

Electronic Supporting Information

Theoretical Insights into the Metal-free and Formal [2+2+2] Cycloaddition Strategy via Intramolecular Cascade Propargylic Ene/Diels-Alder Reactions with Tautomerization

Xinyao Li, and Jiayi Xu*

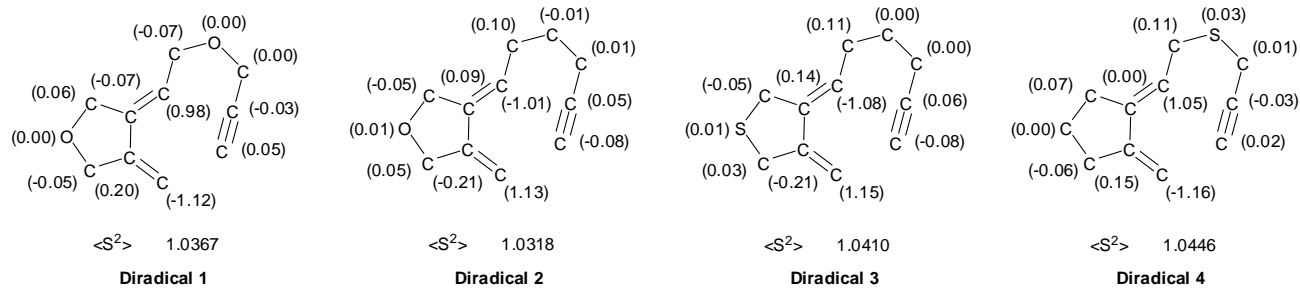
*State Key Laboratory of Chemical Resource Engineering, Department of Organic Chemistry,
Faculty of Science, Beijing University of Chemical Technology, Beijing 100029, P.R. China*

E-mail: jxxu@mail.buct.edu.cn

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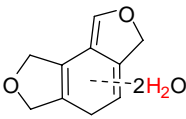
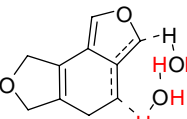
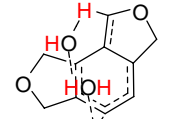
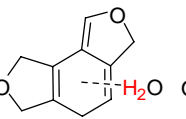
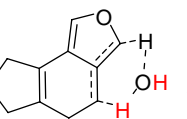
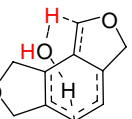
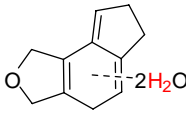
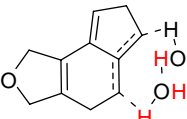
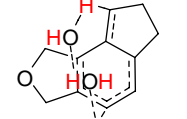
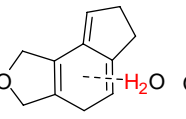
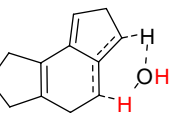
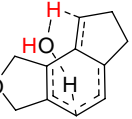
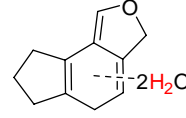
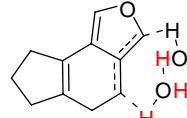
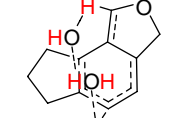
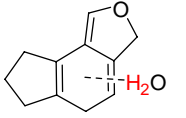
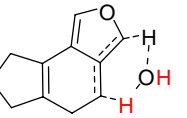
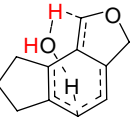
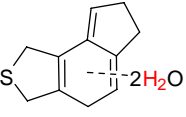
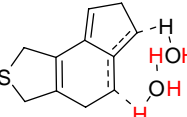
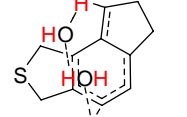
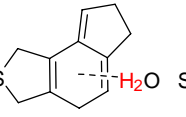
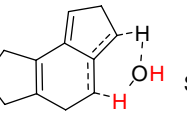
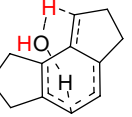
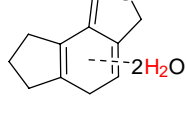
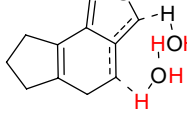
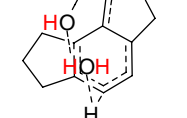
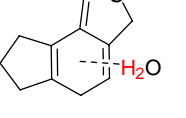
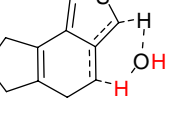
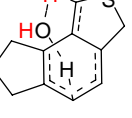
1. The Computed Spin Distribution of the Diradical Species.



Singlet and Triplet Diradical Energies and the Spin Correction Energies Using Yamaguchi-Houk Method

	Diradical 1	Diradical 2	Diradical 3	Diradical 4
E_{ele} (singlet)	-537.367336	-501.4711351	-824.4565929	-824.4534394
E_{ele} (triplet)	-537.366473	-501.4701311	-824.4559668	-824.4527621
ΔE (kcal/mol)	38.3	39.9	42.2	43.8

2.The Tautomerization Assisted by One or Two Water Molecules.

	H-transfer assisted by two water molecules			H-transfer assisted by one water molecule		
structures						
	9-2H₂O	TS4	TS5	9-H₂O	TS4-H₂O	TS5-H₂O
ΔG	-95.0	-55.8	-51.9	-97.1	-47.7	-39.4
(ΔE_0)	-110.4	-74.5	-71.0	-109.0	-63.3	-55.7
$[\Delta G_{sol}]$	-92.5	-57.7	-55.1	-95.7	-49.8	-42.0
structures						
	12-2H₂O	TS10	TS11	12-H₂O	TS10-H₂O	TS11-H₂O
ΔG	-87.0	-40.7	-47.7	-88.7	-33.4	-34.6
(ΔE_0)	-102.3	-59.9	-67.3	-101.2	-49.5	-51.3
$[\Delta G_{sol}]$	-84.0	-42.7	-50.4	-87.4	-35.6	-36.9
structures						
	12-c-2H₂O	TS10-c	TS11-c	12-c-H₂O	TS10-c-H₂O	TS11-c-H₂O
ΔG	-89.1	-50.5	-45.7	-90.6	-42.0	-33.7
(ΔE_0)	-104.7	-69.7	-65.7	-103.7	-58.3	-50.7
$[\Delta G_{sol}]$	-86.0	-52.5	-48.5	-89.0	-44.3	-36.0
structures						
	12-2H₂O	TS10	TS11	12-H₂O	TS10-H₂O	TS11-H₂O
ΔG	-89.6	-41.4	-48.4	-89.6	-33.8	-35.4
(ΔE_0)	-101.5	-60.1	-67.5	-101.5	-49.5	-51.5
$[\Delta G_{sol}]$	-88.7	-46.9	-51.4	-88.7	-36.5	-37.9
structures						
	12-2H₂O	TS10	TS11	12-H₂O	TS10-H₂O	TS11-H₂O
ΔG	-87.5	-48.4	-48.7	-88.8	-41.6	-37.9
(ΔE_0)	-103.3	-67.4	-68.5	-102.1	-57.5	-54.5
$[\Delta G_{sol}]$	-85.3	-50.1	-51.5	-86.6	-43.6	-40.2

3. Computed Energy Surface for the Metal-free [2 + 2 + 2] Cycloaddition

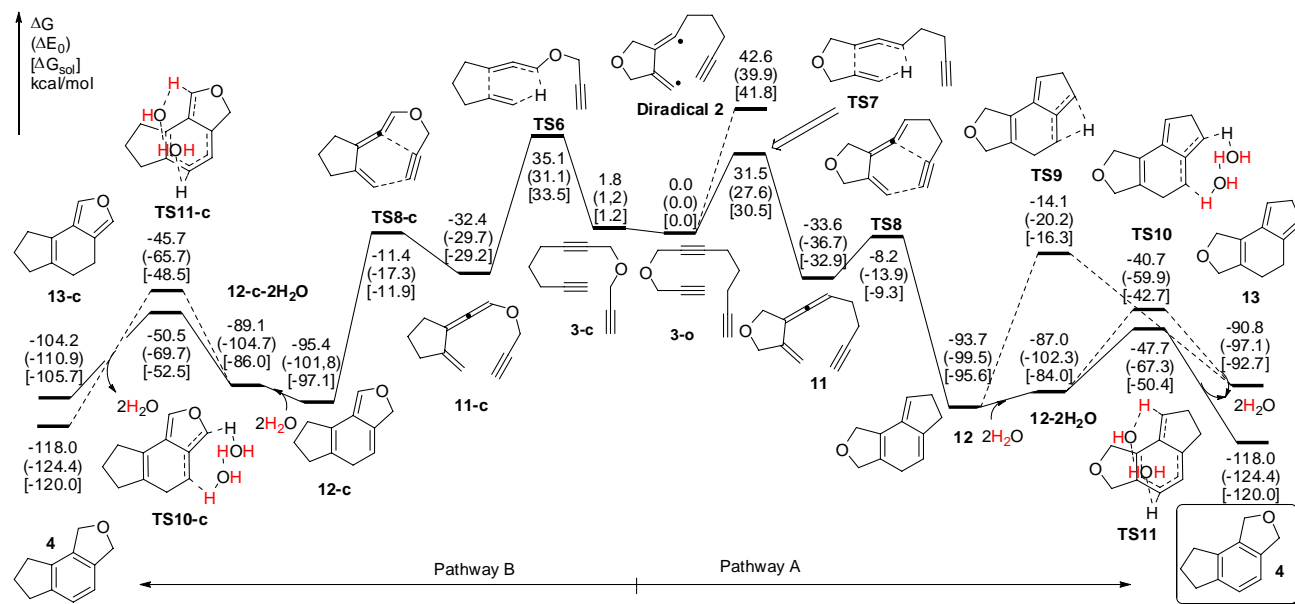


Figure S1. DFT computed full energy surface for the metal-free [2 + 2 + 2] cycloaddition of model system II

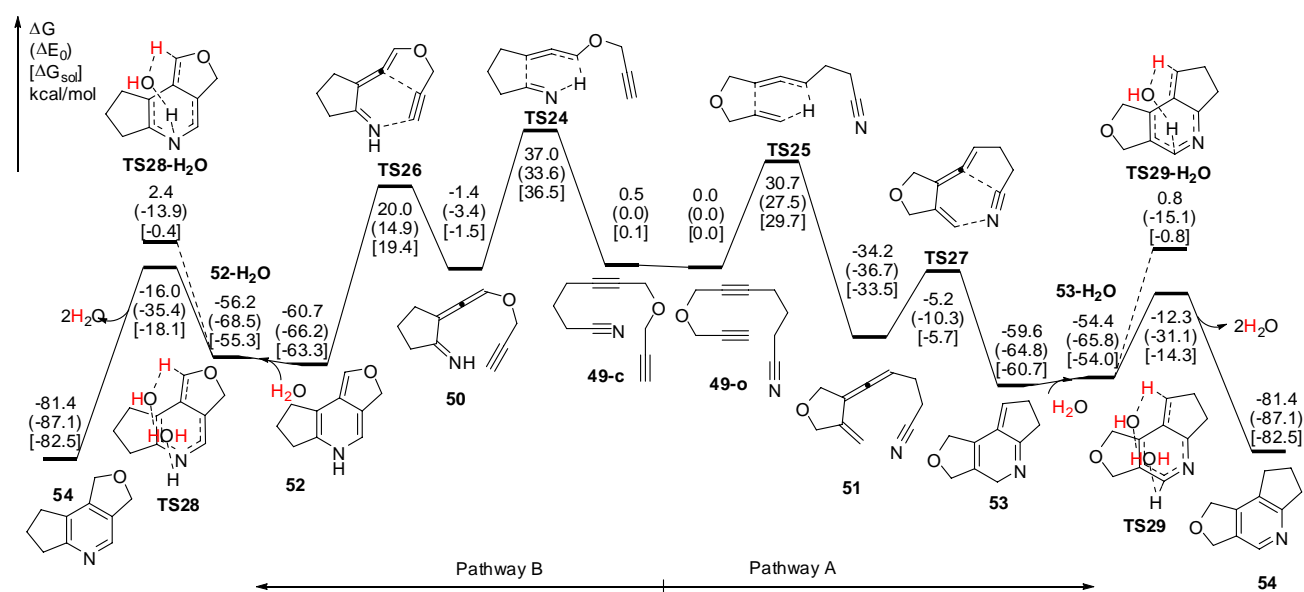


Figure S2. DFT computed full energy surface for the metal-free [2 + 2 + 2] cycloaddition of Danheiser's experimental model.

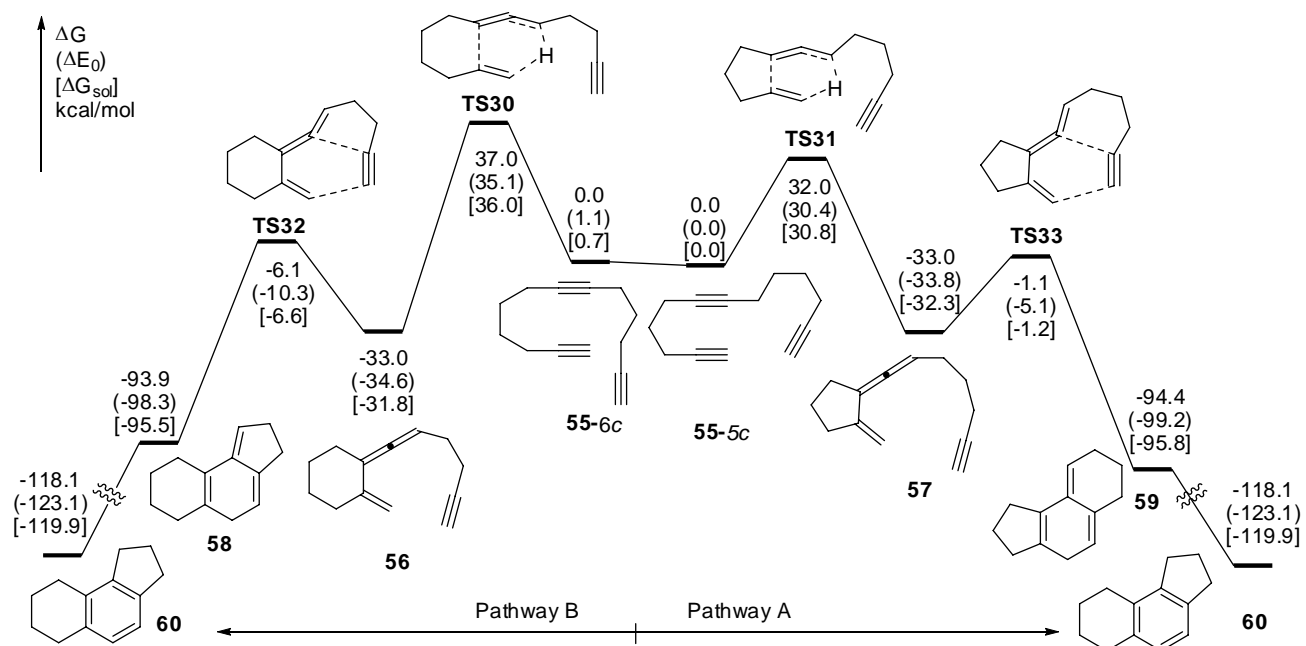


Figure S3. DFT computed full energy surface for the metal-free [2 + 2 + 2] cycloaddition of the unsymmetric triyne with five and six-member ring precursors

4. Computed Energies of All Stationary Points

Table S1. Model system **I**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_s, which equals to E_s + TCGFE, in a.u., solvent = toluene)

	E	H	G	TCGFE	G_s
1	-537.259509	-537.244808	-537.303902	0.124843	-537.302588
H₂O	-76.437180	-76.433400	-76.454823	0.003640	-76.460402
2H₂O	-152.879954	-152.873281	-152.906028	0.020198	-152.914736
Diradical 1	-537.198498	-537.185025	-537.239927	0.127409	-537.238217
TS1	-537.216699	-537.203830	-537.255614	0.126805	-537.255587
8	-537.319695	-537.306549	-537.360448	0.130846	-537.357981
TS2	-537.296263	-537.284720	-537.332304	0.135747	-537.331796
9	-537.430648	-537.420057	-537.466048	0.142393	-537.467391
9-H₂O	-613.870416	-613.855726	-613.913438	0.157961	-613.915573
9-2H₂O	-690.315457	-690.298088	-690.361302	0.180491	-690.364769
TS5	-690.252531	-690.238014	-690.292713	0.179223	-690.305097
TS5-H₂O	-613.797638	-613.785512	-613.834735	0.158270	-613.842287
TS3	-537.307550	-537.296650	-537.343042	0.135405	-537.344846
2	-537.445020	-537.434750	-537.479900	0.143957	-537.480950
TS4	-690.258251	-690.243783	-690.29892	0.178493	-690.309237
TS4-H₂O	-613.785470	-613.773692	-613.821569	0.159721	-613.829983
10	-537.465439	-537.455026	-537.500802	0.143442	-537.502440

Table S2. Model system **II**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_s, which equals to E_s + TCGFE, in a.u., solvent = toluene).

	E	H	G	TCGFE	G_s
3-o	-501.341972	-501.327033	-501.387254	0.148206	-501.383886
Diradical 2	-501.278370	-501.264671	-501.319345	0.151790	-501.317268
TS7	-501.298056	-501.284980	-501.337056	0.150977	-501.335301
11	-501.400493	-501.387209	-501.440750	0.155515	-501.436382
TS8	-501.364177	-501.352439	-501.400269	0.159407	-501.398661
12	-501.500463	-501.489551	-501.536502	0.165442	-501.536173
12-H₂O	-577.940450	-577.925502	-577.983505	0.181729	-577.983565
12-2H₂O	-654.384985	-654.367014	-654.431943	0.202628	-654.432437
TS9	-501.374230	-501.363139	-501.409758	0.158784	-501.409874
TS10	-654.317385	-654.302638	-654.358153	0.20112	-654.366663
TS10-H₂O	-577.857981	-577.845533	-577.895239	0.180972	-577.901000
13	-501.496762	-501.486096	-501.531919	0.166234	-501.531660
TS11	-654.329236	-654.314537	-654.369376	0.203557	-654.379000
TS11-H₂O	-577.860923	-577.848884	-577.897283	0.183190	-577.903034
4	-501.540234	-501.529768	-501.575311	0.167965	-501.575063
3-c	-501.340123	-501.325202	-501.384409	0.149073	-501.382051

TS6	-501.292393	-501.279311	-501.331375	0.150356	-501.330502
11-c	-501.393658	-501.380350	-501.434524	0.154735	-501.430377
TS8-c	-501.369604	-501.357977	-501.405456	0.160036	-501.402845
12-c	-501.504249	-501.493609	-501.539344	0.166981	-501.538604
12-c-H₂O	-577.944343	-577.929710	-577.986466	0.183305	-577.986144
12-c-2H₂O	-654.388809	-654.370975	-654.435235	0.203588	-654.435711
TS10-c	-654.333074	-654.318413	-654.37378	0.202878	-654.382364
TS10-c-H₂O	-577.872040	-577.859784	-577.908982	0.182836	-577.914918
13-c	-501.518656	-501.508303	-501.553330	0.168382	-501.552276
TS11-c	-654.326624	-654.312134	-654.366143	0.203585	-654.375848
TS11-c-H₂O	-577.859995	-577.848137	-577.895857	0.183859	-577.901708

Table S3. Model system **III**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_s, which equals to E_s + TCGFE, in a.u., solvent = toluene).

	E	H	G	TCGFE	G_s
5-s	-824.334299	-824.318704	-824.379758	0.144258	-824.376758
Diradical 3	-824.267044	-824.252799	-824.309478	0.147115	-824.308246
TS13	-824.284690	-824.270985	-824.324775	0.145839	-824.324087
15	-824.389516	-824.375725	-824.431057	0.151020	-824.427418
TS15	-824.353960	-824.341779	-824.390987	0.155468	-824.390231
17	-824.493105	-824.481738	-824.530109	0.161493	-824.530772
17-H₂O	-900.933167	-900.917719	-900.977436	0.177419	-900.978444
17-2H₂O	-977.37799	-977.36037	-977.424308	0.2001	-977.425916
TS17	-977.310053	-977.294851	-977.351707	0.197198	-977.366183
TS17-H₂O	-900.850422	-900.837551	-900.888489	0.177214	-900.895256
19	-824.489399	-824.478317	-824.525367	0.162496	-824.526075
TS19	-977.321883	-977.306739	-977.362882	0.199701	-977.373367
TS19-H₂O	-900.853590	-900.841059	-900.890986	0.179196	-900.897575
6	-824.532408	-824.521461	-824.568589	0.163778	-824.569345
5-c	-824.331942	-824.316344	-824.377296	0.144371	-824.374913
Diradical 4	-824.264552	-824.250138	-824.307779	0.145660	-824.304647
TS12	-824.284954	-824.271128	-824.325477	0.144954	-824.324530
14	-824.386559	-824.372660	-824.428081	0.150556	-824.423704
TS14	-824.353844	-824.341666	-824.390594	0.155649	-824.389029
16	-824.494160	-824.482947	-824.530533	0.162373	-824.530853
16-H₂O	-900.934114	-900.919197	-900.976048	0.180556	-900.975177
16-2H₂O	-977.378867	-977.360889	-977.425298	0.200825	-977.427366
TS18	-977.321588	-977.306516	-977.362895	0.198404	-977.37141
TS18-H₂O	-900.863139	-900.850379	-900.900872	0.178181	-900.906588
7	-824.509911	-824.499094	-824.545306	0.164288	-824.545245
TS16	-977.32334	-977.308449	-977.363461	0.201342	-977.373508
TS16-H₂O	-900.858344	-900.846036	-900.894965	0.180666	-900.901152

Table S4. Intramolecular propargylic ene reactions with different diynes. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.).

	E	H	G
20	-271.386964	-271.377435	-271.421428
TS(20)	-271.311587	-271.303903	-271.341891
21	-310.680069	-310.669198	-310.716767
TS(21)	-310.630011	-310.621434	-310.661398
22	-349.973377	-349.961242	-350.011696
TS(22)	-349.917034	-349.907156	-349.950371
23	-389.269803	-389.256405	-389.309887
TS(23)	-389.203616	-389.192445	-389.238615
24	-77.329619	-77.325876	-77.349225
	-116.637296	-116.632410	-116.661494
TS(24)	-193.913763	-193.907225	-193.941705
25	-389.273413	-389.259889	-389.312279
TS(25)	-389.225591	-389.214217	-389.260016
26	-384.734866	-384.723348	-384.773257
TS(26)	-384.684526	-384.675024	-384.718318
27	-366.009928	-365.997855	-366.047740
TS(27)	-365.962244	-365.952362	-365.995235
28	-346.600107	-346.589466	-346.636750
TS(28)	-346.554565	-346.546177	-346.585895
29	-669.592483	-669.581148	-669.630307
TS(29)	-669.541138	-669.532151	-669.573546
30	-464.487916	-464.474326	-464.528927
TS(30)	-464.444087	-464.431419	-464.482123
31	-499.245954	-499.232101	-499.289332
TS(31)	-499.206083	-499.193981	-499.243452
32	-577.622676	-577.607945	-577.667179
TS(32)	-577.582597	-577.569581	-577.621855
33	-422.743566	-422.731284	-422.783302
TS(33)	-422.703530	-422.693014	-422.738131
34	-445.865676	-445.854562	-445.903871
TS(34)	-445.821304	-445.812122	-445.854337
35	-551.151396	-551.138575	-551.193440
TS(35)	-551.109198	-551.098120	-551.145681
36	-692.389122	-692.370198	-692.439713
TS(36)	-692.347477	-692.330009	-692.393917
37	-695.527009	-695.507993	-695.578554
TS(37)	-695.479565	-695.462021	-695.526222
38	-949.311695	-949.287461	-949.369416
TS(38)	-949.268233	-949.245336	-949.321873
39	-460.882933	-460.871257	-460.921570
TS(39)	-460.869471	-460.859104	-460.904382

40	-500.183626	-500.170592	-500.224512
TS(40)	-500.170993	-500.159829	-500.206703
41	-463.253497	-463.240753	-463.293039
TS(41)	-463.237829	-463.226766	-463.273038
42	-502.545447	-502.531345	-502.587175
TS(42)	-502.523791	-502.511680	-502.560306

Table S5. Our designed model systems. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.).

	E	H	G
43	-690.843515	-690.826418	-690.891774
TS20	-690.828871	-690.813232	-690.872371
44	-690.977640	-690.962430	-691.021205
TS21	-690.946182	-690.932183	-690.985679
45	-691.037225	-691.024514	-691.074906
46	-653.912975	-653.896158	-653.960020
TS22	-653.896102	-653.880571	-653.939347
47	-654.028377	-654.013176	-654.072208
TS23	-654.002128	-653.988515	-654.040773
48	-654.134461	-654.122043	-654.171780

Table S6. Danheiser's experimental model. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_s, which equals to E_s + TCGFE, in a.u., solvent = toluene).

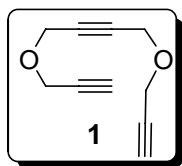
	E	H	G	TCGFE	G_s
49-o	-517.455302	-517.440716	-517.499342	0.139141	-517.498919
TS25	-517.411478	-517.398698	-517.450398	0.140623	-517.451581
51	-517.513722	-517.500753	-517.553846	0.145301	-517.552331
TS27	-517.471660	-517.460276	-517.507644	0.149269	-517.508023
53	-517.558565	-517.547845	-517.594273	0.154393	-517.595657
53-H₂O	-593.997273	-593.982069	-594.040865	0.169292	-594.045447
TS29	-593.916560	-593.904696	-593.952869	0.171954	-593.960659
54	-517.594156	-517.583836	-517.629137	0.156387	-517.630376
49-c	-517.455305	-517.440793	-517.498496	0.139991	-517.498817
TS24	-517.401804	-517.389182	-517.440418	0.140503	-517.440758
50	-517.460725	-517.447634	-517.501538	0.144032	-517.501297
TS26	-517.431499	-517.420010	-517.467390	0.148826	-517.467981
52	-517.560773	-517.549981	-517.596024	0.155338	-517.599841
52-H₂O	-594.001593	-593.986818	-594.043686	0.171917	-594.047466
TS28	-593.914677	-593.903083	-593.950370	0.174417	-593.959977

Table S7. The unsymmetric triyne with five and six-member ring precursors. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_s, which equals to E_s +

TCGFE, in a.u., solvent = toluene).

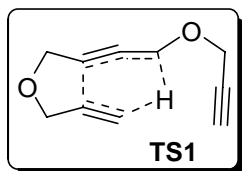
	E	H	G	TCGFE	G_s
55-5c	-504.716780	-504.701146	-504.760689	0.201969	-504.756017
TS31	-504.668276	-504.653586	-504.709713	0.200411	-504.706940
57	-504.770658	-504.755778	-504.813199	0.205502	-504.807441
TS33	-504.724921	-504.711845	-504.762479	0.210735	-504.757960
59	-504.874892	-504.863147	-504.911104	0.219132	-504.908643
60	-504.913029	-504.901523	-504.948942	0.220529	-504.947018
55-6c	-504.714961	-504.698596	-504.760749	0.200428	-504.754980
TS30	-504.660808	-504.646187	-504.701784	0.200782	-504.698644
56	-504.771996	-504.757611	-504.813351	0.207819	-504.806694
TS32	-504.733201	-504.720375	-504.770445	0.211609	-504.766592
58	-504.873444	-504.861526	-504.910360	0.218090	-504.908236

5. Coordinates of All Stationary Points [imaginary frequencies (in brackets, cm^{-1}) for the transition states occurring in the thermal cycloaddition]



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.193641	1.381209	0.191817
2	6	0	2.712758	2.476410	0.073519
3	1	0	2.272468	3.437244	-0.036000
4	6	0	3.858138	0.082677	0.336752
5	1	0	3.834965	-0.228880	1.390315
6	1	0	4.907678	0.192885	0.050488
7	6	0	2.264848	-1.705598	0.053353
8	1	0	2.178004	-2.582962	-0.592133
9	1	0	2.534841	-2.060265	1.058850
10	6	0	0.975075	-1.019052	0.106900
11	6	0	-0.111368	-0.503069	0.145508
12	6	0	-1.396662	0.171656	0.219333
13	1	0	-1.238017	1.261109	0.201261
14	1	0	-1.897223	-0.073255	1.165526
15	6	0	-3.460478	0.462896	-0.929019
16	1	0	-3.918840	0.170187	-1.876038
17	1	0	-3.301793	1.551430	-0.957310
18	6	0	-4.363218	0.133168	0.179234
19	6	0	-5.109368	-0.136334	1.082698
20	1	0	-5.768745	-0.378779	1.880338
21	8	0	3.341891	-0.950370	-0.496027
22	8	0	-2.214833	-0.218691	-0.884706

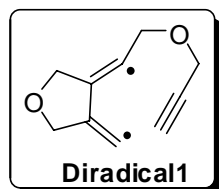


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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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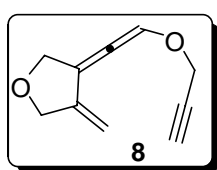
1	6	0	-1.756237	1.101152	-0.187609
2	6	0	-0.737958	1.811885	-0.269039
3	1	0	-0.262406	2.767999	-0.333619
4	6	0	-3.237689	0.948344	-0.170151
5	1	0	-3.610338	1.069378	-1.198653
6	1	0	-3.694632	1.713654	0.458860
7	6	0	-2.834683	-1.347836	-0.166769
8	1	0	-3.007436	-2.229527	0.451464
9	1	0	-3.126071	-1.579493	-1.202367
10	6	0	-1.422212	-0.926231	-0.122001
11	6	0	-0.193172	-1.100203	-0.076673
12	6	0	0.999163	-0.360074	-0.160016
13	1	0	0.448034	0.757416	-0.238373
14	1	0	1.562024	-0.470482	-1.094138
15	6	0	2.970061	0.443819	0.893699
16	1	0	3.443051	0.380075	1.875552
17	1	0	2.658335	1.485930	0.740245
18	6	0	3.931337	0.062359	-0.144831
19	6	0	4.729403	-0.244500	-0.989901
20	1	0	5.434453	-0.520952	-1.735799
21	8	0	-3.647862	-0.304688	0.357624
22	8	0	1.831226	-0.408598	0.971947



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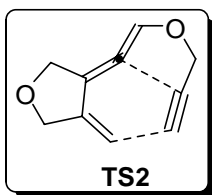
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1	6	0	-1.816519	0.932262	0.282227
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3	1	0	-2.053458	3.063468	0.921139
4	6	0	-3.143083	0.498805	-0.362592
5	1	0	-3.174149	0.832493	-1.410337
6	1	0	-4.023876	0.869197	0.160849
7	6	0	-1.796986	-1.353169	-0.459126
8	1	0	-1.696170	-2.339215	-0.005383
9	1	0	-1.543537	-1.419453	-1.527422
10	6	0	-0.941154	-0.269570	0.214701
11	6	0	0.300264	-0.401029	0.625995

12	6	0	1.347780	-1.434912	0.697309
13	1	0	0.909353	-2.429485	0.532667
14	1	0	1.808178	-1.443463	1.696733
15	6	0	3.315220	-0.283779	-0.070227
16	1	0	4.148511	-0.503731	-0.741836
17	1	0	3.694304	-0.339682	0.960681
18	6	0	2.823839	1.071314	-0.334379
19	6	0	2.467358	2.197107	-0.560344
20	1	0	2.127599	3.185523	-0.751910
21	8	0	-3.141297	-0.920984	-0.289777
22	8	0	2.366137	-1.319192	-0.298614



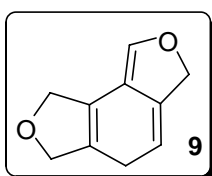
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3	1	0	-3.072340	2.782592	-0.417198
4	6	0	-3.695316	0.044889	-0.136712
5	1	0	-4.118665	-0.108390	-1.141730
6	1	0	-4.441720	0.540046	0.485808
7	6	0	-2.061404	-1.566632	0.050953
8	1	0	-1.623474	-2.212040	0.811943
9	1	0	-2.087821	-2.108624	-0.906643
10	6	0	-1.326023	-0.240163	-0.114920
11	6	0	-0.028118	-0.080731	-0.145575
12	6	0	1.270573	0.036804	-0.219314
13	1	0	-1.234390	2.556580	-0.416086
14	1	0	1.801094	-0.034391	-1.167055
15	6	0	3.359595	0.753769	0.645997
16	1	0	3.791166	0.915858	1.635217
17	1	0	3.266726	1.730507	0.154677
18	6	0	4.231216	-0.118549	-0.141620
19	6	0	4.959771	-0.826626	-0.783928
20	1	0	5.600871	-1.458357	-1.349509
21	8	0	-3.379399	-1.212220	0.461761
22	8	0	2.063032	0.203244	0.896777



