Supporting Information

Mechanisms of Cascade Reactions in the Syntheses of Camptothecin-Family Alkaloids: Intramolecular [4$^+$+2] Reactions of *N*-arylimidates and Alkynes

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Content

1. Computational Details

All of the DFT calculations were performed with the Gaussian 03 program package.[1] The geometry optimization of all the minima and transition states involved were performed at the B3LYP levels of theory[2] with the 6-31G(d) basis set.[3] The vibrational frequencies were computed at the same level of theory to check whether every optimized geometrical structure is an energy minimum or a transition state, and to evaluate its zero-point vibration energy (ZPVE). IRC calculations[4] were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. Solvent effects were computed by the CPCM model[5] in CH_2Cl_2 at the B3LYP/6-31G(d) level using the gas phase optimized structures.

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

[2] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[3] Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

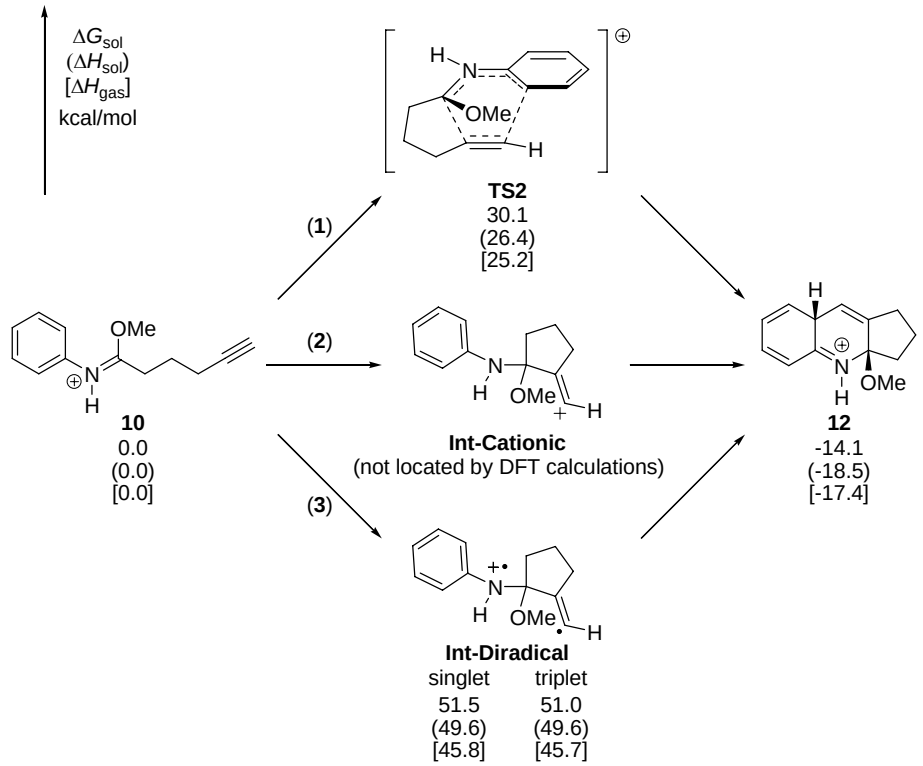
[4] (a) Fukui, K. *J. Phys. Chem.* **1970**, *74*, 4161. (b) Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys.* **1989**, *90*, 2154. (c) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.

[5] (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669. (c) Takano, Y.; Houk, K. N. *J. Chem. Theory Comput.* **2005**, *1*, 70.

2. Discussions on Stepwise Mechanisms

There are several possible mechanisms for the intramolecular aza-Diels-Alder reaction of the *N*-arylimidate and the alkyne (Scheme S1): (1) a concerted [4^++2] mechanism via transition state **TS2** (for details, see Figures 2 and 3 in the paper), (2) a stepwise mechanism involving an olefinic cation intermediate, and (3) a stepwise mechanism proceeding through a diradical intermediate. The two stepwise mechanisms can be ruled out by calculations. The key intermediate involved in the mechanism (2) is a highly unstable olefinic cation (**Int-Cationic**, Scheme S1). After many attempts, this olefinic cationic species cannot be located. All attempted optimizations led to either starting material **10** or product **12**. In addition, the key diradical intermediate involved in the mechanism (3) can be located (UB3LYP/6-31G(d)), but it is even about 20 kcal/mol higher in energy than concerted transition state **TS2** (**Int-Diradical** versus **TS2**, Scheme S1). These results indicate that stepwise mechanisms are extremely disfavored in the present [4^++2] reaction. This conclusion also gets supports from previous theoretical studies on both [4^++2] reactions of *N*-protonated 2-aza-1,3-butadiene and [4+2^+] reactions of iminium cations (for details, see ref. 13 in the paper), where the aza-Diels-Alder reactions all take place via a concerted not a stepwise mechanism.

Scheme S1. Possible Mechanisms for the Intramolecular Aza-Diels-Alder Reaction of the *N*-arylimidate and the Alkyne



3. Figure S1

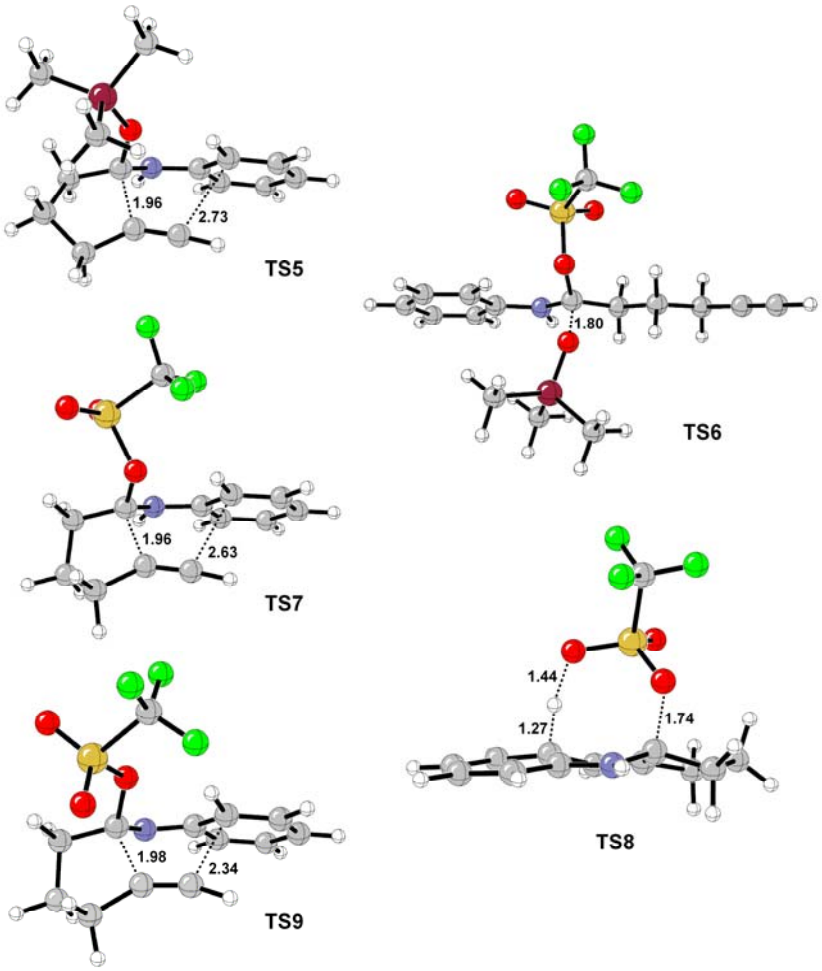


Figure S1. Transition state structures in model system **II**.

4. FMO Analysis

The molecular orbital energies in Table 1 were computed at the HF/6-31G(d) level based on the B3LYP/6-31G(d) gas phase geometries. The molecular orbital coefficients of $2p_z$ (shown in italics in Figure S2) were also computed at the HF/6-31G(d) level based on the B3LYP/6-31G(d) gas phase geometries. According to the FMO analysis (Table 1), *N*-protonated *N*-phenylimidates **32** is the most active azadiene due to its lowest LUMO energy. This is in agreement with the computational results that the activation enthalpy in gas phase of the IADA reaction of **18** is only 17.0 kcal/mol (Figure 4), much lower than those required in the IADA reactions of **10** (25.2 kcal/mol, Figure 2) and **22** (20.9 kcal/mol, Figure 4). But the generation of dicationic imidate **18** is not favored thermodynamically (for details, see the paper and Figure 4).

