

Synthesis and Photoinduced Electron Transfer in Platinum(II) Bis(*N*-(4-ethynylphenyl)carbazole) Bipyridine Fullerene Complexes

Supporting Information

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S1. Computational Studies.

Table S1. Selected singlet excited states (S_n) in the complexes computed by TDDFT/CPCM (CH_2Cl_2)

Complex	S_n	Excitation ^a	Coefficient ^b	Vertical excitation energy [eV] (λ [nm])	f^c
(Cbz) ₂ -Pt(bpy)	S_1	$H \rightarrow L$	0.66	2.56 (484)	0.0609
	S_2	$H-1 \rightarrow L$	0.67	2.75 (451)	0.1591
(Cbz) ₂ -Pt(bpy)-C ₆₀ '	S_1	$H-2 \rightarrow L$	0.70	1.99 (624)	0.0034
	S_2	$H \rightarrow L$	0.69	2.06 (601)	0.0003
	S_{15}	$H \rightarrow L+3$	0.60	2.48 (500)	0.0452
	S_{20}	$H-3 \rightarrow L$	0.43	2.66 (467)	0.0922
		$H-1 \rightarrow L+3$	-0.48		
	S_{21}	$H-3 \rightarrow L$	0.47	2.66 (466)	0.0788
		$H-1 \rightarrow L+3$	0.46		

^a The orbitals involved in the excitations (H = HOMO and L = LUMO).

^b The coefficients in the configuration interaction (CI) expansion. The excitations with the coefficients that are less than the absolute value of 0.3 are not listed.

^c Oscillator strengths.

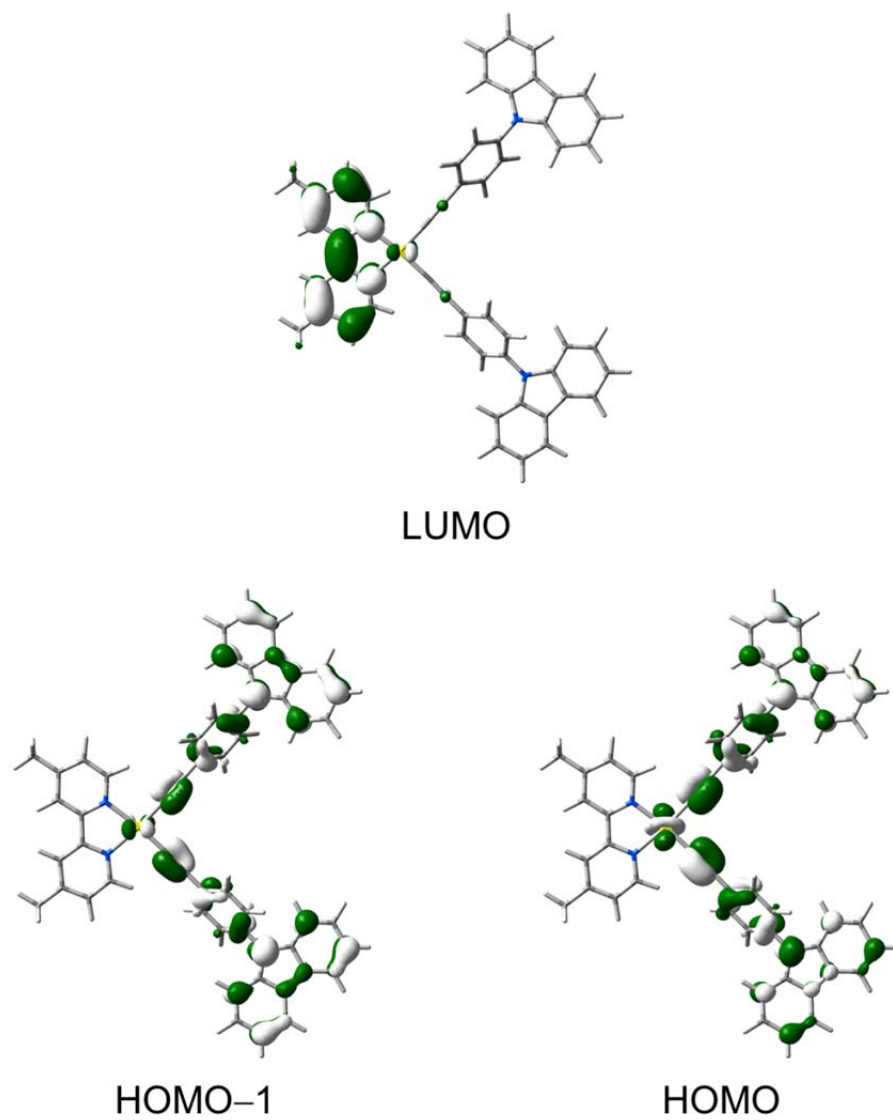


Figure S1. Spatial plots (isovalue = 0.03) of selected molecular orbitals of $(\text{Cbz})_2\text{-Pt}(\text{bpy})$ obtained from PBE0/CPCM calculation.

