Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

[Ag(IPr)(bpy)][PF_6]: Brightness and Darkness Playing with Aggregation Induced Phosphorescence for Light-emitting Electrochemical Cells

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Emission spectrum of $[Cu(IPr)(bpy)][PF_6]$

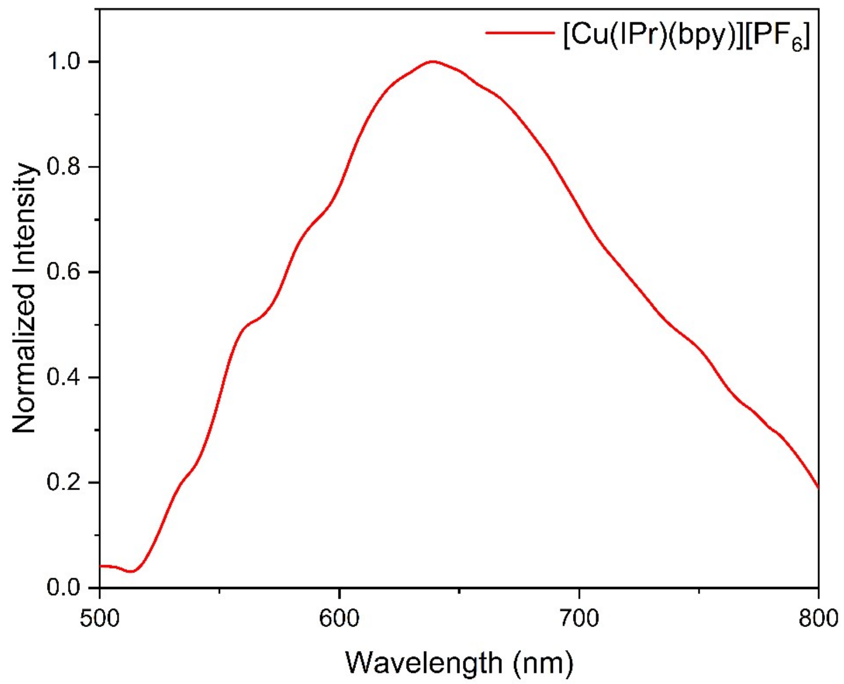


Figure S1. Emission spectrum of $[Cu(IPr)(bpy)][PF_6]$ recorded at 298 K (λ_{ex} = 365 nm).

Synthesis and NMR spectra

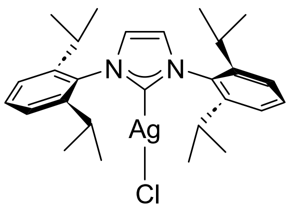
General considerations

Synthesis: All the commercially available compounds were purchased from the supplier and used without further purification. All the reactions were performed under dry argon atmosphere, using standard Schlenk technique. Purchased solvents were degassed bubbling Ar directly in bulk. ^{1}H, ^{13}C, ^{31}P and ^{19}F NMR spectra were recorded at 298 K on 500 MHz and 600 MHz Brüker spectrometers. The spectra are reported in the following format: multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; qui, quintet; sex, sextet; sept, septet; m, multiplet), coupling constant(s) (*J*) in Hertz (Hz), integration. The prefix "br" is occasionally used in case of broad signals. HRMS were performed by LCMT analytical service. 2,2'- bipyridine was commercially available and purchased from Sigma-Aldrich.

Synthesis of the [AgCl(IPr)] precursor.

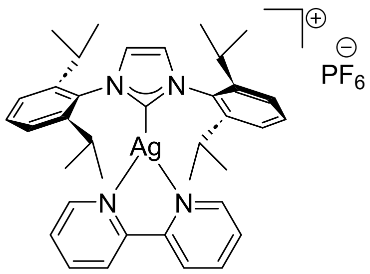
General procedure: In an anhydrous and degassed Schlenk flask, 1,3-bis(2,6-di-iso-propylphenyl) imidazolium chloride salt (1 eq.) and Ag_2O (0.65 eq.) were suspended together in anhydrous and degassed dichloromethane and stirred overnight at room temperature. The reaction mixture was filtered through a pad of diatomaceous earth and the filtrate was concentrated under reduced pressure. The addition of n-pentane caused the precipitation of the product, which was collected by filtration and then dried in vacuum.