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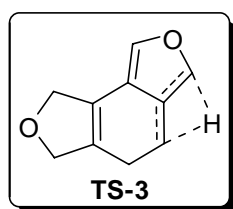
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1	6	0	-2.815698	0.372205	-0.115927
2	6	0	-1.605353	-1.614336	-0.307645
3	1	0	-3.597360	0.309754	0.655472
4	1	0	-3.101813	1.149064	-0.830895
5	1	0	-1.121689	-2.131738	-1.138773
6	1	0	-1.948808	-2.366870	0.418613
7	6	0	-0.708802	-0.590198	0.364607
8	6	0	-1.457455	0.606152	0.508595
9	6	0	-0.951094	1.792797	0.952250
10	1	0	-0.085702	1.817482	1.597528
11	1	0	-1.538839	2.703589	0.893759
12	6	0	0.634633	-0.651298	0.482187
13	6	0	1.782060	-1.194726	0.841058
14	1	0	1.928016	-1.883088	1.664437
15	6	0	2.716536	0.084306	-0.831600
16	1	0	3.639903	0.649365	-0.958593
17	1	0	2.506757	-0.485471	-1.744208
18	6	0	1.564631	0.964154	-0.531838
19	6	0	0.959520	2.037503	-0.566895
20	1	0	0.691667	3.048365	-0.764010
21	8	0	-2.717017	-0.872020	-0.815035
22	8	0	2.956267	-0.834205	0.244774



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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2	6	0	1.704517	-1.608331	0.000164

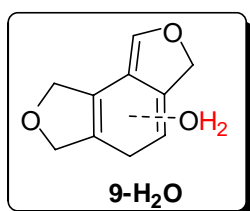
3	1	0	3.314782	0.889498	-0.886655
4	1	0	3.314648	0.889529	0.887137
5	1	0	1.620143	-2.249114	0.888200
6	1	0	1.620277	-2.249151	-0.887857
7	6	0	0.704208	-0.487284	0.000066
8	6	0	1.339341	0.694601	0.000094
9	6	0	0.664647	2.035327	0.000019
10	1	0	0.998469	2.622674	-0.870233
11	1	0	0.998333	2.622703	0.870304
12	6	0	-0.736146	-0.542410	-0.000049
13	6	0	-1.652419	-1.530593	-0.000111
14	1	0	-1.537584	-2.604487	-0.000089
15	6	0	-2.923364	0.362136	-0.000224
16	1	0	-3.458559	0.700873	-0.890603
17	1	0	-3.458682	0.700863	0.890084
18	6	0	-1.457658	0.732486	-0.000123
19	8	0	2.984609	-0.959707	0.000249
20	6	0	-0.846617	1.922956	-0.000096
21	1	0	-1.414981	2.848086	-0.000154
22	8	0	-2.947815	-1.095077	-0.000229



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	0.763928	-0.550056	0.039133
2	6	0	-0.671661	-0.493298	0.022870
3	6	0	-1.319745	0.682985	0.018701
4	6	0	-0.682250	2.044075	0.079463
5	6	0	0.803373	1.987711	-0.203030
6	6	0	1.510956	0.749758	0.012374
7	6	0	1.676569	-1.541703	0.016267
8	6	0	2.893046	0.307753	-0.080946
9	6	0	-1.657458	-1.628022	-0.025738
10	6	0	-2.796525	0.430395	-0.021838
11	1	0	3.821681	0.841545	0.020197
12	1	0	1.588784	-2.615817	0.022090
13	1	0	-3.320478	0.854028	0.846824

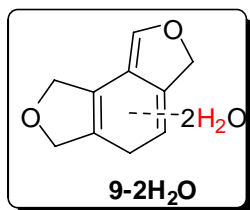
14	1	0	-3.262318	0.848897	-0.926042
15	1	0	-1.578163	-2.297513	0.840987
16	1	0	-1.551436	-2.237039	-0.934096
17	1	0	-0.934009	2.504227	1.056502
18	1	0	1.788898	1.005471	1.101769
19	1	0	1.360095	2.916050	-0.239501
20	1	0	-1.167401	2.703140	-0.656930
21	8	0	-2.944596	-0.995845	-0.017318
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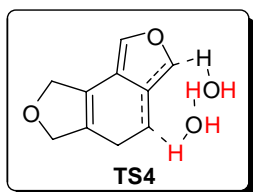
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3	1	0	-3.207457	1.569553	0.575943
4	1	0	-3.514539	0.882501	-1.030046
5	1	0	-2.323401	-2.279698	0.052120
6	1	0	-2.002574	-1.625120	1.671390
7	6	0	-1.015985	-0.542869	0.060877
8	6	0	-1.464024	0.654191	-0.348470
9	6	0	-0.616339	1.724851	-0.972843
10	1	0	-0.715950	2.664770	-0.408043
11	1	0	-1.000426	1.968356	-1.976216
12	6	0	0.378113	-0.886773	-0.071077
13	6	0	1.128104	-1.969019	0.221997
14	1	0	0.856590	-2.918904	0.658816
15	6	0	2.639372	-0.513858	-0.665304
16	1	0	3.366498	0.016167	-0.046383
17	1	0	3.046684	-0.647212	-1.670084
18	6	0	1.266524	0.119879	-0.654629
19	8	0	-3.301213	-0.503282	0.504353
20	6	0	0.843744	1.324375	-1.066956
21	1	0	1.530822	2.041207	-1.506483
22	8	0	2.448039	-1.839124	-0.088508
23	8	0	2.331587	2.196220	1.812234
24	1	0	1.966193	1.838376	2.627053

25 1 0 1.769828 1.842467 1.108977



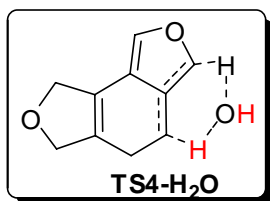
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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3	6	0	-1.810153	-0.729711	0.383795
4	6	0	-0.883762	-1.566658	1.218518
5	6	0	0.496194	-0.945099	1.349486
6	6	0	0.769787	0.265734	0.834491
7	6	0	0.408034	2.192157	-0.306717
8	6	0	2.014665	1.120411	0.900806
9	6	0	-2.679499	1.008681	-0.903482
10	6	0	-3.222117	-1.087158	0.024505
11	1	0	2.902808	0.661550	0.460685
12	1	0	2.241300	1.451162	1.917632
13	1	0	0.040971	3.025052	-0.889086
14	1	0	-3.288785	-2.016319	-0.560069
15	1	0	-3.865217	-1.206601	0.908814
16	1	0	-2.458771	1.162985	-1.968029
17	1	0	-3.043804	1.959810	-0.492301
18	1	0	-0.814315	-2.583579	0.800161
19	8	0	2.064669	-2.041353	-1.359052
20	1	0	1.884279	-2.986344	-1.363187
21	1	0	1.484673	-1.662550	-0.678513
22	1	0	1.235375	-1.483058	1.935734
23	1	0	-1.317998	-1.718938	2.220072
24	8	0	-3.699236	0.008253	-0.768424
25	8	0	1.689724	2.314407	0.121931
26	8	0	4.432754	-0.720111	-0.564372
27	1	0	3.742860	-1.267293	-0.978532
28	1	0	5.004770	-0.432863	-1.281448



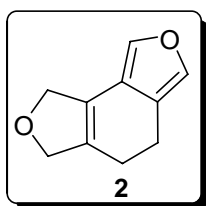
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.072591	1.039876	0.143728
2	6	0	-1.404138	0.519343	-0.093264
3	6	0	-1.737576	-0.696301	0.357698
4	6	0	-0.835384	-1.597028	1.151244
5	6	0	0.647966	-1.171845	1.073865
6	6	0	0.886309	0.216492	0.782210
7	6	0	0.566549	2.227892	-0.133412
8	6	0	2.145174	0.941512	0.779259
9	6	0	-2.560437	1.142627	-0.821824
10	6	0	-3.157968	-0.990338	-0.023900
11	1	0	2.872051	0.386116	0.014470
12	1	0	2.699115	1.047927	1.711419
13	1	0	0.204344	3.123457	-0.619435
14	1	0	-3.230318	-1.850927	-0.704251
15	1	0	-3.798838	-1.195452	0.844249
16	1	0	-2.343449	1.308298	-1.886671
17	1	0	-2.875523	2.101103	-0.387915
18	1	0	-0.930524	-2.628641	0.794557
19	8	0	1.869827	-2.150945	-1.164711
20	1	0	2.139499	-3.073605	-1.204984
21	1	0	1.146922	-1.686178	0.105808
22	1	0	1.254933	-1.563794	1.892746
23	1	0	-1.182895	-1.612084	2.194590
24	8	0	-3.625436	0.194049	-0.685043
25	8	0	1.834161	2.253275	0.255529
26	8	0	3.700532	-0.604801	-0.823640
27	1	0	2.868536	-1.407156	-1.059681
28	1	0	4.076044	-0.275058	-1.645599



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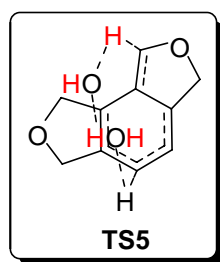
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			X	Y	Z
1	6	0	-0.291568	0.890208	-0.203358
2	6	0	1.098837	0.518446	-0.031071
3	6	0	1.473109	-0.762178	-0.157942
4	6	0	0.568871	-1.908498	-0.516840
5	6	0	-0.915624	-1.509182	-0.596204
6	6	0	-1.213405	-0.116947	-0.607433
7	6	0	-1.037868	2.014596	0.046560
8	6	0	-2.535166	0.439903	-0.443299
9	6	0	2.280523	1.375216	0.322744
10	6	0	2.949048	-0.870570	0.091253
11	1	0	-2.847124	-0.280161	0.520308
12	1	0	-3.326832	0.316861	-1.177777
13	1	0	-0.744830	3.001521	0.375043
14	1	0	3.181397	-1.517996	0.948646
15	1	0	3.495275	-1.262254	-0.778374
16	1	0	2.169746	1.866137	1.299902
17	1	0	2.477197	2.155364	-0.425126
18	1	0	0.699357	-2.722241	0.208539
19	8	0	-2.850935	-1.591126	1.233487
20	1	0	-2.621888	-1.453968	2.159352
21	1	0	-1.644431	-1.705357	0.436576
22	1	0	-1.505132	-2.121730	-1.281509
23	1	0	0.902139	-2.328879	-1.476276
24	8	0	3.388090	0.467140	0.366672
25	8	0	-2.349082	1.827329	-0.129629



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.779823	0.460117	-0.088668
2	6	0	1.681661	-1.611932	0.143803
3	1	0	3.249510	0.782320	-1.029987
4	1	0	3.288149	0.987434	0.731118

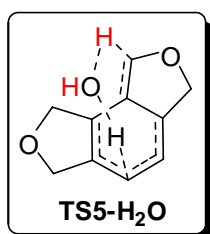
5	1	0	1.608965	-2.167204	1.088067
6	1	0	1.598825	-2.334802	-0.679672
7	6	0	0.672161	-0.504545	0.040796
8	6	0	1.295433	0.675868	-0.085349
9	6	0	0.581883	1.983779	-0.291638
10	1	0	0.516344	2.182191	-1.370869
11	1	0	1.157141	2.812618	0.133243
12	6	0	-0.773851	-0.572104	0.021099
13	6	0	-1.686359	-1.575453	-0.108251
14	1	0	-1.612938	-2.644565	-0.214313
15	6	0	-2.833640	0.299278	0.004230
16	1	0	-3.761617	0.846118	0.017983
17	6	0	-1.530336	0.657951	0.094943
18	6	0	-0.839541	1.972875	0.326199
19	1	0	-1.426570	2.808218	-0.063309
20	1	0	-0.745522	2.130417	1.407967
21	8	0	-2.950245	-1.060736	-0.121105
22	8	0	2.955784	-0.953983	0.075703



(Nimag=1) -984.3528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.622898	-0.741955	-0.384190
2	6	0	-0.797876	-0.723034	-0.301714
3	6	0	-1.483878	0.421619	-0.618646
4	6	0	-0.832191	1.633527	-0.988160
5	6	0	0.569429	1.527930	-1.315931
6	6	0	1.262752	0.394995	-1.009120
7	6	0	1.608294	-1.541393	0.174329
8	6	0	2.737990	0.063839	-1.075155
9	6	0	-1.752036	-1.777518	0.174395
10	6	0	-2.951238	0.177747	-0.396715
11	1	0	3.386224	0.864142	-0.701050
12	1	0	3.071111	-0.195745	-2.090319
13	1	0	1.566805	-2.589474	0.438218
14	1	0	-3.383888	0.863970	0.343609

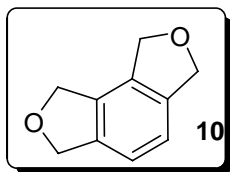
15	1	0	-3.530391	0.275395	-1.324544
16	1	0	-1.567082	-2.082020	1.214903
17	1	0	-1.734977	-2.683226	-0.446535
18	1	0	-0.522021	1.953358	0.601340
19	1	0	0.251239	2.846454	1.778609
20	8	0	-0.220161	2.013661	1.652735
21	1	0	1.261918	-0.617769	1.620515
22	1	0	1.074116	2.387446	-1.748979
23	1	0	-1.411703	2.459950	-1.386992
24	8	0	-3.052136	-1.169134	0.085696
25	8	0	2.898674	-1.096572	-0.227847
26	8	0	1.047743	0.073902	2.391207
27	1	0	1.840166	0.191377	2.926746
28	1	0	0.400655	1.136744	2.005593



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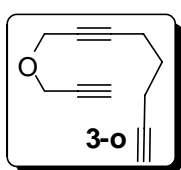
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.625763	-0.632317	-0.346660
2	6	0	-0.796497	-0.542736	-0.369371
3	6	0	-1.357723	0.699761	-0.248018
4	6	0	-0.559155	1.877828	-0.112055
5	6	0	0.801964	1.780286	-0.589216
6	6	0	1.374420	0.553160	-0.734677
7	6	0	1.518253	-1.462363	0.315770
8	6	0	2.819281	0.119960	-0.764833
9	6	0	-1.855036	-1.595198	-0.212209
10	6	0	-2.842199	0.539353	-0.066518
11	1	0	3.518679	0.864386	-0.377149
12	1	0	3.158892	-0.196028	-1.760774
13	1	0	1.423218	-2.497480	0.613329
14	1	0	-3.170257	0.883863	0.925592
15	1	0	-3.426810	1.077609	-0.820996
16	1	0	-1.750150	-2.155546	0.731642
17	1	0	-1.882150	-2.321778	-1.031464
18	1	0	-0.032036	1.263363	1.365380
19	1	0	1.112948	0.958593	2.599504

20	8	0	0.427206	0.523166	2.072377
21	1	0	0.853385	-0.349514	1.561361
22	1	0	1.385521	2.688521	-0.707683
23	1	0	-1.038550	2.850035	-0.078140
24	8	0	-3.092159	-0.865110	-0.212136
25	8	0	2.849064	-1.044610	0.108024



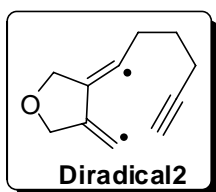
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.857068	0.479723	0.063654
2	6	0	-1.692831	-1.571762	0.034655
3	1	0	-3.299921	0.763270	1.029156
4	1	0	-3.421216	0.979336	-0.730061
5	1	0	-1.559819	-2.293628	-0.778078
6	1	0	-1.662810	-2.122600	0.986442
7	6	0	-0.693686	-0.447003	0.007591
8	6	0	-1.379061	0.767074	0.020379
9	6	0	0.693691	-0.447025	-0.007000
10	6	0	1.692596	-1.571925	-0.033723
11	1	0	1.560556	-2.292239	0.780597
12	6	0	2.857062	0.479923	-0.063358
13	1	0	3.420625	0.978309	0.731602
14	1	0	3.300481	0.765235	-1.028027
15	6	0	1.379064	0.767036	-0.020132
16	6	0	0.699165	1.981995	-0.011650
17	1	0	1.241047	2.921536	-0.023731
18	8	0	2.968960	-0.938638	0.126306
19	6	0	-0.699165	1.982020	0.011607
20	1	0	-1.241016	2.921583	0.023347
21	1	0	1.661102	-2.124577	-0.984358
22	8	0	-2.968663	-0.938432	-0.128684



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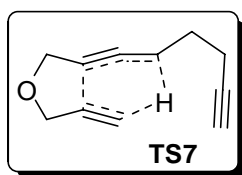
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.152370	1.386627	-0.274547
2	6	0	-2.671275	2.485424	-0.197386
3	1	0	-2.229271	3.449066	-0.126565
4	6	0	-3.820256	0.085579	-0.369121
5	1	0	-3.722227	-0.307890	-1.389818
6	1	0	-4.886988	0.225711	-0.172287
7	6	0	-2.330941	-1.743371	0.133783
8	1	0	-2.261128	-2.513684	0.905460
9	1	0	-2.636114	-2.238559	-0.799949
10	6	0	-1.027222	-1.107092	-0.055100
11	6	0	0.056671	-0.608367	-0.221545
12	6	0	1.359190	0.025377	-0.394688
13	6	0	2.164403	0.120022	0.914710
14	1	0	1.210265	1.031068	-0.807802
15	1	0	1.938870	-0.528432	-1.141219
16	6	0	3.529280	0.814766	0.733734
17	1	0	1.584431	0.679052	1.654273
18	1	0	2.316734	-0.883804	1.319955
19	1	0	4.005192	0.926774	1.713835
20	1	0	3.377719	1.830988	0.349839
21	6	0	4.443696	0.101468	-0.155329
22	6	0	5.189278	-0.497740	-0.884863
23	1	0	5.852795	-1.022888	-1.527486
24	8	0	-3.374125	-0.877945	0.580484



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.754804	0.934845	-0.232895
2	6	0	1.402931	2.129019	-0.643181
3	1	0	1.846611	3.104349	-0.766002
4	6	0	3.143919	0.550203	0.301483
5	1	0	3.226630	0.833464	1.361456
6	1	0	3.965362	0.998630	-0.256506

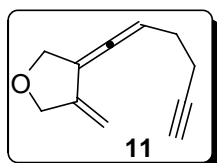
7	6	0	1.917618	-1.384077	0.383854
8	1	0	1.844364	-2.347602	-0.121461
9	1	0	1.746685	-1.528098	1.461670
10	6	0	0.955766	-0.321243	-0.171800
11	6	0	-0.296992	-0.513832	-0.516333
12	6	0	-1.318375	-1.567495	-0.580361
13	1	0	-0.862944	-2.536528	-0.313797
14	1	0	-1.666023	-1.674519	-1.617025
15	6	0	-2.543288	-1.343014	0.331727
16	1	0	-3.179249	-2.231739	0.266707
17	1	0	-2.216445	-1.255893	1.371598
18	6	0	-3.402886	-0.116643	-0.038539
19	1	0	-4.344910	-0.168944	0.518664
20	1	0	-3.673152	-0.168148	-1.100339
21	6	0	-2.774795	1.173182	0.234523
22	6	0	-2.278333	2.241707	0.476833
23	1	0	-1.815696	3.176368	0.677945
24	8	0	3.220819	-0.862157	0.155652



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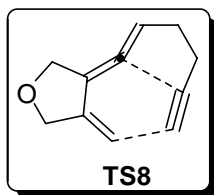
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.694171	1.112888	-0.098749
2	6	0	-0.635135	1.769641	-0.102971
3	1	0	-0.117499	2.705103	-0.060288
4	6	0	-3.183897	1.063216	-0.088463
5	1	0	-3.545511	1.279208	-1.105369
6	1	0	-3.588915	1.812747	0.592824
7	6	0	-2.946692	-1.247686	-0.263033
8	1	0	-3.158624	-2.155554	0.302956
9	1	0	-3.285652	-1.391242	-1.300081
10	6	0	-1.509498	-0.909969	-0.240330
11	6	0	-0.289691	-1.147059	-0.262742
12	6	0	0.958315	-0.502622	-0.247722
13	6	0	1.886151	-0.706289	0.951933
14	1	0	0.487190	0.649253	-0.197517
15	1	0	1.495685	-0.530662	-1.200061
16	6	0	3.058501	0.296953	0.987394

17	1	0	1.308992	-0.603176	1.874889
18	1	0	2.287708	-1.723417	0.933605
19	1	0	3.630677	0.140007	1.907931
20	1	0	2.667002	1.319230	1.039231
21	6	0	3.963748	0.189113	-0.154307
22	6	0	4.705230	0.088040	-1.096187
23	1	0	5.363601	0.002884	-1.925781
24	8	0	-3.677726	-0.192717	0.353591



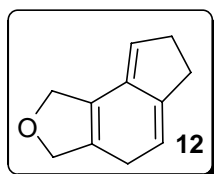
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.141451	0.950076	-0.061067
2	6	0	-1.684012	2.197795	0.054543
3	1	0	-2.358666	3.036654	0.182893
4	6	0	-3.597629	0.520810	-0.049955
5	1	0	-4.055419	0.688475	-1.037293
6	1	0	-4.197456	1.029999	0.705485
7	6	0	-2.398525	-1.424474	-0.309771
8	1	0	-2.125945	-2.313016	0.259572
9	1	0	-2.570691	-1.710700	-1.358432
10	6	0	-1.368401	-0.301892	-0.225594
11	6	0	-0.069062	-0.445092	-0.283441
12	6	0	1.226215	-0.592552	-0.340745
13	6	0	2.123243	-0.817095	0.855790
14	1	0	-0.622720	2.415868	0.020610
15	1	0	1.720045	-0.552684	-1.312027
16	6	0	3.230904	0.255592	0.995365
17	1	0	1.524872	-0.824041	1.769519
18	1	0	2.600940	-1.799303	0.767898
19	1	0	3.786561	0.069279	1.920959
20	1	0	2.769065	1.243208	1.100458
21	6	0	4.169986	0.278492	-0.122902
22	6	0	4.939728	0.280542	-1.047302
23	1	0	5.623589	0.289449	-1.860460
24	8	0	-3.585020	-0.873299	0.256412



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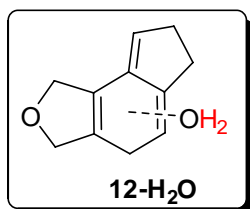
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.815656	0.359450	-0.104407
2	6	0	-1.604059	-1.622555	-0.332364
3	1	0	-3.607903	0.281345	0.654919
4	1	0	-3.090690	1.154057	-0.804651
5	1	0	-1.108407	-2.112502	-1.173353
6	1	0	-1.954674	-2.398324	0.365237
7	6	0	-0.721048	-0.614258	0.382386
8	6	0	-1.463103	0.576356	0.537305
9	6	0	-0.938906	1.765872	0.969745
10	1	0	-0.106114	1.783970	1.657081
11	1	0	-1.525674	2.677499	0.909869
12	6	0	0.623114	-0.691574	0.504549
13	6	0	1.771403	-1.198371	0.899503
14	1	0	1.820476	-1.888799	1.739205
15	6	0	3.048914	-0.752873	0.234740
16	6	0	2.668750	0.150773	-0.951548
17	1	0	3.646471	-1.606610	-0.101839
18	1	0	3.666779	-0.204669	0.957065
19	1	0	3.507604	0.785711	-1.250661
20	1	0	2.405696	-0.473425	-1.812150
21	6	0	1.497301	0.983680	-0.596595
22	6	0	0.841180	2.027395	-0.513161
23	1	0	0.595935	3.051144	-0.678542
24	8	0	-2.712103	-0.869095	-0.830387



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

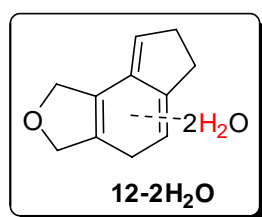
1	6	0	2.849186	0.432367	0.000234
2	6	0	1.694314	-1.620704	0.000072
3	1	0	3.348638	0.849334	-0.886281
4	1	0	3.348122	0.848621	0.887399
5	1	0	1.599341	-2.259587	0.888100
6	1	0	1.599120	-2.260144	-0.887504
7	6	0	0.713836	-0.482179	-0.000065
8	6	0	1.370751	0.686668	0.000016
9	6	0	0.712980	2.031379	0.000057
10	1	0	1.054984	2.613886	-0.869934
11	1	0	1.054946	2.613829	0.870103
12	6	0	-0.733055	-0.525896	-0.000058
13	6	0	-1.604896	-1.554583	0.000053
14	1	0	-1.335973	-2.604455	0.000113
15	6	0	-3.038501	-1.081184	0.000216
16	6	0	-2.931465	0.473791	-0.000243
17	1	0	-3.583066	-1.453213	0.875974
18	1	0	-3.583509	-1.453734	-0.875037
19	1	0	-3.416664	0.907204	-0.878598
20	1	0	-3.417073	0.907830	0.877572
21	6	0	-1.439732	0.764269	-0.000065
22	8	0	2.987234	-0.994799	-0.000417
23	6	0	-0.796570	1.938444	0.000017
24	1	0	-1.347830	2.874578	0.000021



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.501309	-0.826520	-0.079746
2	6	0	-0.924376	-0.594820	0.019563
3	6	0	-1.471618	0.552585	-0.408271
4	6	0	-0.706544	1.683971	-1.021880
5	6	0	0.778680	1.403725	-1.098978
6	6	0	1.312485	0.248098	-0.674989
7	6	0	1.277226	-1.867542	0.284977
8	6	0	2.756680	-0.223981	-0.704639
9	6	0	-1.993298	-1.501221	0.561896

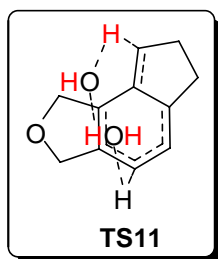
10	6	0	-2.955459	0.513490	-0.189429
11	1	0	3.419057	0.473813	-0.187156
12	1	0	3.113834	-0.298134	-1.735226
13	1	0	0.921938	-2.780587	0.748260
14	1	0	-3.305456	1.314493	0.476968
15	1	0	-3.519844	0.594770	-1.129713
16	1	0	-1.842548	-1.749935	1.620653
17	1	0	-2.068552	-2.443044	0.002102
18	1	0	-0.888509	2.611873	-0.458424
19	1	0	1.119299	1.698846	2.705618
20	8	0	1.587054	2.266697	2.085731
21	1	0	1.407309	1.881322	1.216896
22	1	0	1.404203	2.175781	-1.538337
23	1	0	-1.097410	1.894884	-2.029590
24	8	0	-3.213828	-0.759466	0.417600
25	6	0	2.735347	-1.620779	-0.015348
26	1	0	3.335664	-1.631312	0.902044
27	1	0	3.152629	-2.402659	-0.659681



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.892164	-0.792328	0.039331
2	6	0	-0.542812	-0.984263	0.042300
3	6	0	-1.331366	-0.292433	-0.793643
4	6	0	-0.844388	0.719860	-1.779817
5	6	0	0.662311	0.822537	-1.806575
6	6	0	1.442782	0.132521	-0.966394
7	6	0	1.875998	-1.307201	0.811352
8	6	0	2.956136	0.129642	-0.817830
9	6	0	-1.377067	-1.886245	0.908119
10	6	0	-2.763919	-0.659979	-0.548628
11	1	0	3.342856	1.138076	-0.651923
12	1	0	3.435114	-0.249558	-1.724485
13	1	0	1.732260	-2.018124	1.617098
14	1	0	-3.352646	0.199953	-0.201237
15	1	0	-3.256575	-1.068293	-1.441666

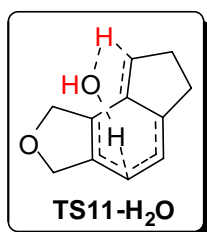
16	1	0	-1.293066	-1.643335	1.977593
17	1	0	-1.122211	-2.947246	0.786438
18	1	0	-1.272511	1.699940	-1.520308
19	8	0	0.476888	1.752427	2.194842
20	1	0	0.187509	1.457825	3.064329
21	1	0	0.777732	0.951202	1.741149
22	1	0	1.096555	1.508990	-2.527905
23	1	0	-1.228732	0.485531	-2.783936
24	8	0	-2.725810	-1.669648	0.472220
25	8	0	-1.473734	3.071502	0.537063
26	1	0	-0.804651	2.668337	1.117760
27	1	0	-1.365999	4.019892	0.649736
28	6	0	3.240350	-0.804382	0.398208
29	1	0	3.739343	-0.270420	1.215663
30	1	0	3.905129	-1.633387	0.130153



(Nimag=1) -923.7705

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.638707	-0.703703	-0.362631
2	6	0	-0.781889	-0.717130	-0.297022
3	6	0	-1.505352	0.401197	-0.629771
4	6	0	-0.883570	1.625572	-0.999713
5	6	0	0.526931	1.561122	-1.295613
6	6	0	1.258359	0.456535	-0.962946
7	6	0	1.602447	-1.557418	0.185651
8	6	0	2.766646	0.266646	-0.929313
9	6	0	-1.707889	-1.796874	0.180056
10	6	0	-2.966241	0.112605	-0.420344
11	1	0	3.219482	0.988242	-0.237212
12	1	0	3.239282	0.428369	-1.901705
13	1	0	1.381221	-2.576646	0.487630
14	1	0	-3.425011	0.784292	0.318128
15	1	0	-3.541727	0.194807	-1.351843
16	1	0	-1.530874	-2.075532	1.228596
17	1	0	-1.648377	-2.711610	-0.424101

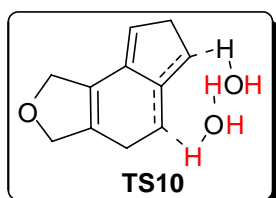
18	1	0	-0.604104	1.938509	0.559292
19	1	0	0.200889	2.841019	1.727563
20	8	0	-0.299257	2.020931	1.629892
21	1	0	1.313445	-0.592545	1.632927
22	1	0	1.015693	2.441750	-1.705012
23	1	0	-1.480076	2.436258	-1.406635
24	8	0	-3.028831	-1.238109	0.056248
25	8	0	1.004645	0.086542	2.382594
26	1	0	1.660983	0.126896	3.085041
27	1	0	0.307220	1.175145	1.983259
28	6	0	2.963126	-1.188649	-0.404711
29	1	0	3.790332	-1.255035	0.309369
30	1	0	3.221530	-1.858245	-1.237022



(Nimag=1) -1370.2204

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.625829	-0.601290	-0.344453
2	6	0	-0.795139	-0.535889	-0.394998
3	6	0	-1.385229	0.692640	-0.252075
4	6	0	-0.604902	1.876080	-0.083847
5	6	0	0.757180	1.808383	-0.575212
6	6	0	1.359626	0.595643	-0.717643
7	6	0	1.478699	-1.468981	0.342575
8	6	0	2.833205	0.239981	-0.779586
9	6	0	-1.832088	-1.610640	-0.232313
10	6	0	-2.863237	0.497030	-0.054807
11	1	0	3.471577	1.038654	-0.393239
12	1	0	3.149413	0.051420	-1.810666
13	1	0	1.213627	-2.477424	0.642128
14	1	0	-3.182416	0.807853	0.951594
15	1	0	-3.470339	1.043099	-0.785296
16	1	0	-1.713963	-2.161452	0.715219
17	1	0	-1.846571	-2.342361	-1.046733
18	1	0	-0.103622	1.270026	1.331418
19	1	0	1.020566	0.972755	2.623418
20	8	0	0.380382	0.514816	2.061372

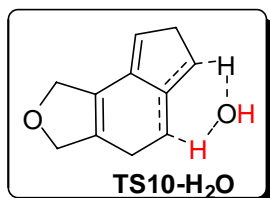
21	1	0	0.864143	-0.346655	1.565458
22	1	0	1.325084	2.728839	-0.675804
23	1	0	-1.098688	2.840532	-0.028050
24	8	0	-3.085324	-0.906946	-0.238462
25	6	0	2.933179	-1.077139	0.065052
26	1	0	3.509157	-0.925765	0.985469
27	1	0	3.458826	-1.857390	-0.494359



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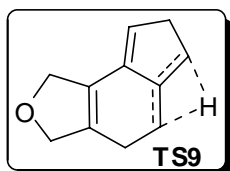
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.036640	1.053490	0.113094
2	6	0	-1.370163	0.534367	-0.110432
3	6	0	-1.741143	-0.655280	0.383177
4	6	0	-0.867391	-1.550076	1.205599
5	6	0	0.618605	-1.155362	1.125888
6	6	0	0.926172	0.202212	0.790345
7	6	0	0.551675	2.247146	-0.169171
8	6	0	2.213542	0.850159	0.800514
9	6	0	-2.510183	1.161622	-0.861095
10	6	0	-3.166941	-0.926084	0.004489
11	1	0	2.836558	0.235504	-0.037390
12	1	0	2.827495	0.710660	1.691220
13	1	0	0.076147	3.073398	-0.684783
14	1	0	-3.257277	-1.808642	-0.645198
15	1	0	-3.815770	-1.085714	0.876369
16	1	0	-2.285897	1.288606	-1.929254
17	1	0	-2.800664	2.140723	-0.457997
18	1	0	-0.984242	-2.589823	0.878989
19	8	0	1.723106	-2.273947	-1.111324
20	1	0	2.015961	-3.189888	-1.076060
21	1	0	1.084809	-1.703445	0.150161
22	1	0	1.230674	-1.566283	1.931281
23	1	0	-1.217253	-1.528130	2.247851
24	8	0	-3.601079	0.244914	-0.699153
25	8	0	3.566921	-0.714735	-0.966283
26	1	0	2.677912	-1.554556	-1.114733

27	1	0	3.836177	-0.356958	-1.817869
28	6	0	1.968715	2.283277	0.311372
29	1	0	2.660099	2.594327	-0.480977
30	1	0	2.086200	3.017527	1.119776



