

Supporting Information

Strategy Towards Tuning Emission of Star Shaped Tetraphenylethene Substituted Truxenes for Sky-Blue and Greenish-White OLEDs

Rekha Sharma,^a Dmytro Volyniuk,^b Charu Popli,^a Oleksandr Bezikonnyi,^b Juozas V. Grazulevicius,^b Rajneesh Misra^{*a}

Department of Chemistry,
Indian Institute of Technology Indore,
Indore- 452 017, India.

rajneeshmisra@iiti.ac.in

Table of Contents

I. PL decay curve of compounds.....	S2
II. EL spectra of compounds.....	S4
III. Major transitions of truxenes.....	S5
IV. Copies of ¹H NMR, ¹³C NMR and HRMS Spectra of the New Compounds	S7
V. DFT Calculations of the truxenes 7-9.....	S12.

Table S1. Fitting results of the photoluminescence decay curves of the solid films of **7**, **8** and **9** prepared by spin-coating of the solutions.

Compounds	7	8	9
Photoluminescence lifetimes (τ) (ns)	1.91 (70%) 4.14 (30%)	2.52 (68%) 4.69 (32%)	0.82 (76%) 2.77 (24%)
χ^2	1.195	1.017	1.031

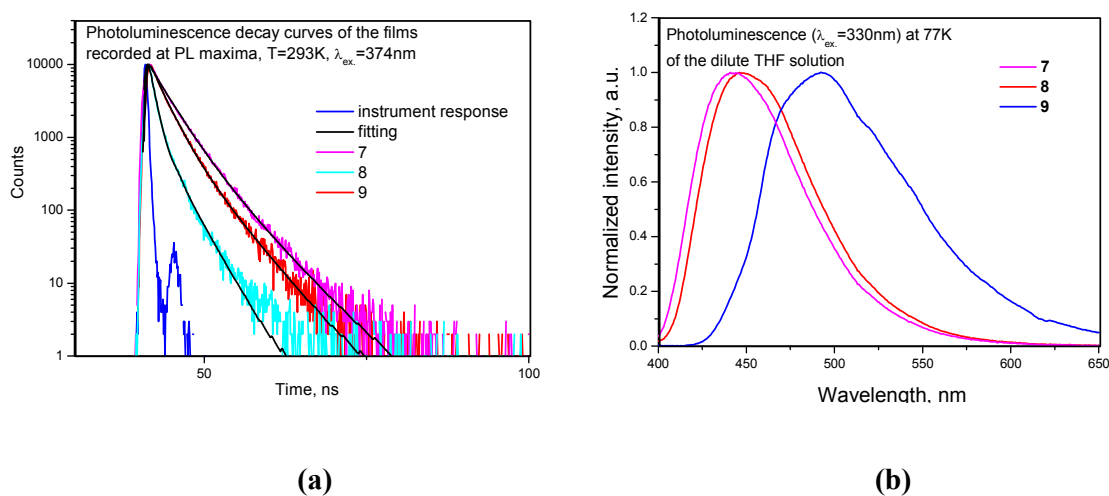
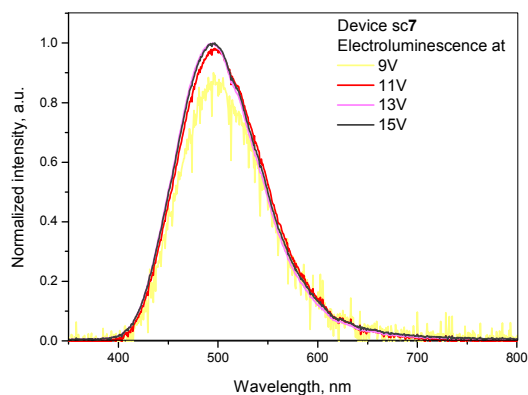


Figure S1. (a) PL decay curves for the films of truxenes **7**, **8** and **9**. (b) PL spectra of the dilute THF solutions of the studied compounds measured at temperature of 77K.



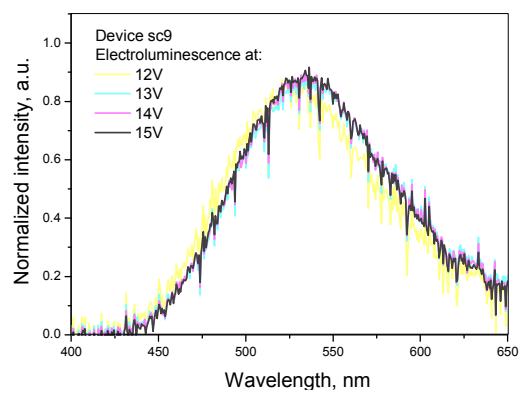
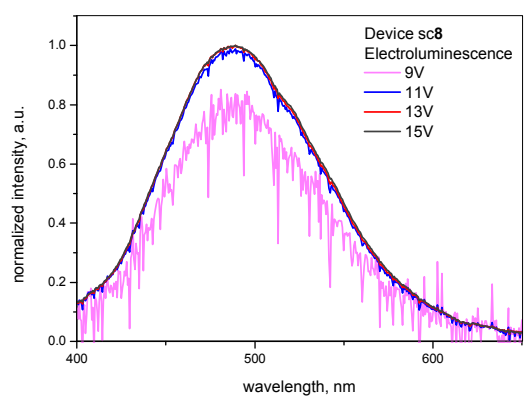


Figure S2. EL spectra of the devices sc7, sc8, and sc9.

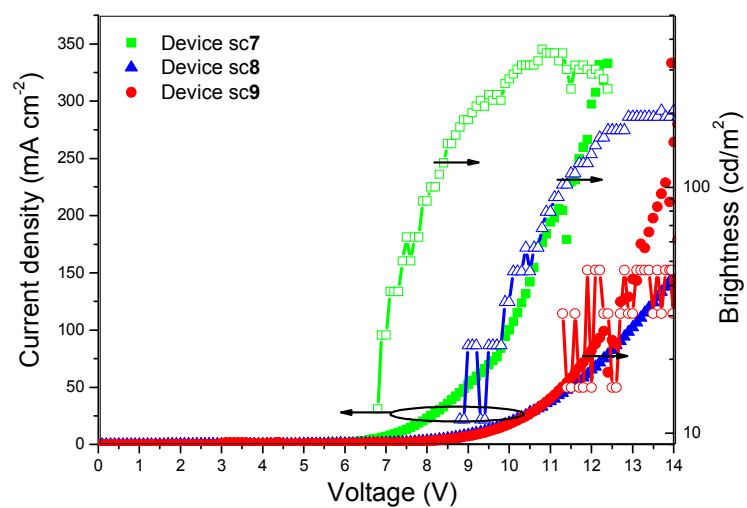


Figure S3. Current density and brightness as functions of voltage for the devices sc7, sc8, and sc9.

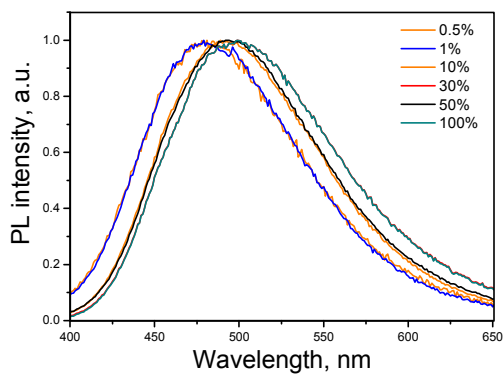


Figure S4. FL spectra of solid solutions of 7 in ZEONEX with different concentrations of dopant (shown in graph in % of dopant dispersed in ZEONEX).

