Supporting Information (I)

Intramolecular 1,3-Dipolar Ene Reactions of Nitrile Oxides Occur By Stepwise 1,1-Cycloaddition/Retro-Ene Mechanisms

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I. The B3LYP/6-31G* optimized structures for reaction (2)

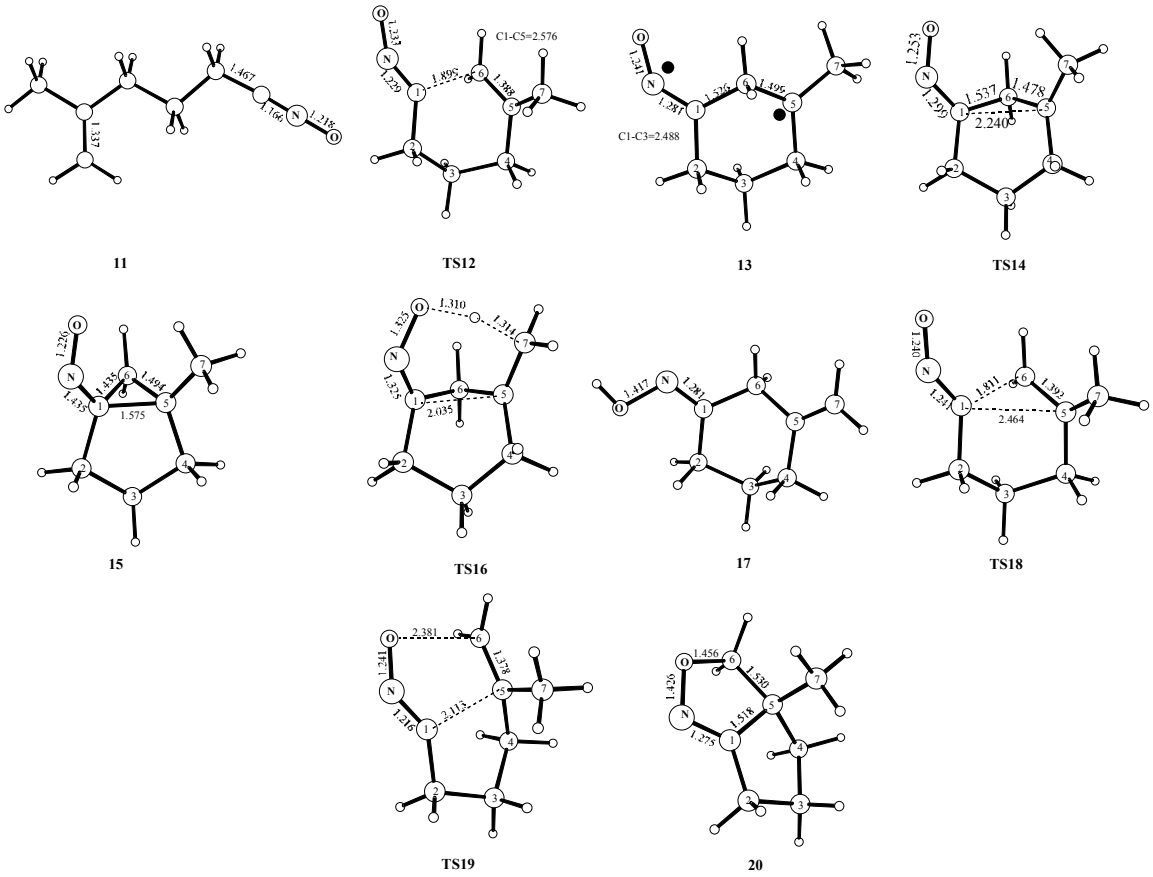
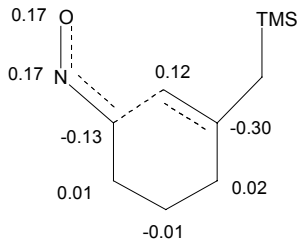


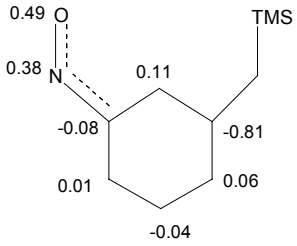
Figure S1. The B3LYP/6-31G* optimized structures for reaction (2)

II. The spin distributions and <S^2> values for all diradical species discussed in the text.



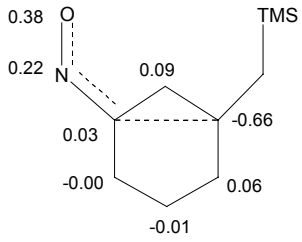
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TS2



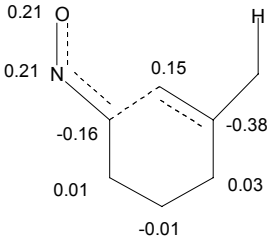
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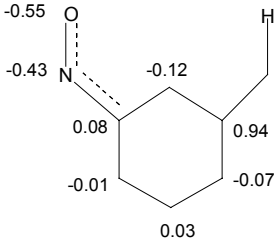
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TS4



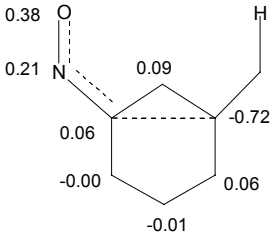
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TS12



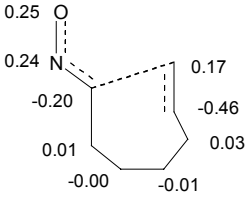
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13



<S^2>=0.69

TS14



<S^2>=0.27

TS24

Figure S2. The spin distributions and <S^2> values for all diradical species discussed in the text.

III. The B3LYP/6-31G* optimized geometries for all species discussed in the text.

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.560650	1.036510	-0.586390
2	6	0	-1.935872	0.638610	-1.076379
3	6	0	0.535606	0.024738	-0.868234
4	14	0	-3.032872	-0.296601	0.190819
5	6	0	-4.612427	-0.834890	-0.708182
6	1	0	-5.300569	-1.349470	-0.026392
7	1	0	-4.391262	-1.521940	-1.534103
8	1	0	-5.147746	0.025529	-1.127654
9	6	0	-3.467577	0.865226	1.619116
10	1	0	-4.063344	0.347668	2.380762
11	1	0	-2.563401	1.248461	2.105447
12	1	0	-4.050726	1.727803	1.274149
13	6	0	-2.148391	-1.827221	0.876204
14	1	0	-2.804596	-2.372148	1.566136
15	1	0	-1.858314	-2.525455	0.081627
16	1	0	-1.243993	-1.555841	1.433382
17	1	0	-1.854420	0.018671	-1.980720
18	1	0	-2.502951	1.532698	-1.368534
19	6	0	-0.339830	2.197001	0.045585
20	1	0	0.636931	2.486106	0.419733
21	1	0	-1.143701	2.910884	0.206973
22	6	0	1.920321	0.332034	-0.291857
23	1	0	0.205565	-0.960850	-0.507115
24	1	0	0.616686	-0.088406	-1.961523
25	1	0	1.863073	0.429775	0.798299
26	6	0	2.935756	-0.775952	-0.647334
27	6	0	4.278163	-0.518356	-0.115087
28	1	0	2.582519	-1.742785	-0.263725
29	1	0	3.002328	-0.883914	-1.738545
30	7	0	5.319800	-0.252654	0.336290
31	8	0	6.414957	0.009886	0.801205
32	1	0	2.289288	1.288918	-0.677986

