Supplementary Information (SI)

Synthesis of Fullerene–Fluorene Dyads through the Platinum-Catalyzed Reactions of [60]Fullerene with 9-Ethynyl-9*H*-fluoren-9-yl Carboxylates

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Table S1. Crystal Data for ***Z*-3b**

Chemical formula	$C_{81}H_{20}O_2$	
Formula weight	1024.97 g/mol	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal size	0.060 x 0.269 x 0.284 mm	
Crystal system	orthorhombic	
Space group	*Pbca*	
Unit cell dimensions	a = 19.3947(6) Å	α = 90°
	b = 17.2114(5) Å	β = 90°
	c = 25.7129(8) Å	γ = 90°
Volume	8583.2(5) $Å^3$	
Z	8	
Density (calculated)	1.586 g/cm^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	4176	

Table S2. Data Collection and Structure Refinement for ***Z*-3b**

Theta range for data collection	2.24 to 27.10°
Index ranges	-24<=h<=24, -22<=k<=21, -25<=l<=32
Reflections collected	76675
Independent reflections	9438 [R(int) = 0.0604]
Max. and min. transmission	0.9940 and 0.9740
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2016/6 (Sheldrick, 2016)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	9438 / 78 / 769
Goodness-of-fit on F^2	1.054
Final R indices	6489 data; $I>2\sigma(I)$ $R_1 = 0.0597$, $wR_2 = 0.1391$
	all data $R_1 = 0.1010$, $wR_2 = 0.1770$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0699P)^2+13.1892P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.645 and –0.628 eÅ^{-3}
R.M.S. deviation from mean	0.075 eÅ^{-3}

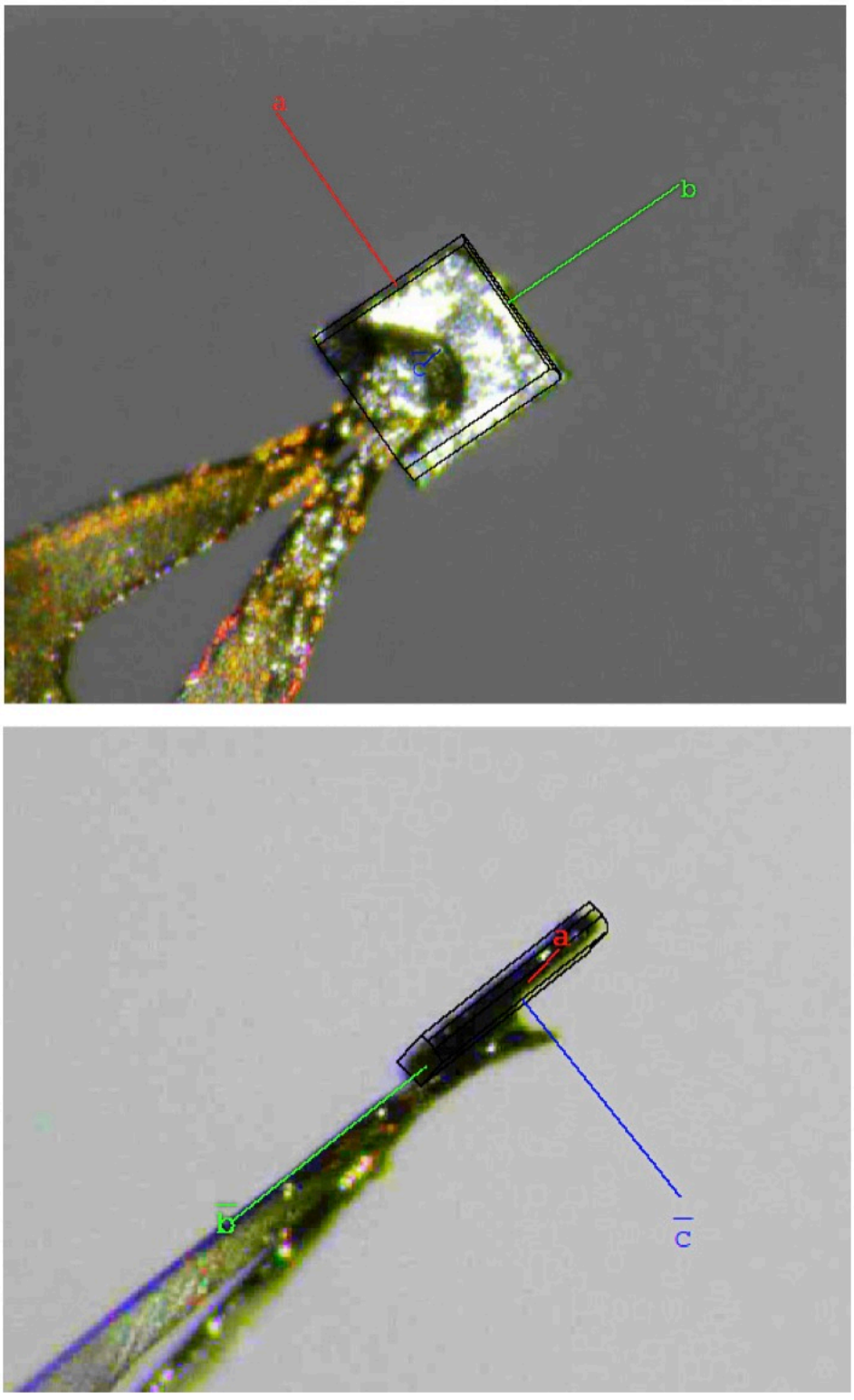

Figure S1. Photographic images of the single crystal of **Z-3b** used for XRD.

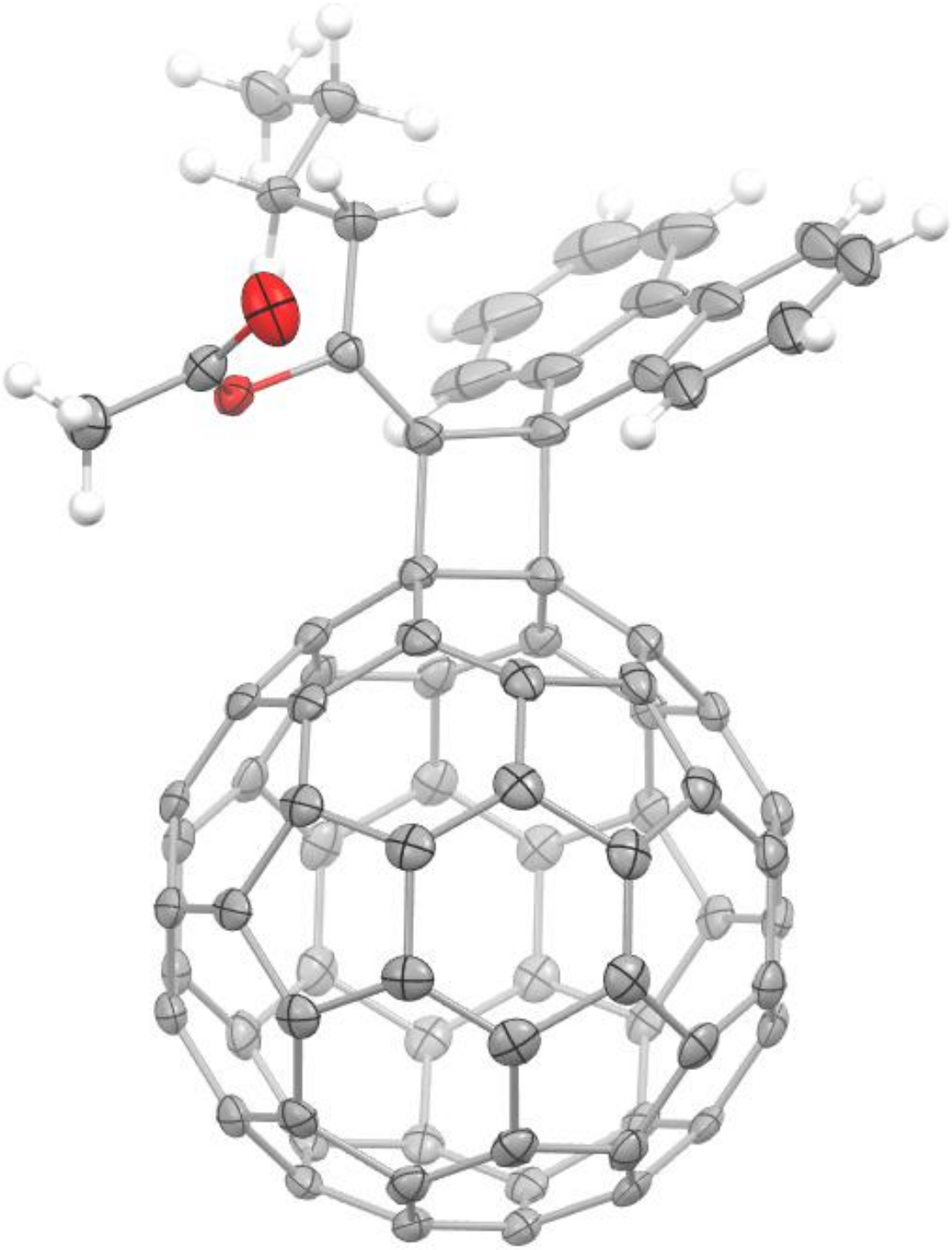

Figure S2. ORTEP drawing of ***Z*-3b** with thermal ellipsoids shown at the 50% probability level. Black plate crystals suitable for data collection were obtained by gradual diffusion of *n*-hexane into a solution of ***Z*-3b** in CS_2/*n*-hexane.

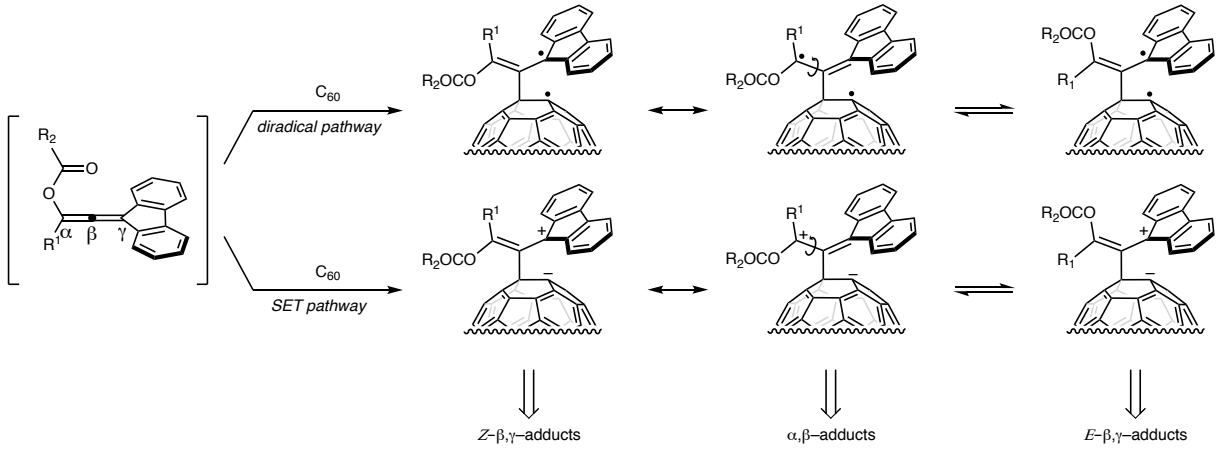

Figure S3. Plausible mechanism for the formal [2+2] cycloaddition of C_{60} with a fluorenylideneallene intermediate.

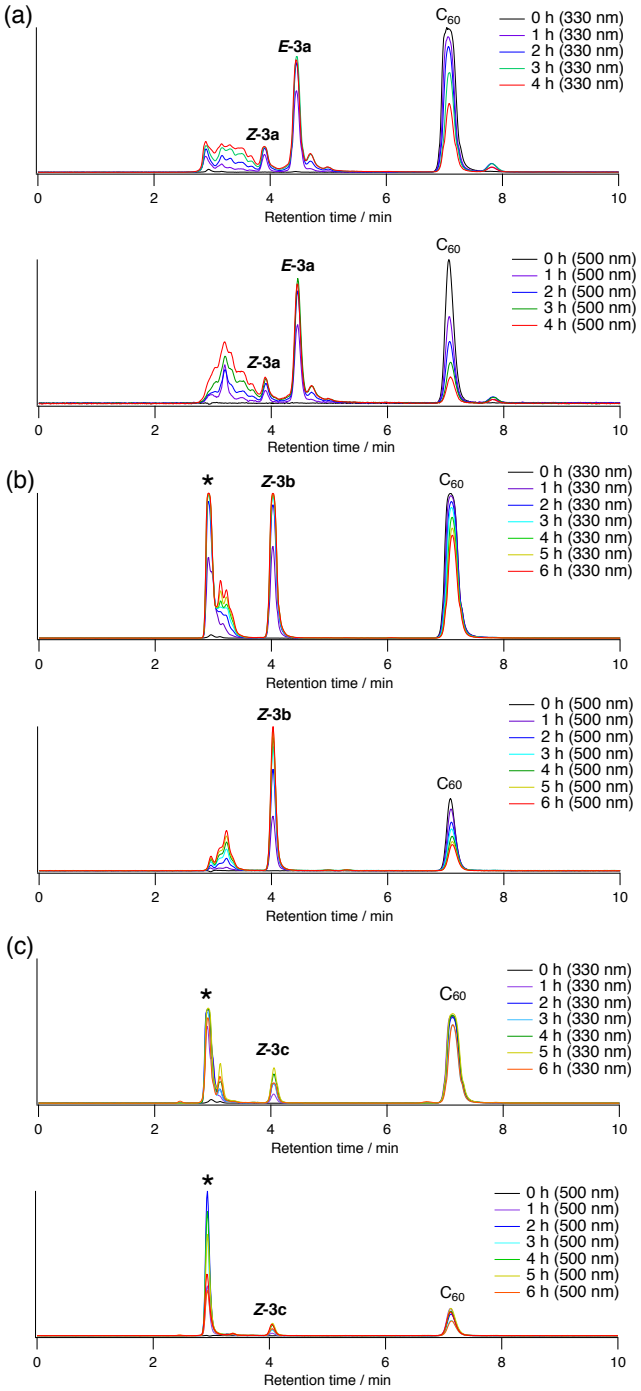

Figure S4. Contrasting HPLC profiles of the reaction mixtures from the reactions of C_{60} with (a) **2a**, (b) **2b**, and (c) **2c** in the presence of $PtCl_2$ monitored at 330 nm and at 500 nm. Conditions: Buckyprep column (4.6 mm 250 mm i.d.); column temp., 40ºC; flow rate, 1.0 mL min^{-1}; eluent, toluene. The peaks marked with astarisks (*) are related to non-fullerene products containing fluorenylideneallene dimers.

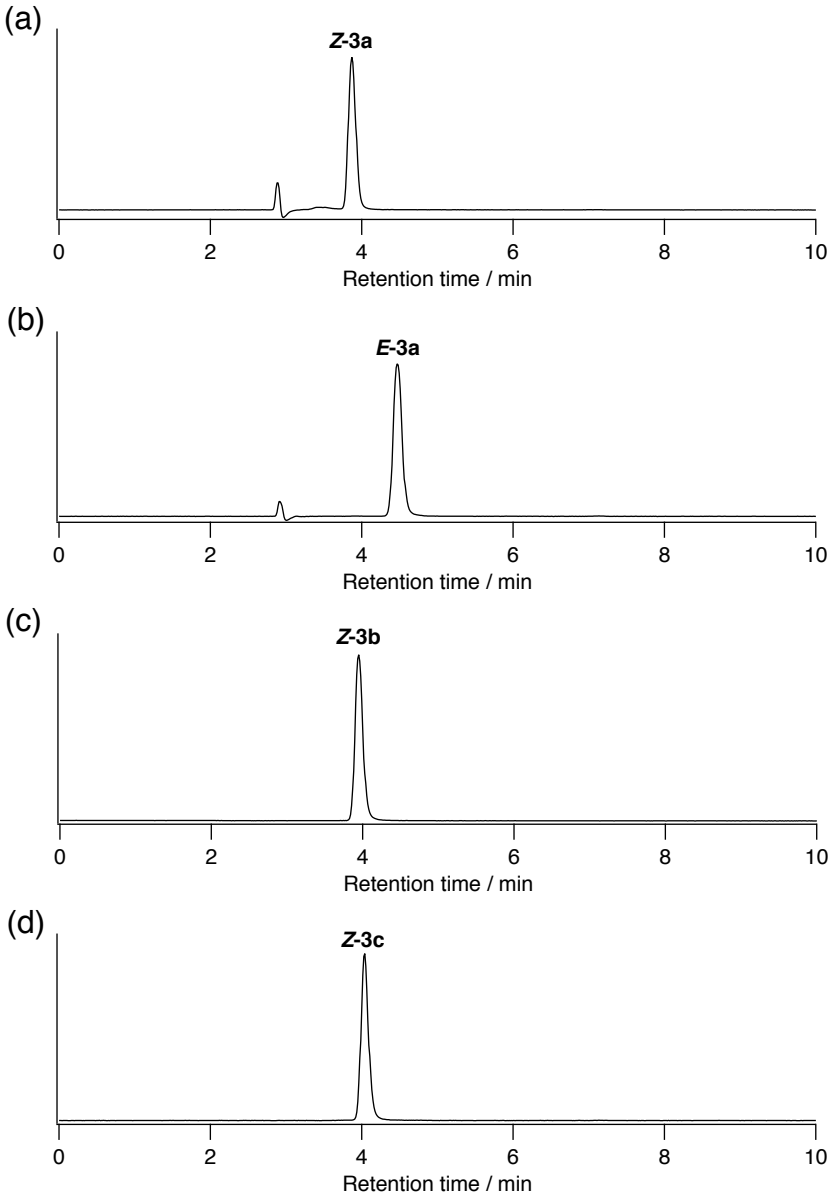

Figure S5. HPLC profiles of isolated (a) ***Z*-3a**, (b) ***E*-3a**, (c) ***Z*-3b**, and (d) ***Z*-3c**. Conditions: Buckyprep column (4.6 mm 250 mm i.d.); column temp., 40ºC; flow rate, 1.0 mL min^{-1}; eluent, toluene.

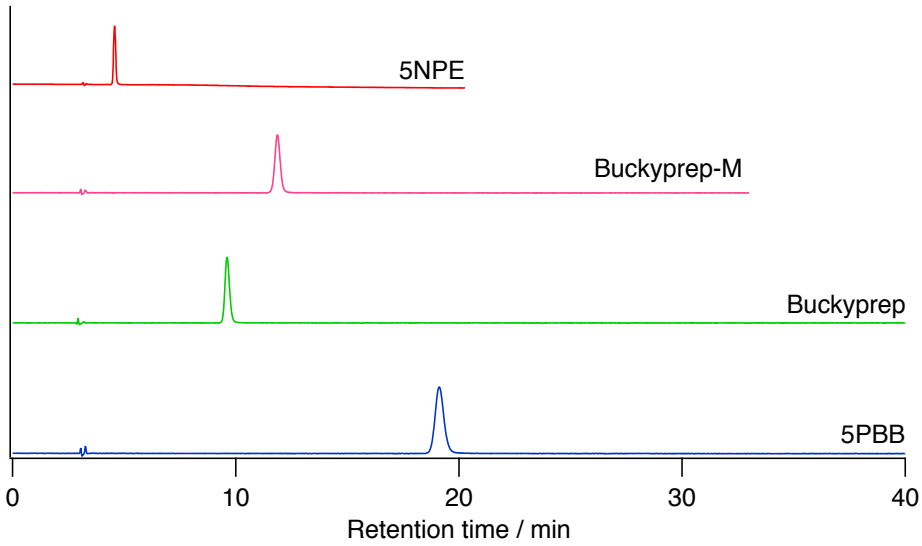

Figure S6. HPLC profiles of ***Z*-3b** using different columns (4.6 mm 250 mm i.d.). Conditions: column temp., 40ºC; flow rate, 1.0 mL min^{-1}; eluent, toluene/*n*-hexane 1:1.

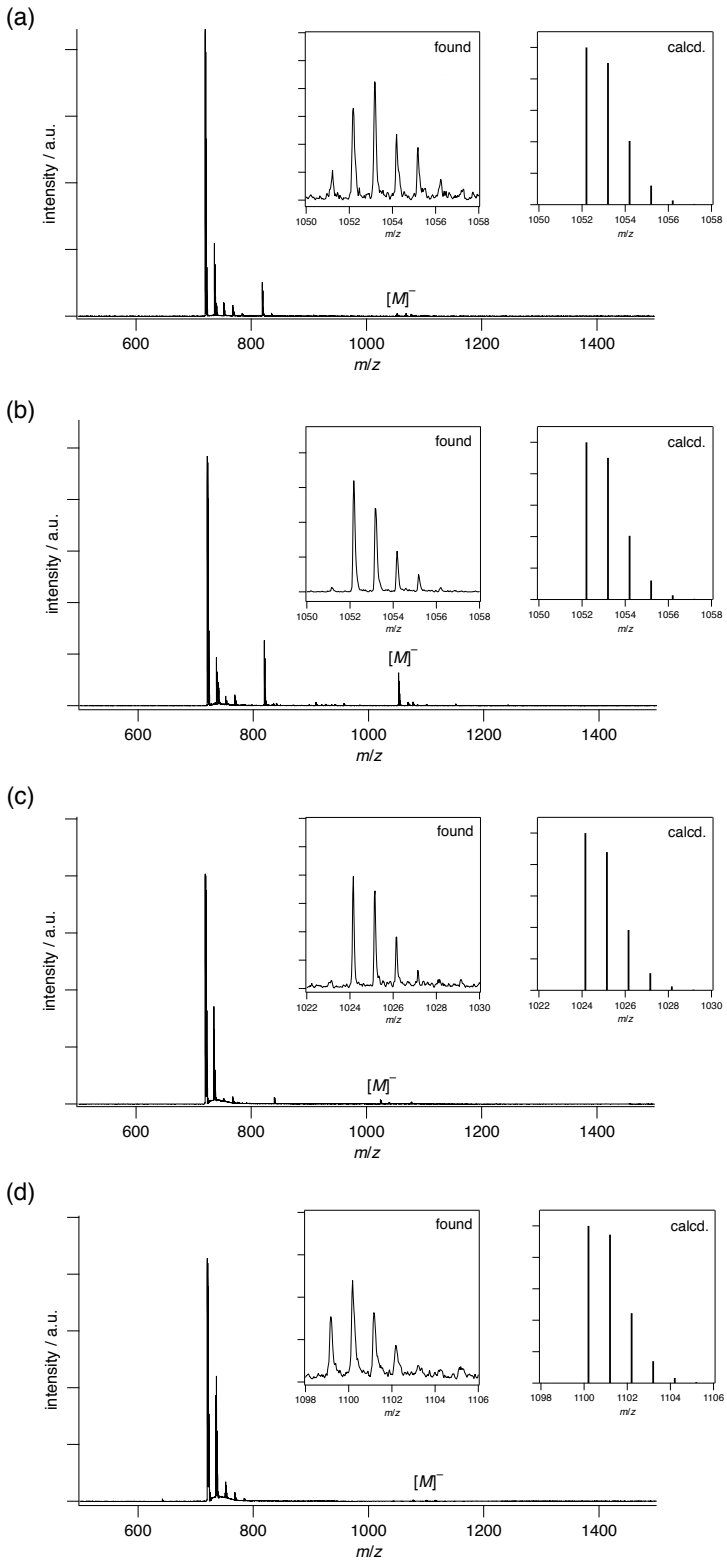

Figure S7. Negative-mode MALDI-TOF mass spectra of (a) ***Z*-3a**, (b) ***E*-3a**, (c) ***Z*-3b**, and (d) ***Z*-3c**. Matrix = 1,1,4,4-tetraphenyl-1,3-butadiene (TPB).

