Spin-Orbit Effects in Square-Planar Pt(II) Complexes with Bidentate and Terdentate Ligands: Theoretical Absorption/Emission Spectroscopy

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Cartesian cooordinates of the optimized geometries of the five complexes $[Pt(bpy)Cl_2]$ **1** , $[Pt(ppy)Cl_2]^-$ **2**, $[Pt(tpy)Cl]^+$ **3** [Pt(phbpyR)Cl] **4** and [Pt(dpybR)Cl] **5** (R = CH_3) in the electronic ground state

Structure of **1**

C	0.015869	1.716152	3.464381
C	0.000611	2.976451	2.885945
C	0.002303	1.923637	0.731437
C	0.020704	0.598319	2.646901
C	0.002303	1.923637	-0.731437
C	0.000611	2.976451	-2.885945
H	-0.005599	3.868671	-3.494940
C	0.015869	1.716152	-3.464381
C	0.020704	0.598319	-2.646901
H	0.023304	1.587765	4.535309
H	-0.005599	3.868671	3.494940
H	0.028940	-0.403645	3.044053
H	0.023304	1.587765	-4.535309
H	0.028940	-0.403645	-3.044053
Pt	0.000644	-0.880236	0.000000
N	0.012956	0.695206	-1.310570
N	0.012956	0.695206	1.310570
C	-0.006533	3.077131	-1.504424
H	-0.017334	4.045604	-1.033048
C	-0.006533	3.077131	1.504424
H	-0.017334	4.045604	1.033048
Cl	-0.025544	-2.560947	-1.650675
Cl	-0.025544	-2.560947	1.650675

Structure of **2**

C	1.718996	-3.474781	0.000000
C	2.985204	-2.900284	0.000000
C	1.945172	-0.730710	0.000000
C	0.609775	-2.648550	0.000000
C	1.920753	0.724896	0.000000
C	2.989433	2.890694	0.000000
H	3.886723	3.494837	0.000000
C	1.729043	3.487143	0.000000
C	0.570388	2.710837	0.000000
H	1.584557	-4.545315	0.000000
H	3.873985	-3.515724	0.000000
H	-0.396012	-3.037063	0.000000
H	1.649665	4.566498	0.000000
H	-0.390966	3.202518	0.000000
Pt	-0.883774	-0.007743	0.000000
C	0.630675	1.312209	0.000000
N	0.711810	-1.310191	0.000000
C	3.080915	1.507665	0.000000
H	4.057488	1.044003	0.000000
C	3.093278	-1.521489	0.000000
H	4.064514	-1.052900	0.000000

Cl	-2.618173	1.609644	0.000000
Cl	-2.644997	-1.806193	0.000000

Structure of **3**

Pt	-0.008180	0.921410	0.000000
Cl	-0.011612	3.279121	0.000000
N	-0.008597	0.575713	-2.023176
N	-0.008597	0.575713	2.023176
C	-0.007155	-1.672671	1.184710
C	-0.007597	-3.060662	1.207092
H	-0.008182	-3.598366	2.140536
C	-0.007759	-3.748266	0.000000
C	-0.007597	-3.060662	-1.207092
H	-0.008182	-3.598366	-2.140536
C	-0.007155	-1.672671	-1.184710
C	-0.008304	-0.756676	-2.333697
C	-0.010404	-1.176584	-3.651549
H	-0.010563	-2.229522	-3.881879
C	-0.012238	-0.231808	-4.669666
H	-0.013719	-0.550174	-5.701538
C	-0.012162	1.113806	-4.340676
H	-0.013549	1.879778	-5.099700
C	-0.010352	1.482511	-3.003119
H	-0.010372	2.514300	-2.689271
C	-0.010352	1.482511	3.003119
H	-0.010372	2.514300	2.689271
C	-0.012162	1.113806	4.340676
H	-0.013549	1.879778	5.099700
C	-0.012238	-0.231808	4.669666
H	-0.013719	-0.550174	5.701538
C	-0.010404	-1.176584	3.651549
H	-0.010563	-2.229522	3.881879
C	-0.008304	-0.756676	2.333697
H	-0.008388	-4.827768	0.000000
N	-0.006575	-1.039109	0.000000

Structure of **4**

Pt	-0.008706	0.979849	-0.041700
Cl	-0.010508	3.346390	-0.008642
N	-0.008869	0.586419	2.086218
C	-0.008137	-1.638227	1.184038
C	-0.007599	-3.026168	1.217354
H	-0.007527	-3.556256	2.154956
C	-0.007286	-3.725468	0.015744
C	-0.007773	-3.044719	-1.191407
H	-0.007889	-3.586821	-2.123243
C	-0.008239	-1.651482	-1.189177
C	-0.009152	-0.743695	-2.335500
C	-0.010776	-1.192799	-3.657246
H	-0.011109	-2.251432	-3.876971
C	-0.011973	-0.278413	-4.701856
H	-0.013222	-0.626761	-5.725209
C	-0.011635	1.085284	-4.418001
H	-0.012514	1.800160	-5.229968
C	-0.010368	1.540591	-3.098295
H	-0.010385	2.604144	-2.905833
C	-0.009830	1.463292	3.090830
H	-0.009418	2.504423	2.802955
C	-0.011410	1.066129	4.419631
H	-0.012162	1.810167	5.200470
C	-0.012226	-0.290418	4.709394
H	-0.013747	-0.637278	5.732264
C	-0.011134	-1.205751	3.666163
H	-0.011856	-2.263845	3.870871
C	-0.009189	-0.744348	2.357222