[AgCl(IPr)] (1,3-bis(2,6-di-*S*-propylphenyl)imidazol-2-ylidene) silver chloride



Following the general procedure, the product was obtained with 88 % yield. **^{1}H NMR ($CDCl_3$, 500 MHz)**: δ 1.22 (d, *J* = 6.9 Hz, 12H), 1.28 (d, *J* = 6.9, Hz 12H), 2.54 (sept, *J* = 6.9 Hz, 4H), 7.21 (d, *J* = 1.9 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 4H), 7.50 (t, *J* = 7.8 Hz, 2H) ppm. In good agreement with the literature.[1]

Synthesis of the complex [Ag(IPr)(bpy)][PF_6].



[AgCl(IPr)] (1.0 eq) and the 2,2'-bipyridine (1.05 eq) were introduced in a flame-dried Schlenk flask under Ar atmosphere. The reagents were dissolved in degassed absolute ethanol and heated at 78 °C for 1h. Afterward, the reaction mixture was allowed to cool down at room temperature and a KPF_6 saturated aqueous solution was added, affording a white precipitate. The solid was washed with distilled water and diethyl ether and then dried under vacuum. The resulting white solid was recrystallized twice by slow diffusion of diethyl ether in a dichloromethane solution of the complex. The clean complex was obtained as white solid in 52 % yield.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 1.15 (d, *J* = 6.9 Hz, 12H), 1.28 (d, *J* = 6.9 Hz, 12H), 2.60 (sept, *J* = 6.9 Hz, 4H), 6.96 (br d, *J* = 4.4 Hz, 2H), 7.28 (m. overlapped with the $CDCl_3$ signal, 2H), 7.42 (d, *J* = 1.9 Hz, 2H), 7.46 (d, *J* = 7.9 Hz, 4H), 7.71 (t, *J* = 7.8 Hz, 2H), 7.98 (td, *J* = 7.9, 1.7 Hz, 2H), 8.19 (d, *J* = 8.1 Hz, 2H) ppm. **^{13}C NMR ($CDCl_3$, 151 MHz):** δ 24.0 (s), 25.1 (s), 28.9 (s), 122.9 (s), 124.0 (d, $J_{\text{Ag-C}}$ = 7.6 Hz, C imidazole), 125.0 (s), 125.8 (s), 130.9 (s), 135.6 (s), 140.2 (s), 146.3 (s), 150.2 (s), 151.4 (s), 186.2 (d, *J* (^{13}C-^{107}Ag) = 246.7 Hz), 186.2 (d, *J* (^{13}C-^{109}Ag) = 284.8 Hz) ppm. **^{31}P NMR ($CDCl_3$, 202 MHz):** δ -144.3 (sept, *J* (^{31}P-^{19}F) = 711.0 Hz, 1P) ppm. **^{19}F NMR ($CDCl_3$, 471 MHz):** δ -73.6 (d, *J* (^{19}F-^{31}P) = 711.2 Hz, 6F) ppm. **HRMS (ESI):** m/z calcd for $C_{37}H_{47}N_4Ag$ [M-PF_6]$^+$ 651.2617, found 651.2612. **IR (neat):** 3167, 3135, 2954, 1738, 1471, 1440, 1366, 837 cm^{-1}.

NMR spectra of the complex [Ag(IPr)(bpy)][PF_6].