TS2 (diradical addition)

Standard orientation:

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

1	6	0	-2.775503	-0.220395	-0.114443
2	6	0	-1.190422	-0.390047	0.928035
3	6	0	-0.292245	0.370203	0.188867
4	6	0	-0.548366	1.861232	0.110592
5	6	0	-2.063232	2.179823	0.194248
6	6	0	-2.931002	1.190543	-0.606931
7	7	0	-3.451043	-1.239701	-0.241576
8	8	0	-3.544566	-2.454105	-0.028479
9	1	0	-3.985190	1.482717	-0.542229
10	1	0	-2.653181	1.245816	-1.670544
11	1	0	-2.391970	2.175436	1.240422
12	1	0	-2.238936	3.194303	-0.180489
13	1	0	-0.146180	2.243841	-0.836786
14	1	0	-0.019630	2.413822	0.902560
15	1	0	-1.066695	-1.470726	0.982185
16	1	0	-1.633950	0.046036	1.823209
17	6	0	0.704814	-0.251527	-0.729569
18	1	0	0.456094	-1.305759	-0.912897
19	1	0	0.719874	0.253405	-1.707449
20	14	0	2.515813	-0.246268	-0.065514
21	6	0	3.097605	1.524857	0.269226
22	6	0	2.595459	-1.265561	1.525455
23	6	0	3.605604	-1.029809	-1.402024
24	1	0	4.653168	-1.075614	-1.080019
25	1	0	3.286232	-2.053424	-1.631499
26	1	0	3.572437	-0.454916	-2.335381
27	1	0	2.514158	2.004329	1.063768
28	1	0	4.148025	1.531351	0.585446
29	1	0	3.021721	2.153530	-0.626187
30	1	0	1.920850	-0.864320	2.290473
31	1	0	2.309883	-2.309255	1.347271
32	1	0	3.609459	-1.267986	1.943466

3 (diradical intermediate)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.086417	2.056077	-0.540950
2	6	0	3.151411	1.120864	0.069227
3	6	0	2.636471	-0.292426	0.177172
4	6	0	1.255327	-0.472595	0.842606
5	6	0	0.306343	0.451681	0.163558
6	6	0	0.719498	1.896726	0.178666
7	7	0	3.311670	-1.290514	-0.255730
8	8	0	3.095855	-2.513028	-0.316178
9	6	0	-0.711821	-0.048512	-0.801512
10	1	0	2.425459	3.097918	-0.479330
11	1	0	1.961255	1.816316	-1.604756
12	1	0	4.073766	1.138925	-0.518778
13	1	0	3.403052	1.488523	1.077490
14	1	0	0.833821	2.256622	1.214602
15	1	0	-0.031545	2.534233	-0.301548
16	1	0	1.376440	-0.209085	1.906998

17	1	0	0.962089	-1.524262	0.777834
18	1	0	-0.450488	-1.049605	-1.173338
19	14	0	-2.483487	-0.190721	-0.050065
20	1	0	-0.791510	0.609254	-1.680520
21	6	0	-3.646872	-0.806034	-1.413628
22	6	0	-2.460543	-1.424100	1.385047
23	6	0	-3.058339	1.505600	0.564844
24	1	0	-4.674603	-0.903552	-1.042719
25	1	0	-3.667835	-0.115382	-2.265315
26	1	0	-3.337943	-1.788224	-1.791103
27	1	0	-3.458957	-1.531456	1.826405
28	1	0	-2.137874	-2.419195	1.055654
29	1	0	-1.780615	-1.101080	2.181966
30	1	0	-4.062092	1.442447	1.002739
31	1	0	-2.387550	1.904210	1.334817
32	1	0	-3.101929	2.237630	-0.250832

TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.431800	0.450089	0.060568
2	6	0	-2.529978	-0.415446	0.131235
3	6	0	-1.280343	-0.286166	1.021640
4	6	0	-3.231542	0.862965	-0.273556
5	6	0	-2.352885	2.079090	0.085829
6	6	0	-0.875569	1.843784	-0.305197
7	6	0	0.602490	-0.257100	-0.736358
8	7	0	-2.913551	-1.571833	-0.312766
9	8	0	-2.325463	-2.675257	-0.210888
10	1	0	-1.511386	0.263959	1.942754
11	1	0	-0.909024	-1.283306	1.265976
12	1	0	0.386012	-1.332891	-0.778761
13	1	0	0.637150	0.111991	-1.772126
14	14	0	2.392683	-0.094869	-0.029361
15	1	0	-0.245380	2.610938	0.175353
16	1	0	-0.741853	1.991848	-1.387220
17	1	0	-2.735406	2.982816	-0.400513
18	1	0	-2.414760	2.263067	1.165139
19	1	0	-3.443894	0.845264	-1.350481
20	1	0	-4.202613	0.955460	0.231914
21	6	0	3.538808	-1.092519	-1.159488
22	6	0	2.921570	1.723916	-0.027368
23	6	0	2.445636	-0.789011	1.729756
24	1	0	4.578236	-1.039321	-0.813048
25	1	0	3.252735	-2.150682	-1.185786
26	1	0	3.514609	-0.716783	-2.189454
27	1	0	3.457632	-0.719749	2.147031
28	1	0	1.773640	-0.241088	2.400646
29	1	0	2.150615	-1.844907	1.753600
30	1	0	3.955751	1.828195	0.323184
31	1	0	2.870418	2.157796	-1.033345