H	-0.006884	-4.805511	0.024312
N	-0.008076	-1.001715	-0.003156
C	-0.009303	0.648938	-2.026220

Structure of **5**

Pt	-0.004448	0.925233	0.000000
Cl	-0.006621	3.423409	0.000000
N	-0.006520	0.553771	-2.042221
N	-0.006520	0.553771	2.042221
C	-0.005111	-1.684879	1.216637
C	-0.006634	-3.082480	1.209001
H	-0.011818	-3.640036	2.136127
C	-0.004190	-3.790085	0.000000
C	-0.006634	-3.082480	-1.209001
H	-0.011818	-3.640036	-2.136127
C	-0.005111	-1.684879	-1.216637
C	-0.009547	-0.781383	-2.368187
C	-0.016389	-1.173646	-3.700317
H	-0.019956	-2.224937	-3.943540
C	-0.018044	-0.216594	-4.703055
H	-0.023194	-0.519351	-5.740411
C	-0.012751	1.128384	-4.356294
H	-0.013145	1.904679	-5.105253
C	-0.007411	1.472878	-3.014653
H	-0.004262	2.500569	-2.685102
C	-0.007411	1.472878	3.014653
H	-0.004262	2.500569	2.685102
C	-0.012751	1.128384	4.356294
H	-0.013145	1.904679	5.105253
C	-0.018044	-0.216594	4.703055
H	-0.023194	-0.519351	5.740411
C	-0.016389	-1.173646	3.700317
H	-0.019956	-2.224937	3.943540
C	-0.009547	-0.781383	2.368187
C	-0.002503	-1.007983	0.000000
C	0.027736	-5.300279	0.000000
H	-0.465467	-5.707206	0.881643
H	1.055906	-5.670117	0.000000
H	-0.465467	-5.707206	-0.881643

Table S1. TD-DFT/B3LYP (without SOC) transition energies (in eV) to the low-lying singlet and triplet excited states of $[Pt(bpy)Cl_2]$ **1** and $[Pt(tpy)Cl]^+$ **3** and associated oscillator strengths f.

	Singlet transition energies	f	Triplet transition energies
$[Pt(bpy)Cl_2]$ **1**	3.13	0.003367	2.81
	3.34	0.004277	2.86
	3.40	0.176000	2.98
	3.40	0.001137	3.00
	3.53	0.000240	3.05
	3.53	0.001389	3.22
	3.56	0.000036	3.28
	3.61	0.001135	3.31
	4.02	0.403000	3.47
	4.10	0.000688	3.95
	4.24	0.284000	4.03
	4.36	0.000255	4.09

	4.47	0.013550	4.10
	4.47	0.171000	4.22
	4.57	0.314100	4.35
	4.57	0.000042	4.38
	4.63	0.015380	4.44
	4.63	0.000257	4.47
	4.75	0.000118	4.52
	4.85	0.000125	4.56
	4.90	0.005373	4.61
	5.12	0.049880	4.62
	5.13	0.009014	4.73
	5.18	0.017930	4.83
	5.33	0.000320	4.88
	5.37	0.000272	5.09
	5.38	0.000002	5.12
	5.39	0.187700	5.26
	5.55	0.015910	5.30
	5.62	0.000108	5.31
	5.72	0.000046	5.41
	5.83	0.019520	5.44
	5.87	0.004438	5.48
	5.87	0.001697	5.49
	5.98	0.002975	5.55
	5.99	0.155400	5.59
	6.01	0.000007	5.72
	6.06	0.450300	5.76
	6.13	0.000006	5.77
	6.14	0.062660	5.80
$[Pt(tpy)Cl]^+$ **3**	3.24	0.075550	2.78
	3.35	0.020200	2.93
	3.35	0.008036	3.12
	3.44	0.000001	3.25
	3.60	0.024890	3.39
	3.80	0.712400	3.39
	3.90	0.000001	3.40
	3.93	0.000002	3.51
	3.99	0.172400	3.54
	3.99	0.001062	3.65
	4.07	0.080320	3.75
	4.15	0.045870	3.88
	4.26	0.000003	3.89
	4.30	0.235600	3.95
	4.58	0.043250	3.97
	4.60	0.006322	4.11
	4.64	0.154100	4.19

4.85	0.138100	4.29
4.88	0.000192	4.40
4.90	0.000838	4.51
4.92	0.000659	4.57
4.93	0.000016	4.68
4.94	0.011620	4.69
4.96	0.740800	4.85
4.98	0.083800	4.87
4.99	0.000094	4.88
5.14	0.000000	4.90
5.32	0.000366	4.91
5.32	0.073900	4.94
5.35	0.001303	4.95
5.36	0.070650	5.03
5.44	0.174900	5.04
5.46	0.007046	5.18
5.60	0.008009	5.20
5.62	0.000085	5.26
5.70	0.000079	5.31
5.71	0.000252	5.41
5.72	0.013940	5.44
5.75	0.000000	5.54
5.81	0.022680	5.56

Table S2. TD-DFT/B3LYP (without SOC) transition energies (in eV) to the low-lying singlet and triplet excited states of $[Pt(ppy)Cl_2]^-$ **2**, [Pt(phbpyR)Cl] **4** and [Pt(dpybR)Cl] **5** (R = CH_3) and associated oscillator strengths f (allowed transitions by symmetry only: A' and A").

