Stereoselectivity in Diels-Alder Reactions of Diene-Substituted *N*-Alkoxy carbonyl-1,2-dihydropyridines.

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Coordinates of the optimized MVK D-A cycloaddition products at the RHF/6-31G* level

C = amide carbonyl cis to C₁, C_k = ketone carbonyl cis to the C₈-methylene in the product, T = amide carbonyl trans to C₁, T_k = ketone carbonyl trans to the C₈-methylene in the product,

15a CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-0.942397	1.842795	1.251182
2 H	-1.288994	2.648421	1.873176
3 C	-0.917903	0.576132	1.619517
4 C	-0.389871	-0.351203	0.544519
5 H	-0.287377	-1.370096	0.872577
6 C	-0.421946	2.080850	-0.149255
7 H	-0.423198	3.130666	-0.416036
8 C	-1.293386	1.268347	-1.134250
9 H	-2.301596	1.655701	-1.145037
10 H	-0.894601	1.367864	-2.138949
11 C	-1.303203	-0.216913	-0.703347
12 C	1.015027	1.536782	-0.214695
13 H	1.663092	2.067438	0.472853
14 H	1.418998	1.652869	-1.213708
15 N	0.934304	0.122832	0.137831
16 C	1.998116	-0.700893	0.188352
17 O	1.963550	-1.859778	0.497662
18 O	3.117036	-0.073878	-0.160001
19 C	4.302129	-0.848118	-0.150573
20 H	4.498814	-1.230786	0.840075
21 H	4.222932	-1.673645	-0.842544
22 H	-0.863735	-0.838253	-1.480491
23 C	-2.703477	-0.779286	-0.471254
24 O	-3.691157	-0.145054	-0.681859
25 C	-2.795100	-2.211165	0.019059
26 H	-3.782631	-2.597173	-0.193364
27 H	-2.641458	-2.238627	1.094350
28 H	-2.041748	-2.845062	-0.435583

29	H	5.090276	-0.177365	-0.456297
30	H	-1.240497	0.206599	2.576092

15a TC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.384199	1.532948	1.397767
2	H	-1.936972	2.096216	2.127877
3	C	-0.807080	0.371355	1.638371
4	C	-0.100311	-0.209870	0.430477
5	H	0.427474	-1.119283	0.650198
6	C	-1.193701	2.028388	-0.018833
7	H	-1.650237	2.996944	-0.180561
8	C	-1.790595	0.978710	-0.983491
9	H	-2.861365	0.919222	-0.855961
10	H	-1.599322	1.279121	-2.008617
11	C	-1.149415	-0.399103	-0.698752
12	C	0.317330	2.119257	-0.282984
13	H	0.792181	2.830390	0.381999
14	H	0.511701	2.435175	-1.301148
15	N	0.858688	0.781622	-0.064759
16	C	2.189052	0.600478	-0.170139
17	O	2.957864	1.461842	-0.490378
18	O	2.568386	-0.646467	0.104842
19	C	3.955881	-0.912020	0.009183
20	H	4.309642	-0.730822	-0.994837
21	H	4.510274	-0.293532	0.699240
22	H	-0.608233	-0.750093	-1.574648
23	C	-2.164809	-1.492806	-0.376233
24	O	-3.341199	-1.301852	-0.396067
25	C	-1.613447	-2.866629	-0.045319
26	H	-2.389579	-3.605059	-0.191289
27	H	-1.305787	-2.894931	0.996406
28	H	-0.747877	-3.113852	-0.650426
29	H	4.070942	-1.954196	0.264808
30	H	-0.825284	-0.141152	2.583275

15a CT_k

Coordinates (Angstroms)			
ATOM	X	Y	Z
1 C	0.669617	2.102570	-0.911962

2 H	0.941733	3.083863	-1.257296
3 C	0.536353	1.046236	-1.690057
4 C	0.145642	-0.210133	-0.941893
5 H	-0.045349	-1.046756	-1.588757
6 C	0.416574	1.814722	0.551648
7 H	0.515240	2.698181	1.171043
8 C	1.424403	0.730856	0.999092
9 H	2.428220	1.131228	0.906923
10 H	1.273964	0.485184	2.045530
11 C	1.231531	-0.533270	0.105045
12 C	-1.006808	1.249576	0.689269
13 H	-1.739975	1.989387	0.392045
14 H	-1.210677	0.972980	1.718239
15 N	-1.073232	0.078117	-0.177168
16 C	-2.191255	-0.647978	-0.365551
17 O	-2.291110	-1.596161	-1.092541
18 O	-3.198432	-0.190272	0.374298
19 C	-4.427143	-0.882711	0.259203
20 H	-4.791536	-0.845661	-0.756834
21 H	-4.312838	-1.914112	0.558922
22 H	0.859920	-1.345750	0.724090
23 C	2.525428	-1.020238	-0.525875
24 O	2.699464	-1.003827	-1.706251
25 C	3.571508	-1.585438	0.412963
26 H	4.507528	-1.704589	-0.114982
27 H	3.239913	-2.558709	0.765695
28 H	3.716446	-0.957548	1.285202
29 H	-5.111347	-0.374140	0.921073
30 H	0.696217	1.034396	-2.751114

15a TT_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-0.815296	1.893685	1.285395
2 H	-1.190400	2.690987	1.901683
3 C	-0.305381	0.769178	1.748463
4 C	0.150302	-0.181134	0.661092
5 H	0.626687	-1.061756	1.048507
6 C	-0.846534	1.971113	-0.225338
7 H	-1.254399	2.908501	-0.583769
8 C	-1.697490	0.785997	-0.735986
9 H	-2.711016	0.900248	-0.367074
10 H	-1.748539	0.797881	-1.819866
11 C	-1.055132	-0.542887	-0.232068

12	C	0.590220	1.803665	-0.744237
13	H	1.218035	2.622418	-0.415962
14	H	0.610506	1.786394	-1.828682
15	N	1.086911	0.540427	-0.210398
16	C	2.385274	0.234189	-0.393627
17	O	3.145292	0.902941	-1.035840
18	O	2.740604	-0.902066	0.200311
19	C	4.091657	-1.293739	0.045101
20	H	4.327277	-1.444518	-0.998163
21	H	4.754651	-0.546385	0.455415
22	H	-0.674921	-1.092662	-1.089376
23	C	-2.041704	-1.460802	0.470632
24	O	-1.918325	-1.758601	1.619909
25	C	-3.160758	-2.037405	-0.372041
26	H	-3.889112	-2.514200	0.269162
27	H	-2.747046	-2.780646	-1.048886
28	H	-3.643388	-1.280355	-0.979889
29	H	4.190009	-2.220570	0.589168
30	H	-0.217983	0.510106	2.786364

16a CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-1.796580	1.966141	0.862314
2 C	-1.394310	1.007380	1.673346
3 C	-0.628516	-0.095643	0.972504
4 C	-1.404241	1.741830	-0.582145
5 H	-1.723454	2.551311	-1.227296
6 C	-2.013823	0.401571	-1.048717
7 H	-3.094776	0.479189	-1.061894
8 H	-1.689634	0.178242	-2.055679
9 C	-1.566468	-0.728595	-0.090429
10 C	0.128655	1.617272	-0.641071
11 H	0.604415	2.536014	-0.319258
12 H	0.451975	1.402724	-1.652199
13 N	0.487997	0.514224	0.246725
14 C	1.750182	0.095016	0.449107
15 O	2.069568	-0.817412	1.163323
16 O	2.622517	0.812683	-0.246841
17 C	3.982516	0.434395	-0.137220
18 H	4.319820	0.520567	0.885119
19 H	4.122634	-0.581396	-0.476127
20 H	4.525979	1.118553	-0.770324
21 H	-1.570559	0.978720	2.733357

22	H	-0.229002	-0.822251	1.657589
23	H	-2.422519	-1.145480	0.433075
24	C	-0.874777	-1.893508	-0.799252
25	C	-0.503144	-3.091381	0.050296
26	H	0.448323	-2.899290	0.535955
27	H	-0.397402	-3.958798	-0.587237
28	H	-1.239809	-3.288128	0.821881
29	O	-0.619304	-1.869846	-1.964594
30	H	-2.346263	2.835895	1.175692

16a TC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-2.228740	-1.274938	-1.061104
2 C	-1.208127	-0.752975	-1.713246
3 C	-0.275673	0.052580	-0.830280
4 C	-2.239442	-0.944122	0.415710
5 H	-3.071451	-1.403251	0.935336
6 C	-2.282492	0.590713	0.568979
7 H	-3.221767	0.971663	0.185256
8 H	-2.223548	0.860993	1.614017
9 C	-1.093241	1.211550	-0.201533
10 C	-0.918135	-1.447836	1.021347
11 H	-0.834249	-2.523902	0.937937
12 H	-0.853192	-1.185550	2.070402
13 N	0.164327	-0.802335	0.278897
14 C	1.417276	-1.273670	0.447162
15 O	1.716387	-2.113698	1.245393
16 O	2.304773	-0.690019	-0.358435
17 C	3.647803	-1.119580	-0.221375
18 H	4.008800	-0.924732	0.777482
19 H	3.732403	-2.175323	-0.431913
20 H	4.211223	-0.547472	-0.942542
21 H	-1.020211	-0.871645	-2.765162
22 H	0.586261	0.408642	-1.364128
23 H	-1.453717	1.832849	-1.017847
24 C	-0.212481	2.114325	0.662398
25 C	0.967220	2.779866	-0.018792
26 H	1.797212	2.082126	-0.066193
27 H	1.271902	3.639767	0.561858
28 H	0.731578	3.084335	-1.033211
29 O	-0.432362	2.308143	1.818047
30 H	-2.988338	-1.886504	-1.514458

16a CT_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-1.690266	2.141849	0.165068
2 C	-1.255292	1.656810	1.312238
3 C	-0.584879	0.304975	1.179372
4 C	-1.397938	1.249302	-1.021992
5 H	-1.732598	1.681937	-1.956993
6 C	-2.063560	-0.126274	-0.789012
7 H	-3.141458	-0.029709	-0.843030
8 H	-1.769447	-0.797182	-1.588114
9 C	-1.646051	-0.669969	0.602969
10 C	0.123855	1.033276	-1.074149
11 H	0.638884	1.975498	-1.214580
12 H	0.389119	0.383009	-1.900457
13 N	0.501384	0.420260	0.198074
14 C	1.787834	0.305885	0.600071
15 O	2.145166	-0.021840	1.694522
16 O	2.630537	0.582319	-0.389902
17 C	4.010270	0.471406	-0.090067
18 H	4.282826	1.152213	0.702706
19 H	4.254350	-0.537851	0.206814
20 H	4.527591	0.730069	-1.001066
21 H	-1.361835	2.138175	2.267297
22 H	-0.174516	-0.061518	2.103648
23 H	-2.490884	-0.646736	1.278544
24 C	-1.148217	-2.114758	0.676520
25 C	-0.451223	-2.767398	-0.498391
26 H	-1.185628	-3.062199	-1.243020
27 H	0.057185	-3.654429	-0.147166
28 H	0.255800	-2.100175	-0.975106
29 O	-1.316763	-2.722318	1.690192
30 H	-2.194246	3.085372	0.055009

