2.804494	-3.481831	-0.221387
45	1	0	2.669309	-2.080701	1.423190
46	1	0	3.966002	-1.761784	0.250854
47	6	0	0.629671	-3.085339	-0.907766
48	1	0	0.273053	-1.657199	0.673789
49	1	0	0.017809	-1.037512	-0.970112
50	1	0	3.414465	-4.172949	0.363504
51	1	0	3.157966	-3.486355	-1.263631
52	1	0	-0.384962	-3.481575	-0.833481
53	1	0	0.935676	-3.083099	-1.964666
54	8	0	1.471464	-3.950269	-0.168146
55	7	0	2.031946	-1.147588	-0.343932

Intermediate: Formation of [2+2] adduct with Enamine 15a and Allene 7a



HF (M062X/6-31+G(d,p)) = -1098.6531182 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.484799 (Hartree/Particle)
Thermal correction = 0.434081 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.439982	0.729523	0.570168
2	6	0	-6.269718	-0.143471	-0.133698
3	6	0	-5.717019	-1.114512	-0.971328
4	6	0	-4.335256	-1.208472	-1.108764
5	6	0	-3.498858	-0.348009	-0.390350

6	6	0	-4.056226	0.620831	0.451038
7	1	0	-5.869996	1.491319	1.212497
8	1	0	-7.347831	-0.065707	-0.032000
9	1	0	-6.364006	-1.791855	-1.519720
10	1	0	-3.889221	-1.946738	-1.768182
11	1	0	-3.406331	1.302628	0.993865
12	6	0	-2.015859	-0.437998	-0.584710
13	6	0	-1.119171	-0.048456	0.541051
14	8	0	-1.562670	-0.818432	-1.657298
15	6	0	-0.007832	0.651549	0.294088
16	6	0	1.117061	0.904449	1.258409
17	6	0	-1.371283	-0.564137	1.949252
18	6	0	-0.384648	0.005134	2.981817
19	1	0	-0.665942	1.040597	3.214948
20	6	0	1.068657	-0.009037	2.476214
21	1	0	1.342401	-1.033655	2.207955
22	1	0	-2.397516	-0.358456	2.270095
23	1	0	-1.281536	-1.660586	1.924384
24	1	0	-0.472349	-0.566465	3.910892
25	1	0	1.757001	0.319752	3.261531
26	1	0	1.106563	1.954060	1.588922
27	6	0	2.772141	3.288331	-0.329390
28	6	0	3.210810	1.850109	-0.047516
29	6	0	2.073045	0.817441	-0.000910
30	6	0	0.803335	1.120076	-0.890914
31	6	0	0.555280	2.608031	-1.210021
32	6	0	1.843887	3.354191	-1.538498
33	1	0	2.254086	3.714014	0.541153
34	1	0	3.899751	1.538971	-0.843458
35	1	0	-0.167761	2.666260	-2.029831
36	1	0	1.618059	4.393961	-1.797036
37	1	0	0.739913	0.531150	-1.808182
38	1	0	0.087027	3.099527	-0.346884
39	1	0	2.335620	2.900374	-2.410118
40	1	0	3.667326	3.898985	-0.487224
41	1	0	3.768765	1.823734	0.895876
42	6	0	3.737680	-0.939709	0.526911
43	6	0	1.723462	-1.639100	-0.537700
44	6	0	4.456765	-2.115201	-0.119781
45	1	0	3.394218	-1.239341	1.532182
46	1	0	4.462205	-0.132750	0.648051
47	6	0	2.495004	-2.784118	-1.177450
48	1	0	1.283546	-2.009024	0.404779
49	1	0	0.896609	-1.362988	-1.194960
50	1	0	5.247722	-2.487422	0.535933
51	1	0	4.901794	-1.788285	-1.072618
52	1	0	1.846424	-3.653829	-1.307821
53	1	0	2.878583	-2.467999	-2.159876
54	8	0	3.576010	-3.199959	-0.357105
55	7	0	2.631501	-0.506825	-0.328206

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