S2. Cartesian Coordinates of the Optimized Structures.

Table S2. Cartesian coordinates of (Cbz)₂-Pt(bpy)

1	C	5.392306	-2.177556	0.045774	51	C	-5.224124	-6.611485	-0.619628
2	C	4.304272	-2.310129	-0.820979	52	H	-4.137458	-4.745894	-0.534245
3	C	3.282808	-1.372133	-0.809272	53	C	-9.887579	-4.077630	0.245038
4	C	3.328680	-0.261261	0.052883	54	C	-9.797570	-1.674297	0.543547
5	C	4.434876	-0.138868	0.912752	55	H	-7.854724	-0.732690	0.445597
6	C	5.446677	-1.087771	0.918115	56	C	-6.469773	-7.251312	-0.541221
7	C	2.285283	0.705960	0.049166	57	H	-8.592352	-7.014191	-0.260331
8	C	1.363835	1.514980	0.027430	58	H	-4.332257	-7.201581	-0.810360
9	Pt	-0.000088	2.882480	0.000318	59	C	-10.529700	-2.868376	0.473255
10	C	-1.363768	1.514731	-0.027044	60	H	-10.453941	-5.003931	0.200922
11	C	-2.285098	0.705582	-0.048936	61	H	-10.318238	-0.739836	0.733147
12	C	-3.328451	-0.261689	-0.052865	62	H	-6.527483	-8.328324	-0.666803
13	C	-3.284103	-1.371084	0.811265	63	H	-11.607449	-2.844615	0.603648
14	C	-4.305558	-2.309096	0.822722	64	N	6.428747	-3.138744	0.041707
15	C	-5.392025	-2.178039	-0.046221	65	C	7.780492	-2.874012	-0.141188
16	C	-5.444859	-1.089737	-0.920507	66	C	6.267542	-4.508025	0.219703
17	C	-4.433099	-0.140789	-0.914933	67	C	8.501428	-4.089479	-0.080601
18	N	1.309126	4.493955	0.015210	68	C	8.417659	-1.657731	-0.387021
19	C	0.736170	5.719439	0.004421	69	C	7.533509	-5.134529	0.150564
20	C	1.515336	6.874113	-0.000347	70	C	5.103634	-5.235601	0.467932
21	C	2.905649	6.789919	0.006395	71	C	9.887450	-4.077378	-0.250196
22	C	3.466936	5.509451	0.017990	72	C	9.796760	-1.674565	-0.552654
23	C	2.646197	4.395752	0.021398	73	H	7.854028	-0.732914	-0.452915
24	C	-0.736891	5.719308	-0.003312	74	C	7.627247	-6.518325	0.313917
25	N	-1.309623	4.493714	-0.014304	75	C	5.225694	-6.610035	0.627049
26	C	-2.646665	4.395251	-0.020570	76	H	4.138752	-4.744665	0.540363
27	C	-3.467624	5.508798	-0.017037	77	C	10.529090	-2.868476	-0.481605
28	C	-2.906583	6.789362	-0.005195	78	H	10.453951	-5.003567	-0.205492
29	C	-1.516278	6.873824	0.001596	79	H	10.317032	-0.740396	-0.744771
30	H	2.436643	-1.478329	-1.480381	80	C	6.471247	-7.249918	0.547544
31	H	4.271638	-3.149307	-1.509411	81	H	8.593311	-7.013143	0.262490
32	H	3.029140	3.379044	0.028299	82	H	4.334207	-7.199861	0.820368
33	H	-1.042337	7.849235	0.012517	83	H	11.606607	-2.844872	-0.613931
34	H	-3.029422	3.378473	-0.027675	84	H	6.529247	-8.326708	0.674879
35	H	1.041193	7.849427	-0.011135	85	H	4.544127	5.374528	0.022864
36	H	-4.544788	5.373660	-0.022027	86	C	-3.769013	8.014899	0.002177
37	H	-2.439146	-1.476119	1.484076	87	H	-4.412564	8.030491	0.887927
38	H	-4.475376	0.699975	-1.600579	88	H	-3.172165	8.929649	-0.000523
39	H	-6.278370	-1.002310	-1.611071	89	H	-4.425265	8.033011	-0.874029
40	H	-4.274140	-3.147101	1.512638	90	C	3.767876	8.015604	-0.000533
41	H	4.478369	0.703057	1.596896	91	H	3.170862	8.930246	-0.001013
42	H	6.281431	-0.999146	1.607021	92	H	4.421516	8.035257	0.877605
43	N	-6.428427	-3.139271	-0.042393	93	H	4.414050	8.029864	-0.884371
44	C	-6.266823	-4.508847	-0.217741					
45	C	-7.780507	-2.874315	0.137674					
46	C	-7.532872	-5.135313	-0.149763					
47	C	-5.102433	-5.236769	-0.462663					
48	C	-8.501261	-4.089929	0.077899					
49	C	-8.418182	-1.657656	0.380306					
50	C	-7.626232	-6.519395	-0.310901					