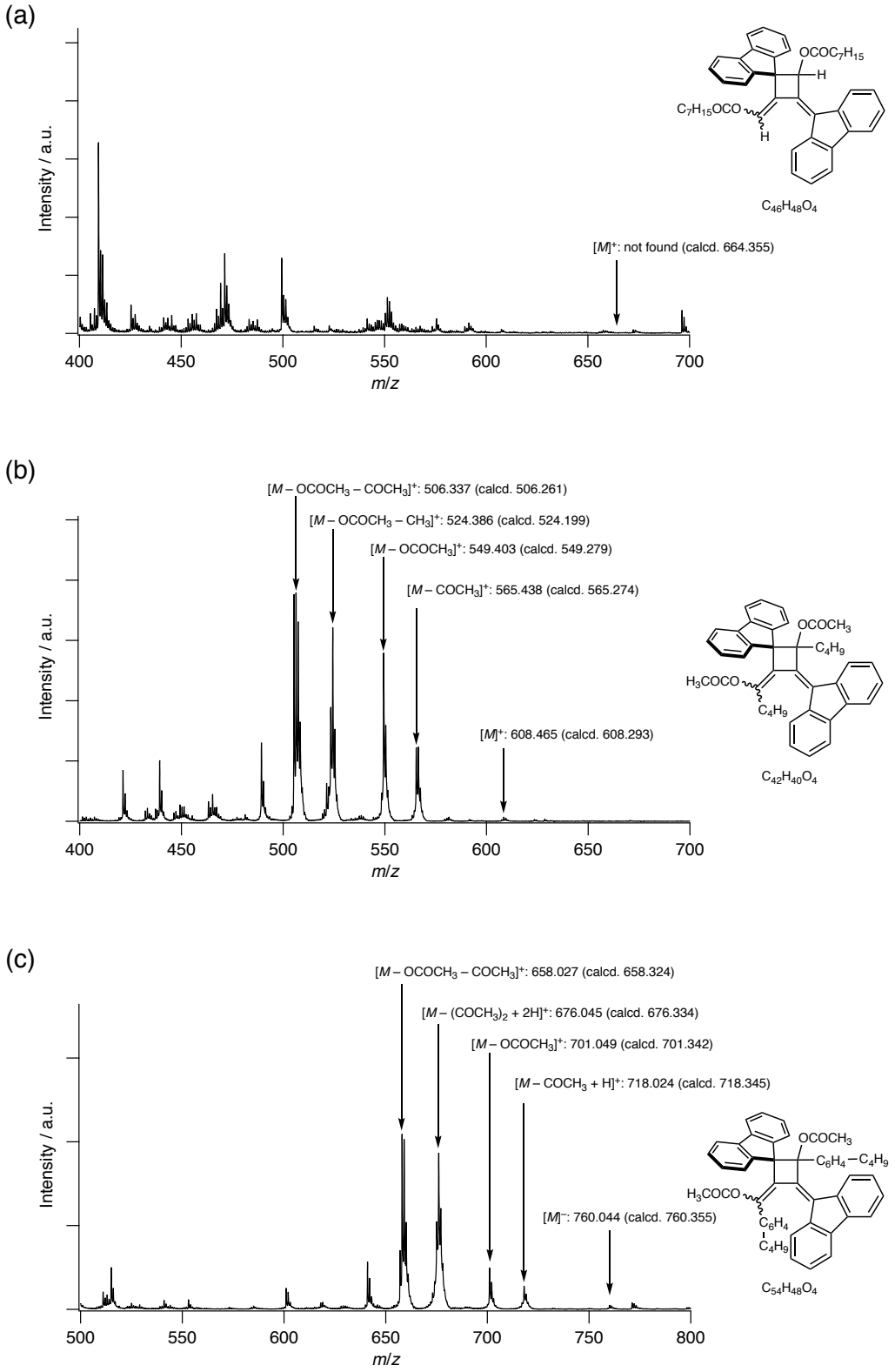

Figure S8. Positive-mode MALDI-TOF mass spectra of fractions containing non-fullerene products from the reactions of C_{60} with (a) **2a**, (b) **2b**, and (c) **2c** in the presence of $PtCl_2$.

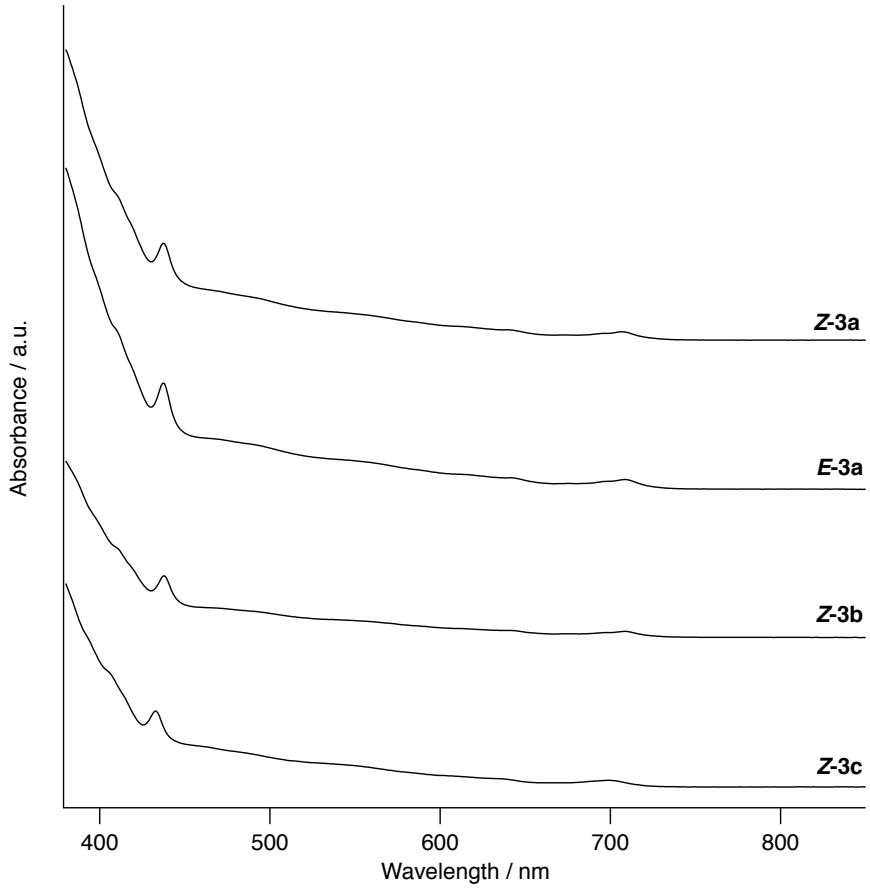

Figure S9. Absorption spectra of ***Z*-3a**, ***E*-3a**, ***Z*-3b**, and ***Z*-3c** in CS_2.

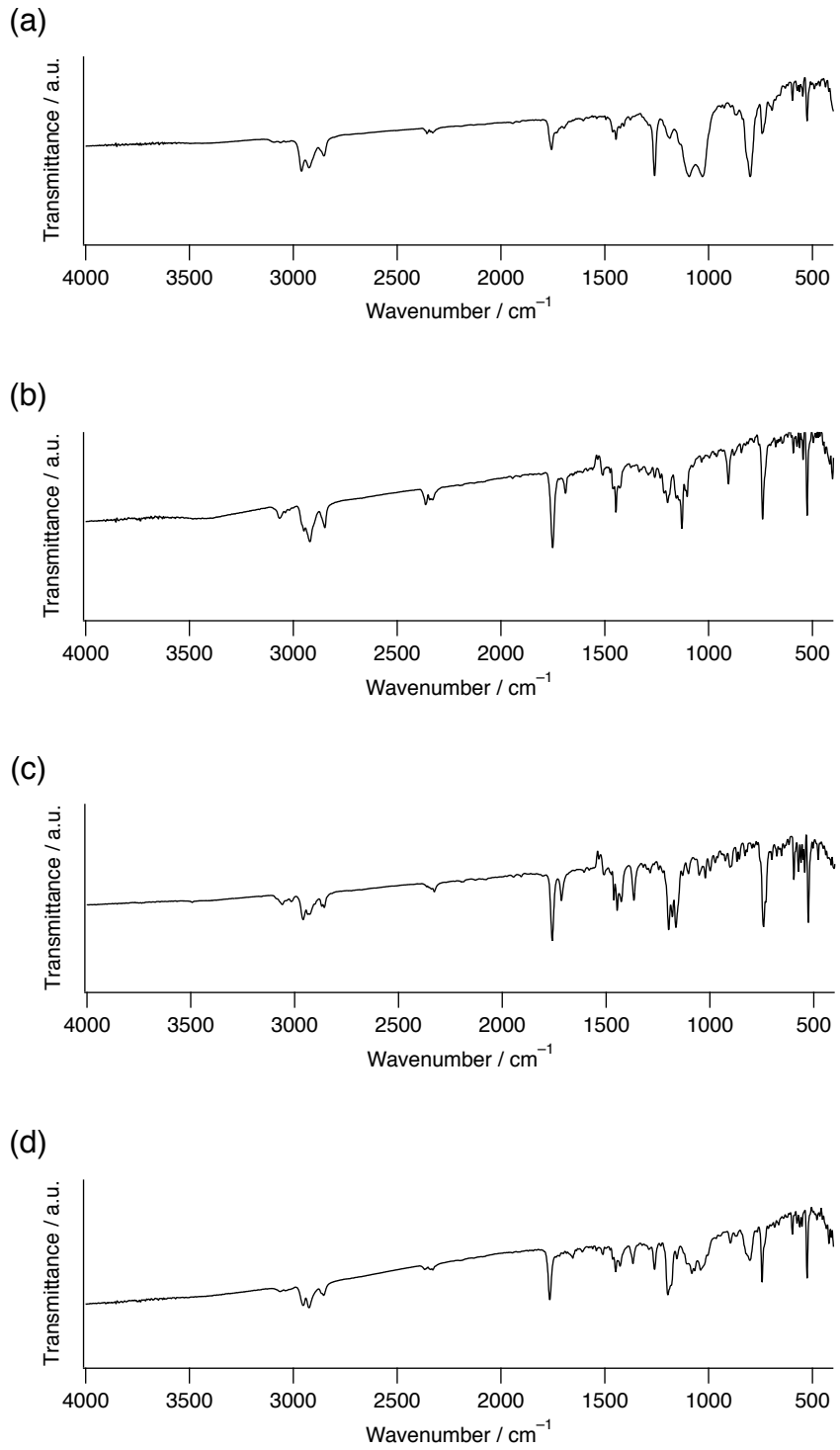

Figure S10. IR spectra of (a) ***Z*-3a**, (b) ***E*-3a**, (c) ***Z*-3b**, and (d) ***Z*-3c**.

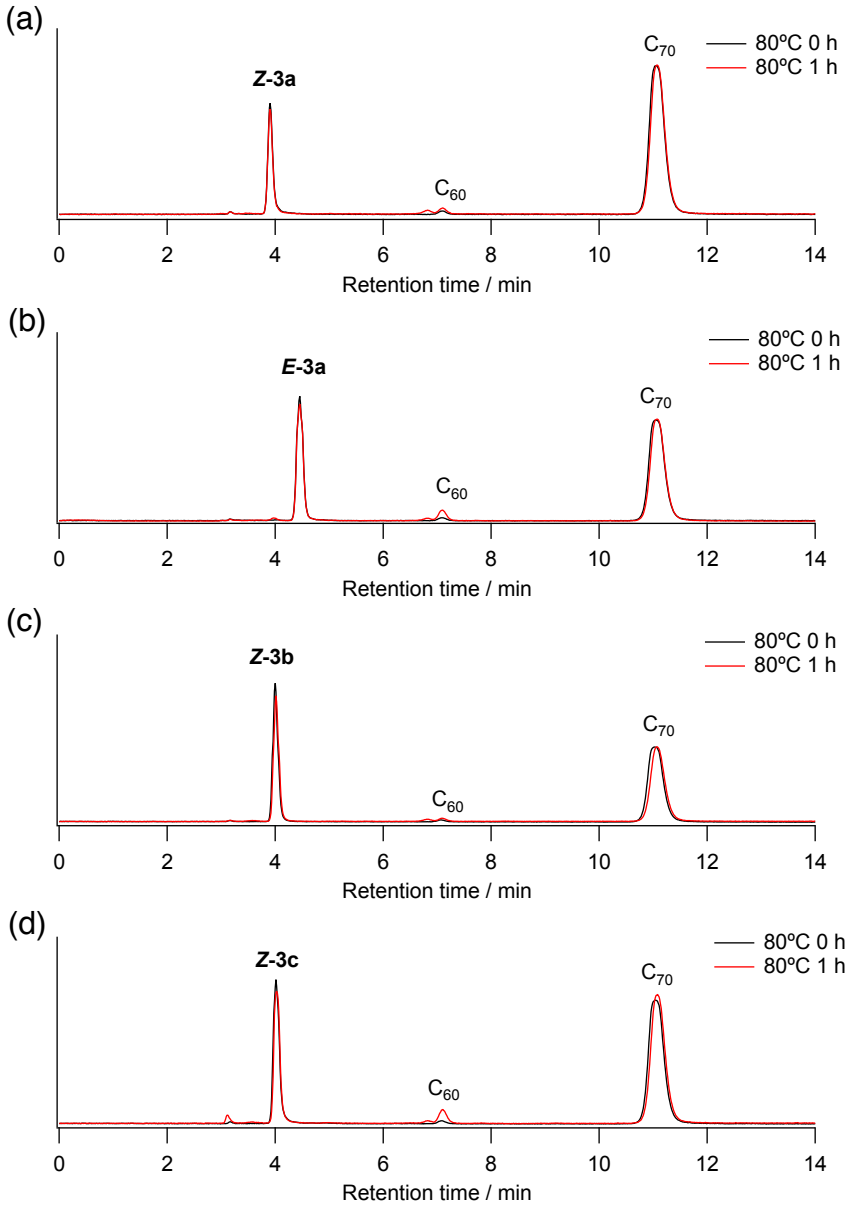

Figure S11. HPLC profiles of (a) ***Z*-3a**, (b) ***E*-3a**, (c) ***Z*-3b**, and (d) ***Z*-3c** before and after heating at 80 ºC for 1 h (C_{70} was added to the solution as an internal standard). Conditions: Buckyprep column (4.6 mm 250 mm i.d.); column temp., 40 ºC; flow rate, 1.0 mL min^{-1}; eluent, toluene; UV detection, 330 nm.

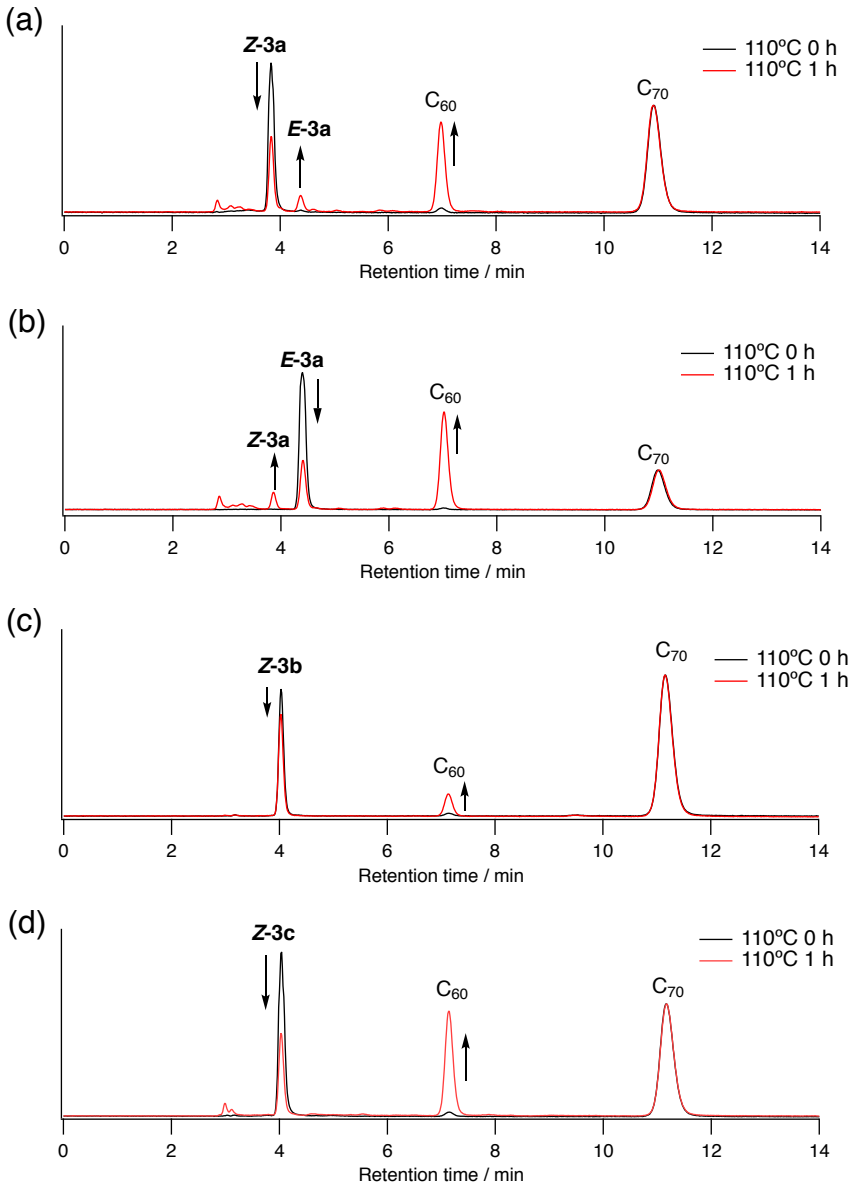

Figure S12. HPLC profiles of (a) ***Z*-3a**, (b) ***E*-3a**, (c) ***Z*-3b**, and (d) ***Z*-3c** before and after heating at 110 ºC for 1 h (C_{70} was added to the solution as an internal standard). Conditions: Buckyprep column (4.6 mm 250 mm i.d.); column temp., 40 ºC; flow rate, 1.0 mL min^{-1}; eluent, toluene; UV detection, 330 nm.

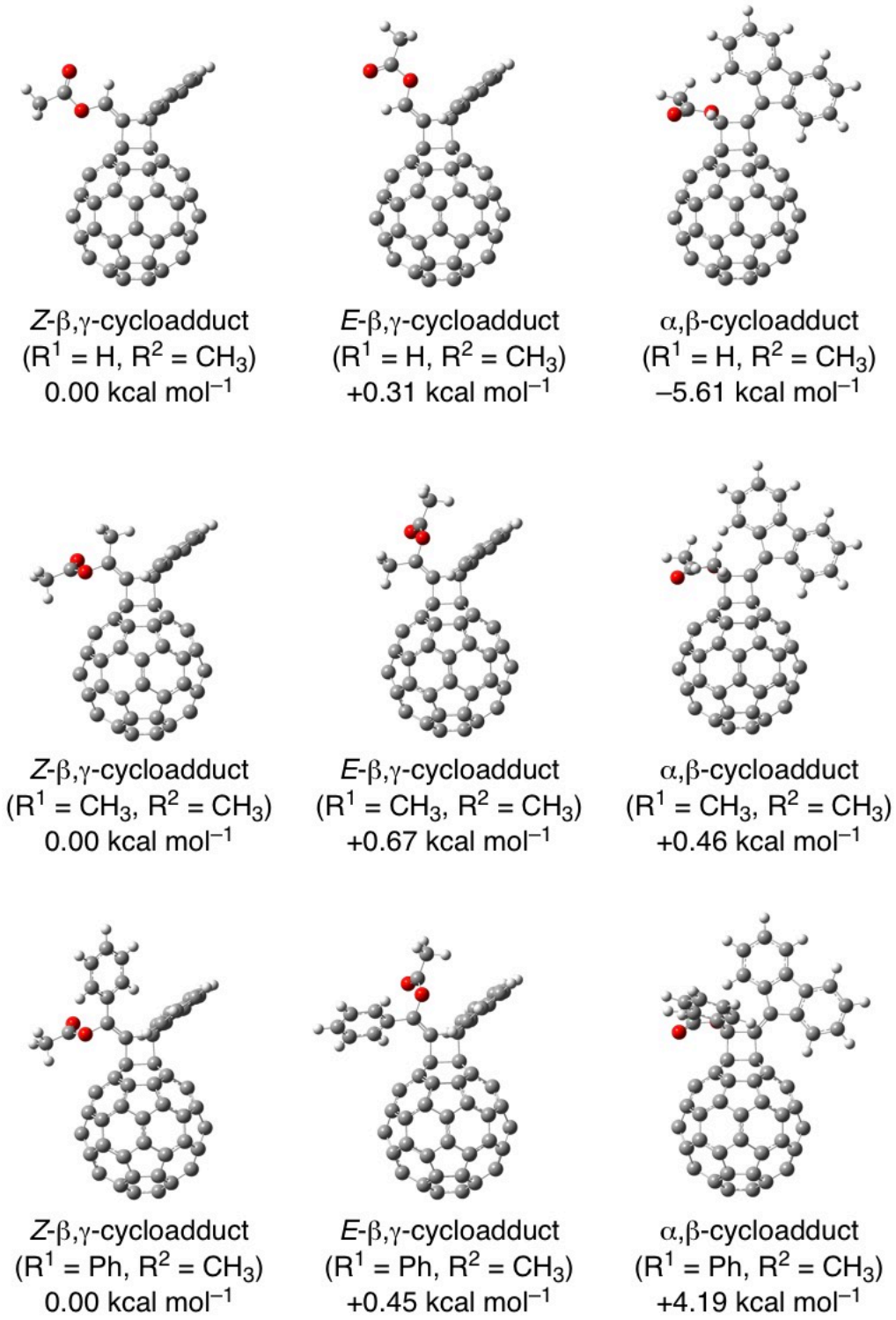

Figure S13. B3LYP/6-31G(d)-optimized structures of possible structural isomers of formal [2+2] cycloadducts. Energies include ZPVE corrections. Calculations were performed using *Gaussian 09* (Rev. D.01).

