Predicting Pt-195 NMR Chemical Shift and $^{1}J(^{195}Pt-^{31}P)$ Coupling Constant for Pt(0) Complexes using the NMR-DKH Basis Sets

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SUPPLEMENTARY MATERIAL

Optimized structure of Pt(0) complexes studied in the present paper - XYZ format

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Complex 01 - $[Pt(PPr^{i}_{3})_2]$

Pt	-0.012491	0.063402	0.010625
P	-2.318739	0.015232	-0.018680
P	2.292419	0.109391	-0.001215
C	-3.020062	-1.209414	-1.267550
H	-4.116683	-1.214501	-1.152019
C	-2.491604	-2.623830	-0.987059
H	-1.394007	-2.652129	-1.074666
H	-2.752219	-2.980674	0.020232
H	-2.917319	-3.338174	-1.712316
C	-2.682003	-0.783479	-2.703659
H	-3.161997	0.165136	-2.987893
H	-1.593269	-0.664746	-2.830967
H	-3.027283	-1.552501	-3.415635
C	-3.070096	1.672723	-0.527092
H	-2.621741	1.821506	-1.523803
C	-4.596070	1.734787	-0.670398
H	-4.890455	2.702666	-1.110384
H	-5.000149	0.944509	-1.321501
H	-5.099815	1.660963	0.306130
C	-2.548827	2.802672	0.372504
H	-2.953952	2.731988	1.395739
H	-1.451114	2.783009	0.440822
H	-2.857060	3.781614	-0.031415
C	-3.162135	-0.390292	1.633696
H	-3.283004	0.610696	2.082943
C	-4.551288	-1.040183	1.549037
H	-4.994264	-1.099353	2.556374
H	-5.249940	-0.479518	0.914652
H	-4.497354	-2.069063	1.162511
C	-2.232851	-1.190119	2.559440
H	-1.253577	-0.700147	2.661606
H	-2.687327	-1.289876	3.560107
H	-2.050920	-2.205957	2.173526
C	3.026779	1.843057	-0.084017
H	4.124926	1.738045	-0.059200
C	2.587662	2.675778	1.129143
H	1.489952	2.767354	1.160509
H	2.915661	2.240298	2.085043
H	3.015629	3.690302	1.065394
C	2.633782	2.546784	-1.391352
H	3.059995	2.057986	-2.280535
H	1.537822	2.568100	-1.508854
H	2.998919	3.587458	-1.384504
C	3.030544	-0.608838	1.586732
H	2.471261	-0.030130	2.341586
C	4.527565	-0.392883	1.848135
H	4.825528	0.663379	1.783444
H	4.776858	-0.737236	2.866031
H	5.157947	-0.963775	1.151608
C	2.634444	-2.079767	1.776269
H	1.560665	-2.232951	1.586603
H	3.200941	-2.744827	1.105756
H	2.852044	-2.398179	2.809756
C	3.042802	-0.739637	-1.514108
H	2.665608	-0.076461	-2.309453
C	4.574104	-0.774654	-1.616966
H	5.013137	-1.509048	-0.925836
H	4.873162	-1.073024	-2.636077
H	5.040111	0.201489	-1.413001
C	2.431831	-2.122915	-1.778753
H	1.330652	-2.087172	-1.719745
H	2.717854	-2.473493	-2.785085
H	2.786388	-2.876979	-1.061837

Complex 2 - $[Pt(Pcy_3)_2]$, cy = cyclohexil

Pt	0.000108	0.028008	-0.008690
P	-2.303969	0.015533	0.012426
P	2.302480	-0.003801	-0.014265
C	-3.245535	4.265844	2.026749
H	-3.790697	5.049828	2.579652
H	-2.265912	4.699555	1.753558
C	-3.020209	3.036584	2.912013
H	-3.993613	2.682233	3.300124
H	-2.414246	3.303383	3.794628
C	-2.334908	1.900371	2.138866
H	-1.326119	2.218010	1.822864
H	-2.180333	1.038526	2.801315
C	-4.002639	3.888562	0.749625
H	-4.103519	4.765693	0.087828
H	-5.031136	3.579292	1.013819
C	-3.315130	2.744676	-0.013896
H	-3.910109	2.507679	-0.907816
H	-2.327798	3.090109	-0.368790
C	-3.124490	1.497670	0.873996
H	-4.131804	1.150038	1.172550
C	-3.149052	-3.887228	2.668467
H	-2.157616	-3.868866	3.157291
H	-3.679028	-4.767448	3.070741
C	-2.958398	-4.016065	1.154059
H	-3.942708	-4.172082	0.673771
H	-2.353213	-4.907064	0.915433
C	-3.905876	-2.601569	3.017617
H	-3.980774	-2.483915	4.112288
H	-4.943651	-2.677402	2.642713
C	-3.243792	-1.353573	2.409668
H	-3.842479	-0.469614	2.674297
H	-2.246414	-1.214744	2.863358
C	-3.088922	-1.479921	0.880881
H	-4.106592	-1.571588	0.456866
C	-2.294402	-2.765606	0.561712
H	-1.277733	-2.647852	0.976195
H	-2.158048	-2.890184	-0.521090
C	-3.411124	-1.378690	-2.316459
H	-4.009869	-2.011843	-1.644772
H	-2.449712	-1.898422	-2.475228
C	-3.150298	0.007372	-1.691982
H	-4.139775	0.475106	-1.528992
C	-4.140666	-1.256814	-3.664675
H	-5.143715	-0.822886	-3.493800
H	-4.306206	-2.262046	-4.088955
C	-3.370864	-0.378346	-4.656321
H	-3.940368	-0.268383	-5.595208
H	-2.421881	-0.879590	-4.922947
C	-3.060640	0.994193	-4.048822
H	-4.003877	1.557601	-3.917564
H	-2.439509	1.588736	-4.740643
C	-2.349729	0.869146	-2.692972
H	-1.358440	0.400467	-2.826490
H	-2.148862	1.869008	-2.282324
C	2.957376	-1.616158	3.859771
H	2.326462	-2.319988	4.429319
H	3.914832	-2.138601	3.674470
C	3.222525	-0.350560	4.681730
H	3.759429	-0.597461	5.613531
H	2.256358	0.093202	4.985571
C	4.012842	0.677081	3.864976
H	5.029303	0.285529	3.672316
H	4.144239	1.609093	4.441207
C	3.334881	0.994682	2.522022
H	2.360538	1.478030	2.713160
H	3.952074	1.723309	1.975788
C	3.108524	-0.280331	1.684344
H	4.104629	-0.712820	1.472538
C	2.286540	-1.288903	2.517935
H	2.104581	-2.216113	1.957188
H	1.289072	-0.848547	2.692832
C	3.094798	-1.361072	-1.082867
H	4.113057	-0.997321	-1.318792
C	2.311585	-1.545384	-2.401084
H	2.179470	-0.587695	-2.922550
H	1.292340	-1.885868	-2.145580
C	2.987388	-2.558494	-3.336809
H	3.971881	-2.164624	-3.653656
H	2.388927	-2.671872	-4.257349
C	3.182998	-3.915578	-2.653129
H	3.723997	-4.611665	-3.316839
H	2.193123	-4.369880	-2.462438
C	3.928537	-3.756702	-1.324252
H	4.966891	-3.430785	-1.524374
H	4.004314	-4.728849	-0.806961
C	3.250592	-2.734155	-0.397463
H	2.252601	-3.111934	-0.111785
H	3.838992	-2.652464	0.528508
C	3.159078	1.576061	-0.634740
H	4.162591	1.570466	-0.169203
C	3.369231	1.658695	-2.160271
H	2.388684	1.622998	-2.666600
H	3.948802	0.798540	-2.525630
C	4.093563	2.952582	-2.564742
H	4.212134	2.982190	-3.661357
H	5.115537	2.941876	-2.142356
C	3.356915	4.201185	-2.071730
H	2.384400	4.276867	-2.591973
H	3.922894	5.111370	-2.333851
C	3.113515	4.130450	-0.560936
H	2.523050	4.999406	-0.224508
H	4.083092	4.192063	-0.032106
C	2.396628	2.832796	-0.160755
H	2.239157	2.814474	0.926213
H	1.387163	2.808291	-0.607170

Complex 3 - $[Pt(PBu^t_2Ph)_2$

Pt	0.008185	0.052728	-0.014029
P	-2.220047	0.681407	-0.060341
P	2.202936	-0.652857	0.080868
C	3.371027	0.788348	-0.182917
C	4.269067	0.944708	-1.256564
C	3.290045	1.850655	0.746023
C	5.044613	2.101157	-1.397644
H	4.375831	0.172391	-2.016123
C	4.089018	2.988678	0.629626
H	2.583716	1.793223	1.575225
C	4.968581	3.127033	-0.450629
H	5.713018	2.194427	-2.258851
H	4.012973	3.779015	1.383467
H	5.580067	4.025884	-0.556942
C	-3.291938	-0.834528	0.111247
C	-2.876725	-1.967660	-0.617379
C	-4.461522	-0.949858	0.884680
C	-3.613933	-3.153348	-0.601137
H	-1.950240	-1.916009	-1.194231
C	-5.178756	-2.150577	0.935950
H	-4.832852	-0.106219	1.465828
C	-4.767117	-3.252925	0.185595
H	-3.277203	-4.007844	-1.196475
H	-6.068470	-2.218491	1.568720
H	-5.334733	-4.186813	0.218800
C	-2.857133	1.421274	-1.734050
C	-2.402655	2.886348	-1.871046
H	-2.987584	3.567562	-1.236890
H	-1.336873	3.011682	-1.632734
H	-2.552343	3.213478	-2.914768
C	-2.186516	0.610936	-2.863284
H	-2.453043	1.062478	-3.835248
H	-1.091363	0.614614	-2.762690
H	-2.526368	-0.434866	-2.884723
C	-4.383715	1.324220	-1.895941
H	-4.934247	1.841828	-1.095998
H	-4.676727	1.791604	-2.852299
H	-4.725092	0.279589	-1.919083
C	-2.619017	1.882694	1.398662
C	-1.555502	3.006487	1.374800
H	-1.767816	3.770463	0.616636
H	-1.544589	3.513232	2.355945
H	-0.551456	2.599392	1.181657
C	-2.402861	1.079507	2.700182
H	-1.364222	0.725159	2.771365
H	-2.598397	1.739371	3.562003
H	-3.065568	0.205388	2.791339
C	-4.013673	2.537761	1.405692
H	-4.086390	3.209818	2.277878
H	-4.188674	3.156337	0.514438
H	-4.841370	1.819410	1.482937
C	2.745524	-1.344144	1.824056
C	2.572611	-1.960330	-1.293128
C	4.246303	-1.160978	2.107996
H	4.550075	-0.104852	2.094585
H	4.472684	-1.556683	3.113638
H	4.878926	-1.702538	1.389401
C	1.921787	-0.595171	2.893777
H	0.843243	-0.690563	2.699132
H	2.146077	-1.026667	3.884290
H	2.156355	0.476933	2.946106
C	2.390906	-2.837559	1.957809
H	1.359597	-3.056698	1.648429
H	3.074742	-3.481746	1.389244
H	2.486464	-3.127303	3.018625
C	4.019566	-2.488231	-1.318450
H	4.265536	-3.032943	-0.395069
H	4.133313	-3.200880	-2.153735
H	4.775519	-1.702187	-1.448769
C	1.610024	-3.160843	-1.121312
H	1.513437	-3.678735	-2.090809
H	1.970806	-3.899278	-0.395841
H	0.605602	-2.829851	-0.815768
C	2.182575	-1.305607	-2.641014
H	2.431415	-2.003236	-3.460263
H	1.099494	-1.115480	-2.666633
H	2.681485	-0.352664	-2.848968

Complex 4 - $[Pt(PBu^t_3)_2$

Pt	-0.001320	0.005206	0.010828
P	2.330531	-0.008064	0.005512
P	-2.334854	0.000859	-0.003191
C	3.008905	0.403737	-1.773675
C	2.746242	-0.812093	-2.687430
H	3.438905	-1.641586	-2.492509
H	1.716845	-1.181017	-2.594359
H	2.904795	-0.507882	-3.736761
C	2.173384	1.604569	-2.322150
H	2.804408	2.496616	-2.475840
H	1.726704	1.347310	-3.298024
H	1.337493	1.877741	-1.659612
C	4.511160	0.742805	-1.862031
H	5.152512	-0.060491	-1.474873
H	4.779676	0.893843	-2.922328
H	4.769437	1.669466	-1.332819
C	2.985497	-1.766267	0.546965
C	2.120881	-2.828950	-0.179313
H	2.471613	-3.022803	-1.203777
H	2.184951	-3.783191	0.372110
H	1.061655	-2.522253	-0.226784
C	2.717260	-1.922255	2.060251
H	2.800017	-2.991171	2.334630
H	3.440734	-1.370263	2.681794
H	1.700205	-1.592781	2.320111
C	4.467983	-2.070045	0.264124
H	4.682078	-3.105736	0.580476
H	4.711786	-2.014154	-0.807949
H	5.157309	-1.410309	0.807851
C	-3.047482	-0.343756	1.781584
C	-2.991867	1.741407	-0.604579
C	-4.505543	-0.834914	1.834285
H	-4.624326	-1.842584	1.415441
H	-4.827103	-0.885709	2.889294
H	-5.202519	-0.163931	1.311035
C	-2.135314	-1.386824	2.467168
H	-1.080304	-1.076738	2.417601
H	-2.427630	-1.471231	3.527922
H	-2.210047	-2.385988	2.021659
C	-2.934845	0.941725	2.625921
H	-1.927383	1.379110	2.578749
H	-3.662993	1.707211	2.331644
H	-3.137480	0.688253	3.680992
C	-4.490891	2.033431	-0.393435
H	-4.805424	1.915173	0.652098
H	-4.685385	3.085211	-0.663656
H	-5.145671	1.411763	-1.019453
C	-2.163144	2.826375	0.137863
H	-2.188242	3.759584	-0.449569
H	-2.571004	3.057896	1.133308
H	-1.108534	2.519652	0.255796
C	-2.663181	1.876395	-2.109972
H	-3.378959	1.342670	-2.755349
H	-2.708425	2.944278	-2.389265
H	-1.645574	1.526160	-2.334354
C	3.044147	1.333097	1.227594
C	2.176548	1.338043	2.506782
H	2.461356	2.207129	3.123702
H	1.109226	1.418434	2.254667
H	2.308515	0.438417	3.120524
C	4.519207	1.145906	1.627416
H	4.832405	2.001247	2.253125
H	4.674933	0.239070	2.228171
H	5.198900	1.104876	0.764394
C	2.869317	2.727622	0.589636
H	1.821744	2.918395	0.318536
H	3.165549	3.490817	1.331166
H	3.491075	2.881509	-0.300449
C	-3.004864	-1.385720	-1.201646
C	-2.694478	-2.757767	-0.562933
H	-2.934374	-3.550455	-1.293018
H	-1.626556	-2.846727	-0.308956
H	-3.282640	-2.960647	0.341517
C	-4.503521	-1.319335	-1.555221
H	-4.792126	-0.354009	-2.004308
H	-4.718643	-2.094870	-2.310213
H	-5.158341	-1.507267	-0.692442
C	-2.191672	-1.330452	-2.519086
H	-1.113136	-1.230224	-2.319615
H	-2.352826	-2.272777	-3.069796
H	-2.503783	-0.513455	-3.180345

Complex 5 - $[Pt(PEt_3)_3]$

Pt	-0.025624	0.057424	-0.021838
P	-2.367138	0.146450	0.073616
P	0.990047	-2.060264	-0.099270
P	1.208818	2.049933	-0.027915
C	2.136788	2.514643	-1.591720
H	2.727153	3.426832	-1.391213
H	1.369023	2.791288	-2.335762
C	2.580118	2.190161	1.240020
H	3.395818	1.537756	0.881795
H	2.979926	3.217893	1.237008
C	0.241353	3.637111	0.271673
H	-0.552290	3.617174	-0.493455
H	-0.278552	3.474575	1.231596
C	0.954617	4.991247	0.267436
H	0.238236	5.804749	0.471749
H	1.739528	5.052001	1.038874
H	1.425290	5.211502	-0.703201
C	2.159638	1.773142	2.653020
H	1.277327	2.337782	2.999168
H	1.900006	0.702790	2.687255
H	2.973583	1.962485	3.375279
C	3.032045	1.403007	-2.150262
H	3.763488	1.050655	-1.403791
H	2.424218	0.537867	-2.456181
H	3.599098	1.757350	-3.028132
C	-3.254953	1.470060	-0.907742
H	-4.344559	1.333444	-0.804957
H	-3.010528	2.427992	-0.413280
C	-3.111784	0.465021	1.757121
H	-2.820852	1.497477	2.020629
H	-4.211294	0.461729	1.673382
C	-3.287627	-1.406410	-0.472730
H	-2.911297	-2.196618	0.197705
H	-2.878136	-1.652474	-1.466188
C	-2.649403	-0.504452	2.847938
H	-2.824289	-1.557085	2.564245
H	-1.570904	-0.389848	3.042366
H	-3.197498	-0.323354	3.789765
C	-4.816856	-1.415596	-0.511662
H	-5.218878	-0.703704	-1.250752
H	-5.190646	-2.414613	-0.792992
H	-5.263489	-1.168234	0.464402
C	-2.844114	1.517875	-2.382347
H	-1.798142	1.846992	-2.488607
H	-2.923004	0.527162	-2.864194
H	-3.490743	2.207893	-2.954655
C	0.470892	-3.161798	-1.518233
H	-0.584855	-3.422188	-1.324509
H	1.039917	-4.105581	-1.475553
C	0.630079	-3.218794	1.324493
H	1.031537	-4.217496	1.078104
H	-0.466674	-3.320363	1.353870
C	2.866190	-2.159745	-0.202801
H	3.132531	-1.633382	-1.135371
H	3.234599	-1.505744	0.604860
C	1.160155	-2.752424	2.683561
H	0.655325	-1.825491	3.004778
H	0.979225	-3.521598	3.456275
H	2.248004	-2.555865	2.660309
C	3.566890	-3.521067	-0.142888
H	3.250215	-4.189677	-0.959317
H	4.659033	-3.397368	-0.231568
H	3.377948	-4.043991	0.808211
C	0.612318	-2.509939	-2.897657
H	-0.053979	-1.633899	-2.989621
H	1.646320	-2.165343	-3.077375
H	0.367994	-3.234549	-3.697417

Complex 6 - $[Pt(PBu^n_3)_3]$

Pt	0.154819	0.032931	-0.069117
P	0.756752	2.292480	0.156009
P	-2.116202	-0.563748	-0.130766
P	1.884802	-1.544705	-0.177839
C	2.132525	-2.475280	-1.782873
H	2.873662	-3.275554	-1.619495
H	2.591389	-1.757754	-2.484483
C	1.822158	-2.962309	1.043596
H	0.984255	-3.605798	0.727068
H	2.738588	-3.570884	0.945144
C	3.626146	-0.885869	0.093569
H	3.728353	-0.071777	-0.644394
H	3.597055	-0.384434	1.076653
C	4.838146	-1.821144	0.010273
H	4.745663	-2.634615	0.751269
H	4.870117	-2.312186	-0.978138
C	1.617336	-2.532226	2.500122
H	2.396577	-1.802793	2.792759
H	0.656772	-1.992431	2.579689
C	0.857288	-3.056980	-2.401177
H	0.366802	-3.734526	-1.678449
H	0.140451	-2.236719	-2.578101
C	2.095002	2.933687	-0.982936
H	2.265655	4.008544	-0.793581
H	3.016143	2.410781	-0.672040
C	1.512967	2.776295	1.796118
H	2.501961	2.288620	1.814030
H	1.700264	3.864769	1.811317
C	-0.603353	3.574502	-0.061607
H	-1.360246	3.300734	0.691725
H	-1.065102	3.337331	-1.036233
C	0.710420	2.349876	3.028493
H	-0.312049	2.769327	2.979397
H	0.585013	1.252776	3.007156
C	-0.269750	5.069702	0.013780
H	0.487202	5.316508	-0.749476
H	0.193276	5.306458	0.988364
C	1.843601	2.684279	-2.473507
H	1.740517	1.595644	-2.639539
H	0.876648	3.127507	-2.777001
C	-3.147938	0.348731	-1.397631
H	-3.161437	1.393757	-1.043880
H	-4.190282	-0.008522	-1.373361
C	-3.101759	-0.169612	1.407868
H	-4.137061	-0.524397	1.275928
H	-3.147159	0.931099	1.454080
C	-2.526748	-2.383939	-0.430077
H	-2.292001	-2.560878	-1.494358
H	-1.735794	-2.913949	0.123471
C	-2.488758	-0.708723	2.705753
H	-1.459301	-0.320489	2.784060
H	-2.393518	-1.809538	2.647228
C	-3.879298	-3.021839	-0.068035
H	-3.744918	-4.117424	-0.145547
H	-4.109991	-2.838214	0.996523
C	-2.600800	0.306600	-2.827390
H	-1.560621	0.680244	-2.823201
H	-2.545350	-0.739569	-3.181547
C	-3.443450	1.119788	-3.820404
H	-3.547699	2.155319	-3.446244
H	-4.469199	0.707261	-3.848214
C	-5.096591	-2.642381	-0.919689
H	-5.361651	-1.584281	-0.754902
H	-4.835021	-2.726661	-1.990630
C	-6.319733	-3.513155	-0.622568
H	-7.186518	-3.218404	-1.235367
H	-6.112895	-4.577523	-0.828455
H	-6.619168	-3.435890	0.437045
C	1.358666	2.774547	4.353317
H	1.411553	3.878367	4.393554
H	2.407353	2.423752	4.375952
C	0.618811	2.252793	5.586323
H	-0.431718	2.591926	5.598558
H	0.607721	1.149377	5.605838
H	1.091580	2.599152	6.520781
C	-1.480216	5.997102	-0.193277
H	-1.112243	7.033963	-0.288264
H	-1.956777	5.757550	-1.161435
C	-2.529879	5.945039	0.919273
H	-2.980278	4.944142	1.018535
H	-2.088468	6.207722	1.895819
H	-3.350780	6.654191	0.725432
C	2.948761	3.248628	-3.374967
H	3.932571	2.894672	-3.014831
H	2.970867	4.349013	-3.270506
C	2.781484	2.877779	-4.851240
H	3.562176	3.341599	-5.474560
H	2.845418	1.785505	-4.997252
H	1.802078	3.205693	-5.241268
C	6.170878	-1.094876	0.239272
H	6.259745	-0.267732	-0.487743
H	6.157054	-0.616843	1.235880
C	7.391751	-2.008556	0.125291
H	7.454360	-2.468948	-0.875371
H	8.329362	-1.455259	0.295674
H	7.350946	-2.827766	0.861975
C	1.640119	-3.701410	3.494780
H	0.905983	-4.465991	3.178628
H	2.627722	-4.197283	3.449883
C	1.348864	-3.274997	4.934671
H	2.059958	-2.501496	5.276038
H	0.333346	-2.851003	5.027252
H	1.421796	-4.124900	5.633852
C	1.106530	-3.822018	-3.707076
H	1.595819	-3.149204	-4.435526
H	1.829417	-4.637274	-3.519879
C	-0.167710	-4.403159	-4.323090
H	-0.665136	-5.101937	-3.628411
H	-0.893492	-3.608757	-4.566555
H	0.045786	-4.955235	-5.253259
C	-2.863463	1.147209	-5.235624
H	-3.527734	1.680236	-5.936222
H	-1.882059	1.652149	-5.256372
H	-2.716082	0.126072	-5.628464
C	-3.268601	-0.343436	3.980424
H	-2.651606	-0.616015	4.854766
H	-3.392237	0.754190	4.028817
C	-4.637996	-1.018861	4.111440
H	-5.121459	-0.764964	5.069065
H	-5.329280	-0.715701	3.307652
H	-4.541265	-2.118212	4.068581

