

Supplementary Materials: Pt(II) Derivatives with Rollover-Coordinated 6-Substituted 2,2'-Bipyridines: Ligands with Multiple Personalities

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Supporting Information

ORTEP diagrams were prepared with ORTEP-3 for Windows⁽¹⁾ and exported as pov files which then have been rendered with POV-Ray™ 3.7.0 for Windows.⁽²⁾

Table S1: Coordinates for the equilibrium geometry for 8a-iso **Figure S1:** optimized geometry of 8a-iso

Pt	-1.870392	0.600396	0.154377
N	-0.388659	2.096207	-0.175672
C	0.941919	1.913906	-0.231081
C	1.801976	2.920773	-0.702622
C	1.260950	4.145281	-1.052065
C	-0.104559	4.367212	-0.888510
C	-0.901359	3.323879	-0.429307
C	-2.328353	3.504382	-0.091977
N	-2.937970	2.442758	0.479269
C	-4.190401	2.577952	0.927869
C	-4.914766	3.757304	0.800058
C	-4.314417	4.841064	0.168077
C	-3.003395	4.712781	-0.276025
O	1.359494	0.745606	0.207125
C	2.729714	0.400110	0.150811
C	-0.770976	-0.967255	-0.553881
P	-3.528006	-0.853781	0.610861
C	-3.903825	-0.913214	2.403791
C	-3.330963	-2.622814	0.180887
C	-5.074642	-0.352865	-0.243118
C	-4.732190	-1.917114	2.930229
C	-5.024782	-1.941887	4.291897
C	-4.484691	-0.976692	5.143555
C	-3.641603	0.008398	4.632302
C	-3.349633	0.039527	3.268573
C	-2.485388	-3.418017	0.967930
C	-2.287278	-4.757728	-0.646682
C	-2.925481	-5.313961	-0.463502
C	-3.766127	-4.527290	-1.248176
C	-3.971168	-3.184300	-0.929171
C	-6.345030	-0.492316	0.329884
C	-7.481094	-0.119595	-0.388190
C	-7.360601	0.386029	-1.682537
C	-6.098117	0.528378	-2.258896
C	-4.959326	0.167908	-1.540856
H	2.870275	2.742154	-0.777506
H	1.905838	4.940615	-1.421144
H	-0.526892	5.343816	-1.098824
H	-4.635865	1.710110	1.406419
H	-5.929903	3.809499	1.184936
H	-4.852520	5.777017	0.029494
H	-2.511760	5.552563	-0.758016
H	2.797014	-0.617472	0.539290
H	3.333100	1.067296	0.778945
H	3.102208	0.415749	-0.881148
H	-0.027107	-0.574984	-1.255946
H	-1.374207	-1.711874	-1.081747
H	-0.236144	-1.477180	0.258138
H	-5.133023	-2.694470	2.280325
H	-5.668583	-2.724386	4.691059
H	-4.711252	-1.002552	6.208402
H	-3.199417	0.748977	5.296695
H	-2.666710	0.791661	2.871671
H	-1.985454	-2.992538	1.837711
H	-1.633036	-5.370226	1.265183
H	-2.768384	-6.361859	-0.713821
H	-4.269597	-4.958135	-2.111967
H	-4.635685	-2.580942	-1.545742
H	-6.455427	-0.881551	1.339913
H	-8.464895	-0.229005	0.065826
H	-8.250683	0.671005	-2.240994
H	-5.998562	0.924186	-3.267935
H	-3.970399	0.294933	-1.982988

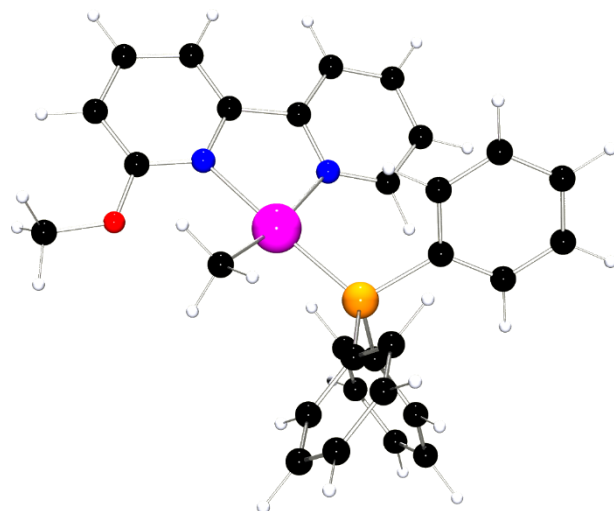


Table S2: Coordinates for the equilibrium geometry for **8a** geometry of **8a**

Pt	0.032405	-0.082094	1.193872
N	0.550379	0.448369	-0.840148
C	1.754275	0.320889	-1.415482
C	1.955952	0.598214	-2.777333
C	0.891296	1.084076	-3.516964
C	-0.334477	1.309044	-2.894615
C	-0.466671	0.987078	-1.547151
C	-1.695780	1.269057	-0.779182
N	-1.635303	1.035485	0.551448
C	-2.697135	1.316366	1.314999
C	-3.874037	1.844738	0.799425
C	-3.956528	2.076694	-0.569545
C	-2.854660	1.783322	-1.364228
O	2.715291	-0.060281	-0.594807
C	4.034837	-0.246436	-1.071529
C	-0.631348	-0.199293	3.114969
P	1.538389	-1.687287	1.721977
C	1.941549	-2.725783	-0.256405
C	3.106024	-1.094556	2.450653
C	0.926941	-2.942553	2.921308
C	0.948284	-2.912921	-0.715019
C	1.178575	-3.741563	-1.812844
C	2.406508	-4.386940	-1.956552
C	3.401209	-4.201566	-0.996318
C	3.170801	-3.378695	0.106271
C	4.028484	-1.970036	3.045927
C	5.213696	-1.477254	3.588697
C	5.482949	-0.108043	3.556513
C	4.561628	0.769713	2.986089
C	3.377659	0.279742	2.435929
C	0.140332	-4.010103	2.468166
C	-0.386850	-4.931449	3.370925
C	-0.134187	-4.800598	4.735846
C	0.648912	-3.742457	5.195013
C	1.174447	-2.815921	4.295723
H	2.928595	0.446021	-3.235213
H	1.021096	1.312589	-4.573128
H	-1.158717	1.739589	-3.453452
H	-2.600997	1.101072	2.375649
H	-4.705268	2.059657	1.466822
H	-4.864481	2.478787	-1.015405
H	-2.900048	1.953873	-2.435771
H	4.631792	-0.512493	-0.196966
H	4.430155	0.679382	-1.507725
H	4.077432	-1.063134	-1.803116
H	-0.972428	0.805536	3.402408
H	0.123096	-0.489760	3.851371
H	-1.466857	-0.907693	3.208040
H	-0.010879	-2.404633	-0.609449
H	0.395170	-3.884959	-2.556047
H	2.587265	-5.035381	-2.812702
H	4.361583	-4.704400	-1.100528
H	3.961225	-3.245014	0.842584
H	3.811795	-3.035653	3.113142
H	5.922970	-2.163454	4.048783
H	6.406004	0.275286	3.988828
H	4.759883	1.840673	2.977749
H	2.649436	0.959787	1.994801
H	-0.056425	-4.136951	1.405031
H	-0.991282	-5.759349	3.003044
H	-0.542994	-5.523810	5.439628
H	0.854887	-3.634737	6.258962
H	1.785757	-1.997727	4.673796

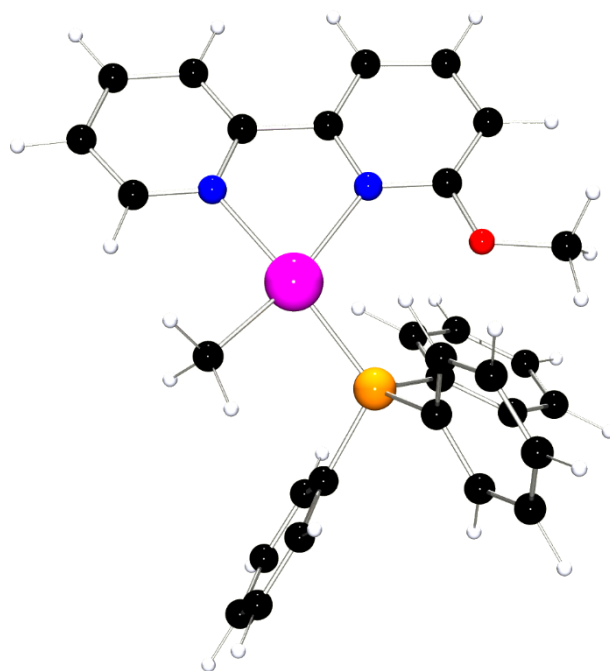
Figure S2: Optimized

Table S3: Selected bond distances, in Å, for **8a** and **8a-iso**.

8a-iso	Bond	8a
2.0451	Pt-CH ₃	2.0359
2.2518	Pt-P	2.2635
2.1312	Pt-N ₁	2.1649
2.1540	Pt-N _{1'}	2.1078
1.3544	N ₁ -C ₂	1.3507
1.4774	C ₂ -C _{2'}	1.4765
1.3509	C _{2'} -N _{1'}	1.3523

Table S4: Selected angles, in degrees, for **8a** and **8a-iso**.

8a-iso	Angle	8a
88.33	P-Pt-CH ₃	87.47
96.36	N ₁ -Pt-CH ₃	168.14
99.03	N _{1'} -Pt-P	166.78
175.17	P-Pt-N ₁	103.52
167.43	N _{1'} -Pt-CH ₃	93.45
76.56	N ₁ -Pt-N _{1'}	76.88
113.70	Pt-N ₁ -C ₂	114.16
115.70	N ₁ -C ₂ -C _{2'}	115.51
115.87	C ₂ -C _{2'} -N _{1'}	116.20
112.63	C _{2'} -N _{1'} -Pt	115.27

Table S5: Coordinates for the equilibrium geometry for **1a**.
geometry of **1a**

Pt	-1.080400	0.194284	-0.099562
N	-2.114254	2.022258	0.289976
C	-3.422301	2.174274	0.530385
C	-3.990982	3.422443	0.765538
C	-3.172906	4.550711	0.749098
C	-1.815897	4.390557	0.499889
C	-1.311698	3.109334	0.273988
C	0.104367	2.837084	0.005417
C	0.457659	1.494588	-0.205344
C	1.826255	1.280525	-0.458390
C	2.717402	2.339348	-0.488031
C	2.219218	3.636096	-0.258514
N	0.949971	3.878712	-0.018564
O	3.100295	4.647464	-0.292447
C	2.608855	5.946947	-0.064117
C	0.183562	-1.370045	-0.506130
S	-2.849931	-1.242847	0.024326
O	-4.230976	-0.741868	0.332624
C	-3.014107	-2.203367	-1.492669
C	-2.543980	-2.562631	1.213692
H	-4.017324	1.259220	0.531197
H	-5.058971	3.494248	0.958522
H	-3.588484	5.541374	0.929513
H	-1.116728	5.222659	0.472002
H	2.202185	0.274114	-0.635534
H	3.779355	2.204170	-0.682767
H	3.471011	6.615566	-0.132702
H	2.148034	6.033569	0.928488
H	1.856767	6.229558	-0.812230
H	0.676929	-1.200811	-1.474000
H	-0.265152	-2.373219	-0.558305
H	0.968661	-1.422323	0.262127
H	-3.284135	-1.482506	-2.269003
H	-3.824902	-2.923933	-1.345021
H	-2.067670	-2.689673	-1.742970
H	-1.602898	-3.072636	0.990279
H	-2.486235	-2.074173	2.190287
H	-3.401445	-3.242620	1.180823