	Singlet transition energies	f	Triplet transition energies
$[Pt(ppy)Cl_2]^-$ **2**			
	3.13	0.036740	2.76
	3.49	0.011200	3.18
	3.59	0.188700	3.27
	3.70	0.000176	3.39
	3.80	0.000369	3.44
	3.85	0.056490	3.48
	3.98	0.018440	3.49
	4.04	0.001125	3.57
	4.08	0.264000	3.69
	4.12	0.163400	3.72
	4.26	0.028800	3.93
	4.28	0.309500	4.00
	4.44	0.000109	4.24
	4.49	0.000011	4.24
	4.65	0.020760	4.40

	4.79	0.049390	4.42
	4.90	0.007532	4.48
	4.91	0.482200	4.61
	5.08	0.000076	4.79
	5.11	0.000610	4.84
	5.13	0.113200	4.95
	5.16	0.033730	5.00
	5.29	0.073590	5.03
	5.32	0.024210	5.05
	5.37	0.000677	5.10
	5.40	0.019400	5.12
	5.57	0.002497	5.25
	5.57	0.023040	5.29
	5.61	0.000182	5.33
	5.65	0.016570	5.39
	5.67	0.000083	5.43
	5.70	0.086260	5.44
	5.84	0.088140	5.56
	5.85	0.424100	5.58
	5.94	0.001174	5.62
	5.97	0.230200	5.66
	6.00	0.016140	5.68
	6.01	0.017640	5.78
	6.02	0.006294	5.83
	6.10	0.097160	5.89
[Pt(phbpyR)Cl] **4**	2.77	0.004346	2.54
	3.12	0.005125	2.72
	3.16	0.056850	2.92
	3.23	0.003563	3.02
	3.43	0.195800	3.15
	3.61	0.350200	3.25
	3.73	0.207500	3.47
	3.77	0.002502	3.62
	3.92	0.001850	3.74
	4.10	0.197100	3.80
	4.22	0.235400	3.81
	4.26	0.000057	3.89
	4.33	0.095570	3.89
	4.37	0.000016	3.92
	4.41	0.071980	3.99
	4.44	0.000282	4.01
	4.45	0.115400	4.04
	4.49	0.352800	4.11
	4.51	0.000346	4.29
	4.54	0.019110	4.34

	4.68	0.000019	4.36
	4.87	0.160700	4.40
	4.89	0.025950	4.47
	5.03	0.160800	4.59
	5.12	0.020230	4.61
	5.14	0.017090	4.67
	5.23	0.001706	4.84
	5.24	0.032920	4.87
	5.27	0.004475	4.99
	5.27	0.434100	5.05
	5.33	0.000074	5.13
	5.36	0.000001	5.16
	5.42	0.130800	5.18
	5.43	0.005331	5.19
	5.45	0.004434	5.25
	5.48	0.019010	5.30
	5.49	0.008696	5.31
	5.62	0.011770	5.34
	5.67	0.061700	5.35
	5.70	0.136700	5.40
[Pt(dpybR)Cl] **5** (R = CH_3)			
	3.17	0.003264	2.68
	3.20	0.099080	2.76
	3.61	0.005118	3.04
	3.61	0.005321	3.25
	3.70	0.000000	3.40
	3.76	0.000000	3.61
	3.91	0.000660	3.67
	3.92	0.043080	3.71
	3.95	0.000121	3.78
	4.21	0.240400	3.84
	4.28	0.015640	3.88
	4.33	0.107500	3.88
	4.35	0.000324	3.98
	4.50	0.000001	4.06
	4.55	0.048460	4.17
	4.55	0.015200	4.20
	4.64	0.011690	4.27
	4.67	0.000049	4.31
	4.76	0.003277	4.38
	4.81	0.000775	4.38
	4.83	0.028340	4.43
	4.87	0.000104	4.43
	4.90	0.000477	4.47
	4.93	0.353600	4.62

4.95	0.000196	4.63
4.97	0.000016	4.72
5.09	0.008831	4.77
5.18	0.000012	4.82
5.20	0.018190	4.82
5.20	0.099720	4.93
5.28	0.000032	4.95
5.30	0.065520	5.06
5.38	0.108900	5.09
5.50	0.373800	5.14
5.56	0.011210	5.20
5.59	0.003514	5.24
5.60	0.000053	5.27
5.69	0.063100	5.35
5.72	0.000108	5.35
5.76	0.022010	5.45

Table S3. TD-DFT/B3LYP transition energies (in eV) to the low-lying SO excited states of $[Pt(bpy)Cl_2]$ **1** and $[Pt(tpy)Cl]^+$ **3** and associated oscillator strengths f.