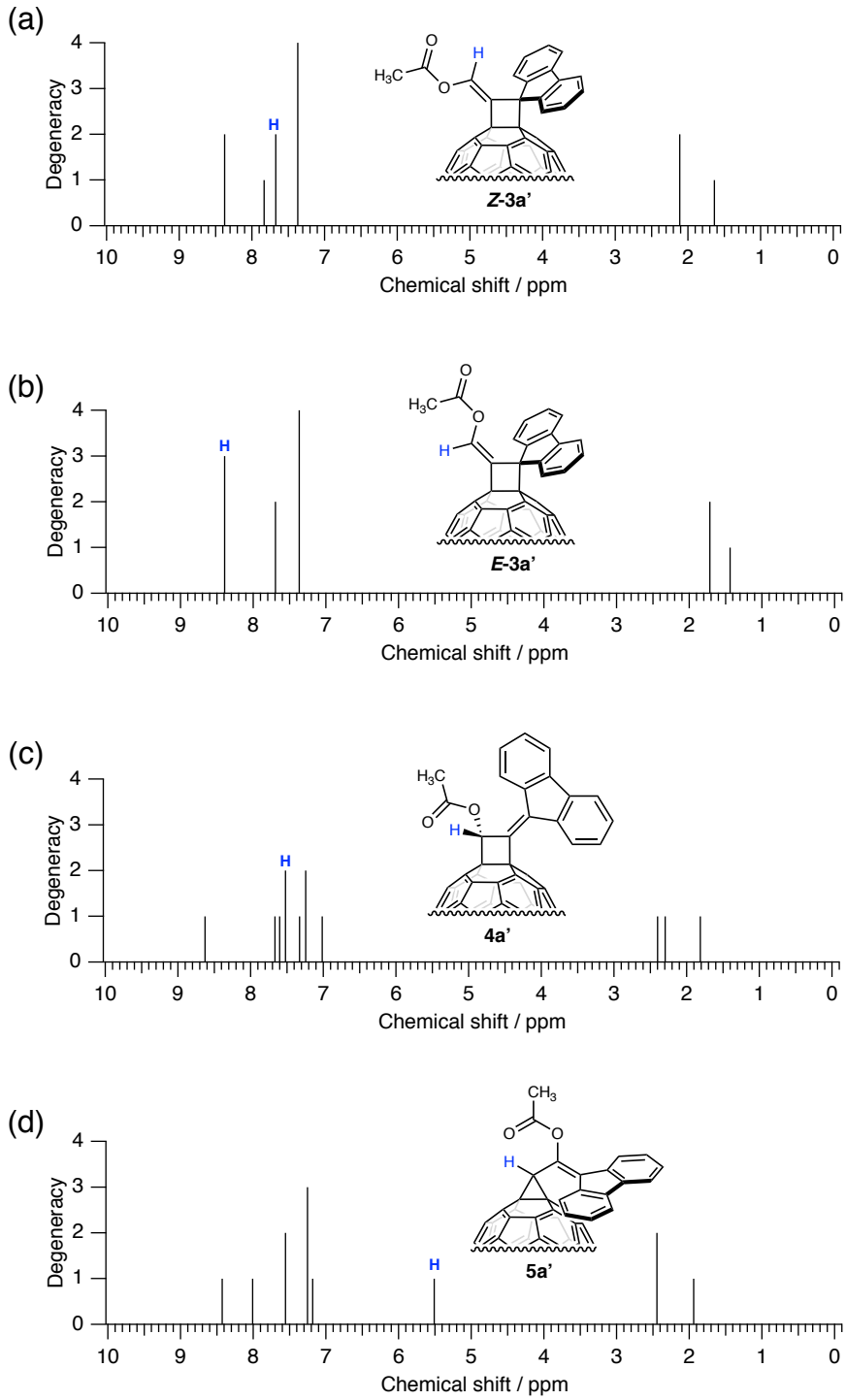

Figure S14. Calculated ^{1}H NMR spectra (degeneracy tolerance = 0.05) of (a, b, c) ***Z*-3a'**, ***Z*-3a'**, and **4a'** where $R^2 = CH_3$, and (d) vinylcarbenoid adduct **5**. Characteristic protons are highlighted in blue and the corresponding signals are marked with blue "H"s. Calculations were performed using *Gaussian 09* (Rev. D.01).

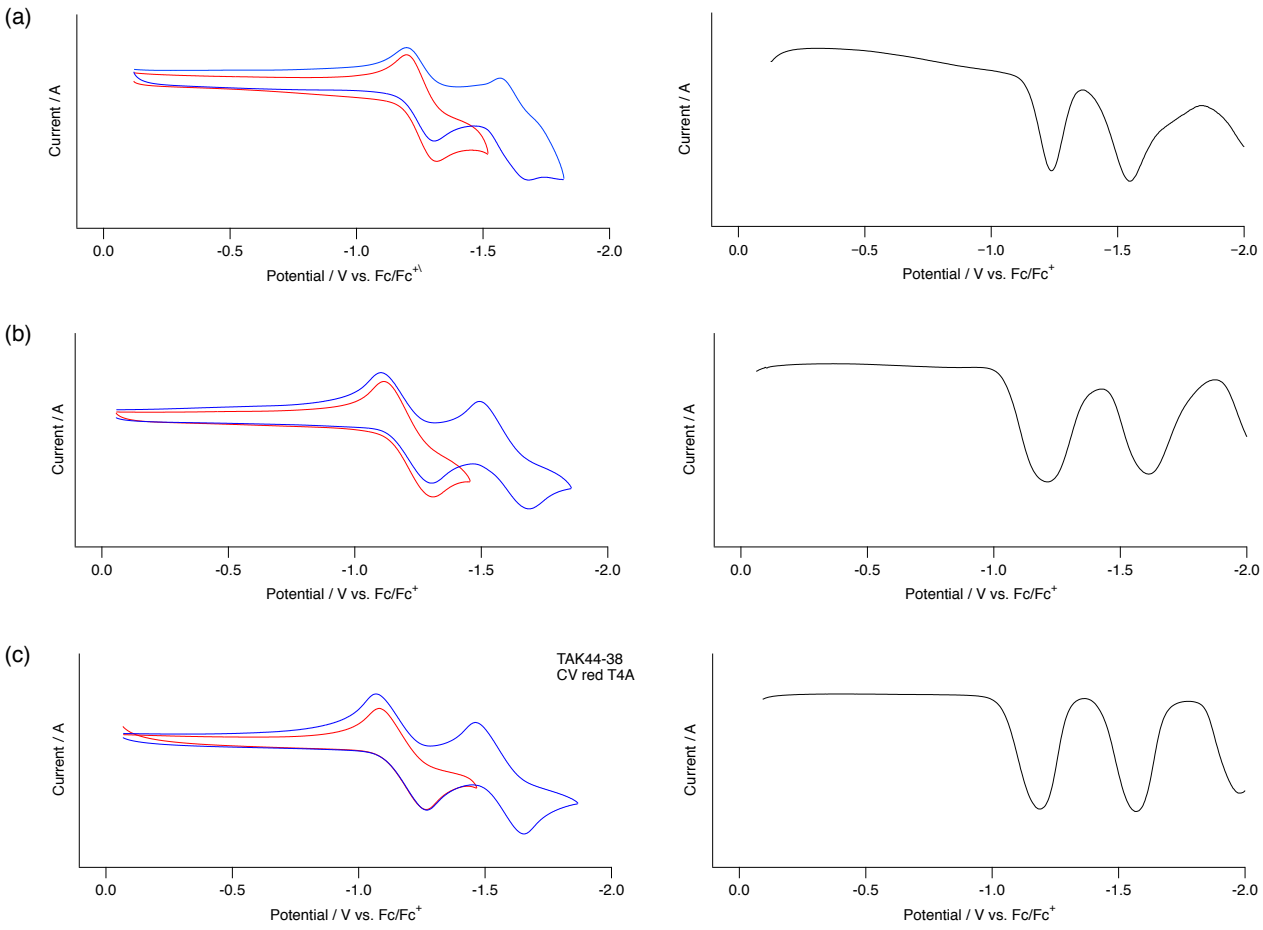

Figure S15. CV and DPV curves of (a) ***E*-3a**, (b) ***Z*-3b**, and (c) ***Z*-3c**.

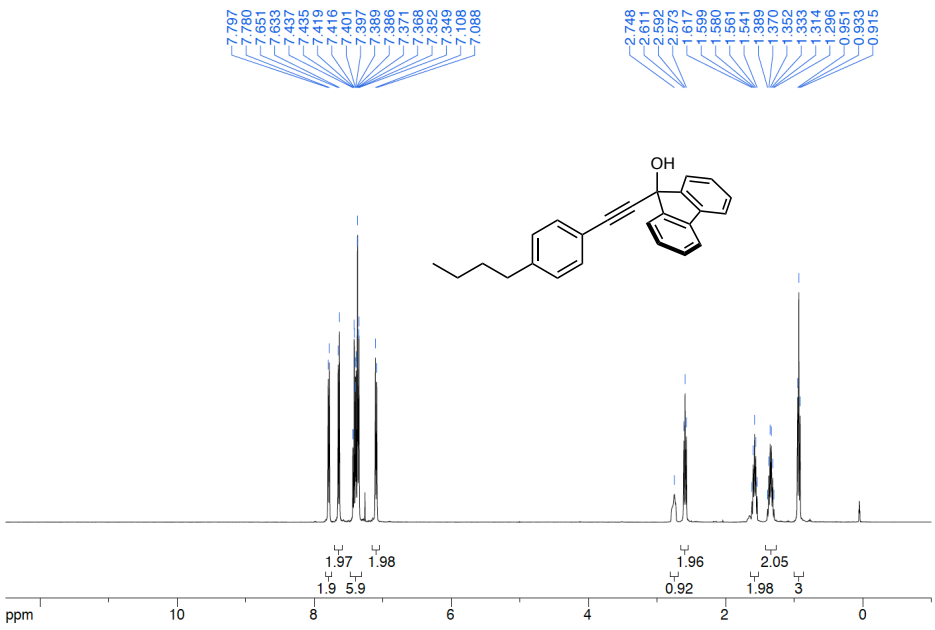

Figure S16. ^{1}H NMR spectrum of **1c** recorded in $CDCl_3$.

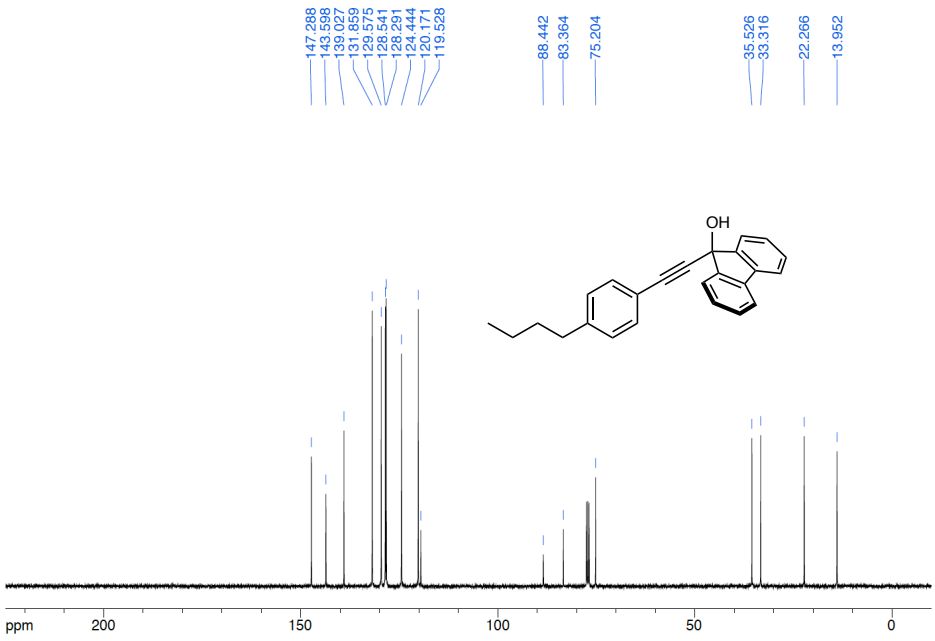

Figure S17. ^{13}C NMR spectrum of **1c** recorded in $CDCl_3$.

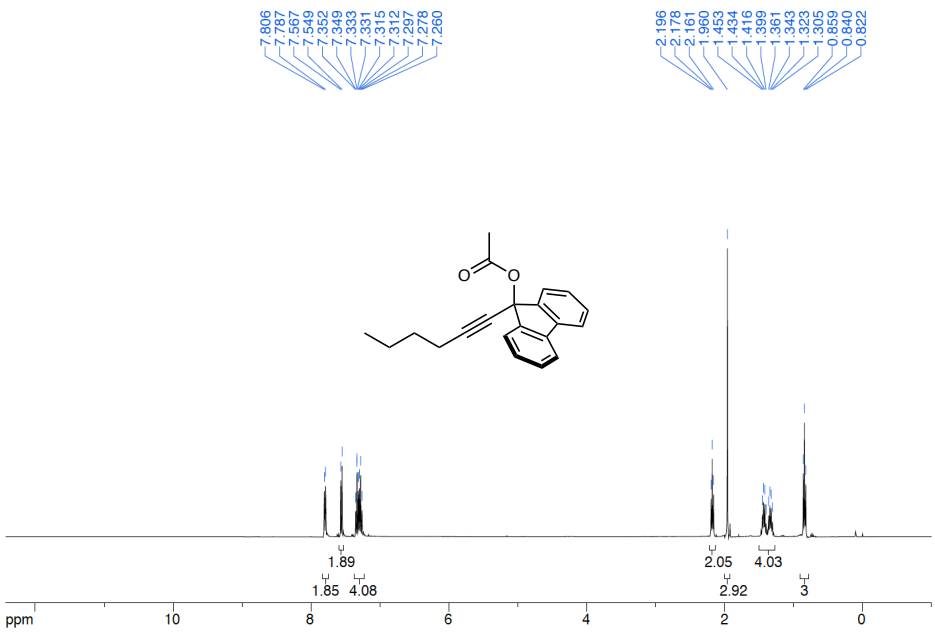

Figure S18. ^{1}H NMR spectrum of **2b** recorded in $CDCl_3$.

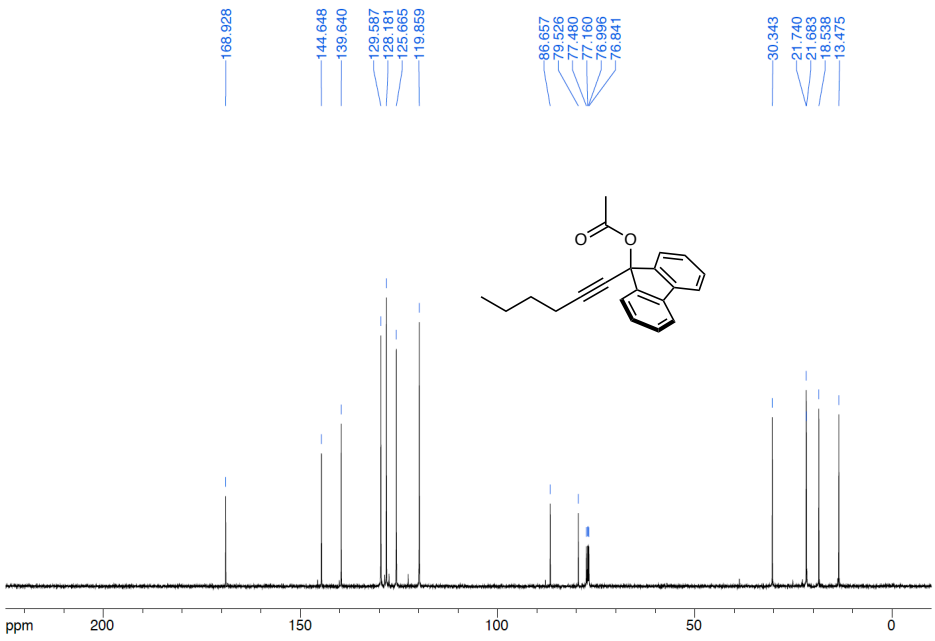

Figure S19. ^{13}C NMR spectrum of **2b** recorded in $CDCl_3$.

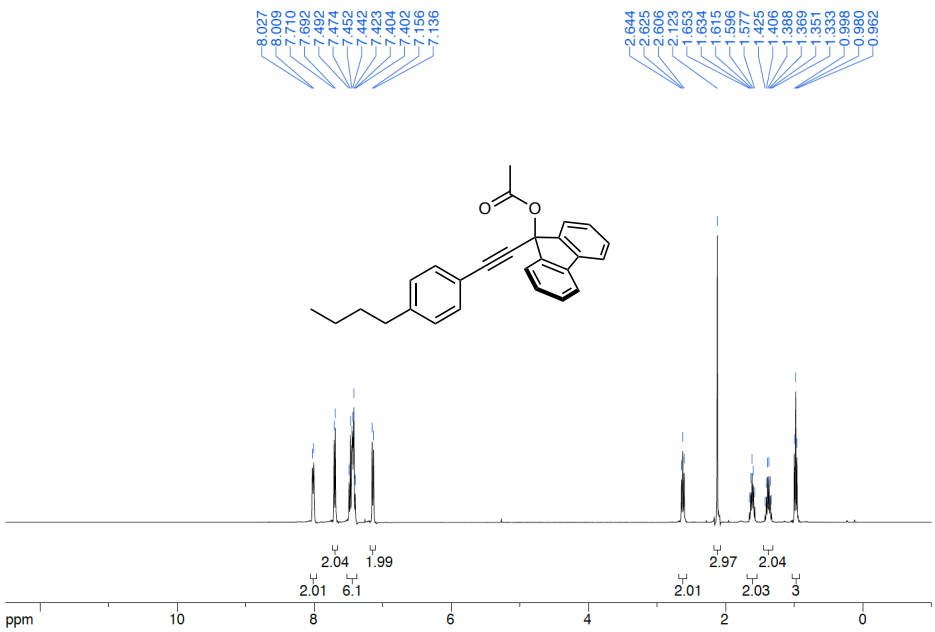

Figure S20. ^{1}H NMR spectrum of **2c** recorded in $CDCl_3$.

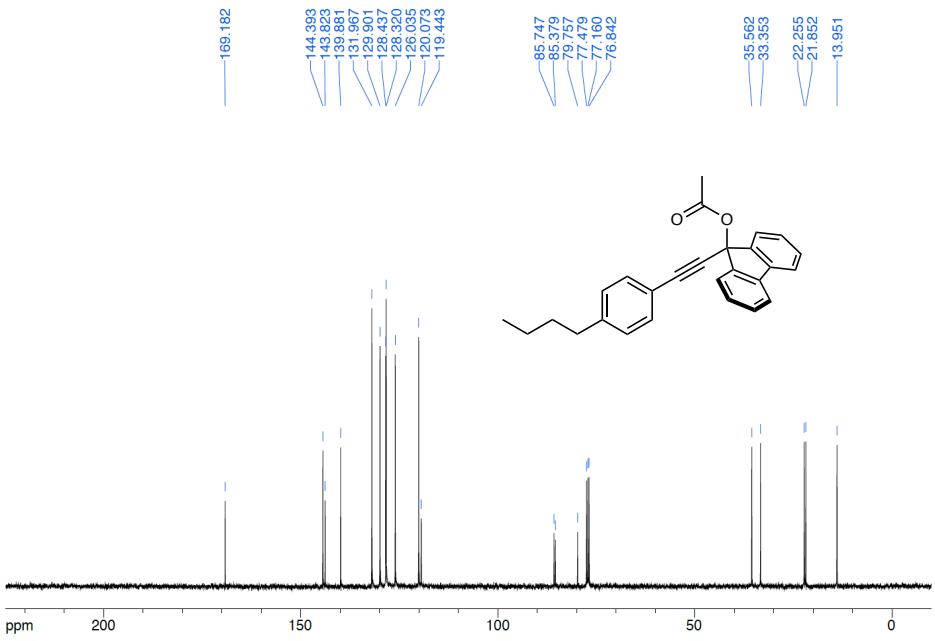

Figure S21. ^{13}C NMR spectrum of **2c** recorded in $CDCl_3$.

