Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Phosphorescent Pt(II) complexes bearing a monoanionic C^N^N luminophore and tunable ancillary ligands

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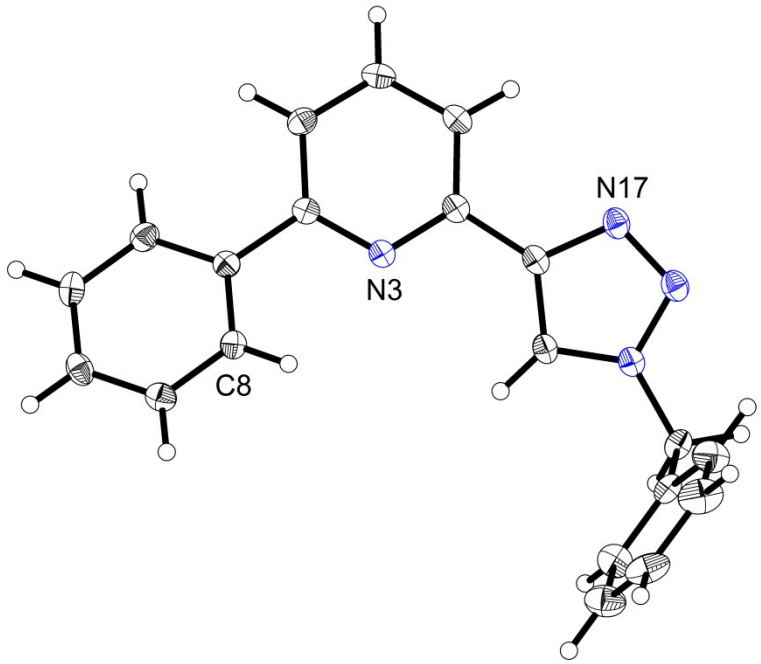


Figure S1. Solid-state structure of **LH**. Displacement ellipsoids are drawn at the 50% probability level.

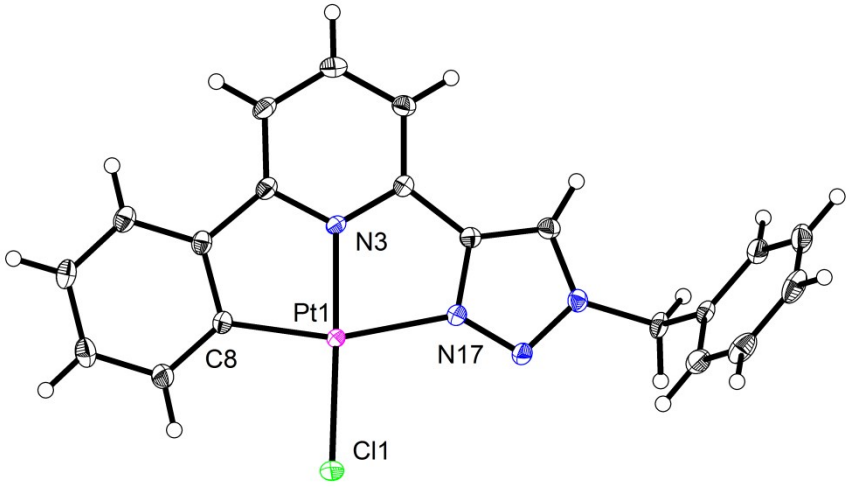


Figure S2. Molecular structure of **[LPtCl]**. Displacement ellipsoids are drawn at the 50% probability level.

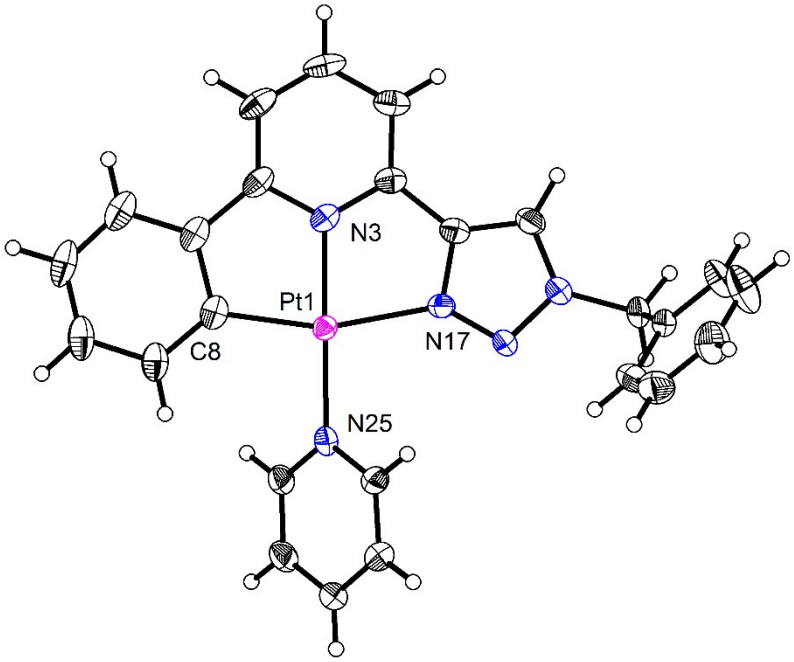


Figure S3. Molecular structure of the cation of **[LPtPy]ClO$_4$**. Displacement ellipsoids are drawn at the 50% probability level and counterion submitted for clarity.

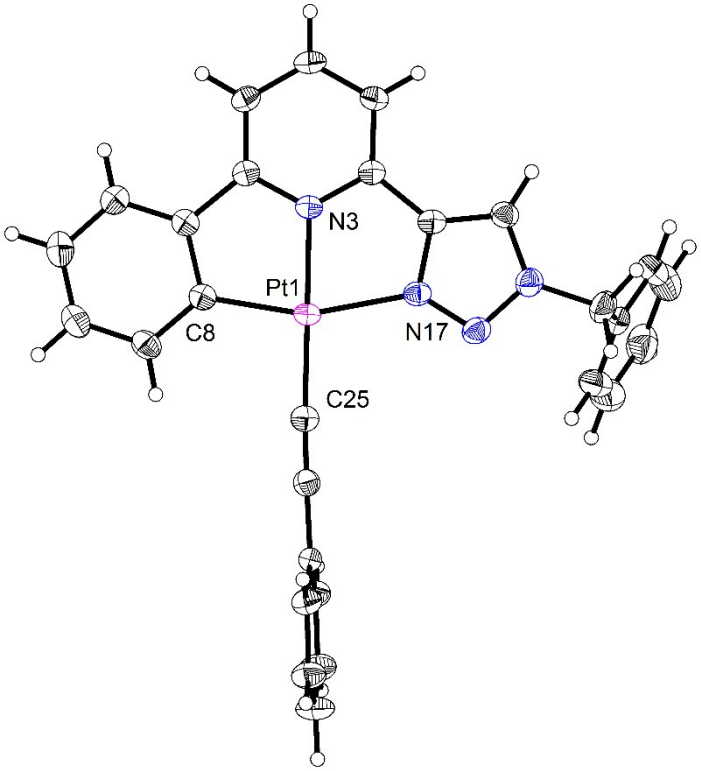


Figure S4. Molecular structure of **[LPt(CCPh)]**. Displacement ellipsoids are drawn at the 50% probability level.

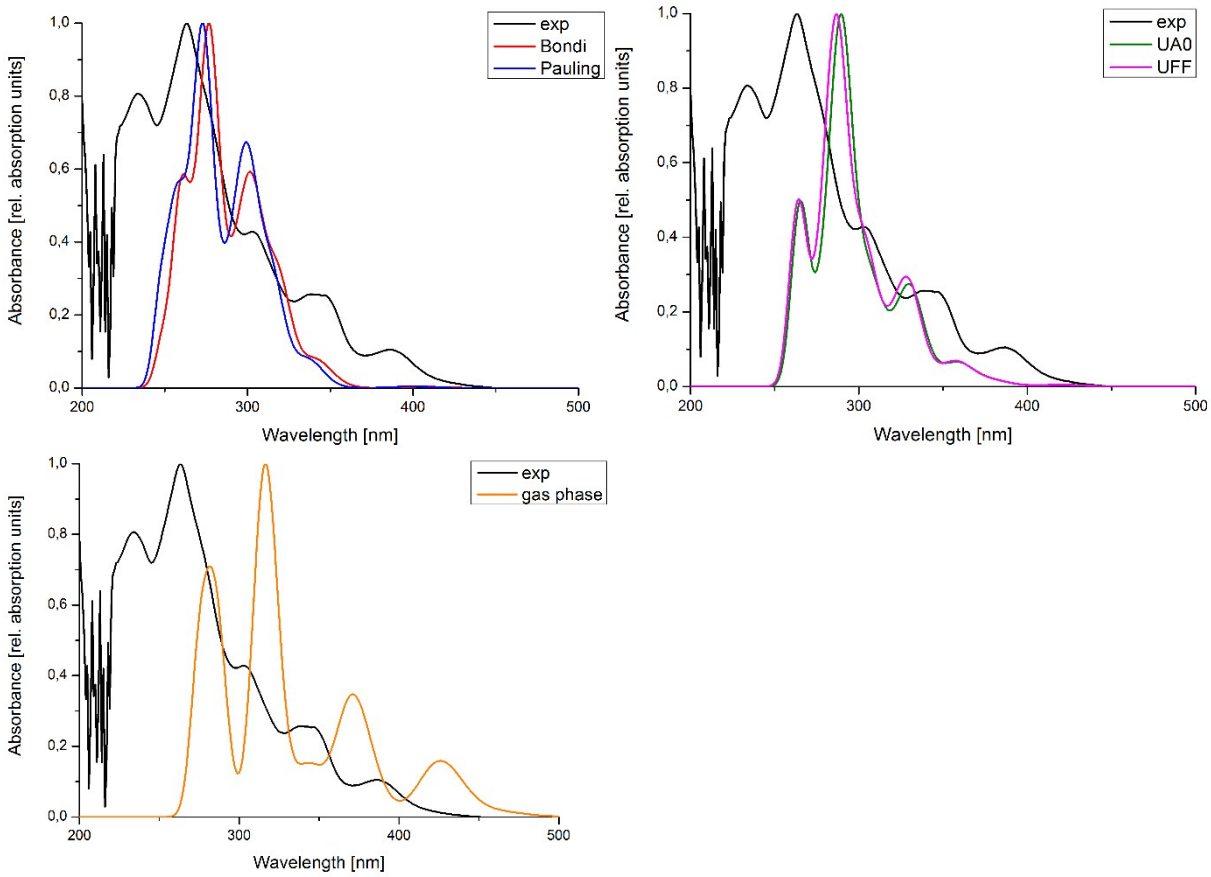


Figure S5. Experimental and computed absorption spectra of **[LPtCl]**. Solvent models as indicated; solvent: methanol; temperature: 298.15 K.

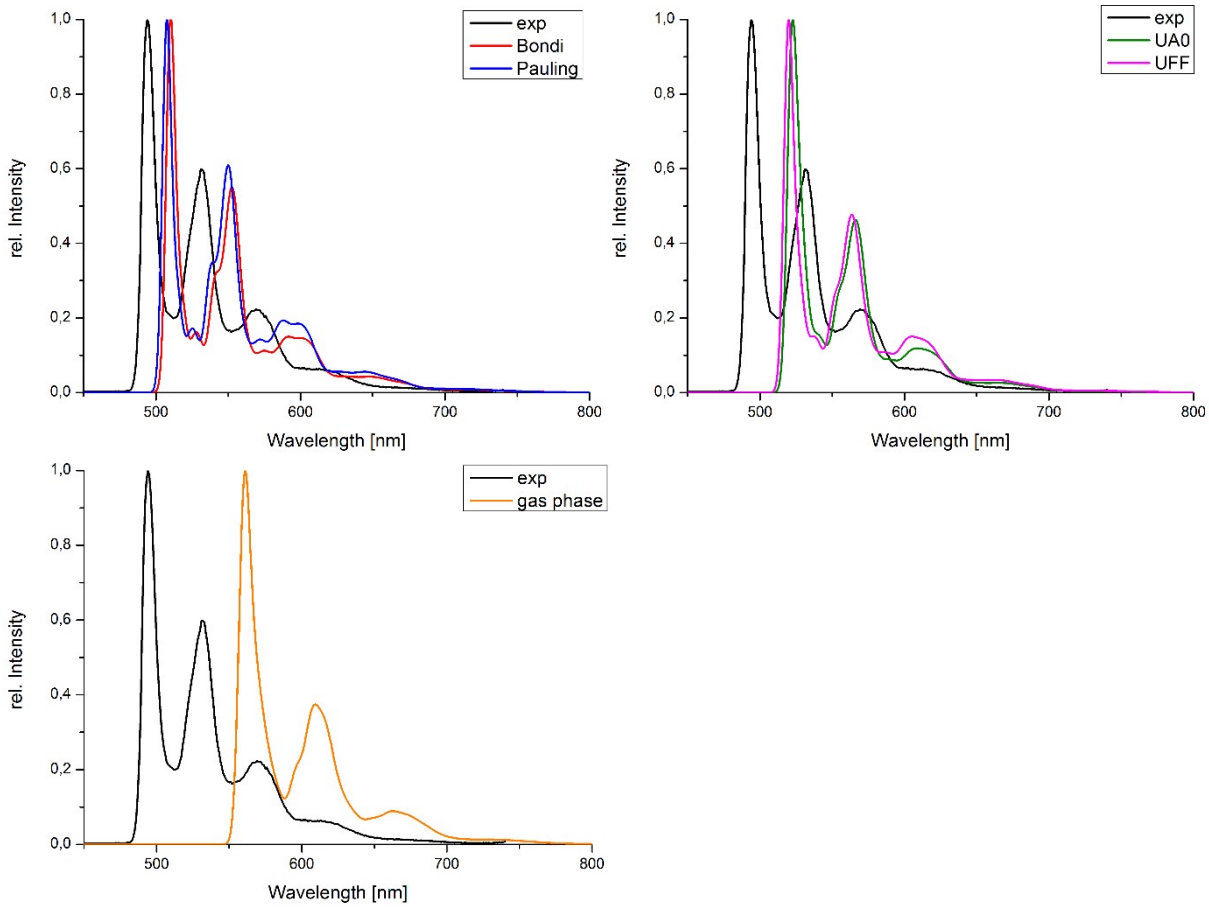


Figure S6. Experimental and computed emission spectra of **[LPtCl]**. Solvent models as indicated; solvent: methanol; temperature: 77 K.