16a TT_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-2.007650	-1.840145	-0.398139
2 C	-1.067399	-1.630261	-1.299071
3 C	-0.192006	-0.433341	-0.991146
4 C	-1.985699	-0.848677	0.745022
5 H	-2.745218	-1.058300	1.488196

6 C	-2.165933	0.574555	0.169787
7 H	-3.164085	0.684071	-0.237737
8 H	-2.078399	1.290775	0.977687
9 C	-1.106967	0.816762	-0.937942
10 C	-0.595429	-0.920923	1.396645
11 H	-0.404659	-1.907105	1.800886
12 H	-0.515108	-0.210393	2.211826
13 N	0.377790	-0.603503	0.353709
14 C	1.682497	-0.847097	0.615472
15 O	2.096653	-1.149243	1.698182
16 O	2.461376	-0.694856	-0.448229
17 C	3.850765	-0.873901	-0.242790
18 H	4.221454	-0.165764	0.483485
19 H	4.058218	-1.877443	0.098255
20 H	4.310410	-0.700208	-1.203208
21 H	-0.915061	-2.223661	-2.182407
22 H	0.600998	-0.290575	-1.700900
23 H	-1.592819	0.895339	-1.902858
24 C	-0.234586	2.073867	-0.848363
25 C	-0.152496	2.893087	0.420068
26 H	-1.105337	3.371614	0.626649
27 H	0.603302	3.654784	0.290004
28 H	0.096909	2.272479	1.273598
29 O	0.393257	2.388274	-1.814164
30 H	-2.724776	-2.640211	-0.442518

15b CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	3.340331	1.811977	-0.349633
2 H	4.116547	2.541710	-0.494825
3 C	3.142192	0.770616	-1.134897
4 H	3.730174	0.533179	-2.002987
5 C	1.985572	-0.102132	-0.694419
6 H	1.768970	-0.901093	-1.380570
7 C	2.358123	1.906319	0.796912
8 H	2.521764	2.785614	1.407895
9 C	2.482688	0.621755	1.647764
10 H	3.454070	0.580381	2.118311
11 H	1.737766	0.635519	2.437144
12 C	2.282648	-0.614626	0.740444
13 C	0.941857	1.953567	0.199482
14 H	0.810517	2.833110	-0.419855
15 H	0.198753	1.983213	0.987509

16	N	0.790337	0.736914	-0.592385
17	C	-0.344316	0.388270	-1.225332
18	O	-0.491165	-0.613319	-1.872693
19	O	-1.295792	1.299759	-1.051261
20	C	-2.587684	1.025884	-1.591317
21	H	-3.010703	2.002261	-1.776332
22	H	-2.476636	0.504295	-2.527601
23	C	-3.448931	0.248596	-0.625791
24	C	-5.033702	-1.167282	1.174202
25	C	-3.547431	-1.134081	-0.711961
26	C	-4.152018	0.913099	0.371996
27	C	-4.939398	0.212131	1.268960
28	C	-4.337305	-1.838318	0.182966
29	H	-2.996422	-1.656472	-1.471837
30	H	-4.084442	1.984862	0.446614
31	H	-5.479836	0.738930	2.035055
32	H	-4.407906	-2.908606	0.105426
33	H	-5.647667	-1.714377	1.867280
34	H	1.408100	-1.178174	1.057735
35	C	3.446236	-1.601929	0.783410
36	O	4.382263	-1.457579	1.508148
37	C	3.354136	-2.811302	-0.127097
38	H	4.015482	-3.583975	0.240218
39	H	3.672147	-2.537871	-1.129542
40	H	2.340679	-3.190825	-0.197136

16b CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	2.838129	2.459231	-0.555433
2 H	3.125992	3.478351	-0.742710
3 C	3.011298	1.468245	-1.407850
4 H	3.460844	1.559320	-2.379991
5 C	2.503223	0.135857	-0.897428
6 H	2.567893	-0.642680	-1.636822
7 C	2.176064	2.036657	0.738129
8 H	2.022087	2.868903	1.414122
9 C	3.053765	0.952247	1.401061
10 H	4.002063	1.384447	1.698800
11 H	2.570062	0.578971	2.293075
12 C	3.280677	-0.207882	0.401838
13 H	4.333177	-0.289188	0.144446
14 C	0.816640	1.405105	0.389456
15 H	0.161833	2.128252	-0.081503

16	H	0.329568	1.038736	1.284671
17	N	1.097414	0.297169	-0.520728
18	C	0.150631	-0.508636	-1.034525
19	O	0.357358	-1.432476	-1.775921
20	O	-1.061569	-0.166140	-0.617795
21	C	-2.146464	-0.976231	-1.062155
22	H	-2.212156	-0.921019	-2.138868
23	H	-1.945319	-2.002979	-0.791423
24	C	-3.406168	-0.469861	-0.409119
25	C	-5.741789	0.437727	0.806532
26	C	-3.564622	-0.558613	0.970588
27	C	-4.427779	0.077117	-1.167991
28	C	-5.593979	0.527585	-0.564877
29	C	-4.721639	-0.106238	1.575308
30	H	-2.776473	-0.980531	1.569272
31	H	-4.317177	0.154551	-2.235521
32	H	-6.379439	0.948364	-1.166853
33	H	-4.832657	-0.179649	2.642445
34	H	-6.643683	0.786675	1.276958
35	C	2.851435	-1.572641	0.941365
36	C	3.149338	-2.778957	0.074477
37	H	2.360382	-2.888932	-0.662756
38	H	3.168808	-3.664946	0.694661
39	H	4.090953	-2.678270	-0.454629
40	O	2.291279	-1.697641	1.987694

15c CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	0.738773	1.043687	-1.746828
2 C	0.484898	-0.230380	-1.970334
3 H	0.609424	-0.729542	-2.912089
4 C	0.004256	-0.975459	-0.745367
5 H	-0.284038	-1.990226	-0.950749
6 C	0.512754	1.491167	-0.314426
7 C	1.421628	0.607943	0.579463
8 H	2.455854	0.824378	0.332345
9 H	1.283126	0.872386	1.623567
10 C	1.087419	-0.897058	0.347947
11 C	-0.952365	1.164014	0.039807
12 H	-1.625510	1.758644	-0.566444
13 H	-1.148638	1.398923	1.081084
14 N	-1.155841	-0.257713	-0.208055
15 C	-2.340458	-0.879240	-0.057372

16	O	-2.550952	-2.038864	-0.278065
17	O	-3.275828	-0.042855	0.386526
18	C	-4.565027	-0.591302	0.585349
19	H	-4.960030	-0.981905	-0.340905
20	H	-4.533478	-1.382166	1.320329
21	H	0.663674	-1.306472	1.261350
22	C	2.311930	-1.735155	0.019851
23	O	2.451869	-2.263182	-1.041061
24	C	3.329435	-1.919480	1.127047
25	H	4.235192	-2.348130	0.720949
26	H	2.921506	-2.598896	1.871097
27	H	3.555501	-0.986104	1.630737
28	H	-5.177239	0.224215	0.938925
29	H	1.088073	1.732863	-2.495985
30	C	0.797759	2.974975	-0.099391
31	H	0.627290	3.263534	0.933442
32	H	0.159773	3.589003	-0.728013
33	H	1.829269	3.208395	-0.344734

16c CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-2.019201	-0.581441	-1.407195
2 C	-1.118264	0.168342	-2.010272
3 H	-1.109805	0.400014	-3.059938
4 C	-0.047967	0.695226	-1.079080
5 H	0.729222	1.227345	-1.598517
6 C	-1.798550	-0.753458	0.084967
7 C	-1.782938	0.660401	0.716684
8 H	-2.772447	1.096753	0.637376
9 H	-1.543337	0.586258	1.768939
10 C	-0.743030	1.557831	0.005897
11 C	-0.385590	-1.349144	0.264839
12 H	-0.331521	-2.338594	-0.174572
13 H	-0.148679	-1.433237	1.318862
14 N	0.556020	-0.445981	-0.390047
15 C	1.885028	-0.650375	-0.432989
16 O	2.680315	0.081565	-0.958818
17 O	2.229627	-1.770753	0.188587
18 C	3.613239	-2.067328	0.235765
19 H	4.012492	-2.178779	-0.761524
20 H	4.151614	-1.286095	0.751670
21 H	3.692415	-2.997119	0.777524
22 H	-1.235348	2.386151	-0.496593

23	C	0.287063	2.171200	0.954996
24	O	0.325793	1.899956	2.116411
25	C	1.283072	3.141358	0.353370
26	H	1.676095	3.776449	1.135773
27	H	0.838312	3.749577	-0.427107
28	H	2.103222	2.581474	-0.084652
29	H	-2.848135	-1.050357	-1.908685
30	C	-2.843426	-1.649354	0.743917
31	H	-2.656449	-1.749816	1.808316
32	H	-2.840036	-2.643902	0.306906
33	H	-3.838808	-1.234167	0.619187

15d CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	0.739305	0.679199	-1.679999
2 C	0.547958	-0.619158	-1.530248
3 C	0.026706	-0.966980	-0.145572
4 H	-0.208526	-2.010893	-0.035766
5 C	0.413027	1.531691	-0.468199
6 C	1.295109	1.023154	0.698079
7 H	2.334437	1.201153	0.441681
8 H	1.087821	1.591614	1.600019
9 C	1.022404	-0.492673	0.931912
10 C	-1.058474	1.251845	-0.099178
11 H	-1.714522	1.602686	-0.886811
12 H	-1.326326	1.774532	0.813776
13 N	-1.195499	-0.188627	0.079951
14 C	-2.365750	-0.802056	0.336381
15 O	-2.519992	-1.985491	0.455615
16 O	-3.359486	0.075166	0.456155
17 C	-4.640268	-0.460475	0.729557
18 H	-4.952469	-1.125233	-0.062391
19 H	-4.636216	-0.999487	1.665588
20 H	0.536336	-0.615394	1.896474
21 C	2.295640	-1.318581	0.982362
22 O	2.551583	-2.146514	0.161489
23 C	3.213347	-1.081335	2.164263
24 H	4.164289	-1.565071	1.988935
25 H	2.759542	-1.509151	3.054563
26 H	3.365558	-0.024715	2.354589
27 H	-5.304312	0.388272	0.789295
28 H	1.088630	1.130844	-2.593287
29 C	0.628281	3.022234	-0.715133

