Supporting Information

Title: Displacement of Ethene from the Decamethyltitanocene-Ethene Complex with Internal Alkynes, Substituent-Dependent Alkyne-to-Allene Rearrangement, and the Electronic Transition Relevant to Ligand Back-Bonding

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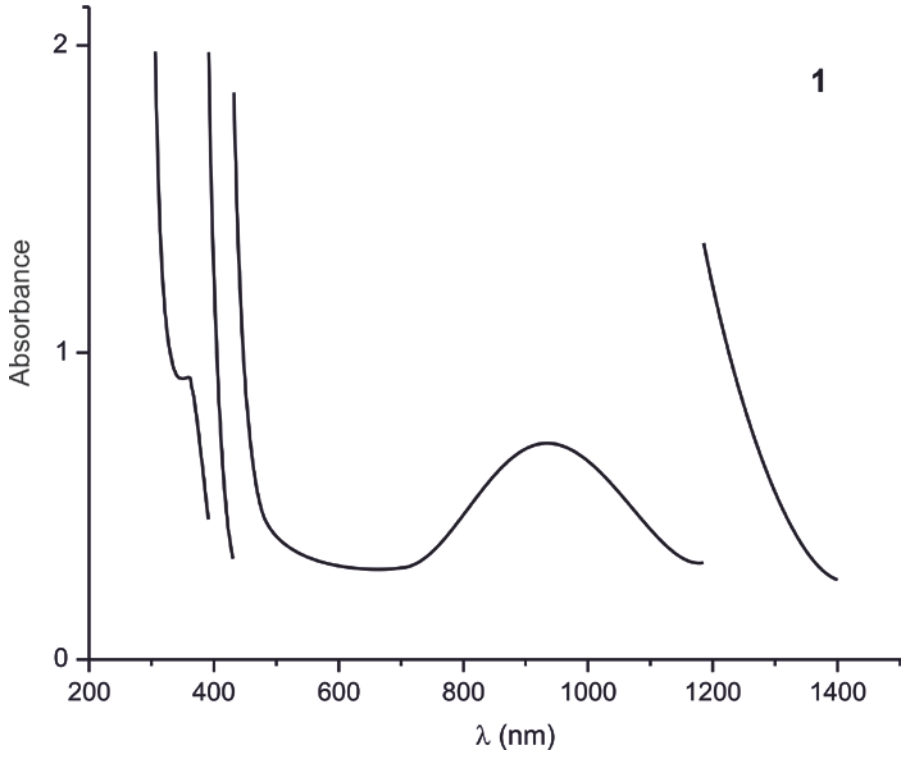
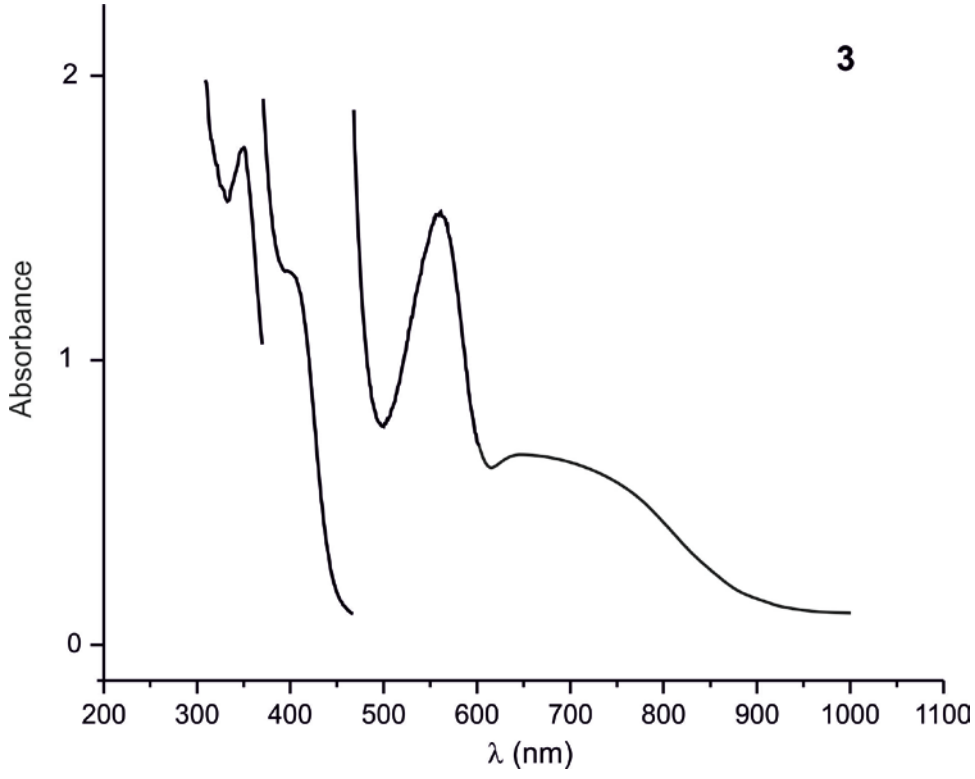
Contents:

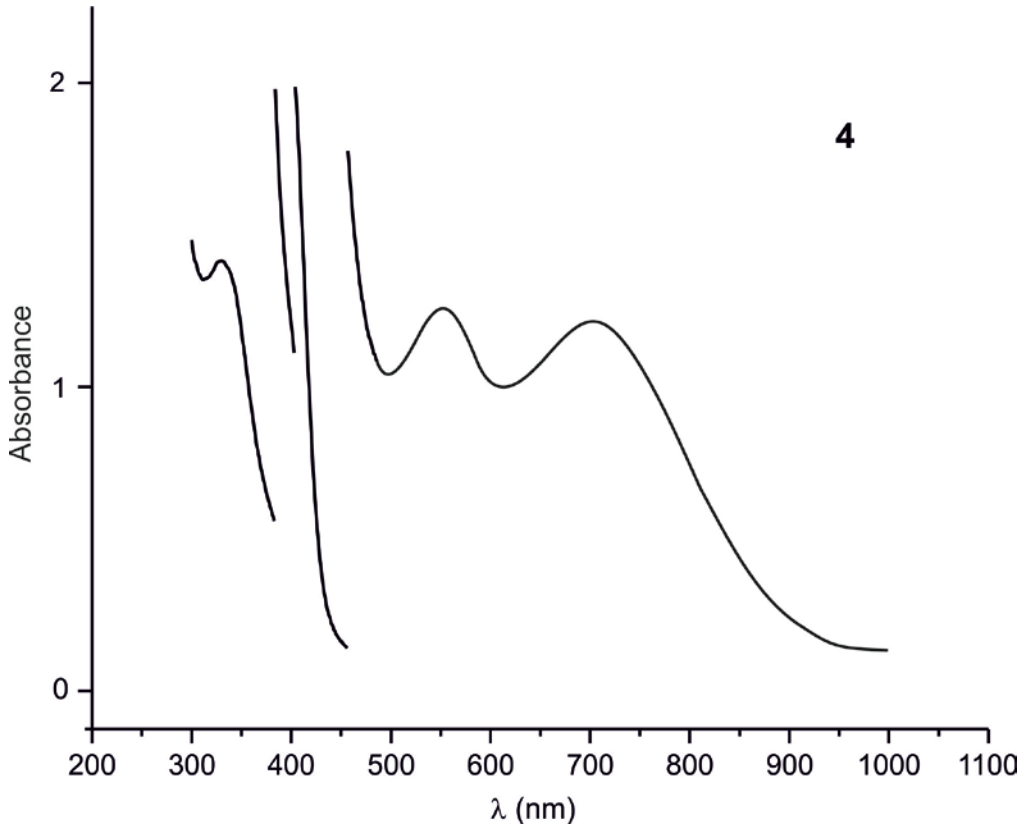
Crystallographic Data and Data Collection and Structure Refinement Details for **4**, **6**, **7**, and **11**