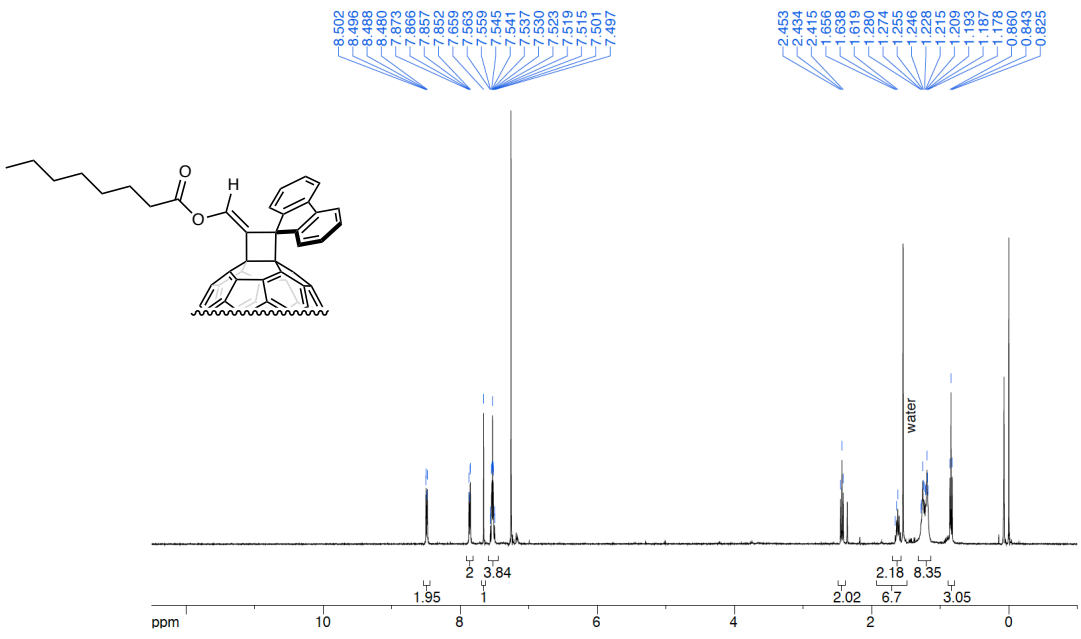

Figure S22. ^{1}H NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

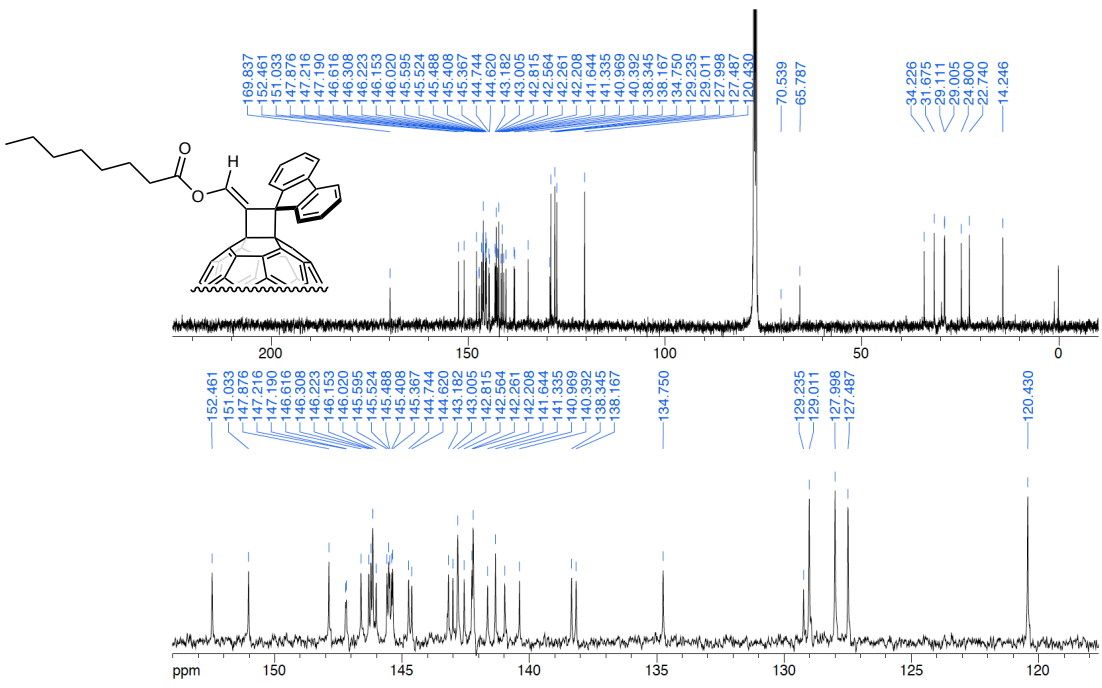

Figure S23. ^{13}C NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

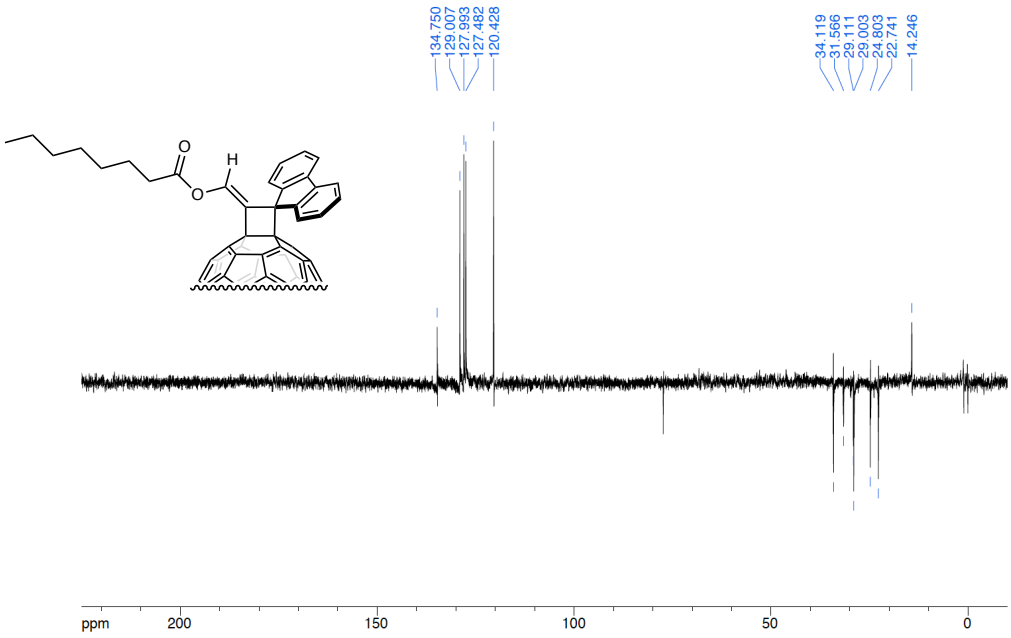

Figure S24. DEPT-135 NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

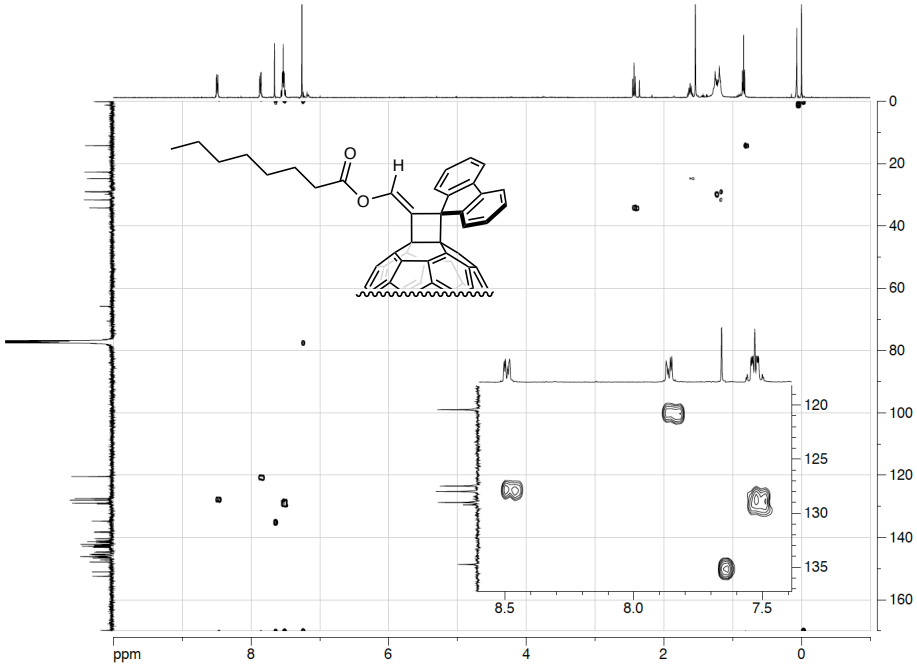

Figure S25. HMQC NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

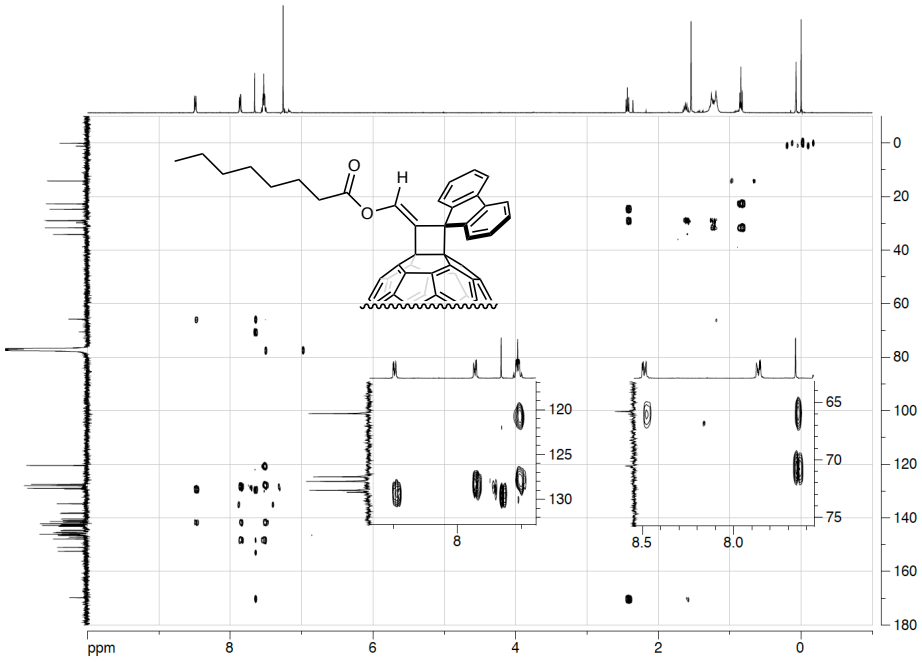

Figure S26. HMBC NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

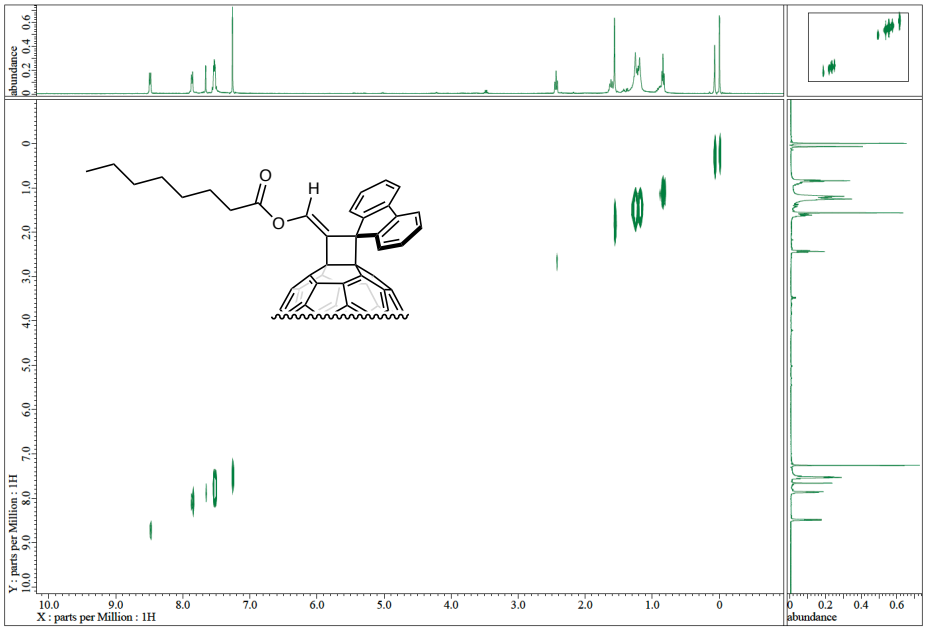

Figure S27. NOESY NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

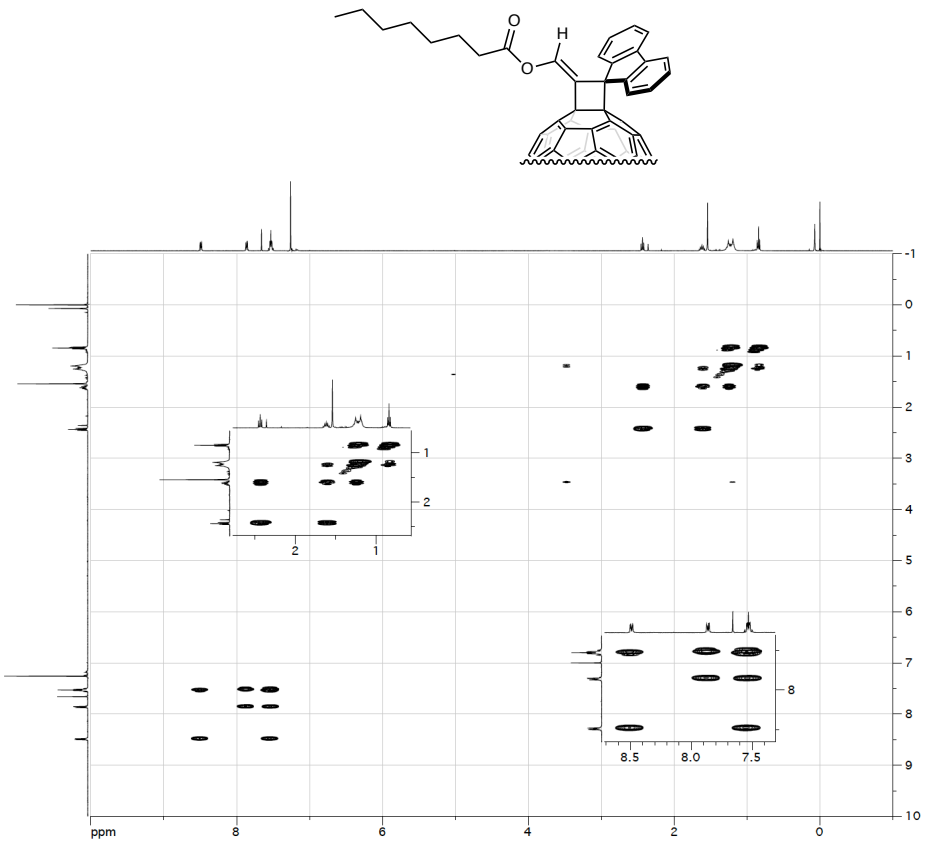

Figure S28. ^{1}H-^{1}H COSY NMR spectrum of ***Z*-3a** recorded in $CDCl_3$.