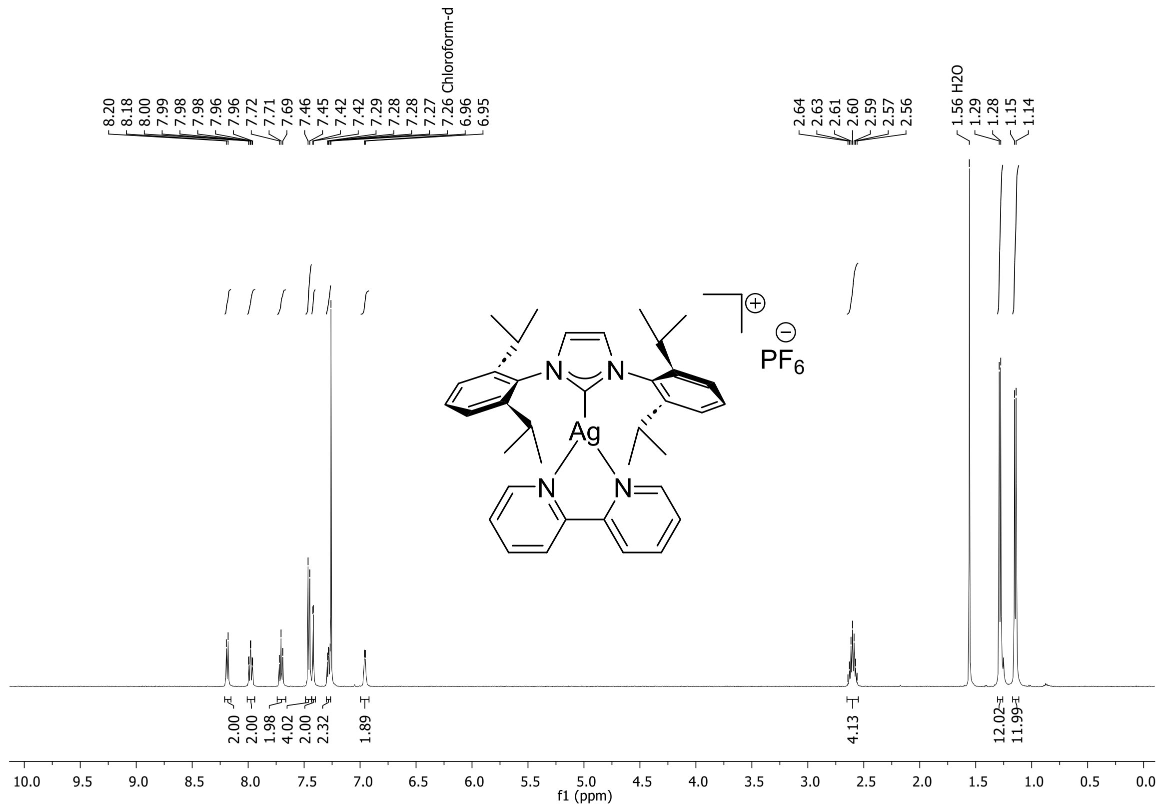


Figure S2. ^{1}H NMR ($CDCl_3$, 500 MHz) of [Ag(IPr)(bpy)][PF_6]