Parameter	**4**	**6**	**7**	**11**
formula	$C_{29}H_{38}Ti$	$C_{31}H_{44}SiTi$	$C_{29}H_{48}SiTi$	$C_{27}H_{42}Ti$
molecular weight	434.49	492.65	472.66	414.51
crystal system	monoclinic	orthorhombic	monoclinic	monoclinic
space group	$P2_1/n$ (No. 14)	$Pca2_1$ (No.29)	$P2_1$ (No. 4)	$P2_1/c$ (No.14)
a (Å)	9.7137(4)	17.9326(6)	19.4682(7)	14.8383(9)
b (Å)	17.1140(6)	9.3275(3)	12.6977(5)	11.7361(7)
c (Å)	14.6646(8)	16.6995(6)	22.4521(9	14.7174(6)
α (°)	90	90	90	90
β (°)	92.480(2)	90	90.201(2)	109.994(2)
γ (°)	90	90	90	90
V (Å^3); Z	2435.56(19); 4	2793.26(16); 4	5550.2(4); 8	2408.5(2); 4
D_{calcd} (g cm^{-3})	1.185	1.171	1.131	1.143
μ (mm^{-1})	0.364	0.366	0.365	0.365
color and habit	green prism	green prism	yellow prism	green prism
cryst size (mm^3)	0.75×0.50×0.22	0.59×0.47×0.34	0.70×0.36×0.32	0.52×0.33×0.24
T (K)	150(2)	150(2)	150(2)	150(2)
$\theta_{min.}$; $\theta_{max.}$ (°)	2.18; 27.50	1.05; 27.50	1.60; 27.50	1.46; 26.00
range of h	−12/12	−17/23	−25/25	−18/18
range of k	−22/21	−12/11	−16/16	−14/10
range of l	−19/12	−21/16	−29/29	−17/18
no. diffrns collected	15753	16306	68429	13395
no. unique diffrns	5604	5418	25472	4742
F(000)	936	1064	2064	904
no. of parameters	282	311	1182	278
$R(F)$; $wR(F^2)$ all data (%)	5.95; 10.17	3.67; 7.68	6.62; 9.74	6.58; 11.15
GooF (F^2), all data	1.018	1.052	1.025	1.045
$R(F)$; $wR(F^2)$ [$I > 2\sigma(I)$]	3.84; 9.23	3.07; 7.44	4.20; 8.68	4.25; 10.12
$\Delta\rho$ (e Å^{-3})	0.429; −0.318	0.272; −0.198	0.301; −0.239	0.487; −0.411