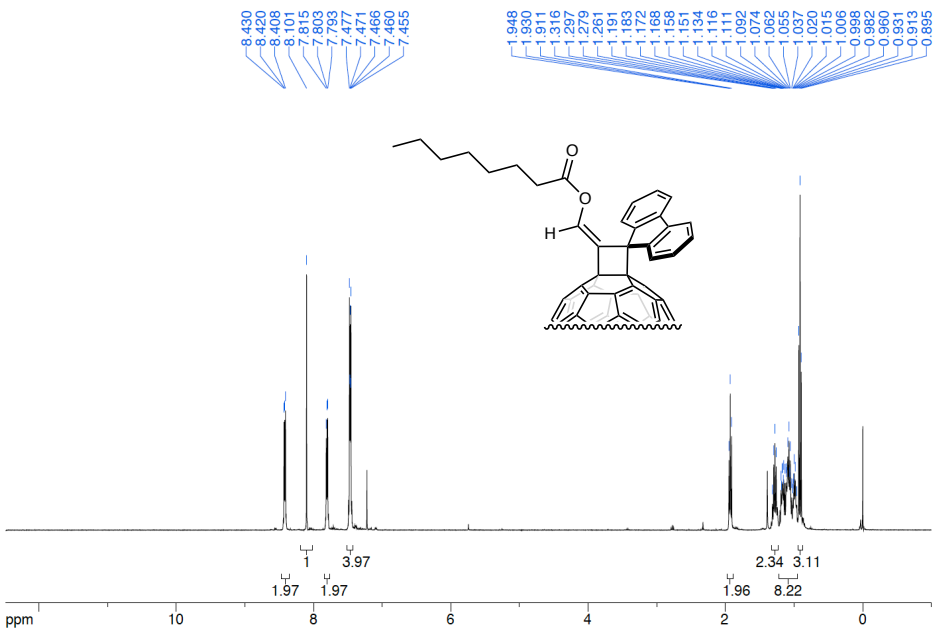

Figure S29. ^{1}H NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

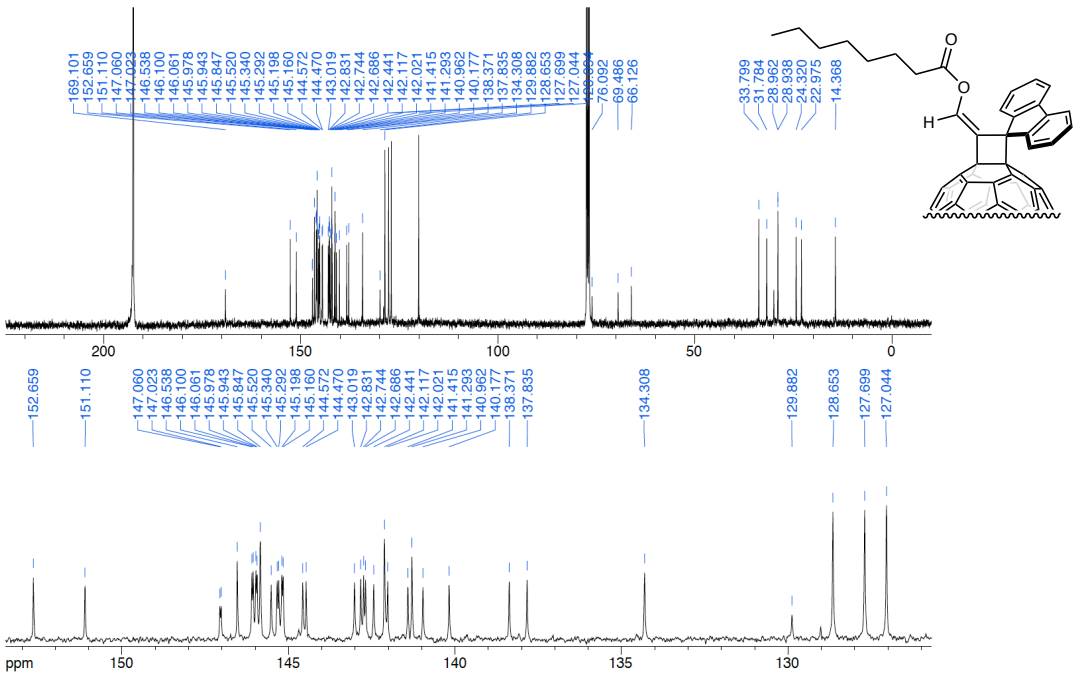

Figure S30. ^{13}C NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

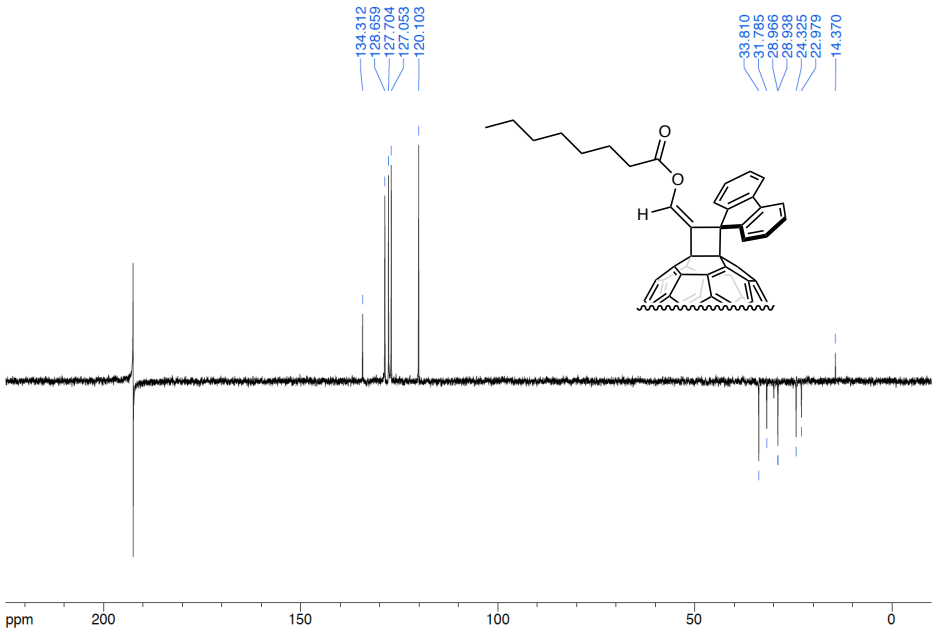

Figure S31. DEPT-135 NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

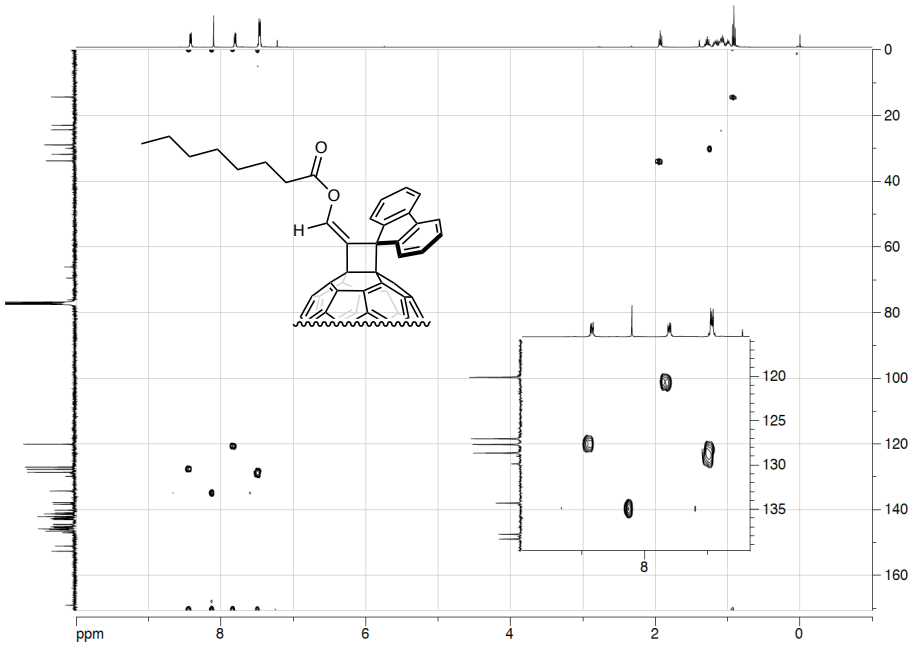

Figure S32. HMQC NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

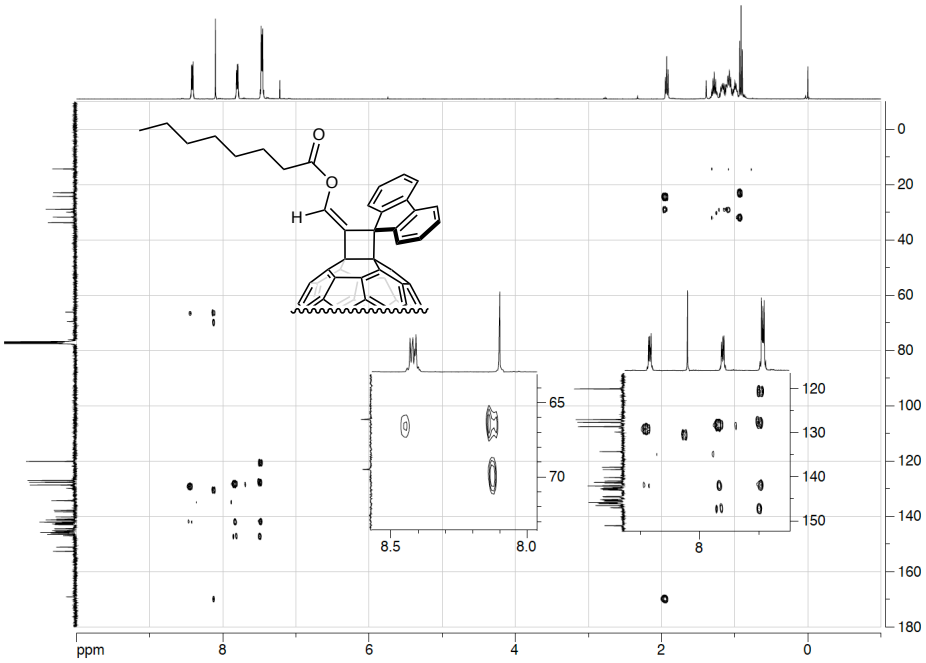

Figure S33. HMBC NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

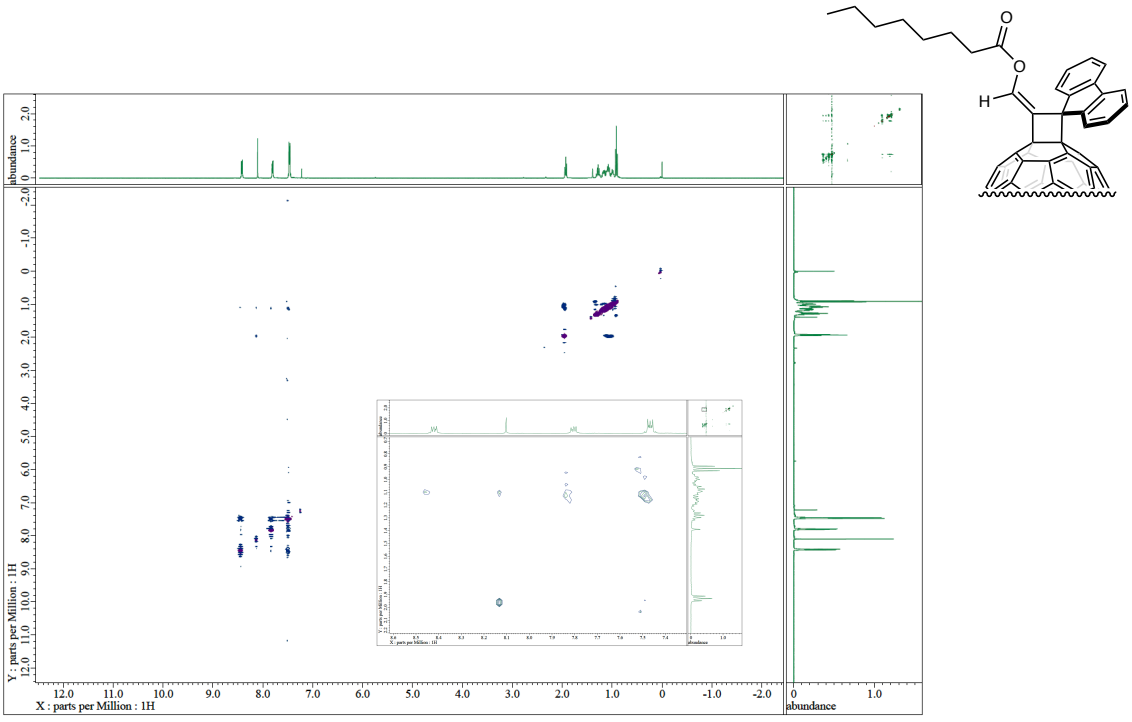

Figure S34. NOESY NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

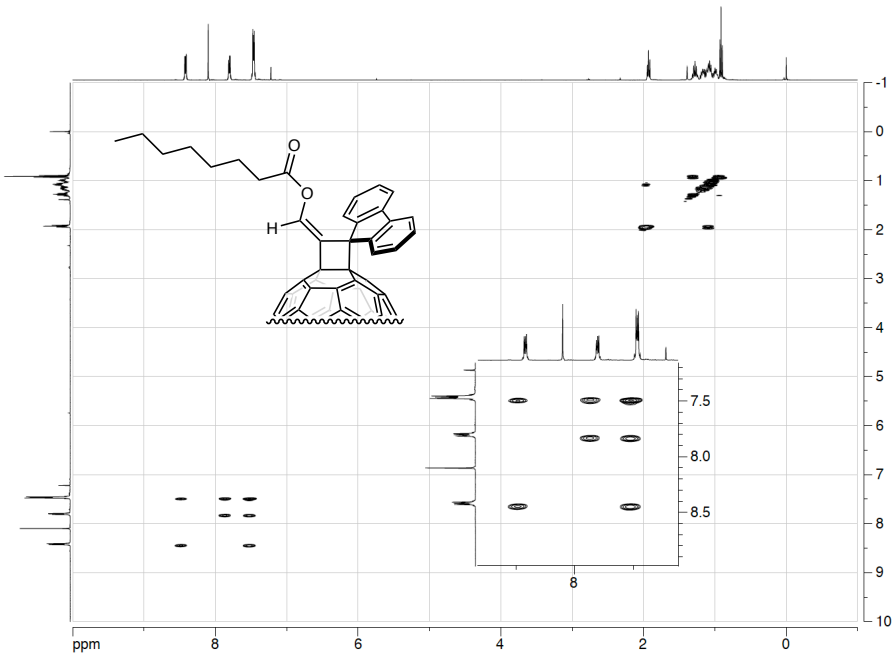

Figure S35. ^{1}H-^{1}H COSY NMR spectrum of ***E*-3a** recorded in $CDCl_3/CS_2$ 1:1.

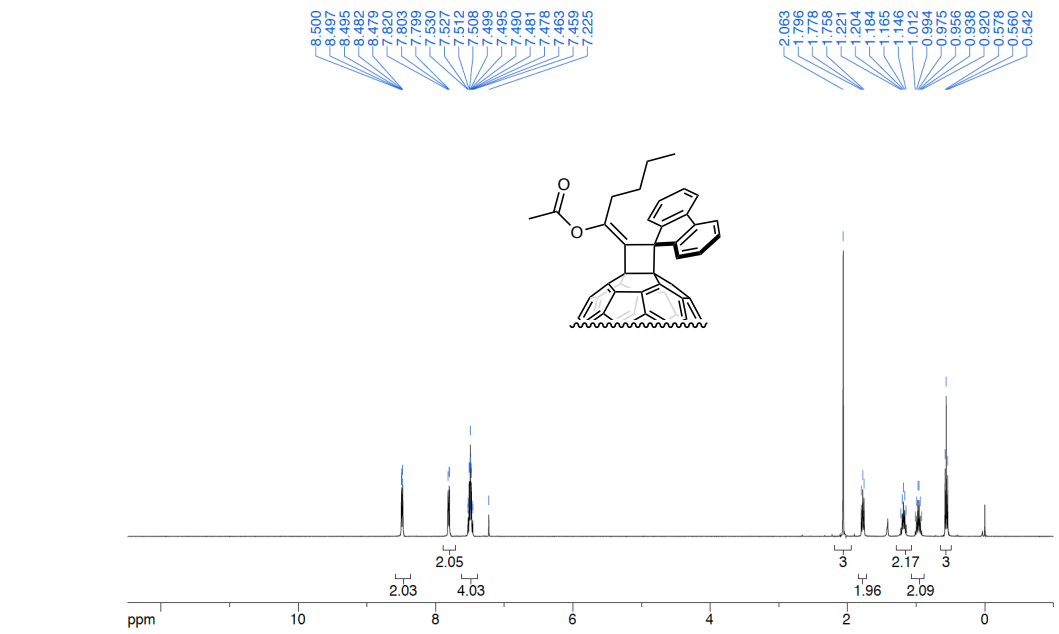

Figure S36. ^{1}H NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

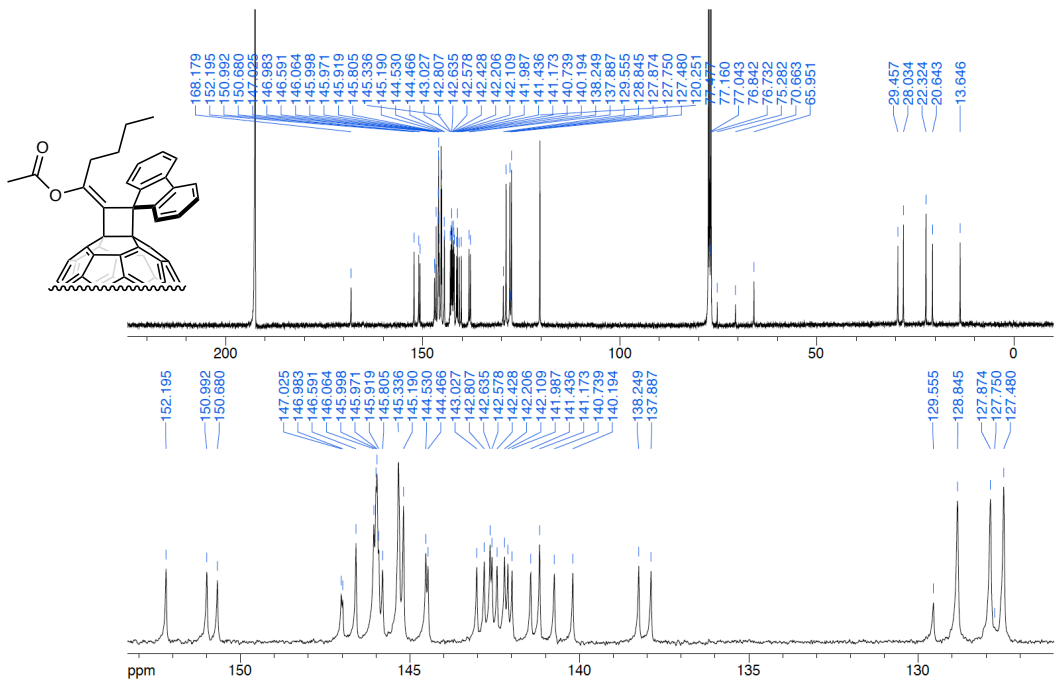

Figure S37. ^{13}C NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

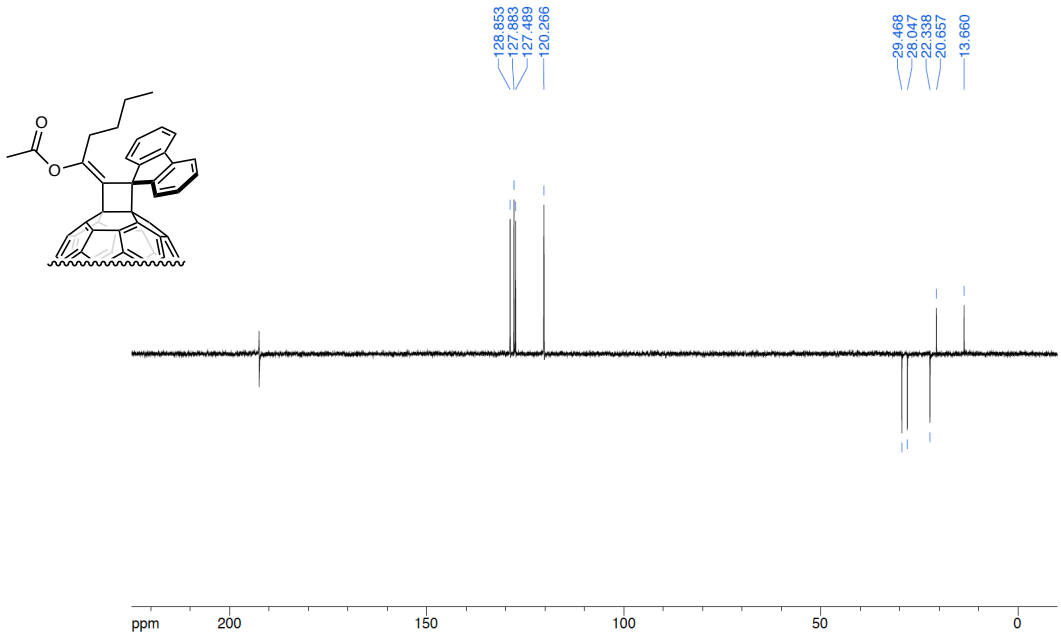

Figure S38. DEPT-135 NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

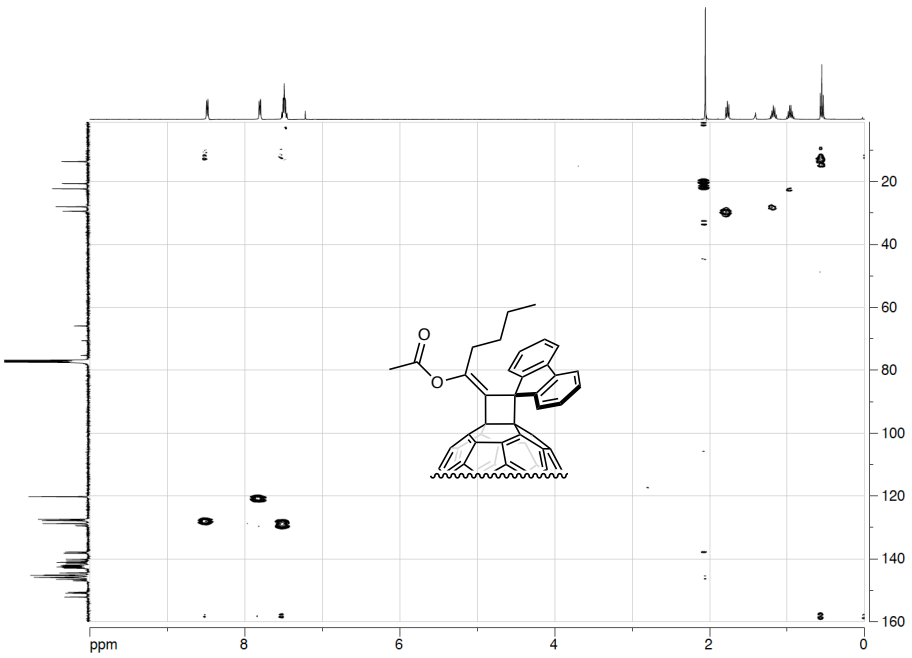

Figure S39. HMQC NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

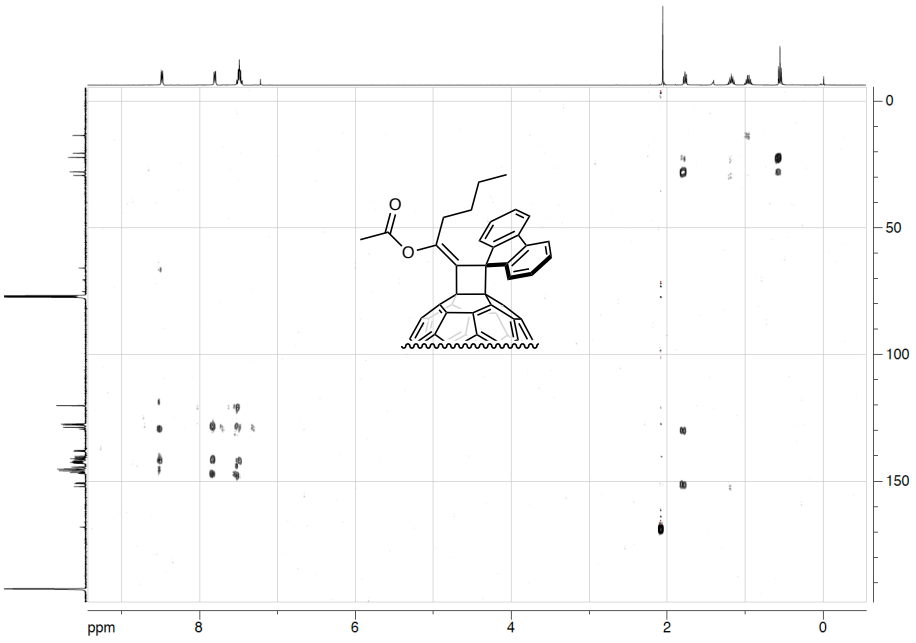

Figure S40. HMBC NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

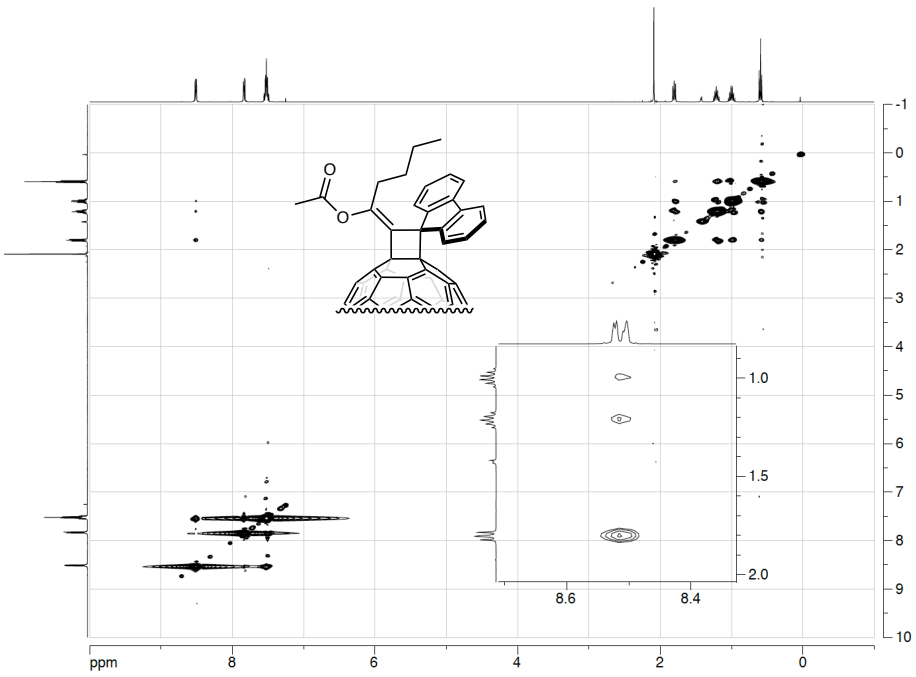

Figure S41. NOESY NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

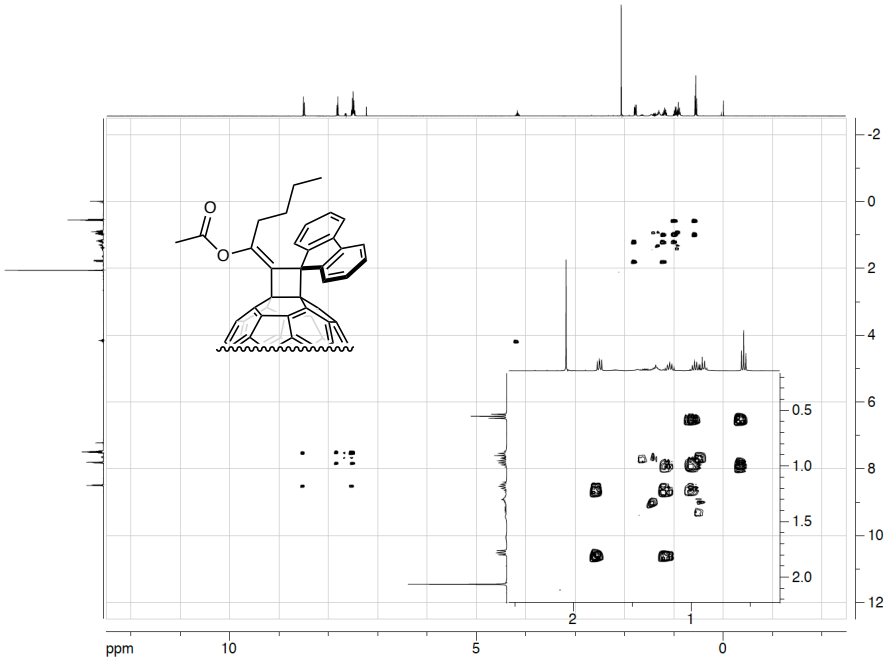

Figure S42. ^{1}H-^{1}H COSY NMR spectrum of ***Z*-3b** recorded in $CDCl_3/CS_2$ 1:1.