Table S3. Cartesian coordinates of (Cbz)₂-Pt(bpy)-C₆₀'

1	C	4.432414	6.101109	-0.176460	81	H	6.681738	11.227746	1.351018
2	C	5.375846	5.284272	-0.805363	82	H	8.671862	7.573007	2.431888
3	C	5.112324	3.937341	-1.004365	83	H	2.222929	11.880759	-1.278050
4	C	3.889187	3.370854	-0.601335	84	H	8.572046	10.042663	2.436493
5	C	2.947515	4.208936	0.022154	85	H	-1.291358	1.615252	-2.511811
6	C	3.218114	5.551552	0.242003	86	C	-3.015663	-0.379955	-3.274865
7	C	3.619955	1.991292	-0.821528	87	N	-3.321522	0.864971	-3.946496
8	C	3.427682	0.796096	-1.017660	88	C	-4.035656	-0.412827	-2.077599
9	Pt	3.008402	-1.059342	-1.354265	89	H	-3.253746	-1.250251	-3.920563
10	C	4.803225	-1.549417	-0.835240	90	C	-4.764827	0.868406	-4.046689
11	C	5.925099	-1.933383	-0.522272	91	C	-2.672341	1.024700	-5.233421
12	C	7.230696	-2.340715	-0.130114	92	C	-3.458147	0.110819	-0.764994
13	C	7.822582	-1.827066	1.038304	93	C	-5.258099	0.445155	-2.643583
14	C	9.089528	-2.229386	1.433597	94	C	-4.392346	-1.834564	-1.665728
15	C	9.812524	-3.140934	0.659590	95	H	-5.123530	0.135159	-4.794571
16	C	9.244592	-3.650757	-0.510535	96	H	-5.139196	1.854903	-4.335667
17	C	7.968259	-3.264177	-0.892377	97	H	-2.941655	0.223599	-5.945474
18	N	1.050549	-0.732813	-1.958305	98	H	-2.964493	1.983887	-5.669411
19	C	0.352295	-1.837806	-2.311364	99	H	-1.586206	1.027207	-5.111921
20	C	-0.960669	-1.738026	-2.765313	100	C	-3.762495	1.332681	-0.216428
21	C	-1.579513	-0.494354	-2.842191	101	C	-3.138167	-0.983636	0.103670
22	C	-0.842113	0.629325	-2.464758	102	C	-5.644817	1.640621	-1.778357
23	C	0.465152	0.470800	-2.037294	103	C	-6.586614	-0.298681	-2.683609
24	C	1.084904	-3.108359	-2.182235	104	C	-5.586663	-2.444075	-1.972578
25	N	2.363780	-2.991207	-1.757071	105	C	-3.715586	-2.186494	-0.453094
26	C	3.107962	-4.096228	-1.607154	106	C	-4.888072	2.125486	-0.740986
27	C	2.611920	-5.360091	-1.872966	107	C	-3.728736	1.517689	1.212326
28	C	1.292894	-5.514809	-2.310289	108	C	-3.074289	-0.818804	1.487059
29	C	0.533596	-4.356825	-2.461013	109	C	-7.070896	1.768536	-1.725481
30	H	5.847316	3.303260	-1.489546	110	C	-6.715184	-1.654751	-2.498570
31	H	6.312443	5.716727	-1.144441	111	C	-7.653401	0.569183	-2.284286
32	H	1.094894	1.304433	-1.739332	112	C	-6.130704	-3.452822	-1.099039
33	H	-0.496030	-4.434661	-2.792742	113	C	-4.212885	-3.179325	0.391832
34	H	4.122747	-3.919950	-1.261505	114	C	-5.521422	2.775701	0.378093
35	H	-1.508157	-2.627512	-3.058045	115	C	-4.809081	2.405323	1.580895
36	H	3.256394	-6.222657	-1.734422	116	C	-3.377182	0.464798	2.056557
37	H	7.263844	-1.115956	1.638139	117	C	-3.606579	-1.842186	2.363198
38	H	7.533525	-3.658174	-1.805902	118	C	-7.701108	2.420202	-0.665117
39	H	9.817209	-4.341234	-1.122574	119	C	-7.925188	-2.197362	-1.934376