Electronic absorption spectra for **1**, and **3**–**9**



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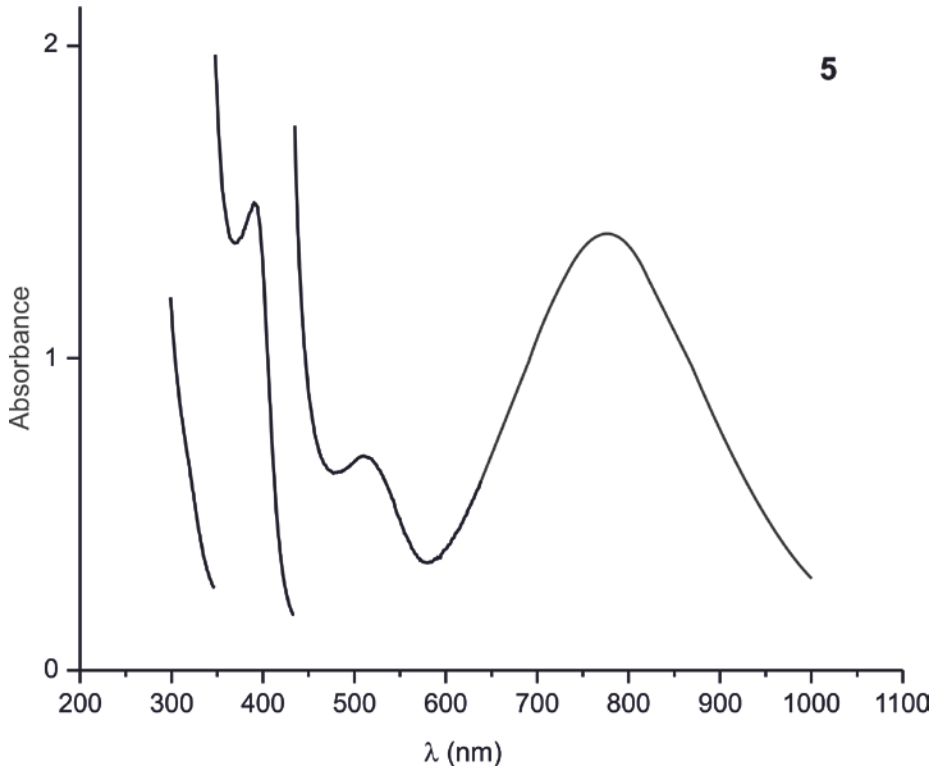
0
1
2
200
300
400
500
600
700
800
900
1000
1100
λ (nm)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1
2
200
300
400
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600
700
800
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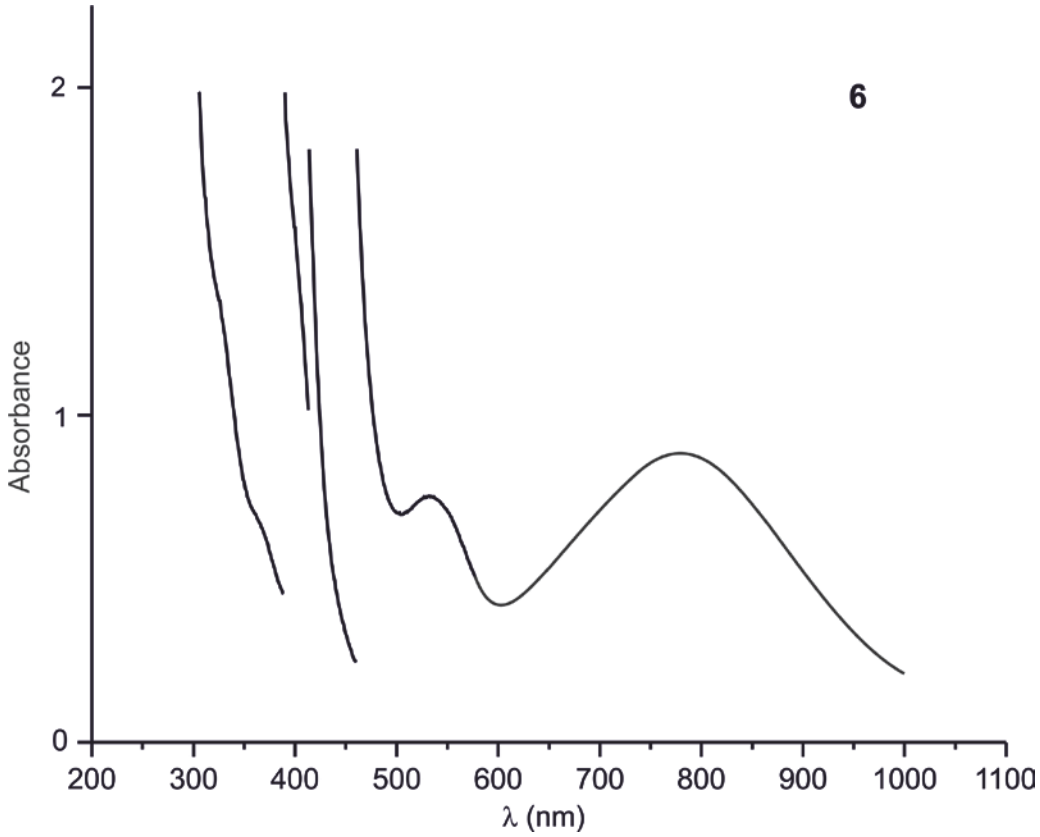
1100
λ (nm)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Absorbance
λ (nm)
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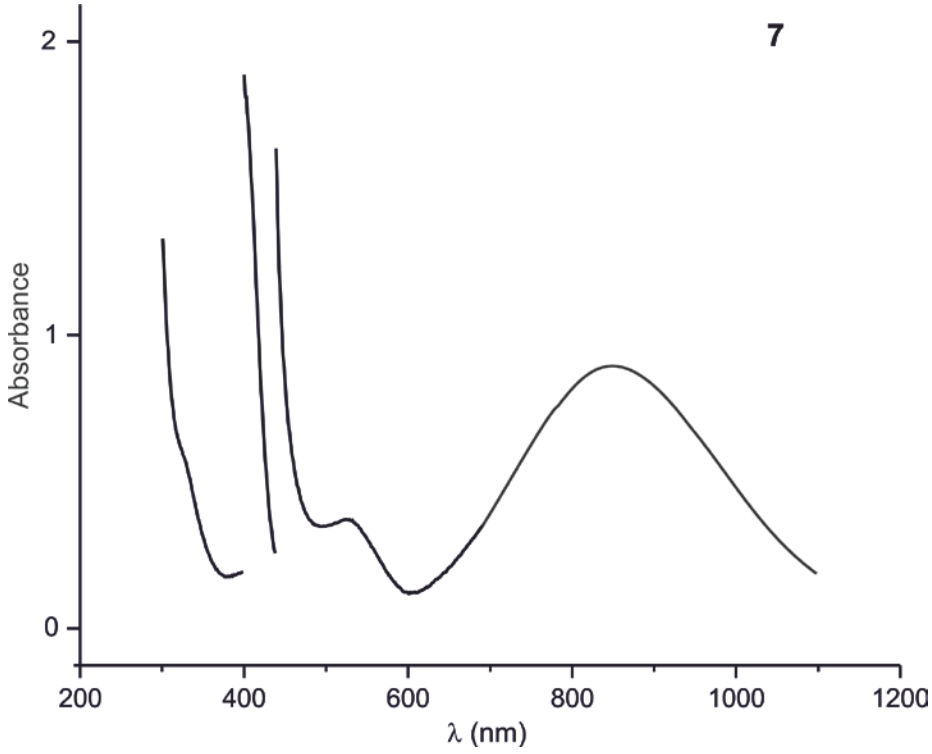
1
2
200
300
400
500
600
700
800
900
1000
1100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Absorbance
λ (nm)
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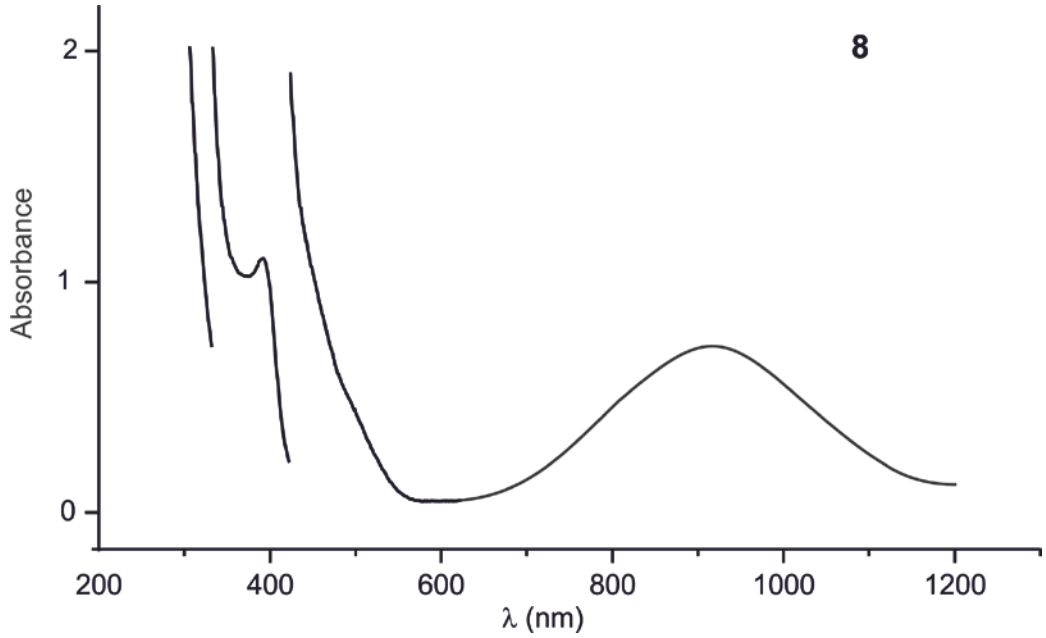
2
200
400
600
800
1000
1200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Absorbance
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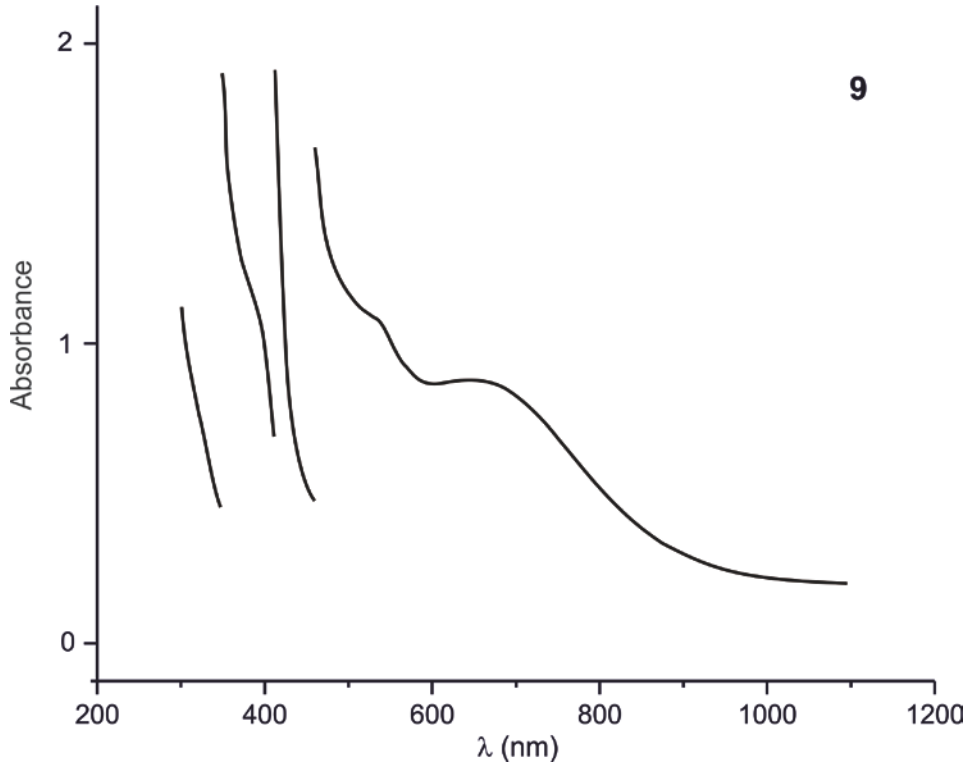
400
600
800
1000
1200
λ (nm)