32	1	0	2.290187	2.332824	0.630291

5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.235124	0.251683	1.285308
2	6	0	2.143055	0.457607	0.091023
3	6	0	0.722292	-0.266910	-0.017283
4	6	0	1.059377	-1.714982	-0.376686
5	6	0	2.540484	-1.939384	-0.007954
6	6	0	3.223798	-0.567537	-0.198420
7	1	0	3.564883	-0.427926	-1.231348
8	1	0	4.099322	-0.451526	0.451993
9	1	0	2.624760	-2.259063	1.037000
10	1	0	3.003319	-2.724890	-0.613429
11	1	0	0.905964	-1.846563	-1.455628
12	1	0	0.397826	-2.428739	0.129174
13	6	0	-0.458781	0.391917	-0.691028
14	1	0	-0.438608	0.168118	-1.767944
15	14	0	-2.205355	-0.037879	-0.029886
16	6	0	-2.357430	0.447004	1.794245
17	6	0	-3.434935	0.965216	-1.065034
18	6	0	-2.598120	-1.882794	-0.223917
19	1	0	-1.976174	-2.509067	0.426068
20	1	0	-2.449872	-2.224213	-1.255549
21	1	0	-3.644976	-2.080426	0.038651
22	1	0	-3.377427	0.698275	-2.127321
23	1	0	-4.466209	0.787476	-0.736319
24	1	0	-3.242979	2.041831	-0.984439
25	1	0	-3.372015	0.255284	2.164974
26	1	0	-1.663704	-0.121509	2.424432
27	1	0	-2.147352	1.512435	1.946862
28	1	0	0.779470	1.167636	1.651469
29	1	0	1.580595	-0.433992	2.056462
30	1	0	-0.367995	1.483345	-0.602996
31	7	0	2.319820	1.735748	-0.513114
32	8	0	1.547276	2.615333	-0.135429

cis-**TS6**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.170894	-1.048232	-0.660500
2	6	0	0.417815	0.236385	-0.705859
3	8	0	-0.448101	-2.168141	-0.346245
4	6	0	-0.738847	0.668428	-0.018003
5	6	0	-2.099903	-0.822389	0.314411

6	7	0	-1.729014	-1.835372	-0.450767
7	6	0	-1.158648	-0.052713	1.223330
8	6	0	-3.425728	-0.161056	0.038077
9	6	0	-3.174473	1.369740	-0.075609
10	6	0	-1.748963	1.635493	-0.607388
11	1	0	-0.384450	-0.680487	1.656951
12	1	0	-1.679296	0.535944	1.981107
13	1	0	-1.445958	2.664536	-0.361950
14	1	0	-1.710611	1.560283	-1.701331
15	1	0	-3.834047	-0.576855	-0.887974
16	1	0	-4.151010	-0.355141	0.839823
17	1	0	-3.282032	1.830377	0.913144
18	1	0	-3.921665	1.848463	-0.717172
19	1	0	0.455155	0.602894	-1.740408
20	14	0	2.191424	0.170541	0.003749
21	6	0	2.275813	-0.545574	1.751605
22	6	0	2.892462	1.932020	0.003536
23	1	0	3.939721	1.938695	0.331093
24	1	0	2.857351	2.377446	-0.997882
25	1	0	2.329425	2.587671	0.678679
26	1	0	1.755461	0.078134	2.487286
27	1	0	1.847798	-1.553308	1.791880
28	1	0	3.324027	-0.617345	2.068021
29	6	0	3.186138	-0.917809	-1.178619
30	1	0	3.154685	-0.531486	-2.204560
31	1	0	4.239699	-0.972226	-0.878641
32	1	0	2.788835	-1.939341	-1.197609

trans-**TS6**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.042275	1.483049	-0.241084
2	6	0	0.496950	0.405179	-0.793084
3	8	0	-0.881178	2.390152	0.103533
4	6	0	-0.731977	-0.316706	-0.810976
5	6	0	-2.289789	0.665868	-0.001485
6	7	0	-1.767082	1.643461	0.732163
7	6	0	-1.910480	0.361145	-1.436459
8	6	0	-3.071811	-0.409424	0.708813
9	6	0	-2.494505	-1.779804	0.257088
10	6	0	-0.998549	-1.619304	-0.082508
11	1	0	-1.645176	1.247458	-2.011724
12	1	0	-2.640163	-0.265627	-1.952627
13	1	0	-0.662941	-2.454742	-0.714987
14	1	0	-0.384368	-1.658582	0.824078
15	1	0	-2.966238	-0.258207	1.787341
16	1	0	-4.141692	-0.358919	0.466529
17	1	0	-3.032404	-2.128311	-0.631822
18	1	0	-2.640526	-2.547468	1.023963
19	1	0	0.672475	0.918649	-1.749096
20	14	0	2.114573	-0.112485	0.060388
21	6	0	2.721925	-1.798818	-0.562352

22	6	0	1.907977	-0.153266	1.943181
23	1	0	2.882258	-0.280009	2.431618
24	1	0	1.470362	0.782708	2.309142
25	1	0	1.265760	-0.973309	2.285124
26	1	0	2.029776	-2.608206	-0.301828
27	1	0	2.839151	-1.800859	-1.652759
28	1	0	3.697112	-2.048474	-0.125689
29	6	0	3.382901	1.214804	-0.399081
30	1	0	3.063713	2.205669	-0.054907
31	1	0	4.358435	1.003886	0.055426
32	1	0	3.531317	1.272586	-1.484367

7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.841306	0.255382	0.641632
2	6	0	2.274862	0.483106	0.221709
3	6	0	3.193632	-0.714326	0.139113
4	6	0	2.416443	-2.031283	0.297165
5	6	0	1.131528	-1.998013	-0.544988
6	6	0	0.176268	-0.889558	-0.112847
7	7	0	2.613276	1.689820	-0.042551
8	8	0	3.984068	1.768091	-0.391432
9	6	0	-1.142672	-0.957628	-0.367739
10	14	0	-2.595053	0.191015	-0.024525
11	6	0	-2.153999	2.026535	0.162985
12	6	0	-3.494511	-0.381563	1.546181
13	6	0	-3.772160	0.012157	-1.500990
14	1	0	3.989211	-0.620017	0.890503
15	1	0	3.705578	-0.684052	-0.831793
16	1	0	2.161963	-2.199573	1.352155
17	1	0	3.048401	-2.873069	-0.007815
18	1	0	0.617051	-2.965309	-0.517318
19	1	0	1.416391	-1.831597	-1.596394
20	1	0	0.846401	-0.005759	1.714151
21	1	0	0.285664	1.188721	0.549664
22	1	0	-1.459002	-1.877816	-0.874246
23	1	0	-3.076551	2.621130	0.151491
24	1	0	-1.639628	2.248565	1.104541
25	1	0	-1.523034	2.385555	-0.658293
26	1	0	-4.065095	-1.033321	-1.657555
27	1	0	-4.690562	0.592393	-1.348632
28	1	0	-3.305999	0.366180	-2.428372
29	1	0	-4.394282	0.220644	1.724853
30	1	0	-3.806547	-1.430030	1.470426
31	1	0	-2.852666	-0.291238	2.430649
32	1	0	4.083773	2.712060	-0.588678