Complex 7 - $[Pt(P(CH_2Ph)_3)_3]$

Pt	-0.026308	-0.074496	0.117452
P	0.077994	2.271228	0.215446
P	1.915046	-1.312232	0.605149
P	-1.961717	-1.134847	-0.696166
C	-0.883794	3.169072	1.571217
H	-0.759622	4.247528	1.369976
H	-0.302702	2.960172	2.482779
C	1.694953	3.138367	0.641096
H	1.476605	4.205711	0.817780
H	1.963962	2.716778	1.625118
C	-0.430416	3.186231	-1.375132
H	-1.484295	2.911511	-1.535588
H	0.137716	2.684390	-2.172175
C	3.246484	-0.476499	1.643206
H	4.049983	-1.209615	1.842003
H	3.685906	0.280159	0.975537
C	2.910090	-1.588841	-0.988598
H	2.219622	-2.089243	-1.682149
H	3.048359	-0.573677	-1.384301
C	2.012904	-3.013975	1.433898
H	3.058206	-3.347574	1.300784
H	1.903973	-2.825949	2.512051
C	-1.701511	-2.181767	-2.237378
H	-1.314241	-3.140419	-1.866606
H	-2.688482	-2.401406	-2.681038
C	-3.447771	-0.042838	-1.176563
H	-3.781146	0.379121	-0.217290
H	-3.005931	0.794255	-1.738055
C	-2.808819	-2.445566	0.374319
H	-3.775044	-2.702866	-0.088524
H	-2.159062	-3.330492	0.288585
C	-4.605522	-0.635909	-1.939832
C	-4.576704	-0.732465	-3.345858
C	-5.758606	-1.100898	-1.281170
C	-5.641338	-1.291750	-4.057485
H	-3.707856	-0.358839	-3.894436
C	-6.827695	-1.663338	-1.987491
H	-5.830616	-1.004369	-0.196716
C	-6.770905	-1.765376	-3.381483
H	-5.590560	-1.351777	-5.147503
H	-7.708193	-2.013355	-1.446285
H	-7.605052	-2.202720	-3.937229
C	-0.764138	-1.653588	-3.302691
C	0.114247	-2.538147	-3.954634
C	-0.757505	-0.308871	-3.713071
C	0.959130	-2.102687	-4.980816
H	0.131554	-3.590767	-3.658356
C	0.081215	0.131321	-4.741957
H	-1.408502	0.411966	-3.218907
C	0.943909	-0.763992	-5.382434
H	1.631533	-2.812626	-5.467280
H	0.059409	1.182519	-5.042282
H	1.600398	-0.421259	-6.186818
C	-2.982004	-2.095053	1.834510
C	-1.945224	-2.339819	2.749917
C	-4.179232	-1.548980	2.330176
C	-2.095124	-2.050248	4.108283
H	-1.015010	-2.783824	2.387291
C	-4.332876	-1.252732	3.687425
H	-5.011236	-1.361197	1.648338
C	-3.292187	-1.501846	4.584163
H	-1.275731	-2.262029	4.799549
H	-5.272103	-0.827335	4.041796
H	-3.412826	-1.274681	5.646387
C	1.085029	-4.139039	1.036182
C	0.632397	-5.034370	2.020890
C	0.699872	-4.386855	-0.292238
C	-0.159101	-6.140406	1.698306
H	0.915556	-4.867270	3.065074
C	-0.090266	-5.493263	-0.623996
H	1.015134	-3.706289	-1.082446
C	-0.522826	-6.377807	0.369290
H	-0.492743	-6.817710	2.488473
H	-0.368647	-5.667113	-1.666383
H	-1.139267	-7.242660	0.109413
C	4.234594	-2.308520	-0.926111
C	5.437900	-1.595041	-0.771204
C	4.312506	-3.709442	-1.037915
C	6.668689	-2.255807	-0.717708
H	5.410855	-0.504088	-0.708751
C	5.541663	-4.373010	-0.984177
H	3.398131	-4.290803	-1.177946
C	6.726481	-3.649428	-0.820336
H	7.588997	-1.676556	-0.602475
H	5.572029	-5.462234	-1.075687
H	7.689269	-4.166055	-0.780883
C	2.855387	0.205457	2.942321
C	3.573017	1.348290	3.344051
C	1.844850	-0.265207	3.799639
C	3.307892	1.982474	4.560973
H	4.352799	1.746375	2.687351
C	1.584177	0.360750	5.021620
H	1.241923	-1.129182	3.515846
C	2.316602	1.486860	5.411873
H	3.880812	2.871702	4.840921
H	0.797682	-0.035481	5.670953
H	2.111544	1.976954	6.366434
C	2.899177	3.045722	-0.274499
C	3.985802	3.908005	-0.028536
C	3.002782	2.154285	-1.353493
C	5.132132	3.880146	-0.824791
H	3.923988	4.619838	0.799877
C	4.149407	2.125531	-2.158597
H	2.178302	1.470372	-1.567077
C	5.219652	2.985487	-1.898034
H	5.958026	4.564286	-0.610485
H	4.201194	1.425008	-2.996875
H	6.112758	2.964091	-2.527600
C	-0.235208	4.681034	-1.458022
C	0.925536	5.221458	-2.042850
C	-1.200152	5.581771	-0.967902
C	1.122650	6.602825	-2.119879
H	1.684805	4.548178	-2.446140
C	-1.005951	6.964471	-1.043881
H	-2.125765	5.201531	-0.530398
C	0.159215	7.482617	-1.616550
H	2.034155	6.992753	-2.580534
H	-1.774821	7.639178	-0.657584
H	0.311567	8.563350	-1.676909
C	-2.341685	2.883519	1.847214
C	-3.344535	3.021598	0.871040
C	-2.749245	2.571071	3.156063
C	-4.697410	2.876736	1.193106
H	-3.075449	3.247144	-0.161216
C	-4.100574	2.432585	3.485216
H	-1.990688	2.447307	3.933875
C	-5.083792	2.589838	2.504910
H	-5.452292	2.993278	0.411041
H	-4.384442	2.201185	4.515165
H	-6.141625	2.488447	2.759287

Complex 8 - $[Pt(Pcy_3)_3]$, cy = cyclohexil

Pt	0.053485	0.110184	0.005758
P	-1.597592	-1.650051	0.062774
P	2.363074	-0.590978	-0.205529
P	-0.792561	2.332102	0.168747
C	-2.686153	2.477271	0.662927
C	-3.013918	3.039103	2.060963
C	-3.642315	3.115301	-0.365425
H	-2.931605	1.402902	0.697748
C	-4.484352	2.824628	2.452993
H	-2.834914	4.124732	2.061342
H	-2.354542	2.599170	2.826480
C	-5.119958	2.930718	0.021832
H	-3.429516	4.195509	-0.454342
H	-3.489535	2.681769	-1.363443
C	-5.423081	3.463408	1.425162
H	-4.661404	3.252541	3.455753
H	-4.700913	1.742692	2.531005
H	-5.760311	3.425778	-0.728901
H	-5.373435	1.855119	-0.016589
H	-6.478465	3.283941	1.690926
H	-5.280169	4.560854	1.435612
C	0.266569	3.359203	1.426219
C	1.607282	3.738459	0.767051
C	-0.246820	4.595472	2.198161
H	0.479232	2.577506	2.177294
C	2.658808	4.191606	1.788879
H	1.427206	4.583004	0.082704
H	1.984798	2.902006	0.164215
C	0.794002	5.086398	3.223070
H	-0.491306	5.410980	1.494799
H	-1.160391	4.368130	2.748605
C	2.155638	5.393317	2.595197
H	3.598499	4.446410	1.268807
H	2.895800	3.356393	2.474162
H	0.401028	5.973315	3.749417
H	0.923182	4.303073	3.993814
H	2.886324	5.678603	3.371543
H	2.058013	6.266312	1.922252
C	-0.528709	3.241588	-1.494670
C	-1.128531	2.460036	-2.685101
C	-0.803583	4.757451	-1.605180
H	0.561708	3.107546	-1.588733
C	-0.718989	3.052197	-4.041002
H	-2.225450	2.459926	-2.632000
H	-0.812780	1.406800	-2.615419
C	-0.393360	5.312404	-2.981069
H	-1.868832	4.978728	-1.428910
H	-0.234741	5.302499	-0.836124
C	-1.051235	4.545938	-4.132701
H	-1.215845	2.492315	-4.854360
H	0.370010	2.915460	-4.189224
H	-0.637265	6.387522	-3.035544
H	0.705456	5.238804	-3.087831
H	-0.727176	4.955992	-5.104953
H	-2.147796	4.684177	-4.083382
C	-3.031074	-1.126829	-1.081455
C	-2.636518	-1.274198	-2.569448
C	-4.453816	-1.650696	-0.802957
H	-3.050982	-0.041695	-0.879778
C	-3.706222	-0.704191	-3.516625
H	-2.476418	-2.334925	-2.825194
H	-1.672436	-0.768066	-2.737544
C	-5.488108	-1.048149	-1.765816
H	-4.487357	-2.748300	-0.890180
H	-4.746527	-1.408241	0.230114
C	-5.098283	-1.280526	-3.228477
H	-3.419499	-0.903312	-4.563565
H	-3.743929	0.395137	-3.407234
H	-6.484678	-1.473618	-1.551995
H	-5.568977	0.039092	-1.581010
H	-5.847909	-0.835199	-3.904357
H	-5.098792	-2.367457	-3.435601
C	-2.393219	-1.838843	1.788953
C	-3.345439	-3.024947	2.062222
C	-1.294893	-1.796116	2.876929
H	-2.976560	-0.902620	1.881504
C	-3.942229	-2.957108	3.478302
H	-2.781958	-3.970964	1.979515
H	-4.153741	-3.078881	1.319319
C	-1.852984	-1.798172	4.308113
H	-0.641083	-2.676258	2.758950
H	-0.656001	-0.913153	2.711587
C	-2.843938	-2.945319	4.543310
H	-4.619326	-3.812941	3.637381
H	-4.558809	-2.046912	3.576800
H	-1.012450	-1.876660	5.024051
H	-2.346898	-0.828719	4.518604
H	-3.279730	-2.879685	5.554548
H	-2.301936	-3.906703	4.501915
C	-1.169367	-3.437276	-0.505325
C	-0.286636	-4.172292	0.525126
C	-2.275648	-4.397610	-0.995668
H	-0.528025	-3.222123	-1.380044
C	0.294134	-5.490255	-0.010841
H	-0.888353	-4.400218	1.418120
H	0.525722	-3.516057	0.864122
C	-1.663955	-5.675372	-1.595515
H	-2.932160	-4.678041	-0.160630
H	-2.916520	-3.920199	-1.744082
C	-0.793969	-6.414413	-0.572641
H	0.851413	-6.001228	0.794070
H	1.028008	-5.270880	-0.805892
H	-2.461378	-6.337081	-1.977519
H	-1.043277	-5.400815	-2.469036
H	-0.338304	-7.312289	-1.023954
H	-1.436719	-6.774052	0.252492
C	3.792231	0.727859	-0.230786
C	5.136627	0.468043	0.483185
C	4.090064	1.362403	-1.607723
H	3.281267	1.502967	0.369281
C	5.945816	1.769370	0.625434
H	5.730083	-0.275228	-0.078520
H	4.978320	0.056447	1.486548
C	4.917358	2.653351	-1.502323
H	4.683967	0.645945	-2.200381
H	3.160715	1.557283	-2.165114
C	6.222897	2.429487	-0.728446
H	6.890754	1.565857	1.160355
H	5.374910	2.472533	1.261240
H	5.140594	3.026635	-2.517118
H	4.321833	3.440050	-1.005669
H	6.763878	3.381525	-0.594921
H	6.891059	1.771979	-1.317656
C	2.454530	-1.792019	-1.718822
C	2.770254	-1.093420	-3.058570
C	3.225925	-3.120626	-1.615057
H	1.385670	-2.064147	-1.757125
C	2.533682	-2.000584	-4.276173
H	3.827816	-0.792550	-3.073464
H	2.176673	-0.171136	-3.159962
C	2.969531	-4.017392	-2.839077
H	4.312156	-2.933486	-1.517507
H	2.912584	-3.669018	-0.713788
C	3.317409	-3.312041	-4.153757
H	2.827737	-1.461409	-5.195819
H	1.453342	-2.223636	-4.376264
H	3.537124	-4.958588	-2.735633
H	1.898764	-4.300132	-2.859045
H	3.114010	-3.969972	-5.016306
H	4.404211	-3.094815	-4.172527
C	2.745749	-1.618649	1.360738
C	4.028312	-2.472456	1.504734
C	2.522714	-0.717106	2.600539
H	1.902916	-2.326923	1.343927
C	4.040321	-3.249407	2.830564
H	4.928527	-1.850216	1.458612
H	4.114475	-3.183005	0.682426
C	2.610732	-1.489209	3.926702
H	3.264845	0.103895	2.615857
H	1.534626	-0.235685	2.508179
C	3.896747	-2.316982	4.034716
H	4.971191	-3.838325	2.900537
H	3.211871	-3.981480	2.836050
H	2.534320	-0.780518	4.772706
H	1.739180	-2.167254	4.009808
H	3.905826	-2.893079	4.975393
H	4.769640	-1.639282	4.076478

Complex 9 - [$Pt(PPh_3)_2(PhCy{\equiv}CPh)$]

Pt	-0.000995	0.574415	0.002869
P	1.893862	-0.885711	-0.039500
C	0.618636	2.556579	0.123294
C	-0.664687	2.541344	-0.117943
P	-1.872307	-0.917862	0.042341
C	-1.985745	-2.065550	1.497438
C	-2.982917	-3.054682	1.594960
C	-1.147194	-1.838986	2.598098
C	-3.117939	-3.812381	2.759861
H	-3.668923	-3.230245	0.763390
C	-1.293462	-2.588291	3.771710
H	-0.381632	-1.063569	2.534168
C	-2.274079	-3.579213	3.853223
H	-3.893157	-4.580712	2.819126
H	-0.632162	-2.396467	4.619770
H	-2.386931	-4.167759	4.767376
C	-2.139270	-1.975223	-1.450073
C	-2.511013	-1.347700	-2.654762
C	-1.882822	-3.355837	-1.464925
C	-2.655733	-2.086303	-3.831075
H	-2.693082	-0.270452	-2.677145
C	-2.022995	-4.094195	-2.645616
H	-1.568913	-3.867141	-0.553475
C	-2.416141	-3.465472	-3.829427
H	-2.955254	-1.581360	-4.752989
H	-1.821662	-5.168381	-2.635652
H	-2.529350	-4.044356	-4.749422
C	-3.520408	-0.080641	0.286330
C	-3.587761	0.934278	1.256154
C	-4.704014	-0.479480	-0.355770
C	-4.807803	1.529836	1.583410
H	-2.674087	1.263469	1.756759
C	-5.923915	0.130440	-0.039799
H	-4.687341	-1.271638	-1.106069
C	-5.980863	1.133067	0.932140
H	-4.839597	2.315875	2.342097
H	-6.834558	-0.188136	-0.554066
H	-6.934950	1.604875	1.180743
C	3.531005	-0.025089	-0.277083
C	3.588526	0.985738	-1.251980
C	4.716450	-0.401656	0.374595
C	4.801504	1.596860	-1.576486
H	2.673006	1.298919	-1.759622
C	5.929033	0.224493	0.061640
H	4.707062	-1.188869	1.130147
C	5.976791	1.221276	-0.916657
H	4.825937	2.378757	-2.339731
H	6.841242	-0.077165	0.583224
H	6.925267	1.705292	-1.163322
C	2.175240	-1.948717	1.446172
C	2.524897	-1.320418	2.657165
C	1.954139	-3.335471	1.449862
C	2.683204	-2.063507	3.828888
H	2.678257	-0.238809	2.687852
C	2.107221	-4.078440	2.626186
H	1.658118	-3.848244	0.533233
C	2.478848	-3.448397	3.816237
H	2.965426	-1.557840	4.755873
H	1.933633	-5.157394	2.607673
H	2.602764	-4.030907	4.732610
C	2.024244	-2.021231	-1.502551
C	3.041799	-2.988388	-1.611026
C	1.174916	-1.806527	-2.597237
C	3.186107	-3.737139	-2.780626
H	3.736768	-3.153050	-0.784670
C	1.330020	-2.546879	-3.775484
H	0.394026	-1.047138	-2.524915
C	2.330709	-3.516659	-3.867674
H	3.977511	-4.488150	-2.848627
H	0.659614	-2.364840	-4.618516
H	2.450476	-4.098238	-4.785479
C	1.737005	3.471703	0.309986
C	2.742173	3.224271	1.266974
C	1.821280	4.659921	-0.450623
C	3.783755	4.133005	1.466125
H	2.690112	2.309382	1.861626
C	2.869558	5.561431	-0.257702
H	1.053407	4.867906	-1.200301
C	3.855394	5.304356	0.703213
H	4.548301	3.922807	2.219104
H	2.916381	6.473077	-0.859856
H	4.674513	6.012019	0.855087
C	-1.808584	3.423535	-0.308055
C	-2.777018	3.169711	-1.300098
C	-1.957453	4.583264	0.484610
C	-3.844808	4.046334	-1.503070
H	-2.674371	2.276186	-1.918918
C	-3.033101	5.451656	0.288930
H	-1.218810	4.795143	1.261323
C	-3.981261	5.189491	-0.707438
H	-4.579170	3.832928	-2.284408
H	-3.130994	6.341315	0.917128
H	-4.821440	5.871449	-0.861660

Complex 10 - $[Pt(PPh_3)_2(PhC{\equiv}CMe)]$

Pt	0.156430	0.859403	-0.125712
P	1.356913	-1.216387	0.062490
C	1.435167	2.520658	-0.225696
C	0.210672	2.895114	-0.464795
P	-2.171988	0.301018	-0.045698
C	-2.836594	-0.643628	1.407888
C	-4.206637	-0.942008	1.533951
C	-1.976003	-0.952621	2.471737
C	-4.696082	-1.559349	2.686400
H	-4.903808	-0.681139	0.733604
C	-2.469844	-1.560449	3.633614
H	-0.916849	-0.705883	2.391887
C	-3.826242	-1.869470	3.741758
H	-5.760984	-1.789857	2.767355
H	-1.783296	-1.790595	4.452757
H	-4.212167	-2.344933	4.647510
C	-2.872281	-0.536673	-1.538509
C	-2.748099	0.122767	-2.777525
C	-3.430931	-1.824910	-1.517141
C	-3.200290	-0.477002	-3.955102
H	-2.290288	1.114716	-2.824621
C	-3.877777	-2.427766	-2.699327
H	-3.516818	-2.372751	-0.577532
C	-3.770850	-1.755601	-3.919320
H	-3.102976	0.054885	-4.905240
H	-4.310120	-3.431330	-2.661571
H	-4.123485	-2.226545	-4.840540
C	-3.258475	1.806221	0.141731
C	-2.959278	2.678366	1.204222
C	-4.377503	2.082097	-0.659710
C	-3.757231	3.794632	1.460013
H	-2.086660	2.483886	1.833973
C	-5.171530	3.209147	-0.409209
H	-4.644197	1.419818	-1.485206
C	-4.866127	4.067547	0.649528
H	-3.507922	4.459738	2.291000
H	-6.036940	3.409738	-1.046604
H	-5.488882	4.944554	0.843864
C	3.183969	-1.111271	-0.295086
C	3.582042	-0.354630	-1.410262
C	4.158905	-1.831959	0.414020
C	4.916186	-0.339156	-1.822547
H	2.837965	0.229097	-1.957480
C	5.499104	-1.800883	0.011753
H	3.880035	-2.428524	1.285689
C	5.881000	-1.061114	-1.111492
H	5.205325	0.247499	-2.698510
H	6.245395	-2.364387	0.577859
H	6.926385	-1.045879	-1.429685
C	1.319156	-2.047168	1.716477
C	1.865432	-1.347736	2.811246
C	0.696954	-3.282828	1.954346
C	1.819805	-1.886321	4.098531
H	2.330187	-0.370170	2.657663
C	0.647611	-3.820308	3.245898
H	0.236311	-3.834605	1.133361
C	1.214131	-3.129199	4.320689
H	2.257210	-1.331546	4.933027
H	0.159392	-4.784231	3.409446
H	1.176922	-3.551467	5.327832
C	0.972884	-2.554471	-1.170919
C	1.610788	-3.809927	-1.133591
C	0.127568	-2.258977	-2.250565
C	1.383009	-4.752470	-2.138469
H	2.302330	-4.053414	-0.323066
C	-0.091184	-3.199844	-3.265793
H	-0.352509	-1.280650	-2.301301
C	0.529972	-4.449256	-3.209064
H	1.882289	-5.723989	-2.092283
H	-0.751953	-2.949200	-4.099944
H	0.358644	-5.185189	-3.999588
C	2.774770	3.071758	-0.067380
C	3.798131	2.388448	0.618873
C	3.067213	4.364918	-0.565171
C	5.050061	2.975329	0.819421
H	3.598039	1.385118	0.995402
C	4.320254	4.946732	-0.374192
H	2.293231	4.916894	-1.104393
C	5.319738	4.257015	0.324943
H	5.822032	2.426792	1.365370
H	4.518372	5.946929	-0.763643
H	6.298997	4.715633	0.483508
C	-0.643072	4.072454	-0.773330
H	-1.602441	3.794056	-1.228797
H	-0.877760	4.634978	0.141901
H	-0.125343	4.761845	-1.456428

Complex 11 - $[Pt(PPh_3)_2(PhC{\equiv}CCO_2Me)]$

Pt	0.196401	0.681956	-0.091547
P	1.284449	-1.447506	-0.000466
C	1.585818	2.229603	-0.053337
C	0.406368	2.712767	-0.349844
P	-2.131482	0.089309	0.003430
C	-2.660552	-0.682105	1.606549
C	-3.975430	-1.141665	1.809014
C	-1.769943	-0.681871	2.689214
C	-4.377655	-1.610889	3.060816
H	-4.697030	-1.124568	0.989571
C	-2.177875	-1.140255	3.947540
H	-0.753233	-0.312967	2.544265
C	-3.479189	-1.609930	4.134899
H	-5.400395	-1.968982	3.201722
H	-1.470754	-1.131910	4.779988
H	-3.797684	-1.970647	5.116330
C	-2.809315	-1.007268	-1.319766
C	-2.939644	-0.488155	-2.622476
C	-3.105931	-2.362414	-1.101944
C	-3.391896	-1.295170	-3.668894
H	-2.689880	0.557116	-2.822793
C	-3.551408	-3.171578	-2.153658
H	-2.990822	-2.797031	-0.107509
C	-3.703484	-2.640186	-3.436703
H	-3.498326	-0.871723	-4.671012
H	-3.780924	-4.223476	-1.964228
H	-4.056404	-3.271984	-4.255792
C	-3.320997	1.525522	0.027546
C	-2.998701	2.619572	0.848807
C	-4.560028	1.521928	-0.633673
C	-3.893418	3.679752	1.009772
H	-2.036628	2.642355	1.367424
C	-5.450093	2.592007	-0.483426
H	-4.846156	0.682614	-1.268940
C	-5.122255	3.671730	0.340263
H	-3.625772	4.520062	1.655797
H	-6.407437	2.573369	-1.011026
H	-5.820395	4.504164	0.460011
C	3.135058	-1.374648	-0.216910
C	3.619590	-0.584034	-1.274112
C	4.049290	-2.127374	0.536695
C	4.981504	-0.556038	-1.578405
H	2.923037	0.018195	-1.863024
C	5.418161	-2.083545	0.242876
H	3.704158	-2.758344	1.357072
C	5.887908	-1.303463	-0.816888
H	5.338478	0.060226	-2.407548
H	6.116937	-2.671326	0.844474
H	6.955195	-1.276801	-1.050052
C	1.057005	-2.478151	1.516799
C	1.607210	-2.019509	2.728633
C	0.280968	-3.649460	1.532532
C	1.423731	-2.735635	3.913616
H	2.187923	-1.093334	2.751417
C	0.089436	-4.361145	2.722608
H	-0.180310	-4.016568	0.614118
C	0.666610	-3.913755	3.913646
H	1.870961	-2.370286	4.841659
H	-0.515205	-5.272041	2.713578
H	0.522810	-4.475248	4.840309
C	0.933340	-2.574113	-1.431431
C	1.470472	-3.874237	-1.502049
C	0.234433	-2.067556	-2.536729
C	1.283195	-4.656131	-2.643539
H	2.049262	-4.278862	-0.667950
C	0.058750	-2.847139	-3.686254
H	-0.167946	-1.053634	-2.496046
C	0.576416	-4.143365	-3.739807
H	1.700267	-5.666181	-2.682288
H	-0.489994	-2.436340	-4.537472
H	0.436085	-4.754443	-4.635365
C	2.967009	2.617049	0.188459
C	3.782256	1.886264	1.077141
C	3.511535	3.765750	-0.430890
C	5.090641	2.291251	1.347147
H	3.372476	0.998424	1.559832
C	4.825345	4.158747	-0.172585
H	2.889219	4.349334	-1.111650
C	5.620265	3.425464	0.719697
H	5.701662	1.714613	2.045444
H	5.231193	5.046858	-0.664597
H	6.647665	3.737847	0.924135
C	-0.251875	3.963197	-0.720298
O	-1.210329	4.069305	-1.457874
O	0.349181	5.037699	-0.156909
C	-0.208579	6.316425	-0.467282
H	-1.199125	6.432142	0.003633
H	0.487489	7.063496	-0.064316
H	-0.319244	6.442748	-1.554969