	transition energies	f
$[Pt(bpy)Cl_2]$ **1**	2.43	0.000000
	2.43	0.000025
	2.54	0.000274
	2.54	0.000109
	2.56	0.001555
	2.66	0.000624
	2.69	0.000001
	2.70	0.000406
	2.72	0.000683
	2.76	0.000002
	2.81	0.001191
	2.82	0.000792
	2.85	0.000616
	2.88	0.001481
	2.90	0.000011
	2.99	0.076480

	3.19	0.000000
	3.20	0.000579
	3.20	0.008916
	3.34	0.001382
	3.36	0.000002
	3.39	0.000145
	3.53	0.000395
	3.55	0.000012
	3.58	0.000782
	3.58	0.000639
	3.59	0.014580
	3.67	0.003031
	3.67	0.000078
	3.69	0.001410
	3.70	0.001971
	3.78	0.070270
	3.78	0.001771
	3.84	0.000270
	3.84	0.014570
	3.86	0.000056
	3.86	0.000033
	3.86	0.022410
	3.87	0.000970
	3.88	0.000077
	3.88	0.004010
	3.93	0.240900
	3.93	0.000352
	3.94	0.000187
	3.94	0.004114
	4.04	0.009674
	4.05	0.000665
	4.05	0.000459
	4.06	0.001349

	4.07	0.250200
	4.08	0.000010
	4.08	0.037480
	4.09	0.001662
	4.10	0.006391
	4.18	0.075060
	4.23	0.000613
	4.23	0.000518
	4.24	0.024260
	4.25	0.188700
	4.36	0.000003
	4.36	0.000062
	4.36	0.000222
	4.36	0.000155
	4.36	0.001908
	4.36	0.005769
	4.47	0.000025
	4.47	0.000408
	4.47	0.002917
	4.50	0.002004
	4.50	0.000080
	4.51	0.000069
	4.63	0.015860
	4.65	0.000090
	4.65	0.025580
	4.65	0.001828
	4.66	0.000052
	4.78	0.013970
	4.78	0.001193
	4.79	0.000064
	4.82	0.011170
	4.83	0.001273
	4.83	0.002248

	4.83	0.001106
	4.84	0.047230
	4.86	0.000308
	4.86	0.000171
	4.87	0.000238
	4.88	0.000046
	4.88	0.026990
	4.89	0.009901
	4.89	0.004511
	4.91	0.014770
	5.01	0.036620
	5.04	0.000020
	5.05	0.000233
	5.08	0.078940
	5.10	0.001318
	5.10	0.017530
	5.11	0.000021
	5.12	0.001098
	5.12	0.000009
	5.12	0.001533
	5.13	0.017320
	5.15	0.028530
	5.20	0.019240
	5.24	0.005444
	5.24	0.004944
	5.25	0.000626
	5.26	0.001691
	5.28	0.000015
	5.29	0.034070
	5.32	0.001888
	5.33	0.012540
	5.33	0.000014
	5.33	0.002297

	5.33	0.000002
	5.37	0.000273
	5.41	0.000582
	5.42	0.064040
	5.45	0.000240
	5.46	0.000062
	5.47	0.000023
	5.48	0.000333
	5.48	0.000054
	5.49	0.035300
	5.49	0.000031
	5.50	0.003183
	5.50	0.000050
	5.51	0.011090
	5.52	0.020590
	5.52	0.000008
	5.54	0.012870
	5.56	0.000005
	5.56	0.000028
	5.57	0.001061
	5.58	0.000016
	5.58	0.000012
	5.59	0.000070
	5.63	0.000103
	5.66	0.000004
	5.68	0.000034
	5.69	0.006479
	5.70	0.013610
	5.72	0.000011
	5.72	0.000742
	5.73	0.000075
	5.77	0.000033
	5.78	0.005099

	5.79	0.000003
	5.80	0.000055
	5.90	0.003764
	5.93	0.000053
	5.96	0.021510
	5.96	0.013870
	6.03	0.002938
	6.04	0.125900
	6.09	0.434500
	6.17	0.061560
	6.21	0.000005
	6.41	0.000027
$[Pt(tpy)Cl]^+$ **3**	2.61	0.000479
	2.61	0.000000
	2.62	0.000847
	2.79	0.000619
	2.79	0.000000
	2.81	0.001573
	2.91	0.040410
	2.95	0.036980
	3.02	0.000000
	3.03	0.000464
	3.04	0.000031
	3.05	0.000005
	3.05	0.010220
	3.11	0.001303
	3.13	0.000014
	3.15	0.000000
	3.16	0.006359
	3.17	0.001003
	3.23	0.003465
	3.33	0.000403
	3.34	0.004794

	3.34	0.000000
	3.37	0.041770
	3.38	0.018940
	3.41	0.000127
	3.41	0.000051
	3.46	0.004273
	3.48	0.000339
	3.50	0.013510
	3.52	0.000003
	3.55	0.137600
	3.60	0.000270
	3.60	0.000003
	3.61	0.053840
	3.62	0.055870
	3.71	0.000001
	3.74	0.002764
	3.75	0.022440
	3.89	0.002835
	3.90	0.000004
	3.92	0.372500
	3.96	0.000121
	3.96	0.000001
	3.97	0.085540
	3.97	0.000276
	4.03	0.003461
	4.03	0.000003
	4.03	0.003094
	4.03	0.000888
	4.09	0.000002
	4.09	0.000125
	4.10	0.009010
	4.11	0.006814
	4.12	0.000008