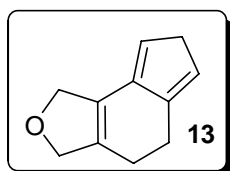
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.299971	0.882709	-0.221278
2	6	0	1.095714	0.514859	-0.059943
3	6	0	1.463140	-0.773037	-0.188095
4	6	0	0.536685	-1.908911	-0.534226
5	6	0	-0.948087	-1.511048	-0.588366
6	6	0	-1.236500	-0.116198	-0.603171
7	6	0	-1.035386	2.015244	0.030492
8	6	0	-2.554137	0.449923	-0.421592
9	6	0	2.264392	1.426011	0.228039
10	6	0	2.953698	-0.936382	-0.017598
11	1	0	-2.861579	-0.246244	0.542388
12	1	0	-3.351580	0.330703	-1.150899
13	1	0	-0.728138	3.002188	0.345601
14	1	0	3.211555	-1.773996	0.639321
15	1	0	3.424572	-1.150923	-0.987313
16	1	0	2.070272	2.120669	1.052358
17	1	0	2.497169	2.041780	-0.650806
18	1	0	0.678490	-2.726497	0.184765
19	8	0	-2.866751	-1.582286	1.277556
20	1	0	-2.620331	-1.445840	2.199088
21	1	0	-1.648525	-1.702154	0.446919
22	1	0	-1.550384	-2.121380	-1.265154
23	1	0	0.852915	-2.328619	-1.500486
24	8	0	-2.351891	1.839301	-0.122125
25	6	0	3.408319	0.430340	0.558435
26	1	0	3.515418	0.348768	1.642935
27	1	0	4.372092	0.754366	0.161644



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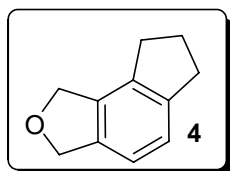
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.758225	-0.536874	-0.019454
2	6	0	-0.683421	-0.486776	-0.014708
3	6	0	-1.355830	0.674507	0.000983
4	6	0	-0.730777	2.034296	0.004832
5	6	0	0.772507	2.004142	-0.095131
6	6	0	1.502799	0.773297	-0.025226
7	6	0	1.633253	-1.557783	-0.010032
8	6	0	2.898212	0.434548	-0.029205
9	6	0	-1.650249	-1.638134	-0.018002
10	6	0	-2.830648	0.398343	0.013144
11	1	0	3.707346	1.149729	-0.021430
12	1	0	1.373934	-2.609378	-0.007661
13	1	0	-3.330570	0.810118	0.901408
14	1	0	-3.339877	0.806373	-0.872171
15	1	0	-1.530895	-2.292908	0.855130
16	1	0	-1.561308	-2.258352	-0.919994
17	1	0	-1.076406	2.584393	0.896877
18	1	0	1.727101	1.138641	1.072609
19	1	0	1.311794	2.942638	-0.128955
20	1	0	-1.137784	2.614026	-0.840564
21	8	0	-2.949823	-1.030043	0.019225
22	6	0	3.057824	-1.061192	0.007282
23	1	0	3.604939	-1.435262	0.887473
24	1	0	3.618934	-1.439921	-0.863421



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.768475	-0.573272	-0.037614

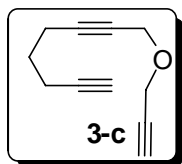
2	6	0	0.677390	-0.505790	-0.052110
3	6	0	1.318947	0.664831	0.090830
4	6	0	0.632973	1.985867	0.286783
5	6	0	-0.784904	1.990609	-0.335022
6	6	0	-1.521367	0.700769	-0.095408
7	6	0	-1.639132	-1.602342	0.083723
8	6	0	-2.836091	0.434659	0.012129
9	6	0	1.674093	-1.626518	-0.145603
10	6	0	2.799684	0.426474	0.107558
11	1	0	-3.645588	1.153098	-0.007791
12	1	0	-1.397326	-2.653135	0.171507
13	1	0	3.323078	0.957638	-0.700403
14	1	0	3.262910	0.733357	1.057403
15	1	0	1.600602	-2.183353	-1.088387
16	1	0	1.575046	-2.345262	0.679381
17	1	0	1.227047	2.798911	-0.144035
18	1	0	-0.675296	2.121403	-1.419379
19	1	0	-1.359700	2.847014	0.026732
20	1	0	0.569000	2.196719	1.363335
21	8	0	2.958271	-0.986682	-0.071743
22	6	0	-3.040637	-1.054624	0.129076
23	1	0	-3.556831	-1.333612	1.058273
24	1	0	-3.663995	-1.443301	-0.688731



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.015289	-0.921288	0.264741
2	6	0	2.857853	0.568206	-0.131074
3	6	0	1.666902	-1.587527	-0.109289
4	1	0	3.871076	-1.399839	-0.215505
5	1	0	3.163282	-0.993095	1.346327
6	1	0	3.210959	0.739897	-1.156007
7	1	0	3.427388	1.238935	0.517510
8	1	0	1.406251	-2.412974	0.559090
9	1	0	1.699627	-2.001669	-1.125642
10	6	0	0.687668	-0.436037	-0.047006
11	6	0	1.362154	0.792338	-0.052631

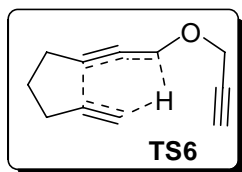
12	6	0	-0.700765	-0.443744	-0.012954
13	6	0	-1.683312	-1.582815	0.010450
14	1	0	-1.560711	-2.280393	-0.825165
15	6	0	-2.876938	0.452672	0.092894
16	1	0	-3.458654	0.947823	-0.691538
17	1	0	-3.311651	0.727182	1.064725
18	6	0	-1.403880	0.759457	0.029064
19	6	0	-0.738999	1.981993	0.029206
20	1	0	-1.290736	2.915458	0.066198
21	8	0	-2.974330	-0.966824	-0.100774
22	6	0	0.658961	1.995338	-0.016345
23	1	0	1.189667	2.941808	-0.020970
24	1	0	-1.621458	-2.160105	0.944830



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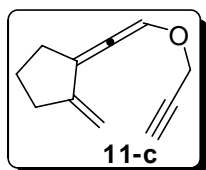
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.170553	1.448994	-0.159715
2	6	0	-2.543479	2.473975	-0.112839
3	1	0	-1.975210	3.370534	-0.074125
4	6	0	-3.986531	0.237716	-0.203078
5	1	0	-4.209493	-0.007149	-1.248864
6	1	0	-4.950895	0.466584	0.264554
7	6	0	-2.250437	-1.712746	-0.261903
8	1	0	-2.110932	-2.706643	0.178951
9	1	0	-2.557728	-1.886978	-1.300733
10	6	0	-0.959531	-1.031020	-0.248131
11	6	0	0.123271	-0.506947	-0.215382
12	6	0	1.403832	0.180961	-0.206981
13	1	0	1.243469	1.262631	-0.076929
14	1	0	1.917378	0.036357	-1.166720
15	6	0	3.457646	0.363372	0.982238
16	1	0	3.906989	-0.010607	1.904859
17	1	0	3.294484	1.444799	1.105257
18	6	0	4.376733	0.137681	-0.139080
19	6	0	5.136963	-0.047728	-1.052004
20	1	0	5.807286	-0.215887	-1.859485
21	6	0	-3.393519	-1.004878	0.495736

22	1	0	-4.206330	-1.729360	0.608682
23	1	0	-3.059534	-0.738648	1.501669
24	8	0	2.216767	-0.315240	0.861214



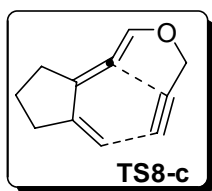
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.741240	1.138398	-0.231527
2	6	0	-0.682453	1.795632	-0.290135
3	1	0	-0.220116	2.761391	-0.338208
4	6	0	-3.223547	1.030461	-0.208208
5	6	0	-3.681442	-0.294378	0.418274
6	1	0	-3.584053	1.090678	-1.242723
7	1	0	-3.643359	1.888562	0.325150
8	6	0	-2.815473	-1.414923	-0.182421
9	1	0	-3.526974	-0.259282	1.500735
10	1	0	-4.744838	-0.471671	0.238704
11	1	0	-2.915513	-2.348459	0.377361
12	1	0	-3.129460	-1.619261	-1.213380
13	6	0	-1.414390	-0.961389	-0.176644
14	6	0	-0.180054	-1.100476	-0.143413
15	6	0	1.008962	-0.364657	-0.202846
16	1	0	0.430837	0.779504	-0.284959
17	1	0	1.595660	-0.460694	-1.122860
18	6	0	2.948699	0.458296	0.891849
19	1	0	3.388975	0.422846	1.890429
20	1	0	2.637698	1.494307	0.700712
21	6	0	3.949093	0.057319	-0.102305
22	6	0	4.779682	-0.265657	-0.909293
23	1	0	5.511954	-0.556670	-1.622568
24	8	0	1.814021	-0.399126	0.951452



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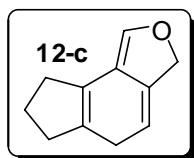
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.346296	0.830685	-0.237143
2	6	0	-3.717012	0.177159	-0.179442
3	6	0	-3.457335	-1.189022	0.484302
4	1	0	-4.092587	0.027980	-1.199957
5	1	0	-4.450296	0.788477	0.350372
6	6	0	-2.062642	-1.588084	-0.033642
7	1	0	-3.427191	-1.071781	1.572122
8	1	0	-4.224368	-1.930406	0.250550
9	1	0	-1.536097	-2.292223	0.611547
10	1	0	-2.145175	-2.048375	-1.025911
11	6	0	-1.327045	-0.255005	-0.162451
12	6	0	-0.025111	-0.108824	-0.181096
13	6	0	1.274560	-0.000709	-0.235902
14	1	0	1.820928	-0.048225	-1.176071
15	6	0	3.340250	0.712216	0.686505
16	1	0	3.757834	0.847359	1.685976
17	1	0	3.230701	1.704595	0.230681
18	6	0	4.244468	-0.107559	-0.122165
19	6	0	4.999277	-0.773132	-0.779652
20	1	0	5.662825	-1.367232	-1.359756
21	6	0	-2.099897	2.140873	-0.313059
22	1	0	-2.904975	2.866377	-0.344471
23	1	0	-1.084904	2.521426	-0.342903
24	8	0	2.056751	0.121304	0.898787



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.727619	-0.849344	0.885216
2	6	0	2.837809	0.437203	0.037855
3	6	0	1.594926	-1.658545	0.216179
4	1	0	3.668050	-1.402069	0.945380
5	1	0	2.430864	-0.589497	1.905960
6	1	0	3.555026	0.299858	-0.781212
7	1	0	3.176383	1.302915	0.613416

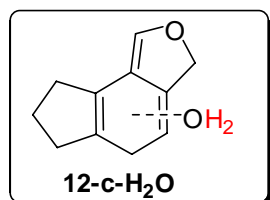
8	1	0	1.055517	-2.306870	0.908906
9	1	0	1.992628	-2.298080	-0.582708
10	6	0	0.703991	-0.584544	-0.398057
11	6	0	1.443708	0.626432	-0.536422
12	6	0	0.897106	1.803488	-0.962901
13	1	0	0.010366	1.814434	-1.579134
14	1	0	1.468989	2.725385	-0.920809
15	6	0	-0.644012	-0.635161	-0.499157
16	6	0	-1.793375	-1.173540	-0.859765
17	1	0	-1.950198	-1.835117	-1.702893
18	6	0	-2.710415	0.052081	0.861035
19	1	0	-3.633379	0.610572	1.018066
20	1	0	-2.484317	-0.540468	1.755408
21	6	0	-1.565117	0.941879	0.563075
22	6	0	-0.970270	2.021562	0.606713
23	1	0	-0.713005	3.032394	0.817626
24	8	0	-2.963594	-0.837816	-0.235079



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.042468	-0.945122	-0.186007
2	6	0	-2.821775	0.565545	0.089446
3	6	0	-1.676651	-1.625286	0.096186
4	1	0	-3.853215	-1.367899	0.410721
5	1	0	-3.306609	-1.085883	-1.237412
6	1	0	-3.189541	0.858622	1.083396
7	1	0	-3.348571	1.201969	-0.630729
8	1	0	-1.452399	-2.419791	-0.623009
9	1	0	-1.647643	-2.086832	1.092005
10	6	0	-0.700405	-0.474860	0.021508
11	6	0	-1.322586	0.719734	0.017771
12	6	0	0.742010	-0.538568	0.008011
13	6	0	1.642948	-1.540948	0.015551
14	1	0	1.509722	-2.612385	0.034593
15	6	0	2.945247	0.329031	-0.030695
16	1	0	3.499975	0.678232	0.843798
17	1	0	3.471197	0.644092	-0.935601

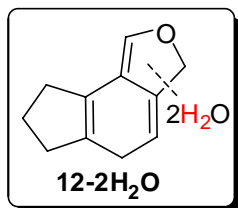
18	6	0	1.485462	0.722586	-0.015584
19	6	0	0.891119	1.921260	-0.017886
20	1	0	1.471556	2.839169	-0.033849
21	8	0	2.947720	-1.126822	-0.003065
22	6	0	-0.617201	2.047306	0.002998
23	1	0	-0.957984	2.638293	-0.862759
24	1	0	-0.932454	2.642914	0.875575



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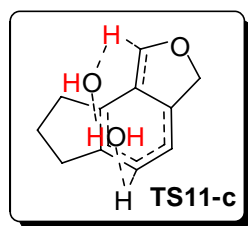
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.943680	0.689190	-0.262706
2	6	0	-2.056236	-1.483032	0.516150
3	1	0	-3.277595	1.632967	0.182899
4	1	0	-3.429814	0.626929	-1.246898
5	1	0	-2.231489	-2.296058	-0.200553
6	1	0	-1.809536	-1.957243	1.471688
7	6	0	-0.962458	-0.569876	0.014332
8	6	0	-1.444282	0.613857	-0.411902
9	6	0	-0.608630	1.703281	-1.025921
10	1	0	-0.760855	2.646038	-0.477406
11	1	0	-0.976304	1.921446	-2.042098
12	6	0	0.449214	-0.857133	-0.091170
13	6	0	1.225697	-1.915518	0.219454
14	1	0	0.973190	-2.874350	0.647598
15	6	0	2.713980	-0.412651	-0.625956
16	1	0	3.406775	0.139250	0.013496
17	1	0	3.154330	-0.527657	-1.619207
18	6	0	1.321023	0.175517	-0.652988
19	6	0	0.866890	1.363067	-1.080316
20	1	0	1.539189	2.104050	-1.503117
21	8	0	2.551520	-1.744418	-0.058214
22	8	0	1.967296	2.204470	1.999930
23	1	0	1.601063	1.648622	2.694527
24	1	0	1.578662	1.863115	1.182248
25	6	0	-3.280145	-0.536083	0.627619
26	1	0	-4.214127	-1.021870	0.338818

27 1 0 -3.392263 -0.209367 1.664700



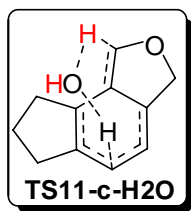
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.040168	-0.673803	-0.144526
2	6	0	0.374843	-0.967154	-0.088053
3	6	0	1.141763	-0.394645	0.860073
4	6	0	0.636546	0.561028	1.902189
5	6	0	-0.857320	0.787983	1.831510
6	6	0	-1.602561	0.212529	0.881471
7	6	0	-2.054338	-1.049872	-0.953562
8	6	0	-3.083391	0.287314	0.583127
9	6	0	1.182136	-1.821098	-1.037516
10	6	0	2.594366	-0.759937	0.694954
11	1	0	-3.433955	1.296366	0.353011
12	1	0	-3.707603	-0.135327	1.374756
13	1	0	-2.066771	-1.699914	-1.816017
14	1	0	3.145717	0.111819	0.320382
15	1	0	3.067203	-1.050623	1.639881
16	1	0	1.264243	-1.335281	-2.019467
17	1	0	0.730658	-2.803419	-1.212853
18	1	0	1.170168	1.517245	1.789073
19	8	0	-0.094502	2.017539	-1.931079
20	1	0	-0.102787	1.809795	-2.870613
21	1	0	-0.493711	1.249896	-1.495819
22	1	0	-1.301946	1.444745	2.573668
23	1	0	0.915230	0.200463	2.904860
24	8	0	2.327135	2.588990	-0.501953
25	1	0	1.519243	2.446251	-1.025395
26	1	0	2.478968	3.537727	-0.525409
27	6	0	2.560959	-1.923094	-0.331033
28	1	0	3.393714	-1.883610	-1.035829
29	1	0	2.627529	-2.878496	0.196213
30	8	0	-3.272998	-0.529422	-0.609749



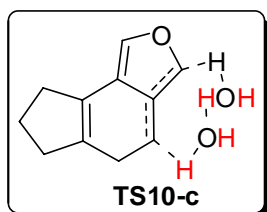
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.602749	-0.757037	-0.345350
2	6	0	-0.815176	-0.707463	-0.231625
3	6	0	-1.481203	0.445083	-0.588556
4	6	0	-0.793288	1.615947	-1.028978
5	6	0	0.594417	1.456586	-1.392224
6	6	0	1.262816	0.320804	-1.044731
7	6	0	1.578567	-1.550170	0.246477
8	6	0	2.727001	-0.054943	-1.120748
9	6	0	-1.750732	-1.737823	0.351422
10	6	0	-2.959911	0.311213	-0.296385
11	1	0	3.402076	0.745802	-0.796905
12	1	0	3.035456	-0.370107	-2.127984
13	1	0	1.507752	-2.585765	0.552519
14	1	0	-3.219519	0.884744	0.603536
15	1	0	-3.586860	0.697463	-1.105684
16	1	0	-1.649741	-1.782062	1.445887
17	1	0	-1.558249	-2.749675	-0.019581
18	1	0	-0.445850	1.998168	0.501049
19	1	0	0.379137	2.930240	1.631957
20	8	0	-0.116744	2.105556	1.559168
21	1	0	1.308985	-0.566051	1.625542
22	1	0	1.109357	2.278942	-1.882177
23	1	0	-1.359589	2.438673	-1.455078
24	8	0	1.130751	0.178595	2.371737
25	1	0	1.943975	0.311812	2.871088
26	1	0	0.493392	1.237963	1.943699
27	6	0	-3.146761	-1.210185	-0.067785
28	1	0	-3.441285	-1.682645	-1.009043
29	1	0	-3.923567	-1.433499	0.666774
30	8	0	2.872700	-1.177409	-0.222742



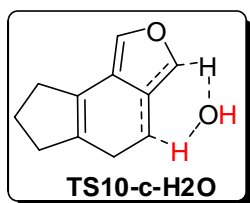
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.625002	-0.635822	-0.332211
2	6	0	-0.798053	-0.539578	-0.329461
3	6	0	-1.345382	0.717269	-0.225202
4	6	0	-0.518612	1.883188	-0.128258
5	6	0	0.831522	1.763573	-0.629542
6	6	0	1.385998	0.526395	-0.757605
7	6	0	1.514555	-1.460092	0.345368
8	6	0	2.824818	0.073303	-0.795037
9	6	0	-1.832627	-1.618158	-0.122035
10	6	0	-2.837073	0.626404	0.008919
11	1	0	3.538037	0.818450	-0.433941
12	1	0	3.148913	-0.269645	-1.787500
13	1	0	1.408846	-2.489611	0.659262
14	1	0	-3.065168	0.855504	1.058651
15	1	0	-3.406555	1.336492	-0.598030
16	1	0	-1.766654	-2.029844	0.897035
17	1	0	-1.722481	-2.463173	-0.808053
18	1	0	0.014524	1.304693	1.332699
19	1	0	1.181441	1.010120	2.560941
20	8	0	0.480878	0.568600	2.059495
21	1	0	0.893436	-0.328600	1.563352
22	1	0	1.423073	2.662715	-0.776568
23	1	0	-0.984864	2.862557	-0.104618
24	8	0	2.851027	-1.070196	0.104189
25	6	0	-3.162803	-0.850296	-0.329210
26	1	0	-3.459886	-0.923652	-1.379025
27	1	0	-3.981972	-1.250360	0.271963



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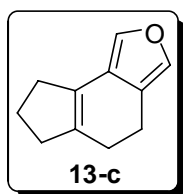
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.074368	1.028303	0.146918
2	6	0	-1.406396	0.504379	-0.096349
3	6	0	-1.728414	-0.720532	0.352817
4	6	0	-0.803955	-1.608991	1.140139
5	6	0	0.675742	-1.172985	1.069816
6	6	0	0.896461	0.220062	0.781756
7	6	0	0.550945	2.224885	-0.130350
8	6	0	2.147240	0.962636	0.784254
9	6	0	-2.526358	1.153314	-0.872613
10	6	0	-3.134013	-1.097717	-0.041724
11	1	0	2.884280	0.424230	0.031608
12	1	0	2.687375	1.079798	1.723594
13	1	0	0.175849	3.114139	-0.618077
14	1	0	-3.107226	-1.872528	-0.819765
15	1	0	-3.706651	-1.519413	0.791637
16	1	0	-2.289369	1.173916	-1.944307
17	1	0	-2.710484	2.190623	-0.572299
18	1	0	-0.889383	-2.639679	0.777825
19	8	0	1.931197	-2.136984	-1.178110
20	1	0	2.216043	-3.054944	-1.219676
21	1	0	1.181316	-1.676881	0.110985
22	1	0	1.283352	-1.556439	1.892722
23	1	0	-1.151792	-1.636560	2.183542
24	8	0	3.744833	-0.574319	-0.813426
25	1	0	2.920857	-1.381861	-1.057889
26	1	0	4.126233	-0.246971	-1.633481
27	8	0	1.818741	2.270033	0.258401
28	6	0	-3.738144	0.232719	-0.563342
29	1	0	-4.383849	0.088717	-1.431248
30	1	0	-4.347155	0.687568	0.221976



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

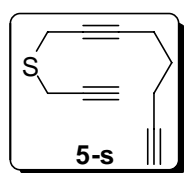
1	6	0	-0.306596	0.887695	-0.172090
2	6	0	1.087620	0.526479	-0.018215
3	6	0	1.498596	-0.740618	-0.179287
4	6	0	0.623164	-1.896297	-0.557779
5	6	0	-0.865662	-1.533550	-0.604393
6	6	0	-1.232217	-0.160441	-0.586902
7	6	0	-1.002554	2.033315	0.044577
8	6	0	-2.571701	0.322229	-0.461503
9	6	0	2.249545	1.403261	0.353405
10	6	0	2.977198	-0.816746	0.066365
11	1	0	-2.798460	-0.447617	0.542364
12	1	0	-3.340076	-0.038113	-1.144205
13	1	0	-0.580269	2.974076	0.377395
14	1	0	3.224367	-1.471470	0.914437
15	1	0	3.531402	-1.184101	-0.808605
16	1	0	2.132030	1.858586	1.346523
17	1	0	2.418134	2.212127	-0.369660
18	1	0	0.785522	-2.727455	0.141293
19	8	0	-2.739000	-1.669413	1.292548
20	1	0	-2.482364	-1.461581	2.197835
21	1	0	-1.548722	-1.745789	0.456323
22	1	0	-1.463692	-2.172922	-1.256822
23	1	0	0.951948	-2.281131	-1.533743
24	8	0	3.384524	0.526316	0.357932
25	6	0	-2.473047	1.819980	-0.177040
26	1	0	-2.845080	2.429601	-1.011245
27	1	0	-3.054998	2.128725	0.701451



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.014883	-0.918792	0.252703
2	6	0	2.778296	0.550574	-0.185014
3	6	0	1.655066	-1.637408	0.049201
4	1	0	3.829268	-1.396515	-0.295675
5	1	0	3.280437	-0.940945	1.312962
6	1	0	3.125988	0.730371	-1.212844

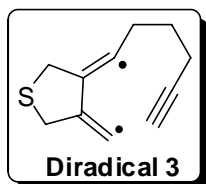
7	1	0	3.312808	1.267461	0.448062
8	1	0	1.442962	-2.363087	0.840867
9	1	0	1.625879	-2.190657	-0.899283
10	6	0	0.668987	-0.494008	0.018985
11	6	0	1.278559	0.700259	-0.104055
12	6	0	0.530916	1.995440	-0.291136
13	1	0	0.444219	2.197372	-1.369191
14	1	0	1.101396	2.832233	0.125075
15	6	0	-0.778989	-0.569282	0.012423
16	6	0	-1.677823	-1.585079	-0.119185
17	1	0	-1.588125	-2.651480	-0.238658
18	6	0	-2.854397	0.268728	0.029213
19	1	0	-3.790264	0.801447	0.059905
20	6	0	-1.555581	0.645915	0.110224
21	6	0	-0.879331	1.965924	0.347189
22	1	0	-1.481995	2.799268	-0.023139
23	1	0	-0.770424	2.111801	1.429482
24	8	0	-2.951957	-1.091361	-0.112607



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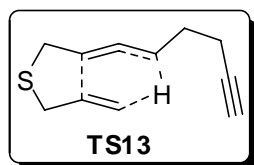
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.714194	1.752789	-0.327868
2	6	0	-2.051473	2.739675	-0.147955
3	1	0	-1.456720	3.604385	0.016384
4	6	0	-3.561344	0.592627	-0.547701
5	1	0	-3.436138	0.203186	-1.561320
6	1	0	-4.611441	0.874577	-0.438229
7	6	0	-2.013434	-1.792471	-0.219411
8	1	0	-1.964082	-2.713447	0.368358
9	1	0	-2.385450	-2.064020	-1.211299
10	6	0	-0.708344	-1.164481	-0.305740
11	6	0	0.373861	-0.642439	-0.393679
12	6	0	1.676781	0.010059	-0.467052
13	6	0	2.408522	0.045365	0.888218
14	1	0	1.541515	1.034386	-0.836400
15	1	0	2.303273	-0.502964	-1.204889
16	6	0	3.778244	0.750163	0.813621

17	1	0	1.786740	0.569275	1.619391
18	1	0	2.542756	-0.975921	1.254191
19	1	0	4.198096	0.821626	1.822686
20	1	0	3.643476	1.781123	0.464233
21	6	0	4.744488	0.077210	-0.051694
22	6	0	5.533633	-0.488528	-0.761890
23	1	0	6.235064	-0.984284	-1.387301
24	16	0	-3.324846	-0.807984	0.638818



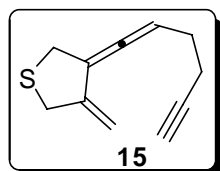
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.356497	1.115540	0.267519
2	6	0	-0.864042	2.220605	0.785519
3	1	0	-1.189612	3.232994	0.968636
4	6	0	-2.767827	1.049837	-0.322821
5	1	0	-2.750738	1.309760	-1.384996
6	1	0	-3.468785	1.705106	0.191821
7	6	0	-1.590819	-1.276745	-0.411144
8	1	0	-1.463224	-2.246245	0.069901
9	1	0	-1.419471	-1.391412	-1.485330
10	6	0	-0.670833	-0.200858	0.179437
11	6	0	0.569320	-0.443847	0.557223
12	6	0	1.532892	-1.547979	0.654989
13	1	0	1.012981	-2.500719	0.457337
14	1	0	1.901629	-1.618202	1.687456
15	6	0	2.743167	-1.454758	-0.298694
16	1	0	3.307604	-2.389156	-0.216180
17	1	0	2.392398	-1.380513	-1.331752
18	6	0	3.712657	-0.291676	-0.001939
19	1	0	4.626572	-0.441601	-0.587560
20	1	0	4.016077	-0.330372	1.051465
21	6	0	3.185560	1.037193	-0.299989
22	6	0	2.772499	2.135995	-0.561955
23	1	0	2.384394	3.100350	-0.779848
24	16	0	-3.309143	-0.694365	-0.120614



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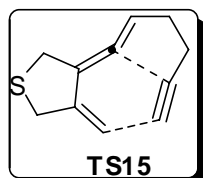
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.303547	1.209172	-0.233679
2	6	0	-0.191535	1.772709	-0.187670
3	1	0	0.350512	2.693523	-0.103096
4	6	0	-2.777538	1.304493	-0.265812
5	1	0	-3.115294	1.428726	-1.298597
6	1	0	-3.114429	2.168749	0.310292
7	6	0	-2.563053	-1.368475	-0.446825
8	1	0	-2.693185	-2.334903	0.042535
9	1	0	-2.916774	-1.449837	-1.478244
10	6	0	-1.164523	-0.932776	-0.397310
11	6	0	0.061951	-1.124878	-0.380175
12	6	0	1.313902	-0.509389	-0.306899
13	6	0	2.170871	-0.705137	0.944177
14	1	0	0.831846	0.674288	-0.272229
15	1	0	1.897219	-0.531857	-1.231177
16	6	0	3.347908	0.289144	1.034823
17	1	0	1.542835	-0.587477	1.831539
18	1	0	2.565368	-1.725365	0.960779
19	1	0	3.866530	0.137337	1.987438
20	1	0	2.963221	1.315012	1.054463
21	6	0	4.314523	0.161795	-0.053313
22	6	0	5.106378	0.044713	-0.951320
23	1	0	5.809342	-0.054762	-1.741807
24	16	0	-3.617451	-0.161353	0.462632



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.722935	1.133224	-0.109083

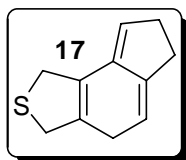
2	6	0	-1.115976	2.303945	0.105498
3	1	0	-1.683062	3.205474	0.305392
4	6	0	-3.230497	0.967346	-0.110096
5	1	0	-3.645036	1.169869	-1.102332
6	1	0	-3.720557	1.619034	0.612438
7	6	0	-2.037857	-1.303160	-0.565049
8	1	0	-1.678745	-2.246861	-0.158076
9	1	0	-2.269369	-1.440866	-1.625236
10	6	0	-1.044773	-0.165079	-0.365160
11	6	0	0.252288	-0.352661	-0.402383
12	6	0	1.541836	-0.548891	-0.425531
13	6	0	2.380416	-0.900148	0.783222
14	1	0	-0.035721	2.391859	0.082745
15	1	0	2.074712	-0.458702	-1.372479
16	6	0	3.520705	0.112466	1.049887
17	1	0	1.744939	-0.953274	1.669922
18	1	0	2.824045	-1.891267	0.636223
19	1	0	4.031360	-0.168893	1.977408
20	1	0	3.091924	1.106297	1.217592
21	6	0	4.504316	0.186630	-0.027085
22	16	0	-3.556840	-0.787887	0.335344
23	6	0	5.310503	0.232099	-0.918717
24	1	0	6.026796	0.278892	-1.702108



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.529243	0.842645	-0.178858
2	6	0	1.373865	-1.564776	-0.074390
3	1	0	3.221383	0.934331	-1.020383
4	1	0	2.716617	1.669139	0.509309
5	1	0	0.886411	-2.200976	0.663819
6	1	0	1.700154	-2.190430	-0.910318
7	6	0	0.467226	-0.446995	-0.559283
8	6	0	1.090912	0.821317	-0.652538
9	6	0	0.390286	1.963172	-0.953034
10	1	0	-0.504791	1.920145	-1.555709
11	1	0	0.874344	2.932632	-0.889910

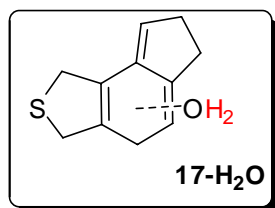
12	6	0	-0.878211	-0.600882	-0.609778
13	6	0	-2.017137	-1.142102	-0.984848
14	1	0	-2.087059	-1.721627	-1.903573
15	6	0	-3.264567	-0.892271	-0.175513
16	6	0	-2.856850	-0.108453	1.085290
17	1	0	-3.763820	-1.829460	0.092614
18	1	0	-3.981738	-0.316548	-0.773931
19	1	0	-3.715193	0.407434	1.525207
20	1	0	-2.470580	-0.805318	1.836581
21	6	0	-1.793404	0.862177	0.747017
22	6	0	-1.228726	1.959706	0.712341
23	1	0	-1.038553	2.979037	0.957812
24	16	0	2.830437	-0.746224	0.708128



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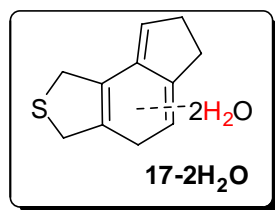
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.499077	0.976793	0.000348
2	6	0	1.416153	-1.496103	0.000510
3	1	0	2.875464	1.501850	-0.883474
4	1	0	2.875178	1.501176	0.884691
5	1	0	1.287102	-2.124103	0.886235
6	1	0	1.286674	-2.124883	-0.884600
7	6	0	0.460752	-0.333962	0.000157
8	6	0	0.998979	0.897654	0.000027
9	6	0	0.186072	2.164123	-0.000335
10	1	0	0.470926	2.777241	-0.870015
11	1	0	0.471130	2.777919	0.868798
12	6	0	-0.983735	-0.504878	0.000037
13	6	0	-1.741711	-1.620539	-0.000148
14	1	0	-1.363102	-2.635851	-0.000223
15	6	0	-3.217449	-1.304268	-0.000453
16	6	0	-3.277380	0.252864	0.000478
17	1	0	-3.719517	-1.733280	0.874638
18	1	0	-3.718822	-1.732159	-0.876501
19	1	0	-3.806231	0.633749	-0.877017
20	1	0	-3.805283	0.632566	0.879062
21	6	0	-1.824653	0.699014	0.000067

22	16	0	3.113724	-0.765780	-0.000314
23	6	0	-1.304410	1.930767	-0.000106
24	1	0	-1.943272	2.809465	-0.000062