30 H	0.379521	3.607838	0.164917
31 H	0.011159	3.373913	-1.536529
32 H	1.664472	3.224527	-0.968294
33 C	0.753640	-1.684608	-2.565336
34 H	-0.178572	-2.208324	-2.762098
35 H	1.474534	-2.415535	-2.218904
36 H	1.107116	-1.258370	-3.497856

16d CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-2.019456	-0.609140	-0.903959
2 C	-1.252162	0.275464	-1.513078
3 C	-0.094036	0.733066	-0.642376
4 H	0.581637	1.384050	-1.170268
5 C	-1.595942	-0.970515	0.508310
6 C	-1.566080	0.337730	1.335023
7 H	-2.577658	0.712333	1.445430
8 H	-1.182655	0.137283	2.326592
9 C	-0.678527	1.391493	0.633420
10 C	-0.145777	-1.491228	0.427038
11 H	-0.102601	-2.408480	-0.148884
12 H	0.235826	-1.696203	1.420405
13 N	0.652400	-0.448637	-0.211620
14 C	1.972902	-0.551463	-0.446267
15 O	2.652369	0.297192	-0.959554
16 O	2.455132	-1.717296	-0.035742
17 C	3.846290	-1.919964	-0.202741
18 H	4.115208	-1.870689	-1.247608
19 H	4.406806	-1.177977	0.346471
20 H	4.045150	-2.905301	0.189535
21 H	-1.274987	2.244946	0.320814
22 C	0.438891	1.941662	1.520424
23 O	0.651725	1.517708	2.615348
24 C	1.291253	3.053136	0.942676
25 H	1.750975	3.604204	1.751955
26 H	0.713827	3.727032	0.318733
27 H	2.074323	2.617580	0.330227
28 H	-2.885242	-1.061823	-1.357783
29 C	-2.502294	-2.016537	1.150762
30 H	-2.173740	-2.252872	2.157965
31 H	-2.508890	-2.937583	0.574772
32 H	-3.524014	-1.654285	1.211036
33 C	-1.421436	0.819632	-2.901593

34 H	-0.553521	0.592228	-3.515008
35 H	-1.527361	1.902034	-2.888169
36 H	-2.298334	0.401219	-3.382289

15e CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	0.643395	-1.535619	-1.404005
2 H	0.914380	-2.342567	-2.062432
3 C	0.551047	-1.652636	-0.091036
4 C	0.125635	-0.351587	0.572556
5 H	-0.029052	-0.453266	1.632182
6 C	0.316382	-0.158434	-1.937264
7 H	0.381814	-0.109496	-3.017804
8 C	1.295258	0.848220	-1.295944
9 H	2.304127	0.596633	-1.605357
10 H	1.093541	1.854721	-1.649252
11 C	1.139416	0.767696	0.253371
12 C	-1.113484	0.195984	-1.495823
13 H	-1.829235	-0.478991	-1.948581
14 H	-1.370834	1.206181	-1.796712
15 N	-1.137377	0.074331	-0.041950
16 C	-2.246626	0.234146	0.703605
17 O	-2.309433	0.107068	1.894506
18 O	-3.293463	0.568359	-0.047167
19 C	-4.517423	0.766556	0.634539
20 H	-4.820406	-0.136197	1.144252
21 H	-4.427979	1.567973	1.353190
22 H	0.710324	1.701004	0.609074
23 C	2.467003	0.601652	0.971388
24 O	2.738340	-0.381719	1.591114
25 C	3.423036	1.775279	0.910732
26 H	4.395342	1.471353	1.273021
27 H	3.044185	2.572239	1.545369
28 H	3.511168	2.175262	-0.093307
29 H	-5.236691	1.025520	-0.127330
30 C	0.779167	-2.891968	0.721878
31 H	-0.122847	-3.161369	1.265791
32 H	1.565447	-2.728918	1.449342
33 H	1.055842	-3.727411	0.088052

16e CC_k

Coordinates (Angstroms)

ATOM	X	Y	Z
1 C	1.879596	1.679540	0.355165
2 H	2.558461	2.512075	0.422958
3 C	1.563035	1.077312	-0.776516
4 C	0.571169	-0.056884	-0.569177
5 H	0.244981	-0.487936	-1.500110
6 C	1.196811	1.107314	1.578608
7 H	1.461942	1.640696	2.483517
8 C	1.575309	-0.384482	1.696738
9 H	2.635546	-0.474863	1.902457
10 H	1.041953	-0.841784	2.518676
11 C	1.220176	-1.104332	0.373929
12 C	-0.323161	1.199587	1.361294
13 H	-0.640462	2.232194	1.278785
14 H	-0.855228	0.744749	2.187984
15 N	-0.603547	0.476262	0.122911
16 C	-1.833350	0.339816	-0.404906
17 O	-2.089592	-0.254744	-1.417832
18 O	-2.754319	0.943231	0.335409
19 C	-4.094147	0.833613	-0.108832
20 H	-4.207031	1.272638	-1.089133
21 H	-4.399332	-0.201798	-0.143058
22 H	-4.684853	1.374209	0.614429
23 C	2.066821	1.405159	-2.151863
24 H	1.246296	1.679333	-2.809753
25 H	2.563721	0.548711	-2.601965
26 H	2.772139	2.227904	-2.124706
27 H	2.119310	-1.473371	-0.113126
28 C	0.299565	-2.310960	0.560602
29 O	-0.162014	-2.603114	1.621438
30 C	-0.022027	-3.128127	-0.674031
31 H	-0.327647	-4.120789	-0.372032
32 H	0.822990	-3.192371	-1.351347
33 H	-0.843112	-2.658788	-1.206514

15f CC_k

Coordinates (Angstroms)			
ATOM	X	Y	Z
1 C	-1.179088	1.565722	0.547352
2 C	-0.942259	0.468145	1.244482
3 C	-0.145889	-0.579578	0.497296
4 C	-0.567272	1.516126	-0.841554
5 H	-0.739280	2.433691	-1.392999
6 C	-1.165568	0.310212	-1.600597
7 H	-2.222382	0.461599	-1.766676

8 H	-0.692409	0.224146	-2.573846
9 C	-0.939547	-0.977501	-0.775377
10 C	0.945839	1.290158	-0.688584
11 H	1.408372	2.104334	-0.142240
12 H	1.419412	1.229585	-1.661589
13 N	1.100334	0.030397	0.029507
14 C	2.288861	-0.526169	0.326363
15 O	2.443432	-1.554376	0.925624
16 O	3.298804	0.204569	-0.136291
17 C	4.600852	-0.291272	0.113161
18 H	4.781925	-0.368265	1.175168
19 H	4.732310	-1.261879	-0.341992
20 H	-0.319601	-1.678736	-1.329519
21 C	-2.226457	-1.730977	-0.450638
22 O	-3.292615	-1.385123	-0.858515
23 C	-2.093722	-2.974381	0.406678
24 H	-1.193860	-3.533494	0.175191
25 H	-2.965472	-3.598688	0.266181
26 H	-2.042428	-2.689316	1.453907
27 H	5.275093	0.425072	-0.330561
28 H	-1.280495	0.301963	2.252180
29 H	0.111965	-1.429185	1.104087
30 C	-1.949951	2.767194	1.009433
31 H	-1.331370	3.660971	0.981227
32 H	-2.313899	2.637199	2.021986
33 H	-2.803631	2.947855	0.361157

16f CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-2.228143	-0.698830	-0.427066
2 C	-1.486635	-0.152376	-1.373795
3 C	-0.203378	0.476098	-0.874611
4 C	-1.605027	-0.555292	0.950658
5 H	-2.207235	-1.025758	1.719944
6 C	-1.419188	0.947124	1.253862
7 H	-2.389013	1.426575	1.324523
8 H	-0.923138	1.073850	2.206235
9 C	-0.576287	1.597489	0.131032
10 C	-0.216254	-1.217012	0.921045
11 H	-0.296088	-2.276415	0.706328
12 H	0.277258	-1.102058	1.878395
13 N	0.543723	-0.535942	-0.122925
14 C	1.811366	-0.843170	-0.450103

15	O	2.458063	-0.296240	-1.302987
16	O	2.283291	-1.835452	0.294449
17	C	3.626008	-2.217854	0.059793
18	H	3.752129	-2.559613	-0.956940
19	H	4.294526	-1.389995	0.244541
20	H	3.824532	-3.020905	0.752665
21	H	-1.739643	-0.141091	-2.419389
22	H	0.421019	0.829748	-1.675993
23	C	-3.540748	-1.401750	-0.614475
24	H	-3.481189	-2.432369	-0.273283
25	H	-3.842144	-1.406143	-1.655689
26	H	-4.324199	-0.919761	-0.034523
27	H	-1.162810	2.338297	-0.405638
28	C	0.673634	2.314660	0.641636
29	C	1.507700	3.054214	-0.384197
30	H	2.172790	2.350725	-0.874766
31	H	2.104612	3.803696	0.117770
32	H	0.893479	3.521348	-1.146734
33	O	0.996986	2.294203	1.790238

15g CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-0.934615	1.333817	0.351057
2 C	-0.621032	0.520874	1.343990
3 H	-0.848620	0.702795	2.377864
4 C	0.077994	-0.749932	0.916282
5 H	0.401226	-1.353394	1.744769
6 C	-0.524740	0.776281	-1.001827
7 H	-0.770684	1.448952	-1.815814
8 C	-1.251417	-0.574419	-1.196209
9 H	-2.321567	-0.395416	-1.203351
10 H	-0.995190	-1.004021	-2.159573
11 C	-0.842733	-1.536321	-0.038803
12 C	0.991579	0.523403	-0.992692
13 H	1.533743	1.453208	-0.869831
14 H	1.308636	0.076080	-1.928988
15 N	1.254180	-0.380214	0.120291
16 C	2.485397	-0.792186	0.473727
17 O	2.740251	-1.515680	1.395367
18 O	3.415381	-0.301539	-0.343107
19 C	4.752250	-0.673515	-0.066974
20 H	5.045334	-0.339269	0.917381
21 H	4.870275	-1.745457	-0.128384