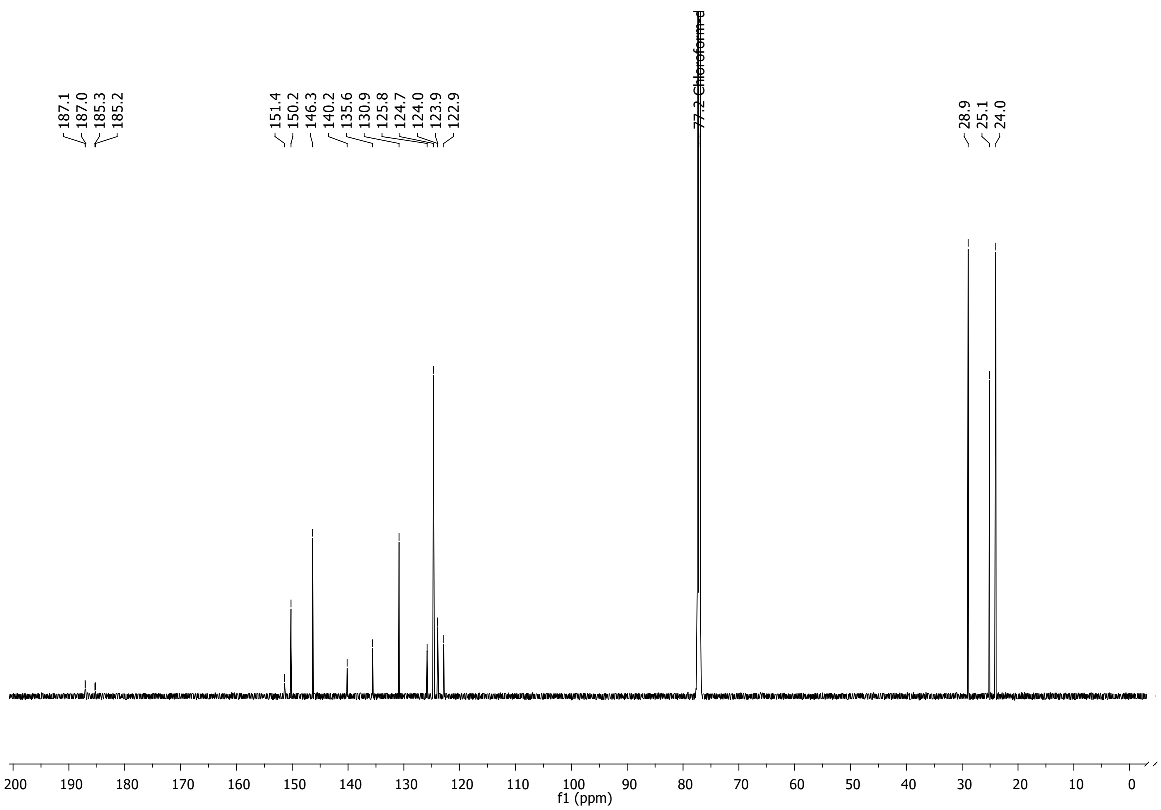


Figure S3. ^{13}C NMR ($CDCl_3$, 151 MHz) of [Ag(IPr)(bpy)][PF_6]

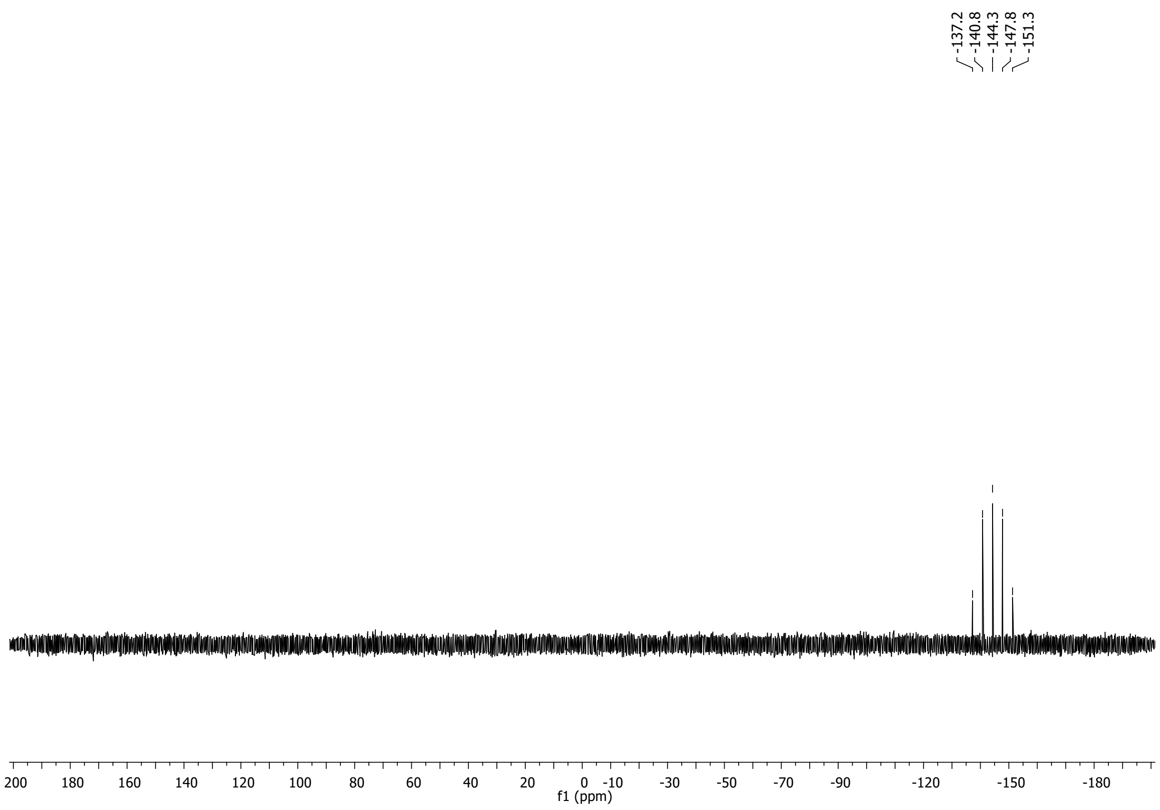


Figure S4. ^{31}P NMR ($CDCl_3$, 202 MHz) of [Ag(IPr)(bpy)][PF_6]