Table S1. Calculated and experimental absorption parameters of **[LPtCl]**: [a]Wavelength computed by DFT calculations; [b]oscillator strength; [c]molecular orbitals with main contribution to excitation and percentage to mixture; [d]local maximum in experimental absorption spectra.

Entry	λ [nm][a]	f[b]	Excitation (contribution)[c]	Nature	λ_{max} [nm][d]
1	256	0.129	HOMO-1 → LUMO+2 (60%)	MLCT/LLCT	234
2	275	0.287	HOMO → LUMO+2 (68%)	MLCT/LLCT	263
3	300	0.237	HOMO-3 → LUMO (56%)	MC/LMCT/IL	303
4	315	0.119	HOMO → LUMO+1 (57%)	MLCT/LLCT	
5	336	0.024	HOMO-1 → LUMO (79%)	MC/LMCT/IL/LLCT	347
6	341	0.008	HOMO-2 → LUMO (95%)	MLCT/LLCT	
7	399	0.002	HOMO → LUMO (98%)	MC/LMCT/IL	387

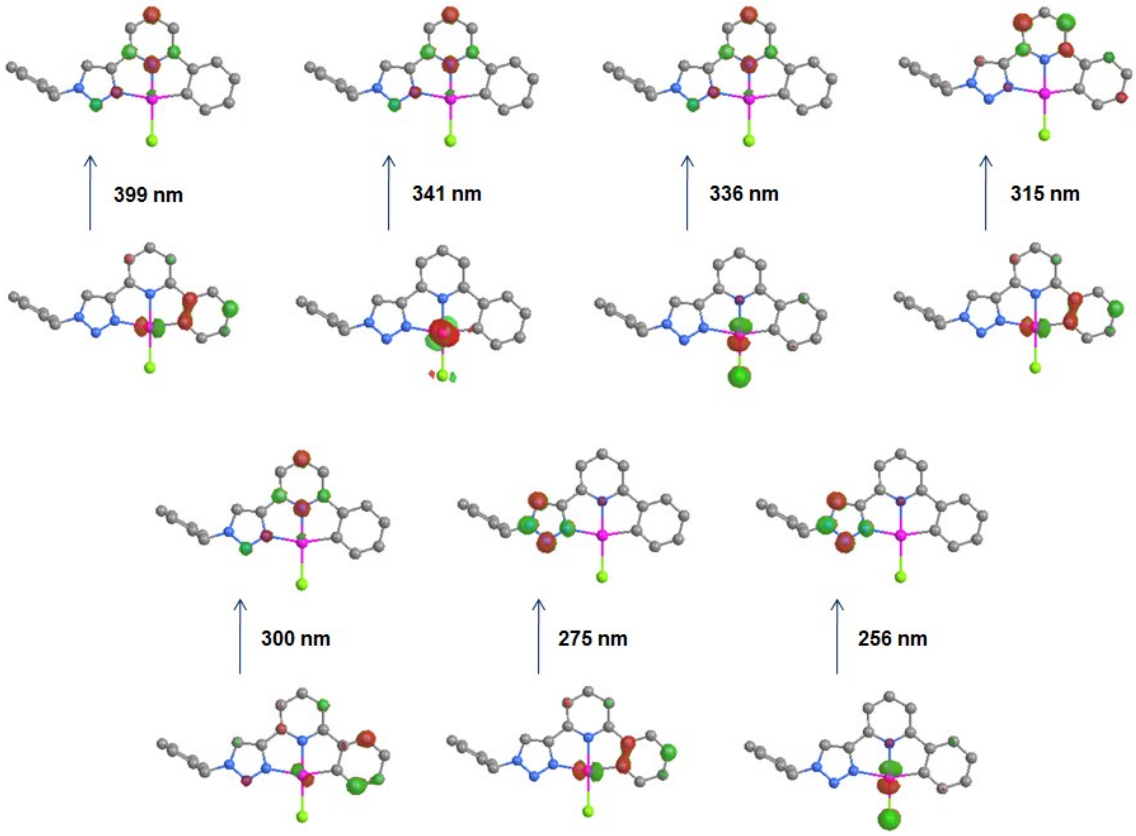


Figure S7. Computed molecular orbitals of the transitions during the absorption process at the denoted wavelength (for **[LPtCl]**); isodensity surface plot value: 0.07.

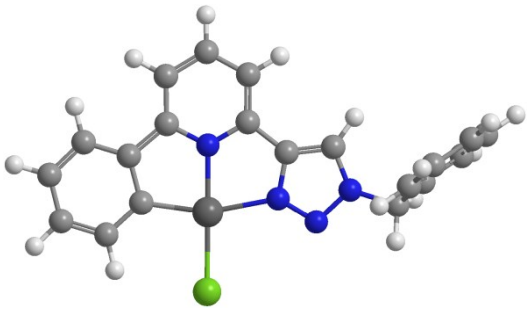
Table S2. Computed bond lengths (Å) and angles (°) for S_0 and T_1 in the gas phase and with solvent model for complex **[LPtCl]**; [a] solvent model: Pauling, solvent: methanol.

	S_0 (gas phase)	T_1 (gas phase)	S_0 (PCM)[a]	T_1 (PCM)[a]
Pt-X	2.358	2.343	2.406	2.419
Pt-$N_{triazole}$	2.117	2.121	2.108	2.100
Pt-$N_{pyridine}$	1.978	1.928	1.976	1.956
Pt-C_{phenyl}	1.987	1.997	2.000	1.960
$N_{pyridine}$-Pt-X	179.6	179.5	179.4	178.7
C-Pt-X	97.7	97.2	98.7	98.4

Table S3. Computed 0-0 transition energies for complex **[LPtCl]** in the gas phase and with solvent model and corresponding transition modes. [a]Solvent model: Pauling; solvent: methanol. [b]Experimental emission wavelength.

ΔE (0-0, gas phase)		ΔE (0-0, PCM)[a]		λ_{max} [eV, nm][b]
Calculated (eV, nm)	Nature	Calculated (eV, nm)	Nature	
2.32, 534	ILCT / LMCT	2.56, 484	ILCT / LMCT	2.50, 500

Compound: **[LPtCl]**; **conditions**: gas phase, singlet



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C	2.43521	0.000347	-0.00165
C	1.214216	-0.695476	-0.000786
C	-1.134535	2.326248	-0.001022
C	-0.792235	3.720417	-0.002887
C	-1.845978	4.650631	-0.003237
C	-3.182022	4.222072	-0.002238
C	-3.502966	2.851149	-0.00105
C	-2.477078	1.902765	-0.000383
Pt	1.169858	4.034409	-0.003299
Cl	1.11097	6.39147	-0.016376
C	3.534294	2.309239	-0.003898
N	3.255735	3.675804	-0.001735
N	4.376668	4.382645	-0.009706
N	5.391935	3.459365	-0.016176
C	4.913654	2.17892	-0.014863
C	6.784015	3.928369	-0.009392
C	7.614756	3.283206	-1.096546

C	8.753912	2.532144	-0.767026
C	9.537479	1.950301	-1.775941
C	9.181295	2.114437	-3.121573
C	8.041594	2.864699	-3.4562
C	7.263872	3.4481	-2.449223
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H	3.381797	-0.528035	-0.003088
H	1.213473	-1.78077	-0.001047
H	-1.60802	5.709657	-0.004486
H	-3.980442	4.960288	-0.002422
H	-4.541493	2.533039	-0.000302
H	-2.724913	0.843516	0.000904
H	5.559445	1.317938	-0.039869
H	7.217924	3.731574	0.97677
H	6.718113	5.01292	-0.138365
H	9.035501	2.405412	0.276187
H	10.419679	1.374622	-1.512017
H	9.786391	1.665818	-3.903915
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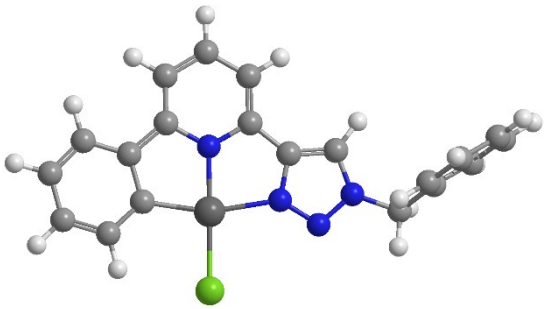
Compound: **[LPtCl]**; **conditions**: gas phase, triplet



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H	7.300177	3.667687	0.966019
H	6.787239	4.984302	-0.101858
H	9.173373	2.464559	0.203322
H	10.55366	1.509997	-1.629216
H	9.844412	1.790017	-4.001291
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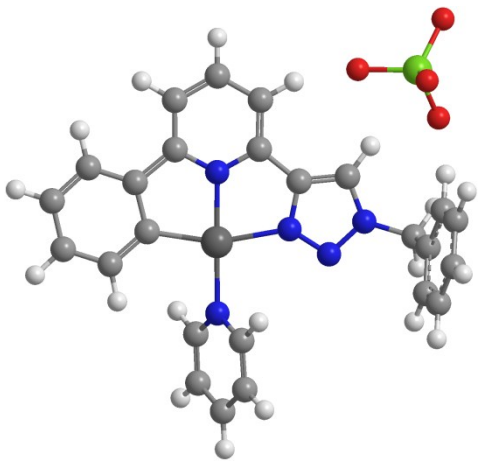
Compound: **[LPtPy]ClO_4**; **conditions**: gas phase, singlet



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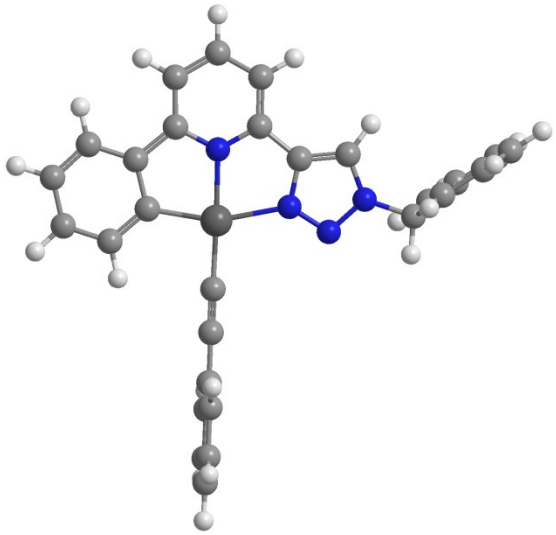
Compound: **[LPt(CCPh)]**; **conditions**: gas phase, singlet



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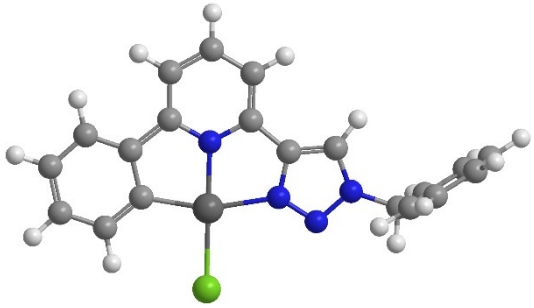
Compound: **[LPtCl]**; **conditions**: PCM (Methanol, Bondi), singlet



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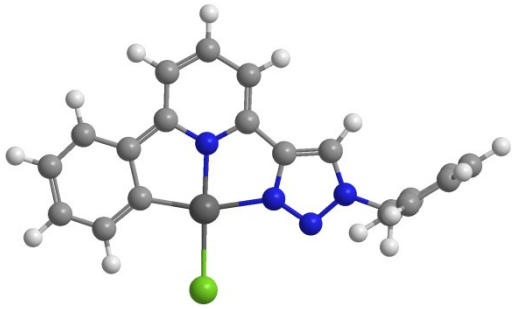
Compound: **[LPtCl]**; **conditions**: PCM (Methanol, Bondi), triplet



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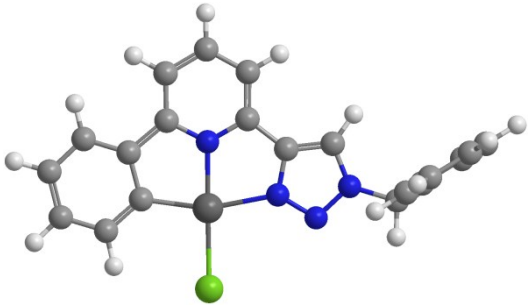
C	-1.742685	3.721627	-5.60628
C	-2.064912	7.936844	-5.562776
C	-2.194127	8.891015	-6.621275
C	-2.2792	10.235344	-6.323495
C	-2.240905	10.706905	-4.957003
C	-2.116194	9.804606	-3.90474

C	-2.022862	8.410238	-4.13627
Pt	-1.84069	6.923432	-2.874939
Cl	-1.821956	8.202837	-0.824341
H	-0.943956	-0.539058	-0.00257
H	1.234228	3.183968	0.00349
H	3.378715	1.93025	-0.003405
H	3.371246	-0.564142	-0.00033
H	1.202644	-1.796196	0.004387
H	-1.390652	2.782115	0.927218
H	-2.157638	1.472094	0.012359
H	-1.434206	1.784955	-2.809656
H	-2.066304	6.265477	-7.888248
H	-1.86854	3.792499	-7.78124
H	-1.655505	2.642625	-5.5488
H	-2.225199	8.558043	-7.654106
H	-2.377291	10.961669	-7.1253
H	-2.310562	11.772893	-4.763091
H	-2.088683	10.171031	-2.882781