22	H	-0.265278	-2.358359	-0.454210
23	C	-2.035026	-2.156227	0.670835
24	O	-2.281096	-1.928087	1.815846
25	C	-2.873166	-3.131488	-0.130770
26	H	-3.790497	-3.344582	0.400448
27	H	-2.315774	-4.056361	-0.255494
28	H	-3.099240	-2.754200	-1.122064
29	C	-1.635628	2.660434	0.476906
30	H	-1.996775	2.773459	1.494113
31	H	-2.513532	2.664826	-0.167535
32	C	-0.746183	3.856511	0.116882
33	H	-0.384279	3.794160	-0.905134
34	H	0.116242	3.906259	0.773530
35	H	-1.297303	4.786821	0.212710
36	H	5.351885	-0.187214	-0.821236

16g CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-1.955138	-0.229626	0.105858
2 C	-1.290938	0.093460	-0.990402
3 H	-1.692419	0.072713	-1.986824
4 C	0.144715	0.509246	-0.748543
5 H	0.683215	0.676075	-1.664757
6 C	-1.101192	-0.095668	1.355625
7 H	-1.644312	-0.383745	2.249019
8 C	-0.614249	1.364690	1.468520
9 H	-1.463404	2.020083	1.626446
10 H	0.042159	1.471327	2.321108
11 C	0.136855	1.756469	0.174054
12 C	0.129353	-1.005232	1.198539
13 H	-0.165473	-2.044622	1.110830
14 H	0.781820	-0.910137	2.057917
15 N	0.818324	-0.561474	-0.009267
16 C	1.945769	-1.123055	-0.479843
17 O	2.532099	-0.774409	-1.469552
18 O	2.353515	-2.124161	0.290528
19 C	3.556204	-2.765843	-0.091470
20 H	3.458472	-3.203636	-1.073936
21 H	4.377339	-2.064313	-0.092433
22 C	-3.383374	-0.692867	0.220594
23 H	-3.905184	-0.023331	0.903243
24 H	-3.389209	-1.665495	0.710666
25 C	-4.152464	-0.780895	-1.094600

26 H	-3.684793	-1.480982	-1.779042
27 H	-4.205856	0.185227	-1.585906
28 H	-5.167775	-1.118903	-0.916107
29 H	3.722164	-3.534990	0.646939
30 H	-0.391946	2.548697	-0.349024
31 C	1.556715	2.266668	0.420640
32 O	2.051674	2.277421	1.506565
33 C	2.330002	2.754666	-0.787167
34 H	3.119146	3.417622	-0.458896
35 H	1.690850	3.265795	-1.499314
36 H	2.777337	1.903227	-1.290008

15h CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-0.766006	2.122360	1.181472
2 C	-0.691037	0.944027	1.761617
3 C	-0.226220	-0.200559	0.872295
4 C	-0.333809	2.104820	-0.262016
5 H	-0.364710	3.086484	-0.719954
6 C	-1.240709	1.123566	-1.034052
7 H	-2.253301	1.512926	-1.038980
8 H	-0.921107	1.056781	-2.069190
9 C	-1.182148	-0.282691	-0.352207
10 C	1.097954	1.568177	-0.300854
11 H	1.766474	2.219258	0.249204
12 H	1.450771	1.518660	-1.323145
13 N	1.082813	0.223170	0.286994
14 C	2.127527	-0.606686	0.062070
15 O	2.175005	-1.786673	0.262279
16 O	3.167215	0.063729	-0.437707
17 C	4.329139	-0.694073	-0.713355
18 H	4.708278	-1.152694	0.187906
19 H	4.120894	-1.463253	-1.442629
20 H	-0.742638	-0.991770	-1.047201
21 C	-2.596282	-0.760334	-0.050934
22 O	-3.093628	-0.695658	1.031372
23 C	-3.361973	-1.325641	-1.230017
24 H	-3.256272	-0.701740	-2.111661
25 H	-4.407346	-1.427011	-0.973228
26 H	-2.959938	-2.304739	-1.477283
27 H	5.047859	0.009053	-1.105943
28 H	-0.963371	0.749221	2.781763
29 H	-1.092821	3.021967	1.671106

30	C	-0.162452	-1.499287	1.677453
31	H	0.641057	-1.456939	2.401413
32	H	-0.000935	-2.365459	1.056056
33	H	-1.098281	-1.608994	2.207360

16h CC_k

ATOM	Coordinates (Angstroms)		
	X	Y	Z
1 C	-1.415353	2.346597	0.721720
2 C	-1.259659	1.307007	1.513433
3 C	-0.586479	0.092474	0.882578
4 C	-0.878017	2.117828	-0.668013
5 H	-0.973916	2.991367	-1.301982
6 C	-1.621018	0.916995	-1.281087
7 H	-2.668111	1.162550	-1.417816
8 H	-1.204273	0.696437	-2.255109
9 C	-1.479958	-0.313715	-0.343749
10 C	0.602749	1.742750	-0.542322
11 H	1.173502	2.567533	-0.132979
12 H	1.005050	1.502670	-1.516865
13 N	0.703904	0.571114	0.336977
14 C	1.869931	-0.111779	0.406131
15 O	2.063053	-1.155357	0.962022
16 O	2.842972	0.547006	-0.219036
17 C	4.110309	-0.080055	-0.241950
18 H	4.486792	-0.216918	0.761175
19 H	4.051161	-1.038700	-0.735590
20 H	4.753962	0.586827	-0.795231
21 H	-1.571643	1.270671	2.542009
22 H	-2.451517	-0.587036	0.053518
23 C	-0.911594	-1.519589	-1.091839
24 C	-1.578361	-2.859727	-0.872078
25 H	-0.984539	-3.641708	-1.324485
26 H	-2.561027	-2.843281	-1.338245
27 H	-1.726185	-3.067433	0.181186
28 O	0.000151	-1.403053	-1.853388
29 H	-1.868552	3.275153	1.019984
30 C	-0.487967	-1.017278	1.931224
31 H	-0.073506	-1.935395	1.553044
32 H	-1.491156	-1.203253	2.304994
33 H	0.129294	-0.700697	2.761767

Coordinates of the optimized MVK/ DHP Diels-Alder cycloaddition transition states at the RHF/3-21G (*) level

N = endo, C = carbonyl cis to C₁ of the cycloadduct, C_k = ketone carbonyl cis to C₈-methylene of the cycloadduct. X = endo, T = amide carbonyl trans to C₁ of the cycloadduct, T_k = ketone carbonyl trans to C₈-methylene of the cycloadduct.

15a NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.307612	-2.011895	-0.806437
2	H	-2.185668	-2.624072	-0.828208
3	C	-1.253537	-0.843652	-1.551743
4	C	-0.283874	0.073363	-1.242080
5	H	-0.272406	1.061060	-1.646748
6	C	-0.331044	-2.196379	0.156777
7	H	-0.361770	-3.073160	0.776394
8	C	-1.113656	0.465514	0.925098
9	H	-0.411161	1.273133	0.940882
10	C	-0.852232	-0.753246	1.533230
11	H	-1.700461	-1.302794	1.888933
12	H	0.044541	-0.867826	2.113530
13	N	0.944862	-0.323443	-0.697529
14	C	1.068510	-1.695374	-0.177598
15	H	1.525343	-2.329242	-0.930559
16	H	1.705215	-1.687090	0.689984
17	C	1.912364	0.613266	-0.533429
18	O	1.790639	1.791481	-0.800470
19	O	3.040157	0.084739	-0.024876
20	C	4.161963	0.983822	0.195352
21	H	3.885035	1.760541	0.890337
22	H	4.466006	1.432049	-0.736974
23	C	-2.491312	0.744569	0.553037
24	O	-3.347786	-0.130631	0.570576
25	C	-2.814674	2.168765	0.141852
26	H	-3.802631	2.203623	-0.295171
27	H	-2.084348	2.551829	-0.560925
28	H	-2.795919	2.807792	1.020337
29	H	4.942899	0.363635	0.598784
30	H	-2.077443	-0.540377	-2.162355

15a NTC_k

Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z

1	C	1.932363	-1.417857	0.999813
2	H	2.982682	-1.522295	1.178086
3	C	1.214986	-0.413113	1.630067
4	C	-0.020766	-0.087101	1.133378
5	H	-0.550860	0.781160	1.449438
6	C	1.314640	-2.073397	-0.053113
7	H	1.849933	-2.839176	-0.582682
8	C	0.849489	0.612411	-0.955643
9	H	-0.139546	0.985694	-1.120922
10	C	1.277387	-0.601534	-1.476398
11	H	2.323889	-0.685630	-1.690485
12	H	0.629556	-1.141092	-2.142154
13	N	-0.810613	-1.038379	0.480866
14	C	-0.183050	-2.310601	0.082350
15	H	-0.380194	-3.063413	0.838629
16	H	-0.628646	-2.636474	-0.843618
17	C	-2.079150	-0.789689	0.069126
18	O	-2.787044	-1.582418	-0.510621
19	O	-2.474486	0.467831	0.370166
20	C	-3.837185	0.839441	0.022555
21	H	-4.538440	0.202434	0.538146
22	H	-3.987343	0.746598	-1.041296
23	C	1.866147	1.515317	-0.448030
24	O	3.023445	1.147603	-0.283518
25	C	1.429053	2.932229	-0.123044
26	H	2.225262	3.443847	0.398635
27	H	0.529326	2.937056	0.481012
28	H	1.213726	3.463518	-1.045499
29	H	-3.938777	1.862536	0.340100
30	H	1.694214	0.264491	2.304658

15a NCT_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.318541	-1.643047	-0.987145
2	H	-2.222752	-2.199123	-1.142150
3	C	-1.100831	-0.454767	-1.665013
4	C	-0.069831	0.351063	-1.235557
5	H	0.066821	1.349498	-1.590366
6	C	-0.491430	-1.924111	0.083855
7	H	-0.683683	-2.790680	0.688909

8	C	-0.981803	0.868136	0.771262
9	H	-0.122304	1.498135	0.885435
10	C	-1.029991	-0.357102	1.411087
11	H	-1.976412	-0.790434	1.663146
12	H	-0.239060	-0.610009	2.091901
13	N	1.067539	-0.208391	-0.637169
14	C	0.979372	-1.558191	-0.052832
15	H	1.481276	-2.267412	-0.702120
16	H	1.480046	-1.567902	0.901190
17	C	2.176324	0.564707	-0.492265
18	O	2.272504	1.722069	-0.836939
19	O	3.176835	-0.119803	0.093690
20	C	4.435431	0.579146	0.299780
21	H	4.293646	1.407165	0.976264
22	H	4.813120	0.948133	-0.640362
23	C	-2.167087	1.592279	0.282534
24	O	-2.074180	2.714904	-0.184989
25	C	-3.512689	0.897999	0.387042
26	H	-4.249577	1.495981	-0.129245
27	H	-3.801167	0.804402	1.429146
28	H	-3.477940	-0.093768	-0.044653
29	H	5.098038	-0.155822	0.722063
30	H	-1.821673	-0.053052	-2.346498