	4.12	0.000224
	4.17	0.008800
	4.21	0.164300
	4.25	0.027530
	4.25	0.000032
	4.25	0.000014
	4.26	0.001533
	4.26	0.000038
	4.26	0.000006
	4.27	0.020310
	4.33	0.000257
	4.37	0.002119
	4.37	0.000027
	4.38	0.000008
	4.38	0.006336
	4.39	0.058010
	4.41	0.089460
	4.42	0.013060
	4.42	0.000029
	4.43	0.000052
	4.45	0.090970
	4.45	0.000100
	4.45	0.002599
	4.46	0.000067
	4.50	0.000005
	4.51	0.017420
	4.51	0.000178
	4.51	0.000019
	4.53	0.013330
	4.54	0.000072
	4.55	0.000008
	4.60	0.092780
	4.61	0.069250

	4.66	0.024780
	4.82	0.003680
	4.82	0.000071
	4.82	0.000036
	4.83	0.011170
	4.85	0.000073
	4.85	0.000026
	4.92	0.439000
	4.94	0.007059
	4.95	0.000019
	4.95	0.012620
	4.95	0.002787
	4.96	0.000020
	4.97	0.006038
	4.97	0.000054
	4.97	0.000025
	4.97	0.009483
	4.98	0.019000
	4.99	0.000276
	4.99	0.107700
	5.00	0.000125
	5.00	0.000221
	5.01	0.053290
	5.01	0.000330
	5.03	0.011390
	5.05	0.000069
	5.05	0.024470
	5.09	0.000011
	5.11	0.051530
	5.11	0.128700
	5.14	0.000066
	5.17	0.000001
	5.19	0.001595

	5.22	0.007783
	5.23	0.000451
	5.24	0.000043
	5.24	0.000033
	5.25	0.000033
	5.27	0.005651
	5.27	0.000086
	5.28	0.007540
	5.29	0.000099
	5.29	0.000010
	5.29	0.019560
	5.30	0.000077
	5.31	0.004218
	5.31	0.000106
	5.32	0.000003
	5.35	0.000314
	5.37	0.024970
	5.38	0.023870
	5.40	0.000043
	5.42	0.000005
	5.43	0.002933
	5.44	0.003506
	5.45	0.063890
	5.46	0.000179
	5.46	0.086860
	5.53	0.004981
	5.56	0.037160
	5.57	0.003140
	5.57	0.001089
	5.57	0.000019
	5.57	0.000004
	5.58	0.016620
	5.60	0.031700

	5.63	0.000087
	5.68	0.005970
	5.71	0.000091
	5.73	0.013310
	5.80	0.000000
	5.83	0.022260
	5.91	0.000170

Table S4. TD-DFT/B3LYP transition energies (in eV) to the SO excited states of $[Pt(ppy)Cl_2]^-$ **2**, [Pt(phbpyR)Cl] **4** and [Pt(dpybR)Cl] **5** (R = CH_3) and associated oscillator strengths f.

	transition energies	f
$[Pt(ppy)Cl_2]^-$ **2**	2.64	0.000019
	2.64	0.000770
	2.65	0.000449
	2.87	0.022460
	2.88	0.000716
	2.89	0.006381
	2.92	0.002645
	2.94	0.002098
	2.96	0.000225
	3.02	0.021670
	3.07	0.017340
	3.09	0.000429
	3.16	0.036080
	3.23	0.000925
	3.27	0.000115
	3.30	0.010480
	3.32	0.021190
	3.33	0.001418
	3.38	0.000559
	3.49	0.000052
	3.49	0.001978

	3.49	0.002077
	3.64	0.009734
	3.65	0.000654
	3.67	0.003272
	3.68	0.035760
	3.69	0.031130
	3.73	0.008840
	3.73	0.004040
	3.74	0.000926
	3.80	0.015380
	3.82	0.002352
	3.85	0.007229
	3.85	0.051680
	3.88	0.001113
	3.89	0.057690
	3.90	0.000682
	3.91	0.013330
	3.93	0.000968
	3.94	0.000857
	3.95	0.085010
	4.07	0.020400
	4.13	0.172700
	4.13	0.000761
	4.14	0.006143
	4.14	0.028010
	4.19	0.000694
	4.21	0.140200
	4.31	0.003682
	4.31	0.039000
	4.33	0.000704
	4.34	0.016200
	4.35	0.002779
	4.42	0.003985

	4.42	0.000157
	4.43	0.001407
	4.44	0.001594
	4.47	0.024350
	4.52	0.000642
	4.52	0.001567
	4.53	0.000269
	4.58	0.002763
	4.59	0.000312
	4.59	0.001792
	4.60	0.002758
	4.60	0.000514
	4.61	0.009612
	4.62	0.067750
	4.65	0.120500
	4.68	0.067340
	4.69	0.005160
	4.71	0.006120
	4.72	0.120200
	4.75	0.091630
	4.82	0.006902
	4.82	0.001194
	4.84	0.011570
	4.84	0.033980
	4.87	0.010210
	4.90	0.001873
	4.91	0.004629
	4.92	0.030090
	4.99	0.001960
	5.00	0.004980
	5.00	0.000923
	5.02	0.001693
	5.02	0.003258