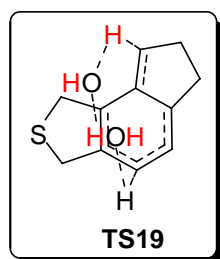
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.736583	-0.803312	-0.131572
2	6	0	-0.679952	-0.476952	-0.072089
3	6	0	-1.117340	0.729260	-0.474275
4	6	0	-0.216868	1.810083	-1.009989
5	6	0	1.242739	1.425705	-1.039355
6	6	0	1.662985	0.216832	-0.642147
7	6	0	1.404409	-1.921658	0.218891
8	6	0	3.063200	-0.373248	-0.625684
9	6	0	-1.716624	-1.448340	0.423200
10	6	0	-2.596928	0.972123	-0.384822
11	1	0	3.751395	0.242087	-0.041442
12	1	0	3.467895	-0.428844	-1.639697
13	1	0	0.952419	-2.818903	0.624935
14	1	0	-2.828725	1.826934	0.258073
15	1	0	-3.030797	1.168945	-1.370540
16	1	0	-1.525907	-1.754855	1.455268
17	1	0	-1.751839	-2.348195	-0.197215
18	1	0	-0.354336	2.728077	-0.418230
19	1	0	1.773422	1.785012	1.315001
20	8	0	1.927571	2.145133	2.199414
21	1	0	1.350133	1.634495	2.775067
22	1	0	1.942833	2.164764	-1.418817
23	1	0	-0.547677	2.088062	-2.023017
24	6	0	2.890287	-1.792450	-0.008250
25	1	0	3.266049	-2.577928	-0.673513
26	1	0	3.445909	-1.898689	0.930806
27	16	0	-3.335393	-0.562518	0.331535



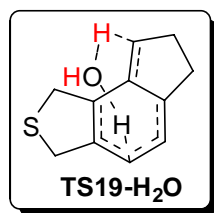
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.101522	-0.760346	-0.038368
2	6	0	-0.349587	-0.787777	-0.139732
3	6	0	-0.988554	0.099481	-0.922555
4	6	0	-0.290418	1.149864	-1.739029
5	6	0	1.212623	1.085241	-1.654605
6	6	0	1.839281	0.206665	-0.865238
7	6	0	1.951217	-1.485743	0.723956
8	6	0	3.324051	-0.005986	-0.618543
9	6	0	-1.201991	-1.764879	0.624208
10	6	0	-2.488148	0.044892	-0.912391
11	1	0	3.815589	0.918321	-0.305483
12	1	0	3.824175	-0.337883	-1.532455
13	1	0	1.660450	-2.269390	1.414133
14	1	0	-2.901630	0.972029	-0.505659
15	1	0	-2.898719	-0.106489	-1.915222
16	1	0	-1.073881	-1.660731	1.706373
17	1	0	-0.968315	-2.799265	0.357305
18	1	0	-0.640810	2.135614	-1.399117
19	8	0	0.502722	1.525196	2.416873
20	1	0	0.147839	1.093096	3.200447
21	1	0	0.859881	0.810332	1.870598
22	1	0	1.773620	1.799814	-2.250458
23	1	0	-0.614207	1.072327	-2.788229
24	8	0	-1.329625	3.052886	0.805237
25	1	0	-0.708872	2.584928	1.391181
26	1	0	-1.336549	3.962404	1.115852
27	6	0	3.393778	-1.103346	0.486392
28	1	0	3.868414	-0.731321	1.402365
29	1	0	3.988972	-1.966896	0.168610
30	16	0	-2.950211	-1.385621	0.164270



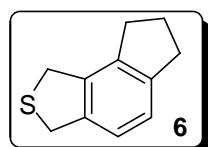
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.804824	-0.671821	-0.405283
2	6	0	-0.614060	-0.518992	-0.339218
3	6	0	-1.183601	0.703234	-0.616852
4	6	0	-0.385123	1.848783	-0.912323
5	6	0	1.006672	1.627938	-1.205549
6	6	0	1.583765	0.420919	-0.936335
7	6	0	1.637792	-1.679686	0.094989
8	6	0	3.051792	0.027650	-0.908372
9	6	0	-1.542929	-1.619381	0.090866
10	6	0	-2.685235	0.765723	-0.508638
11	1	0	3.589947	0.640705	-0.173959
12	1	0	3.553117	0.178881	-1.867985
13	1	0	1.277342	-2.675039	0.335766
14	1	0	-3.009177	1.520447	0.212870
15	1	0	-3.139801	1.002720	-1.474242
16	1	0	-1.323926	-1.963461	1.106530
17	1	0	-1.491677	-2.484046	-0.576995
18	1	0	-0.092590	2.034864	0.667753
19	1	0	0.790168	2.764029	1.898839
20	8	0	0.201159	2.015165	1.742400
21	1	0	1.472588	-0.770572	1.598997
22	1	0	1.606115	2.462255	-1.561336
23	1	0	-0.868951	2.750496	-1.275185
24	8	0	1.253380	-0.101903	2.387589
25	1	0	1.918205	-0.175400	3.079397
26	1	0	0.696860	1.082439	2.049603
27	16	0	-3.248289	-0.905292	0.045410
28	6	0	3.042372	-1.468121	-0.468524
29	1	0	3.845137	-1.688788	0.242439
30	1	0	3.215335	-2.118414	-1.337513



(Nimag=1) -1347.8916

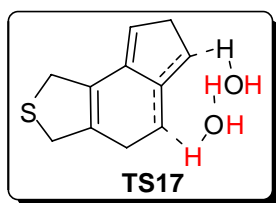
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.848098	-0.588617	-0.311860
2	6	0	-0.571464	-0.412213	-0.324941
3	6	0	-1.048454	0.870397	-0.216306
4	6	0	-0.145032	1.978556	-0.110996
5	6	0	1.190769	1.781759	-0.627863
6	6	0	1.679601	0.516875	-0.744707
7	6	0	1.634655	-1.515360	0.377562
8	6	0	3.111894	0.023786	-0.830296
9	6	0	-1.570471	-1.522167	-0.149839
10	6	0	-2.536171	1.000719	-0.024239
11	1	0	3.831448	0.770259	-0.484093
12	1	0	3.382214	-0.222688	-1.862201
13	1	0	1.285469	-2.485665	0.713861
14	1	0	-2.775164	1.436035	0.950444
15	1	0	-2.989177	1.626878	-0.796634
16	1	0	-1.422907	-2.058060	0.794389
17	1	0	-1.534845	-2.251504	-0.962482
18	1	0	0.335597	1.376182	1.321373
19	1	0	1.467084	1.025987	2.587526
20	8	0	0.770932	0.608455	2.061567
21	1	0	1.160120	-0.307851	1.579368
22	1	0	1.831398	2.647028	-0.772423
23	1	0	-0.553484	2.983418	-0.084088
24	16	0	-3.230129	-0.707339	-0.154356
25	6	0	3.111166	-1.271559	0.052455
26	1	0	3.723919	-1.149234	0.953202
27	1	0	3.545382	-2.114059	-0.494906



(Nimag=0)

Center	Atomic	Atomic	Coordinates (Angstroms)		
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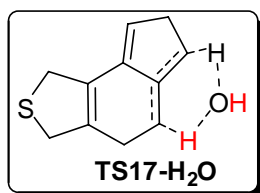
Number	Number	Type	X	Y	Z
1	6	0	3.217882	-1.130351	0.259083
2	6	0	3.208662	0.362522	-0.151731
3	6	0	1.804610	-1.658171	-0.094363
4	1	0	4.015227	-1.699085	-0.223383
5	1	0	3.368444	-1.205622	1.340064
6	1	0	3.565274	0.487939	-1.182140
7	1	0	3.850151	0.979009	0.483456
8	1	0	1.469174	-2.446187	0.585739
9	1	0	1.783639	-2.084668	-1.106103
10	6	0	0.947655	-0.412001	-0.035754
11	6	0	1.744466	0.737233	-0.060704
12	6	0	-0.441462	-0.300732	0.009158
13	6	0	-1.395962	-1.466980	0.043401
14	1	0	-1.239049	-2.151065	-0.793644
15	6	0	-2.531931	0.991901	0.132053
16	1	0	-2.980078	1.603722	-0.653523
17	1	0	-2.871028	1.372529	1.099211
18	6	0	-1.025505	0.969164	0.044131
19	6	0	-0.227401	2.115302	0.025100
20	1	0	-0.688672	3.096970	0.056355
21	6	0	1.162312	2.002316	-0.032879
22	1	0	1.778115	2.895518	-0.052916
23	1	0	-1.299777	-2.038313	0.971250
24	16	0	-3.095710	-0.754498	-0.084333



(Nimag=1) -1361.7155

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.242278	1.019636	0.203231
2	6	0	-1.101257	0.490509	0.018030
3	6	0	-1.423206	-0.721841	0.498972
4	6	0	-0.470287	-1.600935	1.263228
5	6	0	1.001727	-1.191000	1.109949
6	6	0	1.262651	0.179963	0.800957
7	6	0	0.784800	2.236030	-0.076024

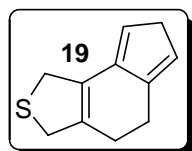
8	6	0	2.532540	0.860644	0.762020
9	6	0	-2.178379	1.254610	-0.700060
10	6	0	-2.833905	-1.177764	0.263668
11	1	0	3.125553	0.283566	-0.121633
12	1	0	3.194311	0.713801	1.616610
13	1	0	0.262052	3.062798	-0.542579
14	1	0	-2.858089	-2.075563	-0.361933
15	1	0	-3.346694	-1.408678	1.202438
16	1	0	-1.917617	1.425468	-1.748675
17	1	0	-2.369140	2.225512	-0.233662
18	1	0	-0.592346	-2.639698	0.936183
19	8	0	1.999755	-2.216448	-1.221006
20	1	0	2.308045	-3.127881	-1.234666
21	1	0	1.419688	-1.700851	0.093089
22	1	0	1.663032	-1.616283	1.867693
23	1	0	-0.764695	-1.591296	2.322929
24	8	0	3.825041	-0.632567	-1.110364
25	1	0	2.941501	-1.482391	-1.245441
26	1	0	4.056880	-0.249158	-1.961769
27	6	0	2.224552	2.298672	0.327522
28	1	0	2.861975	2.649508	-0.492972
29	1	0	2.367572	3.014604	1.148119
30	16	0	-3.699968	0.213594	-0.588858



(Nimag=1) -1859.7707

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.571387	0.846539	-0.211256
2	6	0	0.817419	0.431692	-0.081342
3	6	0	1.158338	-0.861145	-0.229072
4	6	0	0.190629	-1.965243	-0.567129
5	6	0	-1.277406	-1.536939	-0.578293
6	6	0	-1.568553	-0.148113	-0.580869
7	6	0	-1.192396	2.035400	0.002107
8	6	0	-2.873659	0.414394	-0.428421
9	6	0	1.920005	1.400317	0.246517
10	6	0	2.613936	-1.188709	-0.054337

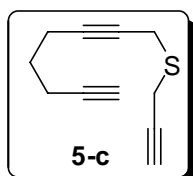
11	1	0	-3.114598	-0.323324	0.597624
12	1	0	-3.680891	0.087964	-1.082700
13	1	0	-0.706237	2.954898	0.305574
14	1	0	2.769012	-1.886299	0.774651
15	1	0	3.034427	-1.643990	-0.956468
16	1	0	1.758032	1.883514	1.214515
17	1	0	2.008898	2.182709	-0.512541
18	1	0	0.333398	-2.795565	0.137087
19	8	0	-3.099810	-1.528929	1.372512
20	1	0	-2.806149	-1.315917	2.265259
21	1	0	-1.939803	-1.689572	0.505995
22	1	0	-1.924318	-2.159446	-1.199749
23	1	0	0.472760	-2.377615	-1.546589
24	6	0	-2.678262	1.907970	-0.175597
25	1	0	-3.036391	2.524661	-1.010721
26	1	0	-3.215501	2.266874	0.712292
27	16	0	3.475866	0.406598	0.297614



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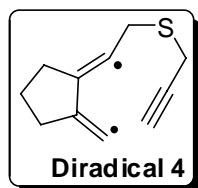
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.443350	0.980236	0.139504
2	6	0	-1.411477	-1.499305	-0.140667
3	1	0	-2.796100	1.402292	1.086536
4	1	0	-2.821359	1.614820	-0.668629
5	1	0	-1.297561	-2.043359	-1.081926
6	1	0	-1.293033	-2.211654	0.680600
7	6	0	-0.432480	-0.361940	-0.032081
8	6	0	-0.946044	0.874163	0.105814
9	6	0	-0.092002	2.105219	0.294078
10	1	0	0.022508	2.290816	1.371186
11	1	0	-0.605189	2.984323	-0.109247
12	6	0	1.008251	-0.562843	-0.021173
13	6	0	1.761425	-1.679734	0.113107
14	1	0	1.406324	-2.695673	0.222343
15	6	0	3.176657	0.208069	-0.012496
16	1	0	4.059931	0.832465	-0.053828
17	6	0	1.898021	0.615096	-0.113549

18	6	0	1.298294	1.968069	-0.363924
19	1	0	1.963552	2.767519	-0.027517
20	1	0	1.174908	2.094051	-1.447361
21	6	0	3.215461	-1.291406	0.135120
22	1	0	3.707262	-1.607338	1.065716
23	1	0	3.782386	-1.764520	-0.679237
24	16	0	-3.093760	-0.737342	-0.061314



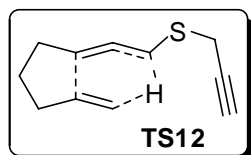
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.430757	1.467009	0.202594
2	6	0	2.797149	2.488536	0.171380
3	1	0	2.223146	3.381902	0.145581
4	6	0	4.254087	0.260133	0.222822
5	6	0	3.660048	-0.976499	-0.486093
6	1	0	4.490129	0.003240	1.262813
7	1	0	5.211804	0.500590	-0.252527
8	6	0	2.542837	-1.712910	0.282686
9	1	0	3.301389	-0.695591	-1.479497
10	1	0	4.477567	-1.690009	-0.630457
11	1	0	2.394711	-2.693130	-0.185218
12	1	0	2.883478	-1.918109	1.305407
13	6	0	1.250860	-1.034261	0.333329
14	6	0	0.168548	-0.507962	0.367396
15	6	0	-1.118500	0.158357	0.399861
16	1	0	-0.986217	1.243852	0.435828
17	1	0	-1.697174	-0.152582	1.273194
18	6	0	-3.650993	0.653663	-0.729046
19	1	0	-4.271838	0.526600	-1.619471
20	1	0	-3.423832	1.719636	-0.639375
21	6	0	-4.351850	0.178788	0.451656
22	6	0	-4.920442	-0.207625	1.438574
23	1	0	-5.427780	-0.555853	2.304850
24	16	0	-2.096900	-0.267120	-1.115755



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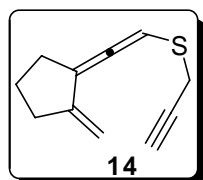
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.133217	0.882457	0.341875
2	6	0	-2.025159	2.024692	0.986262
3	1	0	-2.607146	2.921935	1.131775
4	6	0	-3.326685	0.466626	-0.532478
5	6	0	-3.261572	-1.071252	-0.530386
6	1	0	-3.173153	0.850158	-1.548030
7	1	0	-4.273631	0.865654	-0.166168
8	6	0	-1.754450	-1.382399	-0.501635
9	1	0	-3.737065	-1.459267	0.375693
10	1	0	-3.768929	-1.515638	-1.390026
11	1	0	-1.524688	-2.367859	-0.090088
12	1	0	-1.332013	-1.344941	-1.512758
13	6	0	-1.158301	-0.241245	0.333627
14	6	0	0.020290	-0.267131	0.926719
15	6	0	1.148653	-1.181385	1.107854
16	1	0	0.798495	-2.218140	1.211456
17	1	0	1.719093	-0.950165	2.011978
18	6	0	3.264719	0.321311	-0.093718
19	1	0	4.130079	0.220532	-0.754010
20	1	0	3.642597	0.369782	0.931225
21	6	0	2.514085	1.520239	-0.421679
22	6	0	1.904012	2.522128	-0.684835
23	1	0	1.344174	3.396236	-0.910701
24	16	0	2.351746	-1.270783	-0.304998



(Nimag=1) -1045.8439

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.864702	1.226025	-0.071580

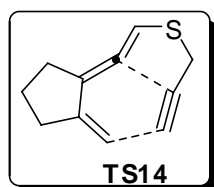
2	6	0	3.348373	1.209205	-0.109278
3	6	0	3.894500	-0.204252	-0.357062
4	1	0	3.718313	1.581112	0.854392
5	1	0	3.698334	1.907400	-0.875980
6	6	0	3.149968	-1.167388	0.585052
7	1	0	3.702037	-0.492451	-1.394625
8	1	0	4.974468	-0.244931	-0.194144
9	1	0	3.311354	-2.210880	0.301492
10	1	0	3.520999	-1.048551	1.610354
11	6	0	1.717967	-0.835179	0.538387
12	6	0	0.493192	-1.014078	0.615125
13	6	0	-0.748562	-0.399438	0.473982
14	1	0	-0.262697	0.757812	0.142807
15	1	0	-1.327812	-0.239252	1.385063
16	6	0	-3.071976	0.323929	-0.910736
17	1	0	-3.725793	0.057587	-1.744986
18	1	0	-2.587175	1.270168	-1.161934
19	6	0	-3.840397	0.450617	0.315544
20	6	0	-4.464680	0.563788	1.337309
21	1	0	-5.022216	0.657247	2.237008
22	16	0	-1.799693	-1.016542	-0.882405
23	6	0	0.750837	1.777827	-0.184687
24	1	0	0.231740	2.683081	-0.433294



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.461304	0.975615	0.065092
2	6	0	3.909872	0.518882	0.122098
3	6	0	3.842939	-0.992107	-0.168401
4	1	0	4.303069	0.685137	1.133167
5	1	0	4.549151	1.069727	-0.570571
6	6	0	2.520653	-1.434141	0.488133
7	1	0	3.792022	-1.159101	-1.248809
8	1	0	4.707092	-1.539963	0.213235
9	1	0	2.097174	-2.341931	0.056347
10	1	0	2.671850	-1.618321	1.558626
11	6	0	1.608907	-0.220556	0.310302

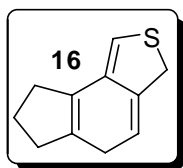
12	6	0	0.299819	-0.246313	0.355291
13	6	0	-1.002072	-0.292820	0.398745
14	1	0	-1.555812	-0.165899	1.326657
15	6	0	-3.402050	0.491261	-0.804018
16	1	0	-4.043377	0.318515	-1.672065
17	1	0	-3.009403	1.507740	-0.875724
18	6	0	-4.151650	0.312332	0.426200
19	6	0	-4.762902	0.172131	1.452421
20	1	0	-5.309210	0.043183	2.354676
21	6	0	2.035954	2.216637	-0.185777
22	1	0	2.734511	3.024039	-0.373892
23	1	0	0.979252	2.458200	-0.211092
24	16	0	-2.005060	-0.705429	-1.028192



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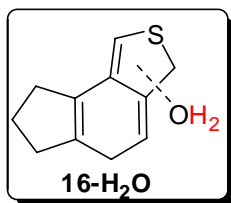
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.154351	0.280971	0.006502
2	6	0	1.770680	-1.714250	0.298002
3	1	0	3.862630	0.055813	-0.800853
4	1	0	3.547400	1.152024	0.537972
5	1	0	1.190854	-2.282787	1.027070
6	1	0	2.118093	-2.424674	-0.463487
7	6	0	0.956544	-0.614264	-0.375810
8	6	0	1.775493	0.529984	-0.579981
9	6	0	1.299139	1.715293	-1.070954
10	1	0	0.424227	1.742070	-1.704207
11	1	0	1.931535	2.597699	-1.088335
12	6	0	-0.391995	-0.587889	-0.489784
13	6	0	-1.547152	-1.057854	-0.911218
14	1	0	-1.642314	-1.723467	-1.763522
15	6	0	-2.310454	0.447753	1.132705
16	1	0	-3.076475	1.144030	1.478584
17	1	0	-2.024641	-0.210241	1.956497
18	6	0	-1.127351	1.157231	0.617411
19	6	0	-0.427024	2.164605	0.483730
20	1	0	-0.101502	3.173548	0.586119
21	6	0	2.959361	-0.948867	0.920640

22	1	0	3.859612	-1.561299	1.009380
23	1	0	2.685699	-0.615282	1.926211
24	16	0	-3.090292	-0.580232	-0.180555



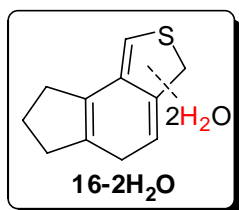
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.220458	-1.199248	0.199813
2	6	0	3.183646	0.322698	-0.095734
3	6	0	1.783410	-1.712916	-0.078881
4	1	0	3.975970	-1.724389	-0.387964
5	1	0	3.462787	-1.356506	1.254088
6	1	0	3.582126	0.556127	-1.093514
7	1	0	3.783718	0.901469	0.615600
8	1	0	1.465182	-2.467416	0.647615
9	1	0	1.700176	-2.177281	-1.070247
10	6	0	0.950845	-0.453047	-0.017614
11	6	0	1.713905	0.656066	-0.026396
12	6	0	-0.495555	-0.366751	-0.004827
13	6	0	-1.401113	-1.368941	-0.031579
14	1	0	-1.186808	-2.428198	-0.065809
15	6	0	-2.607579	0.924571	0.077989
16	1	0	-3.071047	1.454633	-0.754592
17	1	0	-2.996926	1.331117	1.012548
18	6	0	-1.090829	0.974719	0.025494
19	6	0	-0.344075	2.088281	0.012415
20	1	0	-0.815039	3.067264	0.030504
21	6	0	1.164100	2.050458	-0.027182
22	1	0	1.576338	2.615877	0.824135
23	1	0	1.529406	2.594785	-0.913557
24	16	0	-3.091823	-0.866426	-0.018737



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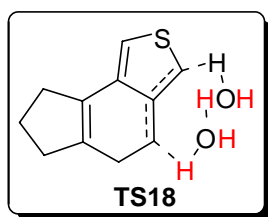
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.227166	-0.516992	-0.264998
2	6	0	-1.205437	-0.491575	-0.046511
3	6	0	-1.898965	0.660260	-0.125703
4	6	0	-1.281477	1.989872	-0.438105
5	6	0	0.200029	1.903785	-0.714959
6	6	0	0.873544	0.743778	-0.657481
7	6	0	1.092317	-1.540594	-0.091573
8	6	0	2.335388	0.538737	-1.002427
9	6	0	-2.082982	-1.653871	0.356207
10	6	0	-3.356414	0.457632	0.207163
11	1	0	2.994990	1.285226	-0.561104
12	1	0	2.484690	0.526875	-2.084069
13	1	0	0.848318	-2.543416	0.230206
14	1	0	-3.584461	0.881412	1.195481
15	1	0	-4.026093	0.957387	-0.501672
16	1	0	-1.877666	-1.944748	1.394592
17	1	0	-1.915264	-2.544201	-0.257984
18	1	0	-1.468118	2.692833	0.389855
19	1	0	1.572038	1.297778	1.860009
20	8	0	2.307068	1.115382	2.456344
21	1	0	2.676809	0.288256	2.121664
22	1	0	0.710913	2.822754	-0.988262
23	1	0	-1.793587	2.449136	-1.298753
24	6	0	-3.516246	-1.084851	0.188986
25	1	0	-4.203750	-1.445763	0.956181
26	1	0	-3.918074	-1.395057	-0.779070
27	16	0	2.795073	-1.143038	-0.361964



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.262524	0.878629	0.072686
2	6	0	-1.622568	0.417631	-0.121702

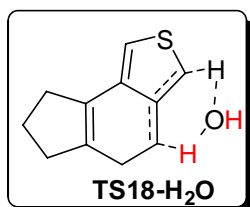
3	6	0	-2.034678	-0.766986	0.368268
4	6	0	-1.157838	-1.702572	1.146200
5	6	0	0.257073	-1.190638	1.301209
6	6	0	0.645237	0.008928	0.829244
7	6	0	0.320466	2.014305	-0.374644
8	6	0	2.011428	0.639328	1.023902
9	6	0	-2.712592	1.116488	-0.900934
10	6	0	-3.467986	-1.058069	-0.001011
11	1	0	2.833870	0.010005	0.679604
12	1	0	2.176102	0.901879	2.070442
13	1	0	-0.155295	2.785617	-0.964962
14	1	0	-3.514505	-1.846143	-0.766346
15	1	0	-4.058346	-1.421919	0.847627
16	1	0	-2.495092	1.081750	-1.976349
17	1	0	-2.809842	2.174062	-0.635737
18	1	0	-1.159541	-2.699131	0.674270
19	8	0	1.734259	-2.298331	-1.471241
20	1	0	1.434430	-3.211659	-1.510790
21	1	0	1.186130	-1.868615	-0.794974
22	1	0	0.951177	-1.805493	1.867836
23	1	0	-1.595430	-1.883304	2.141851
24	8	0	4.250565	-1.422333	-0.504966
25	1	0	3.488850	-1.806519	-0.973048
26	1	0	4.813465	-1.051361	-1.190307
27	16	0	2.016342	2.215069	0.040853
28	6	0	-3.982791	0.302282	-0.539711
29	1	0	-4.663645	0.189621	-1.385603
30	1	0	-4.531747	0.819450	0.251444



(Nimag=1) -1259.7125

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.092485	-0.885578	0.098410
2	6	0	1.485834	-0.520742	-0.108401
3	6	0	1.974469	0.628627	0.388082
4	6	0	1.171397	1.601550	1.200149
5	6	0	-0.345978	1.375757	1.074690

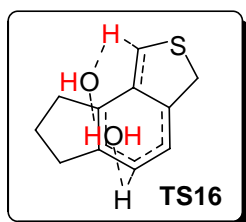
6	6	0	-0.776230	0.042013	0.740884
7	6	0	-0.554906	-2.052903	-0.246104
8	6	0	-2.160765	-0.401974	0.769407
9	6	0	2.516702	-1.294418	-0.894923
10	6	0	3.423342	0.819290	0.018854
11	1	0	-2.745483	0.284575	-0.026623
12	1	0	-2.709522	-0.267075	1.701297
13	1	0	-0.109603	-2.895906	-0.757664
14	1	0	3.514449	1.619369	-0.728167
15	1	0	4.038553	1.125145	0.872333
16	1	0	2.290536	-1.252976	-1.968302
17	1	0	2.552344	-2.355233	-0.623789
18	1	0	1.408498	2.626234	0.891316
19	8	0	-1.333875	2.628047	-1.135356
20	1	0	-1.448874	3.583011	-1.107731
21	1	0	-0.734734	1.988152	0.106223
22	1	0	-0.923278	1.831005	1.882707
23	1	0	1.491608	1.531413	2.250837
24	8	0	-3.389070	1.369955	-0.883336
25	1	0	-2.453092	2.036866	-1.070172
26	1	0	-3.735757	1.074929	-1.731033
27	6	0	3.841719	-0.561819	-0.550621
28	1	0	4.506192	-0.476003	-1.412114
29	1	0	4.378691	-1.124340	0.217314
30	16	0	-2.221586	-2.113251	0.169409



(Nimag=1) -1837.3712

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.201996	-0.696376	-0.157263
2	6	0	-1.233675	-0.521445	-0.003019
3	6	0	-1.802458	0.687547	-0.161690
4	6	0	-1.062022	1.938604	-0.537640
5	6	0	0.459192	1.756604	-0.595022
6	6	0	0.981336	0.430885	-0.567297
7	6	0	0.976835	-1.801778	0.099346
8	6	0	2.405280	0.194255	-0.456975

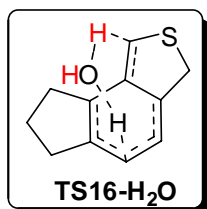
9	6	0	-2.231934	-1.575782	0.412676
10	6	0	-3.284445	0.641045	0.115524
11	1	0	2.569025	0.977454	0.511661
12	1	0	3.081169	0.588326	-1.213546
13	1	0	0.622304	-2.766358	0.436798
14	1	0	-3.506700	1.148012	1.064856
15	1	0	-3.872115	1.158288	-0.651012
16	1	0	-2.086470	-1.849149	1.466366
17	1	0	-2.136750	-2.501071	-0.165281
18	1	0	-1.319716	2.741624	0.166815
19	8	0	2.317352	2.220271	1.237766
20	1	0	2.096998	1.997194	2.149239
21	1	0	1.147541	2.102627	0.448939
22	1	0	0.965934	2.440255	-1.279949
23	1	0	-1.441286	2.289107	-1.509017
24	6	0	-3.597808	-0.876686	0.179961
25	1	0	-4.013129	-1.202490	-0.777025
26	1	0	-4.330594	-1.122440	0.950717
27	16	0	2.675699	-1.551549	-0.092081



(Nimag=1) -948.7389

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.479930	-0.538561	-0.452803
2	6	0	-0.942169	-0.676413	-0.453294
3	6	0	-1.746085	0.426028	-0.636192
4	6	0	-1.204553	1.736685	-0.785778
5	6	0	0.205089	1.820322	-1.056967
6	6	0	1.018123	0.733018	-0.892020
7	6	0	1.425737	-1.405685	0.091722
8	6	0	2.517650	0.688922	-1.101946
9	6	0	-1.750910	-1.926122	-0.199738
10	6	0	-3.205919	0.039559	-0.571074
11	1	0	3.028888	1.585998	-0.749550
12	1	0	2.773322	0.538511	-2.155540
13	1	0	1.303857	-2.476130	0.195379
14	1	0	-3.807798	0.744531	0.010642

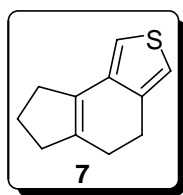
15	1	0	-3.628238	0.029300	-1.584396
16	1	0	-1.378762	-2.504299	0.653313
17	1	0	-1.715417	-2.598017	-1.067687
18	1	0	-0.998858	1.836897	0.813328
19	1	0	-0.357475	2.621444	2.155174
20	8	0	-0.753612	1.780321	1.896174
21	1	0	0.955727	-0.680809	1.618599
22	1	0	0.628495	2.778090	-1.348717
23	1	0	-1.851524	2.558034	-1.078504
24	8	0	0.677212	-0.119324	2.458061
25	1	0	1.487086	0.053625	2.950827
26	1	0	-0.075683	0.934977	2.157154
27	16	0	3.117385	-0.779566	-0.132779
28	6	0	-3.182578	-1.381056	0.050137
29	1	0	-3.959029	-2.030997	-0.358970
30	1	0	-3.357442	-1.306256	1.127237



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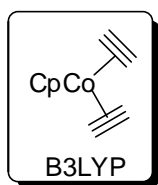
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.416638	-0.482777	-0.367704
2	6	0	-1.011934	-0.515080	-0.378874
3	6	0	-1.680301	0.670646	-0.182093
4	6	0	-0.964012	1.896974	-0.002117
5	6	0	0.378837	1.934390	-0.530021
6	6	0	1.055178	0.769014	-0.745282
7	6	0	1.284024	-1.328711	0.322015
8	6	0	2.527203	0.587041	-1.002377
9	6	0	-1.935034	-1.700834	-0.230933
10	6	0	-3.151833	0.417781	0.056348
11	1	0	3.120409	1.469306	-0.761374
12	1	0	2.742687	0.284312	-2.030721
13	1	0	1.099357	-2.366985	0.568054
14	1	0	-3.386282	0.546722	1.121640
15	1	0	-3.796551	1.110116	-0.493198
16	1	0	-1.819453	-2.161125	0.762348
17	1	0	-1.749903	-2.490104	-0.965296

18	1	0	-0.376234	1.287760	1.392898
19	1	0	0.845938	1.036399	2.584096
20	8	0	0.159490	0.560146	2.095811
21	1	0	0.629284	-0.267135	1.562542
22	1	0	0.875511	2.893290	-0.646682
23	1	0	-1.514695	2.826705	0.095270
24	6	0	-3.335033	-1.055988	-0.385370
25	1	0	-3.629284	-1.083661	-1.438211
26	1	0	-4.107718	-1.575484	0.185138
27	16	0	3.018039	-0.821626	0.123466



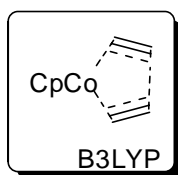
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.190337	-1.184128	0.245250
2	6	0	3.131558	0.293959	-0.220028
3	6	0	1.748917	-1.729971	0.073538
4	1	0	3.930896	-1.770053	-0.302845
5	1	0	3.466546	-1.218688	1.302468
6	1	0	3.477273	0.408683	-1.257803
7	1	0	3.763882	0.951079	0.387260
8	1	0	1.461793	-2.412259	0.879909
9	1	0	1.635869	-2.288940	-0.865272
10	6	0	0.910936	-0.473248	0.038350
11	6	0	1.664427	0.631682	-0.117555
12	6	0	1.075737	2.002208	-0.309811
13	1	0	0.989468	2.203968	-1.387941
14	1	0	1.746812	2.771010	0.087312
15	6	0	-0.541703	-0.391266	0.042317
16	6	0	-1.457205	-1.404704	-0.076226
17	1	0	-1.275694	-2.463972	-0.175889
18	6	0	-2.522806	0.838664	0.059873
19	1	0	-3.239209	1.645335	0.109709
20	6	0	-1.164431	0.908155	0.128139
21	6	0	-0.309471	2.129456	0.360417
22	1	0	-0.818672	3.035150	0.021231
23	1	0	-0.157671	2.238539	1.442407
24	16	0	-3.083691	-0.801543	-0.099133