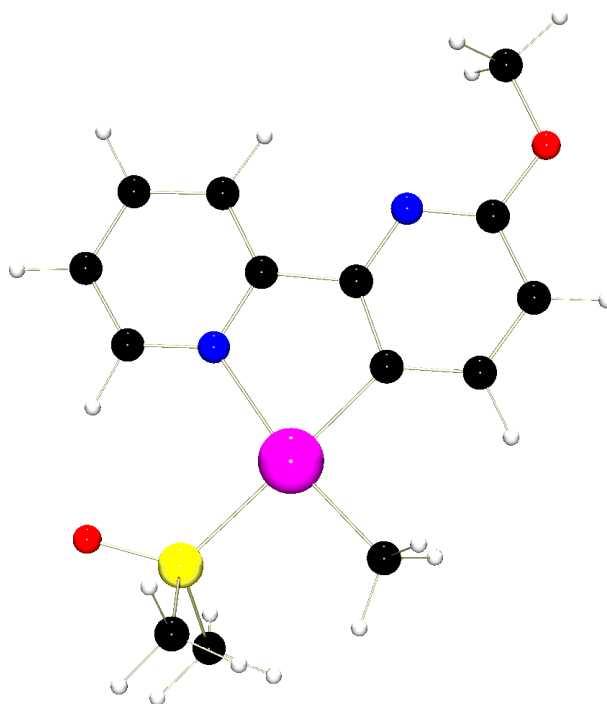
Figure S5: Optimized

Table S6: Coordinates for the equilibrium geometry for 3a

Pt	-1.078398	0.189963	-0.104866
N	-2.137370	2.020545	0.289487
C	-3.445955	2.148374	0.525049
C	-4.040894	3.387155	0.766093
C	-3.249906	4.528644	0.761080
C	-1.885168	4.393675	0.515785
C	-1.354580	3.125685	0.283655
C	0.052460	2.831018	0.013399
C	0.432675	1.510819	-0.205065
C	1.810456	1.309363	-0.463462
C	2.721762	2.348361	-0.497411
C	2.276502	3.654074	-0.267581
N	0.968642	3.849477	-0.021715
O	3.127985	4.653543	-0.295106
C	2.711294	5.988949	-0.068386
C	0.193477	-1.359859	-0.506598
S	-2.843817	-1.272630	0.016669
O	-4.199935	-0.714738	0.319432
C	-3.012837	-2.224408	-1.498542
C	-2.548991	-2.570435	1.224175
H	-4.023434	1.220011	0.517318
H	-5.110863	3.437524	0.954081
H	-3.681954	5.510605	0.945125
H	-1.259377	5.285621	0.510880
H	2.176736	0.300230	-0.644370
H	3.780186	2.199690	-0.696959
H	3.608044	6.604511	-0.154871
H	2.299216	6.110365	0.943136
H	1.987966	6.314131	-0.829471
H	0.674871	-1.195607	-1.481442
H	-0.251179	-2.362455	-0.546787
H	0.980268	-1.401422	0.260571
H	-3.260017	-1.503080	-2.282146
H	-3.842786	-2.923503	-1.353760
H	-2.079304	-2.740636	-1.736837
H	-1.618560	-3.100785	1.003597
H	-2.483566	-2.072800	2.195743
H	-3.416221	-3.238371	1.200928
H	0.645811	4.795336	0.147353

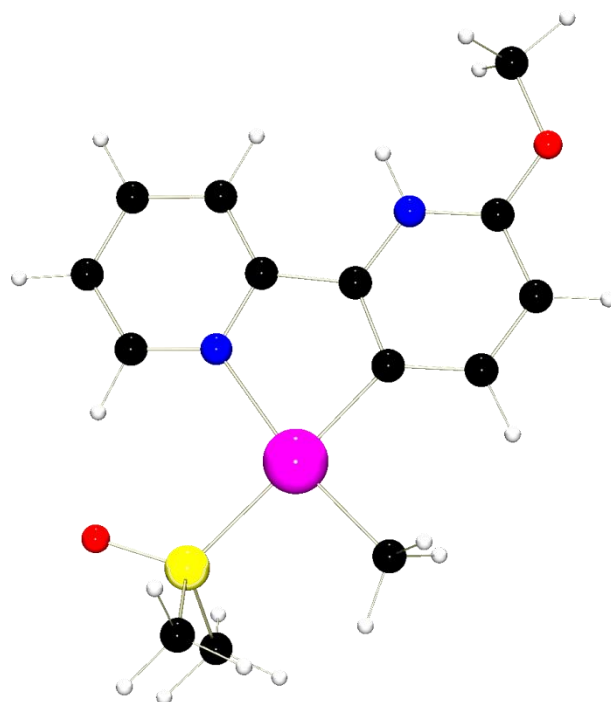
Figure S6: Optimized geometry of 3a

Table S7: Coordinates for the equilibrium geometry for 4a geometry of 4a

Pt	-1.890728	0.291179	-0.193391
N	-2.943468	2.066639	-0.147858
C	-4.276982	2.165672	-0.193341
C	-4.916778	3.398103	-0.158208
C	-4.143270	4.556804	-0.072705
C	-2.760200	4.446379	-0.025473
C	-2.179081	3.178867	-0.065089
C	-0.742722	2.922393	-0.023982
C	-0.356648	1.572241	-0.075074
C	1.034027	1.349068	-0.034570
C	1.908507	2.418355	0.049579
C	1.380515	3.724361	0.093705
N	0.090023	3.970510	0.057877
O	2.254743	4.737587	0.175859
C	1.734462	6.045111	0.223818
S	-0.727373	-1.606285	-0.238100
O	0.760858	-1.634712	-0.184292
C	-1.316655	-2.670329	1.084763
C	-1.213863	-2.544872	-1.691626
Cl	-3.886673	-1.043353	-0.333020
H	-4.815927	1.221346	-0.259194
H	-6.002877	3.438483	-0.198147
H	-4.618490	5.536592	-0.043163
H	-2.097268	5.305447	0.041389
H	1.416263	0.329140	-0.069757
H	2.987730	2.281516	0.083499
H	2.595991	6.714248	0.290846
H	1.083139	6.186196	1.096267
H	1.150348	6.278459	-0.676187
H	-1.025869	-2.180554	2.018180
H	-0.800191	-3.629365	0.980785
H	-2.405399	-2.753421	1.011137
H	-0.861301	-1.971764	-2.553410
H	-2.304502	-2.634068	-1.702875
H	-0.699650	-3.509174	-1.638111

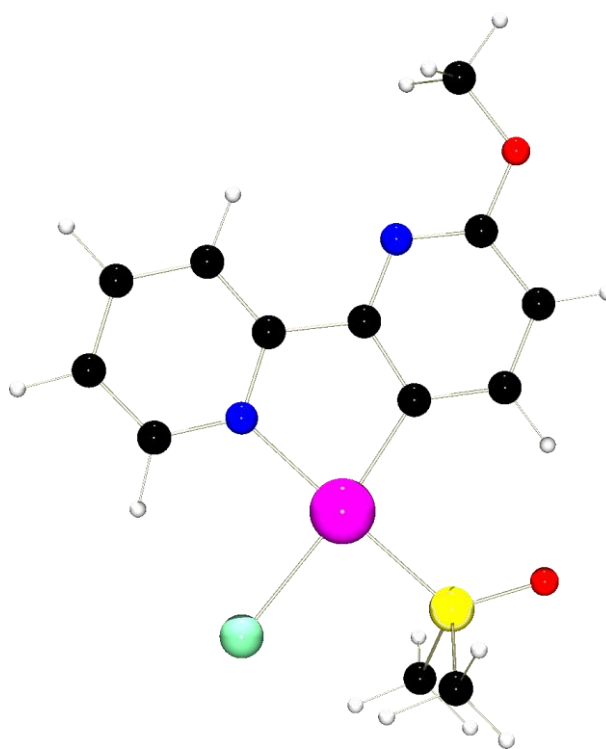
Figure S7: Optimized

Table S8: Coordinates for the equilibrium geometry for 5a geometry of 5a

Pt	-1.924731	0.294349	-0.191932
N	-2.985188	2.073897	-0.146561
C	-4.316722	2.155901	-0.193139
C	-4.977030	3.381679	-0.159574
C	-4.225519	4.548254	-0.074529
C	-2.836195	4.455952	-0.025823
C	-2.234901	3.199870	-0.063740
C	-0.807102	2.911369	-0.022897
C	-0.404541	1.578966	-0.069111
C	0.997475	1.359403	-0.023036
C	1.899862	2.401064	0.059663
C	1.432928	3.721069	0.100330
N	0.105737	3.930759	0.058611
O	2.284710	4.716399	0.177236
C	1.850421	6.064934	0.217681
S	-0.740816	-1.606662	-0.239021
O	0.745642	-1.545200	-0.179971
C	-1.293082	-2.677669	1.088039
C	-1.187291	-2.542908	-1.701043
Cl	-3.872067	-1.025996	-0.336863
H	-4.844516	1.204417	-0.259037
H	-6.063581	3.405928	-0.200355
H	-4.711675	5.521880	-0.045896
H	-2.243321	5.367275	0.041805
H	1.358247	0.328408	-0.055662
H	2.975359	2.242629	0.095250
H	2.754483	6.672087	0.282422
H	1.234496	6.257153	1.107515
H	1.311447	6.336122	-0.701148
H	-1.025821	-2.176074	2.022338
H	-0.740291	-3.616853	0.988910
H	-2.376498	-2.809100	1.012096
H	-0.854268	-1.953499	-2.559726
H	-2.272588	-2.678753	-1.718131
H	-0.638381	-3.488242	-1.651958
H	-0.234142	4.885042	0.088977

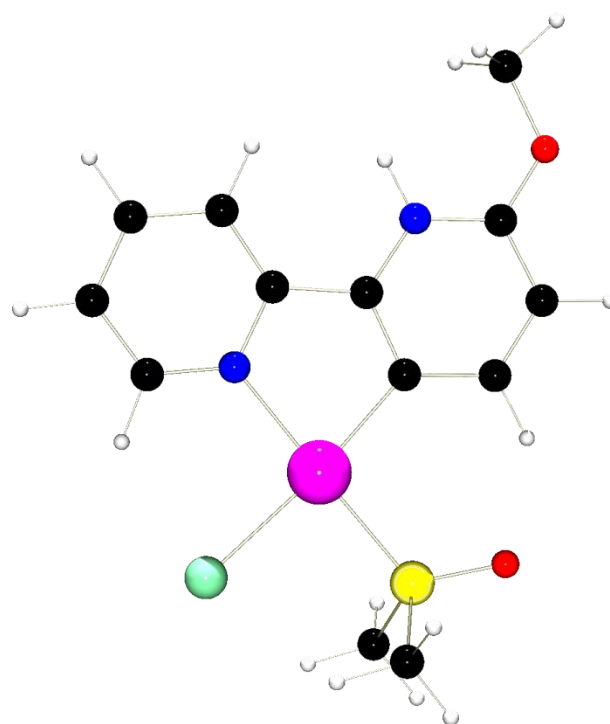
Figure S8: Optimized

Table S9: Coordinates for the equilibrium geometry for 6a geometry of 6a

Pt	-1.157504	-0.431124	0.063958
N	-2.231974	1.431521	0.088962
C	-3.551807	1.617496	-0.010351
C	-4.142989	2.875821	0.011319
C	-3.324332	3.996605	0.142893
C	-1.952473	3.810782	0.237345
C	-1.430579	2.515248	0.202048
C	0.006794	2.235055	0.262256
C	0.387361	0.886333	0.186257
C	1.780750	0.674953	0.215738
C	2.662568	1.736521	0.320008
C	2.131459	3.038552	0.396971
N	0.841546	3.283295	0.366248
O	3.005515	4.053314	0.502745
C	2.480715	5.356599	0.578062
C	0.189167	-1.983309	0.001970
P	-2.800768	-2.065234	-0.051018
C	-4.588416	-1.642617	-0.259577
C	-5.179614	-1.577018	-1.527379
C	-6.502164	-1.156207	-1.671215
C	-7.252117	-0.797233	-0.552367
C	-6.672223	-0.861084	0.715684
C	-5.350606	-1.277988	0.861527
C	-2.505997	-3.171952	-1.496957
C	-2.801565	-4.539481	-1.515731
C	-2.577076	-5.293210	-2.667800
C	-2.060118	-4.689120	-3.813503
C	-1.753287	-3.328795	-3.799745
C	-1.966066	-2.576402	-2.645621
C	-2.876204	-3.161479	1.427758
C	-3.909897	-4.092037	1.619161
C	-3.937272	-4.893991	2.758266
C	-2.939634	-4.769592	3.726645
C	-1.920876	-3.834745	3.554345
C	-1.889796	-3.033362	2.412755
H	-4.161093	0.724925	-0.110249
H	-5.224075	2.960861	-0.074924
H	-3.750953	4.998713	0.167042
H	-1.248779	4.633771	0.333481
H	2.183077	-0.335253	0.153032
H	3.742266	1.600451	0.344028
H	3.339604	6.027686	0.661970
H	1.826044	5.477271	1.451241
H	1.897559	5.608616	-0.317767
H	0.864574	-1.929958	0.868184
H	0.801899	-1.871021	-0.904689
H	-0.222501	-3.000862	-0.021126
H	-4.606577	-1.861392	-2.408683
H	-6.948031	-1.114370	-2.664346
H	-8.285203	-0.472506	-0.666364
H	-7.250379	-0.585928	1.596688
H	-4.907418	-1.321003	1.856166
H	-3.189298	-5.030406	-0.625545
H	-2.803436	-6.358618	-2.666418
H	-1.883842	-5.280637	-4.711169
H	-1.331639	-2.853121	-4.684277
H	-1.689380	-1.521597	-2.615253
H	-4.713207	-4.177170	0.887262
H	-4.745831	-5.611630	2.894309
H	-2.965052	-5.393230	4.619626
H	-1.147487	-3.720714	4.313151
H	-1.104828	-2.289783	2.278347