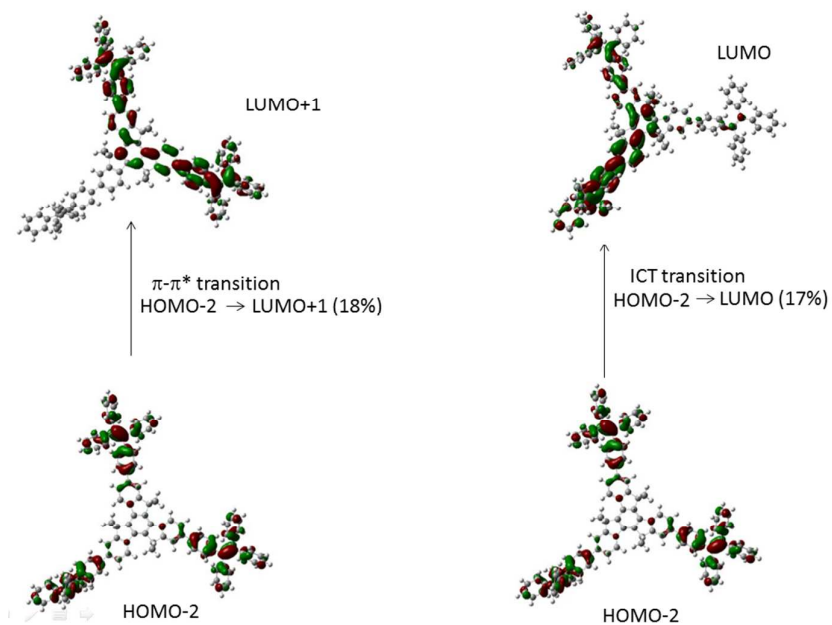


Figure S5. The major transitions in truxene 7

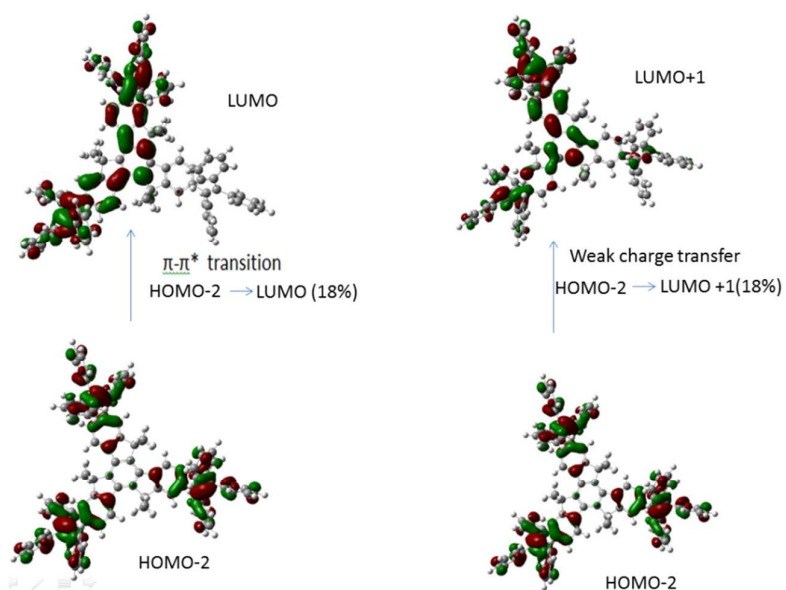


Figure S6. The major transitions in truxene 8

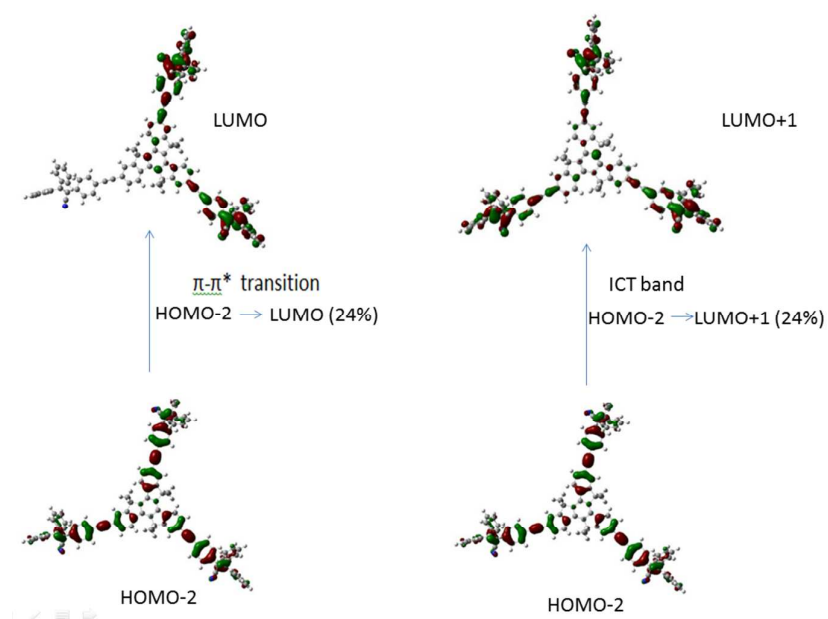


Figure S7. The major transitions in truxene 9

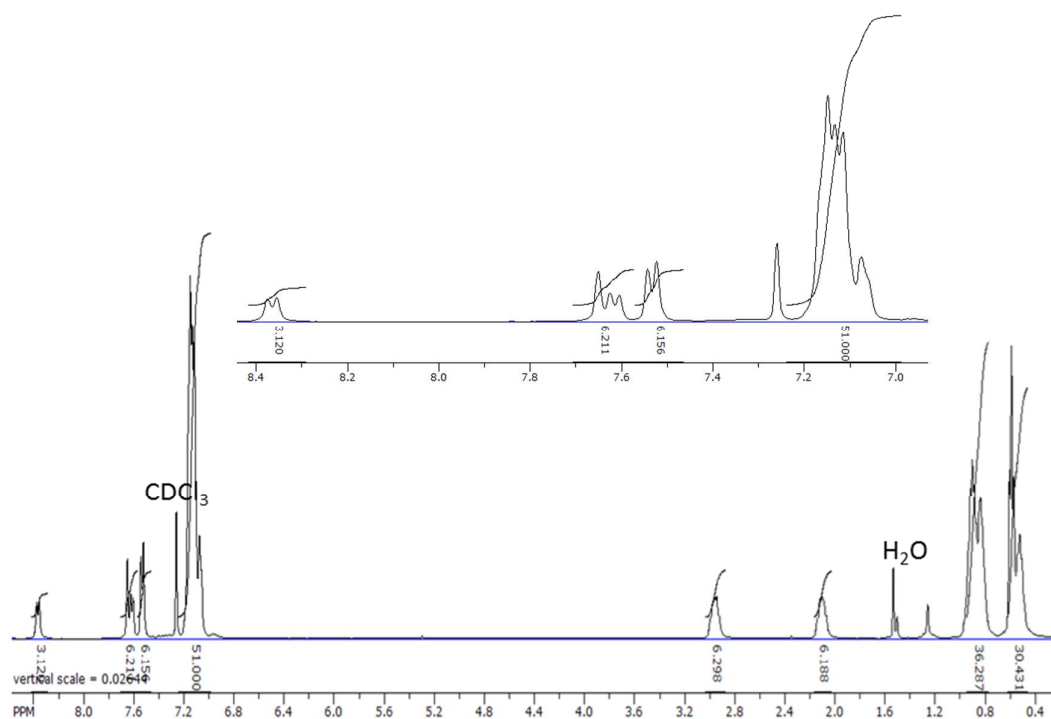


Figure S8. ^1H NMR Spectra of truxene 7.