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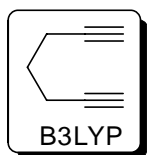
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.216207	-1.527503	0.000000
2	6	0	-0.373240	-1.490547	1.141145
3	6	0	-0.373240	-1.490547	-1.141145
4	6	0	0.989706	-1.511854	0.706093
5	6	0	0.989706	-1.511854	-0.706093
6	1	0	-2.295049	-1.530289	0.000000
7	1	0	-0.700456	-1.460234	2.169109
8	1	0	-0.700456	-1.460234	-2.169109
9	1	0	1.857612	-1.505710	1.347173
10	1	0	1.857612	-1.505710	-1.347173
11	6	0	0.624316	1.573204	1.412475
12	6	0	0.624316	1.573204	-1.412475
13	6	0	-0.618710	1.567844	1.420899
14	6	0	-0.618710	1.567844	-1.420899
15	27	0	-0.007577	0.280061	0.000000
16	1	0	1.611573	1.857941	1.713566
17	1	0	1.611573	1.857941	-1.713566
18	1	0	-1.602734	1.842945	1.741538
19	1	0	-1.602734	1.842945	-1.741538



(Nimag=1) -451.7170

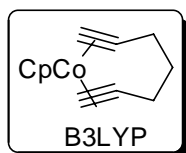
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.484261	1.926657	0.987941
2	6	0	0.484261	1.926657	-0.987941
3	6	0	-0.570761	1.403069	1.475563
4	6	0	-0.570761	1.403069	-1.475563
5	1	0	1.342360	2.544010	1.198704

6	1	0	1.342360	2.544010	-1.198704
7	1	0	-1.229657	1.381873	2.323948
8	1	0	-1.229657	1.381873	-2.323948
9	27	0	-0.089954	0.243187	0.000000
10	6	0	0.471900	-1.540425	1.144476
11	6	0	0.471900	-1.540425	-1.144476
12	6	0	-0.891814	-1.572146	0.708979
13	6	0	-0.891814	-1.572146	-0.708979
14	6	0	1.302692	-1.554068	0.000000
15	1	0	0.804352	-1.507206	2.170653
16	1	0	0.804352	-1.507206	-2.170653
17	1	0	-1.762836	-1.592432	1.345078
18	1	0	-1.762836	-1.592432	-1.345078
19	1	0	2.381125	-1.499979	0.000000



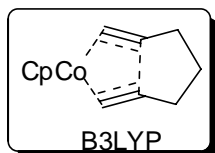
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.669495	0.433370	0.075497
2	6	0	2.011677	1.578117	-0.057699
3	1	0	2.290195	2.596791	-0.171952
4	6	0	1.306919	-0.973692	0.225778
5	6	0	0.000026	-1.412832	-0.469118
6	1	0	1.248117	-1.217427	1.293693
7	1	0	2.128006	-1.578282	-0.175972
8	6	0	-1.306885	-0.973719	0.225770
9	1	0	0.000030	-1.070738	-1.507039
10	1	0	0.000038	-2.507129	-0.492659
11	1	0	-2.127955	-1.578339	-0.175967
12	1	0	-1.248075	-1.217434	1.293689
13	6	0	-1.669508	0.433329	0.075485
14	6	0	-2.011734	1.578065	-0.057692
15	1	0	-2.290294	2.596729	-0.171919



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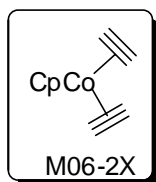
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.583734	0.000512	-0.495373
2	6	0	-2.155863	1.141797	0.235024
3	6	0	-2.156427	-1.141446	0.234242
4	6	0	-1.534548	0.705664	1.446384
5	6	0	-1.534849	-0.706392	1.445893
6	1	0	-3.097414	0.000952	-1.443875
7	1	0	-2.287639	2.170303	-0.064685
8	1	0	-2.288717	-2.169691	-0.066136
9	1	0	-1.121852	1.347625	2.209704
10	1	0	-1.122444	-1.349055	2.208779
11	6	0	1.112916	1.297494	-0.357052
12	6	0	1.112960	-1.297495	-0.356988
13	6	0	0.409325	1.499292	-1.364561
14	6	0	0.409409	-1.499374	-1.364517
15	27	0	-0.433004	-0.000040	-0.315063
16	1	0	0.110354	1.992624	-2.266575
17	1	0	0.110520	-1.992715	-2.266554
18	6	0	2.266573	1.293339	0.558906
19	1	0	2.907735	2.158378	0.351688
20	1	0	1.918253	1.393134	1.593029
21	6	0	2.266622	-1.293293	0.558961
22	1	0	2.907806	-2.158318	0.351755
23	1	0	1.918318	-1.393077	1.593088
24	6	0	3.098627	0.000037	0.412219
25	1	0	3.573335	0.000022	-0.573135
26	1	0	3.896782	0.000091	1.160778



(Nimag=1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.291343	0.985469	-0.320297
2	6	0	1.291340	-0.985417	-0.320347
3	6	0	0.405816	1.468549	-1.106835
4	6	0	0.405747	-1.468365	-1.106968

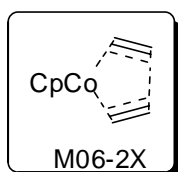
5	1	0	0.166887	2.348170	-1.678687
6	1	0	0.166774	-2.347939	-1.678873
7	27	0	-0.537425	0.000052	-0.289070
8	6	0	-2.035326	1.145073	0.832941
9	6	0	-2.036053	-1.145925	0.830687
10	6	0	-2.511992	0.710077	-0.445126
11	6	0	-2.512457	-0.708177	-0.446607
12	6	0	-1.773261	-0.001292	1.619870
13	1	0	-1.895688	2.170957	1.137504
14	1	0	-1.897044	-2.172491	1.133231
15	1	0	-2.814433	1.346847	-1.261689
16	1	0	-2.815334	-1.343121	-1.264428
17	1	0	-1.373172	-0.002420	2.623030
18	6	0	2.534234	1.230745	0.469620
19	1	0	3.022617	2.138209	0.103766
20	1	0	2.262675	1.407393	1.518229
21	6	0	2.534191	-1.230844	0.469548
22	1	0	3.022565	-2.138282	0.103618
23	1	0	2.262601	-1.407598	1.518132
24	6	0	3.446187	-0.000059	0.362345
25	1	0	4.222356	-0.000103	1.131631
26	1	0	3.941053	-0.000027	-0.613568



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.211291	-1.592032	0.000000
2	6	0	-0.371126	-1.546685	1.139635
3	6	0	-0.371126	-1.546685	-1.139635
4	6	0	0.985005	-1.563914	0.706076
5	6	0	0.985005	-1.563914	-0.706076
6	1	0	-2.290217	-1.609561	0.000000
7	1	0	-0.699409	-1.531002	2.168262
8	1	0	-0.699409	-1.531002	-2.168262
9	1	0	1.853936	-1.564028	1.346651
10	1	0	1.853936	-1.564028	-1.346651
11	6	0	0.612809	1.650272	1.491488
12	6	0	0.612809	1.650272	-1.491488

13	6	0	-0.609246	1.653454	1.493937
14	6	0	-0.609246	1.653454	-1.493937
15	27	0	-0.006331	0.286539	0.000000
16	1	0	1.647123	1.821507	1.693691
17	1	0	1.647123	1.821507	-1.693691
18	1	0	-1.641854	1.827369	1.702850
19	1	0	-1.641854	1.827369	-1.702850



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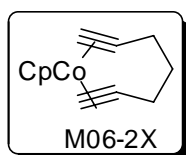
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.443109	1.998451	0.977247
2	6	0	0.443109	1.998451	-0.977247
3	6	0	-0.540638	1.403745	1.512129
4	6	0	-0.540638	1.403745	-1.512129
5	1	0	1.248168	2.694441	1.145431
6	1	0	1.248168	2.694441	-1.145431
7	1	0	-1.136863	1.328260	2.402060
8	1	0	-1.136863	1.328260	-2.402060
9	27	0	-0.093876	0.241912	0.000000
10	6	0	0.477027	-1.560973	1.141388
11	6	0	0.477027	-1.560973	-1.141388
12	6	0	-0.881728	-1.614253	0.706231
13	6	0	-0.881728	-1.614253	-0.706231
14	6	0	1.307169	-1.578031	0.000000
15	1	0	0.808382	-1.528559	2.168045
16	1	0	0.808382	-1.528559	-2.168045
17	1	0	-1.753002	-1.628843	1.342383
18	1	0	-1.753002	-1.628843	-1.342383
19	1	0	2.385021	-1.517681	0.000000



(Nimag=0)

Center	Atomic	Atomic	Coordinates (Angstroms)		
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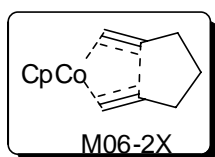
Number	Number	Type	X	Y	Z
1	6	0	1.576337	0.531979	0.068617
2	6	0	1.757614	1.715656	-0.003259
3	1	0	1.898697	2.767889	-0.063802
4	6	0	1.389353	-0.917209	0.146810
5	6	0	0.080237	-1.432147	-0.468388
6	1	0	1.442492	-1.224078	1.196789
7	1	0	2.231555	-1.396718	-0.360295
8	6	0	-1.187202	-1.036799	0.306842
9	1	0	-0.001663	-1.091680	-1.502859
10	1	0	0.135225	-2.523677	-0.485934
11	1	0	-2.004341	-1.702206	0.014207
12	1	0	-1.026814	-1.193601	1.378716
13	6	0	-1.633226	0.339395	0.084781
14	6	0	-2.033891	1.452183	-0.116482
15	1	0	-2.370491	2.445725	-0.290344



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.639093	0.000022	-0.456817
2	6	0	-2.191535	1.139909	0.256355
3	6	0	-2.191390	-1.140067	0.255953
4	6	0	-1.544795	0.705325	1.448126
5	6	0	-1.544706	-0.705812	1.447868
6	1	0	-3.185561	0.000159	-1.387200
7	1	0	-2.343429	2.168951	-0.033558
8	1	0	-2.343129	-2.169028	-0.034330
9	1	0	-1.123950	1.348115	2.207110
10	1	0	-1.123775	-1.348831	2.206610
11	6	0	1.191601	1.379496	-0.427506
12	6	0	1.191491	-1.379398	-0.427773
13	6	0	0.513721	1.588677	-1.423834
14	6	0	0.513687	-1.588259	-1.424175
15	27	0	-0.416426	0.000133	-0.353717
16	1	0	0.083629	1.969447	-2.322828
17	1	0	0.083620	-1.968680	-2.323327

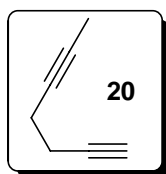
18	6	0	2.213811	1.286582	0.625965
19	1	0	2.877219	2.153545	0.554021
20	1	0	1.722150	1.327331	1.602910
21	6	0	2.213670	-1.286796	0.625744
22	1	0	2.876991	-2.153816	0.553665
23	1	0	1.721977	-1.327665	1.602667
24	6	0	3.044983	-0.000142	0.511338
25	1	0	3.571548	-0.000087	-0.446273
26	1	0	3.797535	-0.000257	1.303430



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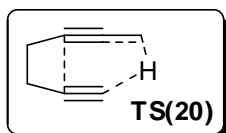
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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3	6	0	0.440761	1.497090	-1.032261
4	6	0	0.440698	-1.495766	-1.035807
5	1	0	0.201833	2.408356	-1.550807
6	1	0	0.203193	-2.407372	-1.554536
7	27	0	-0.544213	-0.000120	-0.276643
8	6	0	-2.068014	1.099188	0.900775
9	6	0	-2.145458	-1.173644	0.684286
10	6	0	-2.525877	0.801721	-0.416425
11	6	0	-2.573519	-0.604089	-0.553324
12	6	0	-1.877963	-0.121481	1.585859
13	1	0	-1.906592	2.087477	1.303284
14	1	0	-2.051390	-2.228402	0.892522
15	1	0	-2.764753	1.522570	-1.182791
16	1	0	-2.860007	-1.149452	-1.438828
17	1	0	-1.511209	-0.230892	2.595456
18	6	0	2.597899	1.214552	0.471517
19	1	0	3.056381	2.137907	0.113349
20	1	0	2.352087	1.350828	1.530833
21	6	0	2.596859	-1.215715	0.470347
22	1	0	3.054857	-2.139166	0.111816
23	1	0	2.350515	-1.352392	1.529517
24	6	0	3.505811	-0.000903	0.298567
25	1	0	4.329571	-0.001541	1.013869

26 1 0 3.925832 -0.000599 -0.710678



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.568091	-0.812580	0.488094
2	6	0	-0.398409	-1.348932	-0.378657
3	1	0	-1.267264	-0.820363	1.540553
4	1	0	-2.412402	-1.504357	0.394600
5	1	0	-0.242950	-2.402188	-0.119874
6	1	0	-0.697119	-1.325401	-1.431804
7	6	0	0.851712	-0.615570	-0.202488
8	6	0	1.879441	-0.008184	-0.044248
9	6	0	3.119661	0.736292	0.139249
10	1	0	2.934033	1.685845	0.649725
11	1	0	3.589633	0.961384	-0.822655
12	1	0	3.838278	0.169282	0.738286
13	6	0	-2.009948	0.528086	0.118606
14	6	0	-2.380863	1.626772	-0.199372
15	1	0	-2.703229	2.600503	-0.475943



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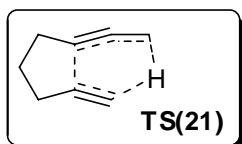
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.433605	0.959248	-0.000222
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3	1	0	0.857365	2.770642	0.000534
4	6	0	-1.855023	0.475036	-0.000178
5	1	0	-2.398762	0.819070	-0.884242
6	1	0	-2.399279	0.819994	0.883202
7	6	0	-1.571516	-1.056679	0.000453
8	1	0	-1.949019	-1.574901	0.885866
9	1	0	-1.950490	-1.575983	-0.883694

10	6	0	-0.094700	-0.909523	-0.000560
11	6	0	1.140882	-1.095349	-0.000123
12	6	0	2.315635	-0.343156	0.000076
13	1	0	1.715751	0.832535	0.000026
14	1	0	2.923166	-0.367554	-0.905646
15	1	0	2.922711	-0.367473	0.906108



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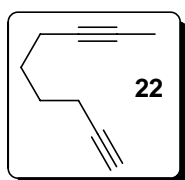
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	0.928579	2.435086	-0.101318
3	1	0	0.468623	3.379015	-0.261253
4	6	0	2.100047	0.076306	0.292816
5	6	0	1.510416	-1.128069	-0.475201
6	1	0	2.118029	-0.149984	1.365956
7	1	0	3.147257	0.197025	-0.006897
8	6	0	0.247003	-1.758462	0.146673
9	1	0	1.309930	-0.840242	-1.510394
10	1	0	2.280057	-1.906246	-0.502154
11	1	0	0.054147	-2.708157	-0.366178
12	1	0	0.458048	-2.020108	1.191464
13	6	0	-0.963487	-0.941778	0.088487
14	6	0	-1.972617	-0.287292	0.033449
15	6	0	-3.171200	0.539311	-0.030005
16	1	0	-2.908191	1.598430	-0.112860
17	1	0	-3.784709	0.417014	0.867564
18	1	0	-3.789077	0.279358	-0.894654



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-0.057638	1.121445	-0.065212
2	6	0	1.008742	1.766632	0.027172

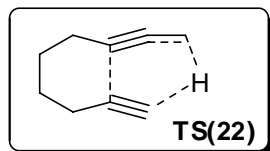
3	1	0	1.468832	2.732079	0.099744
4	6	0	-1.540656	1.071198	-0.183761
5	6	0	-2.097334	-0.242454	0.381367
6	1	0	-1.801693	1.152358	-1.246409
7	1	0	-1.975750	1.939662	0.319346
8	6	0	-1.228841	-1.384805	-0.174331
9	1	0	-2.024955	-0.229098	1.473039
10	1	0	-3.149758	-0.375587	0.118318
11	1	0	-1.383297	-2.314588	0.379168
12	1	0	-1.496416	-1.581040	-1.219878
13	6	0	0.180788	-0.958225	-0.096036
14	6	0	1.411158	-1.118228	-0.010800
15	6	0	2.623451	-0.433259	0.082262
16	1	0	2.109395	0.738568	0.069767
17	1	0	3.288236	-0.482635	-0.781586
18	1	0	3.167388	-0.513547	1.024527



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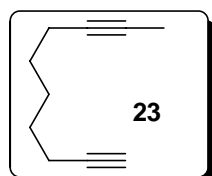
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.146846	1.648687	0.051079
2	6	0	0.898145	2.461222	0.902614
3	1	0	0.660558	3.173506	1.653957
4	6	0	1.501538	0.676601	-0.980331
5	1	0	2.248855	1.141949	-1.632616
6	1	0	0.625730	0.476530	-1.606778
7	6	0	-0.005850	-1.411405	0.975165
8	1	0	-0.328487	-2.341333	1.457147
9	1	0	0.437552	-0.795562	1.765937
10	6	0	-1.190924	-0.741611	0.440053
11	6	0	-2.177836	-0.217660	-0.010141
12	6	0	-3.363223	0.443636	-0.543823
13	1	0	-3.249522	1.531707	-0.521987
14	1	0	-4.253765	0.189115	0.038710
15	6	0	2.079519	-0.654705	-0.434517
16	1	0	2.701479	-0.432692	0.438606
17	1	0	2.754189	-1.061449	-1.195198
18	6	0	1.069423	-1.757758	-0.084740

19	1	0	0.564500	-2.097938	-0.994892
20	1	0	1.643345	-2.614049	0.285645
21	1	0	-3.550252	0.148175	-1.580677



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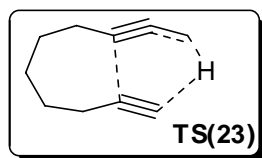
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	1.455432	1.742585	-0.075998
3	1	0	2.001314	2.664896	-0.137003
4	6	0	-1.133425	1.521703	0.201450
5	1	0	-1.329641	2.513979	-0.222299
6	1	0	-1.296032	1.614712	1.282966
7	6	0	-0.878766	-1.669838	-0.153682
8	1	0	-0.855858	-2.629407	0.373647
9	1	0	-1.012823	-1.905632	-1.217316
10	6	0	0.440642	-1.017708	0.004027
11	6	0	1.676374	-1.137202	0.050771
12	6	0	2.920251	-0.520201	0.022174
13	1	0	2.437223	0.689304	-0.039983
14	1	0	3.504512	-0.630426	-0.892100
15	6	0	-2.162300	0.526148	-0.350643
16	1	0	-2.040788	0.424455	-1.435612
17	1	0	-3.155806	0.956484	-0.187628
18	6	0	-2.086844	-0.849989	0.313317
19	1	0	-2.058474	-0.729458	1.402786
20	1	0	-2.992065	-1.421621	0.085119
21	1	0	3.533214	-0.564521	0.922979



(Nimag=0)

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

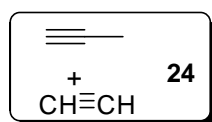
1	6	0	0.512197	-1.510204	-0.596404
2	1	0	1.146441	-2.268308	-1.065324
3	1	0	0.388804	-0.711923	-1.333799
4	6	0	-2.216936	-0.054234	0.617970
5	1	0	-3.270245	0.244623	0.673186
6	1	0	-1.952312	-0.394628	1.627182
7	6	0	-1.429290	1.130729	0.276057
8	6	0	-0.801727	2.119094	-0.009343
9	6	0	-0.037535	3.315251	-0.346431
10	1	0	0.717641	3.528940	0.415897
11	1	0	-0.690205	4.189899	-0.427274
12	6	0	-0.856724	-2.136194	-0.255258
13	1	0	-0.819971	-2.567444	0.754078
14	1	0	-1.019653	-2.984899	-0.928051
15	6	0	-2.100292	-1.237441	-0.372955
16	1	0	-2.177852	-0.850076	-1.394471
17	1	0	-2.978602	-1.873933	-0.218482
18	1	0	0.481914	3.195128	-1.301901
19	6	0	1.275381	-0.951387	0.624610
20	1	0	1.415804	-1.752315	1.360755
21	1	0	0.683733	-0.171739	1.113490
22	6	0	2.580656	-0.397955	0.272825
23	6	0	3.653139	0.050458	-0.039085
24	1	0	4.601283	0.447972	-0.307193



(Nimag=1) -1127.0013

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.668904	1.311372	-0.182517
2	6	0	-1.860804	1.693682	-0.193731
3	1	0	-2.457249	2.586213	-0.260790
4	6	0	0.757757	1.705771	-0.270670
5	1	0	0.780975	2.791750	-0.119693
6	1	0	1.105135	1.541865	-1.297122
7	6	0	0.640514	-1.780260	0.143080
8	1	0	0.454782	-2.794147	-0.225996
9	1	0	0.950552	-1.893330	1.189688
10	6	0	-0.661619	-1.069173	0.096183

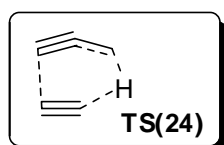
11	6	0	-1.897722	-1.173882	0.137396
12	6	0	-3.169326	-0.633842	0.115627
13	1	0	-2.719827	0.633032	-0.052004
14	1	0	-3.729551	-0.612165	1.050161
15	6	0	1.728873	1.029880	0.722381
16	1	0	1.158411	0.642184	1.570472
17	1	0	2.402295	1.788661	1.132850
18	6	0	1.795445	-1.159115	-0.662924
19	1	0	1.400018	-0.760040	-1.601882
20	1	0	2.491453	-1.956238	-0.943381
21	1	0	-3.790536	-0.823385	-0.759434
22	6	0	2.581714	-0.082496	0.097276
23	1	0	3.166017	-0.561735	0.892085
24	1	0	3.311960	0.365708	-0.587550



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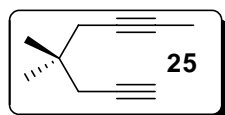
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.420739	-0.000108	0.000001
2	6	0	-0.218528	0.000018	-0.000001
3	6	0	1.238443	0.000039	0.000000
4	1	0	1.629395	1.021244	-0.003286
5	1	0	1.629293	-0.513533	-0.882771
6	1	0	1.629292	-0.507841	0.886059
7	1	0	-2.483033	0.000437	0.000000

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	-0.599706
2	6	0	0.000000	0.000000	0.599706
3	1	0	0.000000	0.000000	-1.662559
4	1	0	0.000000	0.000000	1.662557



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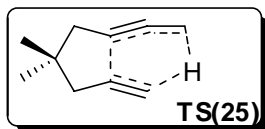
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.463404	0.283821	0.000147
2	6	0	1.382784	-0.955906	-0.000177
3	1	0	1.797581	-1.940776	0.000489
4	6	0	-0.252448	1.361565	0.000088
5	6	0	-1.178890	0.528577	-0.000092
6	6	0	-1.407760	-0.857760	0.000019
7	1	0	-0.246892	-1.214930	-0.000439
8	1	0	-1.867292	-1.267055	-0.901456
9	1	0	-1.866513	-1.266868	0.901990
10	1	0	2.117588	1.132379	-0.000408
11	1	0	0.022990	2.395472	-0.000086



(Nimag=0)

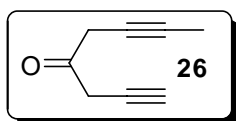
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.179945	1.932492	-0.261833
2	6	0	0.683015	2.715528	0.036079
3	1	0	1.460263	3.390256	0.298449
4	6	0	-1.287256	1.053575	-0.629837
5	6	0	-1.363223	-0.344389	0.058359
6	1	0	-1.282056	0.910839	-1.717157
7	1	0	-2.217288	1.588037	-0.401205
8	6	0	-0.318759	-1.334241	-0.538671
9	1	0	-0.538233	-2.329320	-0.132230
10	1	0	-0.490858	-1.407655	-1.619904
11	6	0	1.091658	-1.038555	-0.300008
12	6	0	2.262547	-0.829585	-0.112410
13	6	0	3.669806	-0.526554	0.114039
14	1	0	3.817232	0.549511	0.250197
15	1	0	4.284582	-0.842067	-0.734254
16	1	0	4.048701	-1.032298	1.007156
17	6	0	-1.184560	-0.217250	1.577568
18	1	0	-1.932666	0.459991	2.000828
19	1	0	-1.302073	-1.192054	2.060742
20	1	0	-0.195952	0.170191	1.828661

21	6	0	-2.757839	-0.920845	-0.252262
22	1	0	-2.928974	-0.996982	-1.331092
23	1	0	-2.870692	-1.921180	0.175324
24	1	0	-3.544656	-0.288324	0.168348



(Nimag=1) -963.3618

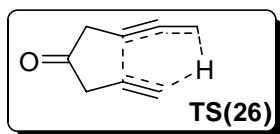
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	0.678369	1.152609	-0.199566
2	6	0	1.773084	1.721020	0.000887
3	1	0	2.290005	2.650454	0.134404
4	6	0	-0.784959	1.203934	-0.458645
5	6	0	-1.513872	-0.066618	0.037178
6	1	0	-0.935602	1.303230	-1.541067
7	1	0	-1.207797	2.100725	0.006143
8	6	0	-0.650515	-1.246299	-0.480626
9	1	0	-0.923268	-2.180805	0.018870
10	1	0	-0.833320	-1.387373	-1.553111
11	6	0	0.771841	-0.930695	-0.261363
12	6	0	1.974973	-1.183925	-0.073408
13	6	0	3.220147	-0.590794	0.142629
14	1	0	2.795243	0.613664	0.116069
15	1	0	3.953956	-0.672165	-0.660859
16	1	0	3.671721	-0.730920	1.125984
17	6	0	-2.935337	-0.138065	-0.533466
18	1	0	-3.440534	-1.054239	-0.212705
19	1	0	-3.539303	0.707832	-0.191258
20	1	0	-2.926269	-0.124375	-1.627819
21	6	0	-1.561961	-0.082356	1.574705
22	1	0	-2.127258	0.774917	1.952998
23	1	0	-2.049943	-0.992080	1.937488
24	1	0	-0.558255	-0.041730	2.004912



(Nimag=0)

Center	Atomic	Atomic	Coordinates (Angstroms)		
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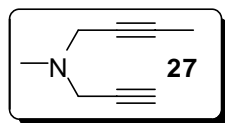
Number	Number	Type	X	Y	Z
1	6	0	-1.785100	1.328895	-0.187371
2	6	0	-2.146338	2.275792	0.459122
3	1	0	-2.464279	3.117832	1.024024
4	6	0	-1.366960	0.164816	-0.959044
5	1	0	-0.476696	0.416294	-1.547781
6	1	0	-2.153588	-0.146849	-1.649495
7	6	0	0.032702	-0.859573	1.015492
8	1	0	-0.391385	-0.172304	1.758159
9	1	0	0.173775	-1.829544	1.497668
10	6	0	1.297988	-0.328938	0.516982
11	6	0	2.344006	0.091816	0.093963
12	6	0	3.614350	0.604699	-0.404798
13	1	0	3.715131	0.430979	-1.480022
14	1	0	4.455723	0.113234	0.092075
15	1	0	3.701955	1.680490	-0.228237
16	6	0	-1.017845	-1.053496	-0.086411
17	8	0	-1.549682	-2.119276	-0.269250



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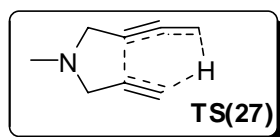
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.350444	1.156205	0.029506
2	6	0	-1.456234	1.730203	-0.042093
3	1	0	-1.989537	2.658604	-0.090081
4	6	0	1.122866	1.228775	0.119838
5	1	0	1.414509	1.637263	1.096163
6	1	0	1.530619	1.911923	-0.630851
7	6	0	0.940453	-1.339374	0.102986
8	1	0	1.210801	-2.039972	-0.692279
9	1	0	1.192939	-1.829571	1.051503
10	6	0	-0.473960	-0.959428	0.053510
11	6	0	-1.696659	-1.172697	0.000883
12	6	0	-2.944157	-0.553937	-0.071355
13	1	0	-2.494952	0.638548	-0.072388
14	1	0	-3.589418	-0.634619	0.804444
15	1	0	-3.497886	-0.665324	-1.004564
16	6	0	1.846500	-0.110754	-0.020064

17 8 0 3.036592 -0.193851 -0.187652



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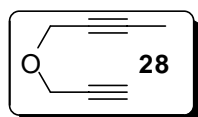
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.208846	1.561272	-0.212045
2	6	0	-0.701173	2.592409	0.142953
3	1	0	-0.237351	3.497575	0.450256
4	6	0	-1.887793	0.318237	-0.624705
5	1	0	-1.872942	0.250994	-1.717078
6	1	0	-2.941804	0.402544	-0.335098
7	6	0	-0.167516	-1.461749	-0.718077
8	1	0	-0.091555	-2.521574	-0.448925
9	1	0	-0.317173	-1.432104	-1.802484
10	6	0	1.106914	-0.801585	-0.385193
11	6	0	2.155675	-0.280425	-0.103065
12	6	0	3.410742	0.379651	0.233124
13	1	0	3.253658	1.448681	0.406029
14	1	0	4.138517	0.276967	-0.577219
15	1	0	3.855332	-0.045139	1.137910
16	7	0	-1.383739	-0.943894	-0.085862
17	6	0	-1.368762	-1.003367	1.370538
18	1	0	-1.138024	-2.024577	1.684710
19	1	0	-0.636302	-0.324354	1.831166
20	1	0	-2.361630	-0.748415	1.750586



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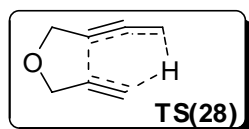
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	-1.535322	1.738479	-0.031108
3	1	0	-2.070750	2.662793	-0.096900
4	6	0	1.027033	1.145916	0.174525
5	1	0	1.272062	1.291419	1.245965

6	1	0	1.435496	1.999408	-0.373934
7	6	0	0.869072	-1.227782	0.180801
8	1	0	1.117693	-2.124635	-0.393289
9	1	0	1.124338	-1.426749	1.240835
10	6	0	-0.565901	-0.910228	0.074770
11	6	0	-1.776212	-1.184064	-0.006042
12	6	0	-3.034268	-0.574411	-0.093145
13	1	0	-2.621996	0.602367	-0.083222
14	1	0	-3.689001	-0.677309	0.774085
15	1	0	-3.579143	-0.706031	-1.029453
16	7	0	1.612671	-0.084970	-0.349517
17	6	0	3.042605	-0.178700	-0.116856
18	1	0	3.430401	-1.093435	-0.571490
19	1	0	3.549221	0.669509	-0.583461
20	1	0	3.304984	-0.189230	0.958064



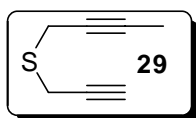
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.505313	1.248344	0.072934
2	6	0	1.209732	2.385489	-0.180861
3	1	0	0.930849	3.384881	-0.409654
4	6	0	1.949694	-0.113404	0.383204
5	1	0	1.729123	-0.345208	1.433980
6	1	0	3.035110	-0.163467	0.257279
7	6	0	0.215175	-1.742590	-0.011614
8	1	0	0.059549	-2.579663	-0.696224
9	1	0	0.381467	-2.162622	0.991478
10	6	0	-0.969661	-0.884804	0.007106
11	6	0	-1.959768	-0.199980	0.026561
12	6	0	-3.134299	0.660758	0.044544
13	1	0	-2.837370	1.712944	0.001077
14	1	0	-3.718095	0.515343	0.957995
15	8	0	1.413667	-1.118181	-0.472174
16	1	0	-3.787088	0.460361	-0.809777



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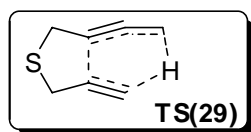
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.087829	1.080222	0.035040
2	6	0	-0.935518	1.791605	-0.006092
3	1	0	-1.402004	2.753287	-0.054064
4	6	0	1.574039	0.977021	0.123936
5	1	0	1.870802	1.116444	1.174665
6	1	0	2.049246	1.751236	-0.479710
7	6	0	1.243198	-1.326726	0.136715
8	1	0	1.446238	-2.203108	-0.479807
9	1	0	1.515041	-1.556385	1.177980
10	6	0	-0.175073	-0.917666	0.060431
11	6	0	-1.402090	-1.109879	-0.002340
12	6	0	-2.614648	-0.408483	-0.054837
13	1	0	-2.120806	0.729422	-0.045255
14	1	0	-3.252467	-0.471531	0.828678
15	8	0	2.052454	-0.267578	-0.362883
16	1	0	-3.192099	-0.495300	-0.976529



(Nimag=0)

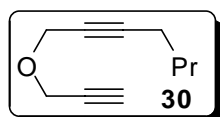
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.087376	1.726024	0.144424
2	6	0	0.552973	2.736445	-0.228371
3	1	0	0.071181	3.621306	-0.565113
4	6	0	1.782027	0.532573	0.597278
5	1	0	1.473869	0.260066	1.609881
6	1	0	2.858338	0.719230	0.626810
7	6	0	0.094786	-1.754340	0.262150
8	1	0	0.027791	-2.709393	-0.266548
9	1	0	0.313509	-1.980610	1.309488
10	6	0	-1.141457	-1.005045	0.137758
11	6	0	-2.165517	-0.378205	0.046789
12	6	0	-3.387374	0.405086	-0.073788
13	1	0	-3.152952	1.456643	-0.264834
14	1	0	-3.981799	0.355395	0.843148
15	16	0	1.591412	-0.958891	-0.482020