15a NTT_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	1.594750	-1.436334	1.108811
2	H	2.605417	-1.664457	1.387409
3	C	0.935094	-0.362058	1.680800
4	C	-0.242127	0.060168	1.100865
5	H	-0.710689	0.978803	1.370353
6	C	1.024941	-2.004320	-0.016466
7	H	1.546686	-2.783976	-0.539453
8	C	0.687176	0.766200	-0.847480
9	H	-0.311478	1.070883	-1.087359
10	C	1.198203	-0.402885	-1.384121
11	H	2.256428	-0.513094	-1.508802
12	H	0.616166	-0.921852	-2.122601
13	N	-1.066034	-0.848997	0.428996
14	C	-0.491113	-2.125737	-0.033752
15	H	-0.809800	-2.925326	0.626521
16	H	-0.870120	-2.338496	-1.021372
17	C	-2.324411	-0.537786	0.017834

18	O	-3.039467	-1.278550	-0.619055
19	O	-2.687648	0.704292	0.392634
20	C	-4.005788	1.175615	-0.001752
21	H	-4.761699	0.471440	0.306427
22	H	-4.045896	1.299395	-1.072439
23	C	1.504300	1.859484	-0.300833
24	O	0.994190	2.905071	0.069188
25	C	3.004862	1.648706	-0.218398
26	H	3.441146	2.479647	0.316895
27	H	3.428277	1.610000	-1.217022
28	H	3.243995	0.721361	0.286202
29	H	-4.125541	2.120626	0.497536
30	H	1.410181	0.272178	2.400434

16a XCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.723911	-0.969792	-0.580052
2	C	-2.127818	-0.191749	-1.555268
3	C	-0.772338	0.010608	-1.480883
4	H	-0.263356	0.704609	-2.113129
5	C	-1.936061	-1.407937	0.476154
6	H	-2.394990	-1.998518	1.248426
7	C	-1.690625	0.334622	1.447257
8	H	-2.716123	0.462297	1.734944
9	H	-1.070773	-0.112977	2.203391
10	C	-1.095873	1.329380	0.670605
11	H	-1.692535	2.090751	0.216069
12	C	-0.489777	-1.792004	0.186640
13	H	-0.439084	-2.802734	-0.201172
14	H	0.116900	-1.728637	1.072308
15	N	0.060770	-0.857680	-0.816725
16	C	1.414502	-0.664683	-0.924964
17	O	1.920927	0.195083	-1.616138
18	O	2.098906	-1.572825	-0.225715
19	C	3.469705	-1.228960	0.136019
20	H	4.045972	-1.025049	-0.751461
21	H	3.439023	-0.361827	0.775724
22	C	0.324343	1.538450	0.762802
23	O	1.080514	0.706316	1.279034
24	C	0.899358	2.802004	0.152950
25	H	0.134701	3.482955	-0.191932
26	H	1.532925	2.508660	-0.676139

27	H	1.523428	3.299441	0.886389
28	H	3.847930	-2.090120	0.658566
29	H	-2.703787	0.379452	-2.252762
30	H	-3.792851	-1.039135	-0.520936

16a XTC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.769426	-0.273845	-0.958959
2	C	-1.694653	0.053581	-1.764519
3	C	-0.426950	-0.213489	-1.298314
4	H	0.446210	0.140872	-1.796581
5	C	-2.500306	-0.798062	0.297170
6	H	-3.320347	-1.023126	0.953965
7	C	-1.728680	0.859176	1.218450
8	H	-2.684942	1.330160	1.335146
9	H	-1.383399	0.320618	2.082305
10	C	-0.761361	1.509592	0.461183
11	H	-1.042504	2.314497	-0.185032
12	C	-1.319871	-1.747369	0.416039
13	H	-1.577682	-2.728355	0.030156
14	H	-0.994229	-1.861983	1.437217
15	N	-0.196878	-1.194933	-0.365945
16	C	1.059739	-1.621525	-0.020050
17	O	1.271295	-2.504973	0.771998
18	O	2.020282	-0.989233	-0.723965
19	C	3.380621	-1.122031	-0.219145
20	H	3.429955	-0.657932	0.752658
21	H	3.649679	-2.162866	-0.148276
22	C	0.638761	1.377291	0.781898
23	O	1.080655	0.509202	1.534781
24	C	1.570755	2.397061	0.148495
25	H	1.683515	3.239306	0.825233
26	H	1.188460	2.767598	-0.793166
27	H	2.544120	1.951386	0.001155
28	H	4.000555	-0.607423	-0.933195
29	H	-1.809099	0.663129	-2.636447
30	H	-3.754274	0.073676	-1.204253

16a XCT_k

Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z

1	C	-2.472114	-1.551128	-0.177692
2	C	-1.994413	-1.089062	-1.393497
3	C	-0.769078	-0.467956	-1.406500
4	H	-0.382799	0.038291	-2.264423
5	C	-1.705752	-1.308235	0.946147
6	H	-2.090207	-1.574096	1.913558
7	C	-1.856124	0.800868	1.015044
8	H	-2.883448	0.757758	1.314868
9	H	-1.166341	0.903611	1.831773
10	C	-1.549869	1.354792	-0.215413
11	H	-2.342994	1.555423	-0.905611
12	C	-0.194215	-1.407258	0.823730
13	H	0.113682	-2.447043	0.852622
14	H	0.300598	-0.898175	1.635486
15	N	0.212596	-0.818547	-0.464868
16	C	1.521717	-0.630390	-0.777729
17	O	1.946132	-0.214930	-1.832122
18	O	2.315402	-0.967638	0.259877
19	C	3.752133	-0.850706	0.066405
20	H	4.069370	-1.483411	-0.747320
21	H	4.013853	0.171695	-0.154659
22	C	-0.348899	2.164184	-0.496958
23	O	-0.242906	2.772502	-1.547878
24	C	0.726816	2.272367	0.570370
25	H	1.016505	1.308429	0.962543
26	H	0.363187	2.879427	1.393070
27	H	1.586448	2.758216	0.131901
28	H	4.187372	-1.170217	0.997116
29	H	-2.631393	-1.000654	-2.249359
30	H	-3.495258	-1.858117	-0.080480

16a XTT_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.713795	-1.187112	-0.197352
2	C	-1.726425	-1.590550	-1.078043
3	C	-0.431178	-1.216831	-0.807031
4	H	0.362880	-1.336084	-1.506759
5	C	-2.335488	-0.384734	0.865972
6	H	-3.090348	0.011140	1.520140
7	C	-1.793656	1.329193	-0.206056

8	H	-2.795739	1.521407	-0.532156
9	H	-1.516244	1.871342	0.678594
10	C	-0.829325	1.039547	-1.160040
11	H	-1.126195	0.857562	-2.172024
12	C	-1.009445	-0.686387	1.546424
13	H	-1.119554	-1.526689	2.223484
14	H	-0.656224	0.154160	2.124724
15	N	-0.011679	-1.025506	0.514866
16	C	1.303660	-0.990399	0.860684
17	O	1.704973	-0.645512	1.951754
18	O	2.097510	-1.373801	-0.153973
19	C	3.500469	-0.979493	-0.147140
20	H	3.570665	-0.007442	-0.609083
21	H	3.871225	-0.959713	0.864035
22	C	0.589008	1.425659	-1.032881
23	O	1.406220	1.130190	-1.892271
24	C	1.023233	2.234377	0.180982
25	H	0.439597	3.143023	0.261745
26	H	2.064697	2.492773	0.053810
27	H	0.919623	1.671491	1.099123
28	H	4.014271	-1.717854	-0.738075
29	H	-1.964136	-1.972424	-2.049545
30	H	-3.748599	-1.281331	-0.463909

15b NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-3.419967	1.609411	-0.484905
2	H	-4.357514	1.711979	-0.991536
3	C	-3.351315	0.936420	0.725921
4	H	-4.227307	0.517301	1.173825
5	C	-2.120493	0.528195	1.167141
6	H	-1.993471	-0.132981	1.995267
7	C	-2.225733	1.880415	-1.129305
8	H	-2.242154	2.368482	-2.085911
9	C	-1.757543	-0.919647	-0.650996
10	H	-0.908773	-1.256342	-0.092270
11	C	-1.638760	-0.014394	-1.694934
12	H	-2.371469	-0.081712	-2.473712
13	H	-0.659447	0.294943	-2.009847
14	N	-0.956639	1.235586	0.830915
15	C	-1.033083	2.233653	-0.249415

16	H	-1.161964	3.222066	0.179264
17	H	-0.111448	2.221762	-0.804691
18	C	0.214525	0.867002	1.402259
19	O	0.338794	-0.064023	2.178862
20	O	1.231455	1.653526	1.013114
21	C	2.580585	1.337040	1.495402
22	H	2.497605	0.966119	2.503353
23	H	3.091647	2.284489	1.483849
24	C	-3.004527	-1.659711	-0.545881
25	O	-3.988868	-1.351085	-1.206041
26	C	-3.028685	-2.830269	0.419470
27	H	-4.050743	-3.138801	0.587619
28	H	-2.556468	-2.578021	1.361139
29	H	-2.480177	-3.661333	-0.014796
30	C	3.257666	0.330851	0.597470
31	C	4.491276	-1.518962	-1.066540
32	C	4.141620	0.750486	-0.383375
33	C	2.988837	-1.024766	0.737479
34	C	3.604613	-1.944286	-0.091155
35	C	4.759048	-0.169841	-1.212900
36	H	4.351701	1.796570	-0.498570
37	H	3.394341	-2.989053	0.024041
38	H	5.444037	0.164545	-1.966536
39	H	4.969559	-2.233867	-1.706315
40	H	2.289237	-1.341746	1.483238

16b NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-3.530956	1.797115	1.173510
2	H	-4.465304	2.268554	1.409247
3	C	-3.063300	0.749279	1.945638
4	H	-3.622164	0.363928	2.772592
5	C	-1.964741	0.058641	1.499948
6	H	-1.626224	-0.839478	1.967722
7	C	-2.926177	2.020768	-0.055198
8	H	-3.297378	2.817355	-0.674267
9	C	-3.625524	0.417785	-1.062682
10	H	-4.655354	0.717344	-1.064870
11	H	-3.085243	0.676504	-1.955530
12	C	-3.293654	-0.798504	-0.468295
13	H	-4.008639	-1.320340	0.130866