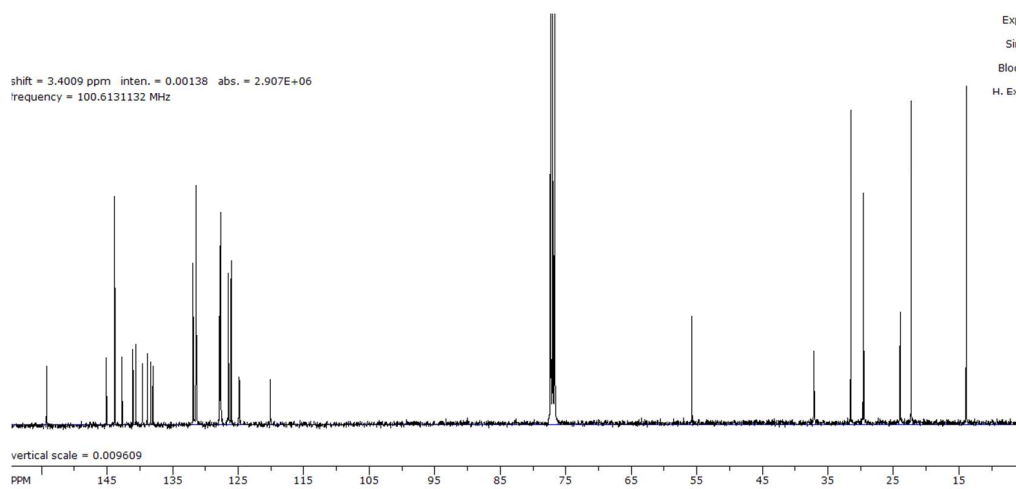


Figure S9. ^{13}C NMR Spectra of **7**.

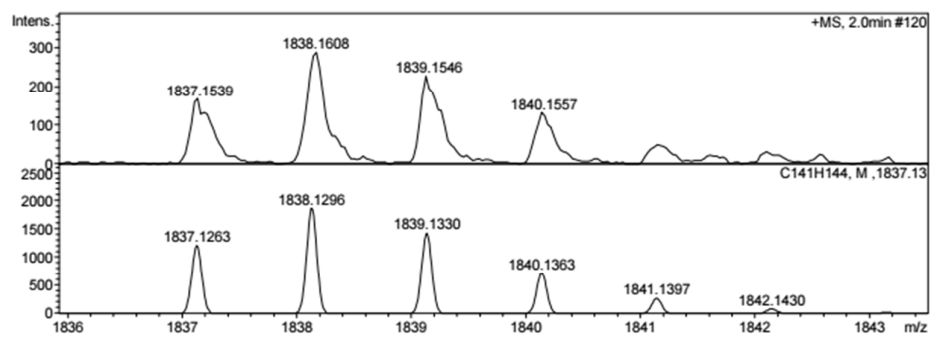


Figure S10. HRMS Spectra of **7**

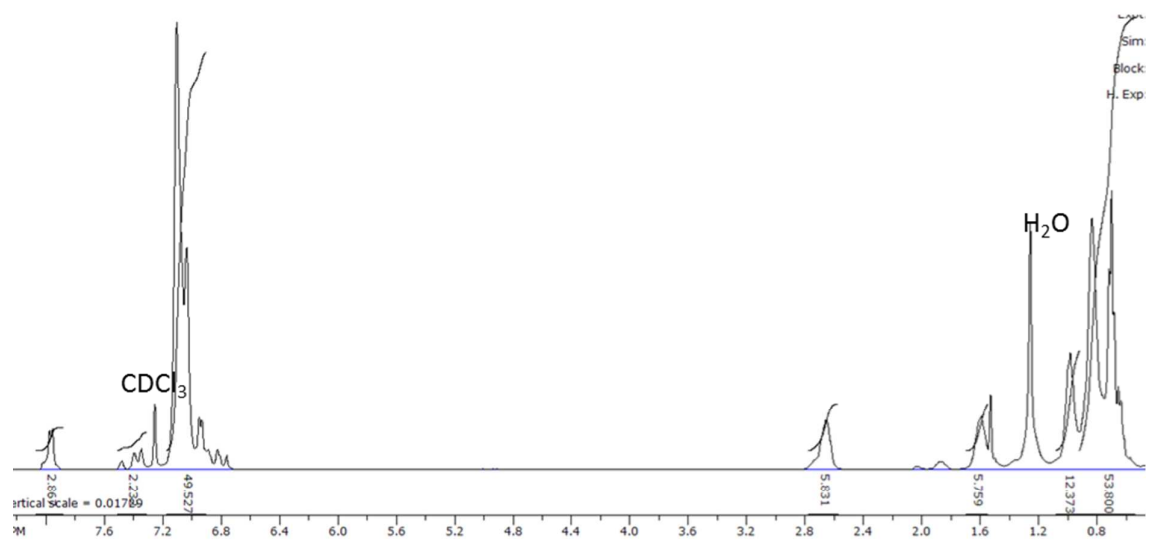


Figure S11. ^1H NMR Spectra of truxene **8**.

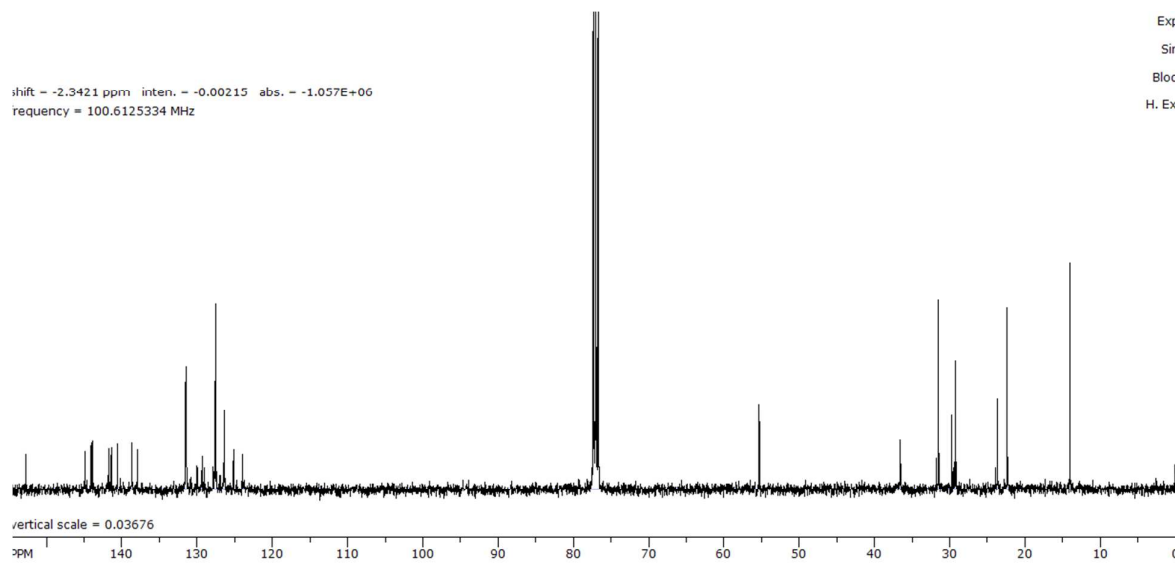


Figure S12. ^{13}C NMR Spectra of **8**.