16 1 0 -4.009407 0.044391 -0.897958



(Nimag=1) -952.9265

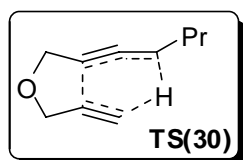
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	-1.386733	1.750995	-0.053920
3	1	0	-1.902273	2.681789	-0.182641
4	6	0	1.164328	1.261547	0.332746
5	1	0	1.371978	1.324781	1.404668
6	1	0	1.562434	2.158085	-0.146547
7	6	0	0.941329	-1.412810	0.337625
8	1	0	1.118490	-2.347217	-0.196812
9	1	0	1.179494	-1.564275	1.393929
10	6	0	-0.442444	-0.957460	0.165119
11	6	0	-1.659224	-1.147314	0.002200
12	6	0	-2.890550	-0.519054	-0.175743
13	1	0	-2.427281	0.668549	-0.141519
14	1	0	-3.607100	-0.589052	0.643747
15	16	0	2.092465	-0.160906	-0.371469
16	1	0	-3.364611	-0.626155	-1.152041



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.931358	1.444937	-0.066119
2	6	0	2.408883	2.524718	-0.143486
3	1	0	1.929496	3.470483	-0.211457
4	6	0	3.645536	0.167300	0.012794
5	1	0	3.750267	-0.133835	1.064057
6	1	0	4.652838	0.305379	-0.390569
7	6	0	2.132051	-1.710041	-0.051387
8	1	0	1.954249	-2.554378	-0.721672
9	1	0	2.603190	-2.106219	0.860378

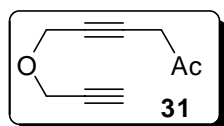
10	6	0	0.862054	-1.070206	0.290750
11	6	0	-0.194225	-0.567132	0.578283
12	6	0	-1.470476	0.063840	0.898939
13	1	0	-1.322639	1.150082	0.943338
14	1	0	-1.781936	-0.241125	1.905585
15	8	0	3.064452	-0.885269	-0.750436
16	6	0	-2.591584	-0.262348	-0.107068
17	6	0	-3.914152	0.430865	0.235234
18	1	0	-2.738413	-1.347648	-0.135491
19	1	0	-2.264583	0.031692	-1.110193
20	6	0	-5.033941	0.108408	-0.758572
21	1	0	-4.226199	0.137582	1.245238
22	1	0	-3.756813	1.516021	0.268210
23	1	0	-5.963738	0.617337	-0.490015
24	1	0	-4.764640	0.420904	-1.772328
25	1	0	-5.239724	-0.966174	-0.787800



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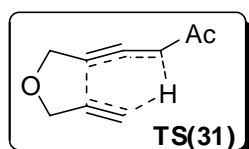
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.517971	1.108255	-0.150899
2	6	0	-0.492109	1.756147	-0.434458
3	1	0	0.018911	2.688112	-0.557162
4	6	0	-2.963462	1.066009	0.208595
5	1	0	-3.554700	1.228318	-0.705615
6	1	0	-3.204705	1.853197	0.924301
7	6	0	-2.754689	-1.253485	0.111685
8	1	0	-2.823163	-2.126570	0.761773
9	1	0	-3.324522	-1.453521	-0.808347
10	6	0	-1.354360	-0.923673	-0.219145
11	6	0	-0.169657	-1.165292	-0.506430
12	6	0	1.044207	-0.526870	-0.812140
13	1	0	0.585018	0.627513	-0.719795
14	1	0	1.339841	-0.609344	-1.863489
15	8	0	-3.331112	-0.161512	0.821227
16	6	0	2.234294	-0.658378	0.142608
17	6	0	3.369976	0.317998	-0.183869
18	1	0	2.615355	-1.685054	0.099131

19	1	0	1.885010	-0.499393	1.168306
20	6	0	4.568739	0.172931	0.757551
21	1	0	3.696663	0.159111	-1.218880
22	1	0	2.990308	1.345093	-0.137322
23	1	0	5.363619	0.878718	0.501680
24	1	0	4.280322	0.359666	1.796609
25	1	0	4.991134	-0.835597	0.708000



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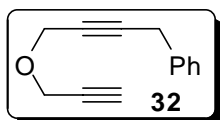
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.579017	1.368113	-0.016158
2	6	0	-2.099220	2.468696	0.042733
3	1	0	-1.663227	3.436480	0.093751
4	6	0	-3.246123	0.064203	-0.074400
5	1	0	-3.383432	-0.235099	-1.122361
6	1	0	-4.239567	0.159841	0.372452
7	6	0	-1.638627	-1.734783	-0.075469
8	1	0	-1.421038	-2.594772	0.562484
9	1	0	-2.095379	-2.117502	-0.999867
10	6	0	-0.397768	-1.030903	-0.401256
11	6	0	0.632260	-0.470333	-0.674731
12	6	0	1.865235	0.231633	-1.000513
13	1	0	1.649129	1.303946	-1.111787
14	1	0	2.273506	-0.102806	-1.957598
15	8	0	-2.594871	-0.971423	0.656288
16	6	0	3.000233	0.132941	0.039513
17	8	0	4.149690	0.135291	-0.335306
18	6	0	2.616201	0.081306	1.498326
19	1	0	1.877501	0.852920	1.733949
20	1	0	2.140086	-0.879293	1.716414
21	1	0	3.504820	0.200102	2.116437



(Nimag=1) -1039.8115

Center	Atomic	Atomic	Coordinates (Angstroms)		
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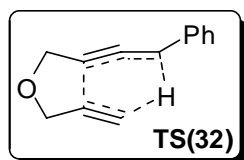
Number	Number	Type	X	Y	Z
1	6	0	-1.298996	1.196409	0.107558
2	6	0	-0.312436	1.954613	0.065331
3	1	0	0.085818	2.930768	0.261864
4	6	0	-2.722489	0.841750	0.324357
5	1	0	-3.297602	1.145097	-0.563477
6	1	0	-3.113971	1.377261	1.191351
7	6	0	-2.241697	-1.344008	-0.368731
8	1	0	-2.232409	-2.360396	0.027752
9	1	0	-2.790357	-1.344170	-1.322095
10	6	0	-0.883154	-0.823057	-0.569141
11	6	0	0.317227	-0.740794	-0.843073
12	6	0	1.442076	0.085254	-0.904817
13	1	0	0.809067	1.137046	-0.449438
14	1	0	1.778651	0.390880	-1.896029
15	8	0	-2.920355	-0.538906	0.593414
16	6	0	2.614466	-0.109602	0.035743
17	8	0	3.698414	0.351039	-0.253474
18	6	0	2.362238	-0.840981	1.334011
19	1	0	1.482687	-0.434113	1.840810
20	1	0	2.149890	-1.894679	1.129074
21	1	0	3.240348	-0.762266	1.973235



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.281915	1.369909	-0.606640
2	6	0	-2.679403	2.276949	-1.115704
3	1	0	-2.130435	3.069102	-1.563276
4	6	0	-4.083227	0.314222	0.018949
5	1	0	-4.347522	-0.444589	-0.729773
6	1	0	-5.015862	0.753164	0.384741
7	6	0	-2.706994	-1.470157	0.880016
8	1	0	-2.466740	-1.878748	1.864282
9	1	0	-3.335366	-2.208216	0.360033
10	6	0	-1.478846	-1.251104	0.116205
11	6	0	-0.461626	-1.091641	-0.508142
12	6	0	0.754919	-0.858464	-1.279733

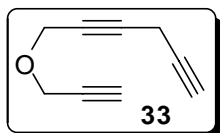
13	1	0	0.517554	-0.154634	-2.089144
14	1	0	1.049043	-1.790186	-1.774774
15	8	0	-3.471636	-0.296009	1.152129
16	6	0	1.940684	-0.318451	-0.487324
17	6	0	3.240641	-0.626159	-0.898929
18	6	0	1.764495	0.515668	0.619165
19	6	0	4.343912	-0.107196	-0.223823
20	1	0	3.392981	-1.279168	-1.752884
21	6	0	2.866591	1.035876	1.295772
22	1	0	0.761054	0.750408	0.955832
23	6	0	4.159736	0.727300	0.877133
24	1	0	5.345349	-0.359640	-0.554556
25	1	0	2.713169	1.680525	2.154232
26	1	0	5.016057	1.129543	1.406593



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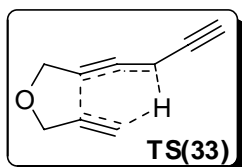
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.244588	0.922276	-0.747181
2	6	0	1.307697	1.701774	-0.998384
3	1	0	0.898768	2.475797	-1.616423
4	6	0	3.608377	0.365637	-0.922298
5	1	0	4.326111	1.040095	-0.430882
6	1	0	3.860481	0.303607	-1.982516
7	6	0	3.177524	-1.043432	0.897894
8	1	0	3.097693	-2.106467	1.129721
9	1	0	3.844767	-0.572493	1.635280
10	6	0	1.864732	-0.381756	0.907698
11	6	0	0.708942	-0.090481	1.236055
12	6	0	-0.374257	0.759157	0.963181
13	1	0	0.229334	1.363146	0.003602
14	1	0	-0.518329	1.554396	1.698772
15	8	0	3.742934	-0.953001	-0.408221
16	6	0	-1.673251	0.230304	0.429146
17	6	0	-1.738526	-0.969068	-0.290286
18	6	0	-2.846736	0.971501	0.606643
19	6	0	-2.947808	-1.413773	-0.816145
20	1	0	-0.836873	-1.554598	-0.430249

21	6	0	-4.058105	0.527356	0.079791
22	1	0	-2.812268	1.901491	1.165555
23	6	0	-4.112918	-0.667854	-0.634025
24	1	0	-2.982166	-2.346453	-1.368403
25	1	0	-4.958077	1.113129	0.230907
26	1	0	-5.054472	-1.017488	-1.042134



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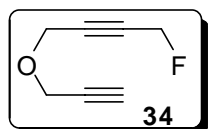
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.267746	1.292925	-0.087527
2	6	0	1.862302	2.414601	-0.236623
3	1	0	1.488794	3.400185	-0.371759
4	6	0	2.841900	-0.045538	0.076794
5	1	0	2.896619	-0.297916	1.144607
6	1	0	3.864420	-0.037059	-0.310894
7	6	0	1.124148	-1.738203	0.066820
8	1	0	0.866151	-2.598004	-0.555827
9	1	0	1.512551	-2.124311	1.020699
10	6	0	-0.073584	-0.935637	0.317006
11	6	0	-1.075586	-0.304263	0.526069
12	6	0	-2.262736	0.512545	0.784933
13	1	0	-1.989976	1.570883	0.686964
14	1	0	-2.579859	0.378463	1.826393
15	8	0	2.166366	-1.072770	-0.642809
16	6	0	-3.393480	0.222965	-0.101977
17	6	0	-4.330059	-0.003128	-0.818738
18	1	0	-5.153539	-0.207679	-1.458258



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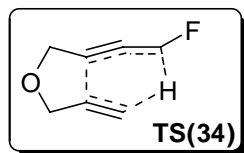
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.936381	1.160260	-0.055641

2	6	0	0.045944	1.901606	-0.239931
3	1	0	0.454275	2.892700	-0.237093
4	6	0	-2.365632	0.866381	0.214286
5	1	0	-2.933024	1.012035	-0.717557
6	1	0	-2.754525	1.552481	0.968957
7	6	0	-1.879581	-1.406771	-0.058772
8	1	0	-1.883138	-2.335125	0.513987
9	1	0	-2.401820	-1.578903	-1.011703
10	6	0	-0.512064	-0.930160	-0.310070
11	6	0	0.697128	-0.935275	-0.558184
12	6	0	1.821209	-0.117194	-0.772233
13	1	0	1.180155	0.988570	-0.562165
14	1	0	2.133653	-0.030314	-1.816831
15	8	0	-2.580599	-0.442125	0.722478
16	6	0	2.939568	-0.168200	0.142442
17	6	0	3.880217	-0.167942	0.891968
18	1	0	4.706772	-0.180672	1.559385



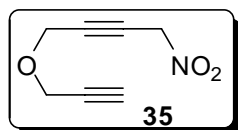
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	1.333077	2.456066	-0.295542
3	1	0	0.933911	3.390911	-0.605394
4	6	0	2.366360	0.129122	0.493693
5	1	0	2.083396	-0.075240	1.535010
6	1	0	3.454901	0.227251	0.461868
7	6	0	0.911404	-1.743124	0.046116
8	1	0	0.950617	-2.646743	-0.566803
9	1	0	0.994507	-2.053882	1.098005
10	6	0	-0.373833	-1.072515	-0.147161
11	6	0	-1.449860	-0.551733	-0.288697
12	6	0	-2.724769	0.110635	-0.489904
13	1	0	-2.593999	1.026074	-1.073792
14	8	0	2.057919	-0.991131	-0.334561
15	1	0	-3.433631	-0.543414	-1.004984
16	9	0	-3.313611	0.476312	0.732376



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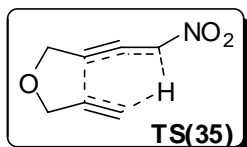
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.598916	1.107523	-0.003670
2	6	0	-0.361282	1.877840	-0.187854
3	1	0	-0.788953	2.852265	-0.296838
4	6	0	2.040970	0.883712	0.296613
5	1	0	2.183518	0.933413	1.386439
6	1	0	2.656804	1.650713	-0.174124
7	6	0	1.559470	-1.389293	0.104406
8	1	0	1.764299	-2.225075	-0.565532
9	1	0	1.688610	-1.728814	1.142930
10	6	0	0.184275	-0.870200	-0.067469
11	6	0	-1.042120	-1.012524	-0.230675
12	6	0	-2.168229	-0.198542	-0.439295
13	1	0	-1.577879	0.886513	-0.403524
14	8	0	2.492462	-0.363998	-0.208603
15	1	0	-2.680120	-0.266921	-1.399885
16	9	0	-3.117553	-0.175689	0.571890



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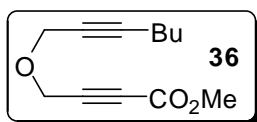
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.205386	1.540289	0.073748
2	6	0	1.689333	2.532969	-0.365286
3	1	0	1.223466	3.405221	-0.754739
4	6	0	2.901875	0.377493	0.628844
5	1	0	2.495186	0.137107	1.619936
6	1	0	3.958216	0.628083	0.757959
7	6	0	1.816335	-1.689440	0.022765
8	1	0	2.061328	-2.572639	-0.571831
9	1	0	1.801336	-1.995082	1.079225
10	6	0	0.485923	-1.202559	-0.342163

11	6	0	-0.619705	-0.814319	-0.612126
12	6	0	-1.920041	-0.308999	-0.972733
13	1	0	-1.866193	0.591905	-1.584978
14	8	0	2.880719	-0.776655	-0.211904
15	1	0	-2.529421	-1.045586	-1.501613
16	7	0	-2.792732	0.094282	0.236106
17	8	0	-3.789174	0.739862	-0.046178
18	8	0	-2.460224	-0.265907	1.346207



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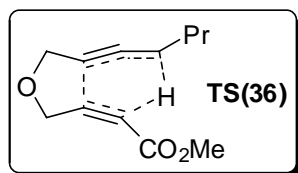
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.241782	1.173845	0.044780
2	6	0	0.260199	1.912626	-0.160120
3	1	0	-0.118284	2.915752	-0.193123
4	6	0	2.630262	0.866063	0.470112
5	1	0	2.647693	0.779927	1.566563
6	1	0	3.298574	1.675642	0.171536
7	6	0	2.220667	-1.390184	0.008577
8	1	0	2.536333	-2.167575	-0.688385
9	1	0	2.249871	-1.797488	1.029677
10	6	0	0.862393	-0.911624	-0.287087
11	6	0	-0.331931	-0.914894	-0.597331
12	6	0	-1.438321	-0.108262	-0.829490
13	1	0	-0.832678	1.023933	-0.559319
14	8	0	3.141821	-0.313262	-0.130941
15	1	0	-1.860916	-0.018485	-1.825318
16	7	0	-2.565039	-0.165053	0.166208
17	8	0	-2.329305	-0.576635	1.288529
18	8	0	-3.641968	0.262177	-0.227805



(Nimag=0)

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

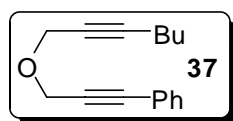
1	6	0	-2.335045	0.998886	-0.189692
2	6	0	-2.234397	-0.201608	-0.167066
3	6	0	-2.531891	2.450063	-0.218017
4	1	0	-2.813183	2.787805	0.790908
5	1	0	-3.370580	2.675678	-0.882511
6	6	0	-0.365388	3.426532	0.207426
7	1	0	0.220123	4.229940	-0.245407
8	1	0	-0.770807	3.806248	1.156654
9	6	0	0.481137	2.261032	0.449764
10	6	0	1.170103	1.288952	0.629552
11	6	0	1.973756	0.083384	0.803403
12	1	0	1.349300	-0.780008	0.543293
13	1	0	2.233702	-0.028957	1.863205
14	8	0	-1.440857	3.205668	-0.714411
15	6	0	3.258996	0.070165	-0.047914
16	6	0	4.080864	-1.208379	0.144132
17	1	0	3.868445	0.944439	0.206863
18	1	0	2.985104	0.179397	-1.102701
19	6	0	5.356513	-1.232502	-0.702658
20	1	0	4.344567	-1.313954	1.203861
21	1	0	3.459582	-2.077048	-0.103841
22	1	0	5.922771	-2.154381	-0.543680
23	1	0	5.123619	-1.165756	-1.769935
24	1	0	6.012708	-0.392306	-0.454404
25	6	0	-1.974511	-1.616916	-0.114420
26	8	0	-0.876035	-2.113361	-0.223603
27	8	0	-3.106507	-2.320487	0.078385
28	6	0	-2.948025	-3.751222	0.154104
29	1	0	-3.950672	-4.141315	0.312296
30	1	0	-2.525815	-4.136643	-0.774787
31	1	0	-2.294348	-4.018013	0.985548



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.611301	0.357151	0.143879
2	6	0	-0.494111	0.911046	0.062828
3	6	0	-3.049729	0.558682	0.525824

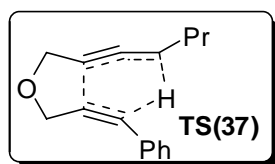
4	1	0	-3.555470	1.094300	-0.291259
5	1	0	-3.120523	1.152038	1.437853
6	6	0	-3.301200	-1.619549	-0.211311
7	1	0	-3.544906	-2.612867	0.165774
8	1	0	-3.854674	-1.447223	-1.146320
9	6	0	-1.844454	-1.463351	-0.449209
10	6	0	-0.735420	-1.899656	-0.812639
11	6	0	0.621590	-1.534015	-0.956188
12	1	0	0.474340	-0.411167	-0.586722
13	1	0	0.943603	-1.443959	-1.999114
14	8	0	-3.690177	-0.678891	0.779467
15	6	0	1.677031	-2.219126	-0.078385
16	6	0	3.025441	-1.490579	-0.102248
17	1	0	1.808824	-3.250606	-0.423843
18	1	0	1.301967	-2.276375	0.948326
19	6	0	4.094826	-2.198161	0.734229
20	1	0	3.371286	-1.402901	-1.139767
21	1	0	2.889007	-0.468613	0.267802
22	1	0	5.043145	-1.655161	0.704980
23	1	0	3.789216	-2.274081	1.782109
24	1	0	4.280512	-3.212671	0.367287
25	6	0	0.462308	1.961065	0.289209
26	8	0	1.199781	2.040953	1.248780
27	8	0	0.463957	2.857889	-0.729332
28	6	0	1.404347	3.939903	-0.601150
29	1	0	1.271876	4.542949	-1.496933
30	1	0	1.192802	4.529034	0.292407
31	1	0	2.424547	3.557236	-0.542919



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.334460	2.251070	-0.100361
2	6	0	-1.849184	1.159440	-0.075020
3	6	0	-0.783914	3.606478	-0.153599
4	1	0	-0.709610	4.016965	0.863471
5	1	0	-1.469427	4.247638	-0.715530
6	6	0	1.622719	3.490735	-0.012419
7	1	0	2.458343	3.869662	-0.605994

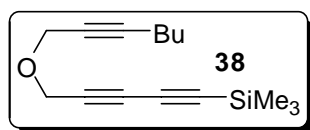
8	1	0	1.561277	4.103750	0.899142
9	6	0	1.866939	2.094276	0.349666
10	6	0	2.105510	0.954084	0.657701
11	6	0	2.370085	-0.440118	0.999417
12	1	0	1.415123	-0.942515	1.195633
13	1	0	2.932910	-0.479047	1.940228
14	8	0	0.469956	3.722613	-0.821842
15	6	0	3.140798	-1.208378	-0.092741
16	6	0	3.406025	-2.668630	0.286364
17	1	0	4.089972	-0.696495	-0.285635
18	1	0	2.569893	-1.164057	-1.026279
19	6	0	4.170551	-3.437828	-0.794782
20	1	0	3.970422	-2.702430	1.226471
21	1	0	2.451196	-3.170138	0.485662
22	1	0	4.347255	-4.474851	-0.496470
23	1	0	3.614104	-3.453177	-1.737049
24	1	0	5.143917	-2.978506	-0.993387
25	6	0	-2.432483	-0.142511	-0.043816
26	6	0	-2.898414	-0.690838	1.164254
27	6	0	-2.553699	-0.899303	-1.222807
28	6	0	-3.469543	-1.958767	1.188644
29	1	0	-2.808615	-0.112335	2.075901
30	6	0	-3.122199	-2.168246	-1.189586
31	1	0	-2.197725	-0.481067	-2.156619
32	6	0	-3.583020	-2.702205	0.013828
33	1	0	-3.826657	-2.368187	2.126997
34	1	0	-3.208374	-2.741119	-2.106110
35	1	0	-4.027913	-3.690551	0.035841



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.662311	-1.516942	-0.136415
2	6	0	0.424353	-0.913708	0.026677
3	6	0	-1.128966	-2.809583	-0.770596
4	1	0	-0.900708	-3.636598	-0.081583
5	1	0	-0.624045	-2.985847	-1.720174
6	6	0	-3.149846	-2.108051	0.067726

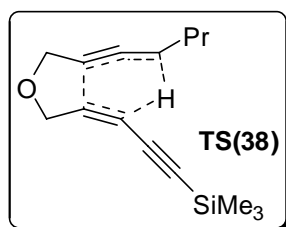
7	1	0	-4.131635	-1.769119	-0.261397
8	1	0	-3.275794	-2.813782	0.902637
9	6	0	-2.282936	-0.963952	0.490769
10	6	0	-2.273914	0.145599	1.084978
11	6	0	-1.280555	1.103814	1.473166
12	1	0	-0.350671	0.607346	1.004862
13	1	0	-1.102374	1.086619	2.554589
14	8	0	-2.518170	-2.748318	-1.029513
15	6	0	-1.408732	2.552631	0.975210
16	6	0	-1.586169	2.689116	-0.539396
17	1	0	-0.511344	3.097436	1.290483
18	1	0	-2.252817	3.026895	1.488862
19	6	0	-1.696071	4.147112	-0.994257
20	1	0	-0.741048	2.208067	-1.045143
21	1	0	-2.479786	2.137390	-0.849205
22	1	0	-1.824451	4.216563	-2.077979
23	1	0	-2.552477	4.643981	-0.527231
24	1	0	-0.799220	4.716477	-0.729439
25	6	0	1.792241	-0.535839	-0.002366
26	6	0	2.670119	-0.908745	1.038870
27	6	0	2.313049	0.211197	-1.081714
28	6	0	4.012311	-0.554202	0.992621
29	1	0	2.283358	-1.478001	1.875850
30	6	0	3.657065	0.560317	-1.116147
31	1	0	1.650399	0.506170	-1.886707
32	6	0	4.514540	0.182407	-0.081541
33	1	0	4.671728	-0.853446	1.799833
34	1	0	4.039171	1.130481	-1.955728
35	1	0	5.562024	0.458890	-0.111942



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.810438	-2.782271	-0.082937
2	6	0	-0.224729	-2.153317	-0.060359
3	6	0	2.007435	-3.621387	-0.088383
4	1	0	2.394860	-3.709380	-1.113082
5	1	0	1.730880	-4.626916	0.244168
6	6	0	4.010120	-2.315190	0.224541

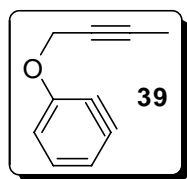
7	1	0	4.770700	-2.205819	1.001022
8	1	0	4.484136	-2.810852	-0.635610
9	6	0	3.510972	-1.002024	-0.180480
10	6	0	3.115361	0.081457	-0.529075
11	6	0	2.611248	1.392423	-0.925266
12	1	0	1.539237	1.303549	-1.139279
13	1	0	3.085928	1.691126	-1.867950
14	8	0	3.034509	-3.188070	0.798390
15	6	0	2.835848	2.489236	0.134794
16	6	0	2.304236	3.855773	-0.308634
17	1	0	3.907255	2.560773	0.351879
18	1	0	2.349954	2.185463	1.067997
19	6	0	2.522853	4.951273	0.738795
20	1	0	2.790363	4.146262	-1.248051
21	1	0	1.233642	3.772663	-0.532215
22	1	0	2.131840	5.913364	0.396661
23	1	0	2.021509	4.704041	1.679667
24	1	0	3.587231	5.083574	0.956560
25	6	0	-1.379474	-1.432292	-0.040766
26	6	0	-2.417498	-0.791300	-0.021412
27	14	0	-3.997024	0.161534	0.021289
28	6	0	-3.942465	1.468575	-1.336001
29	1	0	-4.866598	2.055519	-1.345510
30	1	0	-3.107715	2.158684	-1.185607
31	1	0	-3.824718	1.010506	-2.321890
32	6	0	-4.151969	0.973257	1.714893
33	1	0	-5.078419	1.552799	1.781853
34	1	0	-4.164718	0.224639	2.511695
35	1	0	-3.316128	1.651547	1.906896
36	6	0	-5.418847	-1.039853	-0.272269
37	1	0	-6.379288	-0.514746	-0.251725
38	1	0	-5.325533	-1.532881	-1.243760
39	1	0	-5.443322	-1.816994	0.496473



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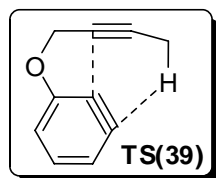
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	1.921153	-1.482072	0.042683
2	6	0	0.730159	-1.085216	-0.050951
3	6	0	2.630039	-2.767727	0.402291
4	1	0	2.576832	-3.444683	-0.464164
5	1	0	2.155831	-3.247188	1.258691
6	6	0	4.480245	-1.512882	-0.132459
7	1	0	5.366850	-1.076696	0.326404
8	1	0	4.758751	-1.960337	-1.098260
9	6	0	3.405542	-0.491802	-0.337568
10	6	0	3.169431	0.701091	-0.652172
11	6	0	2.034123	1.550364	-0.854179
12	1	0	1.197704	0.796975	-0.635662
13	1	0	1.906807	1.829507	-1.906842
14	8	0	3.975000	-2.503174	0.747193
15	6	0	1.877494	2.773348	0.062430
16	6	0	0.523424	3.468485	-0.114416
17	1	0	2.686991	3.481368	-0.146080
18	1	0	2.000567	2.455679	1.103123
19	6	0	0.355301	4.687946	0.796053
20	1	0	0.408738	3.775001	-1.161399
21	1	0	-0.279553	2.749000	0.083099
22	1	0	-0.618098	5.163564	0.648233
23	1	0	0.430526	4.406787	1.851077
24	1	0	1.125586	5.440191	0.598613
25	6	0	-0.612695	-0.942353	-0.048329
26	6	0	-1.832860	-0.809852	-0.045904
27	14	0	-3.665138	-0.645745	-0.026030
28	6	0	-4.194743	0.423151	-1.487216
29	1	0	-5.283629	0.535892	-1.508927
30	1	0	-3.754278	1.422145	-1.427062
31	1	0	-3.884348	-0.022649	-2.436278
32	6	0	-4.168736	0.168494	1.598750
33	1	0	-5.256050	0.285417	1.651954
34	1	0	-3.852671	-0.431816	2.456256
35	1	0	-3.718605	1.159823	1.700145
36	6	0	-4.431133	-2.363254	-0.165839
37	1	0	-4.132867	-2.853630	-1.096588
38	1	0	-4.119373	-3.003077	0.664204
39	1	0	-5.524246	-2.301776	-0.152710



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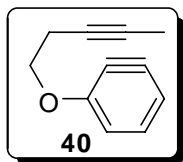
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.983631	-0.298654	0.798408
2	6	0	-3.034440	-1.259289	-0.240682
3	6	0	-1.910875	-1.095528	-1.009034
4	6	0	-0.933481	-0.321101	-0.975073
5	6	0	-0.840777	0.632862	0.036471
6	6	0	-1.930032	0.610570	0.937423
7	1	0	-3.794471	-0.276323	1.519938
8	1	0	-3.833553	-1.976320	-0.355240
9	1	0	-1.931412	1.322679	1.754716
10	8	0	0.131576	1.557538	0.208310
11	6	0	1.281703	1.459066	-0.651108
12	1	0	1.743678	2.446613	-0.605979
13	1	0	0.945325	1.279261	-1.678719
14	6	0	2.224977	0.428219	-0.232870
15	6	0	3.019814	-0.408933	0.108655
16	6	0	3.966159	-1.435068	0.524630
17	1	0	3.840575	-2.349744	-0.061433
18	1	0	4.997025	-1.091425	0.400136
19	1	0	3.823722	-1.687908	1.579178



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.746140	-0.607372	-0.049126
2	6	0	-1.950911	-1.756972	0.096523
3	6	0	-0.575505	-1.510330	0.154670
4	6	0	-0.122382	-0.323193	0.103878
5	6	0	-0.814265	0.858812	-0.045977
6	6	0	-2.202072	0.686306	-0.117962

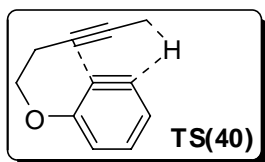
7	1	0	-3.824739	-0.716475	-0.114480
8	1	0	-2.399194	-2.742439	0.142406
9	1	0	-2.842162	1.553860	-0.228135
10	8	0	-0.186542	2.061183	-0.139236
11	6	0	1.215757	1.978523	0.182747
12	1	0	1.350754	2.314205	1.216829
13	1	0	1.733471	2.668875	-0.484306
14	6	0	1.734095	0.604725	0.035001
15	6	0	2.478318	-0.361880	-0.069071
16	6	0	2.807623	-1.760477	-0.126609
17	1	0	3.426526	-2.086246	0.712469
18	1	0	1.818090	-2.275784	-0.050223
19	1	0	3.282481	-2.054305	-1.065115



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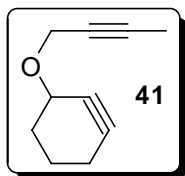
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.272162	1.210517	0.506851
2	6	0	3.979989	0.518356	-0.506686
3	6	0	3.141339	-0.440767	-1.011744
4	6	0	1.969330	-0.794422	-0.770202
5	6	0	1.237269	-0.139295	0.220079
6	6	0	1.956084	0.898643	0.859371
7	1	0	3.777846	2.017033	1.028869
8	1	0	4.996398	0.746521	-0.790564
9	1	0	1.455790	1.458024	1.641666
10	8	0	-0.029026	-0.395079	0.605537
11	6	0	-0.705310	-1.457716	-0.074382
12	1	0	-0.176223	-2.398426	0.114620
13	1	0	-0.699427	-1.263246	-1.151298
14	6	0	-2.132797	-1.540262	0.461359
15	1	0	-2.582299	-2.455964	0.059410
16	1	0	-2.092587	-1.663745	1.549093
17	6	0	-2.967352	-0.391434	0.116707
18	6	0	-3.655577	0.551543	-0.177695
19	6	0	-4.483342	1.699608	-0.528405
20	1	0	-5.214365	1.440604	-1.299899
21	1	0	-5.032557	2.069337	0.342431

22 1 0 -3.871130 2.521868 -0.910140



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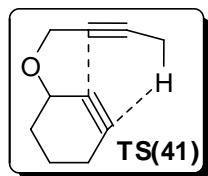
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.948096	0.347603	-0.059157
2	6	0	-2.275592	1.579636	0.035773
3	6	0	-0.892674	1.449382	0.067692
4	6	0	-0.272282	0.338808	0.030032
5	6	0	-0.855100	-0.913661	-0.038183
6	6	0	-2.260559	-0.870563	-0.091400
7	1	0	-4.033225	0.336002	-0.101266
8	1	0	-2.814991	2.518254	0.070936
9	1	0	-2.799667	-1.809667	-0.149407
10	8	0	-0.223112	-2.122981	-0.075445
11	6	0	2.118917	-1.342110	-0.328203
12	1	0	2.035840	-1.602537	-1.388847
13	1	0	3.123323	-1.634160	-0.002512
14	6	0	1.965574	0.108020	-0.154090
15	6	0	2.205018	1.303335	-0.039173
16	6	0	1.885745	2.690363	0.091575
17	1	0	2.190245	3.288965	-0.769881
18	1	0	0.749771	2.692279	0.130147
19	1	0	2.261239	3.145223	1.010845
20	6	0	1.098832	-2.170367	0.463625
21	1	0	1.374724	-3.224063	0.421670
22	1	0	1.078942	-1.849124	1.510919