Compound: **[LPtCl]**; **conditions**: PCM (Methanol, Pauling), singlet

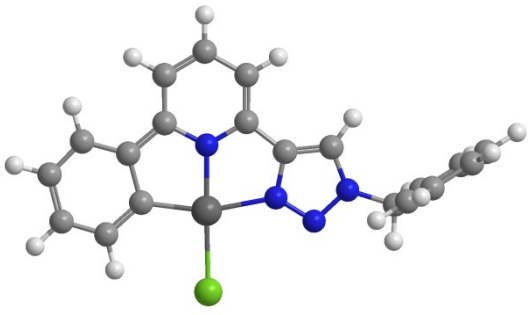


xyz coordinates

C	0	0	0
C	0	1.404847	0
C	1.227334	2.094638	0
C	2.43733	1.386855	-0.00272
C	2.433227	-0.019548	0.000843
C	1.211955	-0.711346	0.004267
C	-1.310397	2.160061	0.034504
N	-1.431881	3.129383	-1.06372
C	-1.400855	2.894528	-2.405598
C	-1.576124	4.136802	-2.994058
N	-1.703169	5.057435	-1.964073
N	-1.615528	4.453011	-0.783719

C	-1.648023	4.647571	-4.354189
N	-1.826293	5.998557	-4.398478
C	-1.916712	6.697756	-5.567724
C	-1.821317	5.995819	-6.77938
C	-1.638792	4.606436	-6.757155
C	-1.550441	3.914633	-5.537375
C	-2.108867	8.137169	-5.349538
C	-2.234114	9.067476	-6.395191
C	-2.416648	10.426807	-6.102813
C	-2.472845	10.848045	-4.763029
C	-2.347806	9.918113	-3.713503
C	-2.163976	8.548061	-3.973911
Pt	-1.960357	7.013168	-2.707751
Cl	-2.116052	8.227611	-0.637022
H	-0.944114	-0.538769	-0.002593
H	1.237525	3.181883	0.002717
H	3.379504	1.927119	-0.003595
H	3.371013	-0.567354	0.000973
H	1.200765	-1.797307	0.00575
H	-1.407369	2.743554	0.95373
H	-2.155113	1.469671	-0.023748
H	-1.25995	1.914318	-2.825632
H	-1.889952	6.525942	-7.720905
H	-1.565336	4.059517	-7.69066
H	-1.407519	2.841991	-5.501743
H	-2.190558	8.741111	-7.430752
H	-2.514169	11.148641	-6.908003
H	-2.61415	11.900904	-4.532896
H	-2.395089	10.269484	-2.686347

Compound: **[LPtCl]**; **conditions**: PCM (Methanol, triplet), singlet



xyz coordinates

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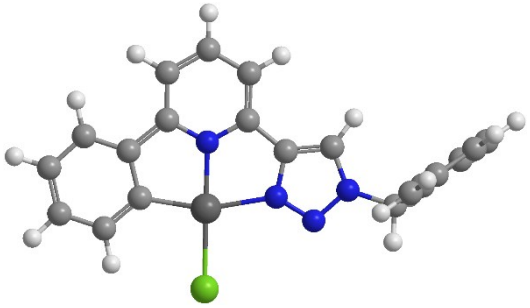
C	2.43322	-0.019676	-0.000696
C	1.21196	-0.711395	0.003218
C	-1.309818	2.160723	0.033569
N	-1.436635	3.118237	-1.075008
C	-1.392861	2.868219	-2.411903
C	-1.586479	4.10058	-3.020234
N	-1.736537	5.033628	-1.996537
N	-1.644744	4.439861	-0.804217
C	-1.666945	4.606484	-4.375912
N	-1.880406	5.960275	-4.406922
C	-1.993968	6.679172	-5.619143
C	-1.879222	5.946017	-6.833622
C	-1.662537	4.574634	-6.808555
C	-1.552869	3.88501	-5.558158
C	-2.208657	8.0578	-5.40855
C	-2.363824	9.038003	-6.443229
C	-2.564525	10.35997	-6.108996
C	-2.62369	10.786185	-4.728322
C	-2.478819	9.859089	-3.698956
C	-2.270149	8.485605	-3.96722
Pt	-2.034672	6.974183	-2.74163
Cl	-2.211863	8.181311	-0.652716
H	-0.944013	-0.538935	-0.002227
H	1.237356	3.181808	0.003027
H	3.379542	1.927068	-0.004792
H	3.370942	-0.567587	-0.00134
H	1.200647	-1.797343	0.004384
H	-1.402346	2.754069	0.946838
H	-2.15502	1.469937	-0.013963
H	-1.232506	1.88503	-2.817792
H	-1.962655	6.468875	-7.779649
H	-1.575466	4.01763	-7.734281
H	-1.382456	2.815445	-5.522643
H	-2.322925	8.741006	-7.486608
H	-2.681961	11.10412	-6.891503
H	-2.782711	11.836616	-4.504879
H	-2.526258	10.192509	-2.66632

Compound: **[LPtCl]**; **conditions**: PCM (Methanol, UA0), singlet



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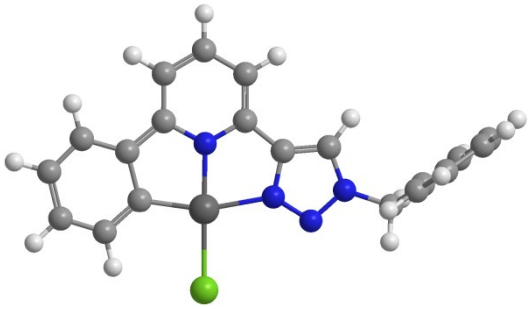
C	0	0	0
C	0	1.404316	0
C	1.225054	2.097591	0
C	2.435049	1.391849	-0.005138
C	2.431423	-0.014089	-0.003987
C	1.212591	-0.708651	0.000461
C	-1.309105	2.162362	0.025605
N	-1.470149	3.04341	-1.144423
C	-1.379929	2.724992	-2.468418
C	-1.629552	3.910119	-3.141946
N	-1.858067	4.884324	-2.177272
N	-1.762404	4.366931	-0.958089
C	-1.693555	4.324933	-4.53663
N	-1.971799	5.653417	-4.673375
C	-2.080108	6.265533	-5.890676
C	-1.896708	5.492712	-7.049335
C	-1.610269	4.12699	-6.930306
C	-1.505043	3.525231	-5.664871
C	-2.38494	7.695014	-5.776869
C	-2.54251	8.541945	-6.888145
C	-2.833144	9.898299	-6.69397
C	-2.964801	10.400411	-5.387176
C	-2.807999	9.555605	-4.273467
C	-2.515709	8.18951	-4.434504
Pt	-2.241492	6.767317	-3.061582
Cl	-2.576327	8.109028	-1.100308
H	-0.944174	-0.541862	-0.000215
H	1.233319	3.18659	0.005073
H	3.377541	1.933423	-0.005382
H	3.370882	-0.561086	-0.00553
H	1.20365	-1.795546	0.001726
H	-1.377251	2.823579	0.895143
H	-2.157164	1.470492	0.055389
H	-1.149266	1.729959	-2.818622

H	-1.977476	5.953279	-8.028383
H	-1.468311	3.526508	-7.824177
H	-1.283748	2.467872	-5.561073
H	-2.4407	8.153227	-7.899525
H	-2.955865	10.5576	-7.549121
H	-3.190415	11.453898	-5.234348
H	-2.913929	9.963554	-3.271767

Compound: **[LPtCl]**; **conditions**: PCM (Methanol, UA0), triplet



xyz coordinates

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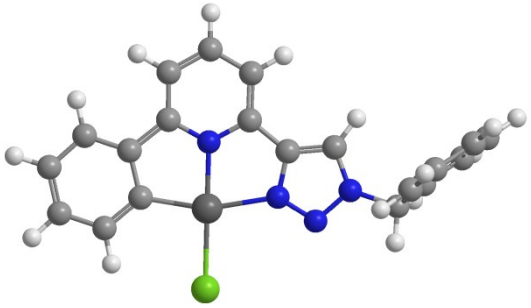
C	1.212494	-0.708889	0.000282
C	-1.308697	2.162777	0.025696
N	-1.47483	3.035879	-1.149744
C	-1.370479	2.706766	-2.468969
C	-1.637294	3.881	-3.160284
N	-1.890568	4.86239	-2.19866
N	-1.792078	4.35124	-0.966903
C	-1.705455	4.296127	-4.546778
N	-2.017053	5.63408	-4.664378
C	-2.1396	6.266984	-5.920708
C	-1.930668	5.483969	-7.079936
C	-1.614856	4.131353	-6.970872
C	-1.499975	3.524637	-5.680659
C	-2.466471	7.64263	-5.796305
C	-2.654589	8.541236	-6.886339
C	-2.971077	9.864308	-6.638082
C	-3.116566	10.360604	-5.292171
C	-2.939937	9.510032	-4.208437

C	-2.614083	8.140049	-4.391753
Pt	-2.312411	6.733541	-3.071527
Cl	-2.674235	8.057129	-1.082917
H	-0.944248	-0.541724	-0.000124
H	1.233395	3.186311	0.004942
H	3.377726	1.932931	-0.005281
H	3.370836	-0.561579	-0.005592
H	1.203415	-1.795792	0.00143
H	-1.373564	2.829357	0.891273
H	-2.156472	1.470813	0.062985
H	-1.119079	1.712824	-2.806728
H	-2.018845	5.946552	-8.059249
H	-1.45508	3.532214	-7.861008
H	-1.254531	2.470694	-5.58618
H	-2.549965	8.189688	-7.909767
H	-3.11454	10.550161	-7.470042
H	-3.365846	11.406999	-5.136757
H	-3.050506	9.8872	-3.195721

Compound: **[LPtCl]**; **conditions**: PCM (Methanol, UFF), singlet



xyz coordinates

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C	1.226257	2.095836	0
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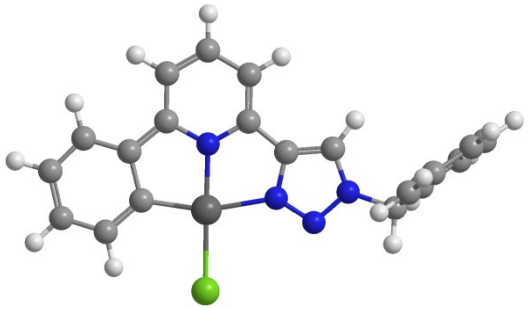
C	2.431499	-0.016564	-0.003371
C	1.211925	-0.709828	0.000743
C	-1.308566	2.163623	0.024049
N	-1.478463	3.022777	-1.16122
C	-1.398851	2.679834	-2.479453
C	-1.653397	3.852007	-3.173521
N	-1.874951	4.843662	-2.225213
N	-1.769772	4.349114	-0.997384

C	-1.725711	4.242875	-4.574677
N	-2.002362	5.56948	-4.73264
C	-2.116067	6.161433	-5.959337
C	-1.94006	5.369619	-7.105818
C	-1.655764	4.005528	-6.965413
C	-1.545218	3.424796	-5.690967
C	-2.418471	7.593359	-5.867321
C	-2.57998	8.422782	-6.990842
C	-2.868059	9.782675	-6.81774
C	-2.993379	10.30616	-5.518775
C	-2.832459	9.478855	-4.392566
C	-2.542503	8.109761	-4.532578
Pt	-2.262556	6.710312	-3.138154
Cl	-2.58787	8.085745	-1.198483
H	-0.943056	-0.541002	-0.000102
H	1.236335	3.183346	0.005487
H	3.377698	1.92979	-0.004381
H	3.369562	-0.563719	-0.004256
H	1.202002	-1.795603	0.002318
H	-1.368252	2.839602	0.881368
H	-2.156434	1.474937	0.073616
H	-1.17254	1.680517	-2.810112
H	-2.024645	5.812023	-8.090862
H	-1.519814	3.390898	-7.84842
H	-1.32613	2.37083	-5.572382
H	-2.483276	8.019397	-7.995415
H	-2.993528	10.427357	-7.682313
H	-3.216955	11.361271	-5.382169
H	-2.933599	9.902533	-3.3974

Compound: **[LPtCl]**; **conditions**: PCM (Methanol, UFF), triplet



xyz coordinates

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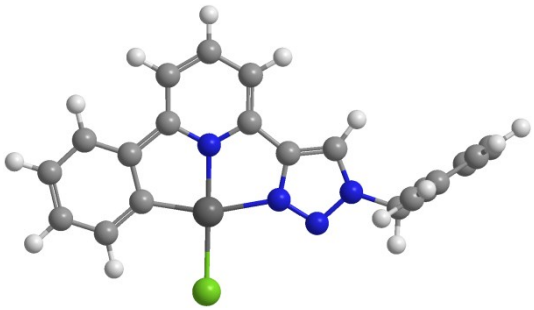
C	0	1.404454	0
C	1.226368	2.095674	0
C	2.435923	1.389062	-0.00483
C	2.431489	-0.016847	-0.00368
C	1.211854	-0.709996	0.000504
C	-1.308282	2.164032	0.023615
N	-1.479417	3.020079	-1.163819
C	-1.393595	2.669192	-2.47856
C	-1.653122	3.835325	-3.185493
N	-1.884362	4.834197	-2.237219
N	-1.778287	4.341935	-0.999136
C	-1.727917	4.230837	-4.578052
N	-2.018825	5.570854	-4.713273
C	-2.142995	6.187807	-5.978439
C	-1.955836	5.382724	-7.127933
C	-1.66109	4.02831	-7.000391
C	-1.544983	3.438709	-5.70121
C	-2.448258	7.568585	-5.872029
C	-2.631755	8.455327	-6.973698
C	-2.926747	9.785936	-6.742452
C	-3.054672	10.303949	-5.403038
C	-2.882077	9.465805	-4.308275
C	-2.578021	8.089443	-4.474073
Pt	-2.286492	6.698073	-3.135119
Cl	-2.620936	8.05769	-1.166499
H	-0.943119	-0.540894	-0.000121
H	1.236291	3.183185	0.005309
H	3.377831	1.929434	-0.004679
H	3.369523	-0.564072	-0.004862
H	1.201819	-1.79578	0.00187
H	-1.367083	2.84185	0.879473
H	-2.156092	1.47534	0.075218
H	-1.160031	1.669219	-2.801663
H	-2.044601	5.829405	-8.112668
H	-1.51865	3.413595	-7.881306
H	-1.316877	2.384237	-5.593431
H	-2.540465	8.089578	-7.991778
H	-3.066228	10.460792	-7.582272
H	-3.287135	11.354911	-5.26113
H	-2.979199	9.858487	-3.300658