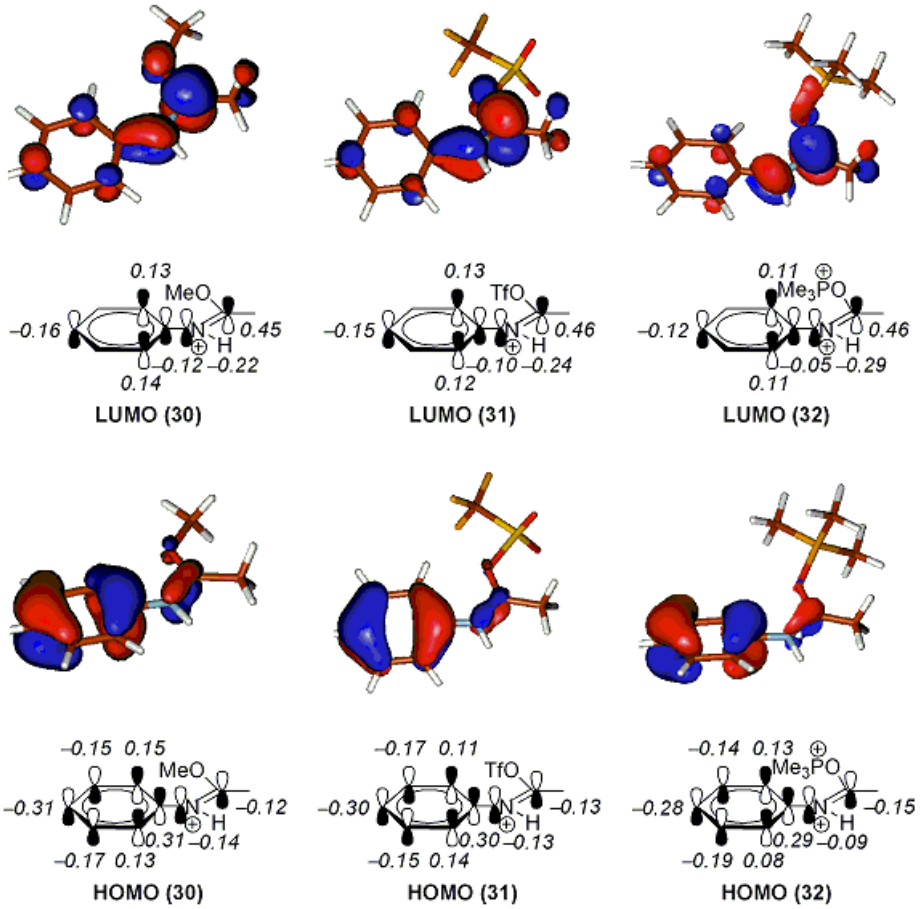
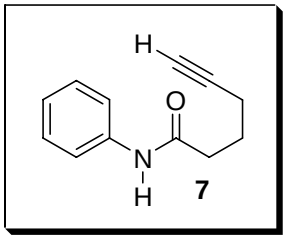


Figure S2. Frontier molecular orbitals of *N*-protonated *N*-phenylimidates **30**, **31**, and **32**.

5. Coordinates of All Stationary Points



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-3.657811	0.643113	0.969359
4	6	0	-2.333508	0.368775	1.298587
5	6	0	-1.468632	-0.208404	0.354655
6	6	0	-1.949988	-0.508128	-0.929429
7	7	0	-0.141926	-0.459794	0.764291
8	6	0	0.906462	-0.982610	0.042441
9	8	0	0.825838	-1.349044	-1.121657
10	6	0	2.203951	-1.153329	0.840512
11	6	0	3.451412	-0.762517	0.032033
12	6	0	3.804509	0.740153	0.099418
13	6	0	2.740162	1.636961	-0.354823
14	6	0	1.857040	2.376139	-0.718732
15	1	0	2.173536	-0.611164	1.794915
16	1	0	2.260778	-2.221510	1.088360
17	1	0	3.291207	-1.065882	-1.007263
18	1	0	4.317376	-1.320300	0.406878
19	1	0	4.073428	0.999757	1.133937
20	1	0	4.707785	0.917116	-0.499982
21	1	0	1.071657	3.013300	-1.056747
22	1	0	-1.283160	-0.949111	-1.656557
23	1	0	-3.643494	-0.462764	-2.239514
24	1	0	-5.174794	0.558624	-0.565187
25	1	0	-4.311063	1.090178	1.714006
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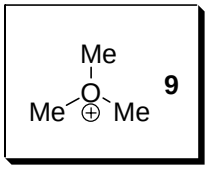

Standard orientation:

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3	1	0	-0.391757	2.030821	0.373379
4	1	0	1.342157	1.572582	0.389635
5	1	0	0.403648	1.476520	-1.154752
6	6	0	1.018840	-1.016071	-0.066433
7	1	0	1.955186	-0.674600	0.371296
8	1	0	0.692706	-1.948077	0.391748
9	1	0	1.075426	-1.089472	-1.154789
10	6	0	-1.389524	-0.374159	-0.066443
11	1	0	-2.033754	0.371755	0.395669
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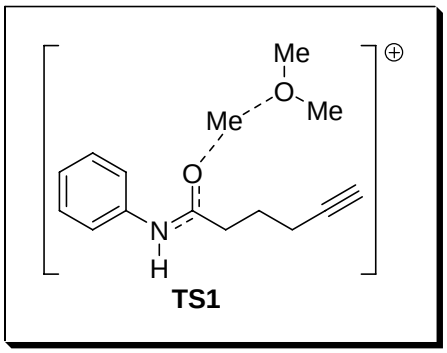

Standard orientation:

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5	6	0	3.525013	-3.360493	0.253934

6	6	0	4.122237	-2.104195	0.373647
7	7	0	1.297951	0.189052	-0.237794
8	6	0	-0.017665	0.453672	-0.252450
9	6	0	-0.379108	1.927734	-0.380118
10	6	0	0.086170	2.797314	0.827866
11	6	0	1.079511	3.916109	0.438369
12	6	0	2.295050	3.417565	-0.209738
13	6	0	3.282896	2.991946	-0.763822
14	8	0	-0.877383	-0.460914	-0.160264
15	6	0	-2.898337	-0.313378	-0.088409
16	1	0	4.117265	-4.261529	0.380073
17	1	0	5.181820	-2.019444	0.595298
18	1	0	3.825329	0.028034	0.316092
19	1	0	0.332455	-2.378071	-0.423250
20	1	0	1.691130	-4.422530	-0.130186
21	1	0	4.178543	2.683269	-1.257285
22	1	0	0.075830	2.304026	-1.304761
23	1	0	-1.459787	2.003366	-0.514021
24	1	0	-0.783820	3.269667	1.294941
25	1	0	0.546639	2.167015	1.596039
26	1	0	1.350697	4.480197	1.339422
27	1	0	0.584901	4.629509	-0.234502
28	1	0	-2.814617	-1.378934	0.058870
29	1	0	-2.815671	0.349750	0.757644
30	1	0	-2.889109	0.089934	-1.088172
31	1	0	1.903350	1.005532	-0.326293
32	8	0	-4.768068	-0.284547	-0.015487
33	6	0	-5.388431	-0.966621	-1.128992
34	6	0	-5.288394	-0.707421	1.265036
35	1	0	-6.463946	-0.775899	-1.097322
36	1	0	-4.966629	-0.540491	-2.039785
37	1	0	-5.191958	-2.043696	-1.081101
38	1	0	-6.362462	-0.507348	1.286822
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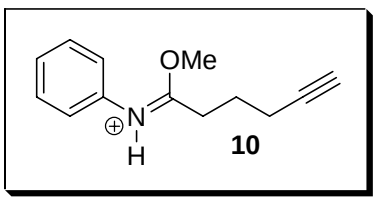

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4	1	0	2.507341	2.654833	0.120271
5	1	0	1.320042	3.141568	1.364041
6	1	0	2.301194	1.665483	1.616932
7	6	0	2.213457	0.402889	-1.357378
8	1	0	2.551036	1.373016	-1.744362
9	1	0	2.002296	-0.214393	-2.237213
10	6	0	3.368755	-0.247972	-0.555099
11	1	0	4.197366	-0.366680	-1.261056
12	1	0	3.723680	0.425431	0.229423
13	6	0	3.036630	-1.621203	0.062413
14	1	0	2.693793	-2.314436	-0.718762
15	1	0	3.964773	-2.053682	0.456636
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17	6	0	1.235253	-1.452432	2.029782
18	1	0	0.530790	-1.410294	2.831384
19	7	0	-0.158376	-0.044217	-1.016713
20	1	0	0.017999	-0.751447	-1.721779
21	6	0	-1.504109	-0.043145	-0.517527
22	6	0	-2.206468	-1.246770	-0.652935
23	1	0	-1.720309	-2.121827	-1.077872
24	6	0	-2.116795	1.091470	0.024461
25	1	0	-1.585671	2.030164	0.102409
26	6	0	-3.528662	-1.321680	-0.224783
27	1	0	-4.071963	-2.255772	-0.325393
28	6	0	-3.442413	0.999284	0.447367
29	1	0	-3.926033	1.876965	0.864535
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Me_2O **11**

Standard orientation:

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5	8	0	0.000000	0.589871	0.000000
6	6	0	-1.171031	-0.195253	0.000000
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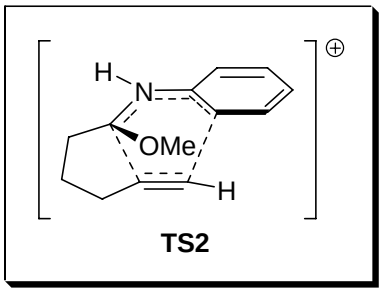

TS2

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6	6	0	1.249153	-0.303316	-0.618801
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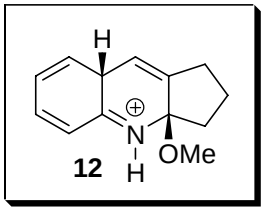