Complex 12 - $[Pt(PPh_3)_2(PhC{\equiv}CH)]$

Pt	0.227174	0.930036	-0.155610
P	1.266879	-1.216201	0.098568
C	1.549662	2.584782	-0.257450
C	0.314154	2.954854	-0.408802
P	-2.122253	0.484872	-0.110840
C	-2.846089	-0.170868	1.467158
C	-4.224613	-0.427219	1.599651
C	-2.022021	-0.298066	2.593813
C	-4.756623	-0.824271	2.827857
H	-4.891994	-0.306370	0.743061
C	-2.558080	-0.685600	3.828324
H	-0.956121	-0.083666	2.503455
C	-3.923454	-0.953696	3.946830
H	-5.827892	-1.023742	2.915524
H	-1.900520	-0.778638	4.695808
H	-4.342728	-1.257509	4.909659
C	-2.812416	-0.589258	-1.448384
C	-2.733859	-0.136293	-2.780030
C	-3.318896	-1.876195	-1.206674
C	-3.189675	-0.932049	-3.833160
H	-2.313666	0.848596	-3.000344
C	-3.764130	-2.677391	-2.264462
H	-3.368583	-2.265585	-0.188732
C	-3.711007	-2.206036	-3.578119
H	-3.132888	-0.556538	-4.858036
H	-4.155106	-3.676337	-2.055013
H	-4.065553	-2.830136	-4.402093
C	-3.150349	2.037644	-0.231163
C	-2.831504	3.084593	0.654296
C	-4.254677	2.194279	-1.084388
C	-3.592089	4.255952	0.682282
H	-1.981597	2.977942	1.332889
C	-5.010569	3.373509	-1.062912
H	-4.541949	1.395903	-1.769778
C	-4.683084	4.407337	-0.182168
H	-3.329595	5.054904	1.381068
H	-5.864924	3.476525	-1.737620
H	-5.275874	5.325681	-0.165406
C	3.127096	-1.241920	-0.039081
C	3.682367	-0.653642	-1.189485
C	3.987045	-1.865490	0.878553
C	5.057974	-0.692776	-1.420840
H	3.030893	-0.156579	-1.913398
C	5.370230	-1.887853	0.654589
H	3.589068	-2.344667	1.773380
C	5.909791	-1.306359	-0.494925
H	5.467654	-0.235293	-2.324374
H	6.024668	-2.372720	1.382775
H	6.988576	-1.331124	-0.670909
C	0.949040	-2.049780	1.718603
C	1.433677	-1.433883	2.889286
C	0.168738	-3.210536	1.844316
C	1.178154	-1.987514	4.146033
H	2.016142	-0.511027	2.820306
C	-0.094601	-3.759103	3.105316
H	-0.241746	-3.696245	0.957557
C	0.415407	-3.156528	4.257927
H	1.573061	-1.501095	5.041879
H	-0.703274	-4.664031	3.182172
H	0.213903	-3.589727	5.241036
C	0.927018	-2.507144	-1.191604
C	1.470434	-3.803765	-1.108382
C	0.219901	-2.142519	-2.345037
C	1.285687	-4.717170	-2.147576
H	2.052589	-4.101942	-0.233386
C	0.046132	-3.054427	-3.393521
H	-0.188645	-1.133864	-2.420720
C	0.573437	-4.343569	-3.294801
H	1.708578	-5.722018	-2.067589
H	-0.506696	-2.751344	-4.285600
H	0.436828	-5.057629	-4.111020
C	2.903942	3.115558	-0.173216
C	3.978741	2.358982	0.334607
C	3.164248	4.445687	-0.577407
C	5.258845	2.910889	0.441228
H	3.800901	1.327718	0.640894
C	4.442835	4.993263	-0.471428
H	2.342988	5.048060	-0.980023
C	5.498525	4.228418	0.039596
H	6.077396	2.302557	0.842138
H	4.618403	6.025617	-0.791814
H	6.500487	4.658700	0.121854
H	-0.353844	3.803826	-0.539432

Complex 13 - $[Pt(PPh_3)_2(EtC{\equiv}CEt)]$

Pt	-0.007788	1.003946	-0.002518
P	1.950344	-0.366526	0.057055
C	0.633457	3.001689	0.037867
C	-0.655589	2.999374	-0.048815
P	-1.955127	-0.379165	-0.051425
C	-2.200035	-1.725951	1.205006
C	-3.407998	-2.444718	1.298703
C	-1.192143	-1.973652	2.146839
C	-3.586263	-3.405622	2.295557
H	-4.220992	-2.246955	0.595930
C	-1.373613	-2.931644	3.152822
H	-0.266226	-1.400181	2.098887
C	-2.567773	-3.651532	3.226326
H	-4.527518	-3.958509	2.353282
H	-0.576771	-3.107191	3.880074
H	-2.712168	-4.397995	4.011578
C	-2.278267	-1.185555	-1.689362
C	-2.251263	-0.360703	-2.831674
C	-2.463091	-2.566698	-1.864093
C	-2.437630	-0.898436	-4.107126
H	-2.072212	0.712559	-2.721788
C	-2.636741	-3.106607	-3.144487
H	-2.462305	-3.235848	-1.002623
C	-2.632405	-2.276050	-4.268037
H	-2.422391	-0.240385	-4.979829
H	-2.774529	-4.185156	-3.259320
H	-2.772267	-2.699106	-5.266077
C	-3.541047	0.550748	0.267033
C	-3.654353	1.221105	1.498948
C	-4.624403	0.595112	-0.623284
C	-4.820779	1.910570	1.833798
H	-2.818269	1.205270	2.203734
C	-5.791341	1.296851	-0.291855
H	-4.571178	0.078679	-1.583158
C	-5.895043	1.954217	0.935769
H	-4.890332	2.422285	2.796983
H	-6.624198	1.320707	-0.999993
H	-6.807058	2.498104	1.194335
C	3.517956	0.567242	-0.335153
C	3.568941	1.239681	-1.570145
C	4.649382	0.599838	0.494135
C	4.721959	1.918723	-1.968448
H	2.693588	1.235393	-2.225695
C	5.801569	1.293985	0.101099
H	4.645091	0.080964	1.454064
C	5.843612	1.952205	-1.130263
H	4.743109	2.430528	-2.934055
H	6.671543	1.311345	0.763349
H	6.744689	2.489356	-1.437420
C	2.312925	-1.101893	1.720171
C	2.377869	-0.225853	2.822356
C	2.430874	-2.482099	1.954111
C	2.586464	-0.715200	4.113923
H	2.261181	0.850769	2.670498
C	2.628793	-2.972432	3.250916
H	2.358828	-3.189254	1.126506
C	2.713925	-2.092813	4.333090
H	2.643210	-0.017944	4.953969
H	2.715301	-4.050728	3.410822
H	2.872264	-2.477113	5.344050
C	2.197574	-1.762905	-1.145162
C	3.392229	-2.508718	-1.182945
C	1.214612	-2.013682	-2.111994
C	3.580573	-3.498547	-2.149636
H	4.187865	-2.310472	-0.459870
C	1.407593	-2.999266	-3.089565
H	0.298384	-1.423406	-2.107230
C	2.587192	-3.745687	-3.107771
H	4.510903	-4.072467	-2.163332
H	0.630768	-3.175183	-3.838320
H	2.740021	-4.514490	-3.870267
C	1.902125	3.778402	0.131955
H	2.566238	3.293589	0.867404
H	2.442991	3.689690	-0.826276
C	-1.927315	3.769989	-0.149985
H	-2.575972	3.293715	-0.904744
H	-2.483927	3.661410	0.797010
C	1.737884	5.260791	0.489427
H	2.723164	5.747182	0.576700
H	1.163613	5.799343	-0.279462
H	1.212743	5.385619	1.450308
C	-1.766855	5.259175	-0.479986
H	-1.206865	5.788194	0.305985
H	-1.228726	5.403426	-1.430988
H	-2.753779	5.741195	-0.573490

Complex 14 - $[Pt(PPh_3)_2(MeC{\equiv}CCO_2Me)]$

Pt	-0.177047	1.087363	-0.111929
P	1.954367	0.047444	0.071235
C	0.123279	3.122197	-0.070478
C	-1.160647	2.929872	-0.214584
P	-1.614092	-0.864594	-0.100171
C	-1.962111	-1.492175	1.612903
C	-2.692479	-2.673943	1.840554
C	-1.574471	-0.713888	2.714288
C	-3.012846	-3.070602	3.140648
H	-3.021022	-3.290614	1.000483
C	-1.905593	-1.106190	4.016879
H	-1.011762	0.207125	2.545346
C	-2.621796	-2.285525	4.233118
H	-3.576863	-3.993087	3.301467
H	-1.598266	-0.486206	4.863166
H	-2.878554	-2.594583	5.249775
C	-1.036794	-2.347840	-1.043032
C	-1.141740	-2.338356	-2.447064
C	-0.426662	-3.449846	-0.423128
C	-0.673670	-3.412700	-3.206388
H	-1.600855	-1.487197	-2.956323
C	0.053041	-4.521203	-1.186767
H	-0.323345	-3.482484	0.662369
C	-0.073595	-4.509700	-2.578235
H	-0.774556	-3.390141	-4.294631
H	0.524122	-5.370629	-0.685416
H	0.295393	-5.349646	-3.172480
C	-3.369451	-0.675619	-0.699212
C	-4.020365	0.538975	-0.441935
C	-4.099029	-1.719288	-1.299551
C	-5.364796	0.718284	-0.781418
H	-3.470323	1.359252	0.011558
C	-5.444757	-1.544405	-1.637039
H	-3.623980	-2.678200	-1.511666
C	-6.081826	-0.323292	-1.380992
H	-5.842300	1.681624	-0.584698
H	-5.995307	-2.370465	-2.103356
H	-7.131760	-0.184871	-1.651098
C	3.371331	1.231652	0.347373
C	3.656326	2.136249	-0.692792
C	4.184999	1.250686	1.490822
C	4.724963	3.028365	-0.592672
H	3.037416	2.139581	-1.597077
C	5.250433	2.155045	1.595702
H	4.007390	0.555189	2.311284
C	5.526222	3.046463	0.556837
H	4.925765	3.714923	-1.417587
H	5.871599	2.151391	2.497018
H	6.359059	3.747408	0.635925
C	2.154078	-1.173718	1.448046
C	1.888785	-0.724605	2.756236
C	2.499231	-2.521841	1.259160
C	2.003272	-1.588461	3.847129
H	1.586063	0.311622	2.925689
C	2.597856	-3.390787	2.352386
H	2.686685	-2.907713	0.256878
C	2.360045	-2.926300	3.648530
H	1.802747	-1.215775	4.854815
H	2.864941	-4.437117	2.184993
H	2.444558	-3.605211	4.500442
C	2.601689	-0.774014	-1.456343
C	3.886683	-1.350661	-1.494568
C	1.849272	-0.713376	-2.637854
C	4.390225	-1.878700	-2.684159
H	4.505854	-1.376267	-0.594600
C	2.361718	-1.229834	-3.834336
H	0.862223	-0.246717	-2.619822
C	3.627640	-1.818478	-3.858212
H	5.386426	-2.328784	-2.698315
H	1.765415	-1.170944	-4.748341
H	4.027477	-2.223863	-4.791075
C	1.124962	4.207889	0.047904
H	1.815957	4.027020	0.885715
H	1.748545	4.274274	-0.857665
H	0.623680	5.177876	0.200297
C	-2.341425	3.770709	-0.390727
O	-3.316112	3.528639	-1.076182
O	-2.231914	4.928793	0.310886
C	-3.309315	5.857958	0.179719
H	-4.252640	5.421728	0.543571
H	-3.039730	6.729428	0.790674
H	-3.446360	6.161532	-0.870914

Complex 15 - $[Pt(PPh_3)_2(MeC{\equiv}CMe)]$

Pt	0.002995	-1.346149	-0.111178
P	-1.881878	0.110914	0.119168
C	-0.645360	-3.327752	-0.134012
C	0.640962	-3.324901	-0.277513
P	1.887110	0.132153	-0.127752
C	2.279371	1.004683	1.464615
C	3.383861	1.870331	1.584344
C	1.526226	0.707292	2.608723
C	3.708425	2.440025	2.816756
H	4.003797	2.094627	0.713014
C	1.857543	1.271348	3.847145
H	0.680222	0.022668	2.525648
C	2.945031	2.141054	3.952923
H	4.566965	3.112449	2.893999
H	1.258593	1.028273	4.728135
H	3.204572	2.582540	4.918707
C	1.892753	1.461869	-1.415555
C	1.943279	1.079039	-2.770273
C	1.764179	2.826564	-1.110289
C	1.909763	2.036695	-3.786378
H	2.010042	0.020566	-3.036453
C	1.716248	3.784802	-2.130230
H	1.700372	3.153294	-0.071194
C	1.799398	3.395767	-3.469286
H	1.963946	1.719190	-4.830970
H	1.617430	4.842224	-1.871104
H	1.769866	4.145763	-4.263790
C	3.552596	-0.684456	-0.362575
C	3.880964	-1.717264	0.534198
C	4.512608	-0.290909	-1.308416
C	5.129943	-2.339495	0.487715
H	3.150643	-2.033867	1.282749
C	5.761563	-0.923886	-1.363581
H	4.302076	0.519320	-2.007081
C	6.075432	-1.948282	-0.467788
H	5.364415	-3.136837	1.198025
H	6.493321	-0.604434	-2.110412
H	7.051673	-2.438355	-0.509914
C	-3.541201	-0.747105	0.102829
C	-3.778123	-1.645755	-0.951893
C	-4.583866	-0.484593	1.006522
C	-5.020079	-2.266119	-1.100146
H	-2.978241	-1.859884	-1.665577
C	-5.825344	-1.117066	0.865992
H	-4.441577	0.219782	1.827112
C	-6.048726	-2.008392	-0.186053
H	-5.183051	-2.959273	-1.929634
H	-6.622294	-0.903279	1.583683
H	-7.019104	-2.498735	-0.295693
C	-1.934324	1.103687	1.678561
C	-2.086441	0.423058	2.902640
C	-1.720595	2.491751	1.705973
C	-2.065525	1.117329	4.114334
H	-2.223402	-0.661621	2.911538
C	-1.690997	3.185096	2.921721
H	-1.575024	3.044213	0.776157
C	-1.871607	2.503753	4.127909
H	-2.197678	0.571876	5.052426
H	-1.527081	4.265907	2.921169
H	-1.854450	3.047613	5.075736
C	-2.249789	1.324603	-1.239095
C	-3.301718	2.255969	-1.147396
C	-1.545466	1.216886	-2.446206
C	-3.621829	3.073568	-2.232926
H	-3.884941	2.338677	-0.227427
C	-1.874325	2.028444	-3.538971
H	-0.737540	0.487542	-2.527650
C	-2.909166	2.960320	-3.433706
H	-4.438315	3.795240	-2.145682
H	-1.314755	1.930345	-4.472272
H	-3.166005	3.595947	-4.285211
C	-1.828023	-4.221974	-0.029221
H	-2.490310	-3.935647	0.802889
H	-2.443933	-4.190458	-0.942104
H	-1.512667	-5.269160	0.125495
C	1.819403	-4.211596	-0.459571
H	2.478391	-3.862539	-1.270075
H	2.440277	-4.254267	0.449939
H	1.499368	-5.242419	-0.694478

Complex 16 - $[Pt(PPh_3)_2(HC{\equiv}CH)]$

Pt	0.002498	-0.819580	-1.254403
P	-1.894662	-0.092834	-0.014721
C	-0.655493	-1.995331	-2.837751
C	0.631675	-1.938276	-2.895330
H	-1.565142	-2.383174	-3.292491
H	1.523399	-2.245281	-3.438394
P	1.898760	0.053104	-0.107396
C	2.369000	-0.813092	1.464667
C	3.542041	-0.479370	2.168046
C	1.577010	-1.870966	1.932355
C	3.903112	-1.180773	3.319237
H	4.183679	0.329979	1.811256
C	1.942040	-2.577592	3.084624
H	0.671200	-2.140347	1.385748
C	3.102259	-2.232826	3.781663
H	4.815767	-0.910020	3.856796
H	1.312566	-3.398481	3.437201
H	3.388586	-2.783944	4.681054
C	1.865269	1.845832	0.350361
C	1.903394	2.809606	-0.675825
C	1.709545	2.282595	1.676278
C	1.825549	4.172046	-0.379519
H	1.999278	2.495752	-1.718794
C	1.615587	3.648350	1.970209
H	1.662130	1.557793	2.490911
C	1.682155	4.596974	0.946614
H	1.870844	4.904923	-1.189384
H	1.495689	3.968631	3.008625
H	1.617360	5.663044	1.178426
C	3.511652	-0.120296	-1.028633
C	3.786504	-1.373646	-1.607143
C	4.485155	0.888303	-1.123115
C	4.996027	-1.610420	-2.264160
H	3.044619	-2.171873	-1.537607
C	5.692941	0.653762	-1.791950
H	4.313354	1.867500	-0.673710
C	5.952990	-0.593739	-2.364941
H	5.190326	-2.593069	-2.702670
H	6.434917	1.454138	-1.858846
H	6.896558	-0.774821	-2.885952
C	-3.522137	-0.738506	-0.660369
C	-3.727422	-0.696944	-2.051157
C	-4.573740	-1.180096	0.159941
C	-4.947737	-1.089385	-2.607322
H	-2.922416	-0.351242	-2.702805
C	-5.792314	-1.584080	-0.398783
H	-4.453349	-1.212955	1.243818
C	-5.983811	-1.540880	-1.782252
H	-5.087648	-1.046499	-3.690664
H	-6.596390	-1.930192	0.256073
H	-6.936114	-1.856002	-2.216569
C	-1.904787	-0.605549	1.761479
C	-2.053324	-1.971536	2.070409
C	-1.657200	0.296817	2.809163
C	-1.991538	-2.415850	3.393257
H	-2.221033	-2.697306	1.270346
C	-1.584679	-0.151798	4.133382
H	-1.518845	1.358967	2.599024
C	-1.759349	-1.505838	4.431204
H	-2.121764	-3.478696	3.613282
H	-1.393689	0.565941	4.935467
H	-1.709463	-1.853000	5.466372
C	-2.308682	1.715188	0.004302
C	-3.382748	2.226291	0.757208
C	-1.599024	2.581100	-0.839484
C	-3.724716	3.577338	0.676812
H	-3.962413	1.566631	1.407070
C	-1.948638	3.934122	-0.927194
H	-0.771066	2.187833	-1.432764
C	-3.008524	4.434988	-0.168186
H	-4.558317	3.962223	1.270006
H	-1.385919	4.596215	-1.589748
H	-3.281300	5.491419	-0.234425

Complex 17 - $[Pt(PPh_3)_2(EtO_2CC{\equiv}CCO_2Et)]$

Pt	-0.559798000	0.121568000	-0.052848000
P	1.244927000	1.690121000	0.088401000
C	-2.400447000	1.052530000	0.031013000
C	-2.588579000	-0.214499000	-0.228676000
P	0.635253000	-1.955652000	-0.077911000
C	1.273429000	-2.450659000	1.589946000
C	1.902399000	-3.695493000	1.786971000
C	1.038891000	-1.625617000	2.699142000
C	2.304184000	-4.091871000	3.063263000
H	2.071163000	-4.365748000	0.940784000
C	1.431675000	-2.029721000	3.981113000
H	0.539024000	-0.665988000	2.555321000
C	2.067397000	-3.259588000	4.165056000
H	2.795016000	-5.058996000	3.201276000
H	1.238246000	-1.377299000	4.836101000
H	2.374214000	-3.575254000	5.165677000
C	2.070691000	-2.128624000	-1.226887000
C	1.827227000	-2.044725000	-2.610696000
C	3.395397000	-2.276910000	-0.784188000
C	2.875756000	-2.145070000	-3.527204000
H	0.808658000	-1.897636000	-2.978944000
C	4.447222000	-2.358866000	-1.704304000
H	3.616576000	-2.328583000	0.282470000
C	4.190830000	-2.302187000	-3.076496000
H	2.664902000	-2.087138000	-4.597910000
H	5.471867000	-2.472721000	-1.341257000
H	5.012851000	-2.372751000	-3.793140000
C	-0.396473000	-3.466047000	-0.434111000
C	-1.480156000	-3.712190000	0.428278000
C	-0.127513000	-4.387719000	-1.457426000
C	-2.271582000	-4.850632000	0.273945000
H	-1.707749000	-3.007606000	1.232692000
C	-0.932737000	-5.522798000	-1.621044000
H	0.714943000	-4.238730000	-2.133803000
C	-2.004017000	-5.759726000	-0.756672000
H	-3.106322000	-5.025686000	0.958174000
H	-0.709798000	-6.225386000	-2.428746000
H	-2.631367000	-6.646520000	-0.881870000
C	0.781586000	3.489810000	0.212477000
C	-0.279455000	3.942713000	-0.587866000
C	1.518098000	4.430660000	0.952612000
C	-0.597873000	5.301961000	-0.651162000
H	-0.862657000	3.223514000	-1.166004000
C	1.193324000	5.790154000	0.893917000
H	2.360506000	4.113160000	1.568913000
C	0.137029000	6.231047000	0.091762000
H	-1.426781000	5.634932000	-1.281537000
H	1.778573000	6.506793000	1.475374000
H	-0.111352000	7.295039000	0.043936000
C	2.449056000	1.452501000	1.467081000
C	2.051228000	1.787155000	2.775874000
C	3.706445000	0.856516000	1.276633000
C	2.904870000	1.564238000	3.858654000
H	1.068098000	2.230814000	2.953314000
C	4.556830000	0.627019000	2.364686000
H	4.033334000	0.567782000	0.276261000
C	4.163483000	0.986195000	3.656230000
H	2.583348000	1.841113000	4.865964000
H	5.534711000	0.168657000	2.195854000
H	4.831951000	0.813317000	4.503385000
C	2.254021000	1.817999000	-1.462826000
C	3.454867000	2.550199000	-1.516959000
C	1.722587000	1.299413000	-2.652394000
C	4.117253000	2.734744000	-2.732150000
H	3.874745000	2.989399000	-0.609598000
C	2.378639000	1.499256000	-3.872502000
H	0.785361000	0.740035000	-2.618046000
C	3.579223000	2.211059000	-3.914396000
H	5.053045000	3.298909000	-2.758424000
H	1.949649000	1.090305000	-4.790644000
H	4.095515000	2.362598000	-4.865818000
C	-3.652248000	-1.168154000	-0.566731000
C	-3.157734000	2.257129000	0.392759000
O	-3.531488000	-2.065077000	-1.375916000
O	-2.781691000	3.078420000	1.206441000
O	-4.792352000	-0.927196000	0.107924000
O	-4.335431000	2.331132000	-0.254619000
C	-5.911491000	-1.796557000	-0.163991000
H	-5.739237000	-2.754702000	0.355020000
H	-5.941642000	-2.008109000	-1.242954000
C	-5.226798000	3.418000000	0.072463000
H	-5.053250000	4.226710000	-0.656711000
H	-4.969535000	3.802764000	1.068834000
C	-7.180081000	-1.120569000	0.313296000
H	-8.039970000	-1.786784000	0.141779000
H	-7.136399000	-0.888658000	1.388813000
H	-7.355981000	-0.184463000	-0.237725000
C	-6.654579000	2.915230000	0.012358000
H	-7.346602000	3.743035000	0.231818000
H	-6.897577000	2.517468000	-0.984954000
H	-6.822063000	2.121017000	0.755417000