Compound: **[LPtCl]**; **conditions**: gas phase, singlet



xyz coordinates

C	0	0	0
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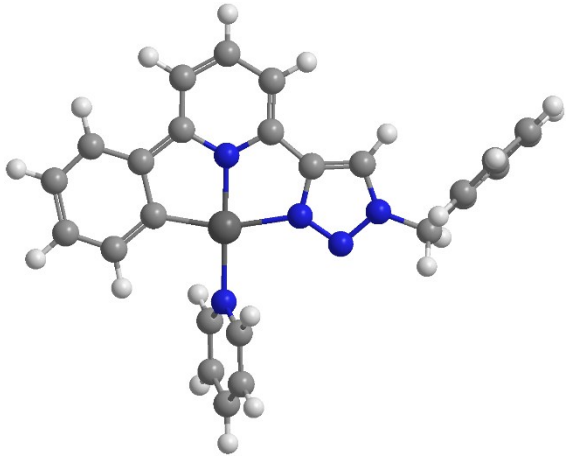
C	2.429168	-0.017564	-0.003467
C	1.21073	-0.710351	0.000437
C	-1.30529	2.168424	0.024469
N	-1.445129	3.074504	-1.122627
C	-1.344081	2.797794	-2.457376
C	-1.569937	4.00718	-3.094603
N	-1.793944	4.955888	-2.09705
N	-1.719775	4.399904	-0.896445
C	-1.614375	4.468065	-4.476117
N	-1.873408	5.803531	-4.565915
C	-1.96061	6.461154	-5.764992
C	-1.775664	5.721389	-6.947202
C	-1.509513	4.349493	-6.874716
C	-1.425185	3.703662	-5.629384
C	-2.242666	7.885209	-5.605694
C	-2.379895	8.775209	-6.687773
C	-2.649625	10.124446	-6.445542
C	-2.781386	10.579611	-5.119711
C	-2.645816	9.697783	-4.036774
C	-2.374452	8.334919	-4.248647
Pt	-2.13645	6.873332	-2.923815
Cl	-2.445472	8.160106	-0.972786
H	-0.94363	-0.541549	0.006127
H	1.233667	3.18215	0.006305
H	3.375883	1.927625	-0.001873
H	3.367186	-0.564887	-0.002745
H	1.201153	-1.796285	0.004577
H	-1.380097	2.813749	0.905003

H	-2.15689	1.479943	0.037195
H	-1.112056	1.815088	-2.830833
H	-1.840029	6.218304	-7.90793
H	-1.366774	3.779454	-7.78716
H	-1.218706	2.641636	-5.561227
H	-2.278226	8.423214	-7.712077
H	-2.757133	10.817875	-7.274585
H	-2.991357	11.629755	-4.931147
H	-2.749405	10.058806	-3.018288

Compound: **[LPtPy]$^{+}$**; **conditions**: gas phase, triplet

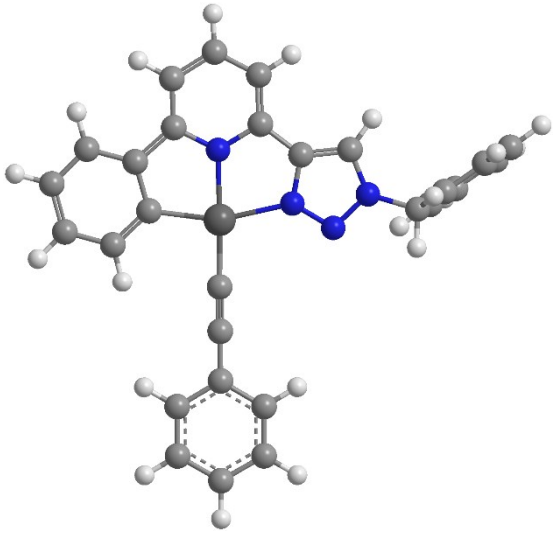


xyz coordinates

C	0	0	0
N	0	1.359531	0
C	1.188236	2.021859	0
C	2.407787	1.344501	-0.00119
C	2.412082	-0.057737	-0.003917
C	1.184957	-0.735917	-0.002961
Pt	-1.773093	2.390558	0.086437
N	-2.494703	1.735248	1.935245
C	-3.712114	2.328927	2.27588
C	-4.06703	1.81358	3.516591
N	-3.063706	0.949918	3.848167
N	-2.09406	0.888965	2.89075
C	-4.265398	3.262941	1.315842
N	-3.454644	3.396909	0.212181
C	-3.778842	4.253179	-0.855353
C	-4.980612	4.99173	-0.772244
C	-5.810986	4.86315	0.340107

C	-5.448981	3.984987	1.402519
C	-2.803095	4.22196	-1.886462
C	-2.863742	4.980371	-3.091107
C	-1.873831	4.837885	-4.041336
C	-0.768047	3.926113	-3.842001
C	-0.672894	3.183985	-2.674474
C	-1.644983	3.293124	-1.647301
C	-2.894621	0.156809	5.088966
C	-4.203993	-0.057074	5.806463
C	-4.513727	0.696461	6.951607
C	-5.727891	0.49624	7.625448
C	-6.64092	-0.458743	7.155013
C	-6.335981	-1.216334	6.01236
C	-5.122018	-1.017432	5.342609
H	-0.970084	-0.48069	0.002252
H	1.134212	3.103154	0.004557
H	3.331493	1.911462	0.002167
H	3.347326	-0.607483	-0.006013
H	1.139318	-1.818701	-0.005615
H	-4.919725	1.978994	4.152355
H	-5.256727	5.659556	-1.581229
H	-6.73319	5.428622	0.401742
H	-6.090498	3.881667	2.271088
H	-3.688651	5.663632	-3.267254
H	-1.920709	5.411156	-4.962681
H	-0.01654	3.830486	-4.619435
H	0.16079	2.499851	-2.54881
H	-2.180616	0.688926	5.725644
H	-2.436568	-0.787438	4.781655
H	-3.803289	1.429678	7.32715
H	-5.955379	1.075513	8.514857
H	-7.578144	-0.619227	7.679001
H	-7.035996	-1.964684	5.653952
H	-4.88457	-1.616485	4.466067

Compound: **[LPt(CCPh)]**; **conditions**: PCM (Methanol, Pauling), triplet



xyz coordinates

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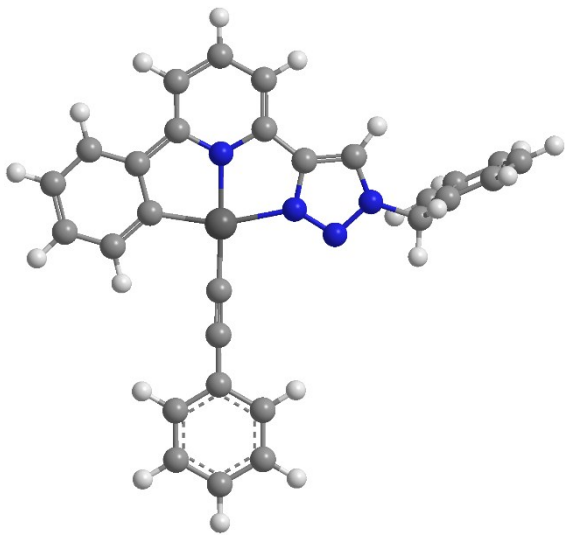
C	2.430443	-0.010859	0.00073
C	1.203109	-0.704552	0.00031
C	-1.2081	2.14528	0.000597
C	-2.289643	2.798455	0.002176
Pt	-3.934062	3.761904	-0.000439
N	-5.374108	2.225397	0.018316
C	-6.689803	2.7132	0.012768
C	-7.51904	1.592888	0.028235
N	-6.683006	0.517869	0.040071
N	-5.36544	0.880569	0.035701
C	-6.857952	4.141578	-0.007238
N	-5.621092	4.804554	-0.016409
C	-5.531307	6.200533	-0.032704
C	-6.699839	6.947719	-0.041931
C	-7.963974	6.29199	-0.033994
C	-8.036585	4.883887	-0.015955
C	-4.139224	6.649736	-0.035686
C	-3.756788	8.007308	-0.051891
C	-2.403635	8.362686	-0.05014
C	-1.416708	7.358061	-0.03228
C	-1.786202	6.002247	-0.017534
C	-3.138502	5.611738	-0.019155
C	-7.035238	-0.909546	0.07053
C	-7.75963	-1.300884	1.341608

C	-7.148191	-1.114952	2.595804
C	-7.812684	-1.493577	3.769665
C	-9.093974	-2.068111	3.700885
C	-9.705725	-2.258673	2.452896
C	-9.040191	-1.873519	1.277361
H	-0.9496	-0.525787	-0.00021
H	1.256286	3.199615	-0.000012
H	3.39579	1.927781	0.00077
H	3.364693	-0.563938	0.001036
H	1.195538	-1.789796	0.00013
H	-8.591223	1.496402	0.034777
H	-6.655407	8.031376	-0.054296
H	-8.875347	6.880094	-0.040763
H	-8.997932	4.380459	-0.008381
H	-4.515063	8.786491	-0.065593
H	-2.116585	9.410326	-0.062475
H	-0.364378	7.630907	-0.030641
H	-1.011937	5.240067	-0.004771
H	-6.086899	-1.444712	-0.029478
H	-7.645961	-1.133136	-0.808266
H	-6.154977	-0.675364	2.654218
H	-7.334462	-1.346091	4.733486
H	-9.607859	-2.363466	4.610902
H	-10.695522	-2.701377	2.393138
H	-9.519528	-2.019051	0.312426

Compound: **[LPt(CCPh)]**; **conditions**: gas phase, triplet



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C	0	0	0
C	0	1.425302	0
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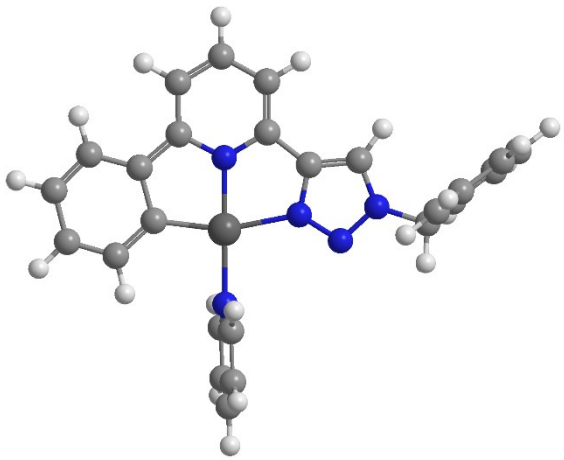
C	2.429758	-0.018141	0.001203
C	1.201893	-0.707465	0.00045
C	-1.210713	2.141291	0.000918
C	-2.308688	2.764896	0.002498
Pt	-3.975769	3.676016	0.005862
N	-5.368643	2.095885	0.031258
C	-6.702246	2.550997	0.04219
C	-7.498688	1.406258	0.073452
N	-6.629156	0.353862	0.077512
N	-5.321444	0.7537	0.054237
C	-6.908449	3.969823	0.026582
N	-5.693106	4.669498	0.010196
C	-5.642296	6.062371	-0.003867
C	-6.827472	6.778452	-0.00283
C	-8.07554	6.086656	0.012585
C	-8.10958	4.683686	0.02733
C	-4.261565	6.551237	-0.017412
C	-3.920941	7.917013	-0.031864
C	-2.579722	8.311664	-0.042253
C	-1.567085	7.336062	-0.038299
C	-1.895907	5.971238	-0.024602
C	-3.234481	5.545361	-0.014358
C	-6.928721	-1.078448	0.115808
C	-7.716635	-1.48076	1.345301
C	-7.292512	-1.078246	2.624738
C	-8.002804	-1.478808	3.762422
C	-9.141699	-2.290919	3.634267
C	-9.56723	-2.696	2.361689
C	-8.857392	-2.288674	1.221268
H	-0.953675	-0.518623	-0.00059
H	1.254525	3.192074	-0.00024
H	3.39627	1.918818	0.001358
H	3.36372	-0.572868	0.001634
H	1.191295	-1.793399	0.000137
H	-8.566414	1.275636	0.112197
H	-6.810116	7.86256	-0.013445
H	-9.002411	6.650938	0.013271
H	-9.057784	4.154553	0.039594
H	-4.702896	8.672821	-0.03487
H	-2.322247	9.367158	-0.053369
H	-0.5228	7.63929	-0.04638

H	-1.103506	5.228655	-0.02214
H	-5.953041	-1.574061	0.090187
H	-7.470785	-1.354786	-0.79502
H	-6.410197	-0.450561	2.728004
H	-7.669562	-1.161559	4.746198
H	-9.691284	-2.602237	4.517813
H	-10.448431	-3.322012	2.255445
H	-9.194284	-2.602276	0.2354