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6	6	0	0.203291	-1.601013	0.430446
7	6	0	1.322549	-0.576566	0.613770
8	6	0	1.211809	0.541014	-0.389883
9	7	0	-0.004997	0.926074	-0.734474
10	6	0	2.701616	-1.126871	0.780290
11	6	0	3.778938	-0.551064	0.204462
12	6	0	3.607422	0.595915	-0.648947
13	6	0	2.380230	1.132582	-0.939124
14	8	0	-1.404907	0.852288	1.169188
15	6	0	-1.792988	2.226658	1.286425
16	1	0	4.778184	-0.938317	0.371980
17	1	0	4.490879	1.045728	-1.094191
18	1	0	2.287782	1.974715	-1.618993
19	1	0	1.106262	-0.075788	1.583629
20	1	0	2.805362	-1.984234	1.439707

21	1	0	0.435824	-2.645441	0.615428
22	1	0	-2.973274	1.361002	-1.009083
23	1	0	-2.134322	0.228595	-2.081347
24	1	0	-4.064328	-1.082258	-1.281662
25	1	0	-3.827655	-0.504810	0.371021
26	1	0	-2.132631	-2.537763	-1.149217
27	1	0	-2.594241	-2.571229	0.549635
28	1	0	-1.774816	2.443892	2.355172
29	1	0	-1.087788	2.895182	0.775799
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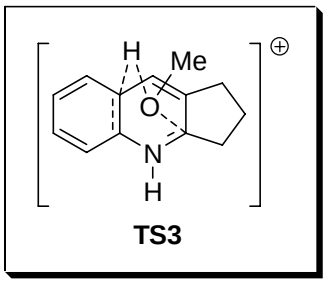

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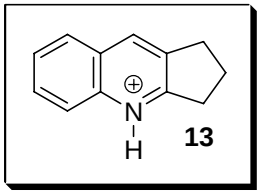
3	6	0	-1.202920	0.385667	-0.066769
4	6	0	-2.625143	0.836889	-0.385989
5	6	0	-3.330249	-0.468015	-0.836811
6	6	0	-0.090117	-1.662394	0.471671
7	6	0	1.101011	-0.749260	0.370746
8	6	0	1.060434	0.203071	-0.732201
9	7	0	-0.192861	0.648553	-1.056281
10	6	0	2.397654	-1.152351	0.841796
11	6	0	3.546502	-0.629459	0.299290
12	6	0	3.462590	0.273959	-0.786839
13	6	0	2.245367	0.694981	-1.298900
14	8	0	-0.673233	0.919162	1.254817
15	6	0	-0.396494	2.339132	1.341003
16	1	0	4.518857	-0.925261	0.678093
17	1	0	4.377668	0.662620	-1.224310
18	1	0	2.203969	1.405178	-2.120037
19	1	0	0.444977	0.200604	1.166889

20	1	0	2.448209	-1.893947	1.634334
21	1	0	0.063736	-2.702418	0.741095
22	1	0	-3.078121	1.208481	0.539404
23	1	0	-2.671156	1.638586	-1.129652
24	1	0	-3.124550	-0.656489	-1.895957
25	1	0	-4.414038	-0.403734	-0.715741
26	1	0	-2.765577	-2.574350	-0.415513
27	1	0	-3.185669	-1.625384	1.012736
28	1	0	-0.122519	2.527198	2.379309
29	1	0	0.423950	2.624384	0.675944
30	1	0	-1.304838	2.891552	1.090246
31	1	0	-0.307636	1.411601	-1.712768



Standard orientation:

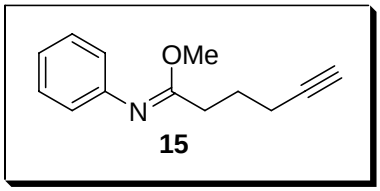
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.474081	0.680897	0.044247
2	6	0	3.435426	-0.733378	0.041756
3	6	0	2.232249	-1.412022	0.014012
4	6	0	1.037817	-0.671970	-0.013870
5	6	0	1.048601	0.755461	-0.011508
6	6	0	2.306517	1.411691	0.019173
7	7	0	-0.192561	-1.306531	-0.040917
8	6	0	-1.353353	-0.647528	-0.060406
9	6	0	-1.380777	0.759152	-0.060730
10	6	0	-0.188202	1.453189	-0.038037
11	6	0	-2.728992	-1.246136	-0.103047
12	6	0	-3.623891	-0.039353	0.292868
13	6	0	-2.818309	1.228940	-0.102124
14	1	0	4.432712	1.188690	0.066402
15	1	0	4.364256	-1.294513	0.061931
16	1	0	2.204389	-2.498299	0.012639
17	1	0	2.330271	2.497246	0.021546
18	1	0	-0.200412	-2.324029	-0.037743
19	1	0	-0.176514	2.540445	-0.035734
20	1	0	-2.843908	-2.113415	0.555992

21	1	0	-2.942047	-1.586993	-1.126819
22	1	0	-4.602178	-0.081047	-0.189448
23	1	0	-3.787083	-0.050762	1.375002
24	1	0	-3.007254	2.073804	0.566457
25	1	0	-3.071303	1.560933	-1.117802

MeOH **14**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.662414	-0.019645	0.000002
2	8	0	-0.749174	0.122374	0.000004
3	1	0	1.078643	0.991299	-0.000982
4	1	0	1.037157	-0.542289	0.893807
5	1	0	1.037005	-0.543948	-0.892885
6	1	0	-1.133900	-0.766183	0.000015



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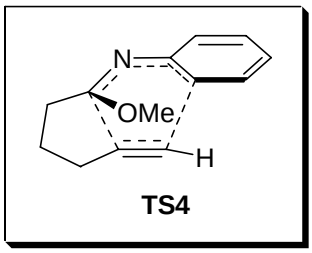
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.204287	-1.133728	-0.203351
2	6	0	3.522508	-0.948171	0.211319
3	6	0	4.073709	0.332955	0.278710
4	6	0	3.294744	1.432237	-0.090200
5	6	0	1.984387	1.251946	-0.527295
6	6	0	1.415208	-0.031304	-0.573581
7	7	0	0.108421	-0.141490	-1.089240
8	6	0	-0.819661	-0.816703	-0.533824
9	6	0	-2.176299	-0.868231	-1.210395
10	6	0	-3.282254	0.053335	-0.645817
11	6	0	-2.853302	1.526886	-0.453906

12	6	0	-2.076738	1.757905	0.765993
13	6	0	-1.463720	1.939716	1.791105
14	1	0	5.099921	0.472387	0.607906
15	1	0	3.713192	2.434969	-0.049626
16	1	0	1.376684	2.098172	-0.833310
17	1	0	1.781723	-2.131687	-0.248933
18	1	0	4.120961	-1.812813	0.488430
19	8	0	-0.593972	-1.527315	0.608261
20	1	0	-0.890749	2.104676	2.675102
21	1	0	-1.982470	-0.578774	-2.246188
22	1	0	-2.548987	-1.900471	-1.227864
23	1	0	-4.114702	0.027037	-1.359485
24	1	0	-3.675595	-0.329526	0.301507
25	1	0	-3.753137	2.155775	-0.423983
26	1	0	-2.270595	1.854971	-1.324767
27	6	0	-1.669845	-1.976073	1.428926
28	1	0	-1.213054	-2.615233	2.187199
29	1	0	-2.164017	-1.130989	1.919117
30	1	0	-2.404500	-2.564171	0.867377

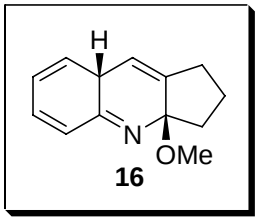


TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.142637	-0.034571	-0.750245
2	6	0	-1.066244	-0.062027	1.316066
3	6	0	0.027123	0.375420	1.746136
4	6	0	1.402852	0.851102	0.122586
5	1	0	0.756282	1.703165	-0.030687
6	6	0	2.719865	1.103282	0.616348
7	1	0	2.910145	2.037410	1.140981
8	6	0	3.736645	0.202487	0.421311
9	1	0	4.733454	0.404780	0.804695
10	6	0	3.496027	-0.987847	-0.320897
11	1	0	4.307671	-1.694539	-0.475160

12	6	0	2.251647	-1.251107	-0.834361
13	1	0	2.044084	-2.165647	-1.381970
14	6	0	1.161291	-0.342112	-0.648012
15	7	0	-0.060799	-0.767091	-1.013810
16	8	0	-1.099023	1.312929	-1.092707
17	6	0	-2.076763	2.214834	-0.590973
18	1	0	-1.777003	3.204110	-0.944971
19	1	0	-3.081917	1.997805	-0.972221
20	1	0	-2.091808	2.211574	0.505395
21	6	0	-2.484492	-0.753741	-0.898874
22	1	0	-3.306548	-0.038966	-1.002989
23	1	0	-2.450450	-1.357679	-1.810521
24	6	0	-2.701715	-1.621662	0.346516
25	1	0	-2.012100	-2.472185	0.315482
26	1	0	-3.723021	-2.015109	0.400217
27	6	0	-2.369317	-0.742284	1.564310
28	1	0	-3.157759	0.012839	1.699823
29	1	0	-2.324947	-1.327075	2.490772
30	1	0	0.666017	0.655086	2.560019