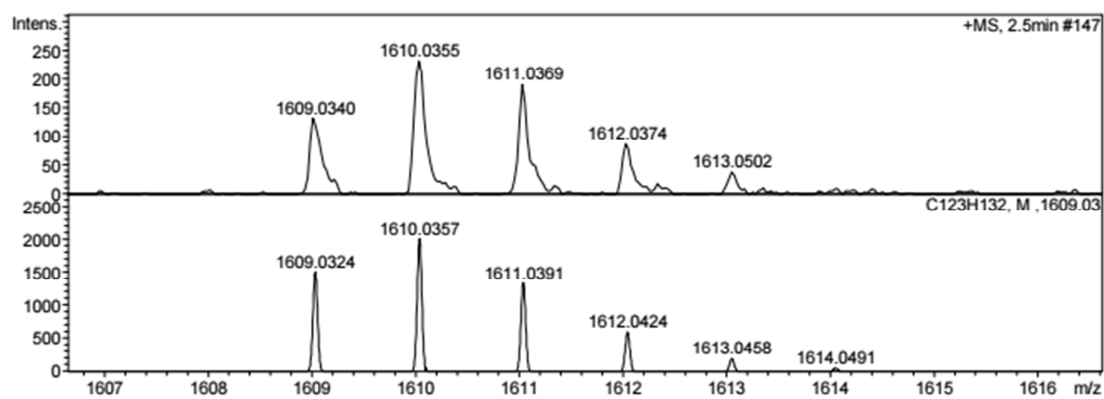


Figure S13. HRMS Spectra of **8**

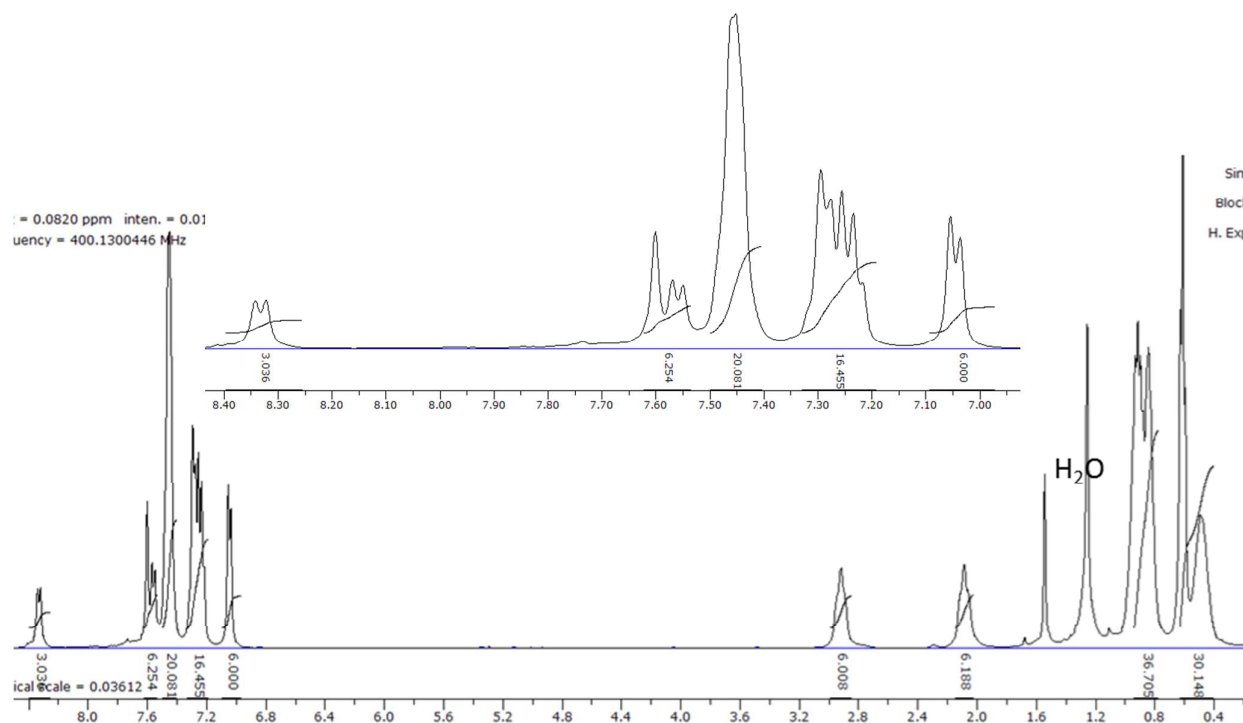


Figure S14. ¹H NMR Spectra of truxene **9**

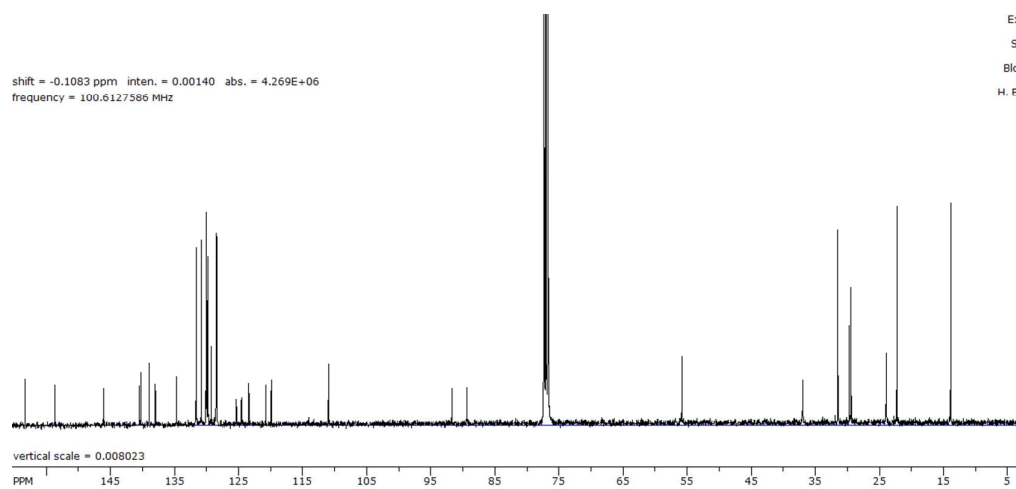


Figure S15. ^{13}C NMR Spectra of **9**.

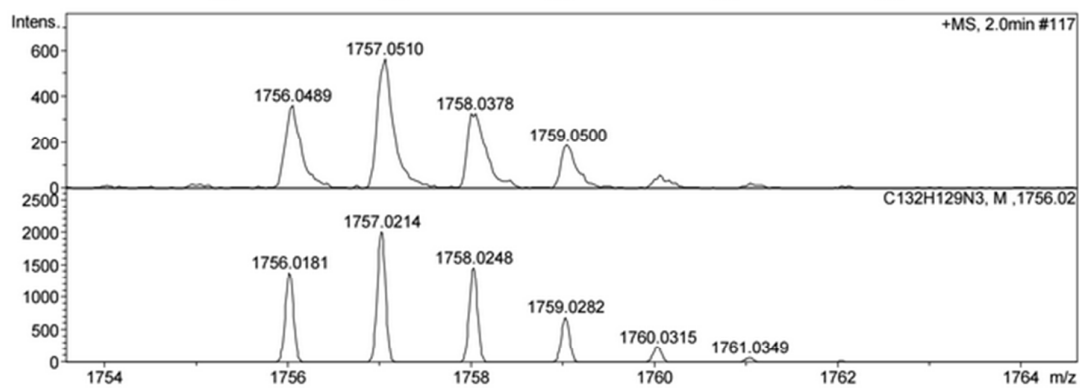


Figure S16. HRMS Spectra of **9**.

DFT Calculations.