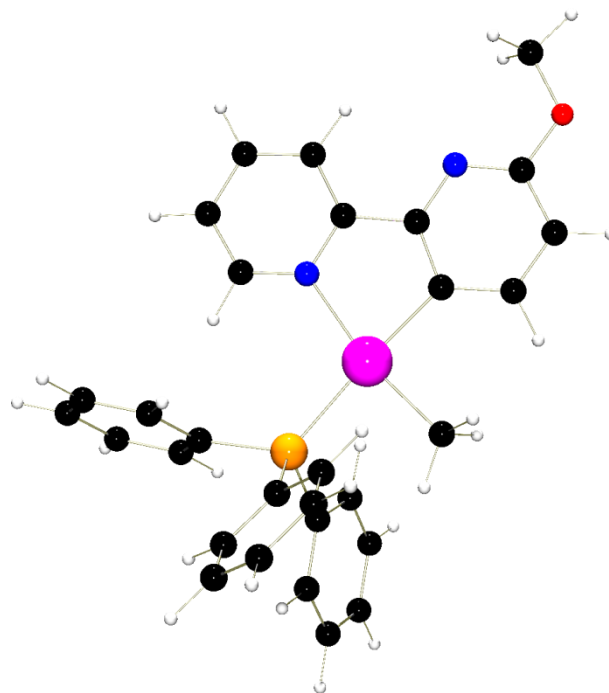
Figure S9: Optimized

Table S10: Coordinates for the equilibrium geometry for 9a

Pt	-1.176282	-0.440785	0.095959
N	-2.265691	1.429600	0.111575
C	-3.587210	1.593426	0.030491
C	-4.200209	2.844816	0.046272
C	-3.404722	3.978840	0.151636
C	-2.024938	3.815285	0.229414
C	-1.480251	2.530572	0.202980
C	-0.051869	2.221510	0.250553
C	0.347055	0.890172	0.196993
C	1.749657	0.682143	0.217830
C	2.660148	1.719432	0.293590
C	2.190246	3.035311	0.352275
N	0.862588	3.241782	0.327631
O	3.041763	4.035577	0.427118
C	2.599266	5.379080	0.478803
C	0.164852	-1.986976	0.053848
P	-2.817940	-2.099355	-0.033519
C	-4.586382	-1.626660	-0.251789
C	-5.157527	-1.511500	-1.525505
C	-6.473257	-1.070022	-1.670516
C	-7.232684	-0.740793	-0.548508
C	-6.672215	-0.857094	0.724779
C	-5.357558	-1.295804	0.874003
C	-2.483674	-3.171659	-1.486989
C	-2.661246	-4.559464	-1.483619
C	-2.407061	-5.301613	-2.637222
C	-1.978734	-4.667119	-3.802289
C	-1.788304	-3.285209	-3.809500
C	-2.029973	-2.542250	-2.655751
C	-2.899231	-3.183165	1.441850
C	-3.918021	-4.139066	1.585601
C	-3.967816	-4.947797	2.718390
C	-3.011151	-4.804059	3.724911
C	-2.009012	-3.844408	3.598371
C	-1.952862	-3.036404	2.462785
H	-4.183391	0.688915	-0.047432
H	-5.283605	2.910941	-0.023363
H	-3.844997	4.974156	0.170521
H	-1.394297	4.700255	0.307767
H	2.134157	-0.335720	0.169065
H	3.736299	1.562911	0.309090
H	3.499364	5.992987	0.536468
H	1.990941	5.564577	1.375542
H	2.047194	5.652522	-0.431889
H	0.840438	-1.919782	0.919370
H	0.767500	-1.892370	-0.861938
H	-0.250988	-3.000776	0.051175
H	-4.580560	-1.779736	-2.409151
H	-6.908510	-0.994604	-2.666068
H	-8.262118	-0.405738	-0.664081
H	-7.262773	-0.614714	1.607006
H	-4.932724	-1.390061	1.873069
H	-2.978821	-5.073417	-0.578958
H	-2.541626	-6.382187	-2.621469
H	-1.781329	-5.250321	-4.700551
H	-1.437713	-2.785889	-4.711601
H	-1.845300	-1.467109	-2.650889
H	-4.688164	-4.242078	0.821011
H	-4.761175	-5.687334	2.819329
H	-3.054977	-5.434538	4.612010
H	-1.268687	-3.719258	4.387465
H	-1.177046	-2.278148	2.365831
H	0.523105	4.195721	0.366289

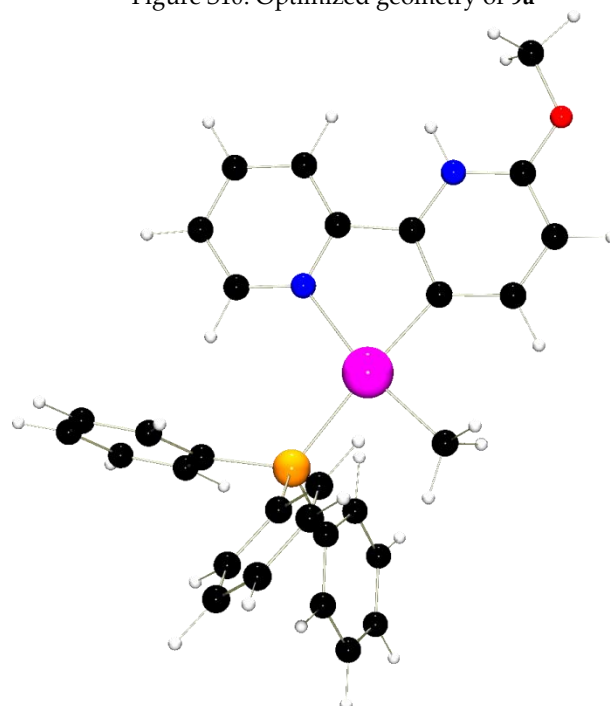
Figure S10: Optimized geometry of 9a

Table S11: Coordinates for the equilibrium geometry for 7a

Pt	-2.734761	0.554845	0.568053
N	-3.539590	2.469212	0.852044
C	-4.649855	2.748331	1.542409
C	-5.112260	4.051004	1.687830
C	-4.393715	5.090781	1.096760
C	-3.241399	4.794364	0.380779
C	-2.834330	3.463608	0.272152
C	-1.648154	3.024387	-0.460998
C	-1.390600	1.638001	-0.465167
C	-0.245614	1.276568	-1.208885
C	0.526949	2.227674	-1.851909
C	0.147466	3.578839	-1.748215
N	-0.911143	3.963853	-1.073408
O	0.913282	4.485328	-2.375094
C	0.533918	5.837390	-2.274155
Cl	-4.478480	-0.425117	1.836143
P	-1.768505	-1.449078	0.224838
C	-1.904869	-2.055837	-1.503781
C	-2.276016	-1.166684	-2.519624
C	-2.378651	-1.608590	-3.838700
C	-2.117770	-2.941128	-4.153016
C	-1.764606	-3.837821	-3.143428
C	-1.664391	-3.401006	-1.824100
C	-2.383450	-2.890503	1.183030
C	-3.657296	-3.399851	0.893588
C	-4.145044	-4.500479	1.590156
C	-3.375464	-5.096421	2.591260
C	-2.115146	-4.586774	2.891366
C	-1.617836	-3.487717	2.188691
C	0.024622	-1.432602	0.631621
C	0.973657	-2.210821	-0.041014
C	2.312560	-2.176209	0.348501
C	2.712116	-1.373738	1.416630
C	1.770769	-0.595301	2.089915
C	0.434393	-0.617276	1.695117
H	-5.155976	1.885283	1.975494
H	-6.021218	4.236396	2.254977
H	-4.731539	6.121861	1.194333
H	-2.633859	5.552690	-0.106370
H	0.059510	0.235043	-1.290980
H	1.411637	1.962767	-2.426931
H	1.273580	6.405908	-2.843681
H	0.526623	6.175990	-1.229870
H	-0.467396	6.006669	-2.691460
H	-2.498558	-0.131383	-2.264499
H	-2.671484	-0.908461	-4.619506
H	-2.202184	-3.286092	-5.182840
H	-1.575680	-4.883663	-3.381878
H	-1.420020	-4.113836	-1.036964
H	-4.270860	-2.928212	0.128331
H	-5.135607	-4.887890	1.357942
H	-3.761571	-5.956316	3.137001
H	-1.509999	-5.044069	3.673011
H	-0.628671	-3.101848	2.426809
H	0.675850	-2.835501	-0.881592
H	3.045310	-2.777524	-0.187809
H	3.758203	-1.349300	1.719446
H	2.078030	0.040646	2.919023
H	-0.301050	0.011671	2.198045