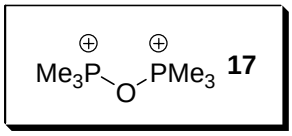


16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.340408	1.189238	-0.860865
2	6	0	1.133564	0.558379	-0.335759
3	6	0	1.315060	-0.597805	0.660045
4	6	0	2.695769	-1.196205	0.674583
5	6	0	3.741291	-0.593202	0.084402
6	6	0	3.562543	0.644236	-0.664695
7	7	0	-0.016126	0.994531	-0.717578
8	6	0	-1.187450	0.333496	-0.154332
9	6	0	-1.004623	-1.155166	0.118028
10	6	0	0.187638	-1.599233	0.506847
11	6	0	-2.405294	0.364192	-1.097361
12	6	0	-3.289802	-0.783578	-0.579601

13	6	0	-2.282400	-1.900788	-0.207626
14	1	0	4.737672	-1.022409	0.149319
15	1	0	4.440762	1.115128	-1.099911
16	1	0	2.197634	2.076280	-1.470618
17	1	0	1.184476	-0.119677	1.651822
18	1	0	2.825453	-2.122143	1.231829
19	8	0	-1.499461	0.911907	1.131422
20	1	0	0.395216	-2.649587	0.704714
21	1	0	-2.908265	1.335116	-1.117636
22	1	0	-2.051504	0.157473	-2.115302
23	1	0	-4.035589	-1.112991	-1.309777
24	1	0	-3.823657	-0.453405	0.318068
25	1	0	-2.121918	-2.574367	-1.060873
26	1	0	-2.630893	-2.523597	0.624267
27	6	0	-1.644836	2.326435	1.167091
28	1	0	-1.912423	2.571401	2.198838
29	1	0	-0.715392	2.841535	0.899057
30	1	0	-2.444222	2.684264	0.503342

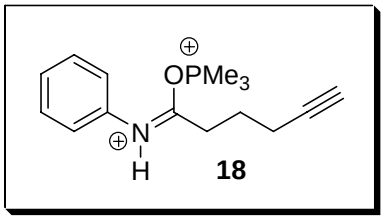


17

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.069766	1.715184	-0.231570
2	15	0	1.589669	-0.003243	0.030521
3	8	0	-0.000355	-0.031991	0.425672
4	15	0	-1.589954	-0.000739	0.030337
5	6	0	-1.912999	1.421717	-1.032548
6	6	0	2.411986	-0.711675	1.466249
7	6	0	1.868160	-0.994337	-1.452664
8	6	0	-2.428364	0.147933	1.615851
9	6	0	-2.007917	-1.547121	-0.799188
10	1	0	3.150247	1.750070	-0.420407
11	1	0	1.555688	2.141038	-1.099040
12	1	0	1.853618	2.311839	0.660536
13	1	0	3.496044	-0.695506	1.299850
14	1	0	2.092049	-1.747659	1.616220
15	1	0	2.182454	-0.122965	2.360199

16	1	0	2.946112	-1.012659	-1.658260
17	1	0	1.532216	-2.024903	-1.299922
18	1	0	1.365908	-0.556270	-2.320964
19	1	0	-2.130024	1.073958	2.117487
20	1	0	-2.186017	-0.709405	2.251822
21	1	0	-3.511692	0.169227	1.445701
22	1	0	-1.755265	-2.402441	-0.164137
23	1	0	-1.496463	-1.630762	-1.762913
24	1	0	-3.089923	-1.560412	-0.982557
25	1	0	-1.615050	2.350233	-0.535073
26	1	0	-2.991288	1.468968	-1.231615
27	1	0	-1.395289	1.323113	-1.991947



18

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.591825	-1.569179	-0.181196
2	6	0	4.541280	-0.682938	0.338002
3	6	0	4.269659	0.686968	0.396064
4	6	0	3.048755	1.175847	-0.061252
5	6	0	2.097690	0.272428	-0.553513
6	6	0	2.359416	-1.100991	-0.631146
7	7	0	0.878399	0.849506	-1.051265
8	6	0	-0.365051	0.462682	-0.978765
9	8	0	-0.558137	-0.743405	-0.409649
10	15	0	-1.781612	-1.615023	0.281823
11	6	0	-1.467473	1.250358	-1.628918
12	6	0	-2.459443	2.007321	-0.704317
13	6	0	-1.823169	3.106647	0.169087
14	6	0	-0.919066	2.585376	1.196914
15	6	0	-0.177033	2.162507	2.054024
16	1	0	-0.999448	1.975694	-2.303094
17	1	0	-2.024111	0.560293	-2.275433
18	1	0	-3.012333	1.311153	-0.063667
19	1	0	-3.199076	2.464072	-1.369664

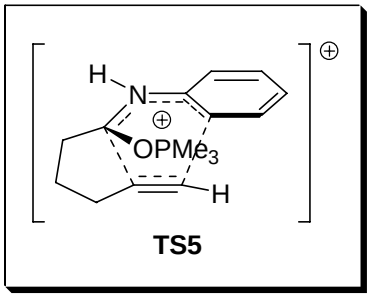
20	1	0	-1.296238	3.833062	-0.464707
21	1	0	-2.630531	3.671001	0.652590
22	1	0	0.476774	1.865180	2.846291
23	1	0	1.648283	-1.782081	-1.082878
24	1	0	3.821175	-2.627352	-0.256295
25	1	0	5.500170	-1.058904	0.680431
26	1	0	5.010912	1.377045	0.785595
27	1	0	2.834437	2.240730	-0.021495
28	6	0	-2.092223	-0.961197	1.933061
29	6	0	-1.046802	-3.256642	0.356447
30	6	0	-3.258632	-1.644635	-0.758792
31	1	0	1.002555	1.767102	-1.476279
32	1	0	-3.946515	-2.382008	-0.324658
33	1	0	-3.768295	-0.679055	-0.788435
34	1	0	-3.004502	-1.971764	-1.772338
35	1	0	-1.736323	-3.929346	0.880366
36	1	0	-0.872273	-3.644204	-0.652147
37	1	0	-0.101853	-3.218205	0.906794
38	1	0	-2.980470	-1.455930	2.344567
39	1	0	-1.232521	-1.179224	2.574530
40	1	0	-2.247731	0.121474	1.914420

Me_3PO **19**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.664979	-0.158415	-0.563852
2	15	0	0.000360	-0.000300	0.192373
3	6	0	-0.695549	1.522626	-0.558994
4	8	0	0.002182	-0.002969	1.693639
5	6	0	-0.971693	-1.361353	-0.562736
6	1	0	1.622089	-0.152891	-1.658435
7	1	0	2.293732	0.671525	-0.226636
8	1	0	2.125810	-1.092893	-0.228894
9	1	0	-0.949165	-1.325152	-1.657353
10	1	0	-2.010207	-1.292792	-0.224168
11	1	0	-0.567104	-2.321812	-0.228499
12	1	0	-0.677230	1.486351	-1.653708
13	1	0	-0.117862	2.388355	-0.220396

14	1	0	-1.729336	1.650418	-0.223119



TS5

Standard orientation:

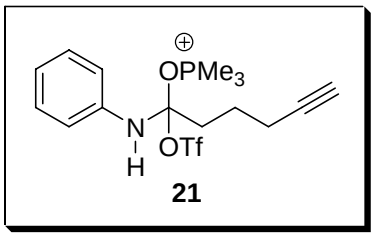
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.282186	0.801740	-0.599963
2	6	0	0.081500	1.575130	1.186574
3	6	0	-0.809731	1.039986	1.873495
4	6	0	-2.009184	-0.905031	0.372620
5	1	0	-1.553441	0.651559	2.538654
6	6	0	1.055579	2.724030	1.111549
7	1	0	0.466203	3.630729	0.925028
8	1	0	1.550573	2.862954	2.076873
9	6	0	2.043301	2.480389	-0.038376
10	1	0	2.860103	1.826804	0.288950
11	1	0	2.510416	3.411346	-0.369366
12	6	0	1.238771	1.837450	-1.177863
13	1	0	1.865276	1.389066	-1.955108
14	1	0	0.635686	2.611111	-1.666367
15	8	0	0.780489	-0.492657	-0.349492
16	15	0	2.197878	-1.235580	-0.063314
17	6	0	1.744185	-2.972407	-0.235027
18	1	0	1.351348	-3.158228	-1.239329
19	1	0	2.632831	-3.594132	-0.078248
20	1	0	0.987929	-3.244935	0.506888
21	6	0	3.465210	-0.821221	-1.286865
22	1	0	3.080860	-0.978834	-2.299599
23	1	0	4.311253	-1.502151	-1.130051
24	1	0	3.828260	0.203565	-1.178789
25	6	0	2.784016	-0.911500	1.617371
26	1	0	3.622617	-1.587823	1.822945
27	1	0	3.131953	0.117106	1.738551
28	1	0	1.984919	-1.113325	2.336748

29	7	0	-0.964921	0.745705	-1.141396
30	1	0	-1.193496	1.546323	-1.723604
31	1	0	-1.058508	-1.330303	0.657789
32	6	0	-3.348662	0.510903	-1.111290
33	1	0	-3.409867	1.275560	-1.881988
34	6	0	-4.501927	-0.042083	-0.587578
35	1	0	-5.468678	0.287123	-0.954806
36	6	0	-4.429476	-1.022373	0.422326
37	1	0	-5.342040	-1.457226	0.817347
38	6	0	-3.193839	-1.446681	0.892725
39	1	0	-3.135567	-2.225267	1.646899
40	6	0	-2.087973	0.090668	-0.630365