DFT calculation data of the truxenes **7-9** Calculation method: B3LYP/6-31+G** for C, H, N with Gaussian 09¹.

Data for truxene **7**:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.397479	5.340748	-0.021377
2	6	0	-0.125562	4.741760	-0.031537
3	1	0	0.759219	5.368762	-0.094073
4	6	0	0.001732	3.360450	0.002055
5	6	0	-1.118857	2.510917	0.045519
6	6	0	-2.389461	3.105838	0.057326
7	1	0	-3.293826	2.518021	0.102078
8	6	0	-2.516920	4.492841	0.024350
9	1	0	-3.510792	4.927953	0.063110
10	6	0	0.784503	1.127570	0.033550
11	6	0	-0.638571	1.105713	0.066400
12	6	0	-1.317051	-0.121217	0.106954
13	6	0	-0.586063	-1.342840	0.117163
14	6	0	0.816050	-1.317692	0.088920
15	6	0	1.508118	-0.074052	0.045468
16	6	0	1.299636	2.570476	-0.013186
17	6	0	1.808229	-2.485678	0.097435
18	6	0	-2.824489	-0.395717	0.143389
19	6	0	2.965148	-0.361226	0.022559
20	6	0	4.115962	0.439942	-0.028149
21	1	0	4.059396	1.517798	-0.051771
22	6	0	5.380945	-0.144726	-0.036306
23	1	0	6.254732	0.499619	-0.046579
24	6	0	5.555076	-1.538284	0.005045
25	6	0	4.399922	-2.338210	0.052054
26	1	0	4.499632	-3.419847	0.054740
27	6	0	3.140456	-1.756543	0.060526
28	6	0	-1.562967	-2.460559	0.158848
29	6	0	-1.442872	-3.857953	0.187318
30	1	0	-0.480502	-4.346728	0.168391
31	6	0	-2.580769	-4.661057	0.227545
32	1	0	-2.459373	-5.739877	0.219658
33	6	0	-3.875441	-4.115008	0.242076
34	6	0	-3.992106	-2.714267	0.212886
35	1	0	-4.977743	-2.259387	0.250479
36	6	0	-2.859283	-1.914268	0.171154
37	6	0	2.051153	2.880902	-1.332190
38	6	0	2.116982	2.943683	1.249413
39	6	0	-3.540536	0.087209	-1.143340
40	6	0	-3.487772	0.135828	1.439022
41	6	0	1.693245	-3.363343	-1.174820

42	6	0	1.734977	-3.310312	1.407548
43	1	0	2.381667	3.924811	-1.344554
44	1	0	2.925491	2.246914	-1.479233
45	1	0	1.385232	2.729269	-2.186438
46	1	0	2.449196	3.985665	1.192431
47	1	0	1.494681	2.837700	2.142575
48	1	0	2.996914	2.314969	1.384540
49	1	0	1.883942	-2.757582	-2.065262
50	1	0	2.436720	-4.166883	-1.149645
51	1	0	0.708509	-3.816608	-1.289367
52	1	0	1.953211	-2.668396	2.265801
53	1	0	0.755473	-3.759520	1.572104
54	1	0	2.478673	-4.114009	1.391266
55	1	0	-3.124884	-0.423404	-2.016703
56	1	0	-4.609019	-0.147972	-1.093748
57	1	0	-3.437548	1.159580	-1.308815
58	1	0	-3.377237	1.213451	1.559875
59	1	0	-4.557439	-0.098831	1.441320
60	1	0	-3.037636	-0.342644	2.313472
61	6	0	6.907252	-2.145232	0.001693
62	6	0	7.181597	-3.313572	0.733683
63	6	0	7.960316	-1.581976	-0.739972
64	6	0	8.445809	-3.892347	0.720661
65	1	0	6.399031	-3.761415	1.338768
66	6	0	9.228557	-2.152675	-0.741592
67	1	0	7.773974	-0.703095	-1.349787
68	6	0	9.504092	-3.316577	-0.003915
69	1	0	8.624349	-4.797987	1.292312
70	1	0	10.017576	-1.700531	-1.333247
71	6	0	10.848762	-3.964861	-0.031139
72	6	0	12.012000	-3.268766	0.141508
73	6	0	10.822374	-5.442669	-0.261452
74	6	0	13.355235	-3.861910	-0.139515
75	6	0	12.044086	-1.855703	0.628453
76	6	0	11.514823	-6.325362	0.584129
77	6	0	10.050303	-5.988444	-1.301881
78	6	0	13.624940	-4.517298	-1.352813
79	6	0	14.403274	-3.725000	0.787815
80	6	0	12.834544	-0.894164	-0.025453
81	6	0	11.337838	-1.463015	1.778053
82	6	0	11.454080	-7.703490	0.384044
83	1	0	12.102166	-5.923149	1.402962
84	6	0	9.999690	-7.365544	-1.510212
85	1	0	9.491063	-5.322604	-1.952322
86	6	0	14.890589	-5.036090	-1.620211
87	1	0	12.833718	-4.615983	-2.088480
88	6	0	15.665459	-4.254771	0.526159
89	1	0	14.219818	-3.202660	1.721891
90	6	0	12.890632	0.420281	0.434299
91	1	0	13.403803	-1.183976	-0.903508
92	6	0	11.403574	-0.151485	2.245267
93	1	0	10.736857	-2.195741	2.306345
94	6	0	10.701282	-8.229596	-0.667190
95	1	0	11.993622	-8.367496	1.053411
96	1	0	9.407477	-7.764482	-2.328945

97	6	0	15.914813	-4.912816	-0.679783
98	1	0	15.077492	-5.534345	-2.567237
99	1	0	16.456683	-4.149099	1.263022
100	6	0	12.175365	0.797487	1.572482
101	1	0	13.497985	1.149618	-0.094243
102	1	0	10.853710	0.128081	3.139444
103	1	0	10.656085	-9.303394	-0.823974
104	1	0	16.900407	-5.319072	-0.887758
105	1	0	12.225060	1.819735	1.936108
106	6	0	-5.074864	-4.984865	0.284594
107	6	0	-5.079290	-6.186150	1.014869
108	6	0	-6.253656	-4.635563	-0.396816
109	6	0	-6.208064	-6.997225	1.060927
110	1	0	-4.196965	-6.471997	1.579542
111	6	0	-7.378856	-5.451842	-0.359487
112	1	0	-6.281832	-3.722102	-0.983181
113	6	0	-7.379376	-6.657961	0.361264
114	1	0	-6.187541	-7.908033	1.651546
115	1	0	-8.271165	-5.157422	-0.901667
116	6	0	-8.594291	-7.522495	0.440145
117	6	0	-9.320792	-7.878734	-0.661725
118	6	0	-8.953824	-7.969248	1.821391
119	6	0	-10.672147	-8.511014	-0.567033
120	6	0	-8.826495	-7.668898	-2.056868
121	6	0	-9.211443	-9.320717	2.106607
122	6	0	-8.985862	-7.049141	2.884000
123	6	0	-11.679723	-7.961220	0.243598
124	6	0	-10.985891	-9.644521	-1.337654
125	6	0	-9.663406	-7.099933	-3.033024
126	6	0	-7.541522	-8.083770	-2.445936
127	6	0	-9.510750	-9.734197	3.403523
128	1	0	-9.174389	-10.047662	1.302088
129	6	0	-9.296791	-7.460294	4.178896
130	1	0	-8.769203	-6.003526	2.686909
131	6	0	-12.948042	-8.536348	0.298448
132	1	0	-11.461763	-7.075928	0.831608
133	6	0	-12.250559	-10.226675	-1.274252
134	1	0	-10.226917	-10.071654	-1.986183
135	6	0	-9.219387	-6.921268	-4.341953
136	1	0	-10.667393	-6.792109	-2.756890
137	6	0	-7.101275	-7.915785	-3.757565
138	1	0	-6.888459	-8.542636	-1.711063
139	6	0	-9.560379	-8.805415	4.444476
140	1	0	-9.701637	-10.785116	3.601477
141	1	0	-9.328523	-6.729779	4.982320
142	6	0	-13.237836	-9.674794	-0.455623
143	1	0	-13.712625	-8.091038	0.928662
144	1	0	-12.466511	-11.109914	-1.868753
145	6	0	-7.935671	-7.328514	-4.710241
146	1	0	-9.878755	-6.467326	-5.076354
147	1	0	-6.105442	-8.248334	-4.036374
148	1	0	-9.795330	-9.127803	5.454694
149	1	0	-14.225930	-10.123568	-0.411477
150	1	0	-7.591520	-7.195992	-5.731819
151	6	0	-1.554631	6.814129	-0.055347