9
Absorbance
2
1
0
200
400
600
800
1000
1200
λ (nm)

Atom coordinates for optimized molecule **1**

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C	0.646317	0.343513	-2.362298
C	0.083444	1.900834	1.029061
C	-1.147261	1.243862	1.330763
C	-1.961784	1.298294	0.167951
C	-1.272629	2.046570	-0.819728
C	0.000000	2.394327	-0.301985
C	1.165299	2.296296	1.982025
C	-1.631179	0.877372	2.694800
C	-3.330922	0.716235	0.023102
C	-1.839296	2.521044	-2.114464
C	1.029481	3.266441	-0.941400
C	-0.646317	-0.343513	-2.362298
C	-0.083444	-1.900834	1.029061
C	1.147261	-1.243862	1.330763
C	1.961784	-1.298294	0.167951
C	1.272629	-2.046570	-0.819728
C	0.000000	-2.394327	-0.301985
C	-1.165299	-2.296296	1.982025
C	1.631179	-0.877372	2.694800
C	3.330922	-0.716235	0.023102
C	1.839296	-2.521044	-2.114464
C	-1.029481	-3.266441	-0.941400
H	0.662552	1.379365	-2.703349
H	-0.662552	-1.379365	-2.703349
H	1.515421	-0.192878	-2.745418
H	-1.515421	0.192878	-2.745418
H	1.975473	-3.610191	-2.085547
H	1.194305	-2.298769	-2.973566
H	2.820696	-2.077034	-2.311764
H	-1.076739	-4.247630	-0.447946
H	-2.032275	-2.823226	-0.882008
H	-0.813804	-3.445137	-1.999676
H	-1.135321	-3.379820	2.163763
H	-1.066584	-1.804268	2.953536
H	-2.168898	-2.073287	1.594647
H	2.130274	-1.743636	3.151304
H	2.361999	-0.062870	2.683105
H	0.821137	-0.589392	3.372393
H	4.114831	-1.474022	0.158168
H	3.473567	-0.268409	-0.968044
H	3.514392	0.070043	0.765135
H	-4.114831	1.474022	0.158168
H	-3.473567	0.268409	-0.968044
H	-3.514392	-0.070043	0.765135
H	-1.975473	3.610191	-2.085547
H	-1.194305	2.298769	-2.973566
H	-2.820696	2.077034	-2.311764
H	1.076739	4.247630	-0.447946
H	2.032275	2.823226	-0.882008
H	0.813804	3.445137	-1.999676
H	1.135321	3.379820	2.163763
H	1.066584	1.804268	2.953536
H	2.168898	2.073287	1.594647
H	-2.130274	1.743636	3.151304
H	-2.361999	0.062870	2.683105
H	-0.821137	0.589392	3.372393