TfO⊖ **20**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.941062	-0.000024	0.000078
2	9	0	-1.445640	0.256881	-1.227697
3	9	0	-1.445419	0.935014	0.836346
4	16	0	0.926237	-0.000010	-0.000021
5	8	0	1.244159	-0.301087	1.414554
6	9	0	-1.445625	-1.191801	0.391480
7	8	0	1.244000	1.375621	-0.446659
8	8	0	1.243931	-1.074601	-0.968057



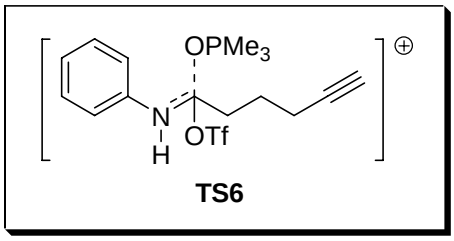
21

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.669559	-0.770719	0.601737

2	6	0	2.391337	-0.447768	-0.733612
3	6	0	3.387487	-0.611043	-1.708410
4	6	0	4.643051	-1.099575	-1.353801
5	6	0	4.928303	-1.414726	-0.023616
6	6	0	3.938133	-1.249192	0.943705
7	7	0	1.144905	0.090265	-1.177333
8	6	0	0.024890	0.387450	-0.395686
9	8	0	-0.442603	-0.686737	0.490446
10	16	0	-0.613231	-2.234874	-0.084070
11	8	0	0.344537	-3.082781	0.594372
12	6	0	-1.131906	0.926522	-1.242207
13	6	0	-2.352726	1.417397	-0.454159
14	6	0	-3.494300	1.845769	-1.401779
15	6	0	-4.633586	2.400840	-0.672953
16	6	0	-5.560343	2.859735	-0.050955
17	8	0	0.371110	1.346444	0.673378
18	15	0	1.256416	2.676719	0.682743
19	6	0	2.188245	2.999605	-0.836571
20	6	0	0.141171	4.069252	0.992732
21	6	0	2.398919	2.510879	2.072303
22	6	0	-2.302286	-2.556662	0.677163
23	8	0	-0.756087	-2.207996	-1.534803
24	1	0	5.905785	-1.797551	0.251673
25	1	0	4.136899	-1.517984	1.977220
26	1	0	1.900770	-0.699810	1.360844
27	1	0	3.172606	-0.367085	-2.746517
28	1	0	5.398071	-1.233566	-2.122625
29	1	0	0.909243	-0.146654	-2.133652
30	1	0	-1.427980	0.118472	-1.920607
31	1	0	-0.734487	1.735427	-1.869950
32	1	0	-2.716293	0.630091	0.209452
33	1	0	-2.084348	2.264639	0.185048
34	1	0	-3.819512	0.980722	-1.995805
35	1	0	-3.123297	2.587487	-2.124146
36	1	0	-6.393803	3.259226	0.482602
37	1	0	0.725394	4.982754	1.146228
38	1	0	-0.532163	4.215866	0.143571
39	1	0	-0.454636	3.870517	1.888517
40	1	0	2.972769	3.435286	2.194299
41	1	0	1.833103	2.313408	2.987706
42	1	0	3.079432	1.676087	1.882523
43	1	0	2.723785	3.946165	-0.700246
44	1	0	2.906191	2.197922	-1.023329
45	1	0	1.516387	3.093658	-1.693103

46	9	0	-2.594317	-3.829354	0.460078
47	9	0	-2.257292	-2.300903	1.976233
48	9	0	-3.203296	-1.772826	0.085369

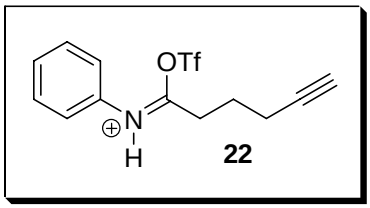


TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.378848	-0.443457	-0.896820
2	6	0	3.398195	-0.495102	-1.856711
3	6	0	4.659012	-0.974415	-1.508027
4	6	0	4.911333	-1.402534	-0.203777
5	6	0	3.891353	-1.348369	0.747204
6	6	0	2.622633	-0.869455	0.414832
7	7	0	1.123938	0.084740	-1.334636
8	6	0	-0.024617	0.299358	-0.659726
9	6	0	-1.147103	0.922230	-1.470071
10	6	0	-2.407125	1.319200	-0.691914
11	6	0	-3.516361	1.806685	-1.648801
12	6	0	-4.711109	2.240385	-0.926451
13	6	0	-5.686702	2.595503	-0.311317
14	8	0	0.216824	1.529211	0.634431
15	15	0	1.178659	2.721134	0.912827
16	8	0	-0.383856	-0.673654	0.269278
17	16	0	-0.758292	-2.242537	-0.277345
18	8	0	-1.444835	-2.148282	-1.554409
19	8	0	0.392669	-3.092589	-0.058025
20	6	0	-2.011529	-2.565197	1.097409
21	9	0	-3.058347	-1.767739	0.932013
22	9	0	-2.372603	-3.833040	0.984165
23	9	0	-1.434998	-2.342456	2.267896
24	1	0	5.891156	-1.782949	0.066603
25	1	0	4.074229	-1.693155	1.760615
26	1	0	1.837157	-0.853884	1.158612
27	1	0	3.202106	-0.178354	-2.879049
28	1	0	5.439844	-1.017273	-2.260969

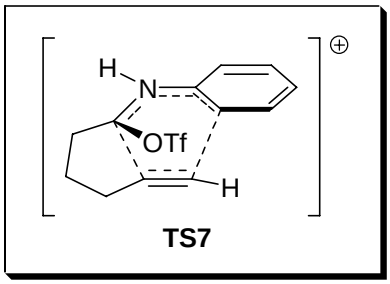
29	1	0	1.168888	0.557141	-2.230423
30	1	0	-1.411089	0.177082	-2.231961
31	1	0	-0.738160	1.792892	-1.998396
32	1	0	-2.780365	0.467231	-0.118801
33	1	0	-2.171461	2.105387	0.029174
34	1	0	-3.779445	1.001502	-2.348682
35	1	0	-3.139910	2.635675	-2.265699
36	1	0	-6.560226	2.906915	0.216621
37	6	0	0.192821	4.148342	1.449926
38	6	0	2.349899	2.323545	2.241142
39	6	0	2.153114	3.244837	-0.534248
40	1	0	0.842202	4.991665	1.706138
41	1	0	-0.491047	4.451142	0.651586
42	1	0	-0.397022	3.871164	2.328600
43	1	0	2.975365	3.192091	2.471837
44	1	0	1.794938	2.034306	3.138666
45	1	0	2.987910	1.490252	1.933891
46	1	0	2.758775	4.117609	-0.269011
47	1	0	2.822631	2.442086	-0.855827
48	1	0	1.489878	3.524170	-1.358723



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.513937	0.039040	-1.187505
2	6	0	2.318387	0.061260	-0.457085
3	6	0	2.140860	-0.757528	0.664788
4	6	0	3.175434	-1.616691	1.032978
5	6	0	4.364920	-1.658970	0.302932
6	6	0	4.533528	-0.827258	-0.806839
7	7	0	1.334933	0.999141	-0.912140
8	6	0	0.035974	1.063470	-0.744947
9	6	0	-0.760934	2.182721	-1.348119
10	6	0	-1.517801	3.078995	-0.332599
11	6	0	-0.608743	3.993961	0.512076

12	6	0	0.294656	3.270977	1.409198
13	6	0	1.033542	2.673697	2.156133
14	8	0	-0.514827	0.091783	-0.027327
15	16	0	-2.173608	-0.496367	-0.234730
16	1	0	5.161525	-2.332829	0.601954
17	1	0	5.457470	-0.849964	-1.375462
18	1	0	3.642226	0.684522	-2.053285
19	1	0	1.232630	-0.720384	1.249307
20	1	0	3.049619	-2.251683	1.904306
21	1	0	1.684089	2.184858	2.847316
22	1	0	-0.091406	2.797149	-1.960176
23	1	0	-1.487783	1.729545	-2.033407
24	1	0	-2.196910	3.704989	-0.920094
25	1	0	-2.141535	2.466591	0.324592
26	1	0	-1.251641	4.655149	1.106955
27	1	0	-0.029746	4.654889	-0.148217
28	8	0	-2.970035	0.110435	0.806285
29	8	0	-2.481468	-0.440229	-1.649154
30	6	0	-1.676444	-2.262665	0.270071
31	1	0	1.725512	1.782328	-1.429041
32	9	0	-2.788104	-2.970412	0.266610
33	9	0	-0.811073	-2.718120	-0.615384
34	9	0	-1.142391	-2.211383	1.477771

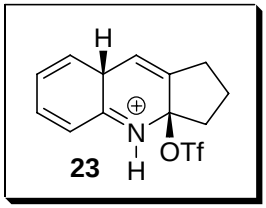


TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.177268	1.308748	-0.289205
2	6	0	-1.151483	2.030064	1.246959
3	6	0	-1.908906	1.219416	1.812162
4	6	0	-1.680397	-1.101416	0.591000
5	1	0	-0.752118	-0.985106	1.130966
6	6	0	-1.914531	-0.401555	-0.616548
7	7	0	-1.096756	0.639328	-1.045060