	5.02	0.010440
	5.04	0.000391
	5.05	0.000747
	5.06	0.000342
	5.10	0.000308
	5.10	0.002778
	5.11	0.001097
	5.11	0.000228
	5.12	0.001561
	5.13	0.020250
	5.15	0.000244
	5.16	0.007813
	5.23	0.000710
	5.23	0.006217
	5.25	0.000293
	5.29	0.068360
	5.30	0.060280
	5.33	0.000514
	5.33	0.002826
	5.34	0.001151
	5.36	0.041590
	5.38	0.000539
	5.40	0.000810
	5.40	0.004968
	5.41	0.018790
	5.43	0.003486
	5.43	0.000814
	5.44	0.000559
	5.45	0.001952
	5.46	0.000151
	5.46	0.003160
	5.50	0.002924
	5.50	0.022040

	5.51	0.000959
	5.51	0.021890
	5.54	0.020840
	5.56	0.001587
	5.57	0.001370
	5.58	0.004945
	5.58	0.000783
	5.59	0.003555
	5.59	0.005993
	5.60	0.007465
	5.60	0.000131
	5.61	0.000968
	5.63	0.001076
	5.64	0.032800
	5.66	0.000514
	5.67	0.002905
	5.67	0.001207
	5.68	0.005034
	5.69	0.018410
	5.69	0.004691
	5.72	0.064440
	5.74	0.000956
	5.75	0.002038
	5.76	0.015900
	5.81	0.002814
	5.82	0.091790
	5.85	0.130000
	5.86	0.136800
	5.91	0.028530
	5.92	0.004052
	5.94	0.039630
	5.94	0.007063
	5.95	0.006752

	5.96	0.111300
	5.98	0.001543
	6.00	0.156600
	6.05	0.021070
	6.07	0.013830
	6.15	0.091130
	6.21	0.006439
[Pt(phbpyR)Cl] **4**	2.40	0.000069
	2.40	0.000226
	2.41	0.000337
	2.50	0.000584
	2.51	0.000068
	2.54	0.001254
	2.58	0.004491
	2.75	0.026920
	2.81	0.000072
	2.82	0.001513
	2.82	0.000188
	3.02	0.001126
	3.03	0.000575
	3.05	0.001219
	3.14	0.008892
	3.22	0.000156
	3.22	0.041790
	3.24	0.002023
	3.28	0.108100
	3.29	0.000118
	3.30	0.016830
	3.30	0.001260
	3.33	0.030710
	3.37	0.081270
	3.39	0.000058
	3.43	0.000859

	3.45	0.018590
	3.47	0.000078
	3.48	0.008266
	3.51	0.000045
	3.51	0.011440
	3.52	0.000143
	3.53	0.000984
	3.54	0.037580
	3.56	0.014490
	3.67	0.265400
	3.71	0.000058
	3.72	0.000067
	3.73	0.004725
	3.74	0.000092
	3.75	0.038920
	3.78	0.000366
	3.81	0.002689
	3.82	0.000207
	3.84	0.001071
	3.85	0.043960
	3.90	0.000094
	3.90	0.005303
	3.90	0.000185
	3.93	0.072150
	3.95	0.000006
	3.95	0.000060
	3.96	0.072500
	4.03	0.054380
	4.05	0.044740
	4.06	0.000173
	4.06	0.000211
	4.09	0.052450
	4.11	0.000310

	4.12	0.000584
	4.12	0.036600
	4.16	0.002086
	4.17	0.000036
	4.17	0.000032
	4.17	0.006967
	4.19	0.000061
	4.23	0.000035
	4.27	0.176000
	4.33	0.000075
	4.33	0.005403
	4.35	0.000037
	4.36	0.003301
	4.36	0.000073
	4.36	0.000039
	4.42	0.023820
	4.44	0.022500
	4.45	0.000029
	4.47	0.205400
	4.49	0.050380
	4.50	0.000387
	4.51	0.053440
	4.54	0.052170
	4.55	0.000049
	4.56	0.008294
	4.58	0.000043
	4.61	0.000072
	4.62	0.009115
	4.62	0.000066
	4.63	0.037740
	4.64	0.000156
	4.69	0.013680
	4.69	0.000107

	4.71	0.000171
	4.72	0.035090
	4.73	0.000171
	4.76	0.070350
	4.77	0.000102
	4.78	0.000141
	4.79	0.054910
	4.80	0.030060
	4.82	0.035960
	4.82	0.001474
	4.83	0.000311
	4.86	0.004314
	4.86	0.000100
	4.87	0.000135
	4.91	0.028240
	4.95	0.009724
	4.96	0.000913
	4.96	0.000136
	4.98	0.065420
	5.00	0.005316
	5.01	0.000140
	5.01	0.000224
	5.04	0.137300
	5.07	0.000223
	5.07	0.025450
	5.07	0.018320
	5.08	0.000079
	5.13	0.000725
	5.14	0.028040
	5.15	0.012410
	5.15	0.000037
	5.17	0.035460
	5.18	0.000307