Compound: **[LPtPy]$^{+}$**; **conditions**: PCM (Methanol, Pauling), triplet

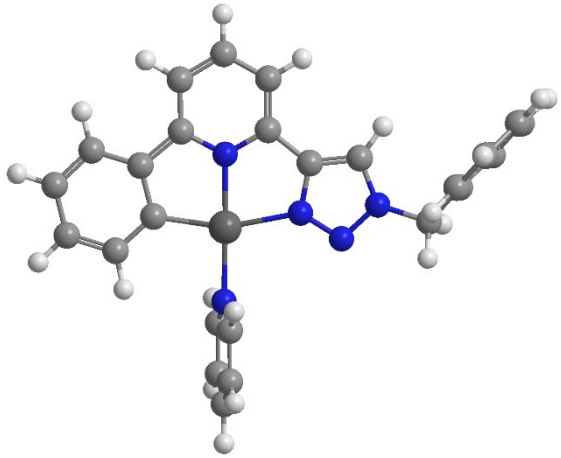


xyz coordinates

C	0	0	0
C	0	1.427355	0
C	1.307123	2.169706	0
C	2.499183	1.400456	0.019974
C	2.464549	0.012217	0.026316
C	1.198067	-0.685641	0.012466
C	-1.161406	2.240778	0.002125
N	-0.852737	3.615122	-0.001079
C	-1.826257	4.585059	-0.00273
C	-3.168899	4.229165	0.003067
C	-3.521589	2.844545	0.008959
C	-2.528586	1.868966	0.008003
Pt	1.049025	4.109375	-0.0236
N	0.139829	5.997624	-0.024059
C	-1.253913	5.917971	-0.012621
C	-1.724008	7.224262	-0.00851
N	-0.608725	8.008107	-0.015411
N	0.540997	7.272184	-0.02419

C	-0.525119	9.480475	-0.033059
C	-1.351016	10.115127	1.063769
C	-1.042227	9.878546	2.416633
C	-1.799505	10.480408	3.429936
C	-2.869513	11.330548	3.099871
C	-3.17817	11.57263	1.75296
C	-2.421501	10.963882	0.73837
N	3.038951	4.634136	-0.059201
C	3.747312	4.571877	-1.218114
C	5.086611	4.958296	-1.280767
C	5.720111	5.421923	-0.118761
C	4.984917	5.483007	1.073928
C	3.648521	5.082199	1.070758
H	-0.937659	-0.546759	-0.007987
H	3.45936	1.907644	0.031249
H	3.385061	-0.562764	0.04024
H	1.198533	-1.771799	0.013886
H	-3.937689	4.993343	0.002625
H	-4.566997	2.559693	0.013831
H	-2.798168	0.818293	0.0125
H	-2.721252	7.629558	0.003907
H	-0.851039	9.829988	-1.016559
H	0.538004	9.71076	0.075825
H	-0.211175	9.227166	2.67728
H	-1.55555	10.293341	4.47138
H	-3.454376	11.799297	3.885705
H	-4.003011	12.228754	1.49209
H	-2.665454	11.150602	-0.304429
H	3.217897	4.206357	-2.088453
H	5.615159	4.893788	-2.224241
H	6.760548	5.726835	-0.141742
H	5.433122	5.832822	1.996124
H	3.042771	5.110532	1.967446

Compound: **[LPtPy]$^+$**; **conditions**: gas phase, singlet



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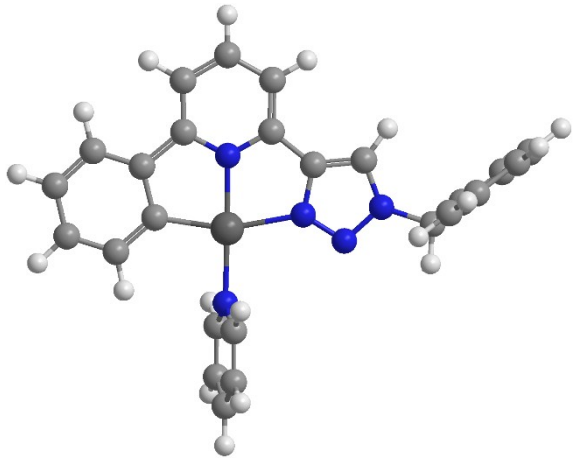
C	0	0	0
N	0	1.359855	0
C	1.185622	2.024422	0
C	2.406288	1.348872	-0.00285
C	2.41249	-0.053161	-0.008828
C	1.186555	-0.733741	-0.007943
Pt	-1.760806	2.388587	-0.028277
N	-3.489056	3.372181	-0.022144
C	-3.937758	3.957101	-1.167969
C	-5.149433	4.647752	-1.174572
C	-5.879393	4.714866	0.025768
C	-5.400621	4.104996	1.189536
C	-4.173298	3.417905	1.158253
C	-3.024283	3.755243	-2.287835
C	-2.988449	4.117845	-3.625638
N	-1.822374	3.5924	-4.106322
N	-1.129405	2.922354	-3.138252
N	-1.86745	3.026501	-2.038858
C	-1.291546	3.62408	-5.48936
C	-1.732889	4.861025	-6.232252
C	-2.733883	4.776343	-7.214929
C	-3.14418	5.92438	-7.909546
C	-2.556024	7.164475	-7.62206
C	-1.553095	7.254275	-6.642673
C	-1.142159	6.107179	-5.952586
C	-3.484524	2.718233	2.244968
C	-2.231428	2.113992	1.896833
C	-1.526463	1.446539	2.90847
C	-2.037249	1.3695	4.216337
C	-3.26801	1.96113	4.54059

C	-3.991567	2.638273	3.552596
H	-0.970248	-0.480086	0.011449
H	1.131409	3.105718	0.005568
H	3.329357	1.916767	0.001357
H	3.348581	-0.601464	-0.011273
H	1.14259	-1.816651	-0.00984
H	-5.516458	5.118159	-2.079078
H	-6.825252	5.245811	0.048194
H	-5.968122	4.160104	2.110369
H	-3.659639	4.691626	-4.241686
H	-1.633199	2.71758	-5.99946
H	-0.204038	3.568422	-5.389815
H	-3.183338	3.814113	-7.450949
H	-3.910643	5.849259	-8.674559
H	-2.868019	8.05256	-8.162982
H	-1.087672	8.211311	-6.428326
H	-0.355087	6.179813	-5.204979
H	-0.567292	0.983777	2.693596
H	-1.471845	0.84815	4.9839
H	-3.655148	1.896751	5.552318
H	-4.942135	3.098626	3.809219

Compound: **[LPtPy]$^{+}$**; **conditions**: PCM (Methanol, Pauling), singlet



xyz coordinates

C	0	0	0
C	0	1.407621	0
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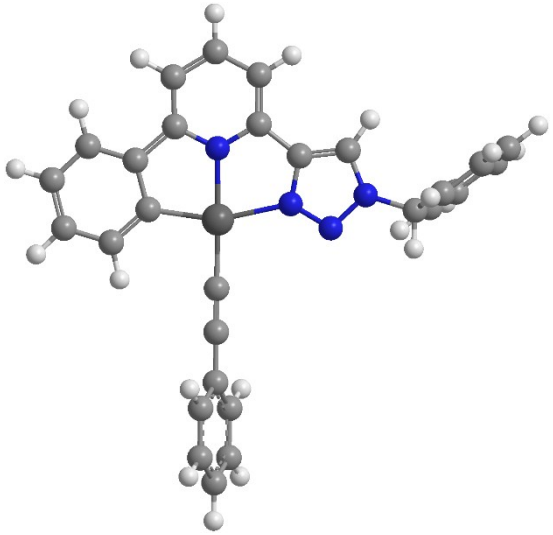
C	2.436623	1.39145	-0.000393
C	2.431853	-0.011412	0.004088

C	1.209756	-0.706397	0.005411
C	-1.303631	2.174208	-0.023031
N	-2.115778	1.933387	1.184604
C	-1.746448	2.040142	2.494108
C	-2.885966	1.727733	3.218317
N	-3.885425	1.450313	2.294302
N	-3.426805	1.571283	1.054052
Pt	-5.701759	0.94441	3.232936
C	-7.052972	0.558221	4.65712
C	-6.516822	0.715493	5.979814
C	-7.309523	0.494748	7.118683
C	-8.649259	0.109931	6.972699
C	-9.189042	-0.054311	5.68612
C	-8.398248	0.168071	4.543813
C	-3.240037	1.629873	4.629714
N	-4.539857	1.263889	4.81386
C	-5.103935	1.112441	6.046891
C	-4.306695	1.340701	7.180508
C	-2.967539	1.715505	7.014642
C	-2.415838	1.865386	5.730947
N	-6.922738	0.624121	1.626714
C	-6.825772	-0.527931	0.910542
C	-7.628546	-0.768053	-0.204944
C	-8.558871	0.203843	-0.600637
C	-8.654008	1.389933	0.141482
C	-7.82511	1.568783	1.249512
H	-0.942616	-0.5425	-0.006338
H	1.229827	3.185162	-0.000106
H	3.377432	1.933442	-0.002297
H	3.369379	-0.559452	0.005054
H	1.202255	-1.792222	0.005234
H	-1.12118	3.249276	-0.1037
H	-1.936732	1.871778	-0.861409
H	-0.750173	2.311917	2.798608
H	-6.894601	0.619053	8.115274
H	-9.264837	-0.061428	7.850313
H	-10.226902	-0.355622	5.570631
H	-8.844322	0.030722	3.562541
H	-4.723413	1.227884	8.173674
H	-2.34818	1.89288	7.886879
H	-1.381285	2.155565	5.596725
H	-6.093781	-1.24874	1.251734
H	-7.52099	-1.70019	-0.746527
H	-9.194223	0.040535	-1.464162
H	-9.358524	2.168166	-0.126328
H	-7.867547	2.464933	1.854843

Compound: **[LPt(CCPh)]**; **conditions**: PCM (Methanol, Pauling), singlet

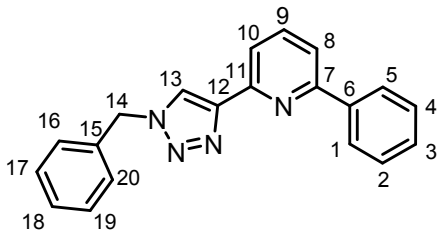


xyz coordinates

C	0	0	0
C	0	1.416831	0
C	1.249046	2.085943	0
C	2.449828	1.364323	-0.001311
C	2.435454	-0.040989	-0.000157
C	1.203517	-0.717354	0.001066
C	-1.228332	2.155562	0.000461
C	-2.286951	2.802104	0.002784
Pt	-3.96156	3.820946	-0.01067
N	-4.682362	3.536677	-1.976729
C	-5.892719	4.186536	-2.201325
C	-6.254359	3.9195	-3.512205
N	-5.25517	3.131995	-4.00591
N	-4.287906	2.89219	-3.069611
C	-6.464181	4.942402	-1.091862
N	-5.685748	4.880906	0.022148
C	-6.007892	5.503751	1.190308
C	-7.199351	6.246981	1.248797
C	-8.015566	6.323964	0.112281
C	-7.656932	5.668799	-1.078509
C	-5.006375	5.28185	2.244317
C	-5.126403	5.828007	3.534469
C	-4.138642	5.580469	4.496485
C	-3.029914	4.784037	4.161825
C	-2.905453	4.235751	2.872861
C	-3.878869	4.46368	1.882042
C	-5.125934	2.545899	-5.35089
C	-6.260787	1.598998	-5.678383

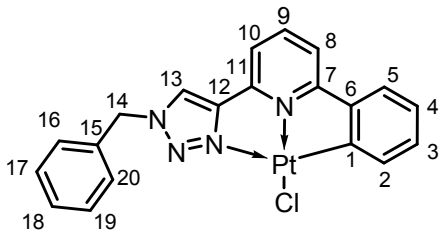
C	-6.46964	0.442893	-4.903109
C	-7.511382	-0.43975	-5.216854
C	-8.351058	-0.178047	-6.313583
C	-8.143731	0.970676	-7.091733
C	-7.102347	1.857434	-6.772549
H	-0.949005	-0.528687	-0.00029
H	1.266549	3.172146	0.000405
H	3.396584	1.897465	-0.002342
H	3.367246	-0.598966	-0.000245
H	1.180855	-1.803676	0.001964
H	-7.108199	4.215152	-4.097778
H	-7.486213	6.75489	2.161513
H	-8.936361	6.895796	0.151503
H	-8.285802	5.724349	-1.958582
H	-5.982573	6.444823	3.794864
H	-4.230519	6.002043	5.492905
H	-2.260711	4.589652	4.90514
H	-2.04153	3.623127	2.632389
H	-4.160896	2.032032	-5.350069
H	-5.077082	3.361617	-6.076967
H	-5.819046	0.231738	-4.057458
H	-7.666475	-1.32941	-4.613808
H	-9.15687	-0.863843	-6.557955
H	-8.788675	1.177853	-7.940384
H	-6.946875	2.748298	-7.37598

NMR assignment



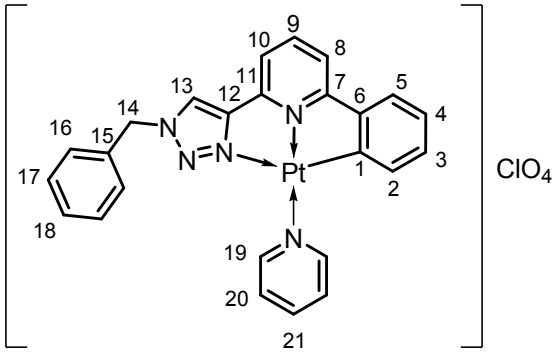
^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.20 (s, 1H, H13), 8.14 (dd, J = 7.8, 1.0 Hz, 1H, H10), 8.06 – 7.98 (m, 2H, H1, H5), 7.82 (t, J = 7.8 Hz, 1H, H9), 7.65 (dd, J = 7.9, 1.0 Hz, 1H, H8), 7.53 – 7.29 (m, 8H, H2, H3, H4, H16, H17, H18, H19, H20), 5.60 (s, 2H, H14).

{^{1}H}^{13}C-NMR (101 MHz, $CDCl_3$): δ (ppm) = 156.8 (C7), 150.0 (C11), 149.0 (C12), 139.0 (C6), 137.5 (C9), 134.5 (C15), 129.0 (C17, C19), 128.9 (C3), 128.6 (C18), 128.5 (C2, C4), 127.9 (C16, C20), 126.8 (C1, C5), 122.1 (C3), 119.4 (C8), 118.3 (C10), 54.2 (C14).