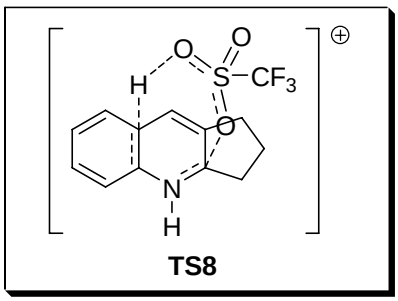
8	1	0	-1.468525	1.172669	-1.825835
9	6	0	0.357421	2.623219	-0.860890
10	1	0	0.365723	2.580689	-1.955138
11	1	0	1.393364	2.736881	-0.530680
12	6	0	-0.484447	3.784769	-0.310563
13	1	0	-1.447139	3.848492	-0.831354
14	1	0	0.024496	4.742706	-0.445754
15	6	0	-0.707865	3.463592	1.171660
16	1	0	0.229159	3.561739	1.734581
17	1	0	-1.452298	4.108386	1.645569
18	1	0	-2.572352	0.623127	2.401063
19	6	0	-2.599008	-2.084171	0.997913
20	1	0	-2.405627	-2.638024	1.911453
21	6	0	-3.716952	-2.370068	0.230165
22	1	0	-4.414649	-3.139492	0.545033
23	6	0	-3.937699	-1.676564	-0.976600
24	1	0	-4.812180	-1.901921	-1.578753
25	6	0	-3.052029	-0.704232	-1.398779
26	1	0	-3.229886	-0.163464	-2.325084
27	8	0	0.724423	0.510995	0.413034
28	16	0	2.166644	0.045352	-0.397848
29	8	0	3.251507	0.799757	0.194131
30	8	0	1.896467	0.004785	-1.824345
31	6	0	2.189220	-1.710082	0.300296
32	9	0	1.197184	-2.397612	-0.251168
33	9	0	3.357742	-2.237221	-0.013381
34	9	0	2.031465	-1.649859	1.615321



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.480606	3.428661	-0.877198
2	6	0	0.948380	2.001821	-0.673536
3	6	0	0.072628	1.342115	0.374258
4	6	0	-0.539060	2.512824	1.150273

5	6	0	-0.752990	3.573312	0.049978
6	6	0	1.967516	1.325274	-1.199410
7	6	0	2.238997	-0.098331	-0.738205
8	6	0	1.843160	-0.317022	0.695455
9	7	0	0.827338	0.386137	1.172658
10	6	0	3.563377	-0.683457	-1.114417
11	6	0	4.221416	-1.534400	-0.297374
12	6	0	3.682981	-1.839173	1.002384
13	6	0	2.537139	-1.263965	1.490497
14	8	0	-0.941505	0.613445	-0.415539
15	16	0	-2.158111	-0.206075	0.351002
16	8	0	-3.431663	0.369616	-0.022257
17	6	0	-1.920479	-1.818715	-0.584264
18	8	0	-1.771610	-0.431273	1.742945
19	1	0	5.154940	-1.994684	-0.602609
20	1	0	4.221565	-2.541110	1.633459
21	1	0	2.189170	-1.479921	2.496319
22	1	0	1.512329	-0.747621	-1.281208
23	1	0	3.936297	-0.449153	-2.107632
24	1	0	2.624026	1.746961	-1.955024
25	1	0	-1.444938	2.245529	1.698728
26	1	0	0.206952	2.859578	1.876587
27	1	0	-0.848499	4.577389	0.468385
28	1	0	-1.672645	3.353691	-0.500241
29	1	0	1.278079	4.122667	-0.584384
30	1	0	0.245659	3.638128	-1.925407
31	1	0	0.440958	0.151364	2.084375
32	9	0	-2.749456	-2.714595	-0.078223
33	9	0	-2.155508	-1.627564	-1.871319
34	9	0	-0.651623	-2.221902	-0.410217



TS8

Standard orientation:

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

1	6	0	2.922132	-1.125692	1.482487
2	6	0	2.136882	-0.194915	0.787824
3	6	0	2.141949	-0.166614	-0.671641
4	6	0	3.118788	-1.009661	-1.341578
5	6	0	3.875626	-1.908758	-0.639658
6	6	0	3.771084	-1.959306	0.773542
7	7	0	1.302308	0.670445	1.432313
8	6	0	0.406809	1.491326	0.758556
9	6	0	0.794383	1.871293	-0.620553
10	6	0	1.650069	1.090947	-1.300027
11	6	0	-0.162187	2.726209	1.426850
12	6	0	-0.777928	3.506121	0.243580
13	6	0	0.133962	3.188112	-0.971917
14	8	0	-1.055494	0.547399	0.664354
15	16	0	-1.383777	-0.388002	-0.548653
16	1	0	4.563714	-2.571928	-1.152343
17	1	0	4.376862	-2.675264	1.321608
18	1	0	2.874499	-1.177949	2.566329
19	1	0	1.091162	-0.864884	-0.805021
20	1	0	3.182658	-0.947788	-2.424294
21	1	0	1.958743	1.314850	-2.317205
22	1	0	-0.869571	2.491498	2.225704
23	1	0	0.682662	3.277451	1.861665
24	1	0	-0.835311	4.576306	0.452202
25	1	0	-1.793029	3.146697	0.056876
26	1	0	0.900797	3.960584	-1.109065
27	1	0	-0.429181	3.120862	-1.907545
28	8	0	-0.258840	-1.368670	-0.771109
29	6	0	-2.732818	-1.438372	0.240234
30	8	0	-1.899766	0.319300	-1.708848
31	1	0	1.198218	0.580901	2.438526
32	9	0	-3.742485	-0.645932	0.563581
33	9	0	-3.109871	-2.337179	-0.653970
34	9	0	-2.240718	-2.030754	1.319661

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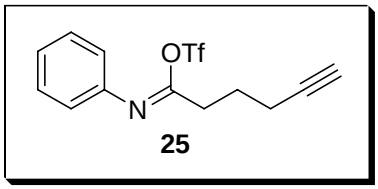
Standard orientation:

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

1	6	0	-1.008504	0.009466	-0.001845
2	9	0	-1.361208	1.220304	0.434605
3	16	0	0.852874	-0.148407	0.075964
4	8	0	1.256787	1.097089	-0.898782
5	8	0	1.261312	0.174482	1.435626
6	8	0	1.215492	-1.373121	-0.604924
7	9	0	-1.543130	-0.923109	0.781369
8	9	0	-1.424597	-0.155617	-1.252410
9	1	0	1.496731	1.855908	-0.331797

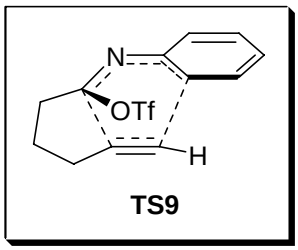


25

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.160066	0.344591	-0.664887
2	6	0	2.143238	-1.014534	-1.008668
3	6	0	3.180012	-1.846659	-0.587368
4	6	0	4.228339	-1.339821	0.182733
5	6	0	4.244756	0.016283	0.517747
6	6	0	3.226488	0.862297	0.082876
7	7	0	1.180539	1.245940	-1.133900
8	6	0	-0.050817	1.169582	-0.916242
9	8	0	-0.571109	0.174395	-0.004067
10	16	0	-1.758700	-0.848110	-0.468108
11	6	0	-1.074427	2.122766	-1.464326
12	6	0	-1.856441	2.937928	-0.413705
13	6	0	-1.001487	3.925965	0.411469
14	6	0	-0.142687	3.296679	1.417202
15	6	0	0.551430	2.778721	2.259068
16	1	0	5.031287	-1.993888	0.510898
17	1	0	5.061493	0.421773	1.109078
18	1	0	3.234255	1.920911	0.322704
19	1	0	1.333335	-1.404705	-1.616970
20	1	0	3.164646	-2.897799	-0.863060
21	1	0	1.161433	2.309181	2.996883
22	1	0	-0.537655	2.789291	-2.145446

23	1	0	-1.793205	1.554408	-2.069693
24	1	0	-2.610792	3.518225	-0.957755
25	1	0	-2.399320	2.264892	0.256268
26	1	0	-1.679028	4.626696	0.917765
27	1	0	-0.387654	4.535149	-0.266986
28	6	0	-1.351643	-2.177120	0.791085
29	8	0	-3.066813	-0.307796	-0.127474
30	8	0	-1.473200	-1.361969	-1.802325
31	9	0	-2.292203	-3.114929	0.686631
32	9	0	-0.160586	-2.703239	0.529064
33	9	0	-1.364473	-1.658838	2.013460