TS8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.728335	-0.248108	-0.099386
2	6	0	-1.211515	-0.355938	0.962075
3	6	0	-0.323494	0.391787	0.195881
4	6	0	-0.589443	1.878098	0.090973
5	6	0	-2.110075	2.177917	0.169038
6	6	0	-2.960512	1.150094	-0.600959
7	7	0	-3.338706	-1.311946	-0.254946
8	8	0	-3.283178	-2.531605	-0.032486
9	1	0	-4.023086	1.400562	-0.504288
10	1	0	-2.719139	1.210818	-1.673133
11	1	0	-2.433894	2.195761	1.216446
12	1	0	-2.302095	3.179256	-0.231562
13	1	0	-0.188211	2.248593	-0.861228
14	1	0	-0.069129	2.447139	0.876603
15	1	0	-1.078101	-1.434505	1.045184
16	1	0	-1.645129	0.103559	1.850763
17	6	0	0.663237	-0.244445	-0.718333
18	1	0	0.417312	-1.302553	-0.879105
19	1	0	0.673902	0.244110	-1.704192
20	14	0	2.480516	-0.223720	-0.064124
21	6	0	3.055256	1.553699	0.246148
22	6	0	2.572765	-1.224668	1.537173
23	6	0	3.560526	-1.018428	-1.401192
24	1	0	4.610961	-1.056595	-1.087668
25	1	0	3.242816	-2.045724	-1.615724
26	1	0	3.516994	-0.454401	-2.340678
27	1	0	2.472488	2.040734	1.036558
28	1	0	4.106533	1.567994	0.559252
29	1	0	2.974693	2.170865	-0.656795
30	1	0	1.905392	-0.814651	2.303875
31	1	0	2.285804	-2.270299	1.373552
32	1	0	3.590562	-1.222162	1.945862

TS9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.478279	-0.000536	0.580717
2	6	0	0.667139	-0.127781	-0.474667
3	6	0	0.870850	-1.326515	-1.130263
4	8	0	2.638890	-2.241342	0.157555
5	7	0	2.946343	-1.124041	0.608156
6	6	0	2.801663	1.445140	0.645422
7	6	0	1.669226	2.179774	-0.122630
8	6	0	1.030301	1.207326	-1.134731
9	1	0	0.345054	-2.229481	-0.845625
10	1	0	1.473219	-1.381524	-2.032003

11	1	0	0.139445	1.673491	-1.573636
12	1	0	1.730135	1.017761	-1.958513
13	1	0	0.911100	2.524721	0.588485
14	1	0	2.058798	3.072659	-0.622603
15	1	0	2.878498	1.803516	1.678762
16	1	0	3.773094	1.620541	0.165924
17	6	0	-0.373164	-0.089185	0.646826
18	1	0	-0.244494	-0.981440	1.274424
19	1	0	-0.194380	0.760946	1.317855
20	14	0	-2.225125	-0.050787	0.151871
21	6	0	-2.711329	-1.663105	-0.714361
22	6	0	-3.214154	0.128329	1.760683
23	6	0	-2.638920	1.410613	-0.985528
24	1	0	-2.165435	1.312523	-1.969321
25	1	0	-2.323531	2.369047	-0.555446
26	1	0	-3.722136	1.467841	-1.151027
27	1	0	-4.293587	0.133098	1.565893
28	1	0	-2.969349	1.063016	2.280071
29	1	0	-3.007998	-0.697186	2.452746
30	1	0	-3.775747	-1.657755	-0.979579
31	1	0	-2.139894	-1.811902	-1.637507
32	1	0	-2.535900	-2.534192	-0.071429

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.006578	1.132847	1.139847
2	6	0	-0.889972	-0.127067	0.252285
3	6	0	-2.213351	-0.043718	-0.493509
4	6	0	-2.663164	1.376613	-0.708223
5	6	0	-1.703739	2.182049	0.226674
6	6	0	-1.104849	-1.515781	0.861074
7	8	0	-2.042951	-2.166422	-0.040618
8	7	0	-2.837902	-1.145135	-0.642232
9	6	0	0.295278	-0.096013	-0.753740
10	1	0	0.209532	-0.990622	-1.386390
11	1	0	0.172676	0.752232	-1.443655
12	14	0	2.104446	-0.009709	-0.121185
13	1	0	-0.215864	-2.147321	0.900511
14	1	0	-1.560891	-1.460053	1.860728
15	1	0	-1.648603	0.909418	2.001520
16	1	0	-0.051047	1.496685	1.528657
17	1	0	-0.955344	2.711618	-0.372763
18	1	0	-2.235233	2.940374	0.809750
19	1	0	-3.715499	1.489193	-0.428519
20	1	0	-2.575795	1.693028	-1.753992
21	6	0	3.197371	-0.686503	-1.514033
22	6	0	2.616232	1.787074	0.215379
23	6	0	2.383756	-1.037418	1.447784
24	1	0	4.259705	-0.633884	-1.246077
25	1	0	2.963466	-1.734820	-1.735516
26	1	0	3.063871	-0.116333	-2.441588
27	1	0	3.689065	1.843788	0.438032

28	1	0	2.430507	2.424200	-0.658191
29	1	0	2.084168	2.229132	1.065630
30	1	0	3.420461	-0.926173	1.789306
31	1	0	1.733582	-0.723236	2.272915
32	1	0	2.212028	-2.106468	1.275577

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.552065	0.682561	-0.000033
2	7	0	-3.468204	0.126440	-0.000005
3	6	0	-1.103451	-1.028117	0.000048
4	1	0	-1.011631	-1.681003	-0.878698
5	1	0	-1.011647	-1.680957	0.878830
6	6	0	0.035460	0.014603	0.000032
7	1	0	-0.070337	0.658517	0.880494
8	1	0	-0.070430	0.658583	-0.880370
9	6	0	1.410940	-0.657905	-0.000064
10	1	0	1.487567	-1.325976	-0.873159
11	1	0	1.487612	-1.326126	0.872912
12	6	0	2.614763	0.263533	-0.000020
13	6	0	2.531174	1.597564	0.000015
14	1	0	1.584282	2.128651	0.000028
15	1	0	3.425267	2.215625	0.000038
16	6	0	3.947730	-0.446127	0.000001
17	1	0	4.051688	-1.095165	0.880524
18	1	0	4.782312	0.261207	-0.000080
19	1	0	4.051641	-1.095320	-0.880411
20	6	0	-2.438679	-0.420819	0.000021

TS12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.029253	0.751358	0.995327
2	6	0	1.009646	-0.426090	-0.072305
3	6	0	-1.215020	0.824183	0.276730
4	7	0	2.199254	-0.144161	-0.197188
5	8	0	3.115530	0.653012	0.016590
6	6	0	-2.038047	-0.437741	0.143981
7	6	0	-1.150912	-1.706290	0.206272
8	6	0	0.162598	-1.557211	-0.585971
9	1	0	-1.710623	-2.560016	-0.191440
10	1	0	-0.913690	-1.951371	1.248637
11	1	0	0.736145	-2.489586	-0.536594
12	1	0	-0.073302	-1.388840	-1.647668
13	1	0	-2.573294	-0.414289	-0.815397

14	1	0	-2.819353	-0.498751	0.918029
15	1	0	0.604564	1.633066	1.075757
16	1	0	0.011319	0.103200	1.871231
17	6	0	-1.525066	1.972880	-0.634835
18	1	0	-0.856996	2.822663	-0.465745
19	1	0	-1.448271	1.684376	-1.695365
20	1	0	-2.559198	2.318039	-0.489050