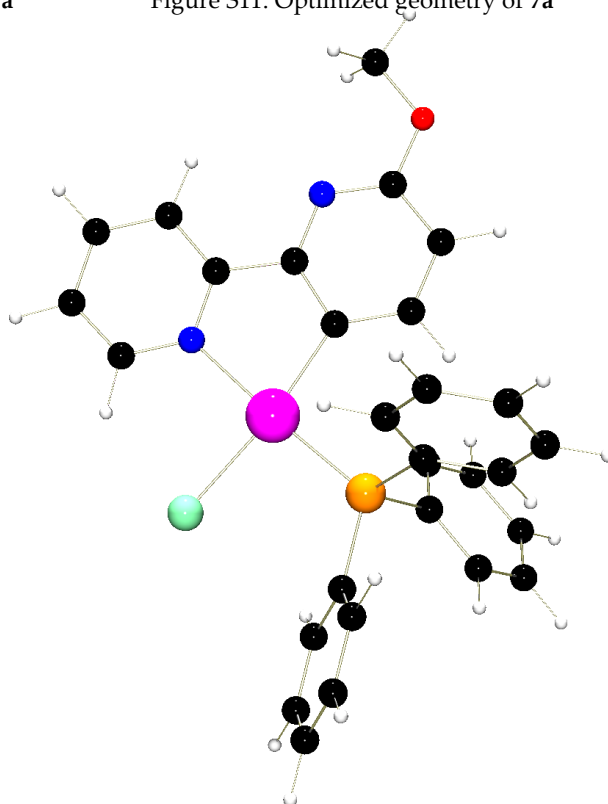
Figure S11: Optimized geometry of 7a

Table S12: Coordinates for the equilibrium geometry for **10a**

Pt	-2.756621	0.540958	0.542358
N	-3.567109	2.463302	0.839685
C	-4.682616	2.723858	1.522533
C	-5.155699	4.023587	1.690096
C	-4.440919	5.076464	1.129644
C	-3.276876	4.798624	0.417027
C	-2.859544	3.473932	0.284640
C	-1.680526	3.002048	-0.431184
C	-1.418123	1.627660	-0.461745
C	-0.266172	1.268945	-1.215688
C	0.537907	2.194219	-1.852008
C	0.222478	3.554135	-1.764764
N	-0.868478	3.906396	-1.065881
O	0.981443	4.448298	-2.359405
C	0.680946	5.830770	-2.292440
Cl	-4.481468	-0.441874	1.763726
P	-1.787409	-1.486445	0.209026
C	-1.940149	-2.069999	-1.518775
C	-2.367414	-1.192095	-2.523131
C	-2.477171	-1.631772	-3.842174
C	-2.166178	-2.951155	-4.166636
C	-1.757892	-3.837190	-3.168190
C	-1.651455	-3.403998	-1.848533
C	-2.388382	-2.905722	1.191570
C	-3.631819	-3.471328	0.874936
C	-4.105389	-4.558813	1.600916
C	-3.350740	-5.084065	2.651591
C	-2.118834	-4.520004	2.973112
C	-1.634516	-3.432986	2.245067
C	0.004622	-1.411076	0.599966
C	0.969740	-2.135062	-0.111178
C	2.311815	-2.068984	0.264410
C	2.698316	-1.291444	1.355557
C	1.741029	-0.569010	2.068670
C	0.400870	-0.621440	1.689591
H	-5.188342	1.849283	1.934943
H	-6.070627	4.193288	2.252285
H	-4.782387	6.103872	1.242988
H	-2.715920	5.621675	-0.023501
H	0.014102	0.221073	-1.302644
H	1.417573	1.910120	-2.424037
H	1.461356	6.339241	-2.860737
H	0.709065	6.194469	-1.255667
H	-0.290458	6.050275	-2.757755
H	-2.641670	-0.171412	-2.259240
H	-2.820378	-0.945609	-4.614618
H	-2.257790	-3.296069	-5.195489
H	-1.533114	-4.873392	-3.415594
H	-1.366252	-4.111449	-1.070380
H	-4.232256	-3.059719	0.065450
H	-5.071036	-4.993863	1.350165
H	-3.725419	-5.934932	3.218403
H	-1.526257	-4.926976	3.790777
H	-0.665927	-3.007314	2.498619
H	0.681809	-2.746926	-0.964513
H	3.055981	-2.632571	-0.296034
H	3.745748	-1.248974	1.650951
H	2.037898	0.036716	2.923657
H	-0.346948	-0.047207	2.237800
H	-1.107040	4.889618	-1.004741

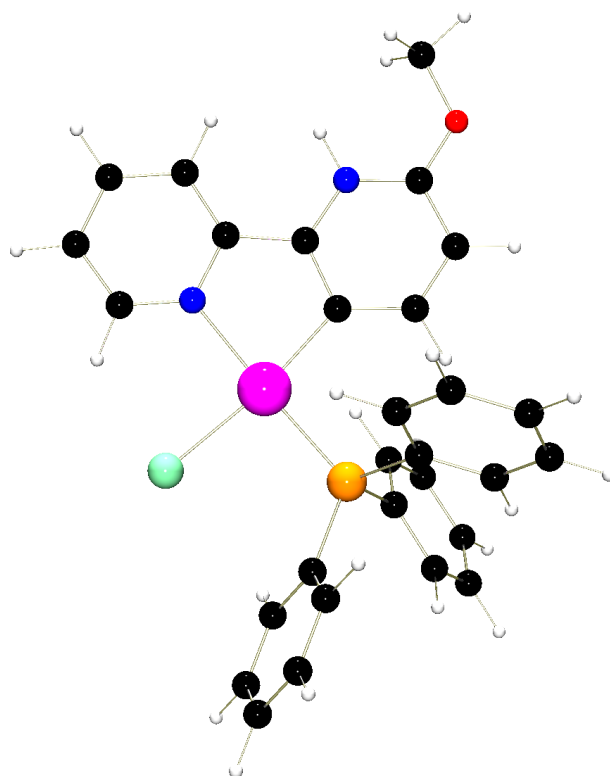
Figure S12: Optimized geometry of

Table S13: Coordinates for the equilibrium geometry for **1b**

Pt	-1.090308	0.165999	-0.100996
N	-2.110125	2.003031	0.282202
C	-3.416856	2.164982	0.526747
C	-3.975707	3.418014	0.756953
C	-3.150033	4.541012	0.731120
C	-1.795311	4.370598	0.477675
C	-1.301287	3.084519	0.257168
C	0.113968	2.802648	-0.015263
C	0.456965	1.451616	-0.219295
C	1.818059	1.228902	-0.473780
C	2.709262	2.294033	-0.510611
C	2.244288	3.602454	-0.292174
N	0.961897	3.834429	-0.048771
C	3.199712	4.772663	-0.333815
C	2.566135	6.123127	-0.049630
C	0.159829	-1.410961	-0.503395
S	-2.873110	-1.258590	0.035067
O	-4.249790	-0.747659	0.346080
C	-3.047510	-2.222175	-1.478702
C	-2.571539	-2.575553	1.228439
H	-4.018361	1.254310	0.534878
H	-5.042456	3.498229	0.953591
H	-3.558427	5.535403	0.907588
H	-1.088007	5.195714	0.441797
H	2.190383	0.220071	-0.645826
H	3.767604	2.122820	-0.710118
H	3.317643	6.920149	-0.096806
H	2.105144	6.141277	0.944212
H	1.775798	6.348117	-0.774128
H	0.653656	-1.250027	-1.472369
H	-0.298607	-2.410056	-0.551504
H	0.945309	-1.467480	0.263904
H	-3.309799	-1.501206	-2.257499
H	-3.866630	-2.932634	-1.328124
H	-2.106717	-2.720231	-1.727075
H	-1.630439	-3.087130	1.009334
H	-2.516433	-2.083384	2.203312
H	-3.429578	-3.254796	1.195988
H	4.013117	4.579628	0.382171
H	3.683602	4.786339	-1.322555

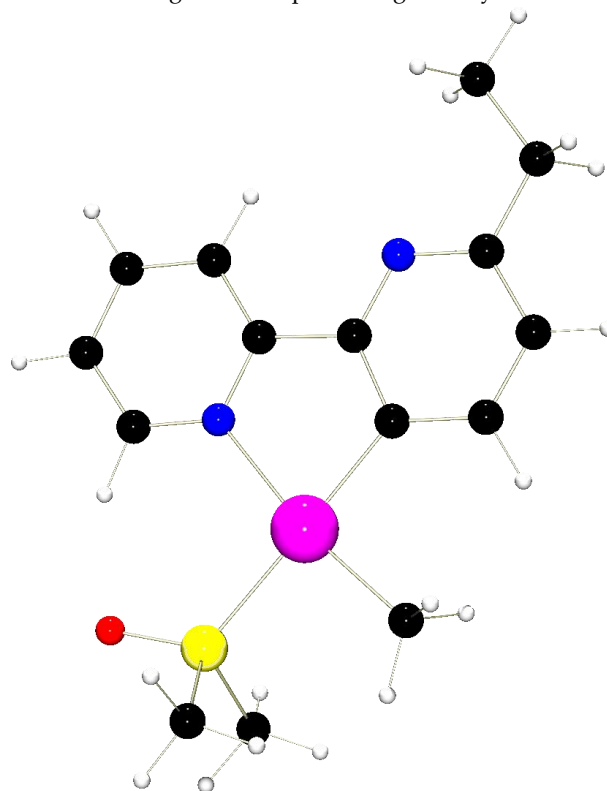
Figure S13: Optimized geometry of **1b**

Table S14: Coordinates for the equilibrium geometry for **3b**

Pt	-1.081742	0.162116	-0.108509
N	-2.118394	2.005683	0.284310
C	-3.424551	2.147381	0.526835
C	-4.005003	3.393310	0.765655
C	-3.202944	4.527053	0.750960
C	-1.841104	4.377575	0.498301
C	-1.325851	3.103132	0.269099
C	0.079115	2.795342	-0.007921
C	0.443651	1.460523	-0.222425
C	1.811255	1.247597	-0.484185
C	2.728929	2.291588	-0.526107
C	2.310781	3.602062	-0.304513
N	1.003155	3.786776	-0.055071
C	3.230025	4.788280	-0.333693
C	2.589523	6.138446	-0.050856
C	0.168599	-1.404920	-0.512494
S	-2.866346	-1.281288	0.027865
O	-4.214142	-0.707643	0.337760
C	-3.054683	-2.233832	-1.484529
C	-2.577591	-2.579460	1.236311
H	-4.011872	1.225266	0.526620
H	-5.073343	3.455240	0.959631
H	-3.624048	5.514102	0.933108
H	-1.204601	5.261475	0.485196
H	2.170104	0.235065	-0.661330
H	3.781008	2.103822	-0.732488
H	3.347251	6.926882	-0.097965
H	2.151356	6.189893	0.955233
H	1.823754	6.400971	-0.793774
H	0.649173	-1.247780	-1.488750
H	-0.290105	-2.401215	-0.550710
H	0.956887	-1.456511	0.252371
H	-3.297446	-1.511203	-2.268323
H	-3.892419	-2.922260	-1.333603
H	-2.128881	-2.762062	-1.726674
H	-1.653839	-3.119538	1.011368
H	-2.501732	-2.080558	2.206484
H	-3.451705	-3.238553	1.219410
H	4.038529	4.596418	0.386076
H	3.716990	4.802642	-1.319343
H	0.701798	4.742621	0.108652

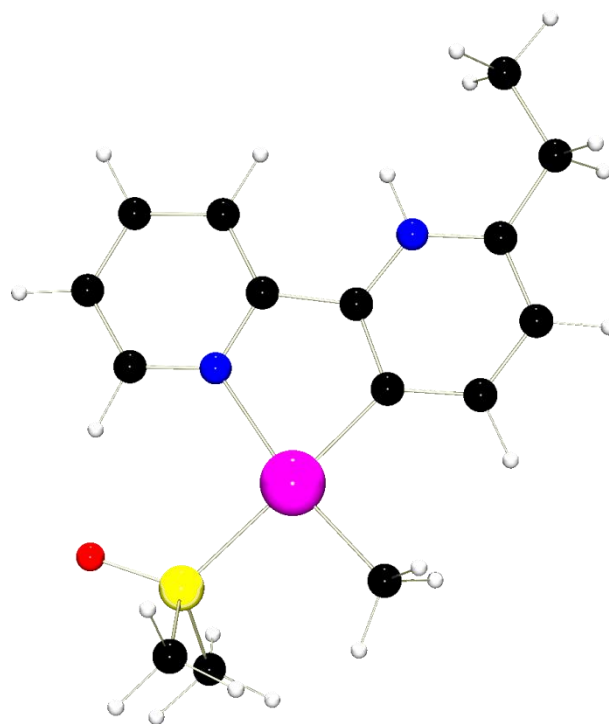
Figure S14: Optimized geometry of **3b**

Table S15: Coordinates for the equilibrium geometry for **4b**

Pt	-1.902830	0.257295	-0.191770
N	-2.936028	2.044544	-0.142655
C	-4.269234	2.158010	-0.184887
C	-4.894470	3.397335	-0.148091
C	-4.107917	4.547750	-0.064681
C	-2.726215	4.422143	-0.020854
C	-2.160231	3.148068	-0.061672
C	-0.724576	2.876825	-0.023561
C	-0.353863	1.517416	-0.075234
C	1.028726	1.281555	-0.038754
C	1.908106	2.354183	0.041863
C	1.418612	3.672369	0.088074
N	0.115308	3.911453	0.054686
C	2.370730	4.841822	0.178624
C	1.706027	6.206972	0.168495
S	-0.762006	-1.654883	-0.240853
O	0.725693	-1.701720	-0.185898
C	-1.365764	-2.716846	1.077294
C	-1.258824	-2.581654	-1.698331
Cl	-3.914007	-1.054888	-0.334404
H	-4.818727	1.219849	-0.249840
H	-5.980193	3.449853	-0.185248
H	-4.572238	5.532716	-0.034161
H	-2.050652	5.271713	0.044064
H	1.403733	0.258949	-0.074649
H	2.984116	2.178123	0.070016
H	2.457285	7.002543	0.233450
H	1.013600	6.314993	1.010795
H	1.123077	6.355580	-0.747561
H	-1.074343	-2.232451	2.013307
H	-0.857665	-3.680154	0.971962
H	-2.455021	-2.788940	0.999300
H	-0.895567	-2.010775	-2.557139
H	-2.350599	-2.655194	-1.712622
H	-0.758903	-3.553594	-1.647071
H	3.089587	4.765414	-0.651710
H	2.973173	4.724543	1.092816