14	C	-1.423075	1.799822	-0.171936
15	H	-0.884999	2.667650	0.190712
16	H	-1.133213	1.612071	-1.190583
17	N	-1.049424	0.622569	0.638721
18	C	0.107827	-0.060399	0.382627
19	O	0.392739	-1.121765	0.909367
20	O	0.896217	0.603950	-0.461029
21	C	1.950724	-0.136576	-1.165155
22	H	1.633637	-1.163812	-1.237089
23	H	1.975194	0.309190	-2.144636
24	C	-2.139679	-1.522368	-0.937338
25	O	-1.268158	-0.991901	-1.634773
26	C	-1.983089	-2.967312	-0.504739
27	H	-2.841233	-3.335045	0.038818
28	H	-1.097899	-3.031435	0.117134
29	H	-1.817414	-3.584749	-1.379840
30	C	3.282744	-0.006337	-0.468640
31	C	5.747619	0.215687	0.794117
32	C	4.302625	0.730742	-1.045511
33	C	3.502392	-0.631254	0.752841
34	C	4.728254	-0.518631	1.379495
35	C	5.533776	0.840476	-0.419845
36	H	2.704487	-1.188189	1.198489
37	H	4.889969	-1.003305	2.322019
38	H	6.316862	1.411810	-0.877691
39	H	6.698826	0.299072	1.281735
40	H	4.138948	1.221087	-1.985949

15c NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.347733	1.410545	1.172625
2	H	-2.254870	1.963309	1.313550
3	C	-1.215527	0.145022	1.720626
4	C	-0.203040	-0.654361	1.262550
5	H	-0.121719	-1.688701	1.513726
6	C	-0.414927	1.818207	0.231922
7	C	-1.065350	-0.758390	-0.919617
8	H	-0.313067	-1.502445	-1.082970
9	C	-0.902779	0.557145	-1.324019
10	H	-1.795208	1.099613	-1.564051
11	H	-0.035502	0.823944	-1.899219

12	N	0.987715	-0.100794	0.772126
13	C	1.015684	1.334359	0.453292
14	H	1.466963	1.886955	1.272620
15	H	1.616922	1.488371	-0.427130
16	C	2.017565	-0.933578	0.480228
17	O	1.985256	-2.143168	0.582742
18	O	3.098931	-0.257897	0.049634
19	C	4.282384	-1.031299	-0.290589
20	H	4.068227	-1.697038	-1.111929
21	H	4.606218	-1.608755	0.560594
22	C	-2.409310	-1.190802	-0.569775
23	O	-3.324105	-0.388458	-0.431795
24	C	-2.624266	-2.681551	-0.385630
25	H	-1.812645	-3.135031	0.169290
26	H	-2.666021	-3.157185	-1.361710
27	H	-3.562994	-2.852540	0.122134
28	H	5.023193	-0.301821	-0.567641
29	H	-2.010205	-0.295665	2.284570
30	C	-0.506880	3.199164	-0.389833
31	H	-0.014053	3.225298	-1.355614
32	H	-0.027640	3.938581	0.247297
33	H	-1.541214	3.488966	-0.528004

16c NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.418396	-0.213993	1.123374
2	H	-3.456432	-0.475945	1.207880
3	C	-1.468748	-0.892700	1.862230
4	C	-0.146430	-0.644431	1.596919
5	H	0.641810	-1.212634	2.041355
6	C	-1.997955	0.597995	0.076705
7	C	-1.380967	-0.858164	-1.181459
8	H	-2.353591	-1.273399	-1.361479
9	H	-1.061615	-0.140966	-1.915741
10	C	-0.391443	-1.690654	-0.662611
11	H	-0.641388	-2.661626	-0.289001
12	C	-0.687936	1.360456	0.258322
13	H	-0.875215	2.286190	0.792401
14	H	-0.246629	1.595705	-0.695066
15	N	0.267267	0.535772	1.020317
16	C	1.610844	0.794632	0.966328

17	O	2.462649	0.064596	1.428301
18	O	1.856893	1.977540	0.395441
19	C	3.206308	2.211378	-0.098854
20	H	3.919914	2.103900	0.701658
21	H	3.409497	1.498358	-0.881804
22	C	0.992759	-1.419190	-0.970709
23	O	1.368350	-0.328483	-1.411132
24	C	2.000552	-2.514367	-0.675423
25	H	2.416862	-2.331414	0.310694
26	H	2.811727	-2.453986	-1.390983
27	H	1.555753	-3.499651	-0.705738
28	H	3.196604	3.217894	-0.479703
29	H	-1.730043	-1.709733	2.501991
30	C	-3.021605	1.369213	-0.737589
31	H	-3.260442	2.312490	-0.253278
32	H	-3.938137	0.801745	-0.845479
33	H	-2.640820	1.593472	-1.727868

15d NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	1.164373	1.493415	-0.829974
2	H	2.045889	2.104131	-0.861198
3	C	1.207705	0.204450	-1.343747
4	C	0.175974	-0.631074	-1.002039
5	H	0.190056	-1.677363	-1.215948
6	C	0.080764	1.874398	-0.053238
7	C	0.677019	-0.594401	1.313847
8	H	-0.057342	-1.369180	1.392784
9	C	0.390307	0.728580	1.614080
10	H	1.208688	1.328956	1.958286
11	H	-0.564534	0.968845	2.044373
12	N	-1.106296	-0.139864	-0.714243
13	C	-1.269019	1.298508	-0.466435
14	H	-1.618467	1.793913	-1.368138
15	H	-2.006876	1.443817	0.304696
16	C	-2.113223	-1.029642	-0.534795
17	O	-1.990287	-2.237521	-0.570475
18	O	-3.287486	-0.415201	-0.298700
19	C	-4.455075	-1.256903	-0.093654
20	H	-4.296165	-1.916482	0.744725
21	H	-4.648081	-1.844641	-0.977178

22	C	2.072136	-0.971880	1.193257
23	O	2.963554	-0.129606	1.138444
24	C	2.379922	-2.456629	1.138001
25	H	1.715077	-2.973150	0.456205
26	H	2.241172	-2.886363	2.126028
27	H	3.407444	-2.601983	0.835525
28	H	-5.262989	-0.572711	0.098882
29	C	0.001914	3.285983	0.499451
30	H	-0.640631	3.327693	1.372037
31	H	-0.404907	3.965609	-0.245363
32	H	0.984618	3.641720	0.783222
33	C	2.467959	-0.338462	-1.986974
34	H	2.354219	-1.384127	-2.250379
35	H	3.301995	-0.240416	-1.303593
36	H	2.690594	0.207580	-2.897773

16d NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.307292	0.366205	0.585244
2	H	-3.374566	0.393980	0.457978
3	C	-1.711637	-0.760365	1.127008
4	C	-0.340665	-0.811681	1.096488
5	H	0.200762	-1.686576	1.383638
6	C	-1.521053	1.312180	-0.060245
7	C	-1.028479	0.209991	-1.684896
8	H	-2.017365	0.173289	-2.099137
9	H	-0.407657	0.992202	-2.082452
10	C	-0.390681	-0.990449	-1.383543
11	H	-0.933413	-1.911953	-1.393047
12	C	-0.133130	1.581428	0.510282
13	H	-0.206103	2.304410	1.316642
14	H	0.524791	1.974206	-0.245686
15	N	0.439805	0.326068	1.022796
16	C	1.790367	0.192076	1.190206
17	O	2.342367	-0.856342	1.458077
18	O	2.420636	1.365043	1.071468
19	C	3.847454	1.319151	0.776689
20	H	4.367578	0.772917	1.546428
21	H	3.979441	0.840548	-0.180423
22	C	1.050684	-1.052286	-1.424048
23	O	1.752155	-0.035773	-1.441126

24	C	1.704035	-2.420189	-1.391337
25	H	2.261312	-2.496068	-0.464976
26	H	2.409931	-2.497444	-2.209967
27	H	0.987335	-3.225962	-1.455680
28	H	4.162193	2.347729	0.747178
29	C	-2.522852	-1.987029	1.496166
30	H	-1.886850	-2.769675	1.892885
31	H	-3.051490	-2.386354	0.635236
32	H	-3.256585	-1.742390	2.257155
33	C	-2.166797	2.551848	-0.653621
34	H	-2.311787	3.308708	0.112961
35	H	-3.132028	2.317678	-1.086641
36	H	-1.540416	2.980878	-1.427700

15e NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.175991	-1.970135	-0.248593
2	H	-2.061492	-2.557661	-0.110406
3	C	-1.206504	-0.868322	-1.095064
4	C	-0.168586	0.021356	-0.984426
5	H	-0.177473	0.973580	-1.467903
6	C	-0.092298	-2.114184	0.601336
7	H	-0.069945	-2.946563	1.280205
8	C	-0.672729	0.610594	1.266917
9	H	0.063771	1.375800	1.133306
10	C	-0.389973	-0.581141	1.919177
11	H	-1.211529	-1.061293	2.411977
12	H	0.563020	-0.697063	2.402083
13	N	1.110273	-0.376950	-0.569058
14	C	1.267256	-1.697709	0.058956
15	H	1.615108	-2.413558	-0.678621
16	H	2.004469	-1.632500	0.840528
17	C	2.121596	0.523756	-0.639774
18	O	2.004803	1.673915	-1.011651
19	O	3.291459	-0.005502	-0.236718
20	C	4.464029	0.853807	-0.274891
21	H	4.307697	1.724895	0.341563
22	H	4.661394	1.165820	-1.288323
23	C	-2.065772	0.939899	1.040297
24	O	-2.957010	0.112177	1.208673
25	C	-2.372126	2.354202	0.583594
26	H	-1.707426	2.664993	-0.213294
27	H	-2.232933	3.036623	1.417207

28	H	-3.399466	2.412342	0.252493
29	H	5.267707	0.248028	0.105881
30	C	-2.460569	-0.507769	-1.865534
31	H	-2.337428	0.427167	-2.401135
32	H	-3.295637	-0.411018	-1.182882
33	H	-2.687694	-1.277585	-2.595919