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.111708	-0.968610	-0.236436

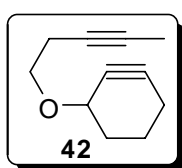
2	6	0	-3.163587	0.072199	0.200728
3	6	0	-2.814609	1.563067	-0.173515
4	6	0	-1.361965	1.604471	0.073425
5	6	0	-0.500755	0.747245	0.146597
6	6	0	-0.661941	-0.725982	0.307013
7	1	0	-2.031796	-0.990497	-1.327355
8	1	0	-3.296358	0.019816	1.286410
9	1	0	-3.406038	2.256212	0.429590
10	1	0	-2.429307	-1.965674	0.084611
11	1	0	-4.127307	-0.186944	-0.250420
12	1	0	-3.037619	1.769717	-1.225004
13	6	0	1.498837	-1.751643	0.128249
14	1	0	1.939970	-2.572271	-0.442253
15	1	0	1.407697	-2.084167	1.172842
16	6	0	2.361925	-0.571809	0.058251
17	6	0	3.085929	0.388740	0.001287
18	6	0	3.925839	1.576230	-0.069594
19	1	0	4.630687	1.517222	-0.903815
20	1	0	3.309930	2.469416	-0.210693
21	1	0	4.501314	1.708546	0.851150
22	1	0	-0.595919	-0.988338	1.373067
23	8	0	0.198369	-1.569560	-0.431769



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.078477	0.803680	-0.307471
2	6	0	2.729845	-0.518327	0.155045
3	6	0	1.871402	-1.792678	-0.137171
4	6	0	0.435590	-1.442535	0.105451
5	6	0	0.018250	-0.280814	0.246373
6	6	0	0.699555	1.034768	0.352837
7	1	0	1.923875	0.796360	-1.390644
8	1	0	2.912231	-0.465201	1.234540
9	1	0	2.218199	-2.627787	0.478159
10	1	0	2.736319	1.646159	-0.072497
11	1	0	3.710570	-0.621579	-0.321876
12	1	0	1.991666	-2.109304	-1.179453

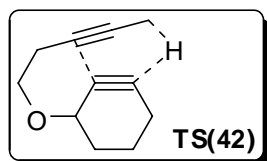
13	6	0	-1.412285	1.948344	0.053269
14	1	0	-1.983554	2.534814	-0.667068
15	1	0	-1.565357	2.375080	1.055151
16	6	0	-1.843161	0.527277	0.047557
17	6	0	-2.570368	-0.462015	-0.029945
18	6	0	-2.728290	-1.885929	-0.092913
19	1	0	-3.277880	-2.307706	0.751718
20	1	0	-3.170884	-2.234359	-1.028737
21	1	0	-1.658602	-2.253019	-0.050548
22	1	0	0.815160	1.321764	1.409802
23	8	0	-0.040729	2.044269	-0.322093



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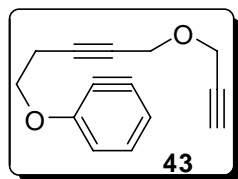
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.489319	-0.349718	1.066872
2	6	0	-2.618847	1.174127	0.830060
3	6	0	-2.906028	1.595432	-0.660286
4	6	0	-2.062649	0.650615	-1.421056
5	6	0	-1.520289	-0.386234	-1.093843
6	6	0	-1.394592	-1.101184	0.195888
7	1	0	-3.452280	-0.826250	0.859287
8	1	0	-1.697530	1.672204	1.147146
9	1	0	-2.662190	2.650328	-0.808217
10	1	0	-2.271652	-0.524903	2.126633
11	1	0	-3.423303	1.560214	1.465681
12	1	0	-3.962443	1.468341	-0.917678
13	1	0	-1.673215	-2.156351	0.121618
14	6	0	0.003467	-1.048275	0.833167
15	1	0	0.354297	-0.013759	0.923741
16	1	0	-0.060969	-1.473458	1.838836
17	8	0	0.956725	-1.843501	0.140015
18	6	0	1.681029	-1.178201	-0.897935
19	1	0	0.992548	-0.728528	-1.623893
20	1	0	2.230104	-1.971134	-1.411182
21	6	0	2.615616	-0.162434	-0.405651
22	6	0	3.391963	0.671672	-0.014256
23	6	0	4.333992	1.676502	0.462949

24	1	0	5.350133	1.455256	0.123788
25	1	0	4.068166	2.674390	0.102292
26	1	0	4.348473	1.707851	1.556378



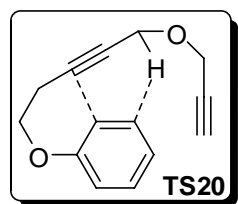
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.261442	-0.642673	0.628566
2	6	0	2.760561	0.406749	-0.384365
3	6	0	2.051486	1.786572	-0.244700
4	6	0	0.590213	1.511751	-0.079621
5	6	0	0.121522	0.396413	0.210013
6	6	0	0.711799	-0.905825	0.588590
7	1	0	2.517688	-0.310382	1.639691
8	1	0	2.597586	0.038983	-1.403177
9	1	0	2.273132	2.412846	-1.113987
10	1	0	2.786597	-1.591100	0.467340
11	1	0	3.842503	0.532198	-0.263368
12	1	0	2.425116	2.332834	0.629549
13	1	0	0.400903	-1.180186	1.602727
14	6	0	0.324755	-2.056644	-0.356858
15	1	0	0.880399	-1.978324	-1.294604
16	1	0	0.586237	-3.013824	0.117340
17	8	0	-1.053455	-2.078275	-0.740418
18	6	0	-1.978759	-1.541712	0.196132
19	1	0	-1.798441	-1.936150	1.204959
20	1	0	-2.962644	-1.890367	-0.122596
21	6	0	-1.967574	-0.061790	0.197864
22	6	0	-2.428042	1.076685	0.101983
23	6	0	-2.244007	2.480805	-0.058937
24	1	0	-2.663614	2.875114	-0.987062
25	1	0	-2.579519	3.081356	0.789555
26	1	0	-1.098692	2.551229	-0.135018



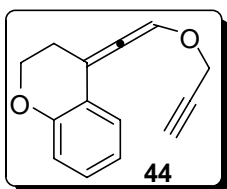
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.677586	-1.645051	-0.738227
2	6	0	5.407804	-1.434427	0.457568
3	6	0	4.779536	-0.433718	1.151581
4	6	0	3.770525	0.272450	0.950691
5	6	0	3.023897	0.096489	-0.213913
6	6	0	3.532903	-0.912553	-1.065190
7	1	0	5.025963	-2.409166	-1.426247
8	1	0	6.293450	-1.991062	0.724988
9	1	0	3.007303	-1.110632	-1.992387
10	8	0	1.915773	0.770986	-0.584606
11	6	0	0.156958	2.364887	-0.254079
12	1	0	0.349533	2.731640	-1.268022
13	1	0	-0.109578	3.240008	0.349811
14	6	0	-0.964726	1.430961	-0.266906
15	6	0	-1.894073	0.666840	-0.255245
16	6	0	-3.003451	-0.274000	-0.278421
17	1	0	-3.621303	-0.104343	-1.170143
18	1	0	-2.618092	-1.303635	-0.334001
19	6	0	1.448500	1.781573	0.314359
20	1	0	2.209394	2.564860	0.402838
21	1	0	1.280730	1.342936	1.302701
22	8	0	-3.794874	-0.119948	0.902763
23	6	0	-4.856868	-1.058773	0.991446
24	1	0	-4.467166	-2.086299	0.934420
25	1	0	-5.285299	-0.921711	1.986686
26	6	0	-5.900832	-0.879588	-0.023552
27	6	0	-6.762440	-0.734781	-0.849576
28	1	0	-7.524034	-0.602755	-1.579135



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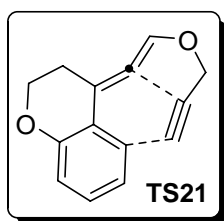
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.659312	2.932719	-0.056451
2	6	0	-0.322906	2.588373	0.220571
3	6	0	-0.120864	1.217075	0.280520
4	6	0	-1.023269	0.337369	0.120432
5	6	0	-2.359991	0.592974	-0.123718
6	6	0	-2.657179	1.964793	-0.220197
7	1	0	-1.930704	3.981053	-0.138260
8	1	0	0.442371	3.341858	0.358717
9	1	0	-3.683295	2.255814	-0.415815
10	8	0	-3.355592	-0.327265	-0.282417
11	6	0	-1.986647	-2.400982	-0.305583
12	1	0	-2.123244	-2.416023	-1.392163
13	1	0	-2.058729	-3.436854	0.043388
14	6	0	-0.648417	-1.883709	0.008748
15	6	0	0.550842	-1.838123	0.252817
16	6	0	1.778458	-1.157086	0.539203
17	1	0	1.446130	-0.064387	0.578865
18	1	0	2.188045	-1.415162	1.526019
19	6	0	-3.135749	-1.601553	0.324241
20	1	0	-4.071095	-2.141810	0.178836
21	1	0	-2.965055	-1.470340	1.398534
22	8	0	2.750777	-1.354657	-0.477404
23	6	0	4.032296	-0.827843	-0.158085
24	1	0	4.382091	-1.236470	0.801581
25	1	0	4.698275	-1.200616	-0.939324
26	6	0	4.096078	0.635379	-0.114116
27	6	0	4.171024	1.834440	-0.079771
28	1	0	4.227528	2.895361	-0.053482



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.938978	2.484482	-0.119441
2	6	0	-1.548852	2.645000	-0.108717

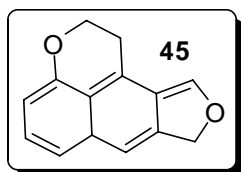
3	6	0	-0.731075	1.526977	-0.062584
4	6	0	-1.264817	0.228215	-0.020648
5	6	0	-2.666017	0.089698	-0.016823
6	6	0	-3.494737	1.214517	-0.071848
7	1	0	-3.588100	3.351956	-0.160524
8	1	0	-1.112640	3.636219	-0.145642
9	1	0	-4.567667	1.064235	-0.069170
10	8	0	-3.294157	-1.124519	0.024923
11	6	0	-1.162961	-2.278167	-0.267713
12	1	0	-1.346138	-2.393146	-1.342606
13	1	0	-0.575728	-3.135976	0.064609
14	6	0	-0.410095	-0.980621	-0.022656
15	6	0	0.891429	-0.958651	0.152980
16	6	0	2.178885	-0.976171	0.361866
17	1	0	0.347545	1.637365	-0.072619
18	1	0	2.600847	-1.057038	1.362982
19	6	0	-2.498495	-2.233554	0.461034
20	1	0	-3.101880	-3.118716	0.258712
21	1	0	-2.344444	-2.151576	1.544528
22	8	0	3.103402	-0.930310	-0.664483
23	6	0	4.431809	-0.590398	-0.263797
24	1	0	4.756030	-1.241536	0.559168
25	1	0	5.057075	-0.811778	-1.130585
26	6	0	4.587863	0.811824	0.123396
27	6	0	4.720568	1.962933	0.442533
28	1	0	4.833997	2.982114	0.722142



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.074030	-1.834848	-0.116628
2	6	0	-1.865831	-2.284599	-0.640384
3	6	0	-0.779672	-1.414995	-0.723232
4	6	0	-0.882160	-0.069303	-0.293204
5	6	0	-2.149574	0.370039	0.189424
6	6	0	-3.219349	-0.505957	0.291313
7	1	0	-3.921760	-2.507331	-0.047388

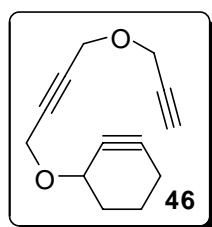
8	1	0	-1.769106	-3.305016	-0.992557
9	1	0	-4.161640	-0.133030	0.674202
10	8	0	-2.350895	1.660668	0.583669
11	6	0	-0.010719	2.234974	0.212667
12	1	0	0.224377	2.320869	1.281641
13	1	0	0.643460	2.938042	-0.312297
14	6	0	0.247448	0.814443	-0.254876
15	6	0	1.535379	0.350224	-0.367352
16	6	0	2.694746	0.724422	-0.924676
17	1	0	0.139505	-1.738094	-1.190527
18	1	0	2.825723	1.321362	-1.817839
19	6	0	-1.463400	2.617501	-0.015168
20	1	0	-1.711835	3.572671	0.446823
21	1	0	-1.686301	2.673971	-1.087983
22	8	0	3.848801	0.193005	-0.447925
23	6	0	3.540936	-0.565690	0.726146
24	1	0	4.256575	-1.382171	0.792379
25	1	0	3.631750	0.088674	1.599524
26	6	0	2.112380	-1.053808	0.617378
27	6	0	1.452523	-2.035939	1.015287
28	1	0	0.713949	-2.758117	1.267903



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.694353	-2.054203	-0.367037
2	6	0	1.453475	-2.460035	-0.051533
3	6	0	0.457101	-1.485049	0.535310
4	6	0	0.765703	-0.033981	0.172250
5	6	0	2.165933	0.299899	-0.028428
6	6	0	3.093066	-0.663582	-0.263928
7	1	0	3.428778	-2.769147	-0.723029
8	1	0	1.160400	-3.501300	-0.130487
9	1	0	4.113432	-0.370234	-0.478388
10	8	0	2.533966	1.613225	-0.139059
11	6	0	0.208520	2.353944	-0.175453
12	1	0	0.185607	2.618033	-1.240241
13	1	0	-0.489312	3.027520	0.335163

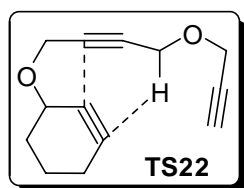
14	6	0	-0.198189	0.915908	0.024446
15	6	0	-1.579334	0.505961	0.006248
16	6	0	-2.740790	1.181964	-0.144416
17	1	0	0.616115	-1.549328	1.633564
18	1	0	-2.938395	2.240440	-0.227259
19	6	0	1.605048	2.567418	0.392399
20	1	0	2.013303	3.542270	0.126420
21	1	0	1.586831	2.478394	1.485773
22	8	0	-3.848926	0.390538	-0.200836
23	6	0	-3.405381	-0.997029	-0.128944
24	1	0	-3.937158	-1.471476	0.698420
25	1	0	-3.693203	-1.482269	-1.065479
26	6	0	-1.909997	-0.917432	0.071101
27	6	0	-0.989385	-1.860334	0.285156
28	1	0	-1.247448	-2.913689	0.341677



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.840888	-0.184771	-0.614799
2	6	0	-4.514320	1.075253	-0.032995
3	6	0	-3.569949	2.332015	0.094698
4	6	0	-2.306199	1.711041	0.525171
5	6	0	-1.849670	0.584520	0.459459
6	6	0	-2.576343	-0.684803	0.162150
7	1	0	-3.518929	-0.001311	-1.644108
8	1	0	-4.909291	0.848786	0.962827
9	1	0	-3.992217	3.056389	0.795254
10	1	0	-4.564997	-1.005027	-0.643558
11	1	0	-5.370244	1.342729	-0.661607
12	1	0	-3.449424	2.836727	-0.868920
13	6	0	-0.918916	-2.404519	-0.029131
14	1	0	-0.726090	-3.243287	-0.702263
15	1	0	-1.299014	-2.817627	0.916557
16	6	0	0.329973	-1.682533	0.213424
17	6	0	1.380537	-1.125588	0.399661
18	6	0	2.609997	-0.395104	0.658786

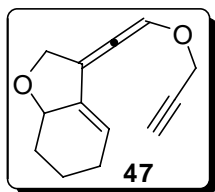
19	1	0	2.415843	0.683078	0.582371
20	1	0	2.958394	-0.597331	1.683292
21	1	0	-2.865052	-1.168381	1.107044
22	8	0	-1.936174	-1.635751	-0.665633
23	8	0	3.616794	-0.785846	-0.277554
24	6	0	4.871824	-0.163180	-0.043071
25	1	0	5.218523	-0.371307	0.980459
26	1	0	5.568789	-0.643602	-0.733147
27	6	0	4.872930	1.285968	-0.269406
28	6	0	4.879116	2.473417	-0.457516
29	1	0	4.880195	3.522641	-0.627286



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.188051	0.946124	-0.547860
2	6	0	-2.728745	2.282546	0.076569
3	6	0	-1.174512	2.477560	0.115664
4	6	0	-0.577688	1.145908	0.424533
5	6	0	-1.169876	0.057713	0.393320
6	6	0	-2.607236	-0.277612	0.198150
7	1	0	-2.862778	0.877529	-1.590207
8	1	0	-3.108085	2.344113	1.102843
9	1	0	-0.911498	3.249475	0.844274
10	1	0	-4.280978	0.888513	-0.537559
11	1	0	-3.183880	3.111861	-0.475392
12	1	0	-0.801155	2.825889	-0.853666
13	6	0	-1.853115	-2.453345	-0.042705
14	1	0	-1.788585	-3.253928	-0.780061
15	1	0	-2.242620	-2.869115	0.897908
16	6	0	-0.515324	-1.852083	0.196278
17	6	0	0.710284	-1.811610	0.315236
18	6	0	1.877936	-1.004219	0.552678
19	1	0	2.348144	-1.223115	1.522260
20	1	0	1.443402	0.039831	0.602767
21	1	0	-3.100886	-0.412231	1.173338
22	8	0	-2.744683	-1.471395	-0.559893
23	8	0	2.831294	-1.112653	-0.497426

24	6	0	4.065311	-0.465813	-0.219923
25	1	0	4.485292	-0.838264	0.726447
26	1	0	4.738571	-0.771668	-1.023754
27	6	0	3.990016	0.997447	-0.171761
28	6	0	3.949315	2.198099	-0.132261
29	1	0	3.902273	3.259208	-0.098157

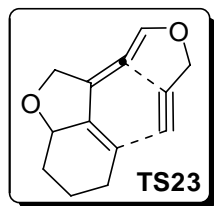


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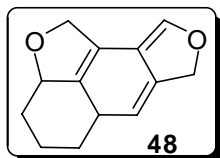
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.811416	0.147307	0.378070
2	6	0	3.787773	1.617933	-0.074803
3	6	0	2.448270	2.311426	0.243425
4	6	0	1.250754	1.412720	0.079832
5	6	0	1.367529	0.111069	-0.196045
6	6	0	2.701522	-0.588920	-0.351837
7	1	0	3.632349	0.070213	1.455606
8	1	0	3.966976	1.656945	-1.155748
9	1	0	2.334007	3.207905	-0.378013
10	1	0	4.782786	-0.308953	0.169370
11	1	0	4.608210	2.168967	0.392753
12	1	0	2.453066	2.679134	1.279469
13	6	0	1.131357	-2.263358	-0.196245
14	1	0	0.751256	-2.972843	0.538876
15	1	0	1.120355	-2.736795	-1.189144
16	6	0	0.344087	-0.950171	-0.227076
17	6	0	-0.958936	-0.836554	-0.267284
18	6	0	-2.257066	-0.733246	-0.359678
19	1	0	0.267818	1.840113	0.261599
20	1	0	-2.764311	-0.700069	-1.322231
21	1	0	2.957997	-0.677248	-1.421954
22	8	0	2.463822	-1.902295	0.169617
23	8	0	-3.080257	-0.665982	0.747297
24	6	0	-4.466942	-0.477503	0.461736
25	1	0	-4.816665	-1.244257	-0.242054
26	1	0	-4.976960	-0.641120	1.412720
27	6	0	-4.786019	0.853525	-0.055649
28	6	0	-5.056348	1.944532	-0.481313

29 1 0 -5.289784 2.911657 -0.855352



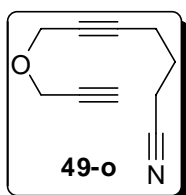
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.938417	0.159448	0.780317
2	6	0	-3.373822	-1.021426	-0.105508
3	6	0	-2.189447	-1.890461	-0.585607
4	6	0	-0.909709	-1.122281	-0.825025
5	6	0	-0.827856	0.218530	-0.571003
6	6	0	-1.993417	1.025640	-0.035928
7	1	0	-2.414350	-0.191709	1.675107
8	1	0	-3.901053	-0.622152	-0.979646
9	1	0	-2.472465	-2.424933	-1.500213
10	1	0	-3.807427	0.736201	1.108659
11	1	0	-4.095535	-1.647009	0.426398
12	1	0	-1.989621	-2.679545	0.151669
13	6	0	-0.104757	2.343309	0.143249
14	1	0	0.564373	2.696069	0.929235
15	1	0	-0.185805	3.126472	-0.627180
16	6	0	0.333921	1.020320	-0.472451
17	6	0	1.600913	0.544973	-0.520146
18	6	0	2.868101	0.629963	-0.886974
19	1	0	-0.121662	-1.617266	-1.375984
20	1	0	3.252578	1.174700	-1.739960
21	1	0	-2.551586	1.471281	-0.877733
22	8	0	-1.389335	2.081064	0.719021
23	8	0	3.830371	-0.097768	-0.245957
24	6	0	3.263430	-0.777322	0.881354
25	1	0	3.881727	-1.657264	1.056911
26	1	0	3.310077	-0.114552	1.753301
27	6	0	1.845453	-1.136516	0.619746
28	6	0	0.884460	-1.896942	0.770361
29	1	0	0.249347	-2.700063	1.060620



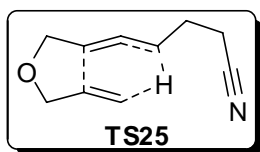
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.037800	0.136546	0.549506
2	6	0	-3.037330	-1.382223	0.288256
3	6	0	-1.631147	-1.997216	0.407131
4	6	0	-0.626067	-1.331520	-0.577599
5	6	0	-0.759393	0.154805	-0.446565
6	6	0	-2.091573	0.834804	-0.436234
7	1	0	-2.681572	0.340695	1.565068
8	1	0	-3.438151	-1.582713	-0.714178
9	1	0	-1.670469	-3.075218	0.217941
10	1	0	-4.047884	0.548216	0.467501
11	1	0	-3.714935	-1.875362	0.991557
12	1	0	-1.257621	-1.863491	1.428672
13	6	0	-0.379655	2.397838	0.019665
14	1	0	-0.140292	2.838174	0.995351
15	1	0	-0.058664	3.104924	-0.758180
16	6	0	0.215618	1.026935	-0.161259
17	6	0	1.570431	0.556438	-0.015500
18	6	0	2.762220	1.129172	0.244875
19	1	0	-0.948488	-1.629465	-1.590377
20	1	0	3.030859	2.163088	0.403884
21	1	0	-2.554521	0.834822	-1.436611
22	8	0	-1.801072	2.195468	-0.067906
23	8	0	3.804521	0.249594	0.320611
24	6	0	3.272019	-1.085908	0.085234
25	1	0	3.787304	-1.497371	-0.786222
26	1	0	3.508619	-1.695287	0.960802
27	6	0	1.788376	-0.889731	-0.132231
28	6	0	0.810682	-1.772453	-0.378134
29	1	0	1.019945	-2.836425	-0.449720



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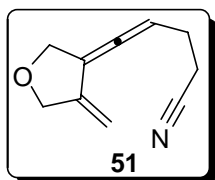
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.145629	1.400555	-0.227222
2	6	0	-2.647185	2.491852	-0.152671
3	1	0	-2.193588	3.450350	-0.085301
4	6	0	-3.835410	0.110469	-0.319998
5	1	0	-3.797351	-0.255888	-1.354887
6	1	0	-4.888068	0.258761	-0.063166
7	6	0	-2.325152	-1.729798	0.068613
8	1	0	-2.248942	-2.544650	0.792387
9	1	0	-2.643304	-2.167514	-0.888887
10	6	0	-1.019480	-1.090361	-0.097121
11	6	0	0.067141	-0.592433	-0.243930
12	6	0	1.372140	0.041022	-0.394633
13	6	0	2.197817	0.022952	0.905958
14	1	0	1.226587	1.077484	-0.723919
15	1	0	1.930426	-0.459784	-1.193693
16	6	0	3.562598	0.726010	0.764598
17	1	0	1.637951	0.526470	1.697927
18	1	0	2.349668	-1.010168	1.227838
19	1	0	4.075206	0.742853	1.730799
20	1	0	3.426195	1.769342	0.460512
21	6	0	4.447126	0.081546	-0.205567
22	7	0	5.133428	-0.438216	-0.973066
23	8	0	-3.356570	-0.886329	0.577961



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.669940	1.113814	-0.080283
2	6	0	-0.607694	1.765594	-0.091018
3	1	0	-0.090990	2.701810	-0.048787
4	6	0	-3.160515	1.073840	-0.051677
5	1	0	-3.532551	1.302516	-1.061855
6	1	0	-3.550867	1.819518	0.642121
7	6	0	-2.941634	-1.234671	-0.256129
8	1	0	-3.151021	-2.148935	0.300270

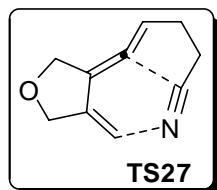
9	1	0	-3.293739	-1.362268	-1.290689
10	6	0	-1.501677	-0.906283	-0.248176
11	6	0	-0.284357	-1.152145	-0.290826
12	6	0	0.967107	-0.515006	-0.286907
13	6	0	1.904855	-0.746984	0.900461
14	1	0	0.505666	0.641203	-0.214925
15	1	0	1.490127	-0.537625	-1.247841
16	6	0	3.067978	0.264633	0.960738
17	1	0	1.337362	-0.668050	1.830972
18	1	0	2.313022	-1.760226	0.855933
19	1	0	3.670549	0.083029	1.855405
20	1	0	2.682206	1.285791	1.039192
21	6	0	3.952968	0.198327	-0.201410
22	7	0	4.643280	0.134487	-1.123160
23	8	0	-3.655659	-0.183110	0.384212



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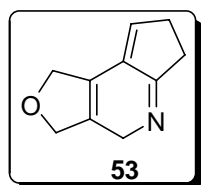
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.107647	0.956851	-0.042502
2	6	0	-1.634008	2.198443	0.070782
3	1	0	-2.296294	3.043576	0.220033
4	6	0	-3.567594	0.541269	-0.001784
5	1	0	-4.046589	0.724968	-0.975869
6	1	0	-4.144109	1.046882	0.773777
7	6	0	-2.395679	-1.411301	-0.316047
8	1	0	-2.120542	-2.313653	0.229598
9	1	0	-2.593807	-1.674216	-1.366104
10	6	0	-1.351088	-0.301562	-0.235380
11	6	0	-0.055451	-0.459777	-0.315506
12	6	0	1.236555	-0.626552	-0.396580
13	6	0	2.142797	-0.884472	0.786809
14	1	0	-0.571871	2.406630	0.011453
15	1	0	1.715672	-0.583884	-1.375353
16	6	0	3.222951	0.207636	0.976907
17	1	0	1.551411	-0.939055	1.702721
18	1	0	2.642061	-1.850957	0.659651
19	1	0	3.813433	-0.008551	1.872456

20	1	0	2.749980	1.182334	1.128166
21	6	0	4.140144	0.310801	-0.156609
22	7	0	4.856912	0.375527	-1.057828
23	8	0	-3.560451	-0.856349	0.287966



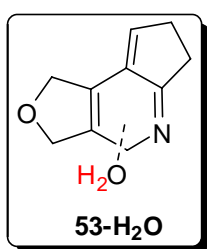
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.832607	0.348097	-0.135305
2	6	0	-1.577536	-1.618944	-0.264574
3	1	0	-3.628262	0.306339	0.621878
4	1	0	-3.109402	1.094665	-0.885227
5	1	0	-1.079666	-2.141818	-1.084319
6	1	0	-1.891471	-2.365589	0.481903
7	6	0	-0.711704	-0.557167	0.384760
8	6	0	-1.484115	0.618534	0.497664
9	6	0	-0.987159	1.825722	0.896911
10	1	0	-0.133775	1.894020	1.551562
11	1	0	-1.549520	2.740262	0.747235
12	6	0	0.650339	-0.589347	0.460846
13	6	0	1.760363	-1.179389	0.877413
14	1	0	1.767173	-1.883701	1.705008
15	6	0	3.053226	-0.764285	0.223540
16	6	0	2.678858	0.196150	-0.915649
17	1	0	3.605965	-1.628531	-0.158139
18	1	0	3.706479	-0.275294	0.956132
19	1	0	3.461348	0.922179	-1.139433
20	1	0	2.463086	-0.365020	-1.829144
21	6	0	1.419992	0.917781	-0.517755
22	7	0	0.894257	1.987173	-0.536011
23	8	0	-2.711212	-0.923829	-0.782810



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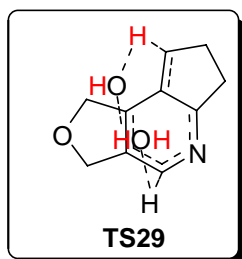
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.824722	0.490587	0.000119
2	6	0	1.745354	-1.607369	0.000073
3	1	0	3.308211	0.924193	-0.886613
4	1	0	3.308013	0.923600	0.887264
5	1	0	1.673711	-2.249043	0.888195
6	1	0	1.673354	-2.249505	-0.887673
7	6	0	0.726926	-0.503612	0.000048
8	6	0	1.338172	0.688678	0.000076
9	6	0	0.604965	1.994747	0.000068
10	1	0	0.902299	2.598192	-0.869583
11	1	0	0.902184	2.598140	0.869795
12	6	0	-0.715131	-0.554377	0.000022
13	6	0	-1.617695	-1.553445	0.000073
14	1	0	-1.380762	-2.611438	0.000140
15	6	0	-3.039599	-1.043564	0.000074
16	6	0	-2.897967	0.501710	-0.000169
17	1	0	-3.589437	-1.407316	0.875502
18	1	0	-3.589573	-1.407597	-0.875148
19	1	0	-3.357262	0.961763	-0.877874
20	1	0	-3.357519	0.962123	0.877209
21	6	0	-1.400296	0.759272	-0.000048
22	7	0	-0.859065	1.911325	-0.000029
23	8	0	3.012942	-0.932270	-0.000379



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.337986	0.852249	-0.570987
2	6	0	-0.667035	2.318365	0.224841
3	1	0	-2.727540	0.910276	-1.597855
4	1	0	-3.105418	0.381685	0.054621
5	1	0	-0.559723	2.626790	1.273274

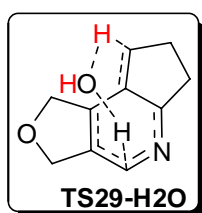
6	1	0	-0.223076	3.102679	-0.403810
7	6	0	-0.078970	0.962785	-0.044904
8	6	0	-1.026016	0.130699	-0.499753
9	6	0	-0.770705	-1.301163	-0.855067
10	1	0	-1.054883	-1.490063	-1.900537
11	1	0	-1.430481	-1.950814	-0.265500
12	6	0	1.269143	0.474329	0.113127
13	6	0	2.423833	1.026094	0.532447
14	1	0	2.545199	2.053450	0.856962
15	6	0	3.572876	0.045087	0.507572
16	6	0	2.945461	-1.274081	-0.015922
17	1	0	4.012218	-0.075429	1.504553
18	1	0	4.383478	0.400564	-0.138917
19	1	0	3.407080	-1.613946	-0.945724
20	1	0	3.037128	-2.092235	0.701975
21	6	0	1.479169	-0.947217	-0.250481
22	7	0	0.609137	-1.769394	-0.682343
23	8	0	-2.060693	2.179316	-0.088915
24	8	0	-3.630746	-2.037798	1.074496
25	1	0	-4.363397	-2.630710	0.879185
26	1	0	-3.511659	-2.091523	2.028293



(Nimag=1) -727.2572

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.582797	-0.775343	-0.304418
2	6	0	-0.830618	-0.747317	-0.223438
3	6	0	-1.499706	0.385516	-0.630632
4	6	0	-0.805557	1.532220	-1.077852
5	6	0	1.182836	0.367678	-0.978287
6	6	0	1.571313	-1.594881	0.238531
7	6	0	2.688714	0.172125	-1.019329
8	6	0	-1.809302	-1.751218	0.308479
9	6	0	-2.974206	0.172221	-0.424493
10	1	0	3.174356	0.958444	-0.429607
11	1	0	3.082044	0.258077	-2.034753

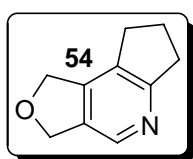
12	1	0	1.377437	-2.592093	0.620292
13	1	0	-3.438663	0.943113	0.201693
14	1	0	-3.514449	0.143226	-1.380863
15	1	0	-1.615381	-2.030191	1.352544
16	1	0	-1.834644	-2.675060	-0.286460
17	1	0	-0.496780	1.987980	0.481064
18	1	0	0.553044	2.917376	1.331667
19	8	0	-0.070121	2.189360	1.463563
20	1	0	1.346169	-0.512064	1.657536
21	1	0	-1.326825	2.366597	-1.536234
22	8	0	1.094975	0.226749	2.354627
23	1	0	1.759203	0.269855	3.049650
24	1	0	0.467159	1.327943	1.883279
25	7	0	0.557087	1.444911	-1.352238
26	8	0	-3.088732	-1.095848	0.236842
27	6	0	2.917636	-1.235194	-0.393408
28	1	0	3.749207	-1.235269	0.318847
29	1	0	3.186096	-1.959244	-1.174154