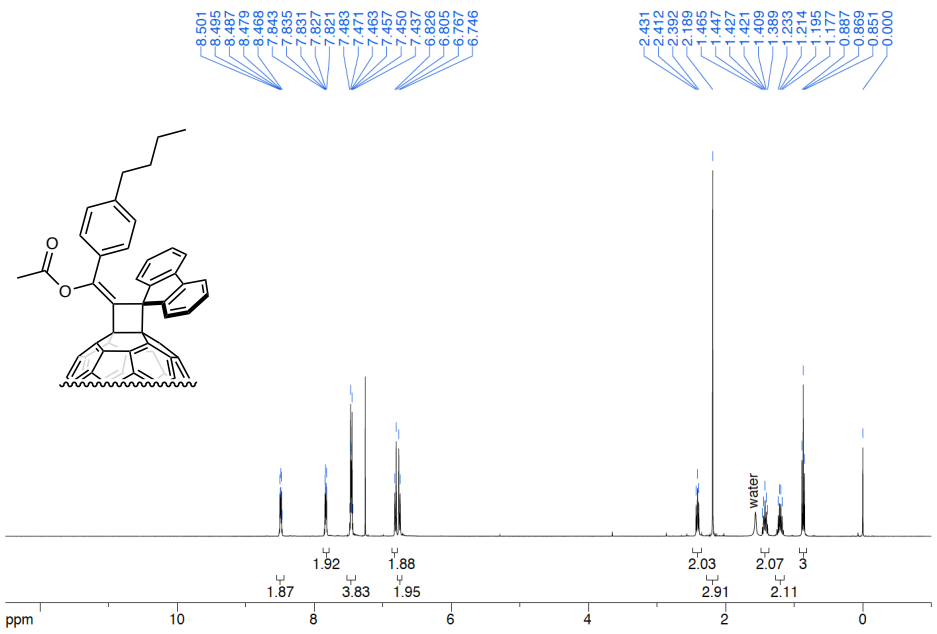

Figure S43. ^{1}H NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

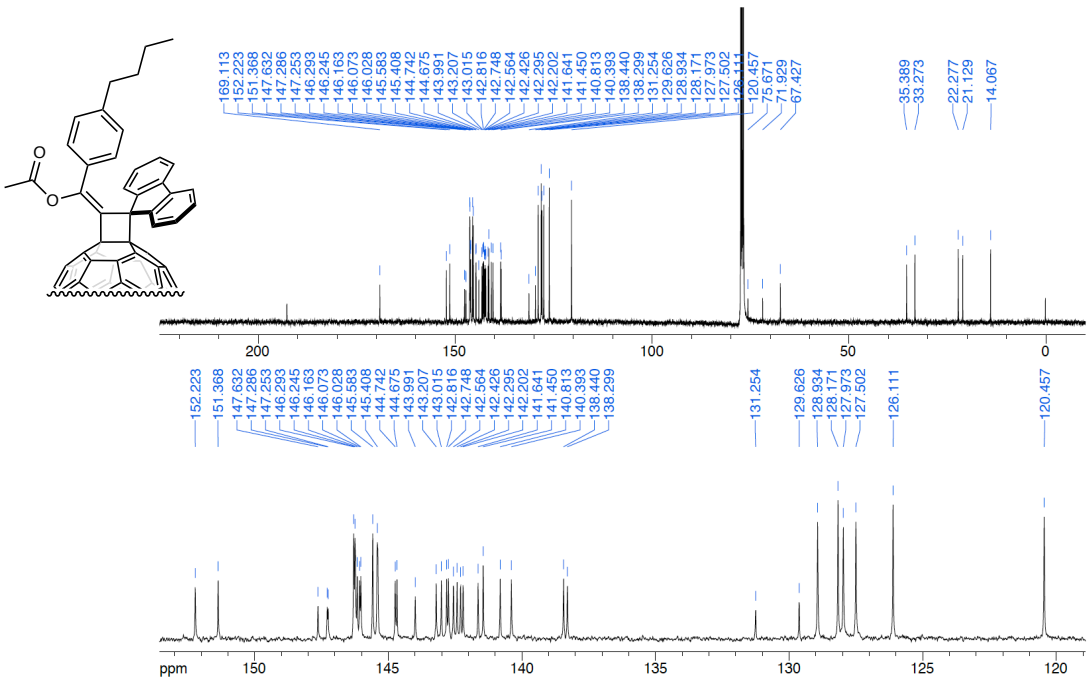

Figure S44. ^{13}C NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

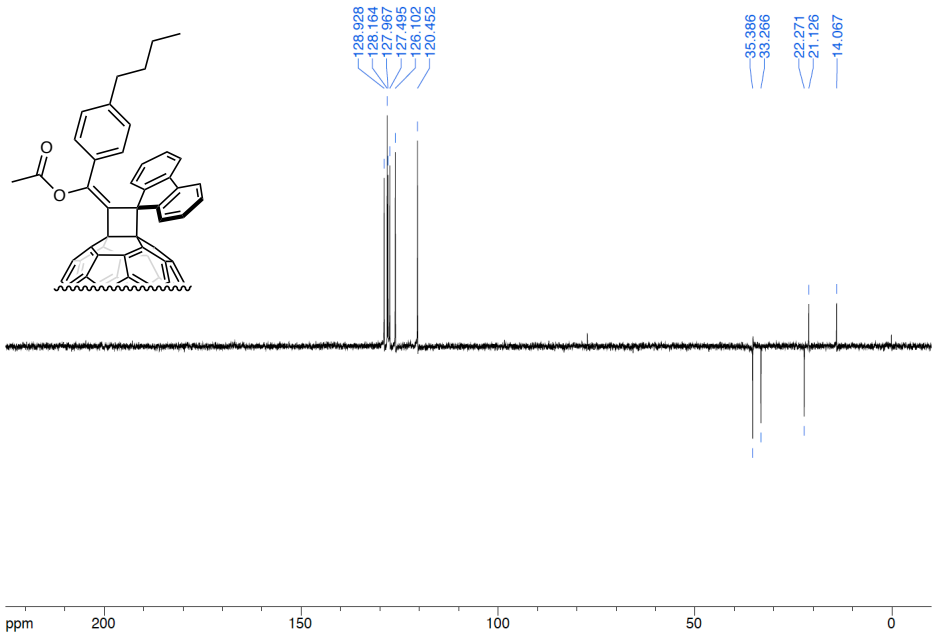

Figure S45. DEPT-135 NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

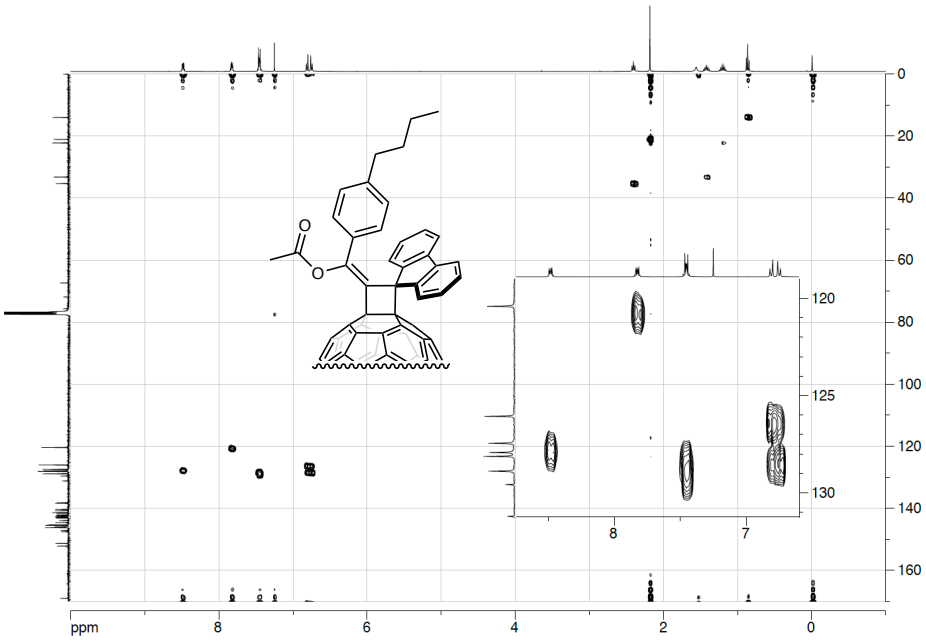

Figure S46. HMQC NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

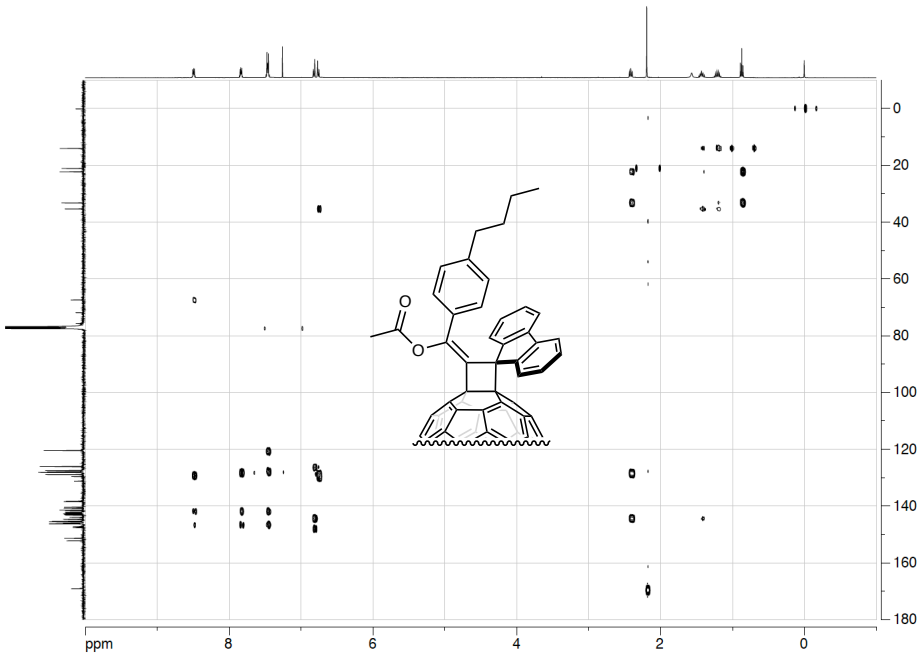

Figure S47. HMBC NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

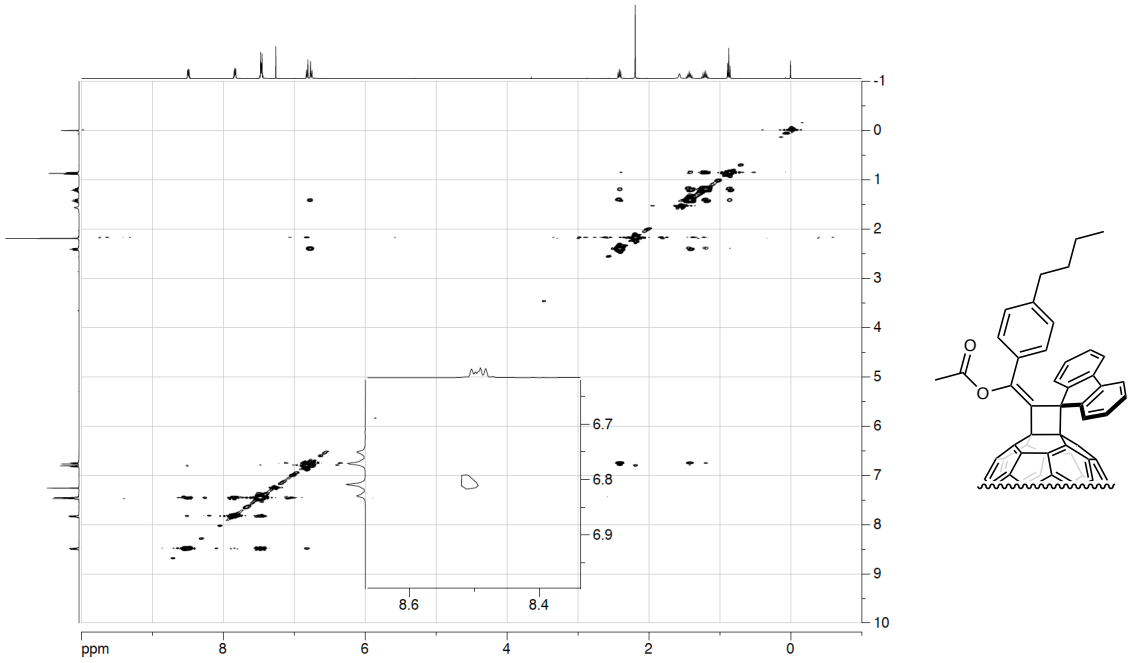

Figure S48. NOESY NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

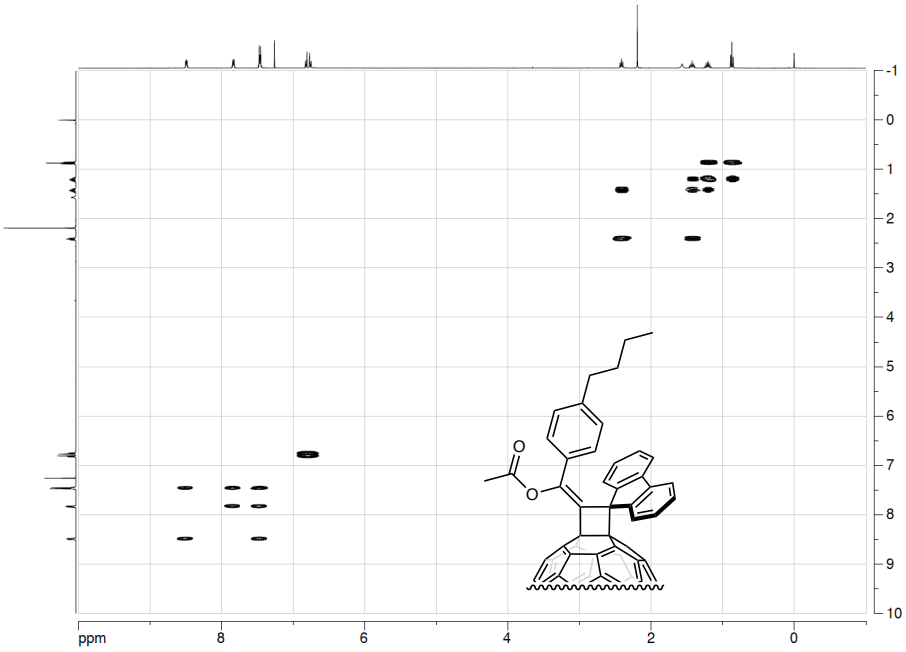

Figure S49. ^{1}H-^{1}H COSY NMR spectrum of ***Z*-3c** recorded in $CDCl_3$.

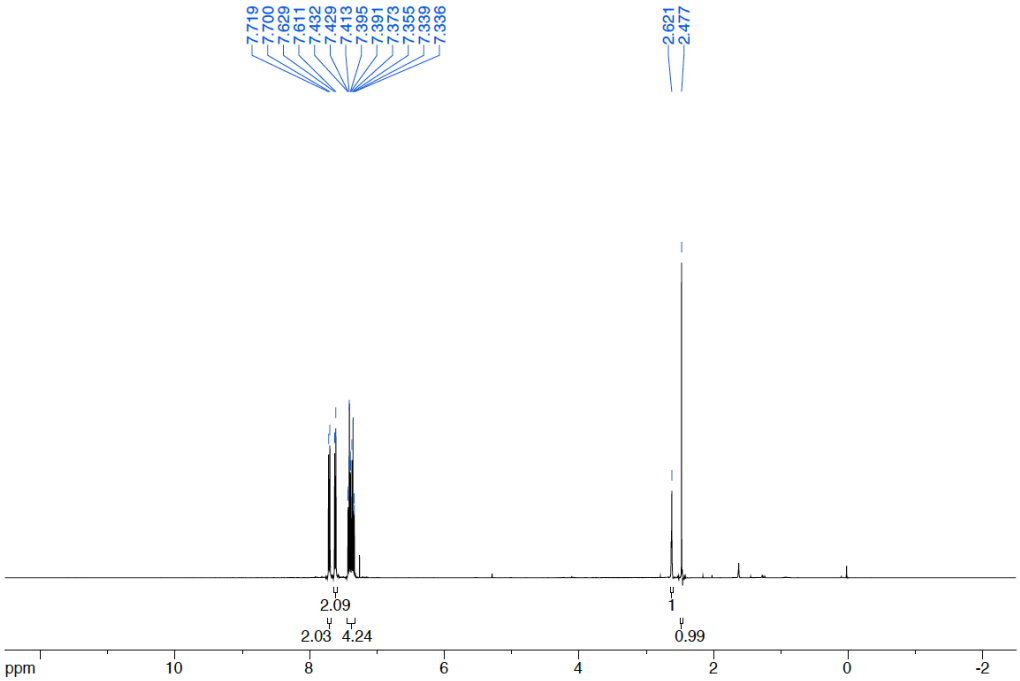

Figure S50. ^{1}H NMR spectrum of **1a** recorded in $CDCl_3$.

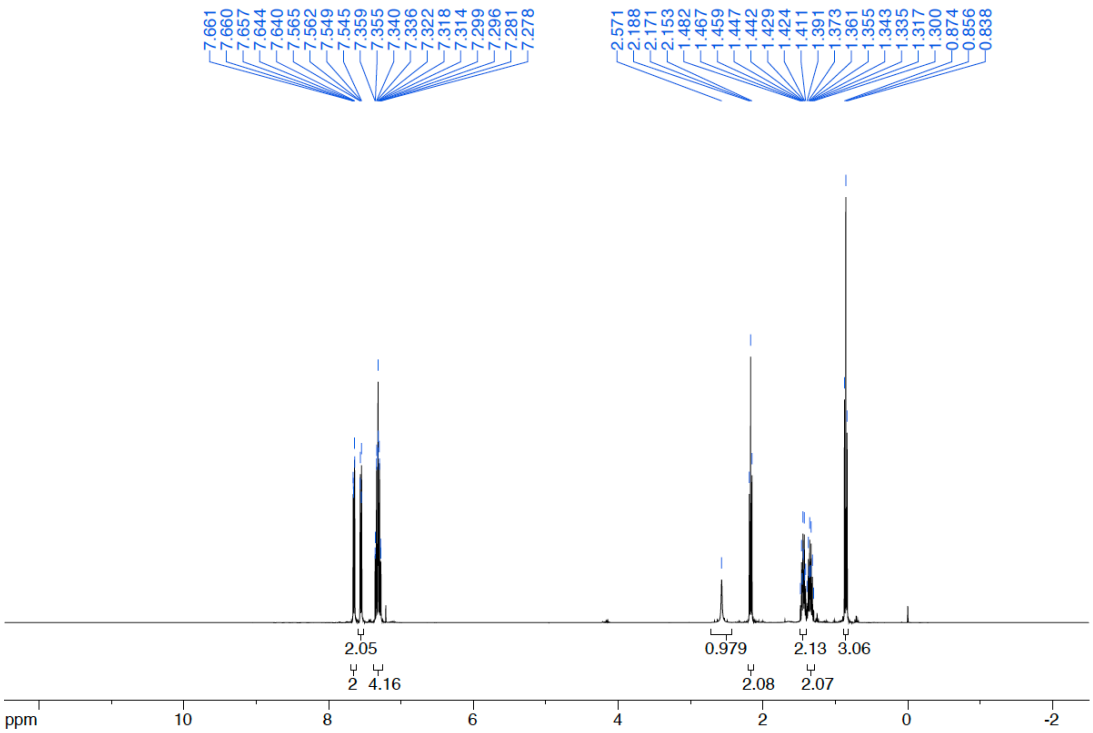

Figure S51. ^{1}H NMR spectrum of **1b** recorded in $CDCl_3$.

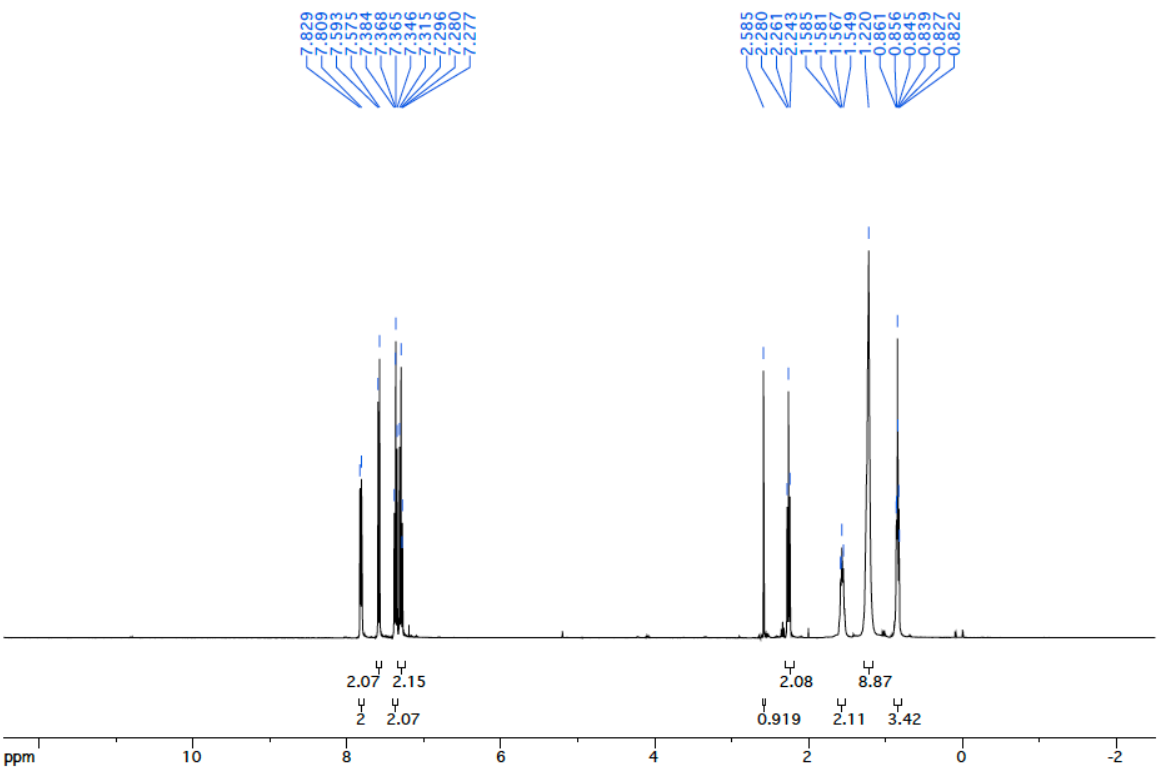

Figure S52. ^{1}H NMR spectrum of **2a** recorded in $CDCl_3$.

Atomic Coordinates of *Z*-β,γ-cycloadduct (R^1 = H)

Zero-point correction= 0.618111 (Hartree/Particle)

Thermal correction to Energy= 0.655483

Thermal correction to Enthalpy= 0.656428

Thermal correction to Gibbs Free Energy= 0.553967

Sum of electronic and zero-point Energies= -3091.028882

Sum of electronic and thermal Energies= -3090.991509

Sum of electronic and thermal Enthalpies= -3090.990565

Sum of electronic and thermal Free Energies= -3091.093025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.550402	2.060271	0.000000
2	6	0	1.056625	1.919250	0.000000
3	6	0	1.644144	1.143049	1.178902
4	6	0	0.895827	0.763969	2.274669
5	6	0	-0.582254	0.888597	2.270132
6	6	0	-1.252012	1.393679	1.174116
7	6	0	-2.454006	0.740777	0.725986
8	6	0	-2.454006	0.740777	-0.725986
9	6	0	-1.252012	1.393679	-1.174116
10	6	0	-0.582254	0.888597	-2.270132
11	6	0	0.895827	0.763969	-2.274669
12	6	0	1.644144	1.143049	-1.178902
13	6	0	2.713136	0.294159	-0.726310
14	6	0	2.713136	0.294159	0.726310
15	6	0	3.060450	-0.868076	1.424635
16	6	0	2.300395	-1.245751	2.591579
17	6	0	1.226979	-0.445190	2.997461
18	6	0	-0.007460	-1.066078	3.442394
19	6	0	-1.116016	-0.243570	2.994311
20	6	0	-2.311882	-0.846844	2.590487

21	6	0	-2.996144	-0.343700	1.423932
22	6	0	-3.547952	-1.476067	0.696967
23	6	0	-3.547952	-1.476067	-0.696967
24	6	0	-2.996144	-0.343700	-1.423932
25	6	0	-2.311882	-0.846844	-2.590487
26	6	0	-1.116016	-0.243570	-2.994311
27	6	0	-0.007460	-1.066078	-3.442394
28	6	0	1.226979	-0.445190	-2.997461
29	6	0	2.300395	-1.245751	-2.591579
30	6	0	3.060450	-0.868076	-1.424635
31	6	0	3.409263	-2.077880	-0.697097
32	6	0	3.409263	-2.077880	0.697097
33	6	0	2.858682	-3.208116	1.424883
34	6	0	2.172305	-2.691933	2.598507
35	6	0	0.982476	-3.285131	3.025669
36	6	0	-0.127608	-2.455125	3.465504
37	6	0	-1.363748	-3.082449	3.025369
38	6	0	-2.433507	-2.293251	2.597629
39	6	0	-3.199207	-2.683857	1.424831
40	6	0	-2.862627	-3.845763	0.727097
41	6	0	-2.862627	-3.845763	-0.727097
42	6	0	-3.199207	-2.683857	-1.424831
43	6	0	-2.433507	-2.293251	-2.597629
44	6	0	-1.363748	-3.082449	-3.025369
45	6	0	-0.127608	-2.455125	-3.465504
46	6	0	0.982476	-3.285131	-3.025669
47	6	0	2.172305	-2.691933	-2.598507
48	6	0	2.858682	-3.208116	-1.424883
49	6	0	2.326578	-4.294239	-0.726990
50	6	0	2.326578	-4.294239	0.726990
51	6	0	1.090999	-4.911322	1.175570
52	6	0	0.433324	-4.416014	2.303474
53	6	0	-1.017190	-4.290615	2.303204

54	6	0	-1.750446	-4.665028	1.175197
55	6	0	-1.063569	-5.173650	0.000000
56	6	0	0.327001	-5.294252	0.000000
57	6	0	1.090999	-4.911322	-1.175570
58	6	0	0.433324	-4.416014	-2.303474
59	6	0	-1.017190	-4.290615	-2.303204
60	6	0	-1.750446	-4.665028	-1.175197
61	6	0	1.131715	3.438655	0.000000
62	6	0	2.157165	4.285007	0.000000
63	1	0	2.069416	5.365588	0.000000
64	8	0	3.447144	3.792333	0.000000
65	6	0	4.482082	4.701186	0.000000
66	6	0	5.801647	3.975922	0.000000
67	1	0	5.875979	3.331337	0.881970
68	1	0	5.875979	3.331337	-0.881970
69	1	0	6.613912	4.703052	0.000000
70	8	0	4.316547	5.895388	0.000000
71	6	0	-0.371288	3.681481	0.000000
72	6	0	-0.990194	4.416990	-1.183789
73	6	0	-0.990194	4.416990	1.183789
74	6	0	-0.708173	4.301591	-2.540648
75	6	0	-1.962774	5.332386	-0.734367
76	6	0	-0.708173	4.301591	2.540648
77	6	0	-1.962774	5.332386	0.734367
78	6	0	-1.430716	5.079280	-3.452976
79	1	0	0.067466	3.629465	-2.894274
80	6	0	-2.686580	6.102318	-1.644971
81	6	0	-1.430716	5.079280	3.452976
82	1	0	0.067466	3.629465	2.894274
83	6	0	-2.686580	6.102318	1.644971
84	6	0	-2.418416	5.963618	-3.009027
85	1	0	-1.217617	4.996661	-4.515130
86	1	0	-3.436897	6.810082	-1.302261