Complex 18 - $[Pt(PPh_3)_2(MeO_2CC{\equiv}CCO_2Me)]$

Pt	0.002742	0.691717	-0.087869
P	1.855538	-0.794028	0.075887
C	0.831557	2.576745	-0.035071
C	-0.451800	2.712357	-0.223701
P	-2.004116	-0.592232	-0.077550
C	-2.317768	-1.569402	1.464247
C	-3.514077	-2.289430	1.648884
C	-1.394459	-1.505454	2.517190
C	-3.763982	-2.948549	2.853705
H	-4.261139	-2.329850	0.852720
C	-1.650520	-2.158884	3.729257
H	-0.476074	-0.931104	2.387862
C	-2.831846	-2.883938	3.897957
H	-4.694229	-3.507817	2.982471
H	-0.920117	-2.096158	4.539408
H	-3.032885	-3.394093	4.843565
C	-2.280979	-1.762419	-1.478660
C	-2.353686	-1.226876	-2.779467
C	-2.342074	-3.155319	-1.316334
C	-2.518104	-2.064447	-3.885013
H	-2.281952	-0.146270	-2.931086
C	-2.497654	-3.993373	-2.426825
H	-2.264878	-3.598119	-0.322143
C	-2.594011	-3.452092	-3.711104
H	-2.583632	-1.631914	-4.886636
H	-2.542713	-5.075886	-2.282078
H	-2.721319	-4.107844	-4.576136
C	-3.552306	0.443932	-0.068922
C	-3.614928	1.506630	0.849408
C	-4.678441	0.169678	-0.860518
C	-4.775172	2.272588	0.976143
H	-2.746406	1.740030	1.470243
C	-5.837380	0.946750	-0.741596
H	-4.664978	-0.654132	-1.575326
C	-5.890981	1.997363	0.177161
H	-4.805561	3.092842	1.698086
H	-6.702903	0.721717	-1.370248
H	-6.796933	2.601405	0.271391
C	3.449850	0.041942	-0.398978
C	3.452503	0.859659	-1.542391
C	4.661689	-0.185928	0.272698
C	4.639046	1.439074	-2.000856
H	2.518596	1.051982	-2.077026
C	5.847307	0.401939	-0.182442
H	4.691454	-0.821699	1.158978
C	5.840534	1.214920	-1.319275
H	4.622673	2.073265	-2.891261
H	6.780457	0.218357	0.356720
H	6.767937	1.672359	-1.673682
C	2.167033	-1.400663	1.789224
C	2.499239	-0.449584	2.774584
C	1.972022	-2.736876	2.173192
C	2.664100	-0.838950	4.105778
H	2.629086	0.600904	2.498959
C	2.133823	-3.121809	3.509017
H	1.685028	-3.487082	1.434697
C	2.485767	-2.177669	4.476800
H	2.930317	-0.092101	4.857977
H	1.980514	-4.166783	3.790339
H	2.615101	-2.481147	5.518711
C	1.990390	-2.266985	-1.039648
C	3.010628	-3.226647	-0.895309
C	1.138642	-2.343811	-2.150582
C	3.152758	-4.253383	-1.830920
H	3.707230	-3.171423	-0.055930
C	1.291965	-3.364823	-3.096326
H	0.357370	-1.593927	-2.280622
C	2.293832	-4.324221	-2.935220
H	3.944670	-4.995967	-1.703464
H	0.620802	-3.406210	-3.957296
H	2.412048	-5.124199	-3.670746
C	2.059529	3.332961	0.215776
C	-1.462749	3.738340	-0.488214
O	2.778973	3.170072	1.179856
O	-2.244988	3.714741	-1.415256
O	2.301448	4.244909	-0.741390
O	-1.418258	4.736371	0.415337
C	3.473501	5.051356	-0.575657
H	4.382543	4.435055	-0.651457
H	3.449093	5.790173	-1.385382
H	3.465042	5.557440	0.400851
C	-2.343884	5.812303	0.224788
H	-3.374900	5.472779	0.407400
H	-2.069497	6.586084	0.952720
H	-2.275967	6.208533	-0.798925

Complex 19 - $[Pt(PPh_3)_2(F_3CC{\equiv}CCF_3)]$

Pt	0.007658	0.873366	-0.004634
P	1.822728	-0.674360	0.093136
C	0.697748	2.814959	0.092584
C	-0.589030	2.850908	-0.102858
P	-1.859854	-0.621225	-0.090280
C	-2.198053	-1.569272	1.463376
C	-3.215127	-2.541332	1.523868
C	-1.522118	-1.218932	2.640493
C	-3.527499	-3.163724	2.733507
H	-3.776318	-2.809599	0.626000
C	-1.844490	-1.835829	3.855120
H	-0.743253	-0.454943	2.605447
C	-2.842474	-2.811608	3.903281
H	-4.316064	-3.920109	2.765587
H	-1.307970	-1.551895	4.763472
H	-3.093095	-3.295104	4.850923
C	-1.835589	-1.865205	-1.452832
C	-2.011420	-1.413961	-2.775265
C	-1.571938	-3.227046	-1.233101
C	-1.965604	-2.310237	-3.845074
H	-2.189015	-0.353465	-2.973939
C	-1.515202	-4.121698	-2.308468
H	-1.410872	-3.600673	-0.220337
C	-1.720852	-3.669188	-3.614390
H	-2.117295	-1.944101	-4.863867
H	-1.312758	-5.179182	-2.118895
H	-1.684303	-4.370777	-4.451583
C	-3.525996	0.191852	-0.267622
C	-3.802072	1.280598	0.575476
C	-4.544846	-0.285276	-1.108805
C	-5.058848	1.887919	0.571339
H	-3.025484	1.665967	1.238314
C	-5.802707	0.328653	-1.117314
H	-4.371176	-1.140433	-1.762760
C	-6.064064	1.415915	-0.279517
H	-5.247464	2.740093	1.228900
H	-6.581534	-0.051363	-1.783746
H	-7.046503	1.894343	-0.289444
C	3.510802	0.098524	0.247376
C	3.830880	1.117400	-0.664627
C	4.503041	-0.347651	1.134593
C	5.104918	1.686785	-0.683525
H	3.074470	1.478038	-1.363889
C	5.779078	0.228930	1.119671
H	4.295648	-1.150818	1.841666
C	6.084778	1.245541	0.212278
H	5.328997	2.483905	-1.396040
H	6.537506	-0.126585	1.821786
H	7.081878	1.693123	0.202417
C	1.771893	-1.899520	1.471170
C	1.933503	-1.429507	2.788614
C	1.504693	-3.263157	1.268909
C	1.871101	-2.309225	3.871253
H	2.112597	-0.366919	2.973237
C	1.429938	-4.140922	2.357151
H	1.354361	-3.651885	0.260370
C	1.622043	-3.669994	3.658393
H	2.012361	-1.928441	4.885973
H	1.224116	-5.199936	2.181245
H	1.571549	-4.358605	4.505602
C	2.130996	-1.643864	-1.452215
C	3.136872	-2.627160	-1.514714
C	1.447585	-1.294029	-2.624930
C	3.430439	-3.261319	-2.723111
H	3.705005	-2.892847	-0.620269
C	1.751419	-1.922378	-3.838551
H	0.678872	-0.520164	-2.584340
C	2.738265	-2.909201	-3.889110
H	4.210585	-4.026079	-2.757788
H	1.209893	-1.638658	-4.744050
H	2.974974	-3.401571	-4.835937
C	1.813107	3.772849	0.270664
C	-1.645019	3.876299	-0.264388
F	-1.147462	5.080393	-0.615664
F	-2.337479	4.067070	0.882077
F	1.389086	4.990952	0.669537
F	2.499212	3.962253	-0.879675
F	2.700877	3.357769	1.195174
F	-2.541015	3.543175	-1.213408

Complex 20 - $[Pt(PPh_3)_2(PhC{\equiv}CCN)]$

Pt	0.290800	0.862191	-0.180400
P	1.169214	-1.320154	-0.009479
C	1.758246	2.310185	-0.151641
C	0.606750	2.913241	-0.361561
P	-2.091126	0.423854	-0.058621
C	-2.693072	0.818002	1.647723
C	-4.031399	1.173975	1.896375
C	-1.798124	0.742765	2.727086
C	-4.462195	1.445215	3.197788
H	-4.743375	1.242666	1.071193
C	-2.231871	1.012650	4.029817
H	-0.755389	0.474058	2.543325
C	-3.563591	1.364765	4.267660
H	-5.504311	1.722075	3.376518
H	-1.523197	0.950261	4.859209
H	-3.901877	1.580087	5.284591
C	-2.815133	-1.249735	-0.391687
C	-2.609923	-1.834673	-1.655133
C	-3.555045	-1.963784	0.566111
C	-3.143447	-3.089923	-1.959368
H	-2.034256	-1.306317	-2.416497
C	-4.080186	-3.225771	0.264034
H	-3.726720	-1.542231	1.557390
C	-3.879681	-3.791640	-0.998308
H	-2.977787	-3.520917	-2.950094
H	-4.651670	-3.766393	1.023185
H	-4.294550	-4.775306	-1.233739
C	-3.142831	1.547138	-1.103307
C	-3.007891	2.931940	-0.895685
C	-4.050724	1.099275	-2.076478
C	-3.753014	3.845022	-1.643785
H	-2.318709	3.306264	-0.138156
C	-4.793778	2.016674	-2.830929
H	-4.194699	0.032825	-2.252657
C	-4.647801	3.389988	-2.619337
H	-3.625403	4.915659	-1.464910
H	-5.494243	1.648420	-3.585202
H	-5.229399	4.103581	-3.208975
C	3.022963	-1.478476	0.031094
C	3.756359	-0.720252	-0.895774
C	3.705670	-2.401127	0.840266
C	5.138935	-0.878377	-1.013987
H	3.241842	0.001282	-1.530650
C	5.092523	-2.552465	0.729486
H	3.162993	-3.016033	1.559414
C	5.812973	-1.792553	-0.197786
H	5.691454	-0.278951	-1.739823
H	5.608881	-3.276479	1.368766
H	6.895425	-1.914083	-0.284685
C	0.605029	-2.228575	1.491814
C	1.095895	-1.801273	2.741471
C	-0.371169	-3.236937	1.460403
C	0.644998	-2.390206	3.924024
H	1.839108	-1.001662	2.794415
C	-0.825611	-3.821593	2.648511
H	-0.794298	-3.568310	0.511864
C	-0.317079	-3.406226	3.880818
H	1.044630	-2.051749	4.883002
H	-1.586080	-4.605080	2.604172
H	-0.671611	-3.867068	4.805945
C	0.875130	-2.408478	-1.479100
C	1.082641	-3.798908	-1.451722
C	0.587759	-1.788429	-2.705441
C	0.969605	-4.553317	-2.622490
H	1.344372	-4.301987	-0.518603
C	0.491084	-2.542372	-3.879615
H	0.442091	-0.705287	-2.734365
C	0.673181	-3.927536	-3.838962
H	1.124190	-5.634625	-2.585943
H	0.269809	-2.044088	-4.826753
H	0.592569	-4.519223	-4.754287
C	3.158597	2.658855	0.038835
C	3.955294	1.993077	0.991305
C	3.735234	3.713857	-0.703382
C	5.278572	2.380996	1.209125
H	3.520503	1.173760	1.566756
C	5.064069	4.085560	-0.495771
H	3.130378	4.236812	-1.448615
C	5.839684	3.423856	0.464181
H	5.877996	1.861063	1.960527
H	5.495852	4.900686	-1.081867
H	6.878644	3.720259	0.629667
C	0.085762	4.199405	-0.486566
N	-0.366742	5.273819	-0.584582

Complex 21 - $[Pt(PPh_3)_2(F_3CH_2CO_2CC{\equiv}CCO_2CH_2CF_3)]$

Pt	-0.313675000	-0.008180000	-0.058883000
P	-1.716139000	-1.924654000	0.060818000
C	1.612871000	-0.744716000	-0.050772000
C	1.667548000	0.548077000	-0.223016000
P	-1.581973000	2.004120000	-0.035845000
C	-2.909881000	2.199626000	1.238543000
C	-3.579295000	3.423602000	1.428872000
C	-3.189569000	1.132572000	2.103446000
C	-4.521845000	3.561987000	2.450002000
H	-3.359363000	4.278810000	0.785584000
C	-4.128089000	1.274414000	3.132197000
H	-2.654441000	0.190664000	1.982039000
C	-4.797836000	2.487486000	3.305271000
H	-5.036272000	4.516427000	2.586205000
H	-4.325846000	0.433006000	3.800951000
H	-5.527945000	2.601765000	4.110749000
C	-2.336734000	2.485083000	-1.651368000
C	-1.485712000	2.549093000	-2.772369000
C	-3.712160000	2.703523000	-1.829912000
C	-2.000458000	2.844327000	-4.036554000
H	-0.413490000	2.368709000	-2.655230000
C	-4.225919000	2.989635000	-3.100786000
H	-4.395114000	2.640873000	-0.981389000
C	-3.373346000	3.063919000	-4.205028000
H	-1.327081000	2.897249000	-4.895620000
H	-5.299771000	3.154160000	-3.222699000
H	-3.776445000	3.288209000	-5.195813000
C	-0.510816000	3.458411000	0.402358000
C	0.330693000	3.333556000	1.522767000
C	-0.540663000	4.678154000	-0.291201000
C	1.120097000	4.406552000	1.942263000
H	0.373280000	2.387465000	2.068849000
C	0.258600000	5.749778000	0.125468000
H	-1.184739000	4.802956000	-1.163707000
C	1.088285000	5.618815000	1.241924000
H	1.765220000	4.294034000	2.817689000
H	0.227446000	6.691526000	-0.428862000
H	1.708640000	6.457876000	1.567391000
C	-0.881645000	-3.379477000	-0.740649000
C	-0.203886000	-3.162674000	-1.952531000
C	-0.959836000	-4.685082000	-0.228273000
C	0.379118000	-4.230505000	-2.640068000
H	-0.128780000	-2.150029000	-2.359588000
C	-0.368053000	-5.750442000	-0.914421000
H	-1.479409000	-4.877149000	0.711735000
C	0.301380000	-5.527805000	-2.120787000
H	0.902896000	-4.047475000	-3.582098000
H	-0.434033000	-6.759319000	-0.500867000
H	0.762227000	-6.362108000	-2.656023000
C	-2.052695000	-2.488626000	1.786805000
C	-0.947041000	-2.822085000	2.594339000
C	-3.337110000	-2.504179000	2.353850000
C	-1.132629000	-3.185336000	3.930336000
H	0.063938000	-2.800021000	2.176351000
C	-3.516591000	-2.860847000	3.696112000
H	-4.207572000	-2.232103000	1.755355000
C	-2.417678000	-3.206880000	4.485212000
H	-0.267104000	-3.450083000	4.542649000
H	-4.524188000	-2.869296000	4.119940000
H	-2.559332000	-3.489812000	5.531836000
C	-3.341832000	-1.984409000	-0.824542000
C	-4.177573000	-3.117464000	-0.772187000
C	-3.699024000	-0.920067000	-1.662087000
C	-5.352810000	-3.164360000	-1.525035000
H	-3.912022000	-3.973218000	-0.147979000
C	-4.871860000	-0.971786000	-2.424877000
H	-3.047324000	-0.049305000	-1.728857000
C	-5.703117000	-2.091482000	-2.354793000
H	-5.995000000	-4.046958000	-1.470378000
H	-5.128711000	-0.132425000	-3.075569000
H	-6.619717000	-2.133995000	-2.949330000
C	2.573332000	1.654462000	-0.511757000
C	2.461449000	-1.909682000	0.174317000
O	2.241879000	-2.773812000	0.994234000
O	2.469866000	2.391481000	-1.465463000
O	3.551356000	-1.918534000	-0.642065000
O	3.551829000	1.771529000	0.425643000
C	4.512620000	-2.944900000	-0.445834000
H	4.581405000	-3.564332000	-1.353101000
H	4.241015000	-3.573770000	0.411286000
C	4.529953000	2.785123000	0.239868000
H	4.479957000	3.502216000	1.073363000
H	4.369581000	3.311614000	-0.711194000
C	5.864877000	-2.305167000	-0.183926000
C	5.905378000	2.142969000	0.226292000
F	6.842345000	3.091393000	0.046221000
F	6.021746000	1.248688000	-0.770016000
F	6.774256000	-3.261169000	0.073372000
F	6.304967000	-1.603912000	-1.238676000
F	5.827156000	-1.476280000	0.871138000
F	6.181081000	1.509659000	1.379188000

Complex 22 - $[Pt(PPh_3)_2(MeC{\equiv}CCN)]$

Pt	-0.012805	1.329085	0.104293
P	1.831204	-0.247109	0.120093
C	0.624052	3.318243	0.224401
C	-0.677730	3.271739	0.078680
P	-1.868232	-0.116980	-0.103311
C	-2.298212	-1.126914	1.386078
C	-3.382506	-2.025054	1.386787
C	-1.607743	-0.893369	2.582343
C	-3.746740	-2.691235	2.558176
H	-3.954805	-2.198590	0.473002
C	-1.983048	-1.551265	3.759954
H	-0.778185	-0.183754	2.583934
C	-3.048042	-2.453954	3.748628
H	-4.586602	-3.390485	2.545804
H	-1.437270	-1.356678	4.685676
H	-3.341044	-2.969635	4.666895
C	-1.796321	-1.290465	-1.527019
C	-1.754371	-0.752014	-2.827716
C	-1.709311	-2.683626	-1.371714
C	-1.666542	-1.586968	-3.943307
H	-1.790572	0.330863	-2.972816
C	-1.605117	-3.517902	-2.491178
H	-1.719931	-3.128632	-0.376001
C	-1.592292	-2.974709	-3.778266
H	-1.646995	-1.150970	-4.945231
H	-1.538272	-4.599920	-2.351394
H	-1.518114	-3.628619	-4.650679
C	-3.508667	0.743321	-0.317683
C	-3.898392	1.624629	0.707785
C	-4.393901	0.519770	-1.384036
C	-5.137494	2.264779	0.668937
H	-3.227043	1.808663	1.550759
C	-5.633138	1.171626	-1.427753
H	-4.133568	-0.170332	-2.187391
C	-6.009694	2.043836	-0.404054
H	-5.421915	2.942344	1.478436
H	-6.307694	0.986490	-2.268099
H	-6.978705	2.547511	-0.438105
C	3.492668	0.440915	0.608233
C	3.849689	1.693110	0.080334
C	4.437174	-0.258414	1.379548
C	5.112992	2.239203	0.320489
H	3.134079	2.247694	-0.527644
C	5.700167	0.292391	1.625413
H	4.199519	-1.239521	1.793430
C	6.042471	1.541408	1.098186
H	5.362336	3.219084	-0.094403
H	6.420172	-0.263404	2.231860
H	7.029306	1.969411	1.292879
C	1.654991	-1.733982	1.204080
C	1.752367	-1.570944	2.598814
C	1.343404	-3.005626	0.696128
C	1.577145	-2.657094	3.458565
H	1.973422	-0.587909	3.022147
C	1.154899	-4.090398	1.560487
H	1.248285	-3.160721	-0.379497
C	1.279266	-3.922728	2.941790
H	1.668652	-2.511807	4.537847
H	0.915593	-5.073117	1.146347
H	1.140026	-4.772524	3.614482
C	2.286986	-0.909063	-1.551412
C	3.293972	-1.880009	-1.711884
C	1.697845	-0.346523	-2.693444
C	3.685053	-2.290031	-2.988063
H	3.784195	-2.315605	-0.837692
C	2.098753	-0.750368	-3.973214
H	0.925352	0.416818	-2.576314
C	3.088587	-1.724275	-4.123012
H	4.464968	-3.048148	-3.098241
H	1.632143	-0.300611	-4.853760
H	3.400818	-2.041383	-5.121742
C	-1.848051	4.171467	-0.054052
H	-2.510322	3.853197	-0.873107
H	-2.457262	4.151986	0.864001
H	-1.530833	5.212588	-0.231830
C	1.663061	4.237008	0.351749
N	2.557876	4.982763	0.451885

Complex 23 - $[Pt(PPh_3)_2(HC{\equiv}CCN)]$

Pt	0.013823	1.372318	-0.009511
P	1.813323	-0.226219	0.088326
C	0.609882	3.399046	0.043168
C	-0.686879	3.280536	-0.043507
P	-1.913102	0.004757	-0.090520
C	-2.509428	-0.618117	1.544929
C	-3.765297	-1.243554	1.671483
C	-1.742112	-0.391971	2.696902
C	-4.231483	-1.645579	2.924170
H	-4.388783	-1.409107	0.789583
C	-2.213863	-0.790597	3.953153
H	-0.775452	0.106662	2.605381
C	-3.456446	-1.418069	4.068402
H	-5.207376	-2.130656	3.008673
H	-1.607170	-0.604173	4.842398
H	-3.827370	-1.724726	5.049377
C	-1.880859	-1.465847	-1.208290
C	-1.593001	-1.253225	-2.569684
C	-2.083938	-2.781273	-0.759927
C	-1.545143	-2.323868	-3.464953
H	-1.405379	-0.240909	-2.935427
C	-2.022395	-3.854154	-1.656694
H	-2.287797	-2.979912	0.292648
C	-1.760843	-3.629491	-3.010598
H	-1.329090	-2.137118	-4.519615
H	-2.183805	-4.871197	-1.290588
H	-1.719888	-4.468003	-3.709991
C	-3.422860	0.946870	-0.640587
C	-3.818802	2.041215	0.151934
C	-4.188080	0.625527	-1.771398
C	-4.945522	2.794876	-0.180933
H	-3.246506	2.301616	1.044923
C	-5.314888	1.387254	-2.108455
H	-3.920574	-0.225668	-2.397563
C	-5.697144	2.473038	-1.317924
H	-5.238654	3.637952	0.450286
H	-5.897825	1.120550	-2.993638
H	-6.576510	3.068602	-1.579710
C	3.495513	0.446684	0.524112
C	3.847119	1.705909	0.013404
C	4.454421	-0.281437	1.247269
C	5.126222	2.231200	0.222046
H	3.118698	2.280751	-0.558294
C	5.730419	0.247255	1.461546
H	4.215156	-1.265066	1.650528
C	6.071741	1.504231	0.952047
H	5.375315	3.217063	-0.179342
H	6.463926	-0.330359	2.030227
H	7.070578	1.915302	1.123121
C	1.577657	-1.591441	1.310004
C	1.740225	-1.306184	2.679404
C	1.138353	-2.872092	0.936779
C	1.500751	-2.285290	3.645951
H	2.064365	-0.312075	2.997065
C	0.891695	-3.849811	1.908001
H	0.986125	-3.118417	-0.115172
C	1.077707	-3.563236	3.262829
H	1.643862	-2.047565	4.703334
H	0.554997	-4.842482	1.598570
H	0.890975	-4.330331	4.018763
C	2.246238	-1.044983	-1.517081
C	3.139916	-2.129624	-1.588968
C	1.763791	-0.483312	-2.708856
C	3.523095	-2.649996	-2.826916
H	3.548656	-2.569844	-0.676636
C	2.157509	-0.998146	-3.949325
H	1.082588	0.369317	-2.661083
C	3.032712	-2.085047	-4.010780
H	4.213917	-3.496105	-2.868247
H	1.775190	-0.547845	-4.868605
H	3.337876	-2.491113	-4.978628
C	1.650878	4.324223	0.106247
N	2.557313	5.059256	0.153885
H	-1.593917	3.882044	-0.108166

Complex 24 - $[Pt(PPh_3)_2(NCC{\equiv}CCN)]$

Pt	0.011283	-1.196259	-0.000630
P	1.872758	0.265886	-0.018660
C	0.637216	-3.166545	-0.051317
C	-0.683833	-3.146499	-0.051616
P	-1.845123	0.292163	0.040320
C	-2.779549	0.279605	-1.553467
C	-4.105168	0.747919	-1.627759
C	-2.171184	-0.224082	-2.713723
C	-4.797348	0.724125	-2.840853
H	-4.605651	1.127101	-0.734052
C	-2.866328	-0.248199	-3.928214
H	-1.153175	-0.615978	-2.659734
C	-4.178691	0.227599	-3.994259
H	-5.826368	1.089917	-2.884406
H	-2.380658	-0.647590	-4.821810
H	-4.723861	0.205244	-4.941457
C	-1.616532	2.079453	0.455011
C	-0.947572	2.409925	1.648139
C	-2.098889	3.119552	-0.355888
C	-0.794662	3.743073	2.036313
H	-0.543687	1.623622	2.288042
C	-1.935716	4.454947	0.029517
H	-2.604437	2.897991	-1.296180
C	-1.291898	4.771092	1.228609
H	-0.280133	3.977047	2.971748
H	-2.317831	5.250497	-0.615187
H	-1.171350	5.814699	1.530023
C	-3.145603	-0.260870	1.249216
C	-3.775730	-1.496195	1.006595
C	-3.517237	0.472509	2.387124
C	-4.744986	-1.988488	1.881976
H	-3.517268	-2.081210	0.122451
C	-4.486882	-0.025436	3.266941
H	-3.062552	1.441118	2.597865
C	-5.101903	-1.255295	3.020096
H	-5.219115	-2.951064	1.672694
H	-4.762206	0.560111	4.148082
H	-5.858479	-1.641056	3.708132
C	3.382933	-0.488715	-0.796059
C	3.944964	-1.616717	-0.171669
C	3.986353	0.010891	-1.960994
C	5.080624	-2.231710	-0.700975
H	3.494438	-2.020787	0.737545
C	5.123355	-0.610201	-2.492271
H	3.580186	0.889935	-2.461891
C	5.673323	-1.730890	-1.866037
H	5.497041	-3.111464	-0.204841
H	5.580649	-0.208113	-3.400125
H	6.560498	-2.214303	-2.282647
C	1.671185	1.844683	-0.953862
C	1.135656	1.752714	-2.251754
C	2.038143	3.106678	-0.461919
C	0.998625	2.890687	-3.049699
H	0.830599	0.780989	-2.646530
C	1.889523	4.247525	-1.259091
H	2.433304	3.213318	0.548441
C	1.377994	4.143065	-2.555060
H	0.589357	2.798117	-4.058672
H	2.174215	5.223777	-0.859068
H	1.267671	5.035420	-3.176250
C	2.516387	0.688359	1.659627
C	3.740568	1.363757	1.828790
C	1.809289	0.266135	2.797596
C	4.223329	1.642407	3.109604
H	4.329310	1.664129	0.958648
C	2.298272	0.540109	4.080236
H	0.881141	-0.298821	2.675385
C	3.500747	1.235059	4.237975
H	5.172406	2.172111	3.227255
H	1.739176	0.201731	4.956369
H	3.883278	1.449363	5.239200
C	1.674008	-4.103338	-0.071498
N	2.560862	-4.861929	-0.089463
C	-1.751204	-4.046749	-0.089906
N	-2.668085	-4.769504	-0.105910