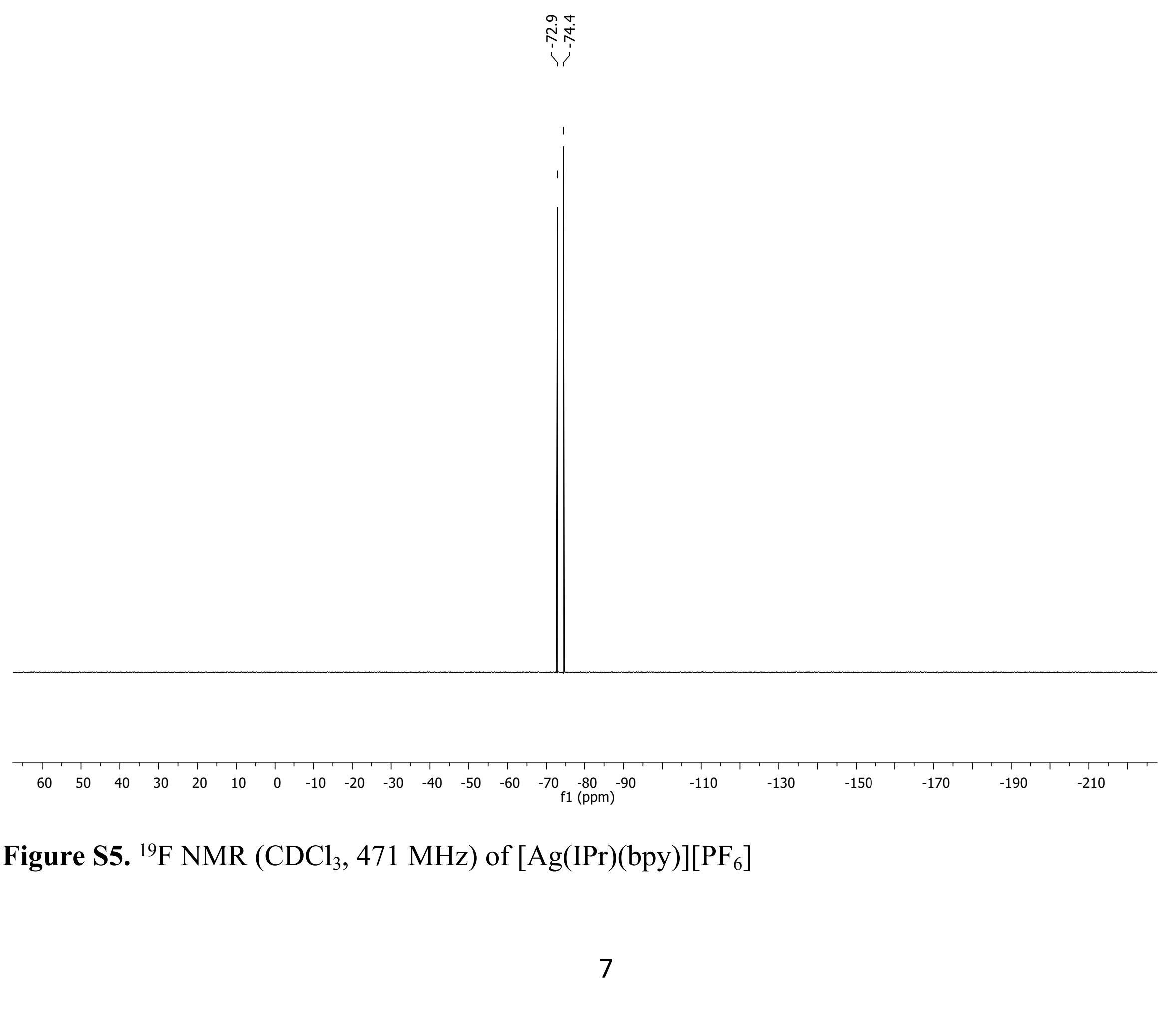


Figure S5. ^{19}F NMR ($CDCl_3$, 471 MHz) of [Ag(IPr)(bpy)][PF_6]

XRD details and structures

Table S1. Crystallographic data of complex [Ag(IPr)(bpy)][PF_6]