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.548676	1.666018	0.228805
2	6	0	1.033137	0.239669	0.209197
3	6	0	0.061607	-0.839531	0.679158
4	6	0	-1.295786	-0.625438	0.079544
5	6	0	-1.835461	0.775332	0.105369
6	6	0	-0.819640	1.788212	-0.469331
7	7	0	2.216125	-0.039830	-0.194705
8	8	0	2.863247	-1.090436	-0.323265
9	6	0	-2.147521	-1.788838	-0.311789
10	1	0	-1.202079	2.810183	-0.358424
11	1	0	-0.693439	1.601678	-1.543345
12	1	0	1.292272	2.319379	-0.237661
13	1	0	0.440447	1.993075	1.275701
14	1	0	-2.072033	1.078457	1.144230
15	1	0	-2.779355	0.835073	-0.449840
16	1	0	0.015693	-0.773126	1.785655
17	1	0	0.462549	-1.829414	0.440595
18	1	0	-1.545391	-2.625898	-0.686715
19	1	0	-2.732580	-2.183398	0.539814
20	1	0	-2.875015	-1.516256	-1.086675

TS14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.684436	1.060561	0.243504
2	6	0	0.634050	-0.747946	0.147771
3	6	0	0.206463	0.322792	1.164091
4	6	0	-0.429175	-1.705048	-0.344623
5	6	0	-1.827059	-1.168652	0.030840
6	6	0	-1.926088	0.351688	-0.226414
7	6	0	-0.206443	2.313679	-0.422092
8	7	0	1.844806	-0.780389	-0.322037
9	8	0	2.760271	0.058891	-0.157070
10	1	0	-0.293929	-0.127173	2.030099
11	1	0	1.078734	0.893367	1.487973

12	1	0	0.879180	2.291672	-0.573969
13	1	0	-0.691090	2.477107	-1.391320
14	1	0	-0.420722	3.198451	0.200464
15	1	0	-2.828221	0.750673	0.268640
16	1	0	-2.070400	0.548610	-1.299150
17	1	0	-2.603786	-1.703139	-0.526135
18	1	0	-2.018335	-1.368748	1.091777
19	1	0	-0.338626	-1.829130	-1.431148
20	1	0	-0.292494	-2.702530	0.095133

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.487518	-0.574149	-0.053821
2	6	0	-0.147453	0.870229	0.130513
3	6	0	0.216495	0.139491	1.382303
4	6	0	0.239068	-0.656092	0.093513
5	7	0	1.466962	-1.059688	-0.528954
6	6	0	-1.625755	0.922047	-0.251777
7	6	0	-2.184438	-0.500818	-0.039030
8	6	0	-0.993632	-1.449867	-0.303882
9	1	0	-0.912083	-1.704427	-1.367649
10	1	0	-1.085573	-2.391542	0.250326
11	1	0	-3.039717	-0.712903	-0.688004
12	1	0	-2.536350	-0.618195	0.992133
13	1	0	1.201087	0.347166	1.792676
14	1	0	-0.545925	-0.119649	2.113663
15	1	0	-2.171684	1.677061	0.328579
16	1	0	-1.700816	1.213109	-1.307678
17	6	0	0.767129	1.945965	-0.405633
18	1	0	0.607972	2.103580	-1.478869
19	1	0	1.819415	1.695746	-0.244857
20	1	0	0.566319	2.895333	0.106886

TS16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.909976	0.543188	-0.469384
2	6	0	1.249419	1.657495	-0.250022
3	8	0	2.226684	-0.711343	-0.264308
4	7	0	1.077514	-1.318007	-0.523672
5	6	0	0.076911	-0.954066	0.265251
6	6	0	0.181340	0.092697	1.356882
7	6	0	0.058745	1.080668	0.241752
8	1	0	1.175377	2.282794	-1.140287
9	1	0	1.953186	2.029732	0.499055
10	1	0	1.155351	0.109896	1.844982
11	1	0	-0.639742	0.051448	2.074822

12	6	0	-1.323419	-1.326799	-0.150560
13	1	0	-1.766782	-2.063438	0.532512
14	1	0	-1.277678	-1.778738	-1.145843
15	6	0	-2.178414	-0.027074	-0.143709
16	6	0	-1.284520	1.194016	-0.447216
17	1	0	-1.121988	1.314921	-1.525759
18	1	0	-1.782470	2.115325	-0.109794
19	1	0	-3.005453	-0.091290	-0.858151
20	1	0	-2.636212	0.101324	0.843752

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.632472	-0.476443	-0.049105
2	6	0	0.400986	-0.967821	0.698045
3	6	0	-0.862691	-0.283624	0.232441
4	6	0	-0.842403	1.222952	0.098188
5	6	0	0.565140	1.797287	0.328466
6	6	0	1.613358	0.991388	-0.455492
7	7	0	-1.869891	-1.031102	-0.025515
8	8	0	-2.986900	-0.256281	-0.425496
9	6	0	2.660688	-1.284526	-0.315436
10	1	0	2.646175	-2.338229	-0.047734
11	1	0	-1.574819	1.661440	0.788949
12	1	0	-1.202455	1.479645	-0.907242
13	1	0	0.810244	1.779760	1.398826
14	1	0	0.589618	2.849122	0.022132
15	1	0	2.611469	1.429788	-0.339381
16	1	0	1.370184	1.062619	-1.527042
17	1	0	0.531375	-0.734688	1.768770
18	1	0	0.287555	-2.052505	0.623504
19	1	0	3.557457	-0.922244	-0.813470
20	1	0	-3.647655	-0.942023	-0.607383

TS18

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.071446	0.635908	1.051418
2	6	0	0.912209	-0.542187	-0.036846
3	6	0	-1.054902	0.907641	0.280325
4	7	0	2.122099	-0.328651	-0.214510
5	8	0	3.010332	0.508134	0.002761
6	6	0	-2.059219	-0.204773	0.096491
7	6	0	-1.368281	-1.592642	0.162997
8	6	0	-0.010483	-1.609034	-0.563855
9	1	0	-2.025177	-2.349608	-0.278645
10	1	0	-1.219242	-1.884578	1.209404
11	1	0	0.461574	-2.591402	-0.447710

12	1	0	-0.174402	-1.465255	-1.642377
13	1	0	-2.555413	-0.083128	-0.875940
14	1	0	-2.861393	-0.158424	0.849722
15	1	0	0.825709	1.411547	1.186131
16	1	0	-0.044143	-0.018553	1.916628
17	6	0	-1.131107	2.095956	-0.626452
18	1	0	-0.335428	2.818639	-0.424950
19	1	0	-1.069090	1.803588	-1.686515
20	1	0	-2.098319	2.607445	-0.510737