40	H	9.526058	-1.846698	2.351304	120	C	-8.842856	0.061078	-1.762102
41	H	2.004937	3.785129	0.354900	121	C	-5.451773	-3.827721	0.060907
42	H	2.495910	6.182771	0.751127	122	C	-7.569061	-3.303753	-1.073844
43	N	11.108685	-3.542302	1.055407	123	C	-4.163143	-2.997863	1.828035
44	C	12.177177	-2.692552	1.318258	124	C	-6.906585	2.936717	0.414768
45	C	11.529998	-4.852600	1.246590	125	C	-5.500492	2.088219	2.771303
46	C	13.302934	-3.466370	1.684001	126	C	-4.103134	0.249744	3.287696
47	C	12.242647	-1.302055	1.229595	127	C	-4.245036	-1.178801	3.478911
48	C	12.889097	-4.848075	1.638457	128	C	-8.926428	1.881295	-0.111688
49	C	10.805676	-6.039400	1.134310	129	C	-8.982137	-1.357720	-1.581964
50	C	14.508600	-2.829164	1.985162	130	C	-9.485723	0.727430	-0.648477
51	C	13.453957	-0.694241	1.533900	131	C	-6.182196	-4.051647	1.288403
52	H	11.380228	-0.716967	0.927694	132	C	-8.274815	-3.530296	0.102627
53	C	13.534167	-6.058283	1.901541	133	C	-5.384777	-3.538130	2.382682
54	C	11.471564	-7.228644	1.402526	134	C	-7.629018	2.717678	1.647500
55	H	9.757537	-6.032103	0.853860	135	C	-5.145163	1.103595	3.638141
56	C	14.576642	-1.444893	1.912364	136	C	-6.940446	2.360302	2.803421
57	H	15.381428	-3.411095	2.268511	137	C	-5.421796	-1.696118	4.012817
58	H	13.531083	0.387620	1.473561	138	C	-8.880639	2.065506	1.322441
59	C	12.822631	-7.243686	1.778240	139	C	-9.708562	-1.583581	-0.352679
60	H	14.578118	-6.069573	2.202837	140	C	-10.021462	-0.293031	0.225410
61	H	10.929968	-8.166946	1.321780	141	C	-7.566395	-3.904582	1.309542
62	H	15.507246	-0.936238	2.145375	142	C	-9.362209	-2.648635	0.474218
63	H	13.312588	-8.191783	1.978627	143	C	-6.003242	-2.898757	3.453548
64	N	4.704613	7.471651	0.036577	144	C	-6.364455	0.566856	4.195249
65	C	3.910765	8.531881	-0.383784	145	C	-7.474354	1.343621	3.678972
66	C	5.811564	7.986133	0.701934	146	C	-6.501805	-0.806308	4.378854
67	C	4.514191	9.747227	0.015629	147	C	-9.393205	1.083234	2.165054
68	C	2.722256	8.511293	-1.113692	148	C	-9.974593	-0.119449	1.605767
69	C	5.729839	9.397928	0.710337	149	C	-8.207921	-3.245908	2.422661
70	C	6.861182	7.310295	1.324193	150	C	-9.317897	-2.469137	1.906287
71	C	3.901001	10.959497	-0.307380	151	C	-7.441532	-2.750390	3.474065
72	C	2.134006	9.731268	-1.421976	152	C	-8.677260	0.716027	3.366835
73	H	2.277442	7.574993	-1.434279	153	C	-7.750507	-1.457888	4.047388
74	C	6.731266	10.142331	1.337510	154	C	-9.616950	-1.228408	2.462392
75	C	7.843103	8.075060	1.940851	155	C	-8.815777	-0.712506	3.551766
76	H	6.905451	6.226219	1.331778	156	C	0.724386	-6.871001	-2.598629
77	C	2.710920	10.945216	-1.021661	157	H	0.749398	-7.499686	-1.702487
78	H	4.353102	11.900602	-0.006264	158	H	-0.310494	-6.811085	-2.942668
79	H	1.207392	9.742442	-1.988996	159	H	1.311379	-7.382464	-3.368410
80	C	7.785703	9.476419	1.946508					