	[Ag(IPr)(bpy)][PF_6]
Formula	$C_{37}H_{44}AgF_6N_4P$
M/g·mol^{-1}	797.60
Crystal system	orthorhombic
Space group	*P* bca
a/ Å	15.6677(4)
b/ Å	17.2396(5)
c/ Å	27.1830(5)
α/ °	90
β/ °	90
γ/ °	90
V/ Å^3	7342.3(3)
Z	8
μ/ mm^{-1}	0.655
ρcalcd/ g·cm^{-3}	1.443
λ (Mo K_α)/ mm^{-1}	0.71073
T/ K	123(2)
N° of reflections	16143
N° of unique reflection	11798
R_{int}	0.075673
R1, wR_2 (I > 2σ(I))	0.034554
R1, wR_2 (all data)	0.059722
GOF	1.01699

Theoretical details

Table S2. Absolute energies (au) calculated of the different states of the dimer of [Ag(IPr)(bpy)][PF_6] at the (TD)-CAM-B3LYP-D3BJ/def2-TZVP level of theory.[a]

State	E[b]	E[c]
X ^1A_g	-5486.147648	-5486.147250
1 ^3A_g	-5486.051782	-5486.052476
1 ^1A_g	-5486.005830	-5486.005039
1 ^1A_u	-5486.005847	-5486.005085
1 ^3A_u	-5486.052168	-5486.051709

[a] The core electrons of Ag were described using the def2-ECP pseudopotential.
[b] Calculated at the equilibrium structure of T_{1A} (1 ^3A_u).
[c] Calculated at the equilibrium structure of T_{1B} (1 ^3A_g).

Table S3. Vertical excitation energies with respect to the ground state (eV) and oscillator strengths (length representation) of the dimer of [Ag(IPr)(bpy)][PF_6] calculated at the TD-CAM-B3LYP-D3BJ/def2-TZVP level of theory.[a]

State	ΔE[b]	*f*[b]	ΔE[c]	*f*[c]
1 ^3A_g	2.61	0.000	2.58	0.000
1 ^1A_g	3.86	0.000	3.87	0.000
1 ^1A_u	3.86	<0.001	3.87	0.001
1 ^3A_u	2.60	0.000	2.60	0.000

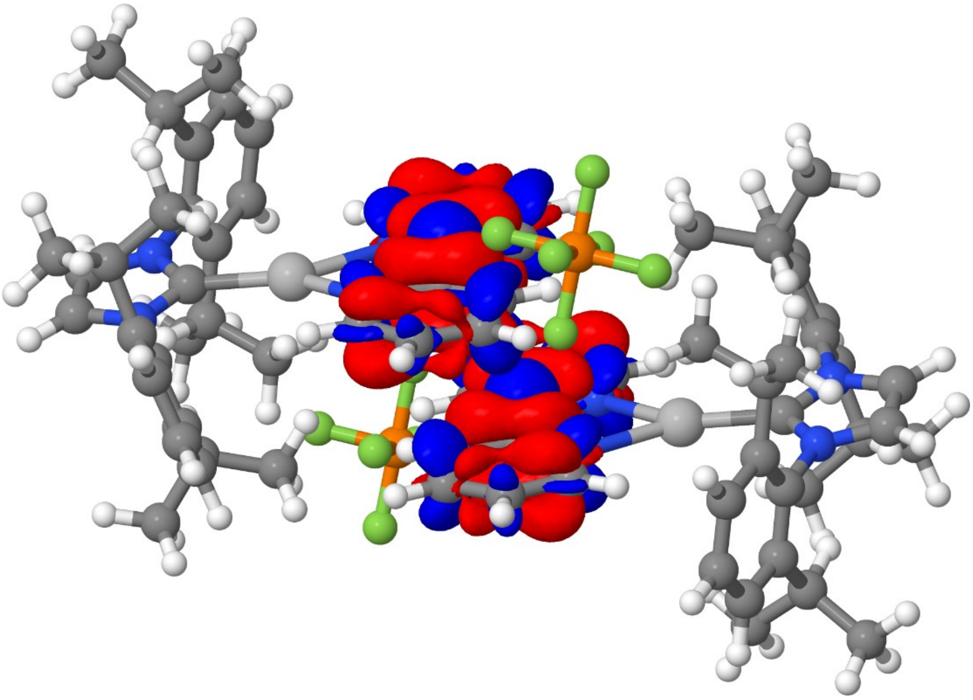
[a] The core electrons of Ag were described using the def2-ECP pseudopotential.
[b] Calculated at the equilibrium structure of T_{1A} (1 ^3A_u).
[c] Calculated at the equilibrium structure of T_{1B} (1 ^3A_g).