152	6	0	-0.647670	7.660746	0.605370
153	6	0	-2.613759	7.417790	-0.755503
154	6	0	-0.793671	9.043291	0.567672
155	1	0	0.169141	7.228502	1.175680
156	6	0	-2.767832	8.799434	-0.781531
157	1	0	-3.308453	6.796341	-1.312531
158	6	0	-1.867617	9.645102	-0.111375
159	1	0	-0.074701	9.670493	1.086019
160	1	0	-3.590852	9.235005	-1.338280
161	6	0	-2.001633	11.131202	-0.162192
162	6	0	-3.184852	11.774817	0.070215
163	6	0	-0.736856	11.861617	-0.483501
164	6	0	-3.388032	13.224738	-0.231291
165	6	0	-4.378117	11.085499	0.650085
166	6	0	-0.292154	12.932546	0.309933
167	6	0	0.070519	11.453166	-1.559607
168	6	0	-3.038790	13.767454	-1.479507
169	6	0	-3.991874	14.071933	0.714665
170	6	0	-5.648556	11.248888	0.070338
171	6	0	-4.276358	10.308730	1.816547
172	6	0	0.905945	13.585320	0.025227
173	1	0	-0.893540	13.250880	1.155064
174	6	0	1.262641	12.113419	-1.851912
175	1	0	-0.246124	10.614294	-2.172170
176	6	0	-3.265255	15.112984	-1.763808
177	1	0	-2.588928	13.124968	-2.229093
178	6	0	-4.207393	15.420092	0.435093
179	1	0	-4.288236	13.666171	1.677224
180	6	0	-6.770928	10.630095	0.617842
181	1	0	-5.750450	11.863317	-0.819178
182	6	0	-5.400624	9.699813	2.371362
183	1	0	-3.306875	10.186641	2.288133
184	6	0	1.685933	13.182702	-1.060136
185	1	0	1.232198	14.407863	0.655331
186	1	0	1.864029	11.789187	-2.696544
187	6	0	-3.845100	15.946828	-0.806124
188	1	0	-2.991982	15.509321	-2.737608
189	1	0	-4.663581	16.058959	1.186033
190	6	0	-6.651836	9.852601	1.771401
191	1	0	-7.740699	10.759560	0.145654
192	1	0	-5.299015	9.108082	3.276667
193	1	0	2.618643	13.692730	-1.282856
194	1	0	-4.019969	16.995677	-1.027526
195	1	0	-7.527449	9.376618	2.203178

HF=-4280.6046343

Data for truxene **8**:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.805458	5.129814	-0.271012
2	6	0	-0.488153	4.637989	-0.307984
3	1	0	0.338875	5.339360	-0.370413
4	6	0	-0.245484	3.272728	-0.257228
5	6	0	-1.291790	2.334728	-0.188126
6	6	0	-2.607726	2.821465	-0.180315
7	1	0	-3.459495	2.159128	-0.149038
8	6	0	-2.850973	4.192474	-0.220773
9	1	0	-3.876552	4.545531	-0.214375
10	6	0	0.719181	1.113014	-0.195318
11	6	0	-0.696919	0.975030	-0.144116
12	6	0	-1.272207	-0.301666	-0.059306
13	6	0	-0.442514	-1.458243	-0.019597
14	6	0	0.952507	-1.319063	-0.071611
15	6	0	1.539255	-0.024878	-0.163739
16	6	0	1.112974	2.592435	-0.277973
17	6	0	2.038050	-2.401316	-0.044445
18	6	0	-2.751788	-0.697541	0.002000
19	6	0	3.014227	-0.192344	-0.205072
20	6	0	4.092925	0.699942	-0.301487
21	1	0	3.944872	1.766751	-0.373633
22	6	0	5.401686	0.222797	-0.313719
23	1	0	6.219713	0.930968	-0.390260
24	6	0	5.691700	-1.149617	-0.232322
25	6	0	4.607626	-2.043101	-0.160005
26	1	0	4.800894	-3.111026	-0.117217
27	6	0	3.304570	-1.567282	-0.136911
28	6	0	-1.323512	-2.650401	0.071746
29	6	0	-1.088076	-4.031541	0.152595
30	1	0	-0.088784	-4.439535	0.157044
31	6	0	-2.156255	-4.922848	0.232650
32	1	0	-1.950424	-5.986461	0.302509
33	6	0	-3.491507	-4.484047	0.215102
34	6	0	-3.723404	-3.099115	0.153563
35	1	0	-4.744543	-2.732131	0.160248
36	6	0	-2.660127	-2.211446	0.081176
37	6	0	1.811494	2.939578	-1.617340
38	6	0	1.919232	3.056107	0.960986
39	6	0	-3.513633	-0.321284	-1.294420
40	6	0	-3.447664	-0.177768	1.285212
41	6	0	1.971302	-3.333920	-1.279949
42	6	0	2.059082	-3.178018	1.296420
43	1	0	2.051263	4.007303	-1.655306
44	1	0	2.733572	2.379139	-1.771439
45	1	0	1.144621	2.715784	-2.454892
46	1	0	2.157688	4.121894	0.880992
47	1	0	1.325239	2.911670	1.868086