87	6	0	-2.418416	5.963618	3.009027
88	1	0	-1.217617	4.996661	4.515130
89	1	0	-3.436897	6.810082	1.302261
90	1	0	-2.972159	6.559174	-3.729810
91	1	0	-2.972159	6.559174	3.729810

Atomic Coordinates of *Z*-β,γ-cycloadduct ($R^1 = CH_3$)

Zero-point correction= 0.645994 (Hartree/Particle)

Thermal correction to Energy= 0.685038

Thermal correction to Enthalpy= 0.685982

Thermal correction to Gibbs Free Energy= 0.580501

Sum of electronic and zero-point Energies= -3130.319898

Sum of electronic and thermal Energies= -3130.280854

Sum of electronic and thermal Enthalpies= -3130.279910

Sum of electronic and thermal Free Energies= -3130.385391

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.026228	-0.551326	0.009726
2	6	0	-1.862838	1.004285	-0.382293
3	6	0	-1.112973	1.858233	0.640058
4	6	0	-0.780191	1.403504	1.899310
5	6	0	-0.928365	-0.028107	2.256999
6	6	0	-1.407973	-0.944762	1.343186
7	6	0	-0.760140	-2.225067	1.229236
8	6	0	-0.714204	-2.585093	-0.176788
9	6	0	-1.333828	-1.526934	-0.930550
10	6	0	-0.785273	-1.153841	-2.140886
11	6	0	-0.637900	0.276074	-2.506240
12	6	0	-1.041095	1.274819	-1.643503
13	6	0	-0.189268	2.416037	-1.440934
14	6	0	-0.234120	2.776181	-0.033726
15	6	0	0.911049	3.277872	0.596151
16	6	0	1.239827	2.828800	1.927333
17	6	0	0.410231	1.895175	2.558524
18	6	0	0.997504	0.805298	3.316657
19	6	0	0.172172	-0.374015	3.128871
20	6	0	0.769965	-1.636631	3.053527

21	6	0	0.293393	-2.584859	2.076360
22	6	0	1.439309	-3.308220	1.548056
23	6	0	1.483263	-3.653484	0.198341
24	6	0	0.383251	-3.290711	-0.681145
25	6	0	0.933113	-2.921046	-1.962574
26	6	0	0.360970	-1.858601	-2.670812
27	6	0	1.214594	-0.901614	-3.350326
28	6	0	0.599017	0.408930	-3.246182
29	6	0	1.402948	1.543447	-3.091380
30	6	0	1.000105	2.571012	-2.162097
31	6	0	2.191696	3.081083	-1.502852
32	6	0	2.148246	3.426958	-0.153016
33	6	0	3.246194	3.065889	0.726887
34	6	0	2.682901	2.695848	2.015214
35	6	0	3.244095	1.644871	2.743794
36	6	0	2.383135	0.684563	3.415742
37	6	0	3.004733	-0.626544	3.317188
38	6	0	2.213109	-1.763192	3.140332
39	6	0	2.628885	-2.798199	2.207571
40	6	0	3.817434	-2.653512	1.489047
41	6	0	3.863151	-3.013907	0.080929
42	6	0	2.718698	-3.504507	-0.550950
43	6	0	2.377004	-3.051240	-1.889665
44	6	0	3.195886	-2.126904	-2.541891
45	6	0	2.601811	-1.033924	-3.295640
46	6	0	3.434832	0.144661	-3.115831
47	6	0	2.846188	1.407095	-3.016321
48	6	0	3.335703	2.359258	-2.032613
49	6	0	4.391295	2.009752	-1.188040
50	6	0	4.345583	2.370494	0.219979
51	6	0	4.929199	1.280115	0.981222
52	6	0	4.388610	0.925769	2.219299
53	6	0	4.240416	-0.478463	2.573741

54	6	0	4.639778	-1.471239	1.676365
55	6	0	5.194654	-1.100465	0.385445
56	6	0	5.336742	0.245738	0.045386
57	6	0	5.003227	0.697079	-1.295203
58	6	0	4.533620	-0.216413	-2.241622
59	6	0	4.385860	-1.620660	-1.886720
60	6	0	4.713422	-2.053660	-0.600129
61	6	0	-3.382186	1.088384	-0.445634
62	6	0	-4.196313	2.112788	-0.696718
63	8	0	-3.594233	3.332237	-1.053196
64	6	0	-3.710329	4.391409	-0.187281
65	6	0	-3.032084	5.608008	-0.764875
66	1	0	-1.958300	5.417087	-0.865017
67	1	0	-3.421807	5.823766	-1.764454
68	1	0	-3.194272	6.460129	-0.104250
69	8	0	-4.267224	4.323122	0.880744
70	6	0	-3.643060	-0.369277	-0.089606
71	6	0	-4.344556	-1.267495	-1.102693
72	6	0	-4.417615	-0.674499	1.187803
73	6	0	-4.190554	-1.332136	-2.483532
74	6	0	-5.268331	-2.108604	-0.449303
75	6	0	-4.351512	-0.051248	2.429341
76	6	0	-5.312582	-1.741469	0.972298
77	6	0	-4.939292	-2.267549	-3.207494
78	1	0	-3.509763	-0.662870	-3.000560
79	6	0	-6.008226	-3.045348	-1.171377
80	6	0	-5.155933	-0.528873	3.470528
81	1	0	-3.703660	0.804848	2.590045
82	6	0	-6.107920	-2.221440	2.013225
83	6	0	-5.831829	-3.123373	-2.555062
84	1	0	-4.826879	-2.325103	-4.286611
85	1	0	-6.721903	-3.695190	-0.671589
86	6	0	-6.016544	-1.612029	3.267078

87	1	0	-5.113794	-0.048061	4.443837
88	1	0	-6.799269	-3.044421	1.851387
89	1	0	-6.403848	-3.846117	-3.130659
90	1	0	-6.632285	-1.972311	4.086795
91	6	0	-5.690989	2.085838	-0.732664
92	1	0	-6.102349	2.726271	0.054292
93	1	0	-6.050728	2.460860	-1.698785
94	1	0	-6.064893	1.069505	-0.592297

Atomic Coordinates of *Z*-β,γ-cycloadduct (R^1 = Ph)

Zero-point correction= 0.698670 (Hartree/Particle)

Thermal correction to Energy= 0.740882

Thermal correction to Enthalpy= 0.741827

Thermal correction to Gibbs Free Energy= 0.628277

Sum of electronic and zero-point Energies= -3321.999745

Sum of electronic and thermal Energies= -3321.957533

Sum of electronic and thermal Enthalpies= -3321.956589

Sum of electronic and thermal Free Energies= -3322.070138

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.514795	-0.852719	0.020429
2	6	0	-1.532698	0.756775	0.064618
3	6	0	-0.793059	1.379256	1.252798
4	6	0	-0.317094	0.636600	2.314957
5	6	0	-0.300359	-0.845449	2.266036
6	6	0	-0.758636	-1.524088	1.155968
7	6	0	-0.007917	-2.645867	0.658335
8	6	0	-0.039149	-2.601554	-0.792524
9	6	0	-0.812290	-1.453602	-1.189745
10	6	0	-0.394764	-0.707247	-2.273284
11	6	0	-0.408232	0.775223	-2.232071
12	6	0	-0.828979	1.447410	-1.104101
13	6	0	-0.076328	2.577074	-0.632700
14	6	0	-0.051067	2.534454	0.819278
15	6	0	1.088207	2.968656	1.507454
16	6	0	1.559171	2.213681	2.643105
17	6	0	0.870813	1.057832	3.026608
18	6	0	1.614427	-0.125036	3.421310
19	6	0	0.891052	-1.292244	2.952519
20	6	0	1.595801	-2.412696	2.499216

21	6	0	1.135692	-3.105147	1.320024
22	6	0	2.299342	-3.525666	0.555972
23	6	0	2.270429	-3.482370	-0.837080
24	6	0	1.076936	-3.017590	-1.526440
25	6	0	1.489928	-2.254092	-2.678818
26	6	0	0.768318	-1.109303	-3.033559
27	6	0	1.474759	0.085038	-3.459428
28	6	0	0.750529	1.240975	-2.963941
29	6	0	1.455260	2.372202	-2.537649
30	6	0	1.032170	3.056044	-1.339422
31	6	0	2.217736	3.495901	-0.622288
32	6	0	2.244940	3.452551	0.770974
33	6	0	3.436236	2.989685	1.461221
34	6	0	3.010938	2.222340	2.620759
35	6	0	3.722405	1.081726	2.998486
36	6	0	3.008970	-0.114492	3.416596
37	6	0	3.740526	-1.271831	2.926132
38	6	0	3.046743	-2.397696	2.477342
39	6	0	3.483715	-3.086901	1.273585
40	6	0	4.594117	-2.620521	0.567165
41	6	0	4.564376	-2.576055	-0.885918
42	6	0	3.425147	-2.999037	-1.573819
43	6	0	2.940950	-2.238614	-2.714927
44	6	0	3.617765	-1.086699	-3.121168
45	6	0	2.868561	0.097434	-3.510322
46	6	0	3.599807	1.266947	-3.049534
47	6	0	2.906137	2.381435	-2.573255
48	6	0	3.379519	3.077584	-1.387378
49	6	0	4.524474	2.629947	-0.725720
50	6	0	4.553448	2.585395	0.727515
51	6	0	5.292785	1.400322	1.124716
52	6	0	4.885058	0.664320	2.239326
53	6	0	4.896427	-0.790917	2.194687

54	6	0	5.314841	-1.450535	1.037074
55	6	0	5.732315	-0.683063	-0.124066
56	6	0	5.721912	0.712078	-0.081185
57	6	0	5.245350	1.471899	-1.224465
58	6	0	4.791486	0.805156	-2.364524
59	6	0	4.802625	-0.649994	-2.409128
60	6	0	5.267248	-1.378718	-1.312171
61	6	0	-3.058218	0.687363	0.044551
62	6	0	-3.940543	1.684636	-0.109358
63	8	0	-3.386118	2.968175	-0.280698
64	6	0	-3.511841	3.850833	0.770567
65	6	0	-2.984425	5.204925	0.369395
66	1	0	-1.981011	5.111121	-0.056445
67	1	0	-3.630248	5.639395	-0.401688
68	1	0	-2.966174	5.859054	1.241577
69	8	0	-3.977604	3.546486	1.838139
70	6	0	-3.144030	-0.835581	0.065553
71	6	0	-3.832877	-1.563520	-1.081878
72	6	0	-3.737429	-1.538340	1.283595
73	6	0	-3.811951	-1.283459	-2.443578
74	6	0	-4.557715	-2.667840	-0.591691
75	6	0	-3.624803	-1.218877	2.632803
76	6	0	-4.498727	-2.652397	0.875266
77	6	0	-4.496291	-2.132681	-3.320646
78	1	0	-3.284382	-0.415018	-2.826133
79	6	0	-5.232194	-3.518303	-1.467897
80	6	0	-4.247121	-2.042647	3.578720
81	1	0	-3.081566	-0.335486	2.953904
82	6	0	-5.109413	-3.477370	1.820200
83	6	0	-5.191395	-3.245471	-2.837280
84	1	0	-4.489151	-1.921834	-4.386423
85	1	0	-5.792792	-4.371429	-1.094571
86	6	0	-4.971677	-3.168540	3.175970

87	1	0	-4.168567	-1.799643	4.634639
88	1	0	-5.697577	-4.337110	1.509856
89	1	0	-5.715425	-3.896698	-3.531660
90	1	0	-5.445965	-3.799543	3.922777
91	6	0	-5.406876	1.622845	-0.269056
92	6	0	-6.034308	2.508064	-1.164094
93	6	0	-6.196705	0.704489	0.438927
94	6	0	-7.412376	2.460937	-1.358306
95	1	0	-5.432481	3.223987	-1.714845
96	6	0	-7.575956	0.662569	0.242625
97	1	0	-5.736158	0.044733	1.164323
98	6	0	-8.188818	1.536008	-0.656922
99	1	0	-7.880476	3.146474	-2.059691
100	1	0	-8.173614	-0.049765	0.804687
101	1	0	-9.264634	1.501413	-0.806077

Atomic Coordinates of *E*-β,γ-cycloadduct (R^1 = H)

Zero-point correction= 0.618118 (Hartree/Particle)

Thermal correction to Energy= 0.655506

Thermal correction to Enthalpy= 0.656450

Thermal correction to Gibbs Free Energy= 0.553788

Sum of electronic and zero-point Energies= -3091.028390

Sum of electronic and thermal Energies= -3090.991002

Sum of electronic and thermal Enthalpies= -3090.990058

Sum of electronic and thermal Free Energies= -3091.092720

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.437933	1.938132	0.000000
2	6	0	1.168924	1.784894	0.000000
3	6	0	1.750565	1.002664	1.175381
4	6	0	1.001915	0.629620	2.273065
5	6	0	-0.474912	0.766114	2.271103
6	6	0	-1.142454	1.276704	1.176246
7	6	0	-2.350456	0.633357	0.730445
8	6	0	-2.350456	0.633357	-0.730445
9	6	0	-1.142454	1.276704	-1.176246
10	6	0	-0.474912	0.766114	-2.271103
11	6	0	1.001915	0.629620	-2.273065
12	6	0	1.750565	1.002664	-1.175381
13	6	0	2.809362	0.145256	-0.732037
14	6	0	2.809362	0.145256	0.732037
15	6	0	3.151945	-1.019495	1.418705
16	6	0	2.391234	-1.390910	2.586988
17	6	0	1.325129	-0.581781	2.995294
18	6	0	0.086574	-1.192891	3.442628
19	6	0	-1.016302	-0.361637	2.996489
20	6	0	-2.217612	-0.955378	2.594845

21	6	0	-2.899901	-0.446795	1.429492
22	6	0	-3.462169	-1.574802	0.703722
23	6	0	-3.462169	-1.574802	-0.703722
24	6	0	-2.899901	-0.446795	-1.429492
25	6	0	-2.217612	-0.955378	-2.594845
26	6	0	-1.016302	-0.361637	-2.996489
27	6	0	0.086574	-1.192891	-3.442628
28	6	0	1.325129	-0.581781	-2.995294
29	6	0	2.391234	-1.390910	-2.586988
30	6	0	3.151945	-1.019495	-1.418705
31	6	0	3.487023	-2.231964	-0.703710
32	6	0	3.487023	-2.231964	0.703710
33	6	0	2.931792	-3.357716	1.419372
34	6	0	2.251823	-2.836071	2.594274
35	6	0	1.058196	-3.419733	3.023822
36	6	0	-0.044491	-2.580855	3.465837
37	6	0	-1.286407	-3.198366	3.028023
38	6	0	-2.350736	-2.400777	2.602311
39	6	0	-3.121747	-2.785355	1.431022
40	6	0	-2.795641	-3.949920	0.732756
41	6	0	-2.795641	-3.949920	-0.732756
42	6	0	-3.121747	-2.785355	-1.431022
43	6	0	-2.350736	-2.400777	-2.602311
44	6	0	-1.286407	-3.198366	-3.028023
45	6	0	-0.044491	-2.580855	-3.465837
46	6	0	1.058196	-3.419733	-3.023822
47	6	0	2.251823	-2.836071	-2.594274
48	6	0	2.931792	-3.357716	-1.419372
49	6	0	2.386973	-4.439711	-0.731401
50	6	0	2.386973	-4.439711	0.731401
51	6	0	1.150238	-5.046838	1.173677
52	6	0	0.498703	-4.546222	2.302824
53	6	0	-0.950788	-4.409257	2.305297

54	6	0	-1.689152	-4.777948	1.178774
55	6	0	-1.008609	-5.292141	0.000000
56	6	0	0.380924	-5.423720	0.000000
57	6	0	1.150238	-5.046838	-1.173677
58	6	0	0.498703	-4.546222	-2.302824
59	6	0	-0.950788	-4.409257	-2.305297
60	6	0	-1.689152	-4.777948	-1.178774
61	6	0	1.253510	3.306171	0.000000
62	6	0	2.308749	4.115915	0.000000
63	1	0	3.343001	3.789796	0.000000
64	8	0	2.119138	5.481338	0.000000
65	6	0	3.235380	6.285973	0.000000
66	6	0	2.822355	7.733659	0.000000
67	1	0	2.208842	7.948636	-0.882164
68	1	0	2.208842	7.948636	0.882164
69	1	0	3.711679	8.364292	0.000000
70	8	0	4.363240	5.857832	0.000000
71	6	0	-0.245994	3.556754	0.000000
72	6	0	-0.856103	4.300496	-1.183322
73	6	0	-0.856103	4.300496	1.183322
74	6	0	-0.579827	4.178431	-2.540641
75	6	0	-1.812789	5.231688	-0.732708
76	6	0	-0.579827	4.178431	2.540641
77	6	0	-1.812789	5.231688	0.732708
78	6	0	-1.292149	4.966215	-3.452353
79	1	0	0.183598	3.493100	-2.895430
80	6	0	-2.526699	6.011789	-1.642702
81	6	0	-1.292149	4.966215	3.452353
82	1	0	0.183598	3.493100	2.895430
83	6	0	-2.526699	6.011789	1.642702
84	6	0	-2.264445	5.867061	-3.007266
85	1	0	-1.084032	4.877568	-4.515045
86	1	0	-3.265733	6.730972	-1.299032

87	6	0	-2.264445	5.867061	3.007266
88	1	0	-1.084032	4.877568	4.515045
89	1	0	-3.265733	6.730972	1.299032
90	1	0	-2.811578	6.469239	-3.727663
91	1	0	-2.811578	6.469239	3.727663

Atomic Coordinates of *E*-β,γ-cycloadduct ($R^1 = CH_3$)

Zero-point correction= 0.645892 (Hartree/Particle)

Thermal correction to Energy= 0.684026

Thermal correction to Enthalpy= 0.684970

Thermal correction to Gibbs Free Energy= 0.582046

Sum of electronic and zero-point Energies= -3130.315226

Sum of electronic and thermal Energies= -3130.277092

Sum of electronic and thermal Enthalpies= -3130.276148

Sum of electronic and thermal Free Energies= -3130.379071

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.454951	1.859122	0.000000
2	6	0	1.154614	1.717331	0.000000
3	6	0	1.732278	0.929686	1.179152
4	6	0	0.981605	0.553126	2.274728
5	6	0	-0.495264	0.687211	2.270931
6	6	0	-1.160043	1.195125	1.173578
7	6	0	-2.366838	0.550974	0.725851
8	6	0	-2.366838	0.550974	-0.725851
9	6	0	-1.160043	1.195125	-1.173578
10	6	0	-0.495264	0.687211	-2.270931
11	6	0	0.981605	0.553126	-2.274728
12	6	0	1.732278	0.929686	-1.179152
13	6	0	2.793193	0.069871	-0.726579
14	6	0	2.793193	0.069871	0.726579
15	6	0	3.134074	-1.094473	1.424496
16	6	0	2.372343	-1.466828	2.591497
17	6	0	1.304530	-0.658738	2.996948
18	6	0	0.066150	-1.271451	3.442530
19	6	0	-1.036822	-0.441516	2.994805
20	6	0	-2.236621	-1.036866	2.590827

21	6	0	-2.917023	-0.529257	1.424002
22	6	0	-3.476634	-1.657737	0.696991
23	6	0	-3.476634	-1.657737	-0.696991
24	6	0	-2.917023	-0.529257	-1.424002
25	6	0	-2.236621	-1.036866	-2.590827
26	6	0	-1.036822	-0.441516	-2.994805
27	6	0	0.066150	-1.271451	-3.442530
28	6	0	1.304530	-0.658738	-2.996948
29	6	0	2.372343	-1.466828	-2.591497
30	6	0	3.134074	-1.094473	-1.424496
31	6	0	3.475185	-2.306223	-0.697023
32	6	0	3.475185	-2.306223	0.697023
33	6	0	2.917830	-3.432938	1.425073
34	6	0	2.235071	-2.912252	2.598766
35	6	0	1.041277	-3.497309	3.025761
36	6	0	-0.063231	-2.659694	3.465578
37	6	0	-1.303497	-3.278811	3.025566
38	6	0	-2.367837	-2.482383	2.597693
39	6	0	-3.136153	-2.867861	1.424854
40	6	0	-2.807327	-4.031989	0.727105
41	6	0	-2.807327	-4.031989	-0.727105
42	6	0	-3.136153	-2.867861	-1.424854
43	6	0	-2.367837	-2.482383	-2.597693
44	6	0	-1.303497	-3.278811	-3.025566
45	6	0	-0.063231	-2.659694	-3.465578
46	6	0	1.041277	-3.497309	-3.025761
47	6	0	2.235071	-2.912252	-2.598766
48	6	0	2.917830	-3.432938	-1.425073
49	6	0	2.378588	-4.515393	-0.727064
50	6	0	2.378588	-4.515393	0.727064
51	6	0	1.138922	-5.124182	1.175605
52	6	0	0.484585	-4.624449	2.303566
53	6	0	-0.965025	-4.489220	2.303266

54	6	0	-1.700721	-4.858699	1.175229
55	6	0	-1.017278	-5.371916	0.000000
56	6	0	0.372418	-5.501974	0.000000
57	6	0	1.138922	-5.124182	-1.175605
58	6	0	0.484585	-4.624449	-2.303566
59	6	0	-0.965025	-4.489220	-2.303266
60	6	0	-1.700721	-4.858699	-1.175229
61	6	0	1.222823	3.241640	0.000000
62	6	0	2.238866	4.114377	0.000000
63	8	0	1.815017	5.442533	0.000000
64	6	0	2.620037	6.549994	0.000000
65	6	0	1.749129	7.782952	0.000000
66	1	0	1.099336	7.782809	-0.881106
67	1	0	1.099336	7.782809	0.881106
68	1	0	2.381671	8.671096	0.000000
69	8	0	3.826467	6.537736	0.000000
70	6	0	-0.279127	3.475989	0.000000
71	6	0	-0.898917	4.212392	-1.183552
72	6	0	-0.898917	4.212392	1.183552
73	6	0	-0.620873	4.094238	-2.540892
74	6	0	-1.866010	5.133299	-0.734087
75	6	0	-0.620873	4.094238	2.540892
76	6	0	-1.866010	5.133299	0.734087
77	6	0	-1.340282	4.874886	-3.453214
78	1	0	0.150091	3.417043	-2.895140
79	6	0	-2.587079	5.906809	-1.644456
80	6	0	-1.340282	4.874886	3.453214
81	1	0	0.150091	3.417043	2.895140
82	6	0	-2.587079	5.906809	1.644456
83	6	0	-2.322236	5.765724	-3.008942
84	1	0	-1.130320	4.788598	-4.515795
85	1	0	-3.334710	6.617362	-1.301160
86	6	0	-2.322236	5.765724	3.008942

87	1	0	-1.130320	4.788598	4.515795
88	1	0	-3.334710	6.617362	1.301160
89	1	0	-2.875101	6.362346	-3.729632
90	1	0	-2.875101	6.362346	3.729632
91	6	0	3.694888	3.756087	0.000000
92	1	0	4.208149	4.159445	-0.877310
93	1	0	4.208149	4.159445	0.877310
94	1	0	3.796654	2.669060	0.000000

Atomic Coordinates of *E*-β,γ-cycloadduct (R^1 = Ph)