Atom coordinates for optimized molecule **3**

Ti	-0.854929	-0.024930	-0.002461
C	1.086513	0.654481	-0.090820
C	1.109322	-0.655404	0.056161
C	2.084037	-1.735413	0.072281
C	3.355846	-1.586127	-0.509336
C	4.259610	-2.639581	-0.539137
C	3.925634	-3.870686	0.020367
C	2.670864	-4.039866	0.598089
C	1.761335	-2.990640	0.611412
C	-0.517000	0.048647	-2.428781
C	-1.617921	0.885622	-2.116842
C	-2.673173	0.069638	-1.621340
C	-2.189972	-1.262260	-1.544115
C	-0.853184	-1.273476	-2.043378
C	-0.060081	-2.506412	-2.327822
C	-1.428370	-0.916166	2.179523
C	-2.590123	-0.265214	1.675026
C	-2.285267	1.114523	1.540339
C	-0.945924	1.314660	1.992582
C	-0.438655	0.065458	2.426661
C	0.885993	-0.164086	3.069685
C	2.003805	1.782219	-0.105507
C	3.262138	1.711118	0.518027
C	4.104278	2.814415	0.560360
C	3.720358	4.016626	-0.028490
C	2.478355	4.107158	-0.650538
C	1.630104	3.008221	-0.677346
C	0.751372	0.440163	-3.104543
C	-2.967336	-2.501946	-1.234958
C	-1.360016	-2.364060	2.545477
C	-3.237373	2.235038	1.265867
C	-1.740521	2.349648	-2.395837
C	-0.309820	2.655708	2.162605
C	-4.092746	0.520815	-1.530381
C	-3.938842	-0.903879	1.632468
H	3.624166	-0.626045	-0.951262
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H	4.636712	-4.694804	-0.000849
H	2.394202	-5.001085	1.029622
H	0.764985	-3.131894	1.032517
H	-0.196108	-3.277968	-1.558248
H	1.015611	-2.304667	-2.390088
H	-0.369535	-2.949209	-3.287830
H	1.591970	0.642979	2.841482
H	1.353495	-1.101815	2.744545
H	0.779850	-0.207204	4.163729
H	3.566030	0.773946	0.985614
H	5.071109	2.735171	1.056229
H	4.382490	4.880268	0.003210
H	2.163177	5.045437	-1.105544
H	0.641144	3.086932	-1.131949
H	0.910697	1.525069	-3.100217
H	0.747656	0.106947	-4.152784
H	1.625919	-0.011508	-2.618239
H	-2.506301	-3.107171	-0.438561
H	-3.026120	-3.150754	-2.121452
H	-3.994993	-2.278188	-0.928100
H	-1.623878	-3.026151	1.706364
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H	-0.357394	-2.647536	2.886695
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H	-3.271893	2.919290	2.126396
H	-0.815467	2.758810	-2.819318
H	-1.973844	2.939255	-1.495251
H	-2.546425	2.548268	-3.118010
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Atom coordinates for optimized molecule **4**

Ti	-0.596854	0.013243	0.144853
C	1.415268	0.003411	0.539419
C	0.761711	0.112854	1.676113
C	1.098091	0.235165	3.121431
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C	-0.681274	-2.043665	-1.118486
C	-2.035219	-1.649268	-0.926314
C	-2.292556	-1.646563	0.466994
C	-1.111108	-2.094794	1.131333
C	-1.023730	-2.395794	2.591294
C	-1.484601	2.148109	0.811169
C	-2.293137	1.650475	-0.254775
C	-1.483212	1.591660	-1.419936
C	-0.184828	2.068314	-1.070170
C	-0.211060	2.470419	0.285023
C	0.925288	3.118376	0.995860
C	2.801062	-0.048035	0.100032
C	3.863832	0.205723	0.985140
C	5.183901	0.150277	0.557027
C	5.482164	-0.163635	-0.766561
C	4.444795	-0.417420	-1.659534
C	3.125700	-0.355393	-1.230708
C	1.199463	-2.989459	0.414920
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C	-1.935173	1.389521	-2.830614
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Atom coordinates for optimized molecule **5**

Ti	0.479682	-0.000208	-0.107635
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C	-1.504002	0.181425	-2.888807
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C	0.873052	-1.971094	1.212637
C	2.167790	-1.575607	0.778779
C	2.182795	-1.630305	-0.638607
C	0.920996	-2.131485	-1.075824
C	0.604636	-2.530261	-2.478827
C	1.282746	2.129546	-0.971254
C	2.182358	1.680396	0.040147
C	1.473802	1.658158	1.271818
C	0.148728	2.121642	1.014332
C	0.059439	2.477676	-0.350328
C	-1.124895	3.106495	-0.996038
Si	-3.335741	-0.146089	0.303592
C	-1.195216	-3.048693	0.087755
C	3.365992	-1.468615	-1.538880
C	1.645622	2.305794	-2.411541
C	2.031917	1.489248	2.649258

C	0.391651	-2.060604	2.626045
C	-0.893853	2.344235	2.059932
C	3.359687	-1.424678	1.663839
C	3.660088	1.604951	-0.161233
H	0.993526	-1.806628	-3.209140
H	-0.475846	-2.619643	-2.645129
H	1.053460	-3.506198	-2.722375
H	-1.931797	2.380256	-1.167704
H	-0.868579	3.558021	-1.962533
H	-1.532576	3.904584	-0.360281
H	-1.766339	-2.809869	0.994483
H	-1.073436	-4.142232	0.056781
H	-1.808733	-2.758126	-0.774252
H	3.170344	-0.798783	-2.389755
H	3.655757	-2.439099	-1.969968
H	4.242426	-1.077483	-1.009583
H	1.896222	1.351625	-2.901554
H	2.517894	2.965279	-2.531027
H	0.819956	2.745967	-2.983135
H	3.084366	1.186819	2.634726
H	1.481114	0.748365	3.247879
H	1.977750	2.439382	3.201974
H	-0.616323	-1.634540	2.742215
H	1.054960	-1.527642	3.318752
H	0.338062	-3.104401	2.969751
H	-0.847313	1.578543	2.846874
H	-1.907297	2.318262	1.640511
H	-0.766789	3.320020	2.555199
H	3.120617	-0.975231	2.633323
H	4.157507	-0.829143	1.206453
H	3.788062	-2.416952	1.872770
H	4.181740	1.130479	0.677058
H	4.073946	2.621088	-0.256681
H	3.935899	1.067188	-1.076093
H	-2.601596	0.120086	-2.976240
H	-1.196883	1.157094	-3.297587
H	-1.071050	-0.573401	-3.561005
C	-4.343643	-1.471955	-0.595596
C	-3.453526	-0.503683	2.153778
C	-4.253081	1.477727	-0.023198
H	-5.413346	-1.338477	-0.379206
H	-4.214987	-1.408206	-1.684693
H	-4.066615	-2.487487	-0.285914
H	-4.502928	-0.486396	2.480221
H	-3.051080	-1.494881	2.406251
H	-2.907629	0.241114	2.748144
H	-5.292036	1.386406	0.325687
H	-3.809931	2.344960	0.483505
H	-4.284258	1.701485	-1.098909

Atom coordinates for optimized molecule **6**

Ti	-0.817991	-0.037617	-0.008709
C	1.211791	-0.302803	-0.110839
C	0.997899	0.997778	-0.021990