48	1	0	2.853404	2.509052	1.087745
49	1	0	2.086582	-2.748128	-2.196416
50	1	0	2.783751	-4.067159	-1.246005
51	1	0	1.028270	-3.875939	-1.351230
52	1	0	2.245239	-2.488364	2.124772
53	1	0	1.121479	-3.694341	1.502073
54	1	0	2.862763	-3.921864	1.290597
55	1	0	-3.066047	-0.831370	-2.151946
56	1	0	-4.558841	-0.639922	-1.228431
57	1	0	-3.496033	0.749203	-1.499456
58	1	0	-3.432821	0.909131	1.365706
59	1	0	-4.492203	-0.505707	1.308396
60	1	0	-2.948623	-0.581882	2.170782
61	6	0	7.094343	-1.657921	-0.283731
62	6	0	8.103733	-1.126892	0.470035
63	6	0	7.310934	-2.799748	-1.225370
64	6	0	9.544251	-1.449587	0.233656
65	6	0	7.855607	-0.177226	1.597705
66	6	0	7.964921	-3.972267	-0.811409
67	6	0	6.811886	-2.746739	-2.538680
68	6	0	10.109981	-1.372228	-1.050307
69	6	0	10.385472	-1.784630	1.309474
70	6	0	8.605952	1.006388	1.711210
71	6	0	6.915121	-0.464858	2.601313
72	6	0	8.133490	-5.044788	-1.685631
73	1	0	8.341398	-4.037663	0.204083
74	6	0	6.990730	-3.814076	-3.416858
75	1	0	6.285316	-1.856705	-2.869860
76	6	0	11.462212	-1.641358	-1.254461
77	1	0	9.480975	-1.096410	-1.890094
78	6	0	11.734996	-2.065211	1.104035
79	1	0	9.971800	-1.828932	2.312434
80	6	0	8.398566	1.887718	2.770728
81	1	0	9.352980	1.234746	0.956987
82	6	0	6.716225	0.410274	3.667684
83	1	0	6.339819	-1.382750	2.539488
84	6	0	7.652412	-4.968574	-2.993815
85	1	0	8.638451	-5.943212	-1.342238
86	1	0	6.608844	-3.745797	-4.431605
87	6	0	12.279768	-1.994839	-0.179601
88	1	0	11.878359	-1.570503	-2.255396
89	1	0	12.362989	-2.334732	1.948545
90	6	0	7.452333	1.593331	3.754278
91	1	0	8.980452	2.803127	2.830905
92	1	0	5.987324	0.164964	4.434909
93	1	0	7.785662	-5.803674	-3.675391
94	1	0	13.333068	-2.206231	-0.339472
95	1	0	7.295487	2.275712	4.584589
96	6	0	-4.618293	-5.458858	0.312108
97	6	0	-5.714960	-5.399151	-0.502408
98	6	0	-4.454685	-6.504912	1.367792
99	6	0	-6.958097	-6.188987	-0.247629
100	6	0	-5.764405	-4.534527	-1.721361
101	6	0	-4.637676	-7.867826	1.079492
102	6	0	-4.055453	-6.149806	2.668301

103	6	0	-7.571694	-6.199464	1.016652
104	6	0	-7.580096	-6.896185	-1.291814
105	6	0	-6.871518	-3.702523	-1.963533
106	6	0	-4.737327	-4.567479	-2.679576
107	6	0	-4.449482	-8.838864	2.061479
108	1	0	-4.927420	-8.162450	0.076352
109	6	0	-3.878461	-7.119455	3.653589
110	1	0	-3.889093	-5.103141	2.904608
111	6	0	-8.752307	-6.907538	1.233944
112	1	0	-7.116975	-5.644650	1.830529
113	6	0	-8.754374	-7.613839	-1.072019
114	1	0	-7.132736	-6.883163	-2.281112
115	6	0	-6.931795	-2.904003	-3.104553
116	1	0	-7.685429	-3.681099	-1.245047
117	6	0	-4.802809	-3.778566	-3.826791
118	1	0	-3.883456	-5.217000	-2.517365
119	6	0	-4.074664	-8.469030	3.354300
120	1	0	-4.591794	-9.887060	1.814306
121	1	0	-3.582291	-6.820867	4.655253
122	6	0	-9.346360	-7.622435	0.192423
123	1	0	-9.211221	-6.896639	2.218505
124	1	0	-9.210228	-8.163245	-1.890896
125	6	0	-5.897010	-2.938401	-4.041602
126	1	0	-7.790736	-2.258447	-3.264814
127	1	0	-3.999262	-3.823771	-4.556424
128	1	0	-3.929530	-9.225904	4.119659
129	1	0	-10.265680	-8.175236	0.362530
130	1	0	-5.946973	-2.322325	-4.934668
131	6	0	-2.072578	6.596621	-0.345970
132	6	0	-2.958407	7.231382	0.479656
133	6	0	-1.289000	7.321573	-1.393640
134	6	0	-3.422867	8.632060	0.240241
135	6	0	-3.538188	6.581904	1.694844
136	6	0	-0.566611	8.487161	-1.087751
137	6	0	-1.208710	6.816290	-2.703217
138	6	0	-3.901545	9.038252	-1.016922
139	6	0	-3.445436	9.565754	1.291395
140	6	0	-4.918188	6.655706	1.953994
141	6	0	-2.720637	5.934955	2.637159
142	6	0	0.191429	9.136182	-2.060874
143	1	0	-0.601904	8.881951	-0.077783
144	6	0	-0.460288	7.471287	-3.679598
145	1	0	-1.743427	5.904950	-2.953490
146	6	0	-4.365743	10.336435	-1.221213
147	1	0	-3.909298	8.326454	-1.835666
148	6	0	-3.898208	10.867418	1.084473
149	1	0	-3.100010	9.264305	2.275708
150	6	0	-5.465245	6.073965	3.096278
151	1	0	-5.563247	7.170439	1.248306
152	6	0	-3.265775	5.363510	3.785424
153	1	0	-1.650883	5.884058	2.463366
154	6	0	0.243809	8.634577	-3.362497
155	1	0	0.745572	10.033343	-1.799895
156	1	0	-0.423353	7.069919	-4.688439
157	6	0	-4.360886	11.258791	-0.173392

158	1	0	-4.735907	10.626240	-2.200539
159	1	0	-3.894242	11.575683	1.908220
160	6	0	-4.641022	5.425185	4.017664
161	1	0	-6.536192	6.131824	3.269242
162	1	0	-2.613772	4.872889	4.502552
163	1	0	0.833375	9.141253	-4.121041
164	1	0	-4.721116	12.270868	-0.333428
165	1	0	-5.065502	4.978294	4.911972

HF=-3587.4129205

Data for truxene **9**:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.252878	5.346732	-0.462450
2	6	0	1.249825	4.353324	-0.376067
3	1	0	2.292387	4.653633	-0.338632
4	6	0	0.890052	3.015919	-0.340147
5	6	0	-0.456162	2.604455	-0.386363
6	6	0	-1.447034	3.595854	-0.473206
7	1	0	-2.496793	3.349021	-0.513368
8	6	0	-1.095692	4.941026	-0.510683
9	1	0	-1.870467	5.697460	-0.577881
10	6	0	0.849782	0.652833	-0.246954
11	6	0	-0.491905	1.122008	-0.327630
12	6	0	-1.553675	0.204377	-0.337664
13	6	0	-1.290744	-1.193505	-0.272827
14	6	0	0.033005	-1.652852	-0.194206
15	6	0	1.112095	-0.724159	-0.179598
16	6	0	1.832868	1.828596	-0.246712
17	6	0	0.557880	-3.090239	-0.111506
18	6	0	-3.062168	0.466036	-0.408123
19	6	0	2.377920	-1.493422	-0.085878
20	6	0	3.733440	-1.129727	-0.032456
21	1	0	4.047388	-0.097478	-0.059680
22	6	0	4.720936	-2.104998	0.059315
23	1	0	5.764441	-1.810983	0.101063
24	6	0	4.395131	-3.475260	0.100831
25	6	0	3.035037	-3.843070	0.045426
26	1	0	2.770737	-4.895387	0.076857
27	6	0	2.058673	-2.864601	-0.045336
28	6	0	-2.591918	-1.906581	-0.301441
29	6	0	-2.956015	-3.262682	-0.271326
30	1	0	-2.218313	-4.048558	-0.219379
31	6	0	-4.296231	-3.632460	-0.309519
32	1	0	-4.565015	-4.683276	-0.285620
33	6	0	-5.320326	-2.666999	-0.378840
34	6	0	-4.957269	-1.304975	-0.412121