Complex 25 - $[Pt(F_3CC{\equiv}CCF_3)(PPh_3)_2]$

Pt	0.008616	0.790391	-0.163139
P	1.816403	-0.735193	0.081017
C	0.817059	2.678975	-0.146311
C	-0.465638	2.803060	-0.332116
P	-1.935625	-0.598549	-0.077955
C	-2.264567	-1.341878	1.586977
C	-3.383712	-2.167157	1.810573
C	-1.463367	-0.976218	2.678229
C	-3.675546	-2.632950	3.093203
H	-4.042356	-2.439065	0.982626
C	-1.765283	-1.433730	3.966837
H	-0.605558	-0.320723	2.519938
C	-2.866306	-2.265852	4.176176
H	-4.545195	-3.275963	3.250797
H	-1.132212	-1.135481	4.805729
H	-3.101340	-2.624374	5.181638
C	-2.056027	-1.987161	-1.287435
C	-2.176978	-1.662082	-2.652217
C	-1.976456	-3.338975	-0.919944
C	-2.257336	-2.666258	-3.618763
H	-2.214695	-0.614737	-2.963630
C	-2.048774	-4.344023	-1.891575
H	-1.857031	-3.619245	0.127649
C	-2.198911	-4.012529	-3.239796
H	-2.364572	-2.395686	-4.672167
H	-1.987180	-5.391945	-1.587682
H	-2.262419	-4.799069	-3.995864
C	-3.558248	0.289814	-0.299926
C	-3.748188	1.472952	0.431964
C	-4.622547	-0.203643	-1.072188
C	-4.965629	2.154146	0.387519
H	-2.934927	1.873499	1.038949
C	-5.842230	0.481988	-1.118684
H	-4.513794	-1.126816	-1.642393
C	-6.018242	1.661379	-0.390967
H	-5.085555	3.078940	0.956963
H	-6.658612	0.085733	-1.728314
H	-6.970938	2.195639	-0.430949
C	3.454066	0.003232	-0.397402
C	3.511316	0.792419	-1.557369
C	4.646557	-0.291149	0.283634
C	4.732631	1.287354	-2.020993
H	2.591552	1.033473	-2.095393
C	5.867510	0.211017	-0.177981
H	4.631487	-0.911839	1.181796
C	5.914500	1.001205	-1.331050
H	4.757648	1.908555	-2.920246
H	6.786484	-0.018361	0.367784
H	6.869530	1.394731	-1.688813
C	2.043605	-1.234425	1.841116
C	2.452817	-0.247301	2.759136
C	1.712917	-2.511218	2.321957
C	2.564050	-0.545997	4.118703
H	2.683840	0.761876	2.409045
C	1.826050	-2.807128	3.685128
H	1.357363	-3.283386	1.637991
C	2.257394	-1.830120	4.585553
H	2.890878	0.229008	4.816698
H	1.570119	-3.807913	4.041926
H	2.348269	-2.064241	5.649240
C	1.938108	-2.271538	-0.945108
C	2.820540	-3.323277	-0.635861
C	1.260478	-2.293438	-2.172951
C	2.995934	-4.384118	-1.527379
H	3.390077	-3.314449	0.295275
C	1.451291	-3.347871	-3.072287
H	0.586811	-1.474669	-2.430909
C	2.313580	-4.397933	-2.749297
H	3.680225	-5.196938	-1.271544
H	0.918036	-3.346358	-4.025330
H	2.460547	-5.224173	-3.449630
C	-1.441562	3.901558	-0.511917
C	2.004637	3.549765	0.008697
F	-0.852719	5.053752	-0.896349
F	-2.108042	4.174129	0.633960
F	-2.368421	3.615155	-1.446276
F	1.690149	4.742958	0.555983
F	2.943135	2.999940	0.807487
F	2.599543	3.808984	-1.174541

Complex 26 - $[Pt(F_2C{=}CF_2)(PPh_3)_2]$

Pt	-0.009753	0.903577	-0.085034
P	1.926780	-0.507568	0.003206
C	0.721381	2.814926	0.010959
C	-0.640859	2.846276	-0.307973
P	-1.961984	-0.484060	0.008455
C	-2.098102	-1.633880	1.454952
C	-3.226481	-2.456636	1.638782
C	-1.121496	-1.588781	2.460996
C	-3.353011	-3.236649	2.789887
H	-4.020413	-2.479980	0.887953
C	-1.256594	-2.360747	3.622005
H	-0.257489	-0.933910	2.342515
C	-2.366977	-3.190468	3.785683
H	-4.229369	-3.876714	2.916731
H	-0.487198	-2.307938	4.396883
H	-2.471951	-3.793981	4.691151
C	-2.336291	-1.483213	-1.497284
C	-2.520740	-0.786194	-2.706997
C	-2.369595	-2.886150	-1.513242
C	-2.766076	-1.478257	-3.895356
H	-2.474642	0.306221	-2.718389
C	-2.612059	-3.577309	-2.706642
H	-2.200411	-3.451007	-0.596122
C	-2.816930	-2.877714	-3.897679
H	-2.916699	-0.922075	-4.823353
H	-2.637884	-4.670005	-2.701233
H	-3.010764	-3.420281	-4.826927
C	-3.522583	0.487590	0.282200
C	-3.507311	1.459880	1.297749
C	-4.718984	0.244828	-0.409346
C	-4.663828	2.172477	1.616546
H	-2.578898	1.671549	1.833781
C	-5.875817	0.968801	-0.095943
H	-4.759921	-0.508156	-1.199427
C	-5.852913	1.932368	0.917611
H	-4.634277	2.926604	2.408376
H	-6.798207	0.773731	-0.649120
H	-6.754833	2.501133	1.160496
C	3.430317	0.363141	-0.657533
C	3.282979	1.198575	-1.776072
C	4.714267	0.147125	-0.135196
C	4.397565	1.804341	-2.362492
H	2.285246	1.389628	-2.180134
C	5.827362	0.762456	-0.716439
H	4.857385	-0.496491	0.734703
C	5.673197	1.590834	-1.830881
H	4.265124	2.455305	-3.230234
H	6.821151	0.590563	-0.292967
H	6.545179	2.069649	-2.283831
C	2.419139	-1.004004	1.711734
C	2.823398	0.010039	2.602750
C	2.305245	-2.320270	2.188395
C	3.133948	-0.296368	3.929565
H	2.901217	1.043361	2.254610
C	2.616800	-2.622921	3.519372
H	1.967238	-3.119479	1.526654
C	3.035841	-1.614774	4.391474
H	3.453654	0.500181	4.606699
H	2.528060	-3.654074	3.872286
H	3.281925	-1.853248	5.429643
C	2.019873	-2.035249	-1.039062
C	3.071988	-2.964158	-0.919117
C	1.098386	-2.186101	-2.085849
C	3.183383	-4.026979	-1.816359
H	3.818786	-2.858724	-0.129931
C	1.218062	-3.245520	-2.992304
H	0.287935	-1.464861	-2.201143
C	2.257712	-4.168691	-2.857409
H	4.003551	-4.742241	-1.707714
H	0.492178	-3.343736	-3.803287
H	2.353354	-4.995868	-3.563895
C	-1.587182	3.694619	-0.673553
C	1.724839	3.601176	0.359020
F	-1.439093	5.019020	-0.768406
F	-2.833609	3.378010	-1.018165
F	1.691695	4.935246	0.402591
F	2.937522	3.191023	0.737452

Complex 27 - $[Pt(H_2C{=}CH_2)(PPh_3)_2]$

Pt	0.028533	-1.353261	-0.188424
P	-1.944870	-0.042259	0.001920
P	1.968648	-0.018187	0.019655
C	-2.732510	0.361571	-1.628773
C	-2.457372	-0.470983	-2.728047
C	-3.043078	-0.225166	-3.973850
C	-3.905423	0.862900	-4.142443
C	-4.179277	1.703123	-3.058213
C	-3.597505	1.455637	-1.810519
C	-1.956454	1.608967	0.854324
C	-2.668532	1.857965	2.039137
C	-2.591938	3.107408	2.667753
C	-1.811243	4.126884	2.118184
C	-1.100344	3.889598	0.935511
C	-1.165966	2.641148	0.314430
C	-3.274135	-0.958638	0.919304
C	-4.634349	-0.904621	0.573575
C	-5.584857	-1.617937	1.312815
C	-5.191065	-2.386645	2.412332
C	-3.838417	-2.446386	2.766142
C	-2.887232	-1.745478	2.019574
C	2.033841	1.458903	-1.098793
C	1.437429	1.334891	-2.366928
C	1.448213	2.402897	-3.268212
C	2.042022	3.617890	-2.908269
C	2.628572	3.754616	-1.646337
C	2.628935	2.681510	-0.747830
C	2.373080	0.654703	1.699671
C	1.323066	0.874477	2.607241
C	1.579066	1.383566	3.884738
C	2.889814	1.671728	4.275906
C	3.944330	1.450028	3.383141
C	3.688990	0.945074	2.104466
C	3.543175	-0.909645	-0.406350
C	3.868186	-2.059445	0.338070
C	5.024260	-2.789449	0.057029
C	5.870462	-2.393212	-0.986658
C	5.552267	-1.259795	-1.738265
C	4.398747	-0.518873	-1.447932
C	0.706769	-3.368082	-0.523562
C	-0.723619	-3.345777	-0.547551
H	-1.772795	-1.313070	-2.602238
H	-2.818409	-0.883569	-4.817094
H	-4.359402	1.059020	-5.117456
H	-4.848712	2.558470	-3.182556
H	-3.818643	2.124135	-0.975769
H	-3.291278	1.077552	2.479440
H	-3.152976	3.281754	3.589746
H	-1.754725	5.102425	2.607913
H	-0.484411	4.678631	0.496591
H	-0.594861	2.468461	-0.600153
H	-4.961149	-0.306830	-0.279503
H	-6.638659	-1.570567	1.025333
H	-5.934939	-2.942595	2.988889
H	-3.520093	-3.049815	3.620505
H	-1.828214	-1.816068	2.282852
H	0.950415	0.394570	-2.639479
H	0.982254	2.288400	-4.250239
H	2.043198	4.457330	-3.608269
H	3.090293	4.702088	-1.356204
H	3.090997	2.806290	0.233232
H	0.299371	0.641946	2.308979
H	0.749966	1.550173	4.576495
H	3.091341	2.063462	5.276486
H	4.972935	1.668279	3.683134
H	4.523978	0.770766	1.421370
H	3.207678	-2.385048	1.145673
H	5.263104	-3.675970	0.650767
H	6.772338	-2.968655	-1.211809
H	6.205833	-0.941468	-2.555011
H	4.171598	0.369046	-2.040681
H	1.268979	-3.469703	-1.459798
H	-1.289456	-3.732233	0.307789
H	-1.252017	-3.439062	-1.503561
H	1.226780	-3.779204	0.349186

Complex 28 - [Pt(P(O-o-tolyl)$_3$)]

Pt	0.052448000	0.441580000	-0.141424000
P	-1.557842000	-1.114550000	0.420023000
P	1.995868000	-0.583333000	-0.860108000
P	-0.229701000	2.684498000	0.228462000
O	-2.312083000	-1.732965000	-0.890891000
O	-2.766775000	-0.710133000	1.485371000
O	-1.009265000	-2.528387000	1.130242000
O	2.693690000	-1.499030000	0.300460000
O	1.889917000	-1.707890000	-2.100947000
O	3.240536000	0.372549000	-1.415320000
O	0.825639000	3.767901000	-0.479241000
O	-1.674591000	3.462486000	-0.052287000
O	-0.204359000	3.157326000	1.819065000
C	0.910251000	5.145637000	-0.275242000
C	1.435131000	5.637378000	0.925628000
C	0.561187000	6.014276000	-1.328688000
C	1.581353000	7.013671000	1.114241000
H	1.749970000	4.940161000	1.702819000
C	0.716675000	7.392591000	-1.108802000
C	1.211250000	7.897371000	0.096768000
H	1.994534000	7.387876000	2.055094000
H	0.446312000	8.083291000	-1.914056000
H	1.319044000	8.975796000	0.234155000
C	-4.124820000	-0.959458000	1.636711000
C	-4.605143000	-2.146414000	2.229943000
C	-4.997641000	0.078921000	1.283866000
C	-5.995802000	-2.252271000	2.410988000
C	-6.374324000	-0.054127000	1.485576000
H	-4.574340000	0.992699000	0.862883000
C	-6.878115000	-1.231324000	2.045841000
H	-6.388515000	-3.165659000	2.867505000
H	-7.048188000	0.762216000	1.210183000
H	-7.952406000	-1.352344000	2.211554000
C	3.689634000	-2.458760000	0.427538000
C	4.309566000	-2.534391000	1.689534000
C	4.027065000	-3.336973000	-0.607051000
C	5.281817000	-3.529226000	1.873029000
C	5.000939000	-4.317024000	-0.392505000
H	3.531489000	-3.247008000	-1.569808000
C	5.628486000	-4.419001000	0.853717000
H	5.774983000	-3.602131000	2.845589000
H	5.265068000	-5.002292000	-1.208320000
H	6.389157000	-5.183777000	1.028173000
C	0.949888000	-1.641815000	-3.115841000
C	0.616500000	-0.425950000	-3.722423000
C	0.377722000	-2.856418000	-3.543562000
C	-0.315019000	-0.401131000	-4.764975000
H	1.094097000	0.496057000	-3.388289000
C	-0.549135000	-2.798886000	-4.594419000
C	-0.900769000	-1.589693000	-5.203425000
H	-0.569434000	0.550828000	-5.236890000
H	-1.005568000	-3.730213000	-4.940180000
H	-1.625989000	-1.579808000	-6.020417000
C	4.608502000	0.128860000	-1.499640000
C	5.386705000	0.282974000	-0.348287000
C	5.192807000	-0.165365000	-2.746915000
C	6.769634000	0.100477000	-0.408062000
H	4.896691000	0.547133000	0.589989000
C	6.586193000	-0.340284000	-2.776837000
C	7.371926000	-0.220662000	-1.627265000
H	7.371406000	0.213055000	0.496941000
H	7.062101000	-0.570771000	-3.734234000
H	8.453112000	-0.366179000	-1.687641000
C	-3.191668000	-2.778601000	-1.155360000
C	-4.391528000	-2.457908000	-1.823139000
C	-2.836653000	-4.102013000	-0.876005000
C	-5.245224000	-3.520958000	-2.155253000
C	-3.708661000	-5.138571000	-1.223908000
H	-1.879593000	-4.308401000	-0.399181000
C	-4.920479000	-4.848462000	-1.856701000
H	-6.185160000	-3.294736000	-2.667987000
H	-3.431345000	-6.172938000	-1.004148000
H	-5.607675000	-5.652615000	-2.131152000
C	-0.329406000	-2.625180000	2.328808000
C	0.306462000	-3.857681000	2.591139000
C	-0.301570000	-1.585297000	3.267304000
C	0.946915000	-4.009537000	3.828753000
C	0.347491000	-1.768564000	4.491948000
H	-0.800704000	-0.639647000	3.056176000
C	0.968944000	-2.984352000	4.780638000
H	1.442615000	-4.960100000	4.045951000
H	0.360569000	-0.950177000	5.215276000
H	1.474722000	-3.135508000	5.737024000
C	0.701966000	2.704351000	2.759201000
C	0.222822000	2.546198000	4.074187000
C	2.045230000	2.475355000	2.438657000
C	1.148301000	2.163568000	5.057555000
C	2.942943000	2.097940000	3.442502000
H	2.388685000	2.592785000	1.409605000
C	2.496851000	1.945047000	4.756290000
H	0.795476000	2.037786000	6.087142000
H	3.992549000	1.933092000	3.190324000
H	3.193620000	1.653904000	5.546515000
C	-2.542566000	3.171875000	-1.086030000
C	-3.910960000	3.429120000	-0.861582000
C	-2.089231000	2.683315000	-2.319370000
C	-4.798316000	3.187612000	-1.923883000
C	-2.997532000	2.455469000	-3.357380000
H	-1.024889000	2.488788000	-2.471939000
C	-4.357441000	2.711755000	-3.163264000
H	-5.864699000	3.380430000	-1.767686000
H	-2.633264000	2.080142000	-4.318008000
H	-5.073741000	2.536580000	-3.971205000
C	3.931668000	-1.600282000	2.809239000
H	3.650797000	-0.604843000	2.436920000
H	3.058086000	-1.982772000	3.365252000
H	4.763033000	-1.491234000	3.523583000
C	4.369353000	-0.260176000	-4.004109000
H	3.648985000	-1.091328000	-3.954828000
H	3.783314000	0.660006000	-4.168327000
H	5.015685000	-0.416466000	-4.881002000
C	0.766139000	-4.163440000	-2.904496000
H	0.119044000	-4.979111000	-3.256733000
H	1.809627000	-4.432189000	-3.141909000
H	0.696066000	-4.110691000	-1.807534000
C	0.064565000	5.496961000	-2.654198000
H	0.697224000	4.674780000	-3.028536000
H	-0.960926000	5.101545000	-2.579907000
H	0.058109000	6.299779000	-3.405172000
C	-1.227355000	2.794609000	4.405368000
H	-1.476391000	2.379906000	5.395645000
H	-1.458914000	3.875130000	4.423087000
H	-1.893231000	2.339397000	3.657174000
C	-4.401073000	3.962941000	0.461280000
H	-4.357029000	5.062457000	0.493791000
H	-5.445880000	3.671901000	0.627914000
H	-3.792893000	3.594747000	1.298759000
C	-4.725050000	-1.036752000	-2.188616000
H	-4.853272000	-0.412572000	-1.291375000
H	-3.918566000	-0.576436000	-2.779789000
H	-5.657480000	-0.988464000	-2.768953000
C	0.281516000	-4.974698000	1.580375000
H	0.890400000	-5.824287000	1.920822000
H	-0.744779000	-5.340785000	1.408009000
H	0.671546000	-4.642112000	0.605221000
C	-3.696071000	-3.254060000	2.692960000
H	-3.164780000	-3.722007000	1.850723000
H	-2.929004000	-2.880323000	3.388486000
H	-4.274028000	-4.035061000	3.206652000

Complex 29 - $[Pt(PPh_3)_3]$

P	-2.248093000	0.787555000	0.011033000
P	1.793539000	1.543923000	-0.016589000
C	2.321599000	2.060156000	1.688659000
C	3.627743000	2.485054000	1.991354000
C	1.370990000	2.021167000	2.724552000
C	3.969122000	2.870232000	3.291907000
H	4.388849000	2.514335000	1.208937000
C	1.710638000	2.411788000	4.023779000
H	0.360105000	1.666741000	2.507279000
C	3.011464000	2.837569000	4.311127000
H	4.989534000	3.197183000	3.508659000
H	0.957369000	2.374116000	4.815034000
H	3.280476000	3.136929000	5.327425000
C	1.516839000	3.160400000	-0.893731000
C	0.764132000	3.131895000	-2.080869000
C	2.010980000	4.394598000	-0.440725000
C	0.528948000	4.301035000	-2.809270000
H	0.346986000	2.181850000	-2.426627000
C	1.760512000	5.568987000	-1.160173000
H	2.594443000	4.448994000	0.480218000
C	1.024362000	5.525728000	-2.348006000
H	-0.055751000	4.257552000	-3.731838000
H	2.146767000	6.522108000	-0.788969000
H	0.831416000	6.443538000	-2.909427000
C	3.415238000	1.006875000	-0.764934000
C	4.067788000	-0.108054000	-0.204293000
C	3.990516000	1.621970000	-1.888931000
C	5.266113000	-0.581610000	-0.740926000
H	3.632906000	-0.613112000	0.660747000
C	5.183795000	1.134569000	-2.438625000
H	3.511035000	2.489775000	-2.344880000
C	5.827912000	0.035642000	-1.865764000
H	5.758434000	-1.443866000	-0.283737000
H	5.611987000	1.625699000	-3.316629000
H	6.761209000	-0.340811000	-2.292377000
C	-3.326338000	0.005413000	-1.283179000
C	-2.769482000	-0.192012000	-2.560303000
C	-4.647902000	-0.409799000	-1.053107000
C	-3.518987000	-0.774436000	-3.585543000
H	-1.731866000	0.100295000	-2.742887000
C	-5.394910000	-1.005599000	-2.076877000
H	-5.102313000	-0.271397000	-0.070053000
C	-4.835492000	-1.185989000	-3.345344000
H	-3.070623000	-0.917078000	-4.572257000
H	-6.420866000	-1.327803000	-1.879674000
H	-5.420675000	-1.650093000	-4.143451000
C	-3.155786000	0.442617000	1.597674000
C	-2.808153000	-0.710357000	2.323386000
C	-4.166286000	1.278314000	2.105686000
C	-3.459648000	-1.025860000	3.519387000
H	-2.018020000	-1.360898000	1.942818000
C	-4.812721000	0.966318000	3.306707000
H	-4.452559000	2.182278000	1.564758000
C	-4.462560000	-0.186700000	4.016498000
H	-3.177299000	-1.928980000	4.066652000
H	-5.594023000	1.629244000	3.687966000
H	-4.967757000	-0.428895000	4.955164000
C	-2.628979000	2.596657000	-0.230423000
C	-3.605132000	3.078428000	-1.118156000
C	-1.885525000	3.527415000	0.517206000
C	-3.835106000	4.453979000	-1.248034000
H	-4.195880000	2.381704000	-1.715518000
C	-2.125842000	4.897500000	0.401565000
H	-1.100502000	3.173309000	1.189654000
C	-3.101872000	5.366900000	-0.485619000
H	-4.596130000	4.809680000	-1.947880000
H	-1.539583000	5.602741000	0.996277000
H	-3.284136000	6.440034000	-0.585541000
Pt	-0.015937000	0.030473000	-0.021015000
P	0.434297000	-2.286961000	-0.037348000
C	1.007602000	-2.955153000	-1.673480000
C	0.786054000	-4.282324000	-2.082920000
C	1.696840000	-2.088914000	-2.540229000
C	1.247432000	-4.731154000	-3.324904000
H	0.247571000	-4.973875000	-1.431908000
C	2.162665000	-2.539737000	-3.779101000
H	1.863768000	-1.052956000	-2.237285000
C	1.937856000	-3.862003000	-4.175928000
H	1.064902000	-5.765606000	-3.627892000
H	2.698692000	-1.851707000	-4.437970000
H	2.295817000	-4.213445000	-5.147168000
C	-0.924079000	-3.487210000	0.395727000
C	-2.100185000	-3.460586000	-0.377913000
C	-0.857888000	-4.376459000	1.481091000
C	-3.168946000	-4.309719000	-0.086243000
H	-2.183485000	-2.763849000	-1.215426000
C	-1.937543000	-5.217055000	1.783539000
H	0.040199000	-4.422307000	2.099308000
C	-3.093504000	-5.190671000	1.000229000
H	-4.069388000	-4.276031000	-0.704942000
H	-1.866633000	-5.899668000	2.634699000
H	-3.933523000	-5.849668000	1.234455000
C	1.774715000	-2.811681000	1.140029000
C	2.700477000	-3.831199000	0.863671000
C	1.863058000	-2.136020000	2.370495000
C	3.690172000	-4.165503000	1.795612000
H	2.656895000	-4.369477000	-0.085074000
C	2.840986000	-2.480288000	3.307827000
H	1.164975000	-1.322125000	2.585533000
C	3.761371000	-3.494870000	3.020496000
H	4.407645000	-4.956446000	1.561277000
H	2.891599000	-1.945826000	4.259972000
H	4.534027000	-3.758315000	3.747415000