16e NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	2.285400	-1.355454	-0.002885
2	H	3.300118	-1.594729	-0.261638
3	C	2.028111	-0.351775	0.917533
4	C	0.717893	0.033611	1.061842
5	H	0.437511	0.878790	1.652288
6	C	1.243910	-1.814384	-0.795667
7	H	1.454501	-2.565546	-1.535496
8	C	0.995750	-0.192588	-1.980826
9	H	1.939947	-0.267387	-2.483794
10	H	0.171613	-0.635269	-2.510614
11	C	0.719301	0.965974	-1.259173
12	H	1.491376	1.678837	-1.059499
13	C	-0.141995	-1.929499	-0.176976
14	H	-0.230565	-2.859109	0.373562
15	H	-0.912471	-1.896626	-0.926978
16	N	-0.339951	-0.795543	0.745242
17	C	-1.599303	-0.393899	1.099049
18	O	-1.838712	0.617602	1.726357
19	O	-2.524925	-1.277095	0.712052
20	C	-3.898512	-0.795751	0.628811
21	H	-4.221035	-0.425823	1.588656
22	H	-3.938088	-0.011012	-0.110357
23	C	-0.651360	1.383390	-1.091844
24	O	-1.601453	0.630449	-1.327292
25	C	-0.904284	2.789644	-0.583459
26	H	-0.007644	3.251553	-0.190265
27	H	-1.658772	2.738907	0.191045
28	H	-1.284769	3.399949	-1.397355
29	H	-4.478503	-1.649705	0.325058
30	C	3.146507	0.457593	1.544839
31	H	2.751764	1.223346	2.202475
32	H	3.756078	0.944250	0.788912

33 H 3.792559 -0.182699 2.136395

15f NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.516506	1.474092	0.537571
2	C	-1.174147	0.441432	1.405688
3	C	0.017414	-0.204525	1.220537
4	H	0.266760	-1.110133	1.728034
5	C	-0.567963	1.807918	-0.418340
6	H	-0.797867	2.586795	-1.122953
7	C	-0.570576	-1.029787	-0.935099
8	H	0.347419	-1.579105	-0.893246
9	C	-0.674552	0.167951	-1.632105
10	H	-1.642604	0.413173	-2.023780
11	H	0.151380	0.485231	-2.242511
12	N	1.119384	0.443485	0.656022
13	C	0.897859	1.733857	-0.016338
14	H	1.150012	2.543792	0.660246
15	H	1.544102	1.798360	-0.875085
16	C	2.309024	-0.209026	0.617747
17	O	2.496559	-1.337420	1.023947
18	O	3.274301	0.545357	0.061664
19	C	4.603255	-0.036755	-0.044345
20	H	4.571753	-0.926062	-0.654317
21	H	4.976700	-0.289832	0.935288
22	C	-1.793947	-1.706000	-0.551197
23	O	-2.887644	-1.150669	-0.582630
24	C	-1.657297	-3.145721	-0.088230
25	H	-1.056119	-3.197339	0.813792
26	H	-1.164114	-3.740600	-0.849032
27	H	-2.638678	-3.551129	0.111134
28	H	5.207241	0.726249	-0.503309
29	H	-1.917951	-0.016443	2.024024
30	C	-2.950227	1.938885	0.427895
31	H	-3.511828	1.182571	-0.107842
32	H	-3.022436	2.883827	-0.095664
33	H	-3.388705	2.057569	1.412435

16f NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.410205	-0.594439	-0.428655
2	C	-1.753684	0.048179	-1.469022
3	C	-0.384714	0.061574	-1.480790
4	H	0.171817	0.664873	-2.164448
5	C	-1.617474	-1.098684	0.600507
6	H	-2.109689	-1.618010	1.404380
7	C	-1.139988	0.591726	1.510178
8	H	-2.130728	0.849983	1.836992
9	H	-0.550659	0.089653	2.257334
10	C	-0.453729	1.516092	0.715609
11	H	-0.972852	2.333291	0.262364
12	C	-0.251567	-1.679066	0.255261
13	H	-0.347817	-2.699153	-0.098311
14	H	0.400781	-1.665850	1.109769
15	N	0.367732	-0.852904	-0.800501
16	C	1.734289	-0.814428	-0.953114
17	O	2.304822	-0.039048	-1.691047
18	O	2.334488	-1.775772	-0.249993
19	C	3.740386	-1.568041	0.082808
20	H	4.318935	-1.444881	-0.818289
21	H	3.806480	-0.688616	0.702244
22	C	0.974482	1.535459	0.735078
23	O	1.646857	0.609683	1.217984
24	C	1.682529	2.711948	0.089486
25	H	0.997030	3.474013	-0.253214
26	H	2.259895	2.332411	-0.745793
27	H	2.376038	3.144315	0.802343
28	H	4.036039	-2.452886	0.619334
29	H	-2.285061	0.665717	-2.163676
30	C	-3.902532	-0.445284	-0.255095
31	H	-4.124215	0.475214	0.282580
32	H	-4.320099	-1.272505	0.305258
33	H	-4.397584	-0.394563	-1.217562

15g NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.549508	-0.831482	-0.052261
2	C	-1.044898	-0.070983	-1.102249

3	C	0.290835	0.224118	-1.117124
4	H	0.714389	0.941286	-1.784850
5	C	-0.619769	-1.289667	0.870826
6	H	-0.967196	-1.864946	1.710179
7	C	0.214090	1.464941	0.905383
8	H	1.235303	1.715323	0.705150
9	C	-0.132395	0.460741	1.801742
10	H	-1.079260	0.565000	2.294044
11	H	0.639300	0.008380	2.397744
12	N	1.234529	-0.632486	-0.541934
13	C	0.752495	-1.696333	0.353083
14	H	0.691261	-2.631351	-0.194213
15	H	1.454642	-1.823138	1.159479
16	C	2.551900	-0.351995	-0.705397
17	O	2.989159	0.608191	-1.305865
18	O	3.335656	-1.269188	-0.109356
19	C	4.775071	-1.086242	-0.208510
20	H	5.061651	-0.144802	0.233677
21	H	5.080199	-1.101199	-1.242887
22	C	-0.817682	2.394909	0.492745
23	O	-2.007428	2.187642	0.709534
24	C	-0.352552	3.650238	-0.223479
25	H	0.391395	3.421211	-0.977444
26	H	0.102233	4.324695	0.496940
27	H	-1.200792	4.143751	-0.676191
28	H	5.200484	-1.913637	0.332160
29	H	-1.702750	0.496090	-1.727478
30	C	-3.039181	-0.895523	0.208682
31	H	-3.435685	0.110668	0.188849
32	H	-3.212071	-1.297564	1.200927
33	C	-3.755532	-1.789513	-0.831115
34	H	-3.369330	-2.801911	-0.793591
35	H	-3.607232	-1.405627	-1.833866
36	H	-4.821327	-1.819595	-0.633334

16g NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.002403	-0.668693	-0.113302
2	C	-1.465388	0.018554	-1.195829
3	C	-0.106036	0.061280	-1.345971
4	H	0.364010	0.694541	-2.066554

5	C	-1.096951	-1.182532	0.811988
6	H	-1.493432	-1.731516	1.649317
7	C	-0.564092	0.505910	1.732504
8	H	-1.525446	0.718426	2.162446
9	H	0.108927	-0.010837	2.393654
10	C	0.012826	1.471194	0.906283
11	H	-0.571221	2.282682	0.528108
12	C	0.242385	-1.715027	0.321137
13	H	0.139126	-2.727134	-0.053743
14	H	0.974081	-1.708839	1.108835
15	N	0.734393	-0.843332	-0.764082
16	C	2.078068	-0.761401	-1.046997
17	O	2.553708	0.046438	-1.816617
18	O	2.769248	-1.719904	-0.428879
19	C	4.196974	-1.483453	-0.239246
20	H	4.679913	-1.357393	-1.194402
21	H	4.309568	-0.598628	0.365758
22	C	1.434304	1.527060	0.774274
23	O	2.176301	0.608062	1.157563
24	C	2.041516	2.738727	0.092074
25	H	1.302825	3.480633	-0.174675
26	H	2.556608	2.395183	-0.796993
27	H	2.778118	3.184726	0.750577
28	H	4.561425	-2.358425	0.270171
29	H	-2.066568	0.638917	-1.823974
30	C	-3.479925	-0.643670	0.235429
31	H	-3.587152	-0.204762	1.224997
32	H	-3.823662	-1.670822	0.313102
33	C	-4.383818	0.114445	-0.753571
34	H	-5.416826	0.042259	-0.433684
35	H	-4.310541	-0.307178	-1.749127
36	H	-4.120867	1.164510	-0.800569

15h NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.221734	-1.959986	-1.028244
2	H	-2.086062	-2.583967	-1.111915
3	C	-1.239611	-0.672463	-1.531039
4	C	-0.289259	0.246304	-1.142669

5	C	-0.147567	-2.296347	-0.215194
6	C	-0.997915	-0.003028	1.220911
7	H	-0.378654	0.856101	1.368197
8	C	-0.541287	-1.301483	1.456091
9	H	-1.281941	-2.002077	1.788815
10	H	0.427673	-1.429480	1.905681
11	N	0.980422	-0.200303	-0.718495
12	C	1.175689	-1.664659	-0.624550
13	H	1.493078	-2.045043	-1.589227
14	H	1.948485	-1.860685	0.093694
15	C	1.909901	0.643211	-0.187062
16	O	1.754936	1.814708	0.089876
17	O	3.080982	0.010962	0.033979
18	C	4.162916	0.790193	0.614805
19	H	3.872590	1.168246	1.582422
20	H	4.411789	1.617764	-0.030187
21	C	-2.410314	0.150429	1.000928
22	O	-3.134749	-0.829784	0.822392
23	C	-2.987213	1.555109	0.996133
24	H	-2.240155	2.307178	0.786802
25	H	-3.410523	1.758661	1.975848
26	H	-3.790418	1.615247	0.272902
27	H	4.986674	0.103002	0.698211
28	H	-2.106945	-0.305239	-2.037221
29	H	-0.072232	-3.298950	0.164001
30	C	-0.444334	1.691409	-1.572064
31	H	-0.251145	2.376108	-0.767200
32	H	-1.442608	1.840675	-1.955608
33	H	0.269531	1.908183	-2.361012

16h NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.661308	1.059221	0.496074
2	H	-3.717836	1.206665	0.378759
3	C	-2.194781	0.035506	1.287005
4	C	-0.841194	-0.252857	1.350578
5	C	-1.761403	1.726065	-0.328770
6	C	-1.586923	0.460864	-1.779167
7	H	-2.593480	0.501603	-2.153845
8	H	-0.905011	1.092918	-2.322978
9	C	-1.080604	-0.804242	-1.430085