	5.21	0.000552
	5.21	0.130700
	5.23	0.000562
	5.23	0.018580
	5.24	0.032830
	5.26	0.001328
	5.27	0.023720
	5.29	0.014440
	5.29	0.001332
	5.29	0.001514
	5.30	0.006581
	5.31	0.000251
	5.31	0.006344
	5.32	0.009559
	5.33	0.004991
	5.33	0.000358
	5.34	0.000347
	5.38	0.001766
	5.38	0.028670
	5.39	0.000271
	5.39	0.082980
	5.40	0.000856
	5.43	0.027150
	5.45	0.000672
	5.47	0.004089
	5.50	0.019330
	5.54	0.058950
	5.57	0.006892
	5.62	0.064120
	5.66	0.000934
	5.69	0.039770
	5.70	0.069260
	5.70	0.004638

	5.74	0.006997
	5.76	0.088040
[Pt(dpybR)Cl] **5** ($R = CH_3$)	2.60	0.000003
	2.60	0.000222
	2.61	0.000155
	2.69	0.000022
	2.69	0.000000
	2.70	0.000181
	2.95	0.002757
	2.96	0.000000
	2.97	0.000079
	2.97	0.001702
	3.00	0.000001
	3.01	0.001055
	3.05	0.001301
	3.06	0.075260
	3.19	0.016480
	3.41	0.013250
	3.42	0.000059
	3.43	0.000016
	3.43	0.002971
	3.48	0.000000
	3.50	0.001176
	3.52	0.000630
	3.56	0.000000
	3.60	0.002450
	3.60	0.001210
	3.61	0.001390
	3.66	0.000187
	3.68	0.000001
	3.70	0.002116
	3.70	0.001372

	3.72	0.000000
	3.77	0.000986
	3.78	0.000059
	3.78	0.013110
	3.82	0.016930
	3.82	0.000002
	3.82	0.001294
	3.83	0.000204
	3.83	0.002646
	3.84	0.000004
	3.84	0.000608
	3.86	0.008773
	3.87	0.010190
	3.91	0.000001
	3.92	0.000428
	3.94	0.000643
	3.96	0.002589
	3.97	0.000001
	3.98	0.000489
	3.99	0.009936
	4.00	0.000205
	4.07	0.000041
	4.13	0.051830
	4.13	0.017650
	4.15	0.013270
	4.16	0.000005
	4.16	0.000271
	4.17	0.002656
	4.18	0.001685
	4.18	0.000001
	4.18	0.000073
	4.22	0.000457
	4.22	0.000007

	4.24	0.048150
	4.30	0.085090
	4.35	0.000002
	4.35	0.000077
	4.36	0.008985
	4.37	0.000004
	4.37	0.000083
	4.38	0.036070
	4.39	0.027610
	4.41	0.001024
	4.42	0.000013
	4.42	0.000290
	4.46	0.000021
	4.46	0.000004
	4.51	0.056490
	4.51	0.024280
	4.52	0.000007
	4.53	0.006945
	4.57	0.000034
	4.58	0.000001
	4.59	0.008740
	4.60	0.003422
	4.60	0.000095
	4.61	0.060790
	4.64	0.012180
	4.71	0.000002
	4.72	0.000184
	4.73	0.002290
	4.73	0.000044
	4.76	0.000030
	4.76	0.000006
	4.78	0.025290
	4.79	0.005336

	4.80	0.000242
	4.80	0.001597
	4.81	0.004075
	4.81	0.000168
	4.82	0.000078
	4.82	0.002327
	4.85	0.000166
	4.89	0.000363
	4.93	0.000822
	4.93	0.000075
	4.93	0.004257
	4.94	0.000221
	4.95	0.013540
	4.95	0.000094
	4.96	0.003218
	4.97	0.047850
	4.97	0.020900
	5.00	0.002058
	5.00	0.000073
	5.00	0.000071
	5.06	0.116100
	5.06	0.005670
	5.08	0.000057
	5.10	0.064000
	5.10	0.001080
	5.10	0.008547
	5.14	0.007894
	5.15	0.000023
	5.15	0.000066
	5.17	0.045050
	5.17	0.000328
	5.20	0.000009
	5.21	0.006986

	5.21	0.000009
	5.22	0.003665
	5.22	0.014380
	5.24	0.000135
	5.25	0.011220
	5.25	0.050420
	5.25	0.004854
	5.27	0.000024
	5.28	0.000004
	5.29	0.000128
	5.33	0.000002
	5.33	0.000003
	5.36	0.011970
	5.39	0.000038
	5.39	0.000034
	5.39	0.068000
	5.41	0.005260
	5.41	0.016170
	5.43	0.000112
	5.44	0.000004
	5.48	0.076810
	5.51	0.000003
	5.51	0.000026
	5.53	0.259700
	5.54	0.066910
	5.63	0.028160
	5.63	0.000378
	5.65	0.003724
	5.72	0.001812
	5.73	0.057530
	5.77	0.021600