TS19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.216544	-1.025773	0.331163
2	6	0	0.028381	1.021140	-0.131246
3	6	0	-1.173979	1.273125	-0.754623
4	8	0	-2.433362	-0.635628	-0.090264
5	7	0	-1.404411	-1.257890	0.216219
6	6	0	1.144826	-1.607568	0.238894
7	6	0	2.092095	-0.447517	-0.173821
8	6	0	1.280399	0.630898	-0.919721
9	6	0	0.277225	1.661459	1.230154
10	1	0	-0.667513	1.881549	1.735910
11	1	0	0.866638	1.025588	1.899014
12	1	0	0.828037	2.605820	1.114944
13	1	0	-1.954024	1.851401	-0.273706
14	1	0	-1.338315	1.012593	-1.795757
15	1	0	0.986221	0.260396	-1.909844
16	1	0	1.912129	1.515466	-1.082783
17	1	0	2.545764	-0.011451	0.722712
18	1	0	2.914471	-0.825124	-0.790256
19	1	0	1.147259	-2.398984	-0.521173
20	1	0	1.462686	-2.061588	1.184730

20

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.036341	-0.816631	0.272905
2	6	0	-0.124180	0.662239	-0.057387
3	6	0	-1.508393	0.638642	-0.708642
4	8	0	-2.158065	-0.529494	-0.131846
5	7	0	-1.135732	-1.460569	0.218199
6	6	0	1.385587	-1.304398	0.352162
7	6	0	2.190777	-0.110210	-0.257479
8	6	0	1.145125	0.834282	-0.921057
9	6	0	-0.093369	1.529559	1.217539

10	1	0	-0.941761	1.288764	1.866570
11	1	0	0.826404	1.375960	1.792355
12	1	0	-0.150859	2.592831	0.954948
13	1	0	-2.137421	1.502306	-0.479024
14	1	0	-1.450339	0.504584	-1.798798
15	1	0	0.939688	0.501685	-1.946225
16	1	0	1.499736	1.869658	-0.973377
17	1	0	2.724589	0.422317	0.537164
18	1	0	2.946884	-0.446148	-0.973498
19	1	0	1.504434	-2.229474	-0.220793
20	1	0	1.698051	-1.523443	1.379801

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.051989	-1.126842	-0.478475
2	6	0	-2.928097	-0.840766	0.180173
3	6	0	-2.530876	0.536510	0.642980
4	6	0	-1.281865	1.107038	-0.064327
5	6	0	0.007442	0.320878	0.204552
6	6	0	1.228278	0.976168	-0.477856
7	6	0	2.480770	0.250457	-0.240251
8	7	0	3.434978	-0.378196	-0.008253
9	8	0	4.442290	-1.022918	0.224237
10	1	0	-2.340717	0.519094	1.726969
11	1	0	1.055940	1.041978	-1.560703
12	1	0	1.343031	2.008880	-0.121459
13	1	0	0.192129	0.260503	1.284818
14	1	0	-0.087290	-0.709029	-0.158025
15	1	0	-1.470733	1.143571	-1.145961
16	1	0	-1.142099	2.146494	0.264635
17	1	0	-2.233378	-1.650297	0.407256
18	1	0	-4.289825	-2.138879	-0.795128
19	1	0	-4.782740	-0.357861	-0.722934
20	1	0	-3.369466	1.225599	0.483629

TS22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.296839	-1.031446	0.150693
2	6	0	0.373160	1.108317	0.619540
3	6	0	1.682958	1.410230	0.349766
4	8	0	2.493261	-0.663188	-0.447166
5	7	0	1.415222	-1.238701	-0.265028
6	6	0	-1.057865	-1.615415	0.278674

7	6	0	-2.139410	-0.508498	0.295163
8	6	0	-1.831641	0.607255	-0.716479
9	6	0	-0.788234	1.635474	-0.215201
10	1	0	-0.390496	2.183837	-1.077871
11	1	0	-1.314984	2.379032	0.401422
12	1	0	-2.753916	1.144592	-0.968416
13	1	0	-1.479765	0.147815	-1.650339
14	1	0	-2.223831	-0.085201	1.304346
15	1	0	-3.105076	-0.976875	0.074321
16	1	0	-1.130479	-2.235191	1.182266
17	1	0	-1.228996	-2.277046	-0.580923
18	1	0	0.129269	0.864130	1.654055
19	1	0	1.972005	1.896412	-0.577184
20	1	0	2.458786	1.299409	1.097913

23 (2+3product)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.286490	-0.768976	0.139041
2	6	0	0.416549	0.672594	0.594149
3	6	0	1.809208	0.969749	0.023777
4	8	0	2.403532	-0.323582	-0.234249
5	7	0	1.368245	-1.280693	-0.313022
6	6	0	-1.022689	-1.507834	0.184073
7	6	0	-2.210344	-0.512820	0.145629
8	6	0	-1.846944	0.760754	-0.632196
9	6	0	-0.754359	1.568514	0.097926
10	1	0	-0.368923	2.353167	-0.565103
11	1	0	-1.205852	2.082506	0.954830
12	1	0	-2.733123	1.390766	-0.773452
13	1	0	-1.496442	0.482179	-1.636104
14	1	0	-2.495785	-0.233665	1.169298
15	1	0	-3.085466	-1.002063	-0.296169
16	1	0	-1.077751	-2.126531	1.090362
17	1	0	-1.061153	-2.199333	-0.664536
18	1	0	0.438867	0.683135	1.694015
19	1	0	1.738678	1.522062	-0.925593
20	1	0	2.473516	1.509402	0.703209

TS24

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.996884	0.216631	0.325404
2	6	0	-0.249531	-1.512061	-0.013012

3	6	0	1.030974	-1.503191	0.524013
4	6	0	-0.017629	1.186904	0.897909
5	6	0	1.105533	1.612101	-0.082083
6	6	0	1.756324	0.483579	-0.906302
7	6	0	2.185689	-0.757979	-0.096820
8	7	0	-2.170475	0.326964	-0.025148
9	8	0	-3.163979	-0.199792	-0.520721
10	1	0	-0.998136	-2.151882	0.451794
11	1	0	-0.372934	-1.432398	-1.093713
12	1	0	1.176789	-1.904641	1.525544
13	1	0	2.894357	-0.461672	0.688966
14	1	0	2.754441	-1.428742	-0.762624
15	1	0	2.634473	0.894720	-1.419797
16	1	0	1.067032	0.172315	-1.700562
17	1	0	1.874185	2.126169	0.510935
18	1	0	0.703266	2.356018	-0.780644
19	1	0	-0.549768	2.076650	1.251871
20	1	0	0.434591	0.707154	1.775382

TS25

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.935274	0.241958	0.419482
2	6	0	-0.415641	-1.408977	0.175300
3	6	0	0.927208	-1.500177	0.553885
4	6	0	0.057333	1.224322	0.947551
5	6	0	1.175410	1.575260	-0.074937
6	6	0	1.652076	0.413479	-0.966974
7	6	0	2.056364	-0.871198	-0.211243
8	7	0	-2.079827	0.434352	-0.047508
9	8	0	-2.938649	-0.213388	-0.657943
10	1	0	-1.121817	-1.999721	0.761547
11	1	0	-0.674664	-1.448564	-0.891910
12	1	0	1.158104	-1.901895	1.539137
13	1	0	2.887786	-0.657840	0.474140
14	1	0	2.460336	-1.591702	-0.943860
15	1	0	2.507724	0.756797	-1.561524
16	1	0	0.863370	0.168144	-1.688408
17	1	0	2.025394	1.992526	0.481730
18	1	0	0.811769	2.373385	-0.733226
19	1	0	-0.464824	2.137581	1.251882
20	1	0	0.509949	0.789914	1.848209