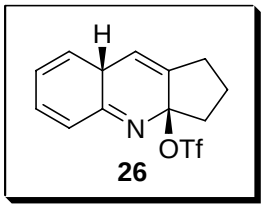


TS9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.377170	1.236149	-0.633392
2	6	0	-0.675279	1.472839	1.304420
3	6	0	-1.274479	0.518703	1.846975
4	6	0	-1.837677	-1.084499	0.235182
5	1	0	-0.781399	-1.275408	0.344579
6	6	0	-2.746565	-2.054906	0.731978
7	1	0	-2.375453	-2.826595	1.402173
8	6	0	-4.069097	-2.046680	0.348614
9	1	0	-4.756387	-2.797270	0.729337
10	6	0	-4.531444	-1.073956	-0.574501
11	1	0	-5.575509	-1.075033	-0.876277
12	6	0	-3.673259	-0.127156	-1.079881
13	1	0	-4.014094	0.641658	-1.766259
14	6	0	-2.298172	-0.100892	-0.695947
15	7	0	-1.569108	0.962738	-1.098593
16	8	0	0.597624	0.087253	-0.699389
17	6	0	0.239747	2.593209	-0.958169
18	1	0	1.331119	2.558468	-0.930157
19	1	0	-0.059661	2.870180	-1.972444

20	6	0	-0.285257	3.578319	0.094960
21	1	0	-1.338700	3.801247	-0.107129
22	1	0	0.269672	4.521845	0.077602
23	6	0	-0.152994	2.869866	1.452348
24	1	0	0.901283	2.811898	1.747063
25	1	0	-0.696604	3.390337	2.247546
26	1	0	-1.692559	-0.068953	2.635540
27	8	0	2.995016	0.463921	-1.399992
28	8	0	2.331491	0.833223	1.017555
29	16	0	2.151183	0.146127	-0.256639
30	6	0	2.324074	-1.689387	0.065994
31	9	0	3.577147	-1.918675	0.454747
32	9	0	1.485079	-2.062503	1.037585
33	9	0	2.060608	-2.380424	-1.038116

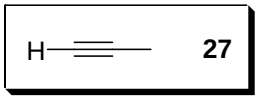


26

Standard orientation:

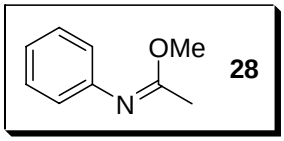
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.313775	-1.412354	1.299939
2	6	0	1.654489	-0.318268	0.602624
3	6	0	2.216707	0.084961	-0.762733
4	6	0	3.630321	-0.366054	-1.013979
5	6	0	4.216143	-1.306952	-0.254197
6	6	0	3.522451	-1.869602	0.895842
7	7	0	0.622010	0.234570	1.148319
8	6	0	0.006119	1.319703	0.443666
9	6	0	0.888047	2.128262	-0.486255
10	6	0	1.945730	1.544533	-1.047383
11	6	0	-0.667648	2.373224	1.324739
12	6	0	-0.846477	3.580145	0.386071
13	6	0	0.418729	3.568889	-0.511885
14	8	0	-1.018866	0.730604	-0.530519
15	16	0	-2.261528	-0.212408	-0.114722
16	8	0	-2.686514	-0.026455	1.265630
17	8	0	-3.194785	-0.130153	-1.226596

18	6	0	-1.510089	-1.934030	-0.229863
19	9	0	-0.915858	-2.279235	0.907813
20	9	0	-2.497925	-2.790811	-0.486540
21	9	0	-0.617955	-1.979836	-1.228348
22	1	0	5.217982	-1.659866	-0.482279
23	1	0	4.014541	-2.658651	1.458990
24	1	0	1.824389	-1.786026	2.193502
25	1	0	1.597509	-0.503705	-1.471819
26	1	0	4.138892	0.057708	-1.877343
27	1	0	2.634275	2.081419	-1.697330
28	1	0	-1.585996	2.012429	1.788190
29	1	0	0.044327	2.606263	2.127168
30	1	0	-0.964818	4.520581	0.931777
31	1	0	-1.742447	3.441590	-0.228249
32	1	0	1.196396	4.226053	-0.100564
33	1	0	0.212503	3.920990	-1.528700



Standard orientation:

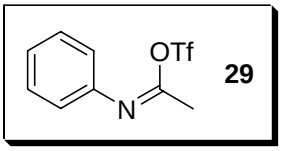
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.116297	-0.382728	1.368901
2	6	0	0.017866	-0.058802	0.210194
3	6	0	-0.101243	0.333154	-1.191522
4	1	0	0.203289	-0.668737	2.391846
5	1	0	0.877775	0.342374	-1.685552
6	1	0	-0.532126	1.337016	-1.287651
7	1	0	-0.746462	-0.360394	-1.744083



Standard orientation:

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

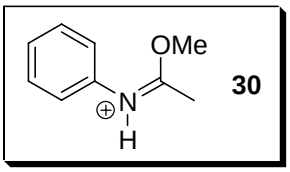
1	6	0	-2.312444	1.316622	-0.478539
2	6	0	-3.307389	0.529579	0.104728
3	6	0	-2.990502	-0.758074	0.543592
4	6	0	-1.696686	-1.251806	0.395436
5	6	0	-0.682237	-0.456665	-0.164411
6	6	0	-1.009508	0.837310	-0.607923
7	7	0	0.578597	-1.064219	-0.326338
8	6	0	1.695862	-0.480972	-0.145480
9	8	0	1.771246	0.824282	0.257186
10	6	0	3.021808	1.397097	0.631822
11	6	0	2.979088	-1.233923	-0.386536
12	1	0	3.598098	-1.288002	0.516899
13	1	0	3.744594	1.381622	-0.191724
14	1	0	2.802375	2.433880	0.893485
15	1	0	3.452993	0.893242	1.504792
16	1	0	3.582158	-0.756707	-1.168652
17	1	0	2.725837	-2.245533	-0.702443
18	1	0	-1.444374	-2.260224	0.710026
19	1	0	-0.244094	1.459109	-1.057909
20	1	0	-3.757120	-1.386253	0.990473
21	1	0	-2.549362	2.317033	-0.832881
22	1	0	-4.319203	0.912100	0.208694



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.226174	-1.503623	0.010874
2	6	0	-4.535445	-0.274105	0.596273
3	6	0	-3.631356	0.782673	0.523378
4	6	0	-2.387475	0.612524	-0.103738
5	6	0	-2.080110	-0.623762	-0.696042
6	6	0	-3.002380	-1.667557	-0.641308
7	7	0	-1.559582	1.752240	-0.165076
8	6	0	-0.309750	1.813557	-0.076385
9	6	0	0.480333	3.081381	-0.174444
10	8	0	0.436119	0.615188	0.209138
11	16	0	2.054936	0.456597	-0.007084

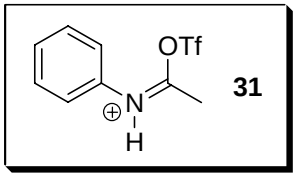
12	8	0	2.777785	0.997638	1.133475
13	6	0	2.030299	-1.410960	0.148958
14	9	0	1.544002	-1.764377	1.331626
15	8	0	2.421883	0.790377	-1.376217
16	9	0	1.288224	-1.933225	-0.825575
17	9	0	3.287557	-1.831878	0.029364
18	1	0	1.153494	3.056755	-1.038233
19	1	0	-4.936066	-2.324840	0.054682
20	1	0	-5.489023	-0.131795	1.097413
21	1	0	-3.867303	1.752109	0.951206
22	1	0	-1.132358	-0.765395	-1.201371
23	1	0	-2.758629	-2.617719	-1.109194
24	1	0	-0.216548	3.912505	-0.283556
25	1	0	1.092531	3.226087	0.722621



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.378233	0.561155	0.022597
2	6	0	-3.130685	-0.811654	0.090631
3	6	0	-1.822855	-1.283481	0.063181
4	6	0	-0.758161	-0.376171	-0.029918
5	6	0	-0.993493	1.002349	-0.102576
6	6	0	-2.311545	1.456289	-0.074771
7	7	0	0.544861	-0.974486	-0.057670
8	6	0	1.762786	-0.475829	-0.021007
9	6	0	2.946667	-1.389747	-0.057127
10	1	0	3.558852	-1.255179	0.841667
11	8	0	1.884026	0.822307	0.046763
12	6	0	3.190907	1.463928	0.103289
13	1	0	3.754404	1.246662	-0.806031
14	1	0	2.968522	2.527147	0.164796
15	1	0	3.730368	1.138242	0.994470
16	1	0	3.575866	-1.163755	-0.925362
17	1	0	2.644688	-2.437128	-0.114417
18	1	0	0.514209	-1.988253	-0.100490

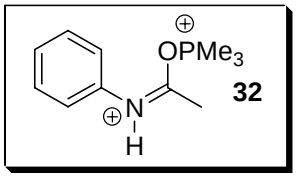
19	1	0	-1.632383	-2.353431	0.117413
20	1	0	-0.181245	1.709193	-0.183810
21	1	0	-3.952608	-1.516313	0.164334
22	1	0	-2.500939	2.523486	-0.132135
23	1	0	-4.398297	0.931243	0.043371