Complex 30 - [Pt(dvtms)(PPh_3)], dvtms = divinyltetramethyldisiloxane

Pt	-0.693555	0.011700	-0.536172
Si	-3.661238	1.551161	0.172107
Si	-3.657747	-1.624072	-0.033735
P	1.606345	0.017665	0.049072
N	-4.398324	-0.031076	-0.017362
H	-5.409303	-0.041239	0.113233
C	-2.129846	1.640135	-0.912984
H	-2.332422	1.609089	-1.993937
C	-0.882584	2.197966	-0.525611
H	-0.754184	2.615332	0.478925
H	-0.218636	2.640113	-1.276554
C	-2.117397	-1.573985	-1.107760
H	-2.308730	-1.430732	-2.181559
C	-0.866298	-2.151496	-0.765078
H	-0.185893	-2.508790	-1.546512
H	-0.738257	-2.656445	0.198489
C	-4.941776	2.827151	-0.391336
H	-5.212448	2.678239	-1.449756
H	-4.552538	3.853055	-0.281362
H	-5.866920	2.756379	0.206608
C	-3.207263	1.917410	1.974894
H	-2.467531	1.193659	2.354212
H	-4.103751	1.843038	2.613423
H	-2.791150	2.931180	2.100203
C	-4.930367	-2.812225	-0.778955
H	-5.193560	-2.516764	-1.807978
H	-5.860419	-2.829833	-0.185017
H	-4.536976	-3.842031	-0.811201
C	-3.217694	-2.236707	1.704324
H	-2.451409	-1.600335	2.175700
H	-2.835727	-3.271579	1.686980
H	-4.111115	-2.221143	2.351493
C	1.993008	0.394917	1.817835
C	1.018511	1.031189	2.604330
H	0.047819	1.266784	2.164881
C	1.277673	1.346480	3.942300
H	0.507836	1.839697	4.541045
C	2.511877	1.022892	4.512820
H	2.713225	1.265011	5.559477
C	3.486078	0.379203	3.741525
H	4.450630	0.117089	4.183321
C	3.229218	0.065345	2.404076
H	3.995325	-0.447117	1.818023
C	2.582256	1.246837	-0.932753
C	3.639203	2.005050	-0.403824
H	3.924589	1.898397	0.643928
C	4.334441	2.912640	-1.210823
H	5.150145	3.500327	-0.781255
C	3.988877	3.069727	-2.556045
H	4.534350	3.778322	-3.184376
C	2.934716	2.321674	-3.091757
H	2.651295	2.443770	-4.140368
C	2.230919	1.424754	-2.283809
H	1.391342	0.860171	-2.699374
C	2.524785	-1.567859	-0.224818
C	2.244778	-2.659313	0.619092
H	1.541099	-2.542577	1.447129
C	2.865697	-3.893405	0.418029
H	2.640054	-4.727813	1.087226
C	3.770466	-4.063168	-0.636787
H	4.253951	-5.030268	-0.796332
C	4.051135	-2.987781	-1.482767
H	4.758083	-3.107935	-2.307825
C	3.435142	-1.746949	-1.278336
H	3.674122	-0.917192	-1.945919

Complex 31 - [Pt(ICy)(dvtms)], dvtms = divinyltetramethyldisiloxane

Pt	0.465523	0.006023	-0.410318
N	2.948795	0.160118	1.441310
C	2.449036	0.041206	0.180128
N	3.550031	-0.079360	-0.612564
C	4.715421	-0.045234	0.140495
H	5.703105	-0.123362	-0.305638
C	4.335874	0.106393	1.437782
H	4.926815	0.186976	2.346074
C	2.127724	0.298406	2.635558
H	2.777660	0.505669	3.495927
H	1.560742	-0.625117	2.824060
C	3.503164	-0.266258	-2.055740
H	4.504328	-0.090735	-2.474553
H	2.791933	0.444423	-2.499560
C	0.266293	2.156921	-0.594021
H	0.358764	2.653098	0.379206
H	0.933300	2.571069	-1.359718
C	-0.973888	1.557381	-0.980012
H	-1.147189	1.469465	-2.063203
Si	-2.527136	1.531459	0.066682
O	-3.132142	-0.034755	0.174123
C	-3.896648	2.549868	-0.738534
H	-4.829190	2.492872	-0.152222
H	-4.115331	2.180052	-1.754308
H	-3.609086	3.611516	-0.819704
C	-2.195239	2.179992	1.808248
H	-3.099645	2.081792	2.431725
H	-1.912073	3.245907	1.792352
H	-1.383375	1.620033	2.299097
H	1.415936	1.125558	2.510639
H	3.180596	-1.289093	-2.306124
C	0.345984	-2.162314	-0.354984
H	0.450710	-2.542743	0.668142
H	1.036774	-2.628167	-1.067969
C	-0.910758	-1.655881	-0.808890
H	-1.078336	-1.692053	-1.895673
Si	-2.469937	-1.579476	0.227005
C	-3.797736	-2.722553	-0.474039
H	-4.736018	-2.637382	0.099507
H	-4.021202	-2.466323	-1.523177
H	-3.474528	-3.776559	-0.444738
C	-2.116146	-2.037799	2.023550
H	-3.019901	-1.901995	2.641024
H	-1.802605	-3.091518	2.112155
H	-1.317056	-1.408983	2.448426

Complex 32 - [Pt(Mes-NHC-Pr^n-SO_3Na)(dvtms)],
dvtms = divinyltetramethyldisiloxane

Pt	-0.842545	0.917069	0.186008
N	-0.098665	-1.772256	1.441727
C	-1.083013	-1.076372	0.799789
N	-2.194462	-1.879878	0.919834
C	-1.895022	-3.016814	1.675766
H	-2.645184	-3.763144	1.922853
C	-0.577992	-2.951813	1.991583
H	0.050323	-3.634490	2.559565
C	1.301091	-1.356117	1.490120
H	1.628794	-1.316504	2.541344
C	-1.084063	0.760770	-1.959730
H	-0.314978	0.134806	-2.427877
H	-2.106409	0.467723	-2.228851
C	-0.806517	2.128322	-1.633514
H	-1.675373	2.801735	-1.597631
Si	0.842909	2.979682	-1.906449
O	1.318545	3.792886	-0.508178
C	0.725561	4.325349	-3.227073
H	1.695347	4.840535	-3.342674
H	-0.022560	5.086558	-2.947735
H	0.439024	3.911535	-4.207943
C	2.186458	1.742628	-2.376314
H	3.169459	2.240569	-2.426892
H	1.990102	1.295593	-3.364769
H	2.252728	0.921395	-1.645319
H	1.313490	-0.331592	1.094214
C	-0.658839	1.521620	2.295278
H	0.208062	1.054259	2.774558
H	-1.598428	1.368467	2.836686
C	-0.494304	2.670920	1.476248
H	-1.375106	3.323123	1.370457
Si	1.146552	3.512270	1.140247
C	1.206701	5.201260	1.972018
H	2.159033	5.705037	1.737527
H	0.385118	5.860337	1.645826
H	1.139853	5.089809	3.068443
C	2.606978	2.492630	1.761461
H	3.548154	3.040285	1.591366
H	2.527234	2.293810	2.842207
H	2.689058	1.522859	1.244137
C	2.226937	-2.258724	0.662342
H	2.428092	-3.201689	1.196869
H	1.734612	-2.525228	-0.285169
C	3.545371	-1.554247	0.355535
H	3.397641	-0.706932	-0.332658
H	4.042347	-1.176708	1.262723
S	4.758418	-2.632749	-0.460869
O	4.055079	-3.282060	-1.595685
O	5.253652	-3.578767	0.583420
O	5.846344	-1.687589	-0.912491
Na	7.892997	-2.314901	-0.344135
C	-3.464638	-1.775895	0.233796
C	-3.786192	-2.811238	-0.684010
C	-4.392471	-0.753376	0.517410
C	-5.068825	-2.834175	-1.242287
C	-5.658407	-0.819357	-0.091463
C	-6.030391	-1.856957	-0.949884
H	-5.326137	-3.648934	-1.925870
H	-6.383512	-0.033930	0.139601
C	-4.107715	0.415068	1.426035
H	-3.274115	0.229967	2.110816
H	-3.833715	1.302214	0.829647
H	-5.002936	0.679872	2.010085
C	-2.801752	-3.886683	-1.088942
H	-1.802582	-3.471107	-1.302358
H	-2.670514	-4.652333	-0.309867
H	-3.157648	-4.400385	-1.993174
C	-7.409023	-1.923754	-1.560761
H	-8.135003	-1.327560	-0.988221
H	-7.406927	-1.538742	-2.595410
H	-7.775608	-2.961112	-1.606764

Complex 33 - [Pt(IPr-4-SO_3Na)(dvtms)], dvtms = divinyltetramethyldisiloxane

Pt	0.111043	0.896877	-0.075593
N	-0.712999	-2.134943	-0.224069
C	0.272662	-1.182437	-0.150925
N	1.432702	-1.908004	-0.260532
C	1.169985	-3.267094	-0.417852
H	1.960702	-4.000884	-0.537382
C	-0.176267	-3.410718	-0.385652
H	-0.795752	-4.298584	-0.455594
C	0.878514	1.177095	1.943271
H	0.184636	0.794412	2.699908
H	1.895342	0.783654	2.032842
C	0.673156	2.463151	1.360880
H	1.573838	2.948859	0.954069
Si	-0.690882	3.669573	1.802656
O	-1.404981	4.260488	0.396583
C	0.026452	5.177708	2.679737
H	-0.755880	5.929297	2.879307
H	0.807827	5.656994	2.066459
H	0.479971	4.895149	3.644538
C	-2.023942	2.881969	2.877740
H	-2.822395	3.612265	3.091832
H	-1.613241	2.540312	3.842455
H	-2.483301	2.015878	2.376099
C	-0.660306	1.068046	-2.105384
H	-1.683449	0.686550	-2.161517
H	0.018967	0.627917	-2.843153
C	-0.428789	2.383194	-1.607626
H	0.508096	2.864162	-1.928637
Si	-1.780317	3.575945	-1.094946
C	-1.878921	5.016867	-2.308728
H	-2.623706	5.762260	-1.982932
H	-0.905616	5.527496	-2.397061
H	-2.167574	4.665440	-3.313395
C	-3.461080	2.724966	-0.987456
H	-4.217092	3.429760	-0.602242
H	-3.798050	2.383097	-1.980605
H	-3.441528	1.850610	-0.317477
C	-2.126537	-1.893215	-0.064540
C	-2.638620	-1.755598	1.247751
C	-2.961250	-1.865802	-1.207606
C	-4.008427	-1.494794	1.389558
C	-4.325924	-1.613180	-1.010184
C	-4.833017	-1.407068	0.271192
H	-4.452502	-1.374398	2.377607
H	-5.006670	-1.588379	-1.861387
C	2.776046	-1.396139	-0.126848
C	3.414213	-0.819634	-1.250222
C	3.431608	-1.546763	1.117960
C	4.724934	-0.350356	-1.089035
C	4.746164	-1.069699	1.223905
C	5.378778	-0.476194	0.136001
H	5.242425	0.114647	-1.928995
H	5.292846	-1.153884	2.162974
C	-2.446109	-2.173662	-2.613181
H	-1.364052	-1.971651	-2.620549
C	-2.651554	-3.664968	-2.953495
H	-3.725188	-3.914040	-2.970852
H	-2.235377	-3.890914	-3.948407
H	-2.166740	-4.332517	-2.227265
C	-3.088312	-1.308133	-3.710289
H	-3.030935	-0.234952	-3.480142
H	-2.572763	-1.478802	-4.667991
H	-4.148948	-1.564550	-3.864786
C	2.756833	-0.771811	-2.624954
H	1.675457	-0.895817	-2.477850
C	2.966321	0.566467	-3.352118
H	2.374901	0.585623	-4.280655
H	2.650275	1.417845	-2.729605
H	4.019119	0.723053	-3.637739
C	3.243162	-1.951189	-3.492119
H	2.732288	-1.948328	-4.468708
H	4.328277	-1.884533	-3.677687
H	3.043957	-2.920177	-3.008203
C	-1.773440	-1.980345	2.486290
H	-0.737252	-1.730634	2.218059
C	-1.805119	-3.467733	2.894718
H	-1.142071	-3.641322	3.757587
H	-2.824581	-3.771910	3.183584
H	-1.475389	-4.126995	2.078321
C	-2.157713	-1.094582	3.678989
H	-1.415222	-1.212130	4.484076
H	-2.193938	-0.031233	3.403368
H	-3.137553	-1.370575	4.099983
C	2.796382	-2.253285	2.315186
H	1.710899	-2.291880	2.144252
C	3.306377	-3.704883	2.423391
H	4.393566	-3.724172	2.604336
H	2.814871	-4.221948	3.263113
H	3.110068	-4.284176	1.509429
C	3.020606	-1.519105	3.647778
H	2.684186	-0.473235	3.602077
H	2.456050	-2.022139	4.448736
H	4.080716	-1.523779	3.946929
S	-6.569530	-0.965139	0.490552
S	7.094222	0.062879	0.305333
O	-7.329981	-1.735385	-0.551758
O	-6.917297	-1.306710	1.887156
O	7.376057	0.114019	1.755987
O	7.912370	-0.954456	-0.443493
O	7.189374	1.387417	-0.397790
O	-6.655071	0.506044	0.181396
Na	-8.107441	0.237480	-1.641853
Na	8.763345	0.590572	-1.985073

Complex 34 - [Pt(IXy-4-SO_3Na)(dvtms)], dvtms = divinyltetramethyldisiloxane

Pt	0.190075	0.599371	-0.114847
N	-0.679486	-2.384824	0.288447
C	0.326484	-1.462995	0.169012
N	1.466712	-2.222711	0.222417
C	1.172456	-3.578195	0.365002
H	1.948138	-4.336832	0.415057
C	-0.177384	-3.679984	0.410748
H	-0.826548	-4.544383	0.515966
C	1.199322	1.182073	1.723253
H	0.604336	0.931589	2.609522
H	2.225470	0.802540	1.757443
C	0.909771	2.363606	0.975981
H	1.747501	2.780244	0.395727
Si	-0.427445	3.604823	1.396692
O	-1.312534	3.981791	0.013533
C	0.335683	5.232503	1.969781
H	-0.441806	5.992655	2.155134
H	1.026998	5.633515	1.209488
H	0.905089	5.094537	2.904462
C	-1.604377	2.947895	2.716699
H	-2.392316	3.690093	2.929077
H	-1.076397	2.739365	3.662310
H	-2.096441	2.017865	2.388859
C	-0.831038	0.434267	-2.032599
H	-1.850090	0.058397	-1.895768
H	-0.244907	-0.133366	-2.763862
C	-0.550254	1.812226	-1.796293
H	0.332626	2.221046	-2.311324
Si	-1.839659	3.083028	-1.310811
C	-2.089165	4.328686	-2.705877
H	-2.807997	5.113654	-2.416364
H	-1.137956	4.821102	-2.969751
H	-2.475507	3.832366	-3.612179
C	-3.483390	2.263314	-0.881222
H	-4.199108	3.013690	-0.505729
H	-3.934161	1.783827	-1.766416
H	-3.362998	1.491588	-0.104110
C	-2.091310	-2.108875	0.288782
C	-2.695674	-1.658889	1.483989
C	-2.838715	-2.370901	-0.876696
C	-4.077674	-1.436058	1.479414
C	-4.222160	-2.136298	-0.837844
C	-4.827910	-1.666158	0.324022
H	-4.579273	-1.106367	2.391143
H	-4.830781	-2.340408	-1.721007
C	2.818749	-1.730398	0.182426
C	3.395788	-1.396110	-1.059897
C	3.537136	-1.648346	1.393306
C	4.716809	-0.927575	-1.065826
C	4.857793	-1.180982	1.343195
C	5.434271	-0.819399	0.126095
H	5.181431	-0.642252	-2.011957
H	5.441447	-1.085136	2.260046
S	-6.598252	-1.311195	0.346173
S	7.148141	-0.251490	0.099634
O	-7.210434	-2.152035	-0.739467
O	-7.066223	-1.631630	1.713284
O	7.467643	0.168932	1.482328
O	7.964214	-1.417402	-0.390227
O	7.201380	0.854186	-0.917812
O	-6.728731	0.144390	-0.016194
Na	-8.002263	-0.256221	-1.947395
Na	8.812909	-0.266657	-2.266574
C	2.630172	-1.518554	-2.352478
H	2.039437	-2.446461	-2.391468
H	1.920990	-0.681848	-2.464600
H	3.314831	-1.504582	-3.212246
C	2.914507	-2.024965	2.715146
H	2.084972	-1.343099	2.970634
H	2.496473	-3.045459	2.697761
H	3.660599	-1.977224	3.522855
C	-1.899695	-1.428386	2.742829
H	-1.448916	-0.422004	2.742346
H	-2.546139	-1.510397	3.628726
H	-1.075147	-2.148889	2.844271
C	-2.226105	-2.894117	-2.154076
H	-2.699643	-3.844175	-2.444681
H	-2.396559	-2.186287	-2.980046
H	-1.147019	-3.062514	-2.073672

Complex 35 - *anti*-[Pt(IMes-4-SO_3Na)(dvtms)], dvtms = divinyltetramethyldisiloxane

Pt	0.176721	0.665245	-0.410596
N	-0.758470	-2.083533	0.763526
C	0.233098	-1.335668	0.184562
N	1.271292	-2.221479	0.058546
C	0.931452	-3.483024	0.542502
H	1.629253	-4.314720	0.527534
C	-0.345571	-3.395032	0.990956
H	-0.997549	-4.135539	1.443882
C	1.749129	1.359593	0.929396
H	1.445057	1.290939	1.980316
H	2.705440	0.874378	0.714121
C	1.322176	2.461529	0.130190
H	1.962718	2.701132	-0.732521
Si	0.294746	3.904518	0.739148
O	-1.001392	4.177735	-0.300991
C	1.314643	5.491182	0.703675
H	0.711399	6.361227	1.013988
H	1.695694	5.689682	-0.312183
H	2.181249	5.419257	1.381795
C	-0.365304	3.608263	2.480941
H	-1.013247	4.445992	2.790002
H	0.455837	3.531725	3.213130
H	-0.957812	2.680901	2.539089
C	-1.377508	0.396845	-1.918522
H	-2.328168	0.114776	-1.456345
H	-1.062808	-0.277962	-2.723093
C	-0.973269	1.763773	-1.928876
H	-0.273459	2.056683	-2.726663
Si	-1.989553	3.167197	-1.217624
C	-2.689362	4.252717	-2.592349
H	-3.243174	5.110652	-2.174495
H	-1.887591	4.649634	-3.235872
H	-3.382603	3.679518	-3.229687
C	-3.397716	2.531193	-0.138353
H	-3.938314	3.379614	0.314327
H	-4.125846	1.941085	-0.719094
H	-3.028636	1.890044	0.677907
C	-2.078852	-1.624307	1.108602
C	-2.244148	-0.959979	2.334638
C	-3.159445	-1.907009	0.239347
C	-3.532434	-0.532524	2.664008
C	-4.450187	-1.475246	0.635799
C	-4.642468	-0.753992	1.841198
H	-3.682132	-0.000970	3.607014
C	2.563276	-1.932843	-0.508352
C	2.694970	-2.017475	-1.904406
C	3.648370	-1.626413	0.344955
C	3.948036	-1.733492	-2.450558
C	4.900161	-1.349920	-0.262028
C	5.056481	-1.383450	-1.669793
C	1.537326	-2.394832	-2.791993
H	1.027749	-3.302250	-2.432347
H	0.782385	-1.592915	-2.812797
H	1.876657	-2.573673	-3.821793
C	3.422402	-1.614969	1.841588
H	3.703961	-0.649773	2.281155
H	2.374328	-1.818678	2.085453
H	4.055182	-2.364245	2.335512
C	-1.089923	-0.697799	3.265196
H	-0.479887	0.144199	2.899108
H	-1.451681	-0.445499	4.271927
H	-0.417182	-1.566539	3.342231
C	-2.873735	-2.647201	-1.049370
H	-3.243800	-3.681767	-0.998161
H	-3.388063	-2.186594	-1.898283
H	-1.799280	-2.671059	-1.254156
C	6.350095	-1.067373	-2.382470
H	6.696398	-0.054782	-2.127415
H	7.149092	-1.753829	-2.071644
H	6.213836	-1.131737	-3.470682
C	-5.971103	-0.201927	2.302671
H	-6.397786	0.474553	1.548081
H	-6.704144	-1.004859	2.456947
H	-5.845914	0.355395	3.240586
S	-5.919576	-1.744038	-0.423028
O	-5.582709	-2.697014	-1.503752
O	-7.009295	-2.262974	0.473630
O	-6.299293	-0.377465	-0.935885
Na	-8.596347	-0.676929	-0.400802
H	4.069834	-1.783651	-3.536535
S	6.369639	-0.864199	0.720003
O	6.066010	-0.986925	2.166091
O	7.486424	-1.757652	0.288357
O	6.634892	0.568515	0.322384
Na	8.853137	0.840194	0.723627

Complex 36 - *syn*-[Pt(SIMes-4-SO_3Na)(dvtms)], dvtms = divinyltetramethyldisiloxane

Pt	0.362241	0.615073	0.312022
N	-0.932612	-2.000767	1.368203
C	0.199049	-1.315113	1.084622
N	1.243678	-2.142930	1.334580
C	0.829132	-3.512034	1.701797
H	1.059929	-4.208504	0.877542
C	-0.678188	-3.345082	1.926850
H	-0.954882	-3.369498	2.994171
C	1.419891	1.499377	1.997064
H	0.781953	1.578493	2.885251
H	2.372532	0.992607	2.180397
C	1.332164	2.478215	0.960654
H	2.234536	2.591977	0.339878
Si	0.239936	3.999696	0.986179
O	-0.644905	4.105275	-0.444588
C	1.302855	5.558903	1.042937
H	0.681468	6.469066	0.990914
H	2.010592	5.583017	0.196487
H	1.891200	5.602943	1.975208
C	-0.953166	3.988436	2.449746
H	-1.616305	4.869115	2.409598
H	-0.408242	4.023153	3.407553
H	-1.588483	3.087513	2.452896
C	-0.628187	0.131014	-1.577239
H	-1.684170	-0.100566	-1.410318
H	-0.082723	-0.643206	-2.127788
C	-0.202851	1.488702	-1.635367
H	0.729410	1.683807	-2.187625
Si	-1.351690	2.959780	-1.459196
C	-1.591459	3.827878	-3.117779
H	-2.220070	4.728012	-3.008424
H	-0.624650	4.140496	-3.547225
H	-2.083502	3.158566	-3.843780
C	-3.029762	2.457365	-0.761408
H	-3.658206	3.350661	-0.603082
H	-3.572595	1.782021	-1.443490
H	-2.926670	1.937159	0.204375
C	-2.273607	-1.508637	1.255506
C	-2.789162	-0.710448	2.290343
C	-3.058357	-1.879551	0.132519
C	-4.100403	-0.242967	2.161294
C	-4.380847	-1.378303	0.049298
C	-4.909468	-0.535637	1.058547
H	-4.509711	0.388906	2.953680
C	2.624257	-1.811017	1.141179
C	3.181534	-1.799387	-0.160742
C	3.391337	-1.507987	2.281630
C	4.520031	-1.354570	-0.304927
C	4.716165	-1.113803	2.090332
C	5.295707	-0.987236	0.822608
H	5.318263	-0.855498	2.965890
C	2.335030	-2.285207	-1.315865
H	1.356875	-2.630451	-0.966547
H	2.175404	-1.499782	-2.065260
H	2.839630	-3.104879	-1.842982
C	2.807334	-1.557029	3.670723
H	1.948037	-0.874683	3.765109
H	2.443477	-2.564217	3.929580
H	3.557717	-1.273329	4.422496
C	-1.972824	-0.329505	3.497651
H	-1.370673	0.570503	3.289134
H	-2.625113	-0.105846	4.354714
H	-1.269200	-1.120949	3.792345
C	-2.437624	-2.783123	-0.910039
H	-2.940345	-3.760618	-0.931869
H	-2.544682	-2.369543	-1.918502
H	-1.373079	-2.933291	-0.706254
C	6.704251	-0.447960	0.751089
H	7.053323	-0.161659	1.754245
H	7.397391	-1.185485	0.323384
H	6.743799	0.440574	0.103452
C	-6.287347	0.082485	1.019686
H	-6.394436	0.737131	0.142146
H	-7.067899	-0.684303	0.942293
H	-6.460302	0.685084	1.921415
S	5.268567	-1.091809	-1.954404
S	-5.441890	-1.697940	-1.409166
O	-4.807678	-2.720094	-2.270681
O	-6.780095	-2.146285	-0.884300
O	6.644643	-1.695123	-1.919630
O	4.409637	-1.699977	-2.993343
O	5.383701	0.405760	-2.092952
O	-5.595868	-0.361669	-2.089816
Na	-7.968305	-0.557240	-2.227260
Na	7.617046	0.329992	-2.849691
H	1.358013	-3.865020	2.598204
H	-1.276668	-4.106040	1.405646