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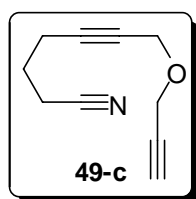
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.605432	-0.638211	-0.298881
2	6	0	-0.807183	-0.568488	-0.351765
3	6	0	-1.366421	0.684630	-0.256738
4	6	0	-0.544917	1.835853	-0.134211
5	6	0	1.301227	0.587172	-0.691425
6	6	0	1.511316	-1.464853	0.364342
7	6	0	2.777679	0.271864	-0.823924
8	6	0	-1.874687	-1.609078	-0.171902
9	6	0	-2.852266	0.534747	-0.075895
10	1	0	3.391329	1.098374	-0.461573
11	1	0	3.047816	0.102811	-1.870698
12	1	0	1.290211	-2.470723	0.705199
13	1	0	-3.182117	0.891531	0.910682
14	1	0	-3.430619	1.066007	-0.839228
15	1	0	-1.780114	-2.138638	0.789865

16	1	0	-1.900888	-2.360052	-0.968221
17	1	0	-0.058424	1.279838	1.335463
18	1	0	1.142905	1.086899	2.538078
19	8	0	0.469773	0.583693	2.057091
20	1	0	0.931423	-0.298181	1.581136
21	1	0	-0.976778	2.830286	-0.109583
22	8	0	-3.106813	-0.870754	-0.207379
23	6	0	2.942331	-1.043946	0.006869
24	1	0	3.567354	-0.890361	0.893321
25	1	0	3.441666	-1.817185	-0.585031
26	7	0	0.779641	1.768249	-0.587990



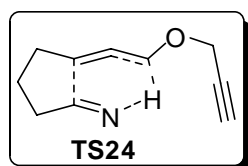
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.024992	-0.872087	0.250065
2	6	0	2.818503	0.615854	-0.124210
3	6	0	1.689828	-1.582859	-0.106925
4	1	0	3.883444	-1.321638	-0.251780
5	1	0	3.196422	-0.953965	1.327231
6	1	0	3.160759	0.824487	-1.145340
7	1	0	3.345421	1.307340	0.536036
8	1	0	1.462753	-2.411210	0.569824
9	1	0	1.724354	-2.002545	-1.120554
10	6	0	0.679507	-0.463797	-0.042153
11	6	0	1.318237	0.787124	-0.049948
12	6	0	-0.704327	-0.464561	-0.005785
13	6	0	-1.719742	-1.572821	0.017351
14	1	0	-1.677975	-2.140960	0.958162
15	6	0	-2.854742	0.498235	0.096034
16	1	0	-3.424343	1.013801	-0.682910
17	1	0	-3.279092	0.773775	1.071462
18	6	0	-1.373269	0.759241	0.032229
19	6	0	-0.646697	1.942948	0.023952
20	1	0	-1.140120	2.910663	0.053085
21	7	0	0.695917	1.963142	-0.021755
22	8	0	-2.988633	-0.918137	-0.112001
23	1	0	-1.607708	-2.280311	-0.810583



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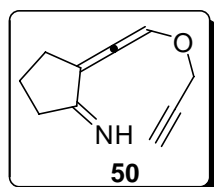
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.786197	1.541070	-0.154196
2	6	0	-3.776501	0.475568	-0.315003
3	6	0	-3.474648	-0.829158	0.453293
4	1	0	-3.886790	0.268645	-1.384874
5	1	0	-4.734751	0.880999	0.024543
6	6	0	-2.392399	-1.724369	-0.184172
7	1	0	-3.199170	-0.592411	1.483736
8	1	0	-4.404978	-1.403369	0.492471
9	1	0	-2.352636	-2.667232	0.372603
10	1	0	-2.695614	-1.989722	-1.204726
11	6	0	-1.058984	-1.132669	-0.210406
12	6	0	0.028296	-0.617655	-0.204711
13	6	0	1.303235	0.081906	-0.223244
14	1	0	1.120659	1.162575	-0.123573
15	1	0	1.813450	-0.083969	-1.181237
16	6	0	3.342547	0.342158	0.973813
17	1	0	3.797296	-0.005996	1.903801
18	1	0	3.144460	1.418968	1.080888
19	6	0	4.273644	0.128787	-0.139835
20	7	0	-2.045460	2.414618	-0.019959
21	6	0	5.042605	-0.045167	-1.047682
22	1	0	5.721237	-0.201272	-1.850609
23	8	0	2.123184	-0.376546	0.854943



(Nimag=1) -1060.4676

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

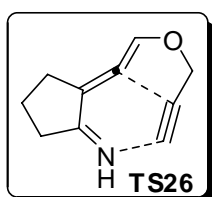
1	6	0	-1.633927	0.997325	-0.244620
2	6	0	-3.136498	1.076555	-0.212875
3	6	0	-3.696087	-0.217478	0.392306
4	1	0	-3.472275	1.193421	-1.249532
5	1	0	-3.440338	1.971694	0.332366
6	6	0	-2.834096	-1.375033	-0.149899
7	1	0	-3.608105	-0.180302	1.481882
8	1	0	-4.752070	-0.350515	0.148854
9	1	0	-2.935762	-2.282473	0.448773
10	1	0	-3.135521	-1.624267	-1.174369
11	6	0	-1.433674	-0.891113	-0.152768
12	6	0	-0.197031	-1.100449	-0.118844
13	6	0	0.999349	-0.385956	-0.198967
14	1	0	0.397075	0.757881	-0.311149
15	1	0	1.582160	-0.502298	-1.119744
16	6	0	2.919889	0.505334	0.869950
17	1	0	3.350733	0.517700	1.872971
18	1	0	2.584304	1.523397	0.634758
19	6	0	3.934482	0.082801	-0.099591
20	7	0	-0.669742	1.709724	-0.326535
21	6	0	4.774362	-0.258512	-0.889195
22	1	0	5.516233	-0.562845	-1.586814
23	8	0	1.802643	-0.378788	0.954346



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.297018	0.869904	-0.245398
2	6	0	-3.698651	0.294566	-0.144051
3	6	0	-3.504920	-1.098016	0.481922
4	1	0	-4.107592	0.206520	-1.158408
5	1	0	-4.358590	0.957519	0.416136
6	6	0	-2.137931	-1.571099	-0.058423
7	1	0	-3.458159	-1.011459	1.571844
8	1	0	-4.312557	-1.791335	0.240133
9	1	0	-1.650377	-2.315840	0.571639
10	1	0	-2.257463	-2.010918	-1.056172
11	6	0	-1.330335	-0.286170	-0.173636

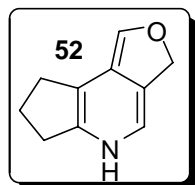
12	6	0	-0.028746	-0.161653	-0.179855
13	6	0	1.271233	-0.031684	-0.222691
14	1	0	-1.042523	2.273701	-0.412650
15	1	0	1.817162	-0.058063	-1.163790
16	6	0	3.324087	0.680287	0.728157
17	1	0	3.739424	0.769328	1.733357
18	1	0	3.208450	1.691985	0.319826
19	6	0	4.226848	-0.099104	-0.118895
20	7	0	-2.052465	2.111208	-0.357680
21	6	0	4.980306	-0.730729	-0.810235
22	1	0	5.644469	-1.294099	-1.419807
23	8	0	2.039471	0.075799	0.915035



(Nimag=1) -431.6646

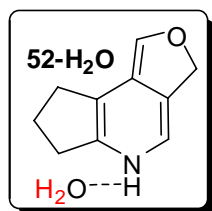
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.006882	-0.946707	0.311691
2	6	0	2.779259	0.577430	0.273672
3	6	0	1.587376	-1.548879	0.435789
4	1	0	3.460464	-1.272056	-0.629462
5	1	0	3.667827	-1.261803	1.121125
6	1	0	3.556564	1.131064	-0.254363
7	1	0	2.714832	0.989787	1.288693
8	1	0	1.295893	-1.646843	1.489576
9	1	0	1.502244	-2.543375	-0.010052
10	6	0	0.705272	-0.521106	-0.254355
11	6	0	1.426376	0.713699	-0.403696
12	6	0	-0.650159	-0.560192	-0.379008
13	6	0	-1.709475	-1.282384	-0.740173
14	1	0	-1.727416	-2.051298	-1.501314
15	6	0	-2.808424	0.056126	0.737737
16	1	0	-3.738710	0.621251	0.734450
17	1	0	-2.655251	-0.406103	1.718848
18	6	0	-1.621189	0.907865	0.406209
19	7	0	0.976793	1.829147	-0.894377
20	1	0	0.113962	1.659375	-1.410462
21	6	0	-1.166028	2.058874	0.465787

22	1	0	-0.827373	3.062490	0.557919
23	8	0	-2.937490	-0.976860	-0.245781



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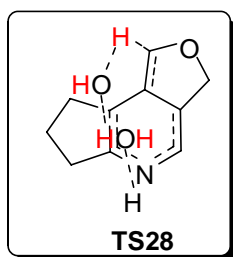
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.046250	-0.894523	0.200007
2	6	0	2.797822	0.608728	-0.095551
3	6	0	1.698773	-1.615398	-0.082216
4	1	0	3.871195	-1.300207	-0.388676
5	1	0	3.308062	-1.016333	1.253930
6	1	0	3.154085	0.896967	-1.093577
7	1	0	3.304737	1.264138	0.622096
8	1	0	1.497665	-2.408030	0.646513
9	1	0	1.690834	-2.093250	-1.071600
10	6	0	0.690334	-0.499101	-0.018219
11	6	0	1.299327	0.708743	-0.025938
12	6	0	-0.754100	-0.564816	-0.010203
13	6	0	-1.683907	-1.539421	-0.035048
14	1	0	-1.598439	-2.613272	-0.074334
15	6	0	-2.927502	0.389764	0.060932
16	1	0	-3.487406	0.797329	-0.786512
17	1	0	-3.419720	0.702261	0.988398
18	6	0	-1.452832	0.721143	0.029265
19	6	0	-0.797258	1.892083	0.019287
20	1	0	-1.277008	2.862035	0.040009
21	7	0	0.607886	1.910106	-0.067173
22	1	0	1.092126	2.755390	0.188631
23	8	0	-2.986598	-1.057622	-0.013571



(Nimag=0)

Center	Atomic	Atomic	Coordinates (Angstroms)		
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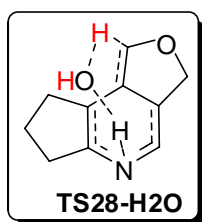
Number	Number	Type	X	Y	Z
1	6	0	2.922766	-0.904175	-0.419565
2	6	0	2.648455	0.598398	-0.694431
3	6	0	1.553551	-1.623582	-0.567964
4	1	0	3.684864	-1.312572	-1.085460
5	1	0	3.283792	-1.022236	0.604440
6	1	0	2.896711	0.882846	-1.725432
7	1	0	3.224933	1.255187	-0.034202
8	1	0	1.428828	-2.422867	0.169933
9	1	0	1.439953	-2.089646	-1.556272
10	6	0	0.557087	-0.506167	-0.393587
11	6	0	1.164250	0.703921	-0.474974
12	6	0	-0.883124	-0.567972	-0.257865
13	6	0	-1.812118	-1.540518	-0.179579
14	1	0	-1.730704	-2.615056	-0.209770
15	6	0	-3.041066	0.393739	-0.014274
16	1	0	-3.661023	0.776127	-0.831146
17	1	0	-3.465391	0.734548	0.935963
18	6	0	-1.573145	0.721025	-0.168497
19	6	0	-0.918537	1.889789	-0.248024
20	1	0	-1.391665	2.861324	-0.190889
21	7	0	0.473600	1.903476	-0.462570
22	1	0	0.980661	2.747290	-0.247780
23	8	0	-3.104673	-1.055980	-0.041376
24	8	0	1.215852	0.068679	2.869726
25	1	0	0.967121	-0.014323	1.937910
26	1	0	0.428569	-0.193290	3.356460



(Nimag=1) -1128.8274

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.638207	-0.879332	-0.191243
2	6	0	-0.781031	-0.835838	-0.146390
3	6	0	-1.395925	0.288410	-0.652950
4	6	0	0.567630	1.156021	-1.514026

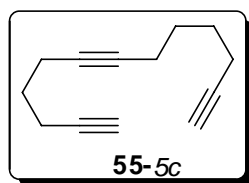
5	6	0	1.270326	0.083992	-1.064071
6	6	0	1.630532	-1.464035	0.580619
7	6	0	2.741027	-0.257858	-1.073383
8	6	0	-1.762763	-1.738160	0.555942
9	6	0	-2.876445	0.272802	-0.348783
10	1	0	3.402450	0.609610	-0.989138
11	1	0	3.038805	-0.832823	-1.962553
12	1	0	1.615812	-2.399051	1.123937
13	1	0	-3.096736	0.974606	0.466467
14	1	0	-3.474985	0.587400	-1.207267
15	1	0	-1.657798	-1.653676	1.647697
16	1	0	-1.625969	-2.796556	0.312113
17	1	0	-0.579978	2.149402	0.070384
18	1	0	0.068309	3.318419	1.067471
19	8	0	-0.300678	2.428323	1.075253
20	1	0	1.225181	-0.168869	1.638081
21	1	0	1.045399	1.956787	-2.073770
22	8	0	1.028691	0.735904	2.191266
23	1	0	1.856361	1.025268	2.591651
24	1	0	0.392517	1.619376	1.616679
25	6	0	-3.135391	-1.193890	0.074840
26	1	0	-3.462984	-1.768293	-0.795966
27	1	0	-3.913211	-1.283201	0.835875
28	8	0	2.920216	-1.094365	0.095756
29	7	0	-0.770858	1.358577	-1.223312



(Nimag=1) -605.7378

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.638005	-0.682088	-0.288270
2	6	0	-0.786054	-0.585821	-0.321365
3	6	0	-1.293856	0.689986	-0.248493
4	6	0	0.752779	1.697553	-0.655215
5	6	0	1.358173	0.486979	-0.775519
6	6	0	1.558054	-1.452004	0.396405
7	6	0	2.807080	0.078104	-0.816214
8	6	0	-1.855205	-1.623458	-0.096593

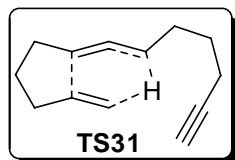
9	6	0	-2.784271	0.662512	-0.003876
10	1	0	3.507243	0.859162	-0.512005
11	1	0	3.122838	-0.318780	-1.790909
12	1	0	1.490913	-2.457589	0.785973
13	1	0	-2.994293	0.936427	1.038787
14	1	0	-3.316842	1.382242	-0.630334
15	1	0	-1.795319	-2.032181	0.923992
16	1	0	-1.783231	-2.476866	-0.777599
17	1	0	-0.020811	1.346158	1.287659
18	1	0	1.137851	1.181856	2.486112
19	8	0	0.429163	0.704300	2.031118
20	1	0	0.835437	-0.189987	1.565681
21	1	0	1.293844	2.627733	-0.812198
22	8	0	2.875552	-1.010632	0.152387
23	6	0	-3.162385	-0.809445	-0.299507
24	1	0	-3.480819	-0.898641	-1.341582
25	1	0	-3.982235	-1.170457	0.324637
26	7	0	-0.549459	1.841095	-0.194911



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.513386	1.642754	-0.127086
2	6	0	-2.768021	2.579831	-0.014968
3	1	0	-2.095664	3.396674	0.079663
4	6	0	-4.473164	0.546887	-0.241443
5	6	0	-4.126669	-0.735076	0.549590
6	1	0	-4.610962	0.296049	-1.300198
7	1	0	-5.443021	0.917848	0.108824
8	6	0	-3.118309	-1.682388	-0.133268
9	1	0	-3.766338	-0.464772	1.545391
10	1	0	-5.055232	-1.298335	0.687194
11	1	0	-3.088790	-2.617506	0.438293
12	1	0	-3.500161	-1.951009	-1.126569
13	6	0	-1.756549	-1.169216	-0.266646
14	6	0	-0.629951	-0.758577	-0.381893
15	6	0	0.723880	-0.225106	-0.503836
16	6	0	1.541264	-0.333455	0.801351

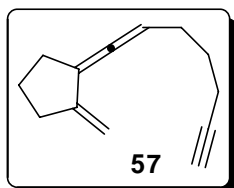
17	1	0	0.664848	0.828694	-0.804851
18	1	0	1.239607	-0.746221	-1.318311
19	6	0	2.941328	0.287399	0.716328
20	1	0	0.981180	0.164127	1.598439
21	1	0	1.615803	-1.387720	1.090723
22	1	0	3.382319	0.311263	1.717155
23	1	0	2.869556	1.329722	0.386706
24	6	0	3.907437	-0.469834	-0.220503
25	1	0	3.519539	-0.475327	-1.244702
26	1	0	3.966501	-1.519726	0.091061
27	6	0	5.251861	0.099723	-0.233724
28	6	0	6.352610	0.584974	-0.230214
29	1	0	7.326831	1.008738	-0.230943



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.072607	1.215953	-0.099026
2	6	0	-0.909223	1.669882	-0.116218
3	1	0	-0.284287	2.538144	-0.046570
4	6	0	-3.546555	1.392916	-0.012254
5	6	0	-4.231995	0.121842	0.508153
6	1	0	-3.921508	1.625335	-1.016867
7	1	0	-3.773736	2.256018	0.620564
8	6	0	-3.634178	-1.072187	-0.256900
9	1	0	-4.025833	0.008075	1.576709
10	1	0	-5.316366	0.174671	0.381871
11	1	0	-3.878649	-2.022006	0.225890
12	1	0	-4.048284	-1.108773	-1.272018
13	6	0	-2.174004	-0.882660	-0.324917
14	6	0	-0.984027	-1.229991	-0.416685
15	6	0	0.330977	-0.752203	-0.427234
16	6	0	1.264871	-1.092348	0.738809
17	1	0	-0.011677	0.479987	-0.307819
18	1	0	0.815056	-0.798178	-1.406903
19	6	0	2.530653	-0.226386	0.806321
20	1	0	0.704034	-0.976891	1.670928
21	1	0	1.550736	-2.149389	0.679454

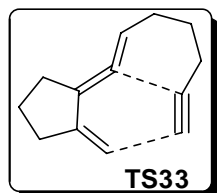
22	1	0	3.052434	-0.434369	1.745090
23	1	0	2.259755	0.833667	0.831280
24	6	0	3.514953	-0.468246	-0.358339
25	1	0	3.038500	-0.231173	-1.315523
26	1	0	3.775036	-1.532962	-0.399838
27	6	0	4.740625	0.316658	-0.240373
28	6	0	5.742891	0.971840	-0.124506
29	1	0	6.630507	1.547421	-0.027246



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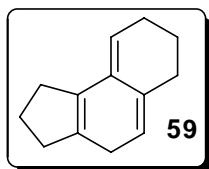
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.135003	-0.639444	-0.130630
2	6	0	-4.265334	0.357183	-0.333966
3	6	0	-3.553716	1.713957	-0.493059
4	1	0	-4.899124	0.374508	0.561962
5	1	0	-4.905230	0.096735	-1.179486
6	6	0	-2.337300	1.601208	0.445652
7	1	0	-3.212510	1.833571	-1.526302
8	1	0	-4.195709	2.564486	-0.253756
9	1	0	-1.514972	2.266702	0.179156
10	1	0	-2.632151	1.838676	1.475107
11	6	0	-1.952004	0.124825	0.355351
12	6	0	-0.771611	-0.367074	0.641797
13	6	0	0.403715	-0.864070	0.916690
14	1	0	0.608342	-1.190296	1.938214
15	6	0	1.540209	-1.014304	-0.071685
16	1	0	1.192214	-0.736756	-1.070887
17	1	0	1.831576	-2.072019	-0.117752
18	6	0	2.767595	-0.172747	0.311293
19	1	0	2.493966	0.886030	0.334662
20	1	0	3.098043	-0.432792	1.322156
21	6	0	3.940633	-0.374952	-0.669170
22	1	0	4.219346	-1.435197	-0.694181
23	1	0	3.617169	-0.119441	-1.685212
24	6	0	5.117921	0.419289	-0.330924
25	6	0	6.077955	1.081791	-0.036769
26	1	0	6.928528	1.664899	0.218479

27	6	0	-3.196727	-1.952863	-0.366344
28	1	0	-2.344006	-2.599924	-0.192792
29	1	0	-4.103480	-2.415968	-0.738787



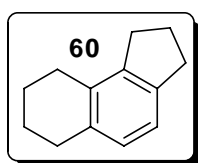
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.963432	-0.794000	1.027347
2	6	0	3.151168	0.308851	-0.038286
3	6	0	1.782577	-1.643188	0.506685
4	1	0	3.868567	-1.382288	1.196417
5	1	0	2.684113	-0.334793	1.980434
6	1	0	3.863297	-0.013650	-0.808600
7	1	0	3.536359	1.244547	0.376675
8	1	0	1.202588	-2.109403	1.305142
9	1	0	2.138998	-2.451016	-0.146464
10	6	0	0.965629	-0.650451	-0.316333
11	6	0	1.770244	0.468579	-0.649896
12	6	0	1.273953	1.586248	-1.265061
13	1	0	0.390165	1.533298	-1.884341
14	1	0	1.894603	2.468362	-1.390786
15	6	0	-0.383813	-0.685793	-0.451295
16	6	0	-1.447031	-1.306607	-0.924686
17	1	0	-1.262726	-2.051175	-1.702470
18	6	0	-2.889134	-1.193158	-0.487317
19	6	0	-2.299676	0.634121	1.223516
20	1	0	-3.087246	-2.018569	0.212633
21	1	0	-3.536910	-1.383535	-1.349379
22	1	0	-2.770375	1.420894	1.823021
23	1	0	-2.038746	-0.179838	1.909284
24	6	0	-1.083319	1.192372	0.589973
25	6	0	-0.366371	2.156354	0.303548
26	1	0	-0.002962	3.157406	0.311464
27	6	0	-3.301017	0.127107	0.168696
28	1	0	-3.419576	0.902489	-0.594679
29	1	0	-4.280011	-0.005353	0.640301



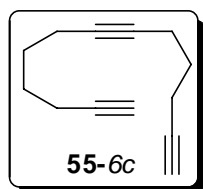
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.256408	-1.119234	-0.180866
2	6	0	-3.173537	0.386927	0.174775
3	6	0	-1.823272	-1.673329	0.026589
4	1	0	-4.003792	-1.652231	0.410566
5	1	0	-3.537754	-1.227159	-1.231819
6	1	0	-3.526177	0.585736	1.197027
7	1	0	-3.787142	1.009088	-0.486674
8	1	0	-1.551448	-2.408646	-0.737212
9	1	0	-1.717054	-2.177319	0.996425
10	6	0	-0.959151	-0.431261	-0.018819
11	6	0	-1.699887	0.687587	0.060157
12	6	0	-1.112468	2.061189	0.097182
13	1	0	-1.399821	2.567919	1.033233
14	1	0	-1.557612	2.684719	-0.694379
15	6	0	0.501638	-0.405018	-0.066175
16	6	0	1.259001	-1.525749	-0.040748
17	1	0	0.767841	-2.493917	-0.022170
18	6	0	2.763379	-1.521717	-0.013253
19	6	0	2.623167	0.972460	-0.338110
20	1	0	3.153438	-1.784833	-1.008324
21	1	0	3.120916	-2.311413	0.657649
22	1	0	3.018978	1.948013	-0.042036
23	1	0	2.833774	0.857951	-1.410681
24	6	0	1.124781	0.934662	-0.130545
25	6	0	0.384428	2.051113	-0.043200
26	1	0	0.877899	3.018994	-0.088957
27	6	0	3.324981	-0.161617	0.419886
28	1	0	3.162730	-0.030226	1.495709
29	1	0	4.405317	-0.122762	0.250395



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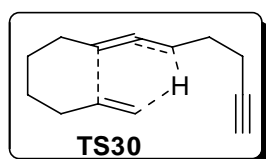
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.756195	-1.380455	-0.343008
2	6	0	-2.570191	1.100187	-0.011486
3	6	0	-1.273555	-1.597676	-0.018670
4	1	0	-3.323835	-2.285220	-0.104577
5	1	0	-2.876515	-1.207839	-1.419751
6	1	0	-2.848324	1.939265	0.634360
7	1	0	-2.902191	1.374464	-1.022242
8	1	0	-0.840273	-2.322337	-0.716078
9	1	0	-1.186713	-2.056744	0.976206
10	6	0	-0.451584	-0.321088	-0.036719
11	6	0	-1.058394	0.948071	-0.017336
12	6	0	0.947703	-0.387451	-0.044169
13	6	0	1.823154	-1.625144	-0.066670
14	1	0	1.829338	-2.069360	-1.071463
15	6	0	3.223394	-1.079868	0.309969
16	6	0	3.206293	0.409804	-0.109762
17	1	0	4.036366	-1.643346	-0.152950
18	1	0	3.354345	-1.146917	1.394216
19	1	0	3.824248	1.038078	0.537598
20	1	0	3.587906	0.534231	-1.131579
21	6	0	1.735994	0.764594	-0.056947
22	6	0	1.134900	2.019941	-0.046305
23	1	0	1.732584	2.925905	-0.049480
24	6	0	-3.304472	-0.172751	0.420792
25	1	0	-3.169564	-0.331429	1.498019
26	1	0	-4.379595	-0.060150	0.250045
27	6	0	-0.254813	2.096589	-0.020185
28	1	0	-0.735242	3.070487	0.002742
29	1	0	1.484058	-2.407598	0.617911



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.824218	1.717068	0.133642

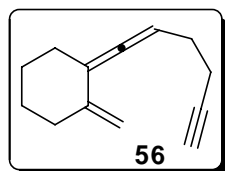
2	6	0	-2.658913	2.589173	-0.678215
3	1	0	-2.494553	3.352902	-1.397981
4	6	0	-3.074835	0.674965	1.126458
5	1	0	-3.697575	1.110304	1.915859
6	1	0	-2.129276	0.390338	1.600402
7	6	0	-1.982253	-1.292740	-1.204553
8	1	0	-1.785917	-2.190634	-1.801503
9	1	0	-2.514173	-0.598262	-1.864667
10	6	0	-0.695480	-0.712069	-0.822404
11	6	0	0.377436	-0.257987	-0.513653
12	6	0	1.673463	0.301197	-0.136565
13	6	0	2.507612	-0.644469	0.747768
14	1	0	1.518701	1.250872	0.391123
15	1	0	2.242651	0.543838	-1.040608
16	6	0	3.871281	-0.047491	1.152614
17	1	0	1.947261	-0.875456	1.658529
18	1	0	2.664919	-1.589173	0.220572
19	1	0	4.364122	-0.726068	1.857198
20	1	0	3.714997	0.894389	1.692433
21	6	0	4.769999	0.193539	0.025854
22	6	0	5.503716	0.381320	-0.908831
23	1	0	6.154679	0.549350	-1.731527
24	6	0	-3.788302	-0.583936	0.569858
25	1	0	-4.521525	-0.267138	-0.178773
26	1	0	-4.360791	-1.031264	1.389189
27	6	0	-2.893075	-1.686563	-0.014665
28	1	0	-2.268199	-2.113252	0.776889
29	1	0	-3.553909	-2.492789	-0.350987



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.292432	1.259552	-0.111975
2	6	0	-0.149506	1.745680	-0.249211
3	1	0	0.404805	2.659235	-0.352706
4	6	0	-2.725297	1.538980	0.163530
5	1	0	-2.942707	2.536689	-0.237027
6	1	0	-2.836327	1.617444	1.252783

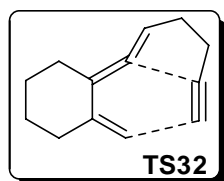
7	6	0	-2.493336	-1.654235	-0.245253
8	1	0	-2.459274	-2.626440	0.258075
9	1	0	-2.669624	-1.864105	-1.308205
10	6	0	-1.163818	-1.017227	-0.122216
11	6	0	0.072188	-1.138593	-0.125076
12	6	0	1.321212	-0.527440	-0.187815
13	6	0	2.255886	-0.582616	1.017914
14	1	0	0.815165	0.675129	-0.263152
15	1	0	1.839555	-0.630650	-1.144376
16	6	0	3.437231	0.406739	0.920553
17	1	0	1.685463	-0.356924	1.923551
18	1	0	2.651805	-1.596512	1.132072
19	1	0	4.010430	0.368135	1.853115
20	1	0	3.054915	1.430251	0.836648
21	6	0	4.340402	0.141469	-0.197016
22	6	0	5.080956	-0.090028	-1.116455
23	1	0	5.736999	-0.290622	-1.927711
24	6	0	-3.779178	0.549559	-0.352614
25	1	0	-3.708376	0.462873	-1.443317
26	1	0	-4.763833	0.977376	-0.137628
27	6	0	-3.675804	-0.836448	0.287240
28	1	0	-3.597481	-0.732205	1.375992
29	1	0	-4.592533	-1.402037	0.092240



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.681549	1.127790	-0.068867
2	6	0	-1.230523	2.314528	-0.486064
3	1	0	-1.698640	3.238413	-0.162586
4	6	0	-2.874532	0.985579	0.854655
5	1	0	-3.367015	1.954062	0.976697
6	1	0	-2.510752	0.684500	1.847047
7	6	0	-2.026688	-1.271331	-0.891890
8	1	0	-1.485426	-2.211887	-1.012836
9	1	0	-2.452509	-1.016252	-1.871840
10	6	0	-1.058430	-0.162253	-0.492408
11	6	0	0.241237	-0.333914	-0.515867

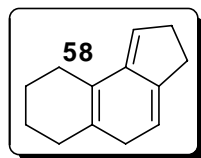
12	6	0	1.532978	-0.525875	-0.527130
13	6	0	2.336594	-1.051518	0.640524
14	1	0	-0.382005	2.394191	-1.155703
15	1	0	2.095011	-0.285201	-1.429308
16	6	0	3.416149	-0.057464	1.135431
17	1	0	1.667413	-1.279841	1.473394
18	1	0	2.832098	-1.985309	0.351645
19	1	0	3.893962	-0.470788	2.030707
20	1	0	2.933810	0.877781	1.439266
21	6	0	4.447809	0.233130	0.143270
22	6	0	5.295768	0.458255	-0.679909
23	1	0	6.046867	0.663495	-1.402731
24	6	0	-3.872718	-0.076747	0.363380
25	1	0	-4.339840	0.267168	-0.567548
26	1	0	-4.677366	-0.193586	1.096317
27	6	0	-3.174072	-1.419054	0.119202
28	1	0	-2.776634	-1.801912	1.067241
29	1	0	-3.891115	-2.161598	-0.245724



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.092226	0.831828	-0.543615
2	6	0	-0.341705	1.911883	-0.946039
3	1	0	-0.777024	2.906783	-0.934826
4	6	0	-2.479705	1.060492	0.042092
5	1	0	-3.006798	1.814780	-0.549155
6	1	0	-2.360884	1.486961	1.048203
7	6	0	-1.287502	-1.676998	-0.004816
8	1	0	-0.634200	-2.364095	0.537589
9	1	0	-1.609576	-2.211544	-0.909299
10	6	0	-0.484251	-0.454478	-0.450047
11	6	0	0.861947	-0.586130	-0.573615
12	6	0	1.985538	-1.119450	-1.004025
13	6	0	3.264572	-0.893468	-0.235817
14	1	0	0.530080	1.786153	-1.570912
15	1	0	2.023266	-1.671995	-1.941720
16	6	0	2.910121	-0.114933	1.045422

17	1	0	3.761821	-1.838924	0.007497
18	1	0	3.968784	-0.319288	-0.850986
19	1	0	3.790907	0.383033	1.461842
20	1	0	2.536396	-0.812491	1.802492
21	6	0	1.853691	0.871975	0.738744
22	6	0	1.304727	1.976630	0.680195
23	1	0	1.141418	3.007409	0.896891
24	6	0	-3.324742	-0.212828	0.150165
25	1	0	-3.630636	-0.542488	-0.850715
26	1	0	-4.243131	0.000399	0.706142
27	6	0	-2.525203	-1.328190	0.827455
28	1	0	-2.219798	-1.000078	1.828694
29	1	0	-3.142199	-2.222604	0.961674



(Nimag=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.770869	-1.394179	-0.366662
2	6	0	-2.530028	1.081640	-0.007780
3	6	0	-1.300552	-1.626941	-0.002140
4	1	0	-3.359650	-2.287634	-0.136660
5	1	0	-2.857119	-1.229584	-1.447761
6	1	0	-2.774904	1.904003	0.675928
7	1	0	-2.840489	1.431193	-1.003902
8	1	0	-0.855041	-2.345089	-0.699152
9	1	0	-1.231080	-2.094665	0.989823
10	6	0	-0.473465	-0.357566	-0.004101
11	6	0	-1.032449	0.872469	-0.012866
12	6	0	0.983950	-0.481239	0.013439
13	6	0	1.760581	-1.585151	0.068515
14	1	0	1.399747	-2.605509	0.111699
15	6	0	3.232690	-1.251235	0.082625
16	6	0	3.273094	0.301042	-0.033238
17	1	0	3.768157	-1.738544	-0.740592
18	1	0	3.712337	-1.602998	1.004381
19	1	0	3.826902	0.756276	0.791791
20	1	0	3.764982	0.616187	-0.957724
21	6	0	1.814982	0.726493	-0.026227

22	6	0	1.277401	1.949179	-0.054171
23	1	0	1.899750	2.839677	-0.083360
24	6	0	-3.322428	-0.173433	0.372076
25	1	0	-3.245078	-0.339860	1.453358
26	1	0	-4.384388	-0.029143	0.150056
27	6	0	-0.213088	2.142244	-0.035700
28	1	0	-0.497370	2.758895	0.832555
29	1	0	-0.525677	2.746851	-0.903065