31

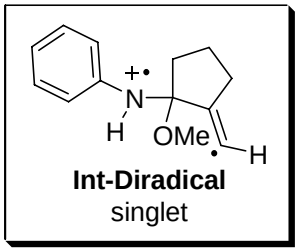
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.751697	-0.197773	0.341411
2	6	0	-3.791006	0.807573	0.303856
3	6	0	-2.474841	0.492235	-0.058652
4	6	0	-2.112131	-0.815771	-0.401439
5	6	0	-3.089705	-1.808527	-0.361391
6	6	0	-4.402003	-1.508675	0.010247
7	7	0	-1.566696	1.603881	-0.087473
8	6	0	-0.257528	1.684105	-0.069153
9	8	0	0.411004	0.545668	-0.016962
10	16	0	2.198829	0.483433	-0.009827
11	6	0	2.184538	-1.419571	0.109555
12	9	0	1.506890	-1.890916	-0.923173
13	6	0	0.423367	3.014585	-0.106150
14	1	0	1.067234	3.080163	-0.990778
15	8	0	2.629660	0.914104	-1.321277
16	8	0	2.634654	1.070958	1.237431
17	9	0	3.446716	-1.791572	0.065356
18	9	0	1.616309	-1.755383	1.248863
19	1	0	-5.151239	-2.293462	0.036257
20	1	0	-5.770097	0.045046	0.626500
21	1	0	-4.062543	1.828455	0.563547
22	1	0	-1.105136	-1.064022	-0.704614
23	1	0	-2.820042	-2.824877	-0.630191
24	1	0	-0.300179	3.831407	-0.137830
25	1	0	1.056999	3.134891	0.779592
26	1	0	-2.035120	2.506207	-0.095604



Standard orientation:

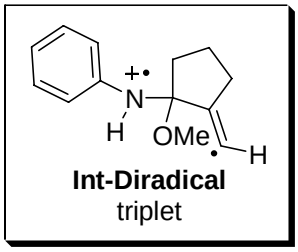
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.877120	-0.805675	-0.563658
2	6	0	3.003923	-1.617224	-0.472842
3	6	0	4.197040	-1.124406	0.068083
4	6	0	4.277429	0.199608	0.509902
5	6	0	3.166808	1.030759	0.415611
6	6	0	1.968195	0.516916	-0.105109
7	7	0	0.887418	1.454184	-0.180813
8	6	0	-0.410987	1.338443	-0.227389
9	6	0	-1.300221	2.531430	-0.346972
10	1	0	-2.056823	2.546241	0.445584
11	8	0	-0.903249	0.081842	-0.220347
12	15	0	-2.396349	-0.564190	0.134279
13	6	0	-3.642047	0.034708	-1.027651
14	6	0	-2.810113	-0.183253	1.849714
15	6	0	-2.081439	-2.319725	-0.098364
16	1	0	-0.730558	3.460973	-0.275313
17	1	0	-1.812025	2.526533	-1.317562
18	1	0	0.973504	-1.183140	-1.023138
19	1	0	2.956964	-2.637098	-0.840727
20	1	0	5.067875	-1.769209	0.130902
21	1	0	5.204677	0.587512	0.918327
22	1	0	3.229419	2.062434	0.754661
23	1	0	1.206433	2.423080	-0.181854
24	1	0	-4.549692	-0.565248	-0.880048
25	1	0	-3.894964	1.084064	-0.854961
26	1	0	-3.300276	-0.106859	-2.058511
27	1	0	-2.994729	-2.877216	0.141706
28	1	0	-1.808769	-2.521161	-1.139293
29	1	0	-1.277891	-2.650516	0.566886
30	1	0	-3.722520	-0.734775	2.111225
31	1	0	-2.002429	-0.509905	2.513026
32	1	0	-3.003143	0.883634	1.995431



Int-Diradical
singlet

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.195572	0.424988	-1.224301
2	6	0	2.260312	1.051895	-0.186405
3	6	0	1.193989	0.000774	0.215361
4	6	0	1.356158	-1.106718	-0.843056
5	6	0	2.862784	-1.076539	-1.157534
6	6	0	2.305420	2.244543	0.348354
7	6	0	-1.802204	-0.947767	-0.423069
8	6	0	-1.396602	0.354382	0.011258
9	7	0	-0.118110	0.708655	0.253084
10	6	0	-3.138419	-1.200998	-0.655402
11	6	0	-4.107700	-0.195327	-0.469016
12	6	0	-3.724562	1.088652	-0.034844
13	6	0	-2.397341	1.366562	0.204738
14	8	0	1.509610	-0.367139	1.537603
15	6	0	0.820349	-1.476071	2.124668
16	1	0	-5.154192	-0.413028	-0.657455
17	1	0	-4.474107	1.859332	0.111863
18	1	0	-2.090295	2.353937	0.539108
19	1	0	-1.070581	-1.730308	-0.562388
20	1	0	-3.445489	-2.189156	-0.982354
21	1	0	2.907370	3.140811	0.388296
22	1	0	1.019067	-2.088082	-0.502087
23	1	0	0.784685	-0.839212	-1.739377
24	1	0	3.098574	-1.604043	-2.085210
25	1	0	3.422502	-1.553551	-0.346449
26	1	0	2.962991	0.830084	-2.217282
27	1	0	4.243663	0.651192	-1.013494
28	1	0	1.146911	-1.497243	3.165165
29	1	0	-0.268816	-1.342330	2.097902
30	1	0	1.088227	-2.425007	1.647609
31	1	0	0.012840	1.652861	0.619235



Int-Diradical
triplet

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.277686	0.396978	-1.113112
2	6	0	2.244804	1.070407	-0.204816
3	6	0	1.188823	0.022408	0.202120
4	6	0	1.380913	-1.097049	-0.835684
5	6	0	2.904262	-1.097786	-1.060600
6	6	0	2.200086	2.315494	0.205139
7	6	0	-1.797856	-0.935265	-0.491126
8	6	0	-1.407110	0.352849	-0.004566
9	7	0	-0.130731	0.720592	0.227374
10	6	0	-3.134269	-1.204380	-0.704906
11	6	0	-4.117456	-0.227183	-0.453536
12	6	0	-3.748327	1.044387	0.026813
13	6	0	-2.421626	1.336886	0.251465
14	8	0	1.480453	-0.326821	1.534862
15	6	0	0.855526	-1.486600	2.096766
16	1	0	-5.163606	-0.456402	-0.629809
17	1	0	-4.508342	1.793911	0.221442
18	1	0	-2.125546	2.314739	0.621740
19	1	0	-1.055065	-1.694502	-0.687607
20	1	0	-3.429780	-2.182286	-1.070994
21	1	0	2.759215	3.238952	0.149534
22	1	0	1.004427	-2.068927	-0.509151
23	1	0	0.865735	-0.820975	-1.763035
24	1	0	3.182875	-1.634266	-1.970902
25	1	0	3.404307	-1.584858	-0.217269
26	1	0	3.178575	0.790141	-2.132164
27	1	0	4.299916	0.598944	-0.782594
28	1	0	1.105854	-1.462598	3.158067
29	1	0	-0.236444	-1.455864	1.988033
30	1	0	1.244561	-2.411579	1.657956
31	1	0	-0.007924	1.659117	0.612499

6. Computed Energies of All Stationary Points

Table S1. Sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Enthalpy (*TCH*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), and total free energy in solution (E_S, in a.u., solvent = dichloromethane)

Structure	*H*	*G*	*TCH*	*TCGFE*	E_S
7	-594.790741	-594.847079	0.237266	0.180928	-595.036308
9	-194.52819	-194.563178	0.129065	0.094077	-194.722261
TS1	-789.329621	-789.404376	0.366733	0.291978	-789.740273
10	-634.41312	-634.472683	0.280755	0.221192	-634.754988
11	-154.939504	-154.970105	0.085541	0.054939	-155.021394
TS2	-634.372822	-634.426509	0.278175	0.224488	-634.71039
12	-634.440733	-634.493201	0.281163	0.228694	-634.784948
TS3	-634.415563	-634.466501	0.276069	0.225132	-634.751384
13	-518.840125	-518.885241	0.224547	0.179431	-519.132475
14	-115.65869	-115.685662	0.055715	0.028743	-115.71783
15	-634.031672	-634.091435	0.266321	0.206557	-634.297881
TS4	-633.976883	-634.029721	0.264058	0.21122	-634.242841
16	-634.052717	-634.105322	0.267342	0.214737	-634.321239
17	-996.642465	-996.700371	0.251017	0.193111	-997.102493
18	-1055.194708	-1055.266317	0.362308	0.290698	-1055.763678
19	-536.226434	-536.265596	0.126554	0.087391	-536.357374
TS5	-1055.167598	-1055.234192	0.360364	0.29377	-1055.728851
20	-961.462598	-961.503229	0.035382	-0.005249	-961.576325
21	-2016.90799	-2017.00009	0.39963	0.30753	-2017.359383
TS6	-2016.906086	-2016.999597	0.39845	0.304938	-2017.351966
22	-1480.672567	-1480.748455	0.271385	0.195497	-1481.002672
TS7	-1480.639301	-1480.708287	0.269253	0.200267	-1480.969546
23	-1480.722134	-1480.788516	0.272675	0.206293	-1481.057974
TS8	-1480.718044	-1480.782847	0.267131	0.202328	-1481.048847
24	-961.951768	-961.993768	0.04735	0.005349	-962.010775
25	-1480.317086	-1480.391325	0.257265	0.183027	-1480.571902
TS9	-1480.264057	-1480.332086	0.255146	0.187118	-1480.519675
26	-1480.344853	-1480.410551	0.258982	0.193285	-1480.609014
Int-Diradical (singlet)	-634.34021	-634.396769	0.277802	0.221243	-634.672991
Int-Diradical (triplet)	-634.340309	-634.397658	0.278045	0.220696	-634.673221