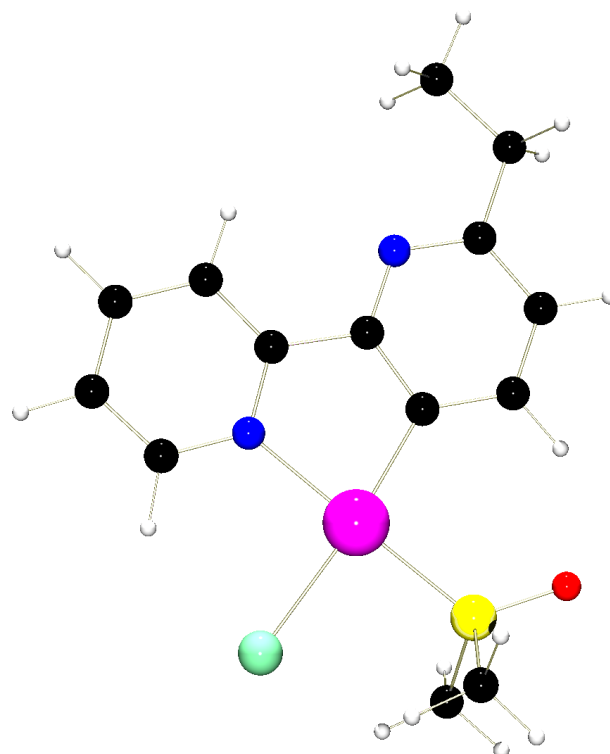
Figure S15: Optimized geometry of **4b**

Table S16: Coordinates for the equilibrium geometry for **5b**

Pt	-1.929099	0.264258	-0.194015
N	-2.962503	2.059660	-0.147011
C	-4.293064	2.160620	-0.188952
C	-4.934717	3.396308	-0.154044
C	-4.166374	4.551987	-0.072667
C	-2.778147	4.439561	-0.028720
C	-2.196990	3.174796	-0.067748
C	-0.770360	2.867450	-0.031469
C	-0.387891	1.520058	-0.078613
C	1.004122	1.285955	-0.038576
C	1.917177	2.329783	0.040217
C	1.481204	3.654685	0.083116
N	0.154306	3.856574	0.045069
C	2.402874	4.835518	0.168894
C	1.738296	6.203071	0.190939
S	-0.776043	-1.656516	-0.241987
O	0.711142	-1.619360	-0.187755
C	-1.342053	-2.715391	1.088967
C	-1.242863	-2.587938	-1.700711
Cl	-3.897863	-1.025884	-0.331323
H	-4.835165	1.217122	-0.252169
H	-6.021014	3.436225	-0.190975
H	-4.637782	5.532808	-0.043162
H	-2.170712	5.341255	0.035937
H	1.354969	0.251783	-0.071926
H	2.986809	2.128937	0.069793
H	2.500763	6.985923	0.248864
H	1.090100	6.338449	1.067719
H	1.160443	6.401691	-0.722439
H	-1.064309	-2.216193	2.021482
H	-0.804588	-3.663503	0.990414
H	-2.427620	-2.829968	1.016322
H	-0.903670	-2.005602	-2.561797
H	-2.330187	-2.707036	-1.713922
H	-0.708667	-3.541677	-1.651590
H	3.102024	4.769050	-0.677364
H	3.023172	4.703671	1.067373
H	-0.160940	4.821372	0.075459

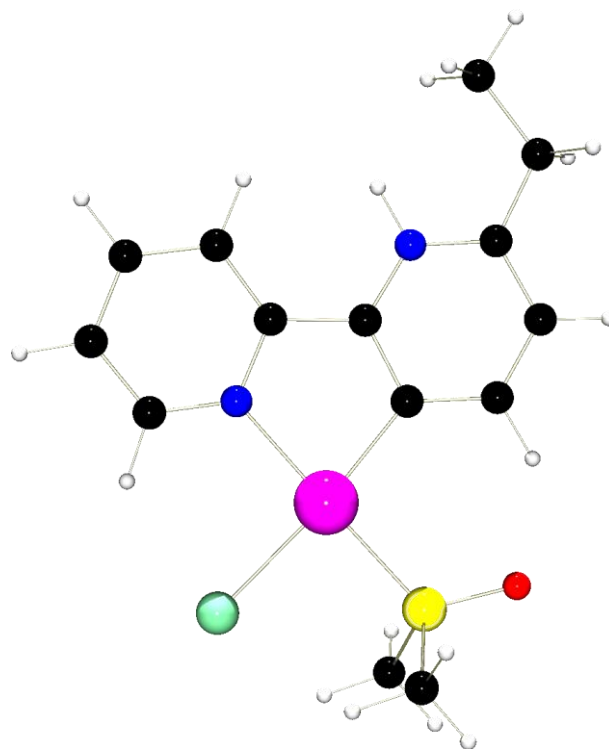
Figure S16: Optimized geometry of **5b**

Table S17: Coordinates for the equilibrium geometry for **6b**

Pt	-1.464608	-0.117506	-0.446161
N	-1.474805	0.554817	1.598201
C	-2.229114	0.104788	2.606777
C	-2.157732	0.622333	3.894938
C	-1.261555	1.659930	4.150439
C	-0.484882	2.139718	3.105691
C	-0.615747	1.571564	1.835910
C	0.143378	2.045869	0.673080
C	-0.122346	1.405055	-0.552200
C	0.603757	1.919595	-1.638146
C	1.500658	2.964585	-1.457377
C	1.685992	3.513238	-0.175880
N	1.005745	3.051006	0.863029
C	2.667424	4.642549	0.040257
C	2.731234	5.166071	1.464514
C	-1.252829	-0.425799	-2.467900
P	-2.928459	-1.919270	-0.483813
C	-4.242226	-1.660526	-1.752292
C	-4.830339	-2.688406	-2.497404
C	-5.846797	-2.404177	-3.409332
C	-6.289017	-1.092986	-3.583099
C	-5.700753	-0.061630	-2.851741
C	-4.677101	-0.342306	-1.948139
C	-2.134946	-3.530289	-0.895659
C	-0.797597	-3.541600	-1.310554
C	-0.164287	-4.745041	-1.622605
C	-0.857514	-5.949390	-1.518370
C	-2.185305	-5.950739	-1.087990
C	-2.818906	-4.750391	-0.773111
C	-3.925501	-2.395866	0.998060
C	-5.230028	-1.922270	1.184635
C	-5.926100	-2.209118	2.359637
C	-5.330387	-2.974435	3.360967
C	-4.031365	-3.453168	3.182916
C	-3.332796	-3.164326	2.012500
H	-2.916160	-0.703216	2.375481
H	-2.796566	0.210475	4.672675
H	-1.175759	2.089448	5.147721
H	0.229161	2.952233	3.219239
H	0.468720	1.504574	-2.636151
H	2.062867	3.364013	-2.302108
H	2.411743	5.460289	-0.650412
H	3.664033	4.298735	-0.277511
H	1.756139	5.546754	1.788744
H	3.464402	5.977486	1.546430
H	3.013445	4.371623	2.164250
H	-0.193337	-0.578802	-2.720364
H	-1.589198	0.482282	-2.989774
H	-1.810635	-1.264029	-2.905349
H	-4.486691	-3.714437	-2.383939
H	-6.291416	-3.211997	-3.988845
H	-7.083383	-0.873995	-4.295853
H	-6.028490	0.967299	-2.993789
H	-4.185739	0.464607	-1.402140
H	-0.256868	-2.598231	-1.374794
H	0.876123	-4.737965	-1.943113
H	-0.362376	-6.888633	-1.761392
H	-2.727582	-6.890331	-0.988851
H	-3.844477	-4.766852	-0.406086
H	-5.709278	-1.330636	0.405767
H	-6.941175	-1.836282	2.487480
H	-5.877184	-3.201935	4.275117
H	-3.558568	-4.054492	3.958594
H	-2.317077	-3.538026	1.886714

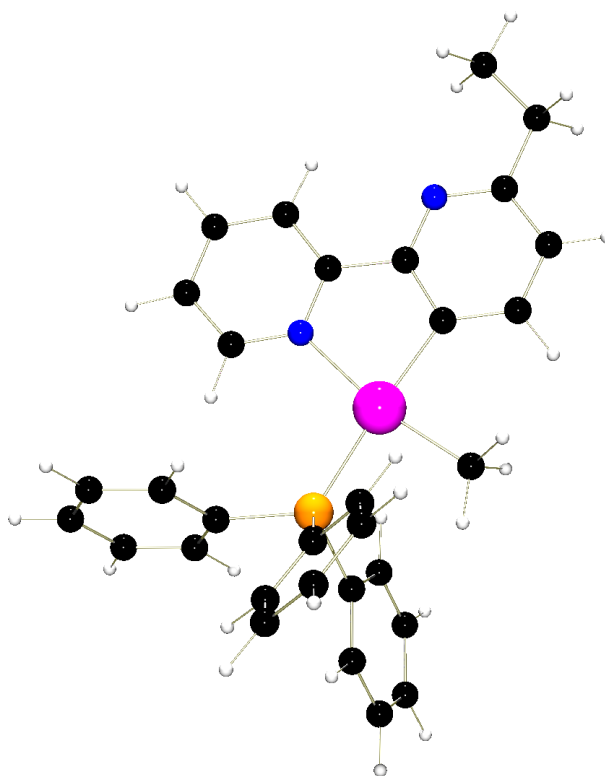
Figure S17 Optimized geometry of **6b**

Table S18: Coordinates for the equilibrium geometry for **9b**

Pt	-1.485598	-0.112762	-0.454368
N	-1.512344	0.566211	1.603192
C	-2.287014	0.115542	2.592012
C	-2.243721	0.630630	3.886159
C	-1.358857	1.664159	4.167483
C	-0.557837	2.148429	3.137571
C	-0.657470	1.584267	1.865074
C	0.098317	2.026682	0.691418
C	-0.154288	1.406724	-0.537915
C	0.582635	1.926071	-1.623212
C	1.497872	2.961810	-1.475408
C	1.721209	3.526731	-0.220875
N	1.005551	3.030683	0.801731
C	2.703032	4.634228	0.032257
C	2.779981	5.147697	1.462087
C	-1.270220	-0.422176	-2.466997
P	-2.943886	-1.942603	-0.503406
C	-4.246508	-1.671524	-1.769168
C	-4.772947	-2.692938	-2.567642
C	-5.787255	-2.413670	-3.483496
C	-6.286047	-1.117587	-3.607511
C	-5.758155	-0.092519	-2.822447
C	-4.737555	-0.365775	-1.914015
C	-2.123536	-3.533969	-0.898480
C	-0.781664	-3.547512	-1.298642
C	-0.148228	-4.753225	-1.600120
C	-0.847056	-5.954712	-1.501179
C	-2.179989	-5.952455	-1.086667
C	-2.814760	-4.751038	-0.780774
C	-3.906564	-2.381483	1.005632
C	-5.206848	-1.901368	1.206092
C	-5.883633	-2.176645	2.395277
C	-5.272122	-2.934879	3.392864
C	-3.977984	-3.421354	3.198354
C	-3.297414	-3.146066	2.013762
H	-2.968045	-0.693390	2.343813
H	-2.899269	0.216145	4.648167
H	-1.294426	2.092946	5.165695
H	0.128657	2.968978	3.342703
H	0.432773	1.504424	-2.616071
H	2.054075	3.344425	-2.329120
H	2.453446	5.458965	-0.649872
H	3.691920	4.279315	-0.292153
H	1.827412	5.575208	1.803335
H	3.521942	5.949734	1.530104
H	3.101386	4.370102	2.169058
H	-0.209540	-0.570494	-2.717953
H	-1.622044	0.480887	-2.987863
H	-1.821211	-1.266222	-2.896406
H	-4.384895	-3.706578	-2.493266
H	-6.186102	-3.214136	-4.104475
H	-7.079177	-0.904241	-4.322804
H	-6.133738	0.924400	-2.925319
H	-4.301739	0.441450	-1.323568
H	-0.233636	-2.609175	-1.364045
H	0.895114	-4.751683	-1.910317
H	-0.352423	-6.895492	-1.737756
H	-2.725685	-6.890335	-0.994322
H	-3.845905	-4.764975	-0.429675
H	-5.701197	-1.322263	0.427301
H	-6.897857	-1.806360	2.534762
H	-5.806757	-3.157877	4.315082
H	-3.499170	-4.025259	3.968066
H	-2.289515	-3.534333	1.869781
H	1.167568	3.444180	1.714223