Si	2.010694	2.551504	0.054956
C	-0.244663	-0.436183	2.370707
C	-1.004328	-1.536311	1.904893
C	-2.316405	-1.073611	1.598501
C	-2.337462	0.332883	1.791552
C	-1.045036	0.724330	2.255641
C	-0.696196	2.099474	2.718382
C	-2.098655	1.027182	-1.733914
C	-2.759118	-0.209766	-1.508067
C	-1.841370	-1.250973	-1.814438
C	-0.647549	-0.655037	-2.315217
C	-0.816127	0.749914	-2.275019
C	0.121524	1.741049	-2.866605
C	2.338797	-1.227593	-0.144449
C	3.667558	-0.792104	-0.016319
C	4.725217	-1.691066	-0.033788
C	4.484987	-3.055168	-0.177821
C	3.175473	-3.510333	-0.300674
C	2.120917	-2.606691	-0.281532
C	1.133587	-0.483743	2.931731
C	-3.523382	1.243972	1.792039
C	-2.677314	2.398167	-1.579868
C	-2.102620	-2.723542	-1.816846
C	-0.596639	-2.974319	1.915989
C	0.478247	-1.364956	-2.988934
C	-3.491627	-1.984732	1.456446
C	-4.224284	-0.361650	-1.266289
H	-1.149490	2.874409	2.084949
H	0.386987	2.268833	2.718372
H	-1.055084	2.275620	3.744679
H	1.166702	1.438819	-2.726793
H	0.000352	2.739374	-2.426632
H	-0.049547	1.837490	-3.950144
H	3.864627	0.272420	0.104919
H	5.746126	-1.325244	0.068260
H	5.314631	-3.760073	-0.190610
H	2.975601	-4.575422	-0.411055
H	1.092229	-2.958210	-0.372665
H	1.673489	-1.390517	2.633339
H	1.099562	-0.462927	4.030988
H	1.738103	0.370951	2.603276
H	-3.410552	2.094048	1.104666
H	-3.679137	1.669873	2.794497
H	-4.445257	0.717867	1.519826
H	-3.671405	2.374604	-1.117022
H	-2.786861	2.894371	-2.555569
H	-2.039516	3.053020	-0.964554
H	-3.074455	-2.973904	-1.375662
H	-1.332946	-3.285358	-1.264939
H	-2.103194	-3.120964	-2.842610
H	0.493523	-3.091248	1.928746
H	-0.973612	-3.520421	1.038167
H	-0.995051	-3.491453	2.802697
H	0.553847	-2.414083	-2.678013
H	1.448484	-0.893857	-2.783029
H	0.336748	-1.356755	-4.081031
H	-3.358951	-2.756782	0.687668

H	-4.417565	-1.444782	1.233488
H	-3.654822	-2.518637	2.405507
H	-4.493517	-1.371325	-0.939546
H	-4.769373	-0.172689	-2.203624
H	-4.619521	0.345262	-0.526785
C	3.216963	2.678006	-1.403680
C	0.952146	4.115651	0.033286
C	3.055673	2.658149	1.633177
H	1.600957	5.002904	0.012092
H	0.299605	4.166966	-0.848943
H	0.316866	4.194333	0.925359
H	4.075809	3.308609	-1.133536
H	3.605136	1.698319	-1.713981
H	2.734706	3.134918	-2.277798
H	3.676384	3.564927	1.583405
H	2.445646	2.734764	2.542990
H	3.731783	1.802624	1.762528

Atom coordinates for optimized molecule **7**

Ti	-0.628212	0.053132	0.003645
Si	2.868653	-1.404222	-0.225090
C	2.071511	2.286357	0.258064
C	1.429934	-0.238967	-0.056850
C	1.196094	1.049426	0.108749
C	2.345852	-3.090932	-0.900855
C	3.764767	-1.733521	1.413171
C	4.229188	-0.789461	-1.389854
C	-2.395116	0.086496	1.663721
C	-2.005704	-1.265910	1.485881
C	-0.665810	-1.394743	1.953054
C	-0.259671	-0.148309	2.482607
C	-1.296625	0.783474	2.249180
C	-3.778772	0.646356	1.631671
C	-2.885927	-2.445317	1.225656
C	0.057003	-2.694418	2.075510
C	1.015022	0.081581	3.209891
C	-1.379958	2.198231	2.722798
C	-0.328668	-0.056264	-2.412565
C	-1.238940	-1.082198	-2.045687
C	-2.444751	-0.466130	-1.609877
C	-2.235291	0.931654	-1.588851
C	-0.930286	1.188391	-2.104781
C	0.975507	-0.227440	-3.106855
C	-1.051719	-2.553202	-2.234350
C	-3.764964	-1.157412	-1.549330
C	-3.249897	2.002627	-1.353150
C	-0.479893	2.535835	-2.563988
H	4.627439	-2.380071	1.201889
H	4.147873	-0.810691	1.864622
H	3.153310	-2.243221	2.166022
H	4.982386	-1.581568	-1.500162
H	3.851899	-0.550115	-2.390945
H	4.742926	0.097314	-1.000152
H	3.151920	-3.818787	-0.741353
H	1.441660	-3.477281	-0.416676
H	2.158355	-3.050495	-1.981334
H	0.879991	0.016095	-4.173932

H	1.749208	0.422363	-2.682657
H	1.340202	-1.258090	-3.039134
H	-1.186102	2.933131	-3.307684
H	-0.416724	3.279135	-1.760113
H	0.497444	2.482507	-3.051597
H	-3.489990	2.520403	-2.292746
H	-4.188211	1.606941	-0.952385
H	-2.888871	2.773205	-0.657028
H	-4.229312	-1.114716	-2.545309
H	-3.675522	-2.215360	-1.290630
H	-4.473531	-0.693712	-0.857065
H	-1.645104	-2.925770	-3.080786
H	-0.005226	-2.807573	-2.428373
H	-1.362233	-3.129084	-1.350985
H	1.042000	-0.520326	4.128418
H	1.883208	-0.201291	2.604441
H	1.137187	1.130668	3.502502
H	-2.192059	2.312981	3.454272
H	-0.454874	2.517232	3.212850
H	-1.579861	2.908559	1.909369
H	-4.202553	0.645485	2.646788
H	-3.804498	1.684335	1.282567
H	-4.461465	0.065917	1.005127
H	-2.930109	-3.072743	2.126820
H	-3.911870	-2.153669	0.986836
H	-2.525473	-3.093438	0.415649
H	-0.221728	-3.214666	3.003985
H	-0.183578	-3.374249	1.248304
H	1.143401	-2.564455	2.088172
C	1.270095	3.479842	0.774344
C	3.230727	2.031077	1.228992
C	2.698645	2.666356	-1.089965
H	3.414460	3.487313	-0.944616
H	3.241754	1.821439	-1.530026
H	1.951359	3.009999	-1.809823
H	1.882795	4.391664	0.774983
H	0.383926	3.664247	0.152662
H	0.925737	3.307805	1.800646
H	3.830799	2.944276	1.344330
H	2.876753	1.734475	2.221821
H	3.896303	1.243197	0.855536