26(R=OMe)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.841527	0.159440	-0.427566
2	6	0	0.212538	-0.921399	-0.386572
3	6	0	1.722216	-0.602063	-0.381242
4	7	0	2.218051	0.760689	-0.391289
5	8	0	1.734541	1.500978	0.450707
6	6	0	1.021618	-1.186121	0.832640
7	1	0	-1.006063	0.488851	-1.467993
8	1	0	1.270010	-2.208042	1.103451
9	1	0	0.909626	-0.489385	1.659439
10	1	0	2.345774	-1.234577	-1.004274
11	1	0	-0.029708	-1.780707	-1.008824
12	1	0	-0.530767	1.037026	0.155028
13	8	0	-2.030672	-0.402389	0.104052
14	6	0	-3.101701	0.518162	0.112878
15	1	0	-3.966571	0.000120	0.535394
16	1	0	-2.875641	1.401663	0.731278
17	1	0	-3.352828	0.863397	-0.903381

TS27(R=OMe)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.211792	0.696333	0.432021
2	6	0	-0.766680	-0.455831	0.363679
3	8	0	0.832839	1.540806	0.523343
4	7	0	1.557477	1.216495	-0.525421
5	6	0	1.960084	-0.051042	-0.525930
6	6	0	0.337293	-1.195553	-0.122939
7	6	0	1.665622	-1.082533	0.528605
8	1	0	1.631423	-0.671613	1.538830
9	1	0	2.303253	-1.964252	0.460872
10	1	0	2.486077	-0.361551	-1.425257
11	1	0	0.248802	-1.737983	-1.059925
12	8	0	-1.919755	-0.522955	-0.409888
13	1	0	-0.942499	-0.548124	1.449203
14	6	0	-2.899678	0.434042	-0.038557
15	1	0	-3.754167	0.280871	-0.701244
16	1	0	-3.224730	0.293935	1.003752
17	1	0	-2.523220	1.459609	-0.157093

26(R=Cl)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.796794	-0.485660	-0.504562
2	6	0	-0.012892	0.780888	-0.449119
3	6	0	-1.561241	0.739741	-0.382832
4	7	0	-2.293333	-0.511012	-0.326470
5	8	0	-1.891681	-1.314603	0.500302
6	6	0	-0.718277	1.215272	0.785081
7	1	0	0.928512	-0.834997	-1.529923
8	1	0	-0.761945	2.271593	1.032098
9	1	0	-0.702188	0.530285	1.629172
10	1	0	-2.082838	1.458810	-1.005392
11	1	0	0.352848	1.565946	-1.107325
12	1	0	0.365100	-1.280152	0.100982
13	17	0	2.474176	-0.183472	0.145403

TS27(R=Cl)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.037089	-0.872477	0.569811
2	6	0	0.801823	0.168141	0.557612
3	8	0	-1.122932	-1.476028	0.553737
4	7	0	-1.663161	-1.050492	-0.568333
5	6	0	-1.816919	0.268535	-0.623552
6	6	0	-0.067009	1.094389	-0.060914
7	6	0	-1.450961	1.257388	0.451216
8	1	0	-1.602387	0.876782	1.462268
9	1	0	-1.897135	2.240455	0.301464
10	1	0	-2.181610	0.645145	-1.575624
11	1	0	0.213735	1.593393	-0.983240
12	17	0	2.373023	-0.135223	-0.224351
13	1	0	0.912890	0.246436	1.641554

26(R=CF_3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.274152	0.388204	-0.596793
2	6	0	-1.652741	0.138536	-0.019829
3	6	0	0.614814	-0.830349	-0.462366

4	6	0	1.314547	-1.159833	0.808819
5	6	0	2.152851	-0.709988	-0.373182
6	7	0	2.809556	0.580625	-0.386683
7	8	0	2.351711	1.405828	0.389264
8	1	0	-0.405237	0.657735	-1.650180
9	1	0	1.408265	-2.197239	1.115402
10	1	0	1.249682	-0.431271	1.612370
11	1	0	2.724065	-1.436047	-0.941541
12	1	0	0.302525	-1.671959	-1.076398
13	1	0	0.149592	1.251131	-0.078049
14	9	0	-2.462529	1.198006	-0.226816
15	9	0	-2.243547	-0.939361	-0.587757
16	9	0	-1.609633	-0.085621	1.311370

TS27 (R=CF_3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.501691	0.885094	-0.565249
2	8	0	-1.653027	1.494573	-0.539895
3	7	0	-2.218217	1.020117	0.548099
4	6	0	-2.369614	-0.300066	0.558448
5	6	0	0.253989	-0.170280	-0.611664
6	6	0	-0.627776	-1.102276	-0.012875
7	6	0	-2.000958	-1.271467	-0.536566
8	1	0	-2.746875	-0.702025	1.495151
9	1	0	-2.148715	-0.873317	-1.541342
10	1	0	-2.454054	-2.253082	-0.399816
11	1	0	-0.355095	-1.612089	0.906374
12	1	0	0.299036	-0.194526	-1.704680
13	6	0	1.607139	0.029884	0.012076
14	9	0	1.529106	0.066235	1.360962
15	9	0	2.166679	1.182583	-0.405170
16	9	0	2.468932	-0.966843	-0.307402

26 (R=TMS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.119468	0.381073	-0.614114
2	14	0	-1.671642	0.092131	-0.007872
3	6	0	1.030386	-0.815417	-0.458513
4	6	0	1.753435	-1.128304	0.803008
5	6	0	2.589374	-0.685484	-0.383519
6	7	0	3.211477	0.607160	-0.432789
7	8	0	2.763283	1.434180	0.353573
8	1	0	0.077007	0.674224	-1.672935

9	1	0	1.867623	-2.160600	1.122901
10	1	0	1.699882	-0.389552	1.598919
11	1	0	3.158692	-1.415731	-0.949210
12	1	0	0.753002	-1.674951	-1.067472
13	1	0	0.527291	1.240996	-0.069724
14	6	0	-2.678064	1.638169	-0.437036
15	6	0	-2.412900	-1.416804	-0.884504
16	6	0	-1.694865	-0.182913	1.865850
17	1	0	-2.720888	-0.320725	2.228688
18	1	0	-1.121101	-1.071346	2.154230
19	1	0	-1.268832	0.674974	2.400036
20	1	0	-3.719967	1.535444	-0.109909
21	1	0	-2.266180	2.530452	0.049698
22	1	0	-2.688006	1.825785	-1.517520
23	1	0	-3.457580	-1.568410	-0.586596
24	1	0	-2.397106	-1.298353	-1.974922
25	1	0	-1.868472	-2.337520	-0.642071