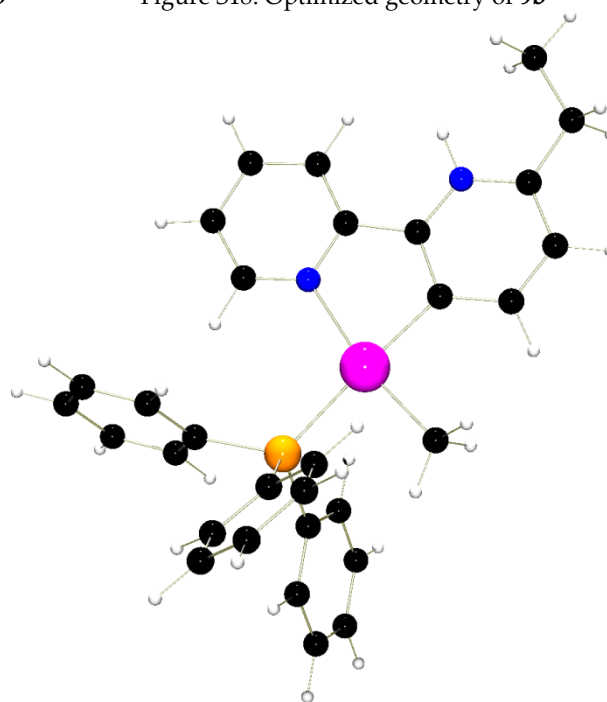
Figure S18: Optimized geometry of **9b**

Table S19: Coordinates for the equilibrium geometry for **7b**

Pt	-2.696416	0.531607	0.614675
N	-3.494952	2.445406	0.919296
C	-4.623735	2.717671	1.583222
C	-5.079052	4.020331	1.745522
C	-4.334653	5.067702	1.200830
C	-3.164159	4.778298	0.512320
C	-2.765545	3.446875	0.384743
C	-1.559464	3.015614	-0.324276
C	-1.313298	1.622264	-0.351420
C	-0.152792	1.271442	-1.065092
C	0.640793	2.243938	-1.659305
C	0.288748	3.599861	-1.550983
N	-0.801464	3.959033	-0.889296
C	1.142270	4.670894	-2.189687
C	0.651253	6.091011	-1.969764
Cl	-4.484725	-0.462544	1.808123
P	-1.736124	-1.473157	0.253771
C	-1.820320	-2.038523	-1.492182
C	-2.159337	-1.126383	-2.498780
C	-2.224779	-1.539430	-3.829591
C	-1.957959	-2.865585	-4.165184
C	-1.636631	-3.785015	-3.165500
C	-1.574266	-3.377240	-1.834640
C	-2.395460	-2.932065	1.154792
C	-3.666277	-3.416866	0.813993
C	-4.187715	-4.530162	1.464652
C	-3.455090	-5.163932	2.470325
C	-2.197834	-4.679530	2.820907
C	-1.666780	-3.567472	2.164615
C	0.042277	-1.482925	0.720742
C	1.009231	-2.245808	0.056120
C	2.334054	-2.233511	0.492304
C	2.701356	-1.469122	1.599226
C	1.742071	-0.706065	2.264855
C	0.420128	-0.705333	1.823612
H	-5.149514	1.849431	1.980732
H	-6.002798	4.200505	2.289985
H	-4.666860	6.099102	1.313278
H	-2.533927	5.540038	0.060181
H	0.150755	0.230660	-1.163288
H	1.538403	1.957857	-2.208045
H	1.210275	4.460251	-3.268206
H	2.169992	4.565187	-1.810185
H	-0.360969	6.224223	-2.367115
H	1.313832	6.810560	-2.464238
H	0.611278	6.333845	-0.902025
H	-2.387064	-0.096105	-2.228428
H	-2.493849	-0.821790	-4.603051
H	-2.013270	-3.187969	-5.204297
H	-1.443558	-4.826055	-3.421027
H	-1.355297	-4.107777	-1.056340
H	-4.251282	-2.916493	0.044817
H	-5.175768	-4.897787	1.193162
H	-3.867434	-6.033496	2.980211
H	-1.621270	-5.166523	3.606163
H	-0.680264	-3.201709	2.441850
H	0.736951	-2.840860	-0.813894
H	3.081217	-2.822659	-0.037582
H	3.736340	-1.462616	1.938803
H	2.024050	-0.100217	3.124779
H	-0.328214	-0.087980	2.321783

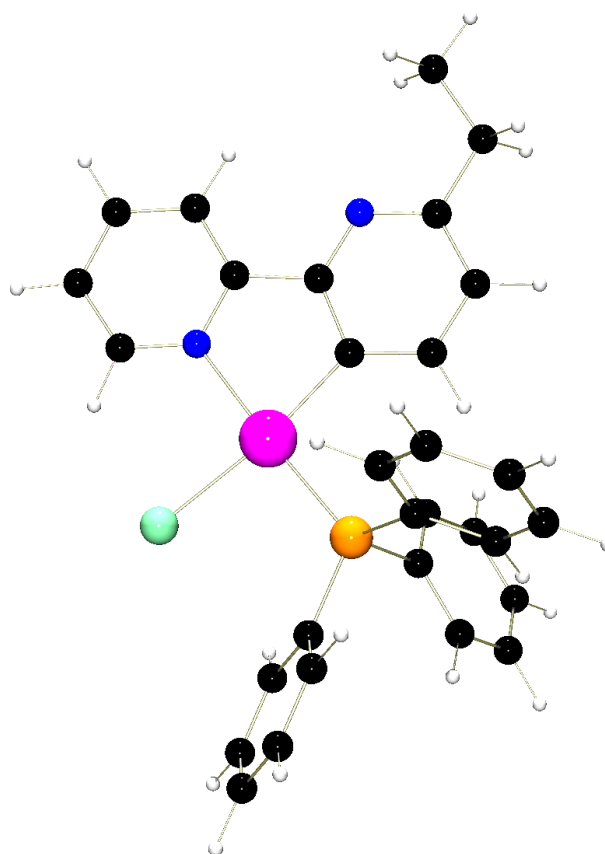
Figure S19: Optimized geometry of **7b**

Table 20: Coordinates for the equilibrium geometry for **10b**

Pt	-2.705676	0.522375	0.589456
N	-3.506413	2.445664	0.905871
C	-4.636795	2.702001	1.565967
C	-5.102084	4.002565	1.747849
C	-4.364885	5.060276	1.226961
C	-3.185771	4.786412	0.537694
C	-2.777896	3.461085	0.389877
C	-1.582142	2.994741	-0.307257
C	-1.331632	1.609461	-0.356925
C	-0.166540	1.261321	-1.081855
C	0.658637	2.207022	-1.676060
C	0.361569	3.565826	-1.578700
N	-0.749474	3.887470	-0.898168
C	1.199625	4.652929	-2.186098
C	0.713049	6.076639	-1.962583
Cl	-4.467163	-0.466596	1.752951
P	-1.748037	-1.508699	0.238147
C	-1.846035	-2.050040	-1.507255
C	-2.242475	-1.150214	-2.504674
C	-2.314393	-1.561800	-3.835415
C	-1.995492	-2.874518	-4.178613
C	-1.617763	-3.782309	-3.187690
C	-1.550037	-3.377479	-1.856606
C	-2.402655	-2.944710	1.160328
C	-3.645387	-3.476879	0.787339
C	-4.161264	-4.577373	1.463155
C	-3.449582	-5.149522	2.519488
C	-2.218331	-4.619416	2.896602
C	-1.691710	-3.519140	2.219155
C	0.028633	-1.463591	0.696192
C	1.015025	-2.167938	-0.005339
C	2.342244	-2.127374	0.422988
C	2.692225	-1.395471	1.557163
C	1.713569	-0.692382	2.260640
C	0.388679	-0.718812	1.829122
H	-5.160156	1.824139	1.948121
H	-6.029200	4.169177	2.290723
H	-4.700263	6.088225	1.352808
H	-2.605509	5.610978	0.126544
H	0.112357	0.214303	-1.182686
H	1.547955	1.900738	-2.223485
H	1.276886	4.447551	-3.263504
H	2.220861	4.539720	-1.795376
H	-0.276683	6.254625	-2.404995
H	1.395736	6.783563	-2.443729
H	0.686794	6.346008	-0.897809
H	-2.522995	-0.134788	-2.227582
H	-2.634849	-0.858993	-4.602674
H	-2.057517	-3.197508	-5.216801
H	-1.387334	-4.813512	-3.450354
H	-1.289617	-4.101880	-1.085435
H	-4.212298	-3.029232	-0.026967
H	-5.126203	-4.985860	1.169043
H	-3.857120	-6.010253	3.047205
H	-1.659103	-5.062872	3.718686
H	-0.723948	-3.120483	2.515948
H	0.755997	-2.744255	-0.891888
H	3.103315	-2.675669	-0.129872
H	3.727763	-1.373708	1.893801
H	1.981641	-0.122404	3.148908
H	-0.375142	-0.159430	2.370498
H	-0.972183	4.875720	-0.828934

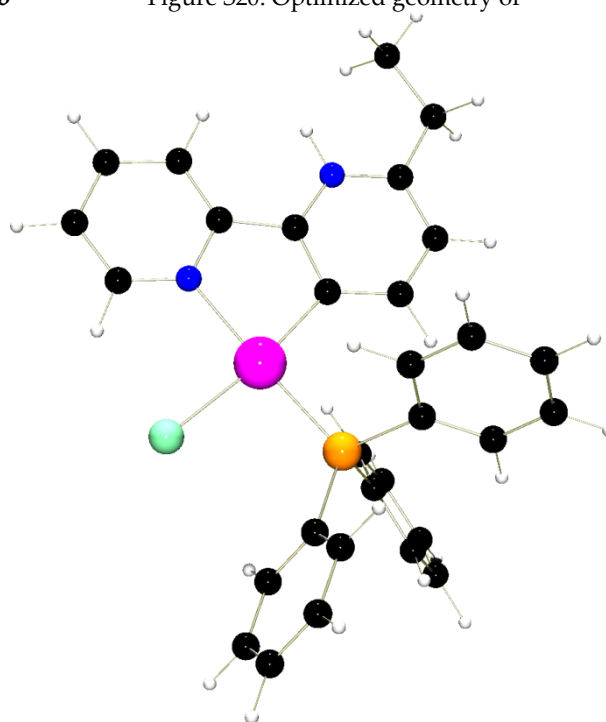
Figure S20: Optimized geometry of

Table S21: Coordinates for the equilibrium geometry for **1e**

Pt	-0.611890	0.445769	0.148517
N	-1.792790	2.222207	0.025186
C	-3.129313	2.308034	0.049028
C	-3.791850	3.528471	-0.031814
C	-3.042718	4.699230	-0.142105
C	-1.657404	4.607537	-0.167793
C	-1.059102	3.350587	-0.081741
C	0.396532	3.154197	-0.099862
C	0.853863	1.820840	-0.000474
C	2.246182	1.672023	-0.023808
C	3.069455	2.790874	-0.136899
C	2.483187	4.055309	-0.225797
N	1.170067	4.235433	-0.208128
C	0.779374	-1.058520	0.252247
S	-2.302576	-1.086872	0.300560
O	-3.739708	-0.655013	0.278330
C	-2.156831	-2.339413	-0.988046
C	-2.134245	-2.111950	1.774349
H	-3.668105	1.362912	0.135043
H	-4.879376	3.547358	-0.007579
H	-3.533877	5.669436	-0.207600
H	-1.002001	5.471323	-0.252100
H	2.697999	0.683783	0.046390
H	4.154149	2.688242	-0.156514
H	3.102987	4.950358	-0.314857
H	1.456550	-0.877768	1.099124
H	1.387674	-1.064702	-0.664164
H	0.394994	-2.081417	0.376600
H	-2.323127	-1.812409	-1.931646
H	-2.946917	-3.078840	-0.823305
H	-1.160320	-2.788790	-0.977717
H	-2.274521	-1.435480	2.621839
H	-1.142551	-2.569768	1.816263
H	-2.934622	-2.858292	1.749226