Table S4. Vertical excitation energies with respect to the ground state including the spin-orbit coupling contribution[a] (eV) and oscillator strengths (length representation) of the dimer of [Ag(IPr)(bpy)][PF_6] calculated at the TD-CAM-B3LYP-D3BJ/ZORA-def2-TZVP level of theory.[b]

State	ΔE[c]	*f*[c]	ΔE[d]	*f*[d]
1 ^3A_g	2.61	0.000	2.58	0.000
1 ^1A_g	3.86	0.000	3.87	0.000
1 ^1A_u	3.86	<0.001	3.87	0.001
1 ^3A_u	2.60	<0.001	2.60	<0.001

[a] Twenty singlet and twenty triplet states were included in the calculation.
[b] The SARC-ZORA-TZVP basis set was used for Ag.
[c] Calculated at the equilibrium structure of T_{1A} (1 ^3A_u).
[d] Calculated at the equilibrium structure of T_{1B} (1 ^3A_g).

a)



b)

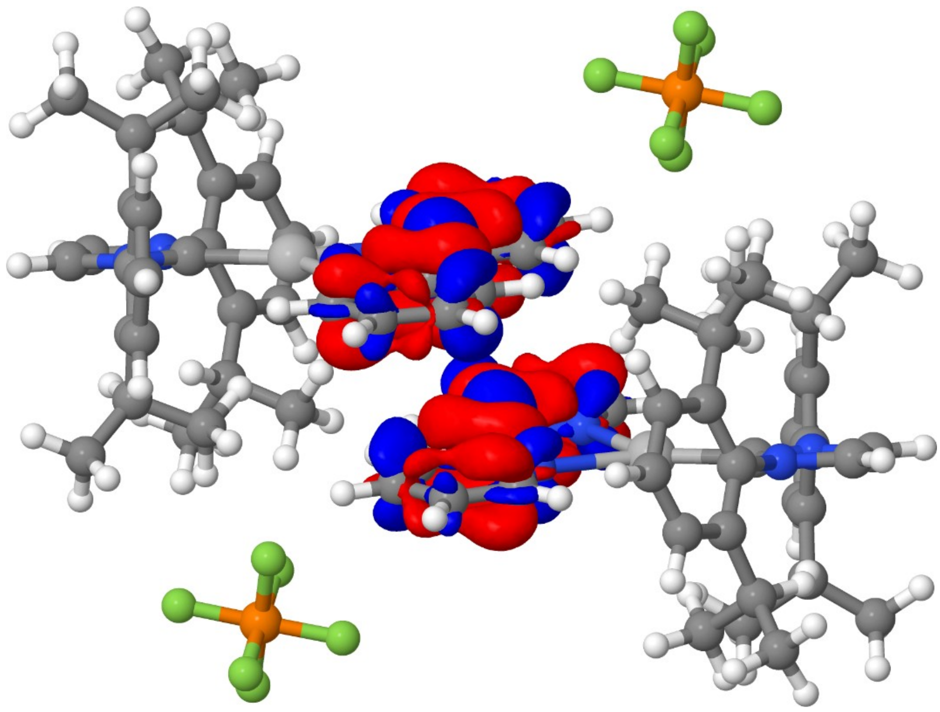


Figure S6. Characterization of the lowest-lying states a) T_{1A} (1 ^3A_u) and b) T_{1B} (1 ^3A_g) of the dimer of [Ag(IPr)(bpy)][PF_6] using density differences (cut-off 0.0008 au) calculated at the TDDFT level using the CAM-B3LYP exchange-correlation functional and the def2-TZVP basis set.

Cartesian coordinates (au). The * indicate unrelaxed (frozen) atoms

T_{1A} (1 ^3A_u)