10	H	-1.740181	-1.636624	-1.305724
11	C	-0.346698	1.887780	0.200599
12	H	-0.288048	2.726341	0.884154
13	H	0.345475	2.040373	-0.603205
14	N	0.087441	0.655731	0.926304
15	C	1.450784	0.399495	0.957222
16	O	1.965251	-0.634539	1.317228
17	O	2.147256	1.487764	0.613656
18	C	3.502977	1.267410	0.119389
19	H	4.099936	0.790676	0.879376
20	H	3.437212	0.648680	-0.760065
21	C	0.316519	-1.024173	-1.467483
22	O	1.146868	-0.094660	-1.544059
23	C	0.823161	-2.453752	-1.385183
24	H	0.031883	-3.165916	-1.198754
25	H	1.566513	-2.507057	-0.598976
26	H	1.314159	-2.707690	-2.318970
27	H	3.878859	2.248456	-0.113594
28	H	-2.871500	-0.628101	1.780548
29	H	-2.113179	2.588158	-0.867836
30	C	-0.429974	-1.501730	2.103618
31	H	0.175677	-2.148748	1.494325
32	H	-1.320370	-2.022930	2.419977
33	H	0.162516	-1.240689	2.969882

Coordinates of the optimized MVK/Diels-Alder cycloaddition transition states at the B3LYP/6-31G* theory level

15a NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.270141	-1.900636	-0.943511
2	H	-2.167913	-2.501318	-1.034785
3	C	-1.116210	-0.736972	-1.711201
4	C	-0.083105	0.128579	-1.424997
5	H	0.005784	1.113246	-1.865549
6	C	-0.372836	-2.087595	0.125440
7	H	-0.420317	-3.031322	0.665835
8	C	-1.281493	0.426107	1.120107
9	H	-0.554268	1.225986	1.219072
10	C	-1.000954	-0.885515	1.547753
11	H	-1.877398	-1.474892	1.803777

12	H	-0.150959	-1.026193	2.214815
13	N	1.036243	-0.267000	-0.711328
14	C	1.055741	-1.616091	-0.112387
15	H	1.587337	-2.304843	-0.786942
16	H	1.618845	-1.572762	0.820926
17	C	2.079589	0.632894	-0.567410
18	O	2.075621	1.770423	-0.999850
19	O	3.108089	0.072955	0.109766
20	C	4.234515	0.943233	0.307741
21	H	3.937269	1.835239	0.864571
22	H	4.657810	1.245901	-0.653344
23	C	-2.584202	0.694379	0.556049
24	O	-3.388302	-0.229480	0.351449
25	C	-2.961287	2.130097	0.212506
26	H	-3.586336	2.141705	-0.685378
27	H	-2.087619	2.773487	0.064042
28	H	-3.558209	2.553942	1.030871
29	H	4.955199	0.355885	0.877239
30	H	-1.890494	-0.409440	-2.395278

16a XCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-2.641227	-1.169379	-0.580413
2	C	-2.019228	-0.553272	-1.669814
3	C	-0.651298	-0.337226	-1.631126
4	H	-0.124683	0.245672	-2.376425
5	C	-1.869524	-1.397647	0.571138
6	H	-2.329502	-1.950958	1.388102
7	C	-1.805078	0.389666	1.440766
8	H	-2.859224	0.460825	1.697085
9	H	-1.173316	0.037784	2.255824
10	C	-1.261288	1.432010	0.666870
11	H	-1.919673	2.096428	0.115299
12	C	-0.407828	-1.768842	0.362174
13	H	-0.314541	-2.837849	0.118137
14	H	0.182435	-1.574202	1.257106
15	N	0.169519	-0.971383	-0.743206
16	C	1.545245	-0.722090	-0.826142
17	O	2.046536	0.025404	-1.643171
18	O	2.215851	-1.475336	0.058957
19	C	3.587952	-1.088805	0.244290
20	H	4.135944	-1.147506	-0.698938

21	H	3.623109	-0.069098	0.635512
22	C	0.152468	1.714963	0.677219
23	O	0.975842	0.945409	1.206367
24	C	0.653082	2.986442	0.004235
25	H	-0.146528	3.571228	-0.460869
26	H	1.396481	2.720100	-0.754801
27	H	1.159724	3.611851	0.748746
28	H	3.990967	-1.795238	0.970609
29	H	-2.587375	-0.134419	-2.493154
30	H	-3.724843	-1.244533	-0.540375

15e NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.164463	-1.937945	-0.283481
2	H	-2.068403	-2.530423	-0.178499
3	C	-1.131552	-0.879977	-1.210899
4	C	-0.040503	-0.033314	-1.171835
5	H	0.005773	0.883732	-1.745642
6	C	-0.144188	-2.015942	0.680258
7	H	-0.132527	-2.892436	1.326087
8	C	-0.826298	0.623932	1.494047
9	H	-0.026511	1.356045	1.433190
10	C	-0.602045	-0.660422	2.022550
11	H	-1.490404	-1.158367	2.402278
12	H	0.287244	-0.799733	2.637549
13	N	1.163486	-0.369919	-0.571561
14	C	1.247903	-1.609955	0.222027
15	H	1.701180	-2.403657	-0.391653
16	H	1.910856	-1.439674	1.072290
17	C	2.235437	0.494017	-0.716932
18	O	2.198787	1.548341	-1.324117
19	O	3.334416	0.003142	-0.098165
20	C	4.501235	0.834600	-0.205365
21	H	4.296403	1.837377	0.176815
22	H	4.824016	0.908061	-1.247162
23	C	-2.152577	0.976087	1.043128
24	O	-3.066901	0.134801	1.014972
25	C	-2.415705	2.415509	0.616369
26	H	-1.539669	2.877661	0.147576
27	H	-2.676238	3.017515	1.497686
28	H	-3.265184	2.447179	-0.071481

29	H	5.263542	0.340117	0.397258
30	C	-2.323829	-0.551159	-2.075239
31	H	-2.119769	0.296105	-2.738202
32	H	-3.188093	-0.305078	-1.447588
33	H	-2.595420	-1.406220	-2.706258

16e NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	2.322298	-1.248205	-0.278940
2	H	3.356013	-1.365366	-0.598313
3	C	2.038214	-0.551094	0.903759
4	C	0.703457	-0.300611	1.190086
5	H	0.397209	0.334680	2.012345
6	C	1.276930	-1.495482	-1.182935
7	H	1.503102	-2.095741	-2.062551
8	C	1.021179	0.256104	-2.091662
9	H	1.974723	0.287964	-2.612873
10	H	0.194657	-0.110187	-2.700023
11	C	0.712660	1.339933	-1.249017
12	H	1.502188	2.005904	-0.913023
13	C	-0.090395	-1.810181	-0.594218
14	H	-0.146149	-2.867317	-0.293557
15	H	-0.884418	-1.620955	-1.316354
16	N	-0.335924	-0.957179	0.587662
17	C	-1.631962	-0.660117	1.019640
18	O	-1.884572	0.143448	1.897118
19	O	-2.529946	-1.434918	0.389680
20	C	-3.893928	-1.013540	0.556822
21	H	-4.164357	-0.990123	1.615028
22	H	-4.018387	-0.021270	0.116038
23	C	-0.652374	1.664193	-0.912956
24	O	-1.598095	0.904400	-1.191246
25	C	-0.939259	2.965374	-0.174749
26	H	-0.037939	3.551858	0.030381
27	H	-1.443542	2.732807	0.769578
28	H	-1.629810	3.573124	-0.771251
29	H	-4.492210	-1.751283	0.020900
30	C	3.125585	0.022925	1.782432
31	H	2.705304	0.632687	2.588810
32	H	3.821359	0.652319	1.213710
33	H	3.718388	-0.774148	2.249680

15h NCC_k

Standard Nuclear Orientation (Angstroms)				
I	Atom	X	Y	Z

1	C	-1.265486	-1.885406	-1.021884
2	H	-2.158044	-2.492747	-1.105997
3	C	-1.223529	-0.607964	-1.600675
4	C	-0.206671	0.292518	-1.329044
5	C	-0.200669	-2.234478	-0.173198
6	C	-1.063653	-0.105629	1.506996
7	H	-0.402776	0.742612	1.657893
8	C	-0.590136	-1.432394	1.560896
9	H	-1.344785	-2.167721	1.828119
10	H	0.382564	-1.600051	2.023504
11	N	0.997636	-0.171516	-0.774064
12	C	1.134562	-1.634479	-0.582629
13	H	1.489014	-2.084626	-1.522751
14	H	1.896506	-1.808394	0.173717
15	C	1.970929	0.693162	-0.293622
16	O	1.862538	1.899175	-0.174109
17	O	3.098465	0.013676	0.035032
18	C	4.145342	0.828133	0.586067
19	H	3.798535	1.347696	1.483098
20	H	4.483991	1.566120	-0.145869
21	C	-2.440580	0.096104	1.152525
22	O	-3.152406	-0.870275	0.815129
23	C	-3.027646	1.501943	1.173338
24	H	-2.260739	2.283810	1.165386
25	H	-3.632467	1.629895	2.080788
26	H	-3.698120	1.634670	0.318219
27	H	4.949740	0.133155	0.830420
28	H	-2.079974	-0.236898	-2.152424
29	H	-0.124305	-3.273812	0.141588
30	C	-0.313589	1.712972	-1.816222
31	H	-0.333549	2.429803	-0.993664
32	H	-1.231392	1.815217	-2.400997
33	H	0.540693	1.985730	-2.445563

16h NCC_k

Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z

1	C	-2.666228	1.038277	0.532353
2	H	-3.741813	1.153665	0.424617
3	C	-2.152454	0.023208	1.337699
4	C	-0.784363	-0.246286	1.405442
5	C	-1.782410	1.696042	-0.330994
6	C	-1.634692	0.482830	-1.887104
7	H	-2.657995	0.575257	-2.243473
8	H	-0.927876	1.135837	-2.398886
9	C	-1.163070	-0.814787	-1.613975
10	H	-1.869483	-1.627747	-1.472511
11	C	-0.363810	1.871214	0.175284
12	H	-0.308479	2.730963	0.859942
13	H	0.322210	2.054588	-0.648752
14	N	0.124607	0.661133	0.895884
15	C	1.511554	0.448966	0.949800
16	O	2.061553	-0.547842	1.372697
17	O	2.163869	1.549860	0.530303
18	C	3.568577	1.350313	0.302323
19	H	4.071040	1.051982	1.225214
20	H	3.706862	0.582387	-0.462149
21	C	0.243909	-1.110149	-1.601390
22	O	1.113111	-0.218107	-1.652948
23	C	0.687487	-2.565832	-1.513735
24	H	-0.144734	-3.264191	-1.380204
25	H	1.394765	-2.675966	-0.684167
26	H	1.225903	-2.835528	-2.430347
27	H	3.942318	2.313301	-0.046327
28	H	-2.816519	-0.650273	1.868138
29	H	-2.146045	2.573490	-0.863244
30	C	-0.330468	-1.453195	2.185218
31	H	0.262757	-2.136081	1.575572
32	H	-1.213527	-1.977712	2.559185
33	H	0.303446	-1.169618	3.030536