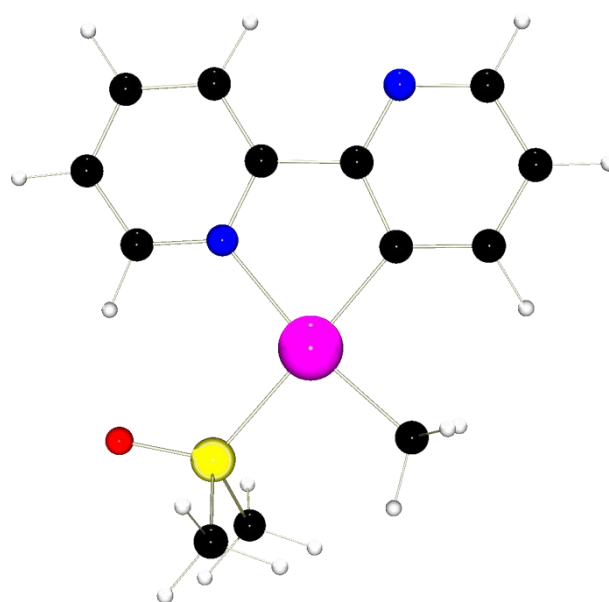
Figure S21: Optimized geometry of **1e**

Table S22: Coordinates for the equilibrium geometry for **3e**

Pt	-0.596373	0.448058	0.148686
N	-1.791865	2.232982	0.025303
C	-3.125783	2.299284	0.050843
C	-3.810256	3.512548	-0.030270
C	-3.086919	4.692786	-0.142401
C	-1.695826	4.621512	-0.169937
C	-1.076097	3.376663	-0.083949
C	0.371664	3.151117	-0.099212
C	0.848161	1.830618	-0.000122
C	2.245979	1.686594	-0.022126
C	3.104033	2.783466	-0.133529
C	2.565428	4.052224	-0.225710
N	1.228858	4.190468	-0.205780
C	0.790273	-1.050990	0.249627
S	-2.291204	-1.101570	0.304219
O	-3.701123	-0.599006	0.282915
C	-2.170422	-2.335055	-0.997148
C	-2.137375	-2.115695	1.779956
H	-3.649066	1.343296	0.138532
H	-4.897846	3.513387	-0.004420
H	-3.590542	5.655535	-0.208099
H	-1.120275	5.542320	-0.258416
H	2.681894	0.691725	0.050196
H	4.184636	2.658571	-0.149111
H	3.155508	4.960399	-0.314692
H	1.459568	-0.878263	1.104493
H	1.398002	-1.054899	-0.667079
H	0.398707	-2.069083	0.365624
H	-2.319061	-1.798180	-1.938268
H	-2.982225	-3.052601	-0.840798
H	-1.189725	-2.818100	-0.984898
H	-2.251780	-1.435972	2.628867
H	-1.162662	-2.609405	1.814697
H	-2.960823	-2.836923	1.761486
H	0.850736	5.129201	-0.275269

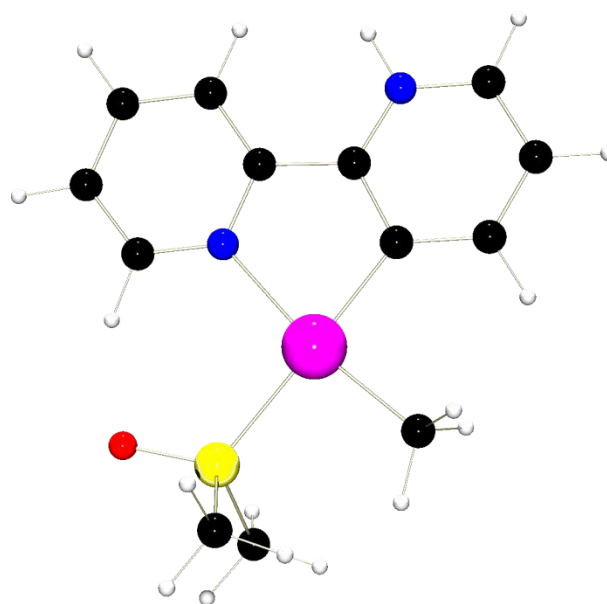
Figure S22: Optimized geometry of **3e**

Table S24: Coordinates for the equilibrium geometry for **5e**

Pt	-0.643178	-0.282601	-0.059131
N	-1.716620	1.490035	-0.052342
C	-3.049605	1.559068	-0.072910
C	-3.718983	2.780862	-0.067421
C	-2.977592	3.956231	-0.039571
C	-1.586276	3.876831	-0.018097
C	-0.977617	2.624972	-0.025207
C	0.457673	2.352404	-0.005772
C	0.872569	1.006765	-0.016728
C	2.265507	0.796386	0.003732
C	3.165578	1.862272	0.032215
C	2.686952	3.160348	0.040879
N	1.359182	3.359038	0.021815
S	0.550106	-2.181838	-0.066513
C	0.034561	-3.205736	1.311170
C	0.075886	-3.169536	-1.484851
O	2.036710	-2.108902	-0.043800
Cl	-2.582363	-1.617944	-0.109200
H	-3.571100	0.602083	-0.094187
H	-4.806496	2.794536	-0.085069
H	-3.471551	4.926274	-0.034487
H	-0.999442	4.794161	0.004007
H	2.632437	-0.232995	-0.003576
H	4.239656	1.689435	0.047784
H	3.318941	4.044214	0.062449
H	-1.049134	-3.347335	1.264535
H	0.319111	-2.668395	2.220135
H	0.591842	-4.144324	1.233916
H	-1.008470	-3.312877	-1.472810
H	0.632069	-4.109408	-1.415958
H	0.385664	-2.608390	-2.370833
H	1.024034	4.316477	0.028737

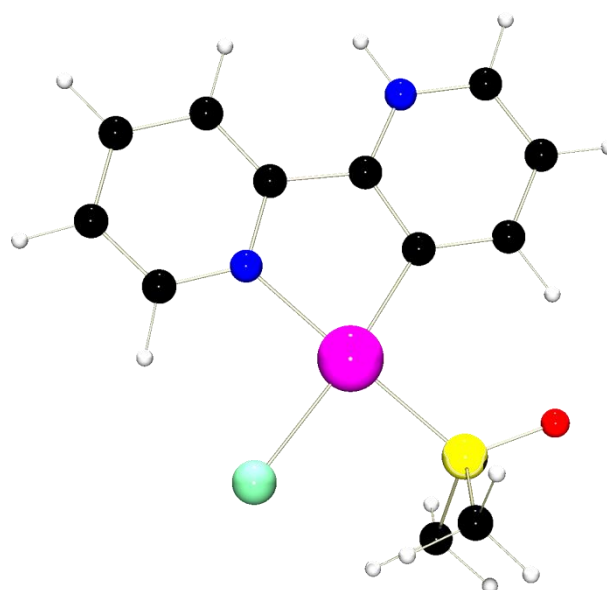
Figure S24: Optimized geometry of **5e**

Table S25: Coordinates for the equilibrium geometry for **6e**

Pt	-0.599778	-0.297491	0.181081
N	-0.891730	0.808832	2.003627
C	-1.702438	0.511324	3.025265
C	-1.813804	1.307941	4.159136
C	-1.049393	2.471840	4.238472
C	-0.214452	2.791431	3.177391
C	-0.158747	1.942140	2.069633
C	0.678594	2.227140	0.898171
C	0.616688	1.294656	-0.160854
C	1.411232	1.620192	-1.269013
C	2.184081	2.779419	-1.267520
C	2.154072	3.611083	-0.144947
N	1.413021	3.342290	0.919982
C	-0.126208	-1.037725	-1.678296
P	-1.924106	-2.191260	0.418881
C	-3.078961	-2.346974	-1.010238
C	-3.585137	-1.153155	-1.543203
C	-4.495392	-1.179243	-2.598434
C	-4.895272	-2.397844	-3.145742
C	-4.379551	-3.588161	-2.634855
C	-3.477874	-3.565040	-1.571148
C	-0.981316	-3.771447	0.486584
C	0.396869	-3.749320	0.240681
C	1.142832	-4.927339	0.290508
C	0.521828	-6.138009	0.591301
C	-0.848516	-6.168007	0.855269
C	-1.594900	-4.992569	0.808612
C	-3.067790	-2.403874	1.855867
C	-2.571329	-2.893319	3.074521
C	-3.393227	-2.964093	4.197862
C	-4.721583	-2.542129	4.123742
C	-5.222501	-2.052690	2.918248
C	-4.402791	-1.984886	1.790937
H	-2.283505	-0.400426	2.933301
H	-2.490314	1.009929	4.957109
H	-1.109069	3.119504	5.112422
H	0.407411	3.683537	3.153233
H	1.429885	0.970202	-2.143613
H	2.803495	3.041314	-2.124949
H	2.749372	4.526473	-0.114523
H	0.964320	-1.145154	-1.770558
H	-0.452516	-0.308206	-2.434093
H	-0.572145	-2.001536	-1.957044
H	-3.236074	-0.201528	-1.139314
H	-4.879189	-0.244127	-3.003381
H	-5.597003	-2.419607	-3.978732
H	-4.674702	-4.542134	-3.069425
H	-3.072098	-4.502130	-1.196203
H	0.879231	-2.798055	0.020604
H	2.214038	-4.894266	0.097116
H	1.105129	-7.057224	0.631505
H	-1.336830	-7.108636	1.106956
H	-2.657222	-5.023678	1.048948
H	-1.534919	-3.221781	3.145743
H	-2.993601	-3.351946	5.134000
H	-5.364062	-2.599781	5.001456
H	-6.258801	-1.725207	2.849508
H	-4.808364	-1.607882	0.853292

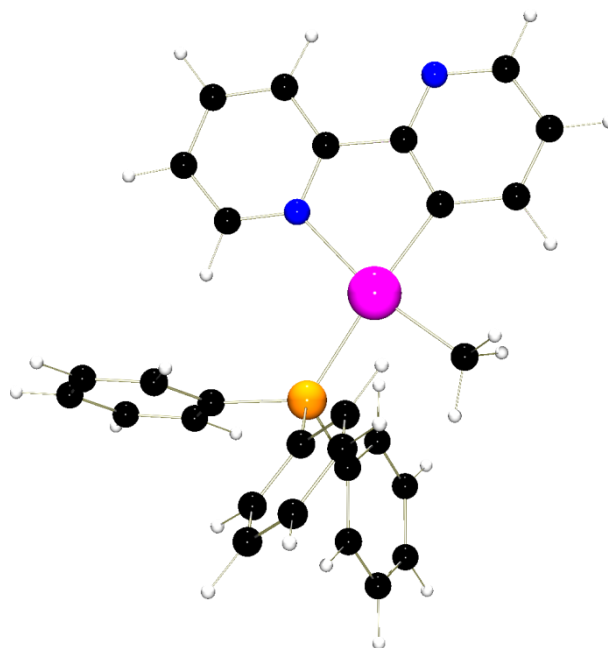
Figure S25: Optimized geometry of **6e**