Atom coordinates for optimized molecule **8**

Ti	0.793976	-0.016793	-0.006201
Si	-2.481601	1.986131	0.033582
Si	-2.545978	-1.947151	-0.068828
C	-1.177954	0.651677	0.004018
C	-1.184745	-0.671810	-0.043350
C	-1.771150	3.681184	-0.395204
C	-3.319205	2.164893	1.722348
C	-3.887643	1.641614	-1.183155
C	-1.937953	-3.680487	0.364203
C	-3.917736	-1.531738	1.164469
C	-3.399171	-2.087034	-1.754884
C	2.490044	-0.647860	1.593583
C	2.307361	0.757359	1.675857
C	0.988145	0.996120	2.163795

C	0.380711	-0.255884	2.421832
C	1.279142	-1.268998	2.011702
C	3.780139	-1.385290	1.457135
C	3.363588	1.812915	1.620746
C	0.457627	2.347419	2.509624
C	-0.945389	-0.461441	3.062029
C	1.082371	-2.746948	2.105019
C	0.489343	0.470158	-2.375475
C	1.563735	1.267278	-1.906460
C	2.639927	0.402290	-1.564974
C	2.191322	-0.932916	-1.722004
C	0.856134	-0.889674	-2.221223
C	-0.765270	0.950758	-3.012823
C	1.630724	2.760215	-1.877594
C	4.050827	0.858962	-1.401423
C	3.006429	-2.183444	-1.656656
C	0.089616	-2.081467	-2.685861
H	-4.672302	-2.329316	1.152114
H	-3.545925	-1.438462	2.191095
H	-4.423500	-0.593964	0.904033
H	-2.729674	-4.409887	0.149171
H	-1.052159	-3.968508	-0.215240
H	-1.689356	-3.773743	1.428052
H	-4.374151	-2.571592	-1.610345
H	-3.582342	-1.114197	-2.226870
H	-2.829084	-2.706974	-2.455864
H	-4.154935	2.869577	1.614264
H	-3.732476	1.216640	2.085930
H	-2.658853	2.566632	2.498908
H	-4.651331	2.425205	-1.090928
H	-3.545909	1.631334	-2.224533
H	-4.374978	0.679872	-0.981012
H	-2.521861	4.459696	-0.208530
H	-0.887769	3.914843	0.211247
H	-1.483326	3.751862	-1.451257
H	-0.711343	0.828797	-4.103140
H	-1.639910	0.393666	-2.659091
H	-0.946595	2.012694	-2.812481
H	0.515654	-2.491636	-3.613106
H	0.091393	-2.890328	-1.942818
H	-0.954010	-1.826924	-2.890786
H	3.131288	-2.611500	-2.661223
H	4.008005	-2.007371	-1.252820
H	2.532433	-2.962872	-1.043969
H	4.513867	0.960407	-2.393625
H	4.119581	1.839277	-0.920561
H	4.673162	0.159956	-0.834088
H	2.336648	3.147128	-2.625397
H	0.655383	3.213572	-2.080458
H	1.963019	3.140315	-0.900772
H	-0.866360	-0.336069	4.150359
H	-1.693656	0.250029	2.697018
H	-1.334260	-1.469256	2.875709
H	1.721941	-3.187649	2.882408
H	0.046017	-3.000685	2.345983
H	1.325402	-3.258790	1.162710
H	4.216603	-1.547743	2.453527

H	3.649596	-2.375963	1.008433
H	4.527330	-0.844447	0.870503
H	3.533802	2.221470	2.626902
H	4.320742	1.420967	1.266667
H	3.094326	2.666415	0.984123
H	0.899489	2.722551	3.444301
H	0.681270	3.088508	1.730202
H	-0.628075	2.333084	2.643465

Atom coordinates for optimized molecule **9**

Ti	0.015752	0.147180	-0.002504
C	0.359925	2.045962	0.651844
C	-1.914382	-0.931855	-0.935008
C	-2.155419	0.474195	-0.966550
C	-2.284093	0.927273	0.367164
C	-2.045245	-0.174904	1.227834
C	-1.882734	-1.338125	0.423365
C	0.359077	2.044230	-0.662339
C	1.415094	-1.608967	0.826799
C	2.121188	-0.390464	1.057008
C	2.503322	0.143239	-0.195636
C	1.946077	-0.678346	-1.204747
C	1.322598	-1.797035	-0.575802
C	0.592176	3.075110	1.701277
C	0.598064	3.072283	-1.710962
C	-1.994243	-1.810823	-2.141204
C	-2.407530	1.268372	-2.205634
C	-2.651956	2.313763	0.766537
C	-2.063901	-0.145634	2.723060
C	1.120938	-2.596647	1.908846
C	2.526548	0.111819	2.404606
C	3.340656	1.359926	-0.388350
C	2.061156	-0.499410	-2.684891
C	0.961219	-3.052787	-1.297732
C	-1.981964	-2.740895	0.923296
H	1.446978	2.817137	2.344365
H	0.790861	4.073499	1.274443
H	-0.270572	3.174593	2.377257
H	-0.307116	3.272502	-2.303201
H	0.930477	4.035068	-1.286067
H	1.363144	2.750798	-2.434472
H	2.739215	-1.241433	-3.133271
H	1.088990	-0.612931	-3.188669
H	2.441145	0.494950	-2.947695
H	4.343501	1.208104	0.035832
H	3.470154	1.603295	-1.449758
H	2.902501	2.243918	0.096265
H	3.258642	-0.561522	2.877143
H	2.989288	1.103902	2.340076
H	1.674169	0.192299	3.095538
H	2.058462	-2.955019	2.361089
H	0.526684	-2.163760	2.727181
H	0.585494	-3.477649	1.539088
H	-3.008834	-1.781720	-2.567645

H	-1.312491	-1.496666	-2.945202
H	-1.773472	-2.857514	-1.906287
H	-3.395710	1.036742	-2.633585
H	-2.383734	2.345966	-2.003152
H	-1.662260	1.065233	-2.988179
H	-3.679187	2.545972	0.449834
H	-2.609443	2.451157	1.853920
H	-1.985986	3.060726	0.311646
H	-3.069689	-0.336693	3.126561
H	-1.397830	-0.906309	3.153305
H	-1.733457	0.825216	3.115856
H	-3.035077	-3.062548	0.914047
H	-1.428832	-3.459727	0.307929
H	-1.631405	-2.846913	1.956654
H	1.868311	-3.647801	-1.487721
H	0.277176	-3.693675	-0.729525
H	0.503944	-2.858818	-2.275207