35	1	0	-5.736691	-0.551491	-0.467656
36	6	0	-3.619643	-0.946537	-0.374568
37	6	0	2.748466	1.828167	-1.497053
38	6	0	2.620744	1.933537	1.083676
39	6	0	-3.483925	1.124213	-1.746467
40	6	0	-3.584316	1.229821	0.835044
41	6	0	0.242058	-3.905428	-1.391315
42	6	0	0.111129	-3.804718	1.189338
43	1	0	3.420769	2.692175	-1.475938
44	1	0	3.357557	0.927790	-1.576122
45	1	0	2.141850	1.897142	-2.404429
46	1	0	3.294290	2.796430	1.058371
47	1	0	1.928219	2.072580	1.918654
48	1	0	3.216152	1.045559	1.294899
49	1	0	0.697807	-3.425778	-2.262127
50	1	0	0.656047	-4.915703	-1.308888
51	1	0	-0.826752	-3.992815	-1.585931
52	1	0	0.482640	-3.259796	2.061755
53	1	0	-0.972318	-3.876683	1.282933
54	1	0	0.522780	-4.818546	1.226217
55	1	0	-3.212193	0.475675	-2.584069
56	1	0	-4.568956	1.268861	-1.772116
57	1	0	-3.010308	2.091668	-1.912469
58	1	0	-3.126965	2.212104	0.952809
59	1	0	-4.668656	1.366157	0.768078
60	1	0	-3.373709	0.656266	1.742141
61	6	0	0.597305	6.726179	-0.498857
62	6	0	0.890082	7.907465	-0.528901
63	6	0	5.412941	-4.463682	0.199723
64	6	0	6.278823	-5.314860	0.288469
65	6	0	-6.687310	-3.058026	-0.413911
66	6	0	-7.858230	-3.389927	-0.442349
67	6	0	-9.225017	-3.781266	-0.470407
68	6	0	-9.587561	-5.143058	-0.464956
69	6	0	-10.252579	-2.815927	-0.513578
70	6	0	-10.923853	-5.519491	-0.492173
71	1	0	-8.809694	-5.898875	-0.443054
72	6	0	-11.585787	-3.198986	-0.533414
73	1	0	-9.989165	-1.763792	-0.539954
74	6	0	-11.949072	-4.557353	-0.507265
75	1	0	-11.181226	-6.574034	-0.503543
76	1	0	-12.357870	-2.439109	-0.576474
77	6	0	-13.377652	-4.980796	-0.560454
78	6	0	-14.423791	-4.399497	0.110249
79	6	0	-13.610199	-6.122241	-1.403647
80	7	0	-13.708333	-7.069036	-2.075261
81	6	0	-14.212940	-3.401389	1.195741
82	6	0	-13.302219	-3.642659	2.238699
83	6	0	-14.970850	-2.217788	1.225928
84	6	0	-13.142269	-2.719236	3.269398
85	1	0	-12.726931	-4.562341	2.240754
86	6	0	-14.796525	-1.287039	2.248506
87	1	0	-15.692363	-2.027961	0.437421
88	6	0	-13.882320	-1.535033	3.273998
89	1	0	-12.440559	-2.926501	4.071818

90	1	0	-15.379968	-0.371084	2.247569
91	1	0	-13.753056	-0.814313	4.075970
92	6	0	-15.837398	-4.762982	-0.175796
93	6	0	-16.318818	-4.860818	-1.492636
94	6	0	-16.733445	-4.992208	0.884768
95	6	0	-17.648834	-5.194903	-1.740276
96	1	0	-15.651642	-4.660033	-2.323806
97	6	0	-18.058295	-5.338780	0.634626
98	1	0	-16.379725	-4.910107	1.907401
99	6	0	-18.521170	-5.440166	-0.679256
100	1	0	-18.003260	-5.259512	-2.764534
101	1	0	-18.730894	-5.528228	1.465902
102	1	0	-19.556638	-5.703159	-0.874072
103	6	0	7.289518	-6.309268	0.395749
104	6	0	6.956053	-7.678141	0.423789
105	6	0	8.650480	-5.951211	0.491869
106	6	0	7.945419	-8.645663	0.537464
107	1	0	5.913491	-7.971346	0.360845
108	6	0	9.634307	-6.923437	0.599283
109	1	0	8.922485	-4.900945	0.492671
110	6	0	9.303998	-8.290472	0.610015
111	1	0	7.664825	-9.693636	0.574674
112	1	0	10.672295	-6.622678	0.685275
113	6	0	10.348782	-9.342418	0.766035
114	6	0	11.586597	-9.356574	0.174307
115	6	0	9.951725	-10.425459	1.624866
116	6	0	12.631343	-10.339259	0.568084
117	6	0	11.950915	-8.422139	-0.926965
118	7	0	9.540721	-11.279596	2.302104
119	6	0	12.918792	-10.603342	1.918273
120	6	0	13.376107	-11.009695	-0.419910
121	6	0	11.103669	-8.237244	-2.033086
122	6	0	13.185018	-7.749198	-0.905987
123	6	0	13.906152	-11.522124	2.268590
124	1	0	12.376080	-10.075781	2.695092
125	6	0	14.352810	-11.937009	-0.067475
126	1	0	13.173730	-10.808721	-1.466973
127	6	0	11.472935	-7.392047	-3.077011
128	1	0	10.158016	-8.767259	-2.073360
129	6	0	13.544843	-6.890456	-1.943049
130	1	0	13.857469	-7.898211	-0.066999
131	6	0	14.622122	-12.195808	1.278396
132	1	0	14.117502	-11.707916	3.317254
133	1	0	14.905876	-12.457066	-0.843984
134	6	0	12.690656	-6.709946	-3.032422
135	1	0	10.809789	-7.268308	-3.927971
136	1	0	14.495783	-6.367482	-1.903086
137	1	0	15.389264	-12.913783	1.552827
138	1	0	12.975213	-6.048252	-3.845121
139	6	0	1.224204	9.289264	-0.561960
140	6	0	0.222601	10.270911	-0.700926
141	6	0	2.566428	9.712239	-0.467338
142	6	0	0.552876	11.619155	-0.735783
143	1	0	-0.813906	9.962151	-0.785701
144	6	0	2.888621	11.061465	-0.495152

145	1	0	3.351053	8.967951	-0.381147
146	6	0	1.888099	12.042367	-0.614682
147	1	0	-0.232344	12.358328	-0.860378
148	1	0	3.928194	11.362799	-0.431100
149	6	0	2.227059	13.492875	-0.679914
150	6	0	3.156323	14.145846	0.089523
151	6	0	1.460812	14.221056	-1.654704
152	6	0	3.569894	15.544266	-0.203798
153	6	0	3.777313	13.517506	1.288433
154	7	0	0.774871	14.743256	-2.438268
155	6	0	3.893504	15.954511	-1.508413
156	6	0	3.668731	16.483728	0.839098
157	6	0	2.993547	12.868505	2.258140
158	6	0	5.163422	13.616339	1.501832
159	6	0	4.285700	17.267001	-1.764251
160	1	0	3.850803	15.238099	-2.321629
161	6	0	4.047749	17.797830	0.578949
162	1	0	3.432231	16.179415	1.853592
163	6	0	3.581084	12.321267	3.396388
164	1	0	1.919747	12.803860	2.118643
165	6	0	5.751557	13.052940	2.632768
166	1	0	5.778486	14.132068	0.771048
167	6	0	4.358865	18.193837	-0.723827
168	1	0	4.537458	17.563195	-2.778042
169	1	0	4.102292	18.513346	1.394034
170	6	0	4.962325	12.404650	3.584424
171	1	0	2.958504	11.831840	4.139413
172	1	0	6.825852	13.126547	2.773677
173	1	0	4.661686	19.217097	-0.925196
174	1	0	5.419148	11.974134	4.470574

HF=-4092.6247552

1) Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648-5652.