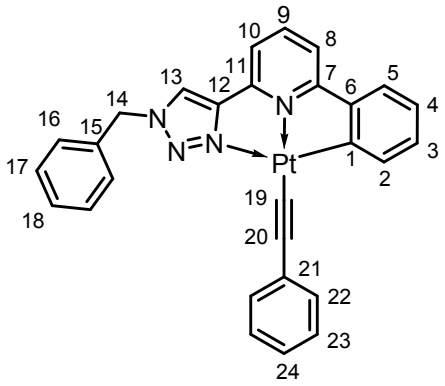
^{1}H-NMR (400 MHz, DMF-d_7): δ (ppm) = 9.21 (s, 1H, H13), 8.09 (t, J = 8.0 Hz, 1H, H9), 7.86 (ddd, J = 7.7, 4.6, 1.0 Hz, 2H, H8, H10), 7.71 (dd, J = 7.6, 1.3 Hz, J(^{195}Pt,^{1}H) = 46.4 Hz), 1H, H5), 7.59 (m, 3H, H2, H16, H20), 7.51 – 7.39 (m, 3H, H17, H18, H19), 7.17 (td, J = 7.4, 1.5 Hz, 1H, H3), 7.09 (td, J = 7.5, 1.4 Hz, 1H, H4), 5.91 (s, 2H, H14).

{^{1}H}^{13}C-NMR (101 MHz, DMF-d_7): δ (ppm) = 166.3 (C7), 150.5 (C12), 148.9 (C11), 147.5 (C6), 140.7 (C9), 140.6 (C1), 135.2 (C15), 134.5 (C2), 130.5 (C3), 129.8 (C16, C20), 129.5 (C18), 129.4 (C17, C19), 126.8 (C13), 125.3 (C5), 124.6 (C4), 118.4 (C8), 118.3 (C10), 56.0 (C14).



^{1}H-NMR (400 MHz, DMF-d_7): δ (ppm) = 9.22 (s, 1H, H13), 9.15-9.12 (m, 2H, H19), 8.39-8.31 (m, 1H, H21), 8.18-8.10 (m, 1H, H9), 7.94-7.80 (m, 4H, H8, H10, H20), 7.70-7.65 (m 1H, H5), 7.59-7.46 (m, 5H, H16, H17, H18), 7.20-7.04 (m, 2H, H4, H3), 6.47-6.43 (m, 1H, H2), 5.89 (s, 2H, H14).

{^{1}H}^{13}C-NMR (101 MHz, DMF-d_7): δ (ppm) = 166.6 (C7), 154.7 (C19), 150.8 (C12), 149.5 (C11), 148.3 (C6), 143.6 (C21), 141.2 (C9), 140.5 (C1), 135.2 (C15), 133.0 (C2), 131.9 (C3), 130.3 (C16), 130.2 (C18), 129.9 (C17), 128.4 (C20), 128.1 (C13), 126.9 (C5), 126.5 (C4), 119.7 (C8), 119.4 (C10), 56.6 (C14).



^{1}H-NMR (400 MHz, DMSO-d_6): δ (ppm) = 9.11 (s, 1H, H13), 8.08 - 8.04 (m, 1H, H9), 7.89 - 7.81 (m, 3H, H2, H8, H10), 7.60 (d, J = 7.0 Hz, 1H, H5), 7.49 - 7.35 (m, 5H, H16, H17, H18), 7.28 – 7.22 (m, 4H, H22, H23), 7.14 - 7.02 (m, 3H, H3, H4, H24), 5.81 (s, 2H, H14).

{^{1}H}^{13}C-NMR (101 MHz, DMSO-d_6): δ (ppm) = 163.8 (C7), 151.1 (C12), 147.5 (C11), 146.7 (C6), 140.7 (C9), 139.7 (C1), 137.1 (C2), 134.3 (C15), 130.9 (C22), 130.4 (C3), 129.0 (C17), 128.9 (C21), 128.8 (C18), 128.5 (C16), 128.1 (C23), 126.2 (C13), 125.0 (C24), 124.7 (C5), 123.6 (C6), 117.7 (C8), 117.4 (C10), 104.5 (C20), 54.7 (C14).

Table S4. Crystallographic data.

	LH	**[LPtCl]**	**[LPtPy]ClO$_4$**	**[LPt(CCPh)]**
empirical formula	$C_{20}H_{16}N_4$	$C_{20}H_{15}ClN_4Pt$	$C_{25}H_{20}ClN_5O_4Pt$	$C_{28}H_{20}N_4Pt$
formula weight	312.37	541.90	685.00	607.57
crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
space group	$P2_1/n$	$P2_1/c$	$C2/c$	$Pbca$
a, b, c / Å	5.7982(1), 11.2478(3), 24.4138(6)	11.387(2), 11.766(2), 13.153(2)	16.6343(8), 21.0742(8), 14.0639(6)	12.0040(5), 15.3488(7), 24.378(1)
β / °	92.459(2)	96.568(3)	108.465(1)	90
V / Å^3	1590.73(6)	1750.7(4)	4676.3(4)	4491.5(3)
Z	4	4	8	8
ρ_{calcd} / g cm^{-3}	1.30	2.06	1.95	1.80
$\mu(Mo_{K\alpha})$ / mm^{-1}	0.1	8.2	6.2	6.3
crystal size / mm	0.23 × 0.10 × 0.04	0.26 × 0.12 × 0.09	0.37 × 0.10 × 0.06	0.16 × 0.10 × 0.03
temperature / K	100(2)	100(2)	153(2)	172(2)
θ_{min}, θ_{max} / °	3.09, 28.21	2.33, 30.11	1.92, 30.03	2.65, 30.10
dataset	–7:7, –14:14, –32:32	–16:16, –16:16, –18:18	–23:22, 0:29, 0:19	–16:16, –21:21, –34:34
tot., uniq. data, R_{int}	24388, 3921, 0.035	26319, 5122, 0.031	12479, 12479, 0.040	51463, 6593, 0.015
observed data [$I > 2\sigma(I)$]	3020	4894	10513	5745
N_{ref}, N_{par}	3921, 217	5122, 235	12479, 326	6593, 298
R_1, wR_2 [$I > 2\sigma(I)$]	0.0441, 0.0979	0.0209, 0.0534	0.0343, 0.0800	0.0191, 0.0442
R_1, wR_2 (all data)	0.0640, 0.1069	0.0221, 0.0540	0.0459, 0.0855	0.0241, 0.0465
S	1.019	1.073	1.025	1.071
min. and max. resd. dens. / e Å^{-3}	–0.22, 0.27	–1.39, 1.58	–1.86, 2.55	–0.58, 1.22
CCDC number	1430086	1430087	1430088	1430089

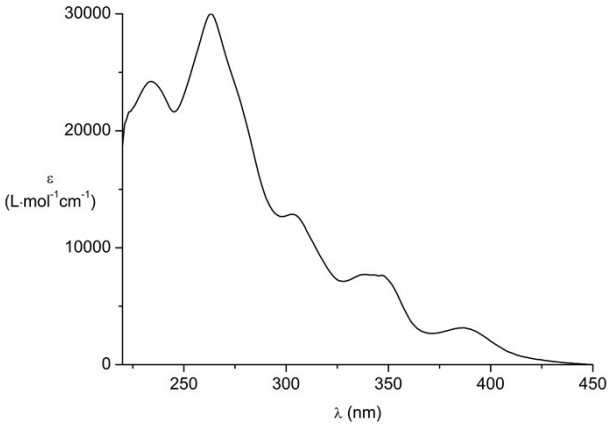


Figure S8: *Absorption spectrum* of **[LPtCl]** at room temperature in CH_2Cl_2.

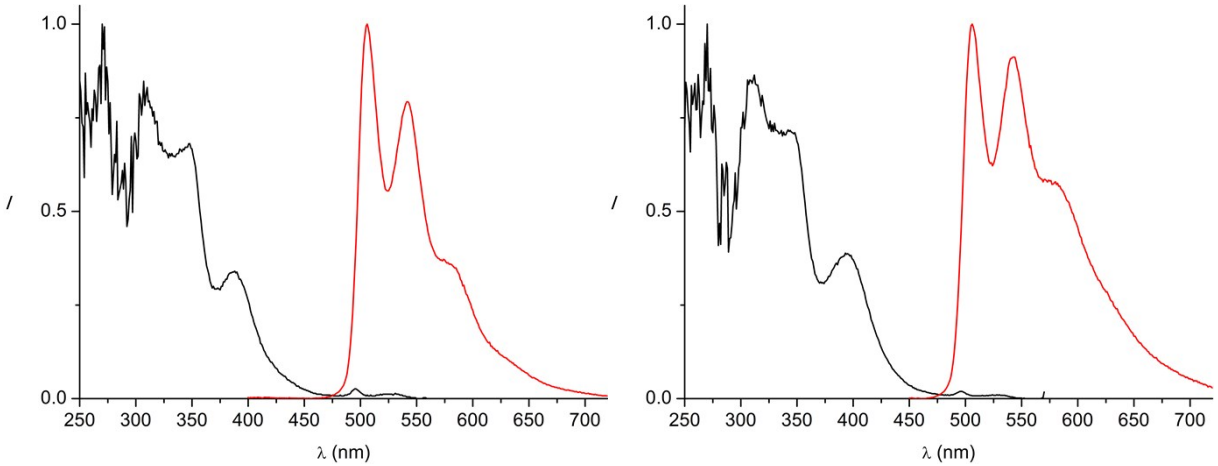


Figure S9: *Excitation* (black) and *Emission* (red) spectra of **[LPtCl]** in *aerated* (left) and *deaerated* (right) CH_2Cl_2 (λ_{exc}= 338nm; λ_{em}=580 nm).

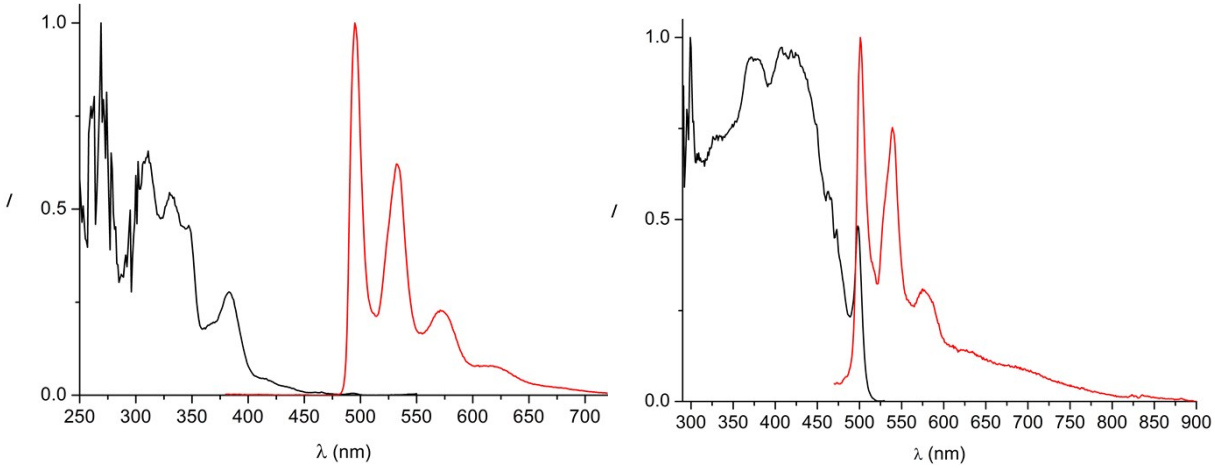
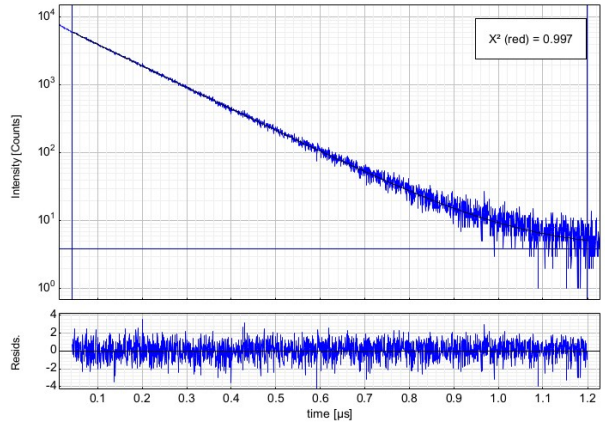
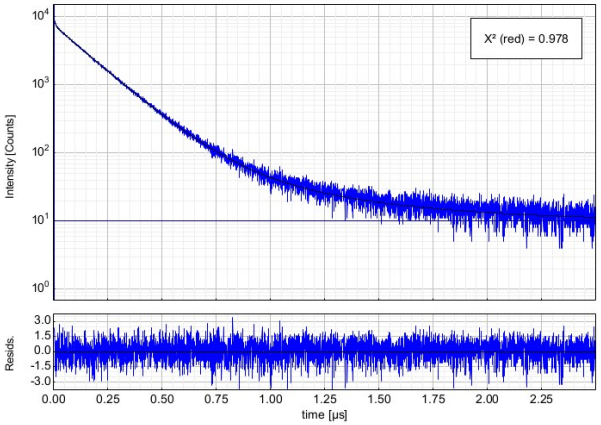


Figure S10: *Excitation* (black) and *Emission* (red) spectra of **[LPtCl]** in a *frozen glassy matrix* at 77K (left, CH_2Cl_2:MeOH 1:1, λ_{exc}=338 nm; λ_{em}= 570 nm) and in the *solid state at room temperature* (right, λ_{exc}=338 nm; λ_{em}=570 nm).