Zero-point correction= 0.698670 (Hartree/Particle)

Thermal correction to Energy= 0.740882

Thermal correction to Enthalpy= 0.741827

Thermal correction to Gibbs Free Energy= 0.628277

Sum of electronic and zero-point Energies= -3321.999745

Sum of electronic and thermal Energies= -3321.957533

Sum of electronic and thermal Enthalpies= -3321.956589

Sum of electronic and thermal Free Energies= -3322.070138

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.514795	-0.852719	0.020429
2	6	0	-1.532698	0.756775	0.064618
3	6	0	-0.793059	1.379256	1.252798
4	6	0	-0.317094	0.636600	2.314957
5	6	0	-0.300359	-0.845449	2.266036
6	6	0	-0.758636	-1.524088	1.155968
7	6	0	-0.007917	-2.645867	0.658335
8	6	0	-0.039149	-2.601554	-0.792524
9	6	0	-0.812290	-1.453602	-1.189745
10	6	0	-0.394764	-0.707247	-2.273284
11	6	0	-0.408232	0.775223	-2.232071
12	6	0	-0.828979	1.447410	-1.104101
13	6	0	-0.076328	2.577074	-0.632700
14	6	0	-0.051067	2.534454	0.819278
15	6	0	1.088207	2.968656	1.507454
16	6	0	1.559171	2.213681	2.643105
17	6	0	0.870813	1.057832	3.026608
18	6	0	1.614427	-0.125036	3.421310
19	6	0	0.891052	-1.292244	2.952519
20	6	0	1.595801	-2.412696	2.499216

21	6	0	1.135692	-3.105147	1.320024
22	6	0	2.299342	-3.525666	0.555972
23	6	0	2.270429	-3.482370	-0.837080
24	6	0	1.076936	-3.017590	-1.526440
25	6	0	1.489928	-2.254092	-2.678818
26	6	0	0.768318	-1.109303	-3.033559
27	6	0	1.474759	0.085038	-3.459428
28	6	0	0.750529	1.240975	-2.963941
29	6	0	1.455260	2.372202	-2.537649
30	6	0	1.032170	3.056044	-1.339422
31	6	0	2.217736	3.495901	-0.622288
32	6	0	2.244940	3.452551	0.770974
33	6	0	3.436236	2.989685	1.461221
34	6	0	3.010938	2.222340	2.620759
35	6	0	3.722405	1.081726	2.998486
36	6	0	3.008970	-0.114492	3.416596
37	6	0	3.740526	-1.271831	2.926132
38	6	0	3.046743	-2.397696	2.477342
39	6	0	3.483715	-3.086901	1.273585
40	6	0	4.594117	-2.620521	0.567165
41	6	0	4.564376	-2.576055	-0.885918
42	6	0	3.425147	-2.999037	-1.573819
43	6	0	2.940950	-2.238614	-2.714927
44	6	0	3.617765	-1.086699	-3.121168
45	6	0	2.868561	0.097434	-3.510322
46	6	0	3.599807	1.266947	-3.049534
47	6	0	2.906137	2.381435	-2.573255
48	6	0	3.379519	3.077584	-1.387378
49	6	0	4.524474	2.629947	-0.725720
50	6	0	4.553448	2.585395	0.727515
51	6	0	5.292785	1.400322	1.124716
52	6	0	4.885058	0.664320	2.239326
53	6	0	4.896427	-0.790917	2.194687

54	6	0	5.314841	-1.450535	1.037074
55	6	0	5.732315	-0.683063	-0.124066
56	6	0	5.721912	0.712078	-0.081185
57	6	0	5.245350	1.471899	-1.224465
58	6	0	4.791486	0.805156	-2.364524
59	6	0	4.802625	-0.649994	-2.409128
60	6	0	5.267248	-1.378718	-1.312171
61	6	0	-3.058218	0.687363	0.044551
62	6	0	-3.940543	1.684636	-0.109358
63	8	0	-3.386118	2.968175	-0.280698
64	6	0	-3.511841	3.850833	0.770567
65	6	0	-2.984425	5.204925	0.369395
66	1	0	-1.981011	5.111121	-0.056445
67	1	0	-3.630248	5.639395	-0.401688
68	1	0	-2.966174	5.859054	1.241577
69	8	0	-3.977604	3.546486	1.838139
70	6	0	-3.144030	-0.835581	0.065553
71	6	0	-3.832877	-1.563520	-1.081878
72	6	0	-3.737429	-1.538340	1.283595
73	6	0	-3.811951	-1.283459	-2.443578
74	6	0	-4.557715	-2.667840	-0.591691
75	6	0	-3.624803	-1.218877	2.632803
76	6	0	-4.498727	-2.652397	0.875266
77	6	0	-4.496291	-2.132681	-3.320646
78	1	0	-3.284382	-0.415018	-2.826133
79	6	0	-5.232194	-3.518303	-1.467897
80	6	0	-4.247121	-2.042647	3.578720
81	1	0	-3.081566	-0.335486	2.953904
82	6	0	-5.109413	-3.477370	1.820200
83	6	0	-5.191395	-3.245471	-2.837280
84	1	0	-4.489151	-1.921834	-4.386423
85	1	0	-5.792792	-4.371429	-1.094571
86	6	0	-4.971677	-3.168540	3.175970

87	1	0	-4.168567	-1.799643	4.634639
88	1	0	-5.697577	-4.337110	1.509856
89	1	0	-5.715425	-3.896698	-3.531660
90	1	0	-5.445965	-3.799543	3.922777
91	6	0	-5.406876	1.622845	-0.269056
92	6	0	-6.034308	2.508064	-1.164094
93	6	0	-6.196705	0.704489	0.438927
94	6	0	-7.412376	2.460937	-1.358306
95	1	0	-5.432481	3.223987	-1.714845
96	6	0	-7.575956	0.662569	0.242625
97	1	0	-5.736158	0.044733	1.164323
98	6	0	-8.188818	1.536008	-0.656922
99	1	0	-7.880476	3.146474	-2.059691
100	1	0	-8.173614	-0.049765	0.804687
101	1	0	-9.264634	1.501413	-0.806077

Cartesian Coordinates of α,β-cycloadduct (R^1 = H)

Zero-point correction= 0.619114 (Hartree/Particle)

Thermal correction to Energy= 0.656300

Thermal correction to Enthalpy= 0.657244

Thermal correction to Gibbs Free Energy= 0.554708

Sum of electronic and zero-point Energies= -3091.037832

Sum of electronic and thermal Energies= -3091.000646

Sum of electronic and thermal Enthalpies= -3090.999702

Sum of electronic and thermal Free Energies= -3091.102237

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.590332	-1.406845	0.239725
2	6	0	-1.938344	0.145271	-0.068138
3	6	0	-1.364816	1.131606	0.953056
4	6	0	-0.817686	0.738190	2.159283
5	6	0	-0.535244	-0.689176	2.448030
6	6	0	-0.798912	-1.665758	1.510344
7	6	0	0.166648	-2.707783	1.279292
8	6	0	0.202690	-2.985294	-0.144846
9	6	0	-0.739763	-2.116721	-0.798684
10	6	0	-0.424465	-1.564640	-2.021799
11	6	0	-0.710337	-0.137022	-2.306156
12	6	0	-1.313754	0.676074	-1.365913
13	6	0	-0.779632	1.995156	-1.146276
14	6	0	-0.813520	2.275373	0.278758
15	6	0	0.188395	3.057427	0.860534
16	6	0	0.728798	2.669687	2.139469
17	6	0	0.240294	1.518273	2.766611
18	6	0	1.164135	0.610781	3.423011
19	6	0	0.686085	-0.744690	3.224956
20	6	0	1.604807	-1.783158	3.035594

21	6	0	1.338493	-2.790155	2.036196
22	6	0	2.595167	-3.141350	1.394064
23	6	0	2.629144	-3.410129	0.026139
24	6	0	1.407770	-3.337846	-0.759340
25	6	0	1.730281	-2.779107	-2.050116
26	6	0	0.831208	-1.897220	-2.660952
27	6	0	1.329827	-0.712544	-3.333598
28	6	0	0.383602	0.366158	-3.111936
29	6	0	0.853057	1.673183	-2.943838
30	6	0	0.256214	2.508945	-1.932084
31	6	0	1.305939	3.309911	-1.322895
32	6	0	1.273027	3.577991	0.044302
33	6	0	2.491862	3.509445	0.830410
34	6	0	2.154122	2.946595	2.128307
35	6	0	3.038879	2.068900	2.756713
36	6	0	2.532804	0.881146	3.426152
37	6	0	3.484974	-0.196596	3.212599
38	6	0	3.028953	-1.502169	3.021317
39	6	0	3.642669	-2.342355	2.004847
40	6	0	4.684481	-1.842633	1.221043
41	6	0	4.719499	-2.122323	-0.205523
42	6	0	3.711899	-2.891505	-0.790888
43	6	0	3.154744	-2.501321	-2.076500
44	6	0	3.630803	-1.360138	-2.724753
45	6	0	2.699575	-0.450990	-3.373720
46	6	0	3.184703	0.905980	-3.179256
47	6	0	2.278971	1.947353	-2.971204
48	6	0	2.559700	2.960986	-1.966662
49	6	0	3.733226	2.892163	-1.212881
50	6	0	3.698370	3.171247	0.214079
51	6	0	4.618044	2.260183	0.872085
52	6	0	4.293996	1.721581	2.119080
53	6	0	4.569999	0.320652	2.401009

54	6	0	5.157974	-0.484798	1.423589
55	6	0	5.487321	0.075091	0.123732
56	6	0	5.223549	1.418917	-0.146309
57	6	0	4.674772	1.808622	-1.434249
58	6	0	4.405966	0.836577	-2.400448
59	6	0	4.681440	-0.564958	-2.119061
60	6	0	5.214038	-0.936890	-0.882746
61	6	0	-3.431727	-0.248252	0.013260
62	6	0	-3.124971	-1.705117	0.267371
63	1	0	-3.465991	-2.125884	1.217001
64	8	0	-3.578386	-2.539784	-0.812078
65	6	0	-3.974677	-4.638147	-1.820084
66	1	0	-4.002955	-5.705610	-1.599487
67	1	0	-4.963778	-4.287229	-2.129892
68	1	0	-3.286144	-4.451010	-2.651155
69	6	0	-3.507817	-3.884590	-0.599938
70	8	0	-3.117476	-4.374050	0.435648
71	6	0	-6.882125	3.297507	-0.192676
72	1	0	-7.946148	3.452073	-0.034049
73	6	0	-6.061506	4.365417	-0.565638
74	1	0	-6.488475	5.356520	-0.692629
75	6	0	-8.264048	0.454443	0.613102
76	1	0	-9.023058	1.232323	0.614030
77	6	0	-8.605611	-0.865758	0.916542
78	1	0	-9.635803	-1.117522	1.153114
79	6	0	-6.295386	-1.563917	0.610072
80	1	0	-5.570953	-2.366810	0.602657
81	6	0	-7.627671	-1.863353	0.914629
82	1	0	-7.901618	-2.888385	1.148500
83	6	0	-4.930304	1.824253	-0.237920
84	6	0	-4.623863	0.389477	0.001365
85	6	0	-5.939325	-0.247245	0.309782
86	6	0	-6.938480	0.756032	0.313008

87	6	0	-6.316009	2.035573	-0.035772
88	6	0	-4.697177	4.161672	-0.786583
89	1	0	-4.067982	4.994012	-1.089282
90	6	0	-4.126615	2.894496	-0.627687
91	1	0	-3.072975	2.763173	-0.825730

Atomic Coordinates of α,β-cycloadduct ($R^1 = CH_3$)

Zero-point correction= 0.646987 (Hartree/Particle)

Thermal correction to Energy= 0.685470

Thermal correction to Enthalpy= 0.686414

Thermal correction to Gibbs Free Energy= 0.583077

Sum of electronic and zero-point Energies= -3130.319171

Sum of electronic and thermal Energies= -3130.280688

Sum of electronic and thermal Enthalpies= -3130.279744

Sum of electronic and thermal Free Energies= -3130.383080

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.546446	-1.365800	0.417317
2	6	0	-1.898731	0.182892	0.109853
3	6	0	-1.262600	1.172275	1.099400
4	6	0	-0.643442	0.782782	2.272607
5	6	0	-0.350080	-0.643752	2.552793
6	6	0	-0.671583	-1.620775	1.634669
7	6	0	0.271202	-2.670007	1.356082
8	6	0	0.224948	-2.951330	-0.065014
9	6	0	-0.751191	-2.081124	-0.667380
10	6	0	-0.499454	-1.541760	-1.910452
11	6	0	-0.789340	-0.114979	-2.189408
12	6	0	-1.328731	0.704412	-1.217461
13	6	0	-0.774127	2.018027	-1.034725
14	6	0	-0.729069	2.304223	0.388076
15	6	0	0.306437	3.085386	0.907304
16	6	0	0.914967	2.703267	2.156569
17	6	0	0.453737	1.558858	2.815288
18	6	0	1.407802	0.649402	3.424199
19	6	0	0.911856	-0.703436	3.259609
20	6	0	1.811301	-1.749302	3.025602

21	6	0	1.482475	-2.758359	2.047616
22	6	0	2.698553	-3.122945	1.339315
23	6	0	2.652792	-3.397198	-0.027106
24	6	0	1.389491	-3.318344	-0.742849
25	6	0	1.643848	-2.770688	-2.053496
26	6	0	0.717707	-1.886972	-2.617665
27	6	0	1.186298	-0.710089	-3.324221
28	6	0	0.261388	0.376476	-3.056922
29	6	0	0.748717	1.680892	-2.921608
30	6	0	0.216178	2.523983	-1.881253
31	6	0	1.302387	3.321653	-1.336449
32	6	0	1.346785	3.596026	0.029004
33	6	0	2.607013	3.524424	0.746111
34	6	0	2.339271	2.971178	2.064183
35	6	0	3.252495	2.090956	2.646706
36	6	0	2.776503	0.910290	3.349622
37	6	0	3.708399	-0.175074	3.089328
38	6	0	3.234232	-1.478646	2.930927
39	6	0	3.784026	-2.328605	1.886215
40	6	0	4.783239	-1.839748	1.042470
41	6	0	4.736253	-2.126642	-0.382285
42	6	0	3.691977	-2.891184	-0.906272
43	6	0	3.066359	-2.504178	-2.161266
44	6	0	3.513333	-1.369692	-2.841375
45	6	0	2.553713	-0.457927	-3.442751
46	6	0	3.057918	0.896822	-3.282506
47	6	0	2.172626	1.945525	-3.029898
48	6	0	2.515798	2.962278	-2.047923
49	6	0	3.728928	2.889225	-1.360161
50	6	0	3.775264	3.175514	0.064953
51	6	0	4.724534	2.261729	0.675451
52	6	0	4.467997	1.731943	1.941860
53	6	0	4.750031	0.330530	2.215742

54	6	0	5.276211	-0.484321	1.211054
55	6	0	5.535699	0.066898	-0.108331
56	6	0	5.266458	1.411133	-0.370670
57	6	0	4.649396	1.798117	-1.628180
58	6	0	4.320153	0.822899	-2.572400
59	6	0	4.601144	-0.578830	-2.298798
60	6	0	5.200031	-0.948022	-1.092558
61	6	0	-3.400210	-0.203811	0.170227
62	6	0	-3.096875	-1.657249	0.537702
63	8	0	-3.584429	-2.549301	-0.497816
64	6	0	-3.851651	-4.563636	-1.686124
65	1	0	-3.643347	-5.632335	-1.626469
66	1	0	-4.931547	-4.390608	-1.729255
67	1	0	-3.418945	-4.153584	-2.605024
68	6	0	-3.245452	-3.868141	-0.490542
69	8	0	-2.546159	-4.392492	0.346000
70	6	0	-6.742544	3.444726	-0.110178
71	1	0	-7.814151	3.613029	-0.043216
72	6	0	-5.866853	4.521270	-0.267592
73	1	0	-6.256268	5.534200	-0.322212
74	6	0	-8.279058	0.601913	0.142581
75	1	0	-9.003929	1.411659	0.143689
76	6	0	-8.704260	-0.726720	0.192451
77	1	0	-9.765252	-0.955778	0.242578
78	6	0	-6.395629	-1.488653	0.093216
79	1	0	-5.697403	-2.309258	0.022463
80	6	0	-7.766236	-1.760922	0.156253
81	1	0	-8.101521	-2.794527	0.167956
82	6	0	-4.829625	1.913496	-0.124597
83	6	0	-4.581360	0.447478	0.023655
84	6	0	-5.951431	-0.163902	0.081005
85	6	0	-6.914484	0.873291	0.077910
86	6	0	-6.222709	2.154962	-0.045671

87	6	0	-4.492335	4.295023	-0.361537
88	1	0	-3.812904	5.132406	-0.494088
89	6	0	-3.970912	2.999188	-0.288738
90	1	0	-2.905687	2.865134	-0.374040
91	6	0	-3.571348	-2.065454	1.935203
92	1	0	-3.235146	-1.326300	2.667010
93	1	0	-4.661958	-2.097739	1.972767
94	1	0	-3.167866	-3.040837	2.209795

Atomic Coordinates of α,β-cycloadduct (R^1 = Ph)

Zero-point correction= 0.699291 (Hartree/Particle)

Thermal correction to Energy= 0.739300

Thermal correction to Enthalpy= 0.740244

Thermal correction to Gibbs Free Energy= 0.633823

Sum of electronic and zero-point Energies= -3321.961151

Sum of electronic and thermal Energies= -3321.921142

Sum of electronic and thermal Enthalpies= -3321.920198

Sum of electronic and thermal Free Energies= -3322.026619

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.390079	-1.103687	-0.192806
2	6	0	-1.606193	0.498117	-0.124941
3	6	0	-0.987060	1.155684	1.118853
4	6	0	-0.496665	0.438342	2.194217
5	6	0	-0.328296	-1.033620	2.126808
6	6	0	-0.639760	-1.724532	0.975062
7	6	0	0.247176	-2.753196	0.503322
8	6	0	0.299972	-2.673843	-0.942953
9	6	0	-0.559212	-1.600045	-1.369230
10	6	0	-0.167570	-0.797991	-2.419392
11	6	0	-0.332569	0.673602	-2.350512
12	6	0	-0.892407	1.275339	-1.240773
13	6	0	-0.264350	2.450198	-0.700575
14	6	0	-0.318136	2.375240	0.748491
15	6	0	0.722626	2.911204	1.511144
16	6	0	1.196633	2.183356	2.661162
17	6	0	0.603093	0.958210	2.982169
18	6	0	1.437040	-0.153136	3.403555
19	6	0	0.863033	-1.375493	2.874800
20	6	0	1.703405	-2.407954	2.444224

21	6	0	1.387410	-3.114539	1.226167
22	6	0	2.629779	-3.401324	0.527789
23	6	0	2.679002	-3.328534	-0.863862
24	6	0	1.488403	-2.965849	-1.615772
25	6	0	1.888863	-2.139522	-2.728981
26	6	0	1.077142	-1.066427	-3.111805
27	6	0	1.684261	0.201105	-3.470443
28	6	0	0.818649	1.266995	-2.999140
29	6	0	1.383140	2.450501	-2.511325
30	6	0	0.826070	3.057818	-1.329133
31	6	0	1.916258	3.598992	-0.534426
32	6	0	1.865769	3.526676	0.856234
33	6	0	3.053708	3.170933	1.611080
34	6	0	2.638932	2.338579	2.729216
35	6	0	3.436528	1.265521	3.129828
36	6	0	2.822090	-0.004121	3.483533
37	6	0	3.694146	-1.071179	3.019742
38	6	0	3.144723	-2.249399	2.510666
39	6	0	3.718828	-2.863812	1.323642
40	6	0	4.816674	-2.274171	0.694061
41	6	0	4.868658	-2.199240	-0.757188
42	6	0	3.820737	-2.717216	-1.520840
43	6	0	3.330564	-1.981737	-2.676254
44	6	0	3.911021	-0.759690	-3.021313
45	6	0	3.071086	0.352537	-3.435193
46	6	0	3.653799	1.577070	-2.909634
47	6	0	2.826143	2.606477	-2.459481
48	6	0	3.156606	3.318251	-1.234735
49	6	0	4.300072	2.972439	-0.511591
50	6	0	4.247370	2.896893	0.939813
51	6	0	5.076114	1.781403	1.361345
52	6	0	4.678427	0.983326	2.436145
53	6	0	4.837820	-0.461835	2.368208

54	6	0	5.387572	-1.050026	1.227134
55	6	0	5.794111	-0.218579	0.106699
56	6	0	5.642469	1.167416	0.172301
57	6	0	5.161009	1.902730	-0.985007
58	6	0	4.844154	1.220617	-2.162006
59	6	0	5.002511	-0.224689	-2.230358
60	6	0	5.471424	-0.928697	-1.119288
61	6	0	-3.130858	0.242821	-0.258523
62	6	0	-2.961736	-1.277314	-0.247693
63	8	0	-3.422527	-1.842816	-1.502142
64	6	0	-3.730144	-3.474299	-3.170873
65	1	0	-3.602885	-4.539336	-3.367263
66	1	0	-4.787909	-3.201107	-3.237757
67	1	0	-3.194690	-2.892277	-3.928694
68	6	0	-3.178521	-3.148189	-1.803404
69	8	0	-2.589843	-3.920665	-1.081950
70	6	0	-6.174464	4.130450	0.170956
71	1	0	-7.233499	4.371469	0.209782
72	6	0	-5.215472	5.130995	0.343598
73	1	0	-5.527090	6.156974	0.519423
74	6	0	-7.921980	1.459433	-0.393142
75	1	0	-8.585933	2.305281	-0.235555
76	6	0	-8.441847	0.201833	-0.704157
77	1	0	-9.516750	0.062293	-0.780286
78	6	0	-6.192019	-0.714050	-0.844161
79	1	0	-5.549507	-1.551025	-1.073440
80	6	0	-7.578799	-0.871070	-0.938256
81	1	0	-7.985443	-1.842402	-1.206671
82	6	0	-4.378936	2.485974	-0.104565
83	6	0	-4.247162	1.012083	-0.312175
84	6	0	-5.656681	0.528926	-0.496528
85	6	0	-6.541123	1.616525	-0.301231
86	6	0	-5.753411	2.823177	-0.056271

87	6	0	-3.857136	4.813799	0.283421
88	1	0	-3.112057	5.594686	0.407835
89	6	0	-3.435620	3.498498	0.062789
90	1	0	-2.379003	3.295595	0.014403
91	6	0	-3.581999	-1.974654	0.977294
92	6	0	-3.880398	-1.237173	2.122994
93	6	0	-3.845945	-3.344110	0.940806
94	6	0	-4.442529	-1.869087	3.232572
95	1	0	-3.672699	-0.157738	2.151709
96	6	0	-4.407502	-3.976029	2.050252
97	1	0	-3.610945	-3.925249	0.037187
98	6	0	-4.705545	-3.238302	3.196614
99	1	0	-4.676953	-1.287535	4.135947
100	1	0	-4.615023	-5.055584	2.022113
101	1	0	-5.148041	-3.736571	4.071384