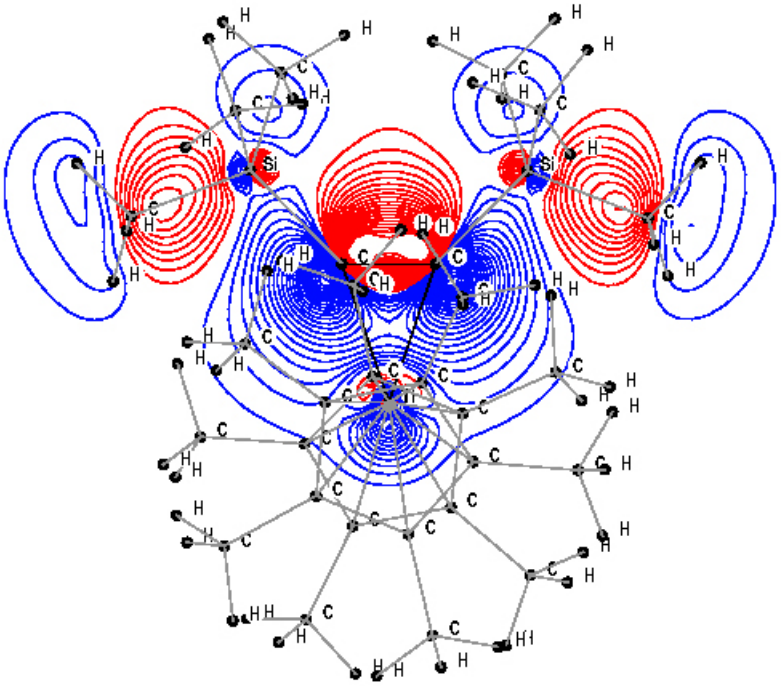
Atom coordinates for optimized molecule **11**

Ti	0.563239	0.001102	-0.164257
C	0.039478	-2.385517	-0.454433
C	1.248330	-2.079271	-1.126621
C	2.208617	-1.683908	-0.154626
C	1.565668	-1.694568	1.120849
C	0.220513	-2.108349	0.925301
C	-1.188129	-2.996382	-1.034731
C	1.516341	-2.177011	-2.593753
C	3.676316	-1.603722	-0.417211
C	2.216801	-1.606986	2.463489
C	-0.766762	-2.359393	2.014929
C	0.934286	2.183416	-1.033978
C	2.174466	1.674347	-0.557601
C	2.085445	1.557201	0.860034
C	0.769808	1.924916	1.243261
C	0.070497	2.348105	0.080764
C	0.700904	2.627998	-2.440083
C	3.400349	1.545255	-1.403668
C	3.242499	1.383914	1.786330
C	0.195890	1.908125	2.623300
C	-1.255896	3.027540	0.077707
C	-1.059042	0.074138	-1.567202
C	-1.515432	0.051290	-0.190848
C	-2.643773	0.036224	0.517397
C	-4.093643	0.067112	0.061105
C	-4.241530	0.070602	-1.454354
C	-4.809259	-1.156972	0.641548
C	-4.751852	1.326722	0.634685
H	-1.332492	-4.003493	-0.622353
H	-1.127660	-3.096551	-2.122995
H	-2.083541	-2.410914	-0.791162
H	2.021354	-1.277052	-2.973563
H	0.591132	-2.287283	-3.167840
H	2.163999	-3.031643	-2.832230
H	4.118075	-2.609620	-0.376779

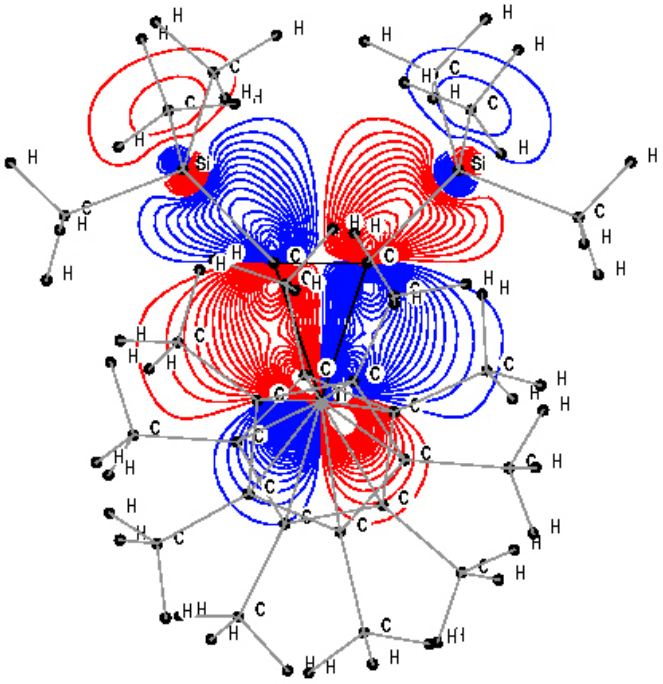
H	4.212609	-0.994173	0.317223
H	3.898418	-1.201830	-1.411830
H	1.669408	-0.959912	3.161411
H	3.243991	-1.237542	2.402465
H	2.257578	-2.602708	2.926640
H	-0.598739	-3.340440	2.482258
H	-1.795427	-2.333388	1.641072
H	-0.691885	-1.606589	2.811131
H	-0.336996	2.932241	-2.607572
H	0.933571	1.838269	-3.166261
H	1.333756	3.493116	-2.683013
H	3.743620	2.531893	-1.744996
H	3.218044	0.946583	-2.307210
H	4.231274	1.080414	-0.863774
H	3.748856	2.350423	1.915876
H	3.995141	0.683280	1.411902
H	2.937490	1.048880	2.781790
H	-0.031413	2.921152	2.980509
H	0.886127	1.457239	3.344577
H	-0.742760	1.336856	2.658219
H	-1.864738	2.728261	0.936607
H	-1.838732	2.806727	-0.823760
H	-1.117409	4.117092	0.121597
H	-1.282470	-0.794736	-2.191527
H	-1.224963	0.995622	-2.130308
H	-2.570812	0.017210	1.617056
H	-5.302972	0.132409	-1.731107
H	-3.828951	-0.841274	-1.902490
H	-3.719702	0.924055	-1.902862
H	-5.882516	-1.134268	0.406333
H	-4.705864	-1.191402	1.734820
H	-4.394542	-2.089444	0.236566
H	-4.310903	2.234900	0.204576
H	-4.625989	1.375174	1.724966
H	-5.829575	1.339257	0.420162

Projections of MO orbitals Ψ1, Ψ2, and Ψ3 onto the plane containing the titanium and acetylenic carbons.

orbital Ψ_1



orbital Ψ_2



orbital Ψ_3