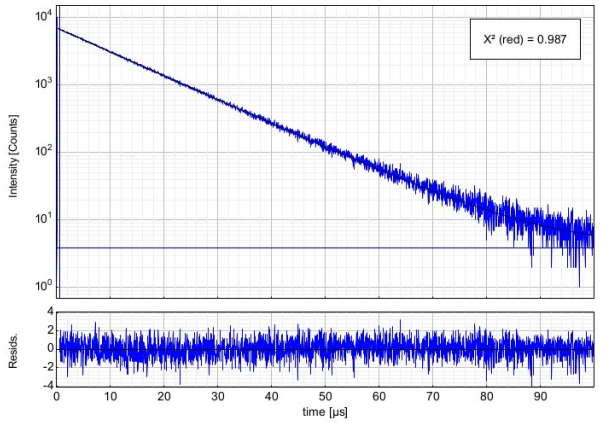
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	6012.3	-35.6	+35.6
τ_1 [µs]	0.136780	-0.000593	+0.000593
Bkgr. Dec [Cnts]	3.864	-0.840	+0.840

Figure S11: Left: Time-resolved luminescence decay of **[LPtCl]** in *aerated* CH_2Cl_2 including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



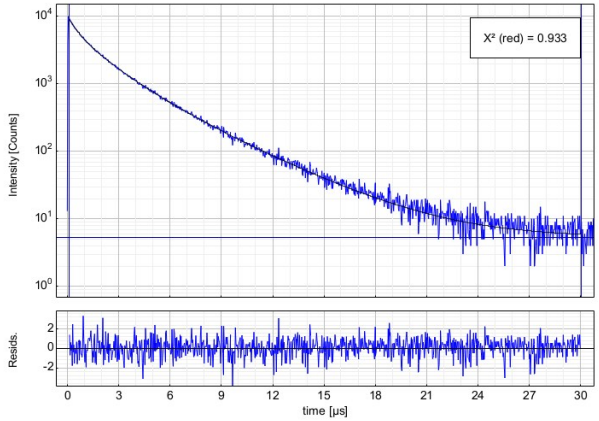
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	1296	-361	+361
τ_1 [µs]	0.00705	-0.00272	+0.00272
A_2 [Cnts]	142.7	-10.2	+10.2
τ_2 [µs]	0.5245	-0.0202	+0.0202
A_3 [Cnts]	7207.6	-54.8	+54.8
τ_3 [µs]	0.156103	-0.000916	+0.000916
Bkgr. Dec [Cnts]	10.162	-0.836	+0.836

Figure S12: Left: Time-resolved luminescence decay of **[LPtCl]** in *deaerated CH_2Cl_2* including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	6714.4	-36.7	+36.7
τ_1 [µs]	12.2407	-0.0486	+0.0486
Bkgr. Dec [Cnts]	3.913	-0.917	+0.917

Figure S13: Left: Time-resolved luminescence decay of **[LPtCl]** in a *frozen glassy matrix (*CH_2Cl_2:MeOH 1:1) including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	4215.4	-59.8	+59.8
τ_1 [µs]	1.6569	-0.0207	+0.0207
A_2 [Cnts]	2719	-138	+138
τ_2 [µs]	0.4915	-0.0299	+0.0299
A_3 [Cnts]	1987.5	-26.4	+26.4
τ_3 [µs]	3.6659	-0.0296	+0.0296
Bkgr. Dec [Cnts]	5.369	-0.727	+0.727

Figure S14: Left: Time-resolved luminescence decay of **[LPtCl]** in the solid state including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

Table S5: Photophysical data of **[LPtCl].**

	λ_{abs} ± 1(nm)	λ_{exc} ± 10 (nm)	λ_{em} ± 10 (nm)	τ ± 0.01 (µs)	Φ ± 0.02	k_r ± 0.1 (10^5 s^{-1})	k_{nr} ± 0.1 (10^5 s^{-1})
aerated	263	270	506	0.14	0.01	0.7	70.7
deaerated	-	270	506	0.18[a)]	0.02	1.1	54.4
77K	-	269	495	12.24	-		
solid	-	299	501	2.50[a)]	0.15	0.6	3.4

a) intensity weighted averaged lifetime.

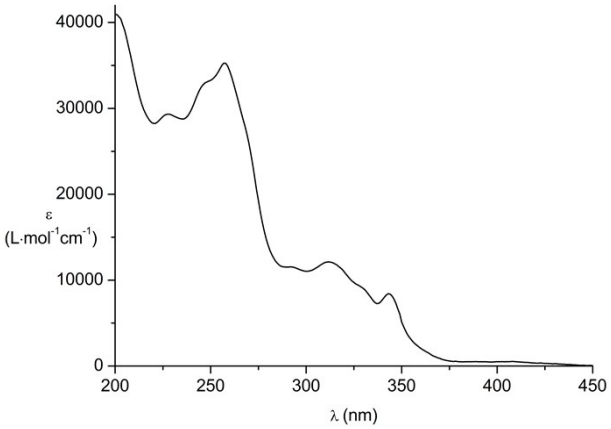


Figure S15: *Absorption spectrum* of **[LPtPy]ClO$_4$** at room temperature in CH_2Cl_2.

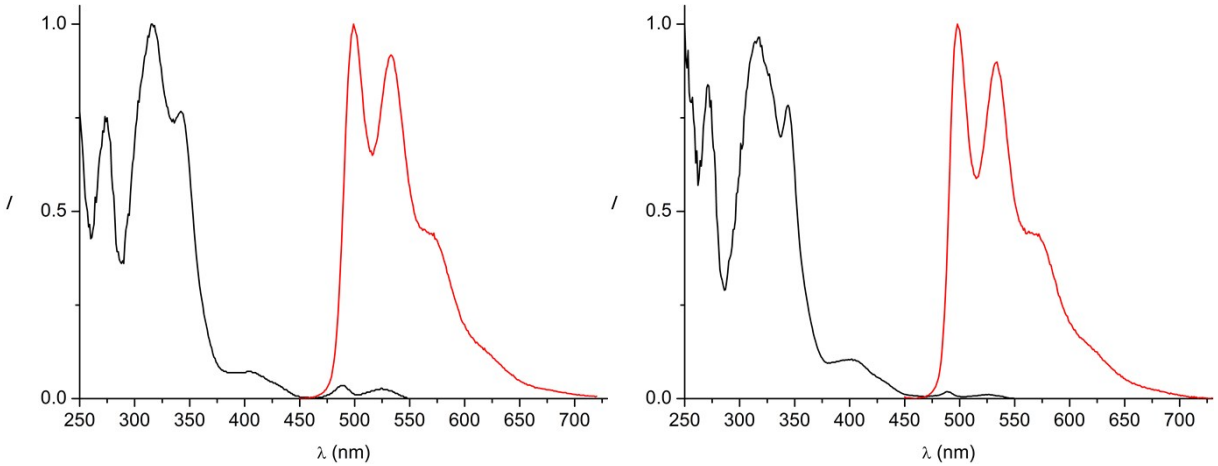


Figure S16: *Excitation* (black) and *Emission* (red) spectra of **[LPtPy]ClO$_4$** in *aerated* (left) and *deaerated* (right) CH_2Cl_2 (λ_{exc}=312 nm; λ_{em}=570 nm).

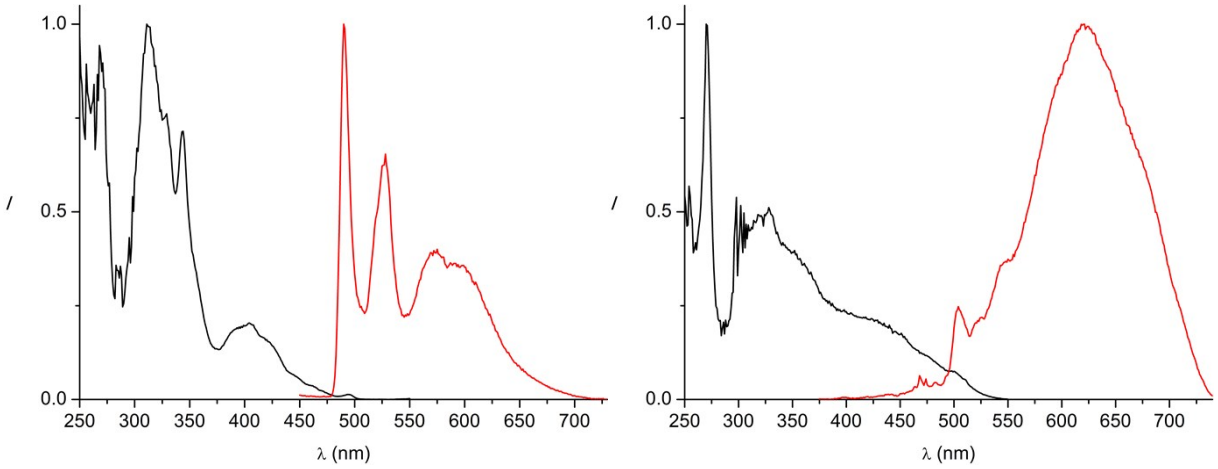
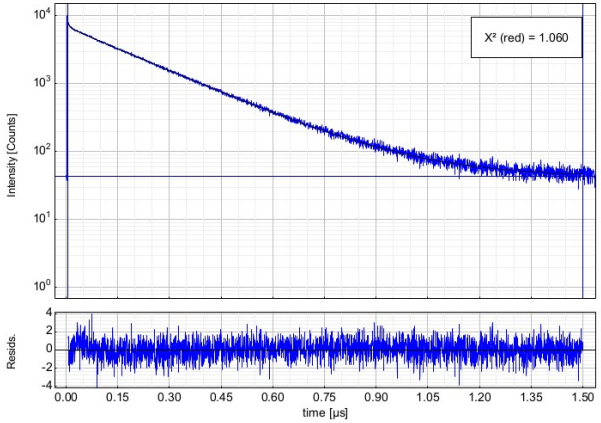
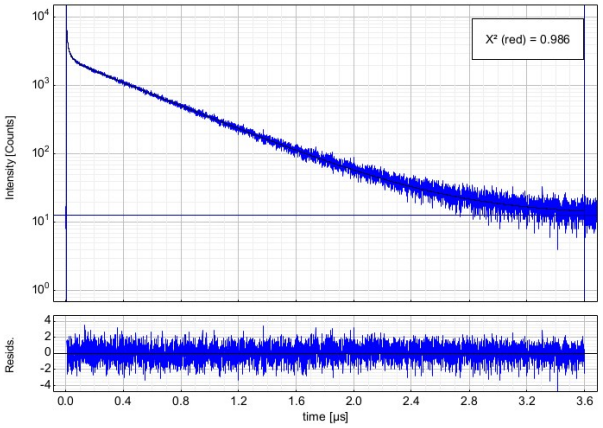


Figure S17: *Excitation* (black) and *Emission* (red) spectra of **[LPtPy]ClO$_4$** in a *frozen glassy matrix* at 77K (left, CH_2Cl_2:MeOH 1:1, λ_{exc}=312 nm; λ_{em}=570 nm) and in the *solid state at room temperature* (right, λ_{exc}=312 nm; λ_{em}=570 nm).



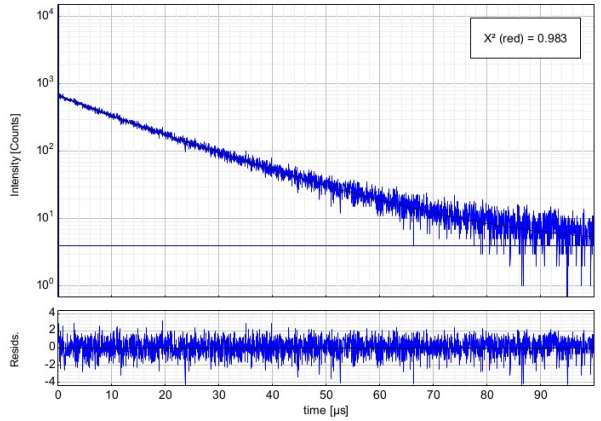
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	6661.7	-37.0	+37.0
τ_1 [µs]	0.199133	-0.000859	+0.000859
A_2 [Cnts]	1150	-290	+290
τ_2 [µs]	0.00642	-0.00227	+0.00227
Bkgr. Dec [Cnts]	43.14	-1.86	+1.86

Figure S18: Left: Time-resolved luminescence decay of **[LPtPy]ClO$_4$** in *aerated CH_2Cl_2* including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



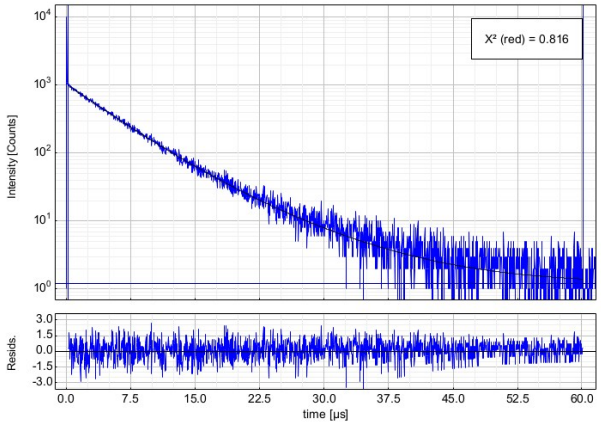
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	2397.1	-21.2	+21.2
τ_1 [µs]	0.50264	-0.00340	+0.00340
A_2 [Cnts]	1380	-151	+151
τ_2 [µs]	0.02892	-0.00374	+0.00374
A_3 [Cnts]	2951	-408	+408
τ_3 [µs]	0.005404	-0.000957	+0.000957
Bkgr. Dec [Cnts]	12.67	-1.09	+1.09

Figure S19: Left: Time-resolved luminescence decay of **[LPtPy]ClO$_4$** in *deaerated CH_2Cl_2* including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