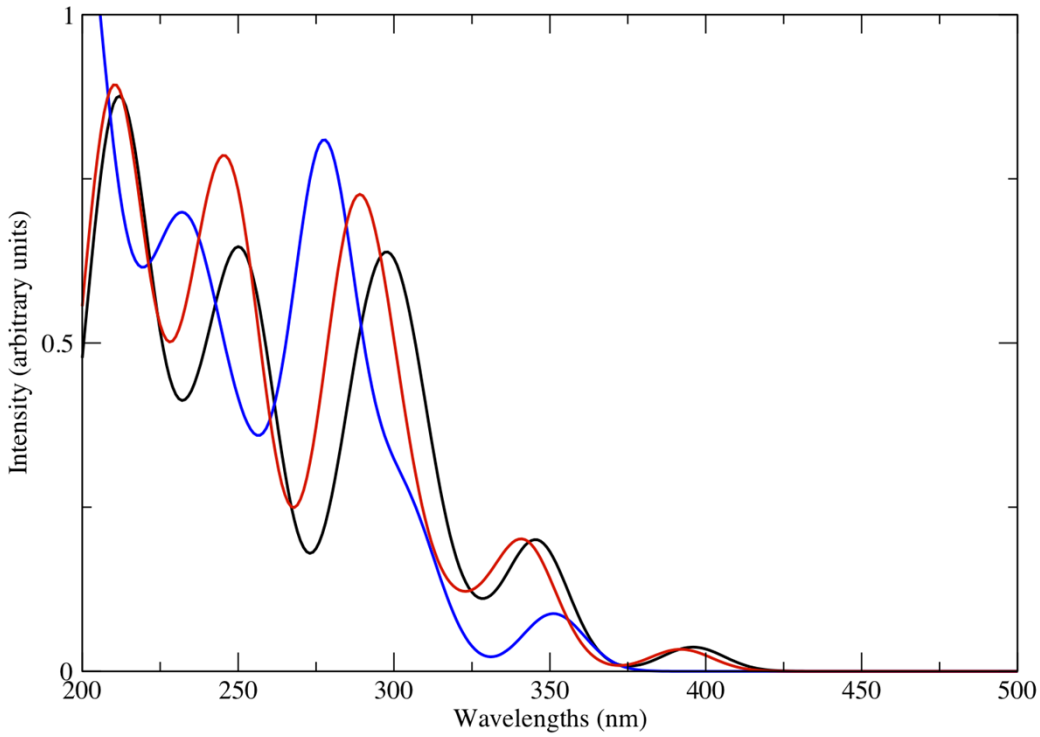

Figure S1. Comparison between the "scalar" TD-DFT theoretical absorption spectra of $[Pt(ppy)Cl_2]^-$ **2** using B3LYP (in black), CAM-B3LYP (in blue) and B3LYP with TDA (in red).

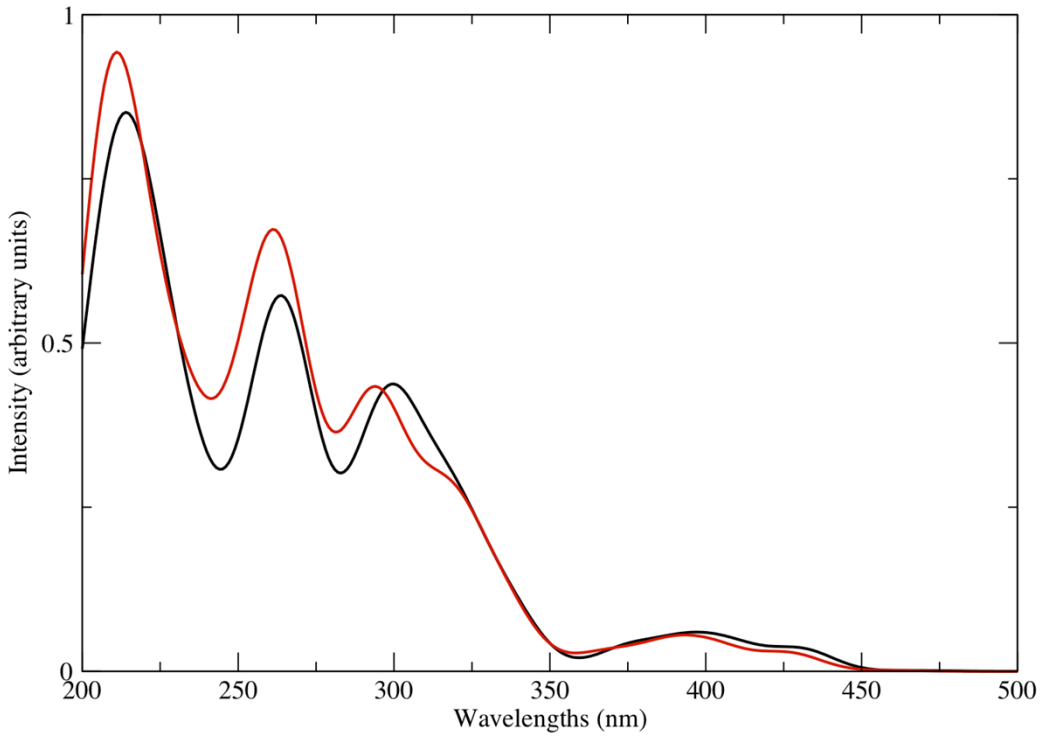

Figure S2. Comparison between the TD-DFT theoretical absorption spectra of $[Pt(ppy)Cl_2]^-$ **2** with SOC computed with B3LYP (in black) and B3LYP with TDA (in red).