TS27(R=TMS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.693551	0.808844	-0.505172
2	6	0	0.115012	-0.216336	-0.977377
3	8	0	1.636929	1.510387	0.173480
4	7	0	2.776945	0.974518	-0.221818
5	6	0	2.877151	-0.328521	-0.017811
6	6	0	1.830643	-1.220001	0.608572
7	6	0	1.107332	-1.175671	-0.689254
8	1	0	3.777594	-0.785487	-0.421264
9	1	0	1.307486	-0.740457	1.434746
10	1	0	2.229593	-2.196397	0.888381
11	1	0	1.508146	-1.807720	-1.480613
12	1	0	-0.096947	-0.131173	-2.049178
13	14	0	-1.512808	0.020769	0.016106
14	6	0	-1.246412	-0.024469	1.886066
15	1	0	-2.182587	0.232944	2.397345
16	1	0	-0.941819	-1.014421	2.244254
17	1	0	-0.487120	0.702394	2.194158
18	6	0	-2.179623	1.712453	-0.494929
19	1	0	-1.478819	2.507891	-0.216101
20	1	0	-3.139169	1.923691	-0.007482
21	1	0	-2.339088	1.774843	-1.578107
22	6	0	-2.718152	-1.344428	-0.503521
23	1	0	-3.692223	-1.211220	-0.016280
24	1	0	-2.341331	-2.336828	-0.228978
25	1	0	-2.887712	-1.340559	-1.586779

26(R=F)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.238897	-0.606862	-0.329088
2	9	0	2.499684	-0.353397	0.211091
3	6	0	0.488484	0.699397	-0.393917
4	6	0	-0.268098	1.230058	0.772130
5	6	0	-1.050393	0.766412	-0.443932
6	7	0	-1.878790	-0.426065	-0.397693
7	8	0	-1.595983	-1.225725	0.479415
8	1	0	1.378756	-1.029173	-1.331244
9	1	0	-0.259108	2.295811	0.979585
10	1	0	-0.364567	0.578031	1.636829
11	1	0	-1.476637	1.496642	-1.123393
12	1	0	0.961745	1.431623	-1.045501
13	1	0	0.728714	-1.338139	0.301285

TS27(R=F)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.409608	-0.975217	0.410034
2	6	0	1.274888	-0.023836	0.369565
3	8	0	-0.826056	-1.446960	0.516425
4	7	0	-1.428616	-0.920923	-0.530383
5	6	0	-1.443775	0.407023	-0.523003
6	6	0	0.454147	1.020633	-0.103495
7	6	0	-0.855513	1.294932	0.539059
8	1	0	-0.951123	0.887160	1.546704
9	1	0	-1.198708	2.327491	0.475988
10	1	0	-1.856726	0.865573	-1.417938
11	1	0	0.711131	1.528321	-1.028713
12	9	0	2.377759	-0.308621	-0.392949
13	1	0	1.516268	-0.026118	1.438989

26 (R=CHO)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.883049	-0.412149	-0.374033
2	6	0	2.179534	-0.078886	0.343133
3	6	0	-0.030381	0.797510	-0.434114
4	6	0	-0.833191	1.250869	0.737492

5	6	0	-1.575096	0.669766	-0.450591
6	7	0	-2.211194	-0.625188	-0.383400
7	8	0	-1.812927	-1.353502	0.514929
8	1	0	1.124185	-0.784992	-1.374227
9	1	0	-0.958416	2.312891	0.926706
10	1	0	-0.841946	0.608578	1.614928
11	1	0	-2.101715	1.325217	-1.135725
12	1	0	0.313819	1.578651	-1.109662
13	1	0	0.392882	-1.218399	0.188305
14	8	0	3.282606	-0.296476	-0.102631
15	1	0	2.048618	0.391542	1.343771

TS27 (R=CHO)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.167676	0.861874	-0.426051
2	8	0	-0.965446	1.543977	-0.492191
3	6	0	0.846719	-0.234196	-0.380449
4	6	0	-0.169576	-1.099722	0.123474
5	6	0	-1.859415	-0.223233	0.517839
6	6	0	-1.473886	-1.208957	-0.559293
7	7	0	-1.651102	1.095071	0.525004
8	1	0	1.010866	-0.272777	-1.463289
9	6	0	2.098033	-0.083391	0.412370
10	8	0	3.165876	0.247096	-0.056490
11	1	0	1.985106	-0.281012	1.503925
12	1	0	-0.018982	-1.652435	1.047646
13	1	0	-1.492520	-0.789979	-1.565690
14	1	0	-2.002668	-2.157754	-0.476557
15	1	0	-2.346453	-0.605006	1.410790

26(R=H)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.445343	1.142329	0.746757
2	6	0	-0.324002	0.819093	-0.521046
3	7	0	-1.453264	-0.079390	-0.515219
4	8	0	-1.543289	-0.799676	0.469259
5	1	0	1.515505	-1.712847	-0.989381
6	6	0	1.403239	-1.177761	-0.039890
7	6	0	1.113279	0.287941	-0.271938
8	1	0	0.760107	2.173486	0.880524
9	1	0	0.060782	0.645046	1.633844
10	1	0	-0.432911	1.568860	-1.297744
11	1	0	1.834957	0.790161	-0.914710

12	1	0	0.612130	-1.661012	0.537898
13	1	0	2.341436	-1.280163	0.518733

TS27(R=H)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.111008	-1.362521	0.031590
2	6	0	1.353008	-1.067741	-0.122410
3	8	0	-1.142010	-1.093008	0.396648
4	7	0	-1.471079	-0.096255	-0.397916
5	6	0	-0.703402	0.979010	-0.277632
6	6	0	1.227297	0.322635	-0.325371
7	6	0	0.475843	1.160284	0.644116
8	1	0	0.342923	0.685985	1.618039
9	1	0	0.789007	2.201617	0.727508
10	1	0	-0.918129	1.766346	-0.996561
11	1	0	1.528179	0.783575	-1.262617
12	1	0	1.832958	-1.648074	-0.908810
13	1	0	1.631219	-1.374207	0.890862

28 (R=H)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.874723	-0.000034	0.094970
2	6	0	-1.670653	-0.159143	-0.454581
3	6	0	0.590550	0.743097	0.119529
4	7	0	1.853978	0.669333	-0.060035
5	8	0	2.315716	-0.662800	-0.055422
6	6	0	-0.393391	-0.386207	0.314460
7	1	0	-3.762642	0.160495	-0.510457
8	1	0	0.084449	-1.323106	0.009476
9	1	0	-0.619873	-0.474783	1.386878
10	1	0	0.211061	1.764328	0.129398
11	1	0	-1.568673	-0.119412	-1.539650
12	1	0	-3.020609	-0.031012	1.173105
13	1	0	3.262019	-0.545712	-0.231403