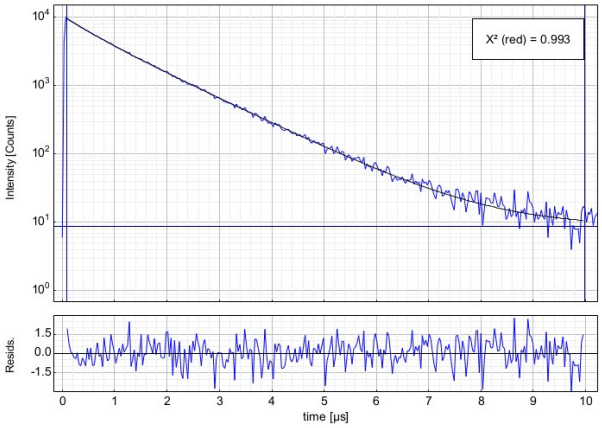
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	516.01	-9.49	+9.49
τ_1 [µs]	16.855	-0.236	+0.236
A_2 [Cnts]	152.4	-16.9	+16.9
τ_2 [µs]	8.240	-0.945	+0.945
Bkgr. Dec [Cnts]	3.997	-0.723	+0.723

Figure S20: Left: Time-resolved luminescence decay of **[LPtPy]ClO$_4$** in a *frozen glassy matrix (*CH_2Cl_2:MeOH 1:1) including the residuals (λ_{exc} = 376.7 nm, λ_{em}= 510 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Parameter	Value	Conf. $_{Lower}$	Conf. $_{Upper}$
A_1 [Cnts]	150.62	-8.31	+8.31
τ_1 [µs]	8.956	-0.295	+0.295
A_2 [Cnts]	836.1	-17.1	+17.1
τ_2 [µs]	4.5840	-0.0787	+0.0787
Bkgr. $_{Dec}$ [Cnts]	1.212	-0.375	+0.375

Figure S21: Left: Time-resolved luminescence decay of **[LPtPy]ClO$_4$** in a *frozen glassy matrix (*CH_2Cl_2:MeOH 1:1) including the residuals (λ_{exc} = 376.7 nm, λ_{em}= 600 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Parameter	Value	Conf. $_{Lower}$	Conf. $_{Upper}$
A_1 [Cnts]	7251.5	-40.5	+40.5
τ_1 [µs]	1.19597	-0.00472	+0.00472
A_2 [Cnts]	2172.9	-79.1	+79.1
τ_2 [µs]	0.5126	-0.0203	+0.0203
Bkgr. $_{Dec}$ [Cnts]	8.79	-1.06	+1.06

Figure S22: Left: Time-resolved luminescence decay of **[LPtPy]ClO$_4$** in the solid state including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

Table S6: Photophysical data of **[LPtPy]ClO_4.**

	λ_{abs} ± 1(nm)	λ_{exc} ± 10 (nm)	λ_{em} ± 10 (nm)	τ ± 0.01 (μs)	Φ ± 0.02	k_r ± 0.1 (10^5 s^{-1})	k_{nr} ± 0.1 (10^5 s^{-1})
aerated	200	320	500	0.21	0.01	0.5	47.1
deaerated		320	500	0.42	0.02	0.5	23.3
77K		310	490	15.77[a)] (490 nm) 5.72[a)] (600 nm)	-		
solid		270	620	2.08[a)] (yellow) 1.12[a)] (orange)	0.36	1.7 3.2	3.1 5.7

a) intensity weighted averaged lifetime.

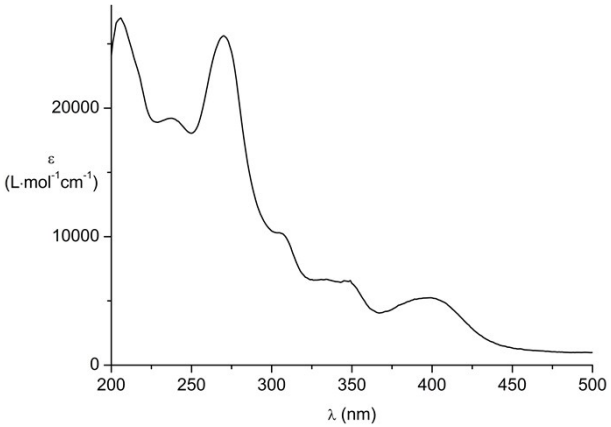


Figure S23: *Absorption spectrum* of **[LPt(CCPh)]** at room temperature in CH_2Cl_2.

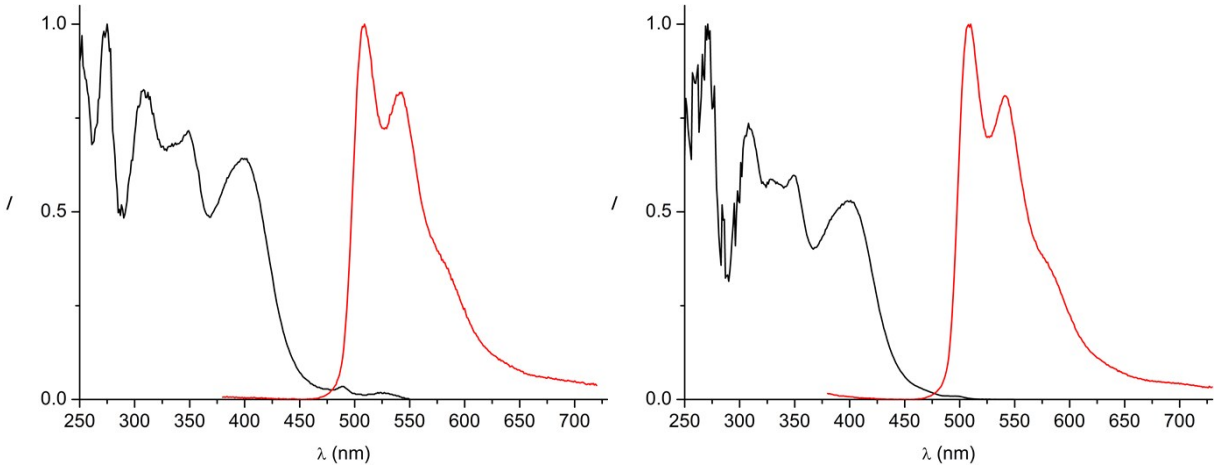


Figure S24: *Excitation* (black) and *Emission* (red) spectra of **[LPt(CCPh)]** in *aerated* (left) and *deaerated* (right) CH_2Cl_2 (λ_{exc}=312 nm; λ_{em}= 570 nm).

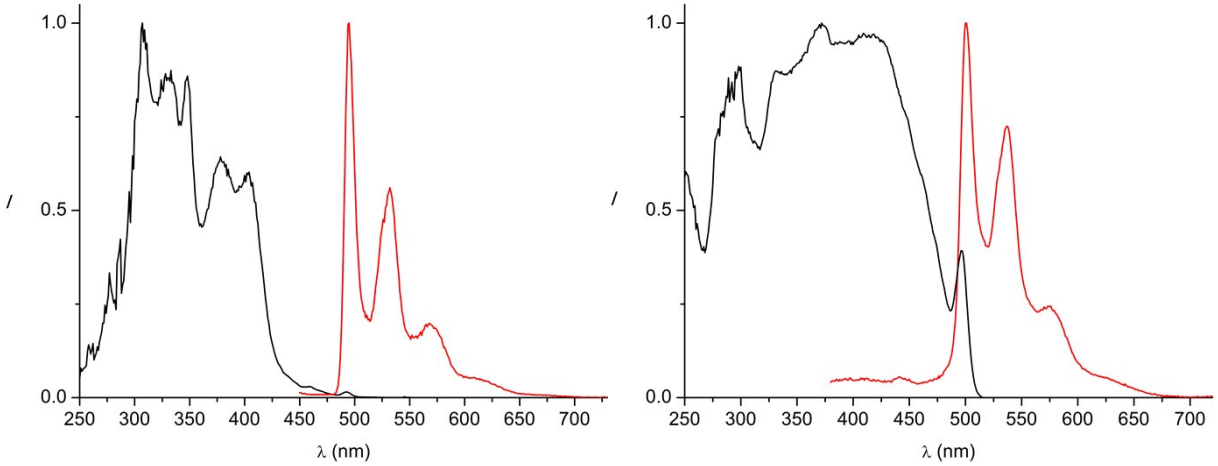
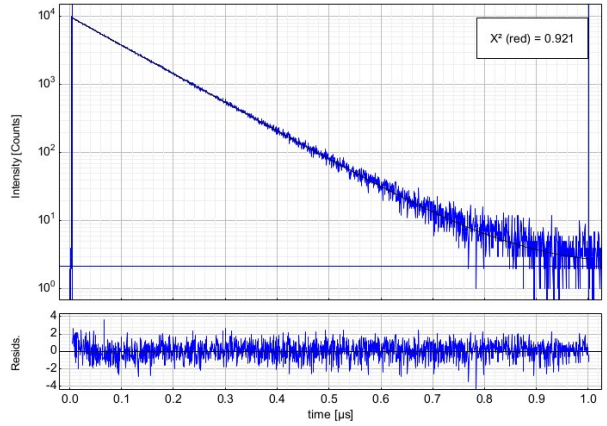
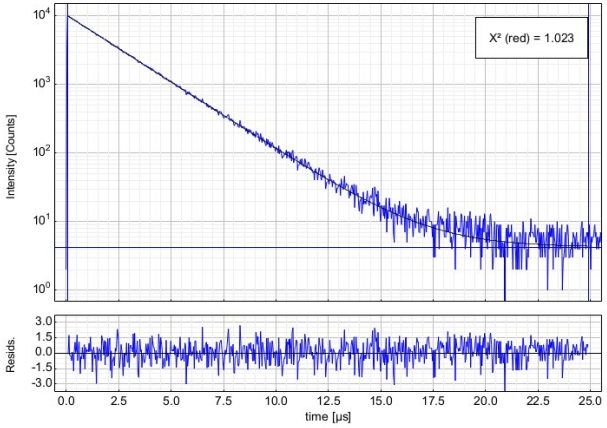


Figure S25: *Excitation* (black) and *Emission* (red) spectra of **[LPt(CCPh)]** in a *frozen glassy matrix* at 77K (left, CH_2Cl_2:MeOH 1:1, λ_{exc}=312 nm; λ_{em}= 570 nm) and in the *solid state at room temperature* (right, λ_{exc}= 312 nm; λ_{em}= 570 nm).



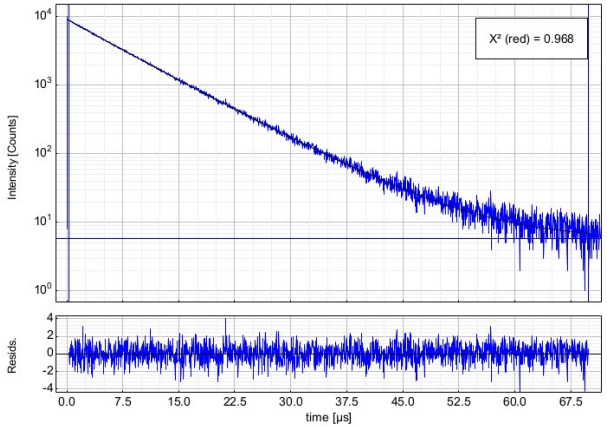
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	9442.4	-45.7	+45.7
τ_1 [µs]	0.103442	-0.000362	+0.000362
Bkgr. Dec [Cnts]	2.136	-0.651	+0.651

Figure S26: Left: Time-resolved luminescence decay of **[LPt(CCPh)]** in *aerated* CH_2Cl_2 including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



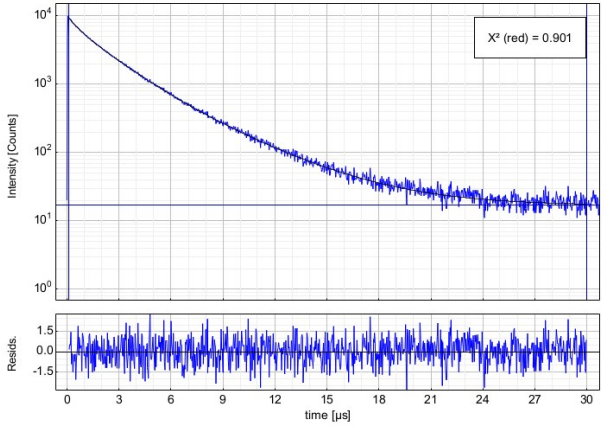
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	9871.3	-52.9	+52.9
τ_1 [µs]	2.21951	-0.00865	+0.00865
Bkgr. Dec [Cnts]	4.268	-0.673	+0.673

Figure S27: Left: Time-resolved luminescence decay of **[LPt(CCPh)]** in *deaerated* CH_2Cl_2 including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	5019.9	-39.6	+39.6
τ_1 [µs]	8.2925	-0.0442	+0.0442
A_2 [Cnts]	3755.8	-53.3	+53.3
τ_2 [µs]	6.0617	-0.0728	+0.0728
Bkgr. Dec [Cnts]	5.816	-0.891	+0.891

Figure S28: Left: Time-resolved luminescence decay of **[LPt(CCPh)]** in a *frozen glassy matrix (*CH_2Cl_2:MeOH 1:1) including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	2121.9	-28.4	+28.4
τ_1 [µs]	3.7775	-0.0314	+0.0314
A_2 [Cnts]	5506.1	-58.3	+58.3
τ_2 [µs]	1.8684	-0.0173	+0.0173
A_3 [Cnts]	1520	-144	+144
τ_3 [µs]	0.4715	-0.0563	+0.0563
Bkgr. Dec [Cnts]	16.89	-1.03	+1.03

Figure S29: Left: Time-resolved luminescence decay of **[LPt(CCPh)]** in the solid state including the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

Table S7: Photophysical data of **[LPt(CCPh)].**

	λ_{abs} ± 1(nm)	λ_{exc} ± 10 (nm)	λ_{em} ± 10 (nm)	τ ± 0.01 (μs)	Φ ± 0.02	k_r ± 0.1 (10^5 s^{-1})	k_{nr} ± 0.1 (10^5 s^{-1})
aerated	206	280	510	0.10	0.03	3.0	97.0
deaerated		270	510	2.22	0.35	1.6	2.9
77K		310	500	7.50[a)]	-	-	-
solid		370	500	2.62[a)]	0.23	0.9	2.9

a) intensity weighted averaged lifetime.