Table S26: Coordinates for the equilibrium geometry for **9e**

Pt	-0.614372	-0.296139	0.171440
N	-0.913677	0.810486	2.008388
C	-1.737022	0.499243	3.011460
C	-1.867760	1.282175	4.157388
C	-1.112582	2.442916	4.267934
C	-0.260255	2.779194	3.220080
C	-0.183031	1.947312	2.102560
C	0.647863	2.204535	0.923507
C	0.588624	1.295420	-0.148290
C	1.383037	1.630045	-1.261373
C	2.181086	2.775096	-1.292953
C	2.198668	3.613848	-0.194208
N	1.436219	3.302538	0.867207
C	-0.142614	-1.032727	-1.680579
P	-1.937782	-2.216589	0.400613
C	-3.081120	-2.352900	-1.029194
C	-3.635011	-1.163305	-1.524330
C	-4.541005	-1.193985	-2.582406
C	-4.888358	-2.411367	-3.167869
C	-4.325303	-3.595075	-2.693555
C	-3.426524	-3.569642	-1.627517
C	-0.973956	-3.772615	0.482806
C	0.407642	-3.750013	0.256128
C	1.151254	-4.928571	0.317460
C	0.523281	-6.137906	0.608663
C	-0.850988	-6.167434	0.852058
C	-1.596229	-4.992397	0.795625
C	-3.055502	-2.380362	1.856741
C	-2.548425	-2.874184	3.069721
C	-3.357170	-2.923280	4.204190
C	-4.678899	-2.477866	4.143729
C	-5.189557	-1.988169	2.942028
C	-4.384548	-1.940270	1.802957
H	-2.313392	-0.414030	2.899325
H	-2.555375	0.971350	4.940594
H	-1.185515	3.080115	5.147375
H	0.327350	3.693250	3.291793
H	1.378414	0.975685	-2.132576
H	2.789288	3.019417	-2.161110
H	2.792459	4.521517	-0.128168
H	0.948642	-1.131106	-1.775907
H	-0.490111	-0.310796	-2.434619
H	-0.579477	-2.001107	-1.948468
H	-3.335743	-0.208299	-1.090207
H	-4.965827	-0.264853	-2.958583
H	-5.588468	-2.436314	-4.001688
H	-4.581602	-4.545860	-3.157834
H	-2.984073	-4.500734	-1.280686
H	0.899492	-2.803552	0.039416
H	2.224952	-4.899029	0.139022
H	1.104375	-7.057775	0.656023
H	-1.343447	-7.108016	1.094042
H	-2.662637	-5.024779	1.016997
H	-1.520526	-3.230913	3.126718
H	-2.955958	-3.320744	5.135408
H	-5.312426	-2.525317	5.028350
H	-6.223399	-1.651843	2.884165
H	-4.800080	-1.570984	0.866669
H	1.461238	3.929953	1.663800

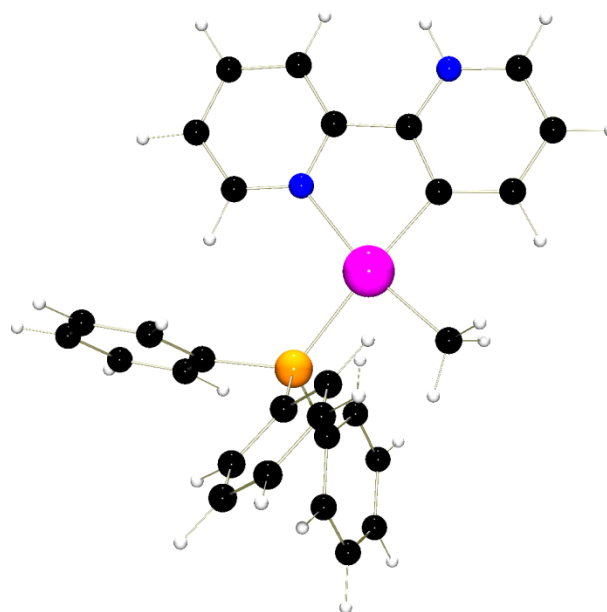
Figure S26: Optimized geometry of **9e**

Table S27: Coordinates for the equilibrium geometry for **7e**

Pt	-1.843521	0.219475	0.074218
N	-2.308659	2.255697	-0.104360
C	-3.435820	2.751172	-0.627622
C	-3.666113	4.119423	-0.700480
C	-2.693937	4.994762	-0.213725
C	-1.526510	4.473662	0.328058
C	-1.360301	3.089090	0.369492
C	-0.173603	2.423682	0.911319
C	-0.173934	1.004555	0.869010
C	0.994259	0.420273	1.386602
C	2.024112	1.211651	1.890344
C	1.882797	2.600558	1.875475
N	0.802158	3.194884	1.391755
Cl	-3.915408	-0.389094	-0.897710
P	-1.261727	-1.941433	0.335110
C	0.100896	-2.489195	-0.768318
C	0.885521	-1.535589	-1.427335
C	1.927069	-1.937773	-2.263547
C	2.190350	-3.293362	-2.452304
C	1.401030	-4.250457	-1.813116
C	0.357017	-3.852582	-0.980725
C	-0.722365	-2.311541	2.053367
C	-1.348853	-1.604819	3.088696
C	-1.023112	-1.868511	4.417917
C	-0.058816	-2.828605	4.724098
C	0.576597	-3.526442	3.697456
C	0.244470	-3.273924	2.366489
C	-2.537800	-3.225904	0.027371
C	-2.968000	-3.448021	-1.288539
C	-3.926434	-4.419916	-1.555955
C	-4.476611	-5.170001	-0.514775
C	-4.061288	-4.945288	0.795119
C	-3.092437	-3.977316	1.067143
H	-4.148266	2.007291	-0.984613
H	-4.595496	4.483272	-1.132523
H	-2.847834	6.072480	-0.257918
H	-0.723587	5.089578	0.726114
H	1.117294	-0.661399	1.408960
H	2.928551	0.756367	2.292465
H	2.671462	3.247048	2.265984
H	0.664283	-0.477784	-1.290442
H	2.528071	-1.186669	-2.773704
H	3.002824	-3.606440	-3.107226
H	1.590877	-5.311300	-1.971932
H	-0.276809	-4.605732	-0.513250
H	-2.080154	-0.834479	2.840786
H	-1.515840	-1.313054	5.214138
H	0.203514	-3.027462	5.762421
H	1.337454	-4.270227	3.931662
H	0.754187	-3.819287	1.574257
H	-2.560077	-2.852539	-2.103027
H	-4.255184	-4.583533	-2.581111
H	-5.231498	-5.926375	-0.727155
H	-4.487987	-5.523896	1.612920
H	-2.769749	-3.813722	2.093656

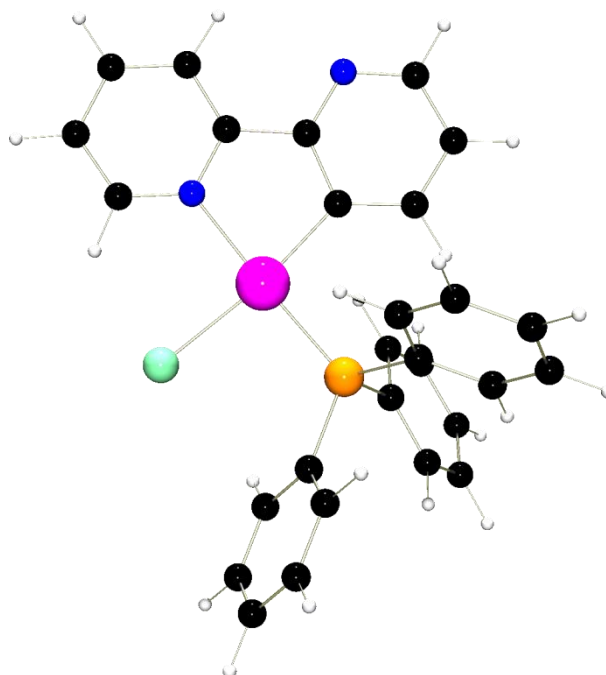
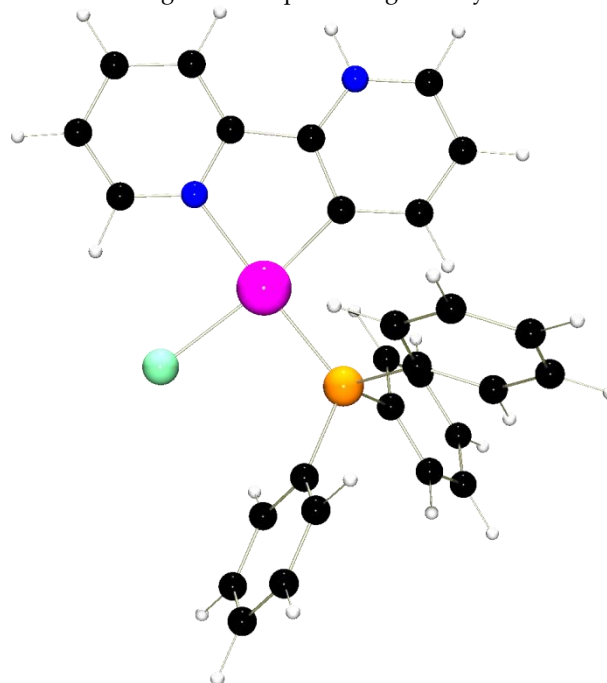
Figure S27: Optimized geometry of **7e**

Table S28: Coordinates for the equilibrium geometry for **10e**

Pt	-1.829941	0.213954	0.068043
N	-2.299773	2.262552	-0.086359
C	-3.425046	2.747860	-0.612643
C	-3.676877	4.117208	-0.670896
C	-2.728011	4.998974	-0.165699
C	-1.554314	4.485699	0.382217
C	-1.365683	3.104763	0.408642
C	-0.198980	2.399434	0.935768
C	-0.180449	0.985232	0.869046
C	0.999008	0.393375	1.373834
C	2.047156	1.141839	1.908353
C	1.945137	2.520317	1.951609
N	0.833419	3.093220	1.464300
Cl	-3.863567	-0.384542	-0.896577
P	-1.265942	-1.975229	0.317994
C	0.099726	-2.491271	-0.784351
C	0.836846	-1.536542	-1.495513
C	1.881550	-1.933267	-2.330161
C	2.194495	-3.284945	-2.463135
C	1.450917	-4.243914	-1.773381
C	0.402627	-3.853040	-0.943867
C	-0.726766	-2.291798	2.043162
C	-1.420677	-1.634953	3.070605
C	-1.091547	-1.871970	4.404039
C	-0.058400	-2.753983	4.722825
C	0.641745	-3.401343	3.705445
C	0.308042	-3.177212	2.369399
C	-2.552044	-3.236641	0.013376
C	-2.935871	-3.501943	-1.309144
C	-3.906107	-4.463177	-1.571111
C	-4.506756	-5.158978	-0.520237
C	-4.131658	-4.893409	0.794503
C	-3.154345	-3.934686	1.064665
H	-4.124474	1.997767	-0.985459
H	-4.607267	4.472927	-1.107349
H	-2.894411	6.074537	-0.195703
H	-0.808088	5.173258	0.776791
H	1.108162	-0.689333	1.359478
H	2.942736	0.659435	2.293368
H	2.709492	3.179701	2.353733
H	0.568324	-0.483669	-1.414332
H	2.442667	-1.185412	-2.888083
H	3.008165	-3.594992	-3.117424
H	1.679254	-5.302047	-1.892209
H	-0.196292	-4.610733	-0.439160
H	-2.219924	-0.935802	2.820547
H	-1.642886	-1.366046	5.194763
H	0.200988	-2.936889	5.764584
H	1.450197	-4.088826	3.950664
H	0.864603	-3.688779	1.586066
H	-2.482263	-2.955113	-2.133937
H	-4.200351	-4.665097	-2.599605
H	-5.268319	-5.909035	-0.729315
H	-4.595894	-5.434729	1.616820
H	-2.862008	-3.742489	2.095136
H	0.771124	4.105253	1.497496

Figure S28: Optimized geometry of

References

1. ORTEP-3 for Windows version 2020.1; L.J. Farrugia, *J. Appl. Chem.*, **2012**, *45*, 849-854.
2. <http://www.povray.org>