Complex 37 - [Pt(Mes-NHC-Prn-SO_3Na)(AE)], AE = diallyl ether

Pt	0.838142	1.139372	-0.125140
N	-0.479081	-1.349103	-1.421621
C	0.605063	-0.817434	-0.787471
N	1.498119	-1.854041	-0.731111
C	0.974222	-3.003065	-1.320101
H	1.536797	-3.930335	-1.380691
C	-0.272169	-2.682878	-1.752354
H	-1.020915	-3.279119	-2.266911
C	-1.745024	-0.651410	-1.630410
H	-2.130954	-0.928559	-2.623706
C	0.076919	0.991984	1.924010
H	-0.999038	0.779771	1.926766
H	0.669322	0.339227	2.571915
C	0.534303	2.315731	1.666847
H	1.497615	2.614655	2.101158
O	0.159028	4.481049	0.562900
H	-1.522852	0.424524	-1.637491
C	1.412484	2.078066	-2.020136
H	0.575835	2.062272	-2.728563
H	2.358825	1.711514	-2.428409
C	1.435981	3.040631	-0.971716
H	2.417104	3.341752	-0.580644
C	-2.766099	-0.984114	-0.538364
H	-2.953580	-2.069709	-0.521465
H	-2.347852	-0.711520	0.442456
C	-4.089845	-0.254778	-0.735303
H	-3.968912	0.839283	-0.712215
H	-4.583754	-0.529616	-1.679634
S	-5.273410	-0.635996	0.584842
O	-4.632049	-0.229827	1.857413
O	-5.550404	-2.114694	0.481698
O	-6.523526	0.131652	0.247480
Na	-7.822524	-1.814875	-0.038841
C	2.796139	-1.801723	-0.111578
C	2.911672	-2.139873	1.252062
C	3.918306	-1.465643	-0.889826
C	4.183927	-2.091927	1.834958
C	5.171123	-1.433451	-0.258536
C	5.325583	-1.736856	1.100209
H	4.286131	-2.344935	2.894434
H	6.050421	-1.166144	-0.851434
C	3.789467	-1.168338	-2.362821
H	3.410068	-2.043492	-2.916549
H	3.080529	-0.346430	-2.545906
H	4.761608	-0.891495	-2.794248
C	1.709306	-2.570476	2.054983
H	0.878962	-1.856297	1.954341
H	1.332260	-3.548853	1.712163
H	1.961617	-2.663701	3.120494
C	6.682789	-1.708833	1.760471
H	7.450971	-1.294445	1.091535
H	6.667056	-1.103950	2.681489
H	7.002148	-2.724068	2.051501
C	0.367224	4.094880	-0.788281
C	-0.392877	3.482126	1.409136
H	-0.585054	3.755589	-1.245712
H	0.664463	5.027227	-1.301062
H	-1.357453	3.116669	1.000939
H	-0.612746	4.009605	2.354683

Complex 38 - [Pt(IXy-4,4-SO_3Na)(AE)], AE = diallyl ether

Pt	-0.022270	1.075943	-0.019027
N	0.952716	-1.859623	-0.453117
C	-0.085902	-0.982077	-0.287951
N	-1.197817	-1.779059	-0.379570
C	-0.856319	-3.112050	-0.603374
H	-1.603905	-3.893949	-0.700524
C	0.496875	-3.162814	-0.652382
H	1.176049	-3.996495	-0.806242
C	-0.969608	1.715180	-1.894704
H	-0.333994	1.478604	-2.755790
H	-2.007267	1.382370	-1.989134
C	-0.674953	2.848245	-1.086545
H	-1.511163	3.320073	-0.553433
O	1.000159	4.400994	-0.177446
C	1.158160	1.236151	1.819635
H	2.191185	0.916625	1.640227
H	0.685339	0.779666	2.694679
C	0.735314	2.528477	1.398316
H	-0.092305	2.997672	1.947001
C	2.351547	-1.537343	-0.362900
C	3.019623	-1.044783	-1.501839
C	3.019673	-1.794590	0.852443
C	4.391330	-0.778486	-1.393845
C	4.393075	-1.520283	0.916379
C	5.064492	-1.009800	-0.193645
H	4.944960	-0.409734	-2.260192
H	4.944509	-1.723560	1.836434
C	-2.560694	-1.333754	-0.276919
C	-3.110634	-1.099881	0.999842
C	-3.313767	-1.194115	-1.460455
C	-4.451330	-0.695599	1.074650
C	-4.652244	-0.790679	-1.343161
C	-5.209527	-0.548057	-0.088254
H	-4.900265	-0.491414	2.048243
H	-5.263106	-0.653431	-2.237196
S	6.820820	-0.606608	-0.081664
S	-6.954758	-0.096368	0.023073
O	7.383232	-1.479151	1.003897
O	7.387023	-0.849934	-1.425399
O	-7.318375	0.481862	-1.287880
O	-7.687977	-1.367308	0.354799
O	-7.065687	0.855168	1.180109
O	6.885609	0.833089	0.354304
Na	8.106344	0.380983	2.304935
Na	-8.548391	-0.538546	2.381210
C	-2.290814	-1.271949	2.254263
H	-1.825564	-2.269343	2.298241
H	-1.472073	-0.534903	2.292574
H	-2.915840	-1.142435	3.149458
C	-2.711738	-1.469775	-2.814962
H	-1.732656	-0.975932	-2.922747
H	-2.542355	-2.547805	-2.968639
H	-3.371990	-1.117125	-3.616496
C	2.293327	-0.815000	-2.802899
H	1.612766	0.045952	-2.724186
H	3.004129	-0.620869	-3.619416
H	1.677806	-1.687307	-3.079909
C	2.296992	-2.327246	2.065846
H	3.015998	-2.692672	2.811384
H	1.693181	-1.534799	2.537091
H	1.609770	-3.149171	1.817738
C	0.477269	3.790463	-1.349095
C	1.655044	3.527807	0.732348
H	0.141369	4.635935	-1.976888
H	1.282087	3.267493	-1.905914
H	2.096143	4.198134	1.491822
H	2.492433	3.000460	0.230765

Complex 39 - [$Pt(PPh_3)_2(MeOPhHC{=}CHCOOPhOMe)$]

Pt	0.238084	-0.166467	0.013030
P	2.193827	0.380911	-1.193366
P	-0.770751	1.732320	1.029329
O	-2.315048	-2.002037	-1.555802
O	-3.360009	-1.790355	0.445974
O	-8.460545	-1.831329	-1.733432
O	4.246355	-5.060331	2.822193
C	3.688761	0.683196	-0.142644
C	3.870719	-0.140475	0.984402
C	4.971845	0.039263	1.825145
C	5.899831	1.053787	1.562640
C	5.721120	1.883169	0.451683
C	4.624242	1.699212	-0.398300
C	2.193978	1.802705	-2.388080
C	3.032122	1.820799	-3.519169
C	3.019656	2.908880	-4.395967
C	2.166694	3.993513	-4.161241
C	1.329673	3.985085	-3.041631
C	1.345082	2.897827	-2.162481
C	2.727853	-1.001286	-2.311096
C	4.018679	-1.550466	-2.301207
C	4.354206	-2.591550	-3.176180
C	3.407196	-3.091345	-4.072893
C	2.116108	-2.548717	-4.089298
C	1.777359	-1.517170	-3.211807
C	0.244565	3.263380	1.293075
C	1.586624	3.097060	1.678639
C	2.403683	4.205692	1.914617
C	1.895808	5.499084	1.751617
C	0.566208	5.675370	1.357430
C	-0.256939	4.566102	1.134085
C	-2.275903	2.357156	0.151183
C	-2.338763	2.212519	-1.246126
C	-3.436254	2.700375	-1.962517
C	-4.491415	3.325574	-1.290285
C	-4.445825	3.459617	0.101872
C	-3.345506	2.980468	0.818742
C	-1.396858	1.389926	2.743670
C	-2.362730	0.380260	2.911968
C	-2.847869	0.065530	4.182732
C	-2.369837	0.743887	5.309853
C	-1.407419	1.744821	5.154319
C	-0.927621	2.070647	3.879452
C	-1.013957	-1.883658	0.472155
C	0.216556	-2.337586	-0.125020
C	-2.235752	-1.894814	-0.353876
C	-4.619875	-1.821302	-0.140114
C	-5.436615	-2.923836	0.095098
C	-6.737906	-2.965243	-0.421189
C	-7.218216	-1.891257	-1.184721
C	-6.384317	-0.781587	-1.414967
C	-5.094540	-0.743370	-0.895993
C	-9.341077	-2.920343	-1.561471
C	1.269996	-3.039006	0.647045
C	1.415237	-2.913253	2.048056
C	2.408300	-3.595797	2.741182
C	3.307105	-4.437255	2.059892
C	3.183163	-4.578291	0.670602
C	2.175847	-3.886770	-0.012329
C	5.177911	-5.916138	2.198399
H	3.144609	-0.926363	1.207116
H	5.098985	-0.613417	2.692683
H	6.757803	1.198941	2.224303
H	6.438557	2.681262	0.241294
H	4.500107	2.357567	-1.259903
H	3.699661	0.979619	-3.720493
H	3.679484	2.906993	-5.268804
H	2.152964	4.840302	-4.852220
H	0.655300	4.824705	-2.849730
H	0.691136	2.900391	-1.290118
H	4.772231	-1.169114	-1.609853
H	5.363913	-3.010060	-3.153860
H	3.670426	-3.902946	-4.756148
H	1.366130	-2.935615	-4.784076
H	0.760676	-1.114763	-3.221489
H	1.997843	2.090250	1.784067
H	3.443712	4.055119	2.214985
H	2.536582	6.367204	1.926242
H	0.162560	6.682680	1.222569
H	-1.293543	4.723795	0.830599
H	-1.529208	1.700206	-1.772290
H	-3.470041	2.579015	-3.048601
H	-5.352748	3.700704	-1.848846
H	-5.271979	3.938302	0.634632
H	-3.324284	3.089285	1.905785
H	-2.741616	-0.165792	2.048270
H	-3.601106	-0.718518	4.291240
H	-2.745157	0.492348	6.305534
H	-1.027041	2.284842	6.028333
H	-0.183372	2.862223	3.779867
H	-1.194797	-2.030941	1.539512
H	0.150562	-2.645118	-1.173409
H	-5.051601	-3.754359	0.689861
H	-7.359661	-3.838107	-0.222628
H	-6.774185	0.046845	-2.009567
H	-4.453247	0.120943	-1.072605
H	-8.933703	-3.850231	-1.997321
H	-10.269779	-2.658996	-2.086447
H	-9.572120	-3.099691	-0.495921
H	0.742935	-2.256586	2.604388
H	2.511754	-3.493904	3.823886
H	3.858385	-5.223060	0.107753
H	2.093454	-4.013358	-1.094703
H	4.683635	-6.767992	1.697127
H	5.831423	-6.302221	2.992297
H	5.796032	-5.380341	1.455708

Complex 40 - [$Pt(PPh_3)_2(PhHC{=}CHCOOPhMe)$]

Pt	0.223719	-0.419875	0.376121
P	-0.651990	1.774125	0.598507
P	2.151346	-0.377202	-0.991442
O	-3.445525	-1.637299	0.900954
O	-2.211161	-2.595285	-0.739072
C	-1.134823	-1.852881	1.286577
C	0.120689	-2.500246	1.000402
C	1.099786	-2.862802	2.052305
C	1.106009	-2.273590	3.335261
C	2.052019	-2.643256	4.293540
C	3.022168	-3.608990	3.999563
C	3.029276	-4.204466	2.733729
C	2.080439	-3.838168	1.776893
C	-2.256624	-2.085289	0.358004
C	-4.616324	-1.756417	0.162050
C	-5.283957	-2.982062	0.089511
C	-6.497122	-3.063192	-0.594238
C	-7.067300	-1.935661	-1.211674
C	-6.374022	-0.719533	-1.123608
C	-5.154469	-0.622982	-0.445587
C	-8.386082	-2.041001	-1.939814
C	-1.561374	2.091099	2.189390
C	-1.236316	3.144931	3.060173
C	-1.946211	3.329179	4.252822
C	-2.995440	2.471093	4.588981
C	-3.330075	1.421766	3.725386
C	-2.616676	1.228091	2.540319
C	0.569713	3.164840	0.589721
C	0.354606	4.382560	-0.073785
C	1.323098	5.392274	-0.033238
C	2.512152	5.201504	0.676562
C	2.733841	3.990996	1.343861
C	1.772472	2.978676	1.294388
C	-1.893414	2.248542	-0.687118
C	-2.957275	3.132004	-0.433066
C	-3.867759	3.452452	-1.445037
C	-3.725747	2.897038	-2.721205
C	-2.671236	2.016519	-2.981888
C	-1.763813	1.689890	-1.970289
C	2.404323	-2.022503	-1.814807
C	3.673253	-2.589923	-2.015640
C	3.804865	-3.826528	-2.657064
C	2.673630	-4.508518	-3.113967
C	1.405149	-3.952504	-2.916456
C	1.269451	-2.724144	-2.262971
C	2.150588	0.780639	-2.444513
C	1.802651	0.346829	-3.735695
C	1.736696	1.252406	-4.800364
C	2.023913	2.604195	-4.596220
C	2.374180	3.046115	-3.316182
C	2.430081	2.146203	-2.249248
C	3.769360	-0.045466	-0.160049
C	4.897050	0.451948	-0.837423
C	6.101061	0.653474	-0.155915
C	6.196438	0.356442	1.207749
C	5.081725	-0.142707	1.888206
C	3.874512	-0.338731	1.210413
H	-1.428563	-1.621502	2.312855
H	0.129327	-3.168737	0.135018
H	0.365602	-1.509613	3.582958
H	2.031029	-2.171713	5.280151
H	3.762379	-3.896093	4.751033
H	3.778562	-4.962847	2.489653
H	2.093363	-4.312436	0.791941
H	-4.850884	-3.862040	0.569854
H	-7.015024	-4.025971	-0.649178
H	-6.790685	0.174915	-1.595603
H	-4.618873	0.326816	-0.387164
H	-8.343210	-2.797196	-2.741455
H	-8.672086	-1.081994	-2.396891
H	-9.198609	-2.343482	-1.257420
H	-0.426434	3.833620	2.815388
H	-1.675544	4.154316	4.917728
H	-3.549884	2.616959	5.519682
H	-4.148924	0.742233	3.976388
H	-2.887461	0.395535	1.888560
H	-0.568863	4.547786	-0.631745
H	1.144103	6.333180	-0.560490
H	3.266538	5.991797	0.706922
H	3.663094	3.829083	1.895698
H	1.961961	2.025706	1.795160
H	-3.081092	3.568882	0.560212
H	-4.692407	4.138358	-1.233838
H	-4.440207	3.146478	-3.509941
H	-2.557772	1.572309	-3.973777
H	-0.951491	0.987577	-2.171253
H	4.568873	-2.073055	-1.668111
H	4.799852	-4.257133	-2.799826
H	2.779203	-5.473867	-3.616217
H	0.511687	-4.480822	-3.258573
H	0.269774	-2.320227	-2.082689
H	1.584988	-0.705918	-3.923166
H	1.464546	0.891976	-5.796208
H	1.977264	3.310128	-5.429424
H	2.604246	4.100322	-3.141143
H	2.701760	2.513924	-1.258760
H	4.838463	0.687290	-1.901923
H	6.969094	1.042735	-0.694826
H	7.138895	0.514507	1.738550
H	5.146527	-0.380894	2.952639
H	3.005128	-0.724691	1.748300

Complex 41 - $[Pt(PPh_3)_2(NO_2PhHC{=}CHCOOPhNO_2)]$

Pt	0.325538	0.102510	-0.089597
P	-0.740291	-1.701832	1.042298
P	2.301980	-0.632797	-1.153478
O	4.553912	5.282210	3.285455
O	5.188757	5.981138	1.339341
O	-2.292409	1.857791	-1.747399
O	-3.257139	1.655074	0.300240
O	-8.958054	3.015299	-1.960318
O	-9.402274	1.238650	-0.809357
N	4.457247	5.318928	2.064707
N	-8.629112	2.081609	-1.242424
C	-1.162745	-1.274084	2.800316
C	-2.036881	-0.194017	3.030005
C	-2.370648	0.186086	4.331434
C	-1.830755	-0.496668	5.427496
C	-0.964120	-1.569111	5.209528
C	-0.634714	-1.959715	3.905932
C	-2.382471	-2.141637	0.316885
C	-3.396252	-2.749994	1.079425
C	-4.610599	-3.106000	0.486198
C	-4.828481	-2.857509	-0.874018
C	-3.830037	-2.246110	-1.637218
C	-2.614535	-1.886717	-1.045171
C	0.114051	-3.337032	1.214115
C	1.452498	-3.338798	1.646298
C	2.150687	-4.538569	1.801482
C	1.528373	-5.756088	1.508259
C	0.203844	-5.764440	1.064281
C	-0.502180	-4.564827	0.922195
C	3.031819	0.663196	-2.260074
C	4.329859	1.170805	-2.101403
C	4.822498	2.144395	-2.980137
C	4.027135	2.616508	-4.026455
C	2.728490	2.116001	-4.190177
C	2.232667	1.151922	-3.310899
C	2.218829	-2.068278	-2.322841
C	3.174426	-2.238399	-3.342969
C	3.096322	-3.327175	-4.214722
C	2.060149	-4.259057	-4.086047
C	1.101719	-4.094222	-3.082519
C	1.180210	-3.004765	-2.209238
C	3.683682	-1.025444	0.011151
C	4.598067	-2.071691	-0.190353
C	5.614904	-2.311800	0.740864
C	5.732490	-1.510313	1.880442
C	4.825730	-0.465426	2.089188
C	3.805427	-0.227738	1.164618
C	0.300411	2.238597	-0.442880
C	-0.917412	1.844911	0.233207
C	1.365812	3.006154	0.231017
C	1.519643	3.037364	1.638507
C	2.523331	3.787108	2.240179
C	3.398777	4.526502	1.435502
C	3.279008	4.522012	0.042993
C	2.270135	3.766601	-0.545030
C	-2.160032	1.794842	-0.549279
C	-4.544561	1.759290	-0.161279
C	-4.959023	2.809867	-0.994143
C	-6.300782	2.912761	-1.350189
C	-7.210354	1.965923	-0.871904
C	-6.807872	0.914770	-0.045542
C	-5.465356	0.812256	0.306960
H	-2.469622	0.349744	2.188510
H	-3.055844	1.022869	4.488984
H	-2.088863	-0.195241	6.445525
H	-0.541152	-2.115133	6.056636
H	0.035340	-2.807712	3.762111
H	-3.237697	-2.948840	2.141785
H	-5.389673	-3.580392	1.088616
H	-5.779519	-3.134093	-1.336117
H	-3.998045	-2.036205	-2.696300
H	-1.843901	-1.391911	-1.641730
H	1.956363	-2.394461	1.861191
H	3.188299	-4.517448	2.143051
H	2.076657	-6.694464	1.621448
H	-0.289447	-6.710542	0.827673
H	-1.536662	-4.594701	0.577415
H	4.966404	0.809504	-1.291320
H	5.835765	2.531585	-2.841072
H	4.414566	3.373597	-4.713120
H	2.098207	2.480979	-5.005566
H	1.214185	0.774796	-3.443119
H	3.981237	-1.512531	-3.466245
H	3.845367	-3.443583	-5.002453
H	1.997734	-5.107779	-4.771953
H	0.284343	-4.812481	-2.977123
H	0.425748	-2.880754	-1.433754
H	4.518819	-2.710587	-1.072275
H	6.317764	-3.131159	0.571259
H	6.527438	-1.700730	2.606355
H	4.908622	0.164863	2.978871
H	3.092152	0.580914	1.342953
H	0.206338	2.448035	-1.512889
H	-1.063847	2.090637	1.287299
H	-4.237372	3.540345	-1.356533
H	-6.654918	3.720888	-1.989176
H	-7.545635	0.194302	0.305087
H	-5.114594	-0.000913	0.943597
H	0.845636	2.456350	2.271394
H	2.640917	3.814496	3.322940
H	3.972459	5.111295	-0.557017
H	2.172771	3.761572	-1.632324

Complex 42 - $[Pt(PPh_3)_2(NO_2PhHC{=}CHCOOPh)]$

Pt	-0.019478	-0.202288	-0.146918
P	1.727052	1.123758	-1.039493
P	-1.573669	1.106846	1.084743
O	6.170026	-4.532397	1.381841
O	5.168406	-4.302192	3.285256
O	-3.065567	-2.697330	-0.301769
O	-1.915791	-2.325992	-2.221787
N	5.201517	-4.217757	2.062648
C	2.982074	1.702430	0.188918
C	3.574655	2.974738	0.147835
C	4.514375	3.349446	1.114981
C	4.877316	2.459455	2.129303
C	4.291444	1.189183	2.178000
C	3.345215	0.816380	1.220267
C	1.310120	2.633729	-2.032359
C	0.127014	3.339367	-1.764748
C	-0.202812	4.484754	-2.494977
C	0.644677	4.939353	-3.508411
C	1.825430	4.242765	-3.786903
C	2.155676	3.098012	-3.057140
C	2.738858	0.170806	-2.268096
C	2.059914	-0.429469	-3.345101
C	2.759575	-1.156067	-4.309881
C	4.148979	-1.305595	-4.207592
C	4.829429	-0.719478	-3.138269
C	4.130249	0.017708	-2.173988
C	-1.122574	2.832041	1.596318
C	0.178149	3.052258	2.083661
C	0.578660	4.325777	2.497097
C	-0.309155	5.403011	2.412323
C	-1.599264	5.197451	1.916749
C	-2.007291	3.919990	1.516135
C	-3.207391	1.307069	0.246384
C	-3.254053	1.256538	-1.156744
C	-4.463090	1.446331	-1.833584
C	-5.639254	1.679278	-1.115782
C	-5.605666	1.717179	0.282941
C	-4.397697	1.531995	0.961427
C	-2.018318	0.312805	2.703519
C	-2.648749	-0.945982	2.678556
C	-2.972683	-1.601059	3.868495
C	-2.663053	-1.018995	5.103095
C	-2.036133	0.228186	5.137056
C	-1.719523	0.893755	3.946646
C	-0.774320	-2.230260	-0.101016
C	0.553060	-2.230209	-0.670342
C	1.732046	-2.729705	0.060797
C	2.888502	-3.107410	-0.659830
C	4.022102	-3.591623	-0.016982
C	4.013864	-3.709380	1.376248
C	2.887964	-3.349592	2.126321
C	1.763365	-2.864625	1.470491
C	-1.920430	-2.404574	-1.015928
C	-4.244819	-3.011456	-0.962192
C	-4.324298	-4.117231	-1.814122
C	-5.552475	-4.444826	-2.393254
C	-6.692924	-3.680943	-2.120742
C	-6.599108	-2.578854	-1.265605
C	-5.373771	-2.236869	-0.686106
H	3.302742	3.683032	-0.636147
H	4.964490	4.344899	1.072066
H	5.612722	2.753889	2.882071
H	4.567280	0.486158	2.967853
H	2.881311	-0.171817	1.276004
H	-0.540845	2.991576	-0.978625
H	-1.129526	5.018497	-2.271138
H	0.385234	5.831278	-4.083502
H	2.492407	4.588435	-4.580441
H	3.076729	2.561839	-3.292852
H	0.973600	-0.333619	-3.425648
H	2.218033	-1.612998	-5.142231
H	4.696567	-1.879291	-4.959773
H	5.912759	-0.832503	-3.048372
H	4.679182	0.472280	-1.347483
H	0.887488	2.223607	2.135116
H	1.592858	4.475253	2.874746
H	0.006362	6.402077	2.726263
H	-2.297971	6.034504	1.840747
H	-3.020183	3.779938	1.136324
H	-2.340058	1.051298	-1.719796
H	-4.485098	1.398220	-2.925036
H	-6.585316	1.822080	-1.644598
H	-6.524535	1.891409	0.849554
H	-4.383247	1.561462	2.053090
H	-2.892553	-1.419203	1.725552
H	-3.466381	-2.575581	3.828774
H	-2.910921	-1.536255	6.033493
H	-1.793322	0.695396	6.094996
H	-1.239098	1.871465	3.997424
H	-0.942473	-2.622429	0.904052
H	0.612333	-2.346166	-1.756318
H	2.888588	-3.017115	-1.747668
H	4.911332	-3.884021	-0.574117
H	2.912458	-3.456714	3.210558
H	0.893532	-2.575500	2.062012
H	-3.433164	-4.711074	-2.018578
H	-5.618170	-5.307733	-3.059883
H	-7.651556	-3.945393	-2.574393
H	-7.484021	-1.975831	-1.048194
H	-5.281374	-1.373877	-0.025174

Complex 43 - $[Pt(PPh_3)_2(MePhHC{=}CHCOOPh)]$

Pt	0.112961	-0.371751	0.039879
P	2.118848	0.511486	-0.838622
P	-1.295809	1.351156	0.869196
O	-3.304170	-2.419078	-0.138014
O	-2.009556	-2.184804	-1.987562
C	2.872814	-0.637789	-2.081423
C	2.035602	-1.175430	-3.076346
C	2.549169	-2.038280	-4.046918
C	3.904250	-2.390045	-4.028951
C	4.740470	-1.869008	-3.038384
C	4.229939	-0.994478	-2.071695
C	2.107618	2.120637	-1.767807
C	1.482282	3.236350	-1.184351
C	1.463386	4.470211	-1.837713
C	2.061422	4.609154	-3.094540
C	2.682939	3.506985	-3.687171
C	2.709156	2.272563	-3.029150
C	3.472951	0.754440	0.402490
C	3.552807	-0.147163	1.479257
C	4.560462	-0.017057	2.438754
C	5.494013	1.020684	2.343362
C	5.417518	1.925595	1.280247
C	4.415011	1.793138	0.313260
C	-0.662025	2.445969	2.228301
C	0.717362	2.502617	2.483329
C	1.223019	3.312094	3.506812
C	0.354589	4.069371	4.295761
C	-1.024150	4.007184	4.063553
C	-1.529525	3.198241	3.042857
C	-1.915024	2.490857	-0.451829
C	-2.241944	3.840741	-0.244203
C	-2.707563	4.627970	-1.303800
C	-2.856580	4.076771	-2.580522
C	-2.531589	2.733891	-2.796890
C	-2.057687	1.947905	-1.742161
C	-2.855276	0.721960	1.652033
C	-2.727226	-0.127902	2.766090
C	-3.857480	-0.641291	3.402219
C	-5.136278	-0.323591	2.928209
C	-5.272870	0.511320	1.818036
C	-4.139326	1.034845	1.183226
C	-4.493115	-2.482424	-0.840768
C	-4.878495	-1.498121	-1.757667
C	-6.128501	-1.593803	-2.375026
C	-6.991333	-2.655277	-2.081672
C	-6.596613	-3.630758	-1.160562
C	-5.346791	-3.548383	-0.540976
C	-2.095465	-2.258430	-0.781465
C	-0.996313	-2.228297	0.200890
C	0.343185	-2.510409	-0.254479
C	1.358974	-3.177325	0.595174
C	1.277536	-3.234339	2.001461
C	2.254783	-3.882320	2.758996
C	3.361704	-4.501518	2.155470
C	3.443674	-4.448806	0.754440
C	2.467785	-3.805460	-0.007120
C	4.431595	-5.179486	2.976709
H	0.971225	-0.925889	-3.084621
H	1.885451	-2.445434	-4.813980
H	4.304652	-3.072574	-4.783255
H	5.798854	-2.142361	-3.013532
H	4.897065	-0.592573	-1.307237
H	1.003489	3.143914	-0.209071
H	0.964717	5.322617	-1.367300
H	2.039766	5.572505	-3.610590
H	3.154158	3.603133	-4.669167
H	3.204693	1.425983	-3.507197
H	2.821682	-0.954687	1.566871
H	4.610119	-0.728628	3.266730
H	6.278050	1.126035	3.098156
H	6.141985	2.740563	1.199609
H	4.368346	2.505185	-0.512959
H	1.401294	1.894855	1.889737
H	2.300481	3.338585	3.689253
H	0.748060	4.699019	5.097928
H	-1.711595	4.585629	4.686030
H	-2.609964	3.142043	2.890733
H	-2.128663	4.289981	0.743726
H	-2.954628	5.678133	-1.127999
H	-3.220516	4.694542	-3.406435
H	-2.635316	2.296644	-3.793273
H	-1.779947	0.905272	-1.920614
H	-1.732735	-0.390669	3.136559
H	-3.741420	-1.298246	4.267985
H	-6.022110	-0.731279	3.421731
H	-6.266370	0.760270	1.437350
H	-4.264887	1.687908	0.317919
H	-4.208853	-0.668273	-1.980957
H	-6.430037	-0.825144	-3.092129
H	-7.967534	-2.720441	-2.568327
H	-7.262899	-4.463977	-0.922542
H	-5.018986	-4.299404	0.181138
H	-1.303215	-2.486067	1.216896
H	0.446360	-2.726176	-1.322461
H	0.437316	-2.762224	2.515102
H	2.152349	-3.911325	3.848152
H	4.287005	-4.926900	0.246583
H	2.560121	-3.788723	-1.096038
H	4.792986	-6.099174	2.489766
H	5.309286	-4.523160	3.114138
H	4.064396	-5.447278	3.978986

Complex 44 - $[Pt(PPh_3)_2(PhHC{=}CHCOOPh)]$

Pt	0.077955	-0.472318	0.303582
P	2.073379	-0.203300	-0.930179
P	-0.959966	1.642110	0.614992
O	-2.045655	-2.795018	-1.093081
O	-3.503246	-2.068570	0.480484
C	-3.092909	0.791647	2.236976
C	-3.946483	0.813327	3.341883
C	-3.773934	1.769592	4.349219
C	-2.744701	2.707102	4.238327
C	-1.893833	2.694833	3.126290
C	-2.057415	1.736282	2.112649
C	-3.185885	3.042671	-0.523794
C	-4.004414	3.431234	-1.588134
C	-3.733304	2.981197	-2.884550
C	-2.642466	2.136588	-3.112876
C	-1.825176	1.742554	-2.048925
C	-2.084216	2.197388	-0.744654
C	-0.035146	4.355562	0.358521
C	0.870746	5.391535	0.614436
C	1.994716	5.164258	1.414444
C	2.213173	3.892777	1.957114
C	1.315097	2.855228	1.693681
C	0.178923	3.075844	0.894441
C	2.050488	2.389441	-2.046624
C	1.967635	3.332687	-3.072875
C	1.861237	2.918605	-4.405053
C	1.844864	1.553593	-4.700566
C	1.938078	0.606158	-3.674392
C	2.041992	1.011453	-2.333055
C	1.520903	-2.576223	-2.335317
C	1.827029	-3.758078	-3.016331
C	3.157757	-4.170311	-3.148297
C	4.180283	-3.390514	-2.600292
C	3.877935	-2.199842	-1.930565
C	2.545086	-1.778501	-1.791666
C	4.672792	0.960169	-0.555463
C	5.812797	1.245610	0.202693
C	5.899343	0.819454	1.531807
C	4.839312	0.107003	2.101575
C	3.695032	-0.172298	1.348537
C	3.600419	0.249205	0.010699
C	2.115852	-3.770844	1.724995
C	3.017514	-4.089666	2.741805
C	2.862551	-3.542714	4.020015
C	1.793060	-2.673633	4.265876
C	0.893464	-2.351808	3.248216
C	1.035415	-2.893526	1.952143
C	0.109515	-2.578187	0.838693
C	-1.218073	-2.057062	1.046181
C	-2.231730	-2.352329	0.017212
C	-4.753033	-1.395731	-1.485911
C	-5.901198	-1.530709	-2.270264
C	-6.882235	-2.471856	-1.938504
C	-6.711128	-3.283799	-0.813078
C	-5.563629	-3.160488	-0.023827
C	-4.592721	-2.216978	-0.365903
H	-3.234477	0.027150	1.471623
H	-4.746704	0.072489	3.416727
H	-4.437980	1.781194	5.217579
H	-2.599476	3.458567	5.019012
H	-1.100924	3.440621	3.056557
H	-3.412020	3.394362	0.485122
H	-4.860222	4.085399	-1.402466
H	-4.376347	3.284256	-3.715019
H	-2.426981	1.776194	-4.121734
H	-0.983110	1.069589	-2.225855
H	-0.908559	4.548603	-0.267349
H	0.694102	6.381480	0.185297
H	2.701178	5.974751	1.612088
H	3.092672	3.703220	2.577869
H	1.502898	1.858738	2.101790
H	2.126409	2.732512	-1.014025
H	1.981219	4.397393	-2.826643
H	1.791982	3.657165	-5.207804
H	1.764308	1.216227	-5.737487
H	1.932026	-0.454425	-3.929609
H	0.474518	-2.284470	-2.210932
H	1.018093	-4.363873	-3.433075
H	3.395993	-5.100291	-3.671242
H	5.222772	-3.708022	-2.691920
H	4.689930	-1.602770	-1.511752
H	4.621558	1.296820	-1.592625
H	6.637618	1.802273	-0.249843
H	6.791702	1.043055	2.122273
H	4.897632	-0.232686	3.138538
H	2.868404	-0.724014	1.801949
H	2.244558	-4.205975	0.730514
H	3.845751	-4.772844	2.535212
H	3.565248	-3.793557	4.818209
H	1.657118	-2.241714	5.261359
H	0.072750	-1.663597	3.460190
H	0.242286	-3.207119	-0.045198
H	-1.614881	-1.900363	2.051890
H	-3.986998	-0.659615	-1.734641
H	-6.029736	-0.890162	-3.146731
H	-7.778341	-2.571082	-2.555768
H	-7.473002	-4.020384	-0.546331
H	-5.409674	-3.785156	0.858365

Complex 45 - [$Pt(PPh_3)_2(NO_2PhHC{=}CHCOOPhOMe)$]

Pt	-0.205915	0.122933	-0.061403
P	0.883849	-1.660011	1.068738
P	-2.125654	-0.651574	-1.208128
O	-4.714675	5.005556	3.352400
O	-5.403010	5.638249	1.402194
O	2.348654	1.981987	-1.654047
O	3.319065	1.852893	0.392217
O	8.580600	2.087360	-1.345603
N	-4.617783	5.044196	2.131420
C	2.503599	-2.126082	0.309615
C	2.711792	-1.868164	-1.055708
C	3.910435	-2.240602	-1.673152
C	4.916153	-2.866803	-0.932112
C	4.723558	-3.115514	0.431797
C	3.525896	-2.746755	1.050457
C	0.011357	-3.280683	1.287259
C	0.612117	-4.524602	1.031908
C	-0.107752	-5.711371	1.210879
C	-1.431378	-5.673488	1.656133
C	-2.038668	-4.439357	1.913672
C	-1.326547	-3.252819	1.721304
C	1.354847	-1.220674	2.811436
C	2.236522	-0.140317	3.006822
C	2.609638	0.247629	4.295201
C	2.101985	-0.427008	5.411635
C	1.227238	-1.499417	5.227280
C	0.858588	-1.898343	3.936651
C	-3.558577	-1.036805	-0.104294
C	-3.761335	-0.199140	1.008449
C	-4.822213	-0.429343	1.887564
C	-5.687535	-1.508666	1.676279
C	-5.487010	-2.351941	0.579779
C	-4.430736	-2.118093	-0.308028
C	-2.000448	-2.103815	-2.354739
C	-0.980760	-3.050413	-2.177029
C	-0.871265	-4.152104	-3.031401
C	-1.779874	-4.320201	-4.079063
C	-2.798108	-3.380006	-4.270015
C	-2.906613	-2.278633	-3.417654
C	-2.800930	0.630763	-2.364522
C	-1.930589	1.149634	-3.341271
C	-2.376135	2.108993	-4.252063
C	-3.696476	2.573365	-4.195285
C	-4.564708	2.068623	-3.224874
C	-4.121578	1.100339	-2.314528
C	0.973322	1.894769	0.322425
C	-0.242819	2.272774	-0.361062
C	-1.355323	2.968814	0.310451
C	-1.519205	2.986471	1.717586
C	-2.576857	3.660977	2.315052
C	-3.499600	4.336609	1.507472
C	-3.369659	4.346555	0.115456
C	-2.305374	3.668930	-0.468216
C	2.232396	1.909827	-0.452732
C	4.609750	1.935175	-0.118638
C	5.494764	0.886686	0.152373
C	6.818930	0.970300	-0.268558
C	7.273380	2.098365	-0.974099
C	6.377963	3.144722	-1.246547
C	5.049514	3.060074	-0.814794
C	9.106414	3.192001	-2.049661
H	1.936300	-1.358558	-1.633134
H	4.061046	-2.027004	-2.733961
H	5.854977	-3.152081	-1.413609
H	5.510208	-3.597662	1.018036
H	3.387853	-2.942375	2.116200
H	1.645845	-4.576617	0.686948
H	0.373763	-6.669825	1.001347
H	-1.991098	-6.601586	1.797000
H	-3.075717	-4.396025	2.255468
H	-1.819376	-2.295977	1.908089
H	2.641965	0.400602	2.149781
H	3.299627	1.085480	4.425779
H	2.390214	-0.118330	6.419743
H	0.828548	-2.038393	6.090713
H	0.182948	-2.746240	3.818028
H	-3.079951	0.635969	1.189101
H	-4.969018	0.234064	2.743494
H	-6.514395	-1.692985	2.367087
H	-6.155873	-3.199731	0.410204
H	-4.288528	-2.788547	-1.157279
H	-0.265509	-2.924900	-1.365650
H	-0.068305	-4.876826	-2.876540
H	-1.692951	-5.178682	-4.750032
H	-3.509422	-3.500297	-5.091061
H	-3.699034	-1.547513	-3.588669
H	-0.894281	0.803519	-3.387238
H	-1.688649	2.499433	-5.006653
H	-4.044105	3.327685	-4.905727
H	-5.596159	2.426531	-3.171104
H	-4.814170	0.714412	-1.564702
H	1.100785	2.122265	1.382725
H	-0.139832	2.507810	-1.424573
H	-0.808791	2.454953	2.353369
H	-2.702955	3.676421	3.397121
H	-4.099883	4.885630	-0.487375
H	-2.199051	3.676728	-1.554540
H	5.138469	0.008346	0.692500
H	7.526379	0.164130	-0.063914
H	6.698997	4.032503	-1.790769
H	4.356914	3.876342	-1.024314
H	9.040202	4.124286	-1.460776
H	8.593002	3.345792	-3.016128
H	10.164290	2.967136	-2.241243

Complex 46 - $[Pt(PPh_3)_2(NO_2PhHC{=}CHCOOPhMe)]$

Pt	0.088909	-0.139988	-0.106099
P	1.984060	0.869268	-1.105108
P	-1.211233	1.457068	1.076924
O	-3.294240	-2.195025	0.049282
O	-2.222105	-2.071082	-1.946155
O	4.774931	-4.899509	3.267843
O	5.622857	-5.338412	1.327071
N	4.753522	-4.856755	2.043098
C	-0.524502	3.145457	1.416295
C	0.815066	3.238634	1.834385
C	1.389963	4.481035	2.114821
C	0.640311	5.651911	1.963366
C	-0.687718	5.571304	1.536162
C	-1.269816	4.326908	1.269179
C	-2.849164	1.794294	0.290683
C	-2.971081	1.637716	-1.100260
C	-4.180203	1.920680	-1.743626
C	-5.283207	2.355017	-1.003191
C	-5.175842	2.500939	0.384671
C	-3.967401	2.222165	1.029491
C	-1.668067	0.859150	2.774003
C	-2.454756	-0.303867	2.882264
C	-2.800358	-0.812758	4.135557
C	-2.357815	-0.178616	5.302669
C	-1.575641	0.973861	5.204433
C	-1.235512	1.493564	3.949825
C	2.820289	-0.273690	-2.302882
C	2.038922	-0.813193	-3.341502
C	2.608341	-1.665624	-4.288844
C	3.965727	-2.001951	-4.207174
C	4.745942	-1.478536	-3.174090
C	4.178225	-0.616718	-2.226477
C	3.334854	1.308593	0.079637
C	3.580948	0.416033	1.139186
C	4.588299	0.678001	2.071175
C	5.354694	1.844154	1.966444
C	5.109413	2.742138	0.924655
C	4.107495	2.477272	-0.016736
C	1.772033	2.373552	-2.167330
C	0.656061	3.204430	-1.987750
C	0.479381	4.344929	-2.777641
C	1.416972	4.668460	-3.761716
C	2.531061	3.843906	-3.954937
C	2.706472	2.703518	-3.167466
C	0.321991	-2.254975	-0.531652
C	-0.955335	-2.020286	0.103292
C	1.449621	-2.905110	0.160958
C	1.534519	-3.006966	1.571049
C	2.605497	-3.641171	2.188509
C	3.623423	-4.188403	1.398144
C	3.575832	-4.108824	0.003186
C	2.496613	-3.473847	-0.601061
C	-2.167388	-2.089207	-0.738667
C	-4.542157	-2.404260	-0.521402
C	-5.575453	-1.532408	-0.172585
C	-6.865471	-1.762757	-0.655517
C	-7.148663	-2.852595	-1.494585
C	-6.088431	-3.707409	-1.835168
C	-4.793591	-3.496344	-1.354886
C	-8.552143	-3.105898	-1.990764
H	1.418156	2.333820	1.935324
H	2.431752	4.531019	2.441043
H	1.091976	6.624961	2.172726
H	-1.280154	6.481134	1.409411
H	-2.309031	4.285586	0.939149
H	-2.117332	1.276033	-1.678769
H	-4.261215	1.787128	-2.824968
H	-6.229825	2.570054	-1.505338
H	-6.037561	2.833123	0.969727
H	-3.897832	2.336758	2.113551
H	-2.805293	-0.815504	1.983905
H	-3.416993	-1.713144	4.199377
H	-2.624041	-0.581886	6.282879
H	-1.227430	1.480325	6.108552
H	-0.631444	2.400364	3.897010
H	0.974977	-0.568887	-3.405803
H	1.988887	-2.073409	-5.091695
H	4.410690	-2.672625	-4.946757
H	5.805187	-1.738125	-3.099641
H	4.802802	-0.214263	-1.427331
H	2.975296	-0.488227	1.236699
H	4.771160	-0.029498	2.883065
H	6.139168	2.053213	2.698855
H	5.701196	3.657342	0.838260
H	3.928992	3.190876	-0.821907
H	-0.080981	2.956477	-1.225451
H	-0.398142	4.977753	-2.622790
H	1.278508	5.557694	-4.381875
H	3.266118	4.086157	-4.727029
H	3.574762	2.063423	-3.339228
H	0.295851	-2.429067	-1.611598
H	-1.118086	-2.326947	1.139085
H	0.749327	-2.575602	2.194066
H	2.668843	-3.723378	3.273065
H	4.380007	-4.548314	-0.586204
H	2.453824	-3.413520	-1.690043
H	-5.360789	-0.677712	0.470919
H	-7.668271	-1.075072	-0.374970
H	-6.276142	-4.562452	-2.490497
H	-3.984124	-4.173245	-1.628951
H	-8.559023	-3.789155	-2.853119
H	-9.048817	-2.170253	-2.293109
H	-9.177953	-3.562669	-1.203932

Complex 47 - $[Pt(PPh_3)_2(NO_2PhHC{=}CHCOOPr^i)]$

Pt	0.121075	-0.308157	-0.331910
P	2.074123	0.294051	0.873196
P	-1.278869	1.567251	-0.666883
O	-6.843889	-3.153832	1.197512
O	-5.659315	-3.713467	2.918859
O	1.244496	-2.320597	-2.980781
O	2.386728	-3.379508	-1.345445
N	-5.770357	-3.304172	1.768793
C	2.376150	-0.851514	2.304162
C	2.348282	-0.430850	3.643291
C	2.543959	-1.348916	4.682241
C	2.777879	-2.696169	4.398538
C	2.814790	-3.122753	3.065274
C	2.611485	-2.212314	2.026239
C	3.637942	0.153534	-0.103058
C	4.889779	-0.029332	0.512122
C	6.054812	-0.092608	-0.257510
C	5.984658	0.024129	-1.650971
C	4.744313	0.194730	-2.271496
C	3.576225	0.254678	-1.503025
C	2.187714	1.970969	1.653887
C	3.315759	2.802497	1.550496
C	3.325789	4.064661	2.155335
C	2.216786	4.508479	2.879901
C	1.088590	3.688049	2.987943
C	1.070022	2.434733	2.370920
C	-0.561435	3.119768	-1.378714
C	0.829613	3.276487	-1.450099
C	1.390100	4.433037	-2.003712
C	0.562488	5.447345	-2.492630
C	-0.828784	5.298546	-2.433253
C	-1.387517	4.141133	-1.886858
C	-2.207876	2.105783	0.838903
C	-2.253559	3.431535	1.299518
C	-2.955258	3.752090	2.467854
C	-3.626551	2.757030	3.184724
C	-3.581575	1.430830	2.736302
C	-2.868783	1.105893	1.579854
C	-2.620614	1.228067	-1.904790
C	-3.986484	1.427289	-1.652469
C	-4.938677	1.148113	-2.641709
C	-4.538241	0.674072	-3.892610
C	-3.175844	0.476564	-4.153937
C	-2.226372	0.746481	-3.166697
C	-0.990849	-1.993448	-1.140933
C	0.333504	-2.417441	-0.753887
C	-2.197817	-2.334368	-0.367651
C	-2.149843	-2.797670	0.970589
C	-3.307460	-3.118051	1.668151
C	-4.548687	-2.974012	1.036263
C	-4.638028	-2.521212	-0.283901
C	-3.470822	-2.210342	-0.971869
C	1.330788	-2.672590	-1.820580
C	3.432870	-3.759247	-2.274423
C	3.036837	-5.047879	-2.987192
C	4.713962	-3.884296	-1.465196
H	2.176629	0.617991	3.888818
H	2.517498	-1.002380	5.718998
H	2.933965	-3.410911	5.210599
H	3.001814	-4.174141	2.830942
H	2.643445	-2.565526	0.993252
H	4.957865	-0.125948	1.598397
H	7.021309	-0.235391	0.233056
H	6.896640	-0.026786	-2.251316
H	4.679020	0.272734	-3.360056
H	2.606086	0.361758	-1.994516
H	4.194446	2.474637	0.993275
H	4.210298	4.700812	2.059483
H	2.228006	5.493158	3.354153
H	0.210806	4.026858	3.544288
H	0.173162	1.814430	2.442094
H	1.475974	2.482738	-1.074584
H	2.476570	4.536432	-2.053359
H	0.997536	6.351347	-2.925910
H	-1.482401	6.085802	-2.819996
H	-2.474195	4.031233	-1.863494
H	-1.731198	4.222789	0.757783
H	-2.975865	4.788114	2.816959
H	-4.179064	3.010802	4.092688
H	-4.101008	0.643285	3.290222
H	-2.824512	0.064787	1.249394
H	-4.319379	1.798661	-0.681712
H	-5.999146	1.303984	-2.427661
H	-5.282295	0.456337	-4.663115
H	-2.851786	0.104996	-5.129334
H	-1.166987	0.574888	-3.377407
H	-1.160661	-1.855175	-2.212679
H	0.470717	-3.036789	0.135079
H	-1.187726	-2.899626	1.474157
H	-3.269764	-3.478249	2.695585
H	-5.617417	-2.423718	-0.750879
H	-3.536290	-1.860874	-2.004031
H	3.527558	-2.949486	-3.014063
H	2.108801	-4.906504	-3.560351
H	2.885295	-5.863268	-2.261236
H	3.828803	-5.353116	-3.689290
H	4.618558	-4.667643	-0.696499
H	4.958290	-2.933363	-0.969495
H	5.552123	-4.153575	-2.126712