	X	Y	Z	
C	-14.77741424770508	-9.95536766148294	-1.69423778420757	*
C	-11.44385563011843	-8.07207440764481	1.13130360835596	*
Ag	-7.38101578966537	-1.64387725730181	0.75543426112115	
N	-12.80615787863992	0.51464947579435	0.69014036553132	*
N	-12.37777586344851	-2.29818140454536	-2.17135663169588	*
N	-4.22849966681473	0.30776730745040	3.01803557446774	
N	-3.85514467560083	-3.98774011022819	0.28737089093894	
C	-11.09520551458212	-1.12118249535732	-0.29992116623037	*
C	-12.25007951030304	2.16642128680724	2.78511531373107	*
C	-15.11398779806527	0.35965791850480	-0.53804933464671	*
C	-11.24034026040563	-4.13363837432412	-3.84316142935593	*
C	-14.83304032539103	-1.41273511104296	-2.36020641196036	*
C	-9.71192221190381	-3.24550489027251	-5.81460687051502	*
C	-1.92557462118329	-0.84864756894031	2.91127471685947	
C	-8.56962245381615	-5.05764641912564	-7.36664460584854	*
C	-12.51779701037878	1.21800175992782	5.23426273220818	*
C	-2.51427112895964	3.57680199452248	5.59993479824739	
C	-11.67451428616903	-6.69773405350997	-3.37518965185361	*
C	-1.71582600259153	-3.12716218508990	1.45166580715731	
C	-11.10212947110275	5.55752347909145	-0.43407849299592	*
C	-11.43514456768880	4.63036337111406	2.25616585363932	*
C	-9.22190299970548	-0.45300557330764	-6.27201885843294	*
C	-8.96765168799383	-7.60916219149985	-6.95873966294357	*
C	-0.14892628016705	2.42212091557482	5.53880651721266	
C	0.63995420146226	-6.64637116404682	-0.22926399708837	
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C	-10.50183340117576	-8.42259858129727	-4.99868738058985	*
C	0.15118111661045	0.21953443574805	4.21082556442283	
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C	-13.19895068172626	-7.61556458361008	-1.12083331257680	*
C	-4.49991201749367	2.41289701145867	4.30350056966618	
C	-12.00515399701642	8.27784659645235	-0.78741948377845	*
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C	11.44385563011843	8.07207440764481	-1.13130360835596	*
Ag	7.38101578966537	1.64387725730181	-0.75543426112115	
N	12.80615787863992	-0.51464947579435	-0.69014036553132	*
N	12.37777586344851	2.29818140454536	2.17135663169588	*
N	4.22849966681473	-0.30776730745040	-3.01803557446774	
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C	11.09520551458212	1.12118249535732	0.29992116623037	*
C	12.25007951030304	-2.16642128680724	-2.78511531373107	*
C	15.11398779806527	-0.35965791850480	0.53804933464671	*
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C	1.92557462118329	0.84864756894031	-2.91127471685947	
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C	12.51779701037878	-1.21800175992782	-5.23426273220818	*
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C	1.71582600259153	3.12716218508990	-1.45166580715731	
C	11.10212947110275	-5.55752347909145	0.43407849299592	*
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C	-0.63995420146226	6.64637116404682	0.22926399708837	
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C	13.19895068172626	7.61556458361008	1.12083331257680	*
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C	10.14801430968370	-0.38698146854076	8.86816807214469	*
C	6.40897385360728	-0.16979335531139	5.99603569628809	*
C	11.07002680369761	-5.26801932652491	-6.76970111326299	*
C	16.03724751132143	1.35598285606820	-7.06161466663843	*
C	8.34615478067465	-5.29980074048886	1.24861848285012	*
C	11.54781381869124	2.95459856092149	-7.29818570072808	*
H	16.00024607477662	10.38056701989590	0.09207508448586	
H	15.96641690353662	9.68123806176219	3.35395908511680	
H	13.60183294199152	11.61589897927798	2.01640253559194	
H	12.52705907348053	8.64782051810993	-2.78748311949943	
H	10.08825345778883	9.56693122976263	-0.70795016958191	
H	10.38308439144912	6.37473369570811	-1.61573010012008	
H	9.84176559849502	-2.40944070442347	9.11124672073491	
H	12.15893609476947	-0.00977590372769	9.11297877463005	
H	9.13763541514423	0.58852781732707	10.37645445399473	
H	6.10565377057388	-2.20011618340956	6.16207047013328	
H	5.29767711530759	0.76577053064308	7.45709738004506	
H	5.71559698806931	0.45138661915764	4.15875431776349	
H	11.95807187291589	-8.77392515175426	2.78459790432034	
H	10.77245224227155	-9.62608261419747	-0.16046291744789	
H	13.92948237944766	-8.53066043869645	0.09386762315083	
H	8.09437699245064	-5.94226896440190	3.18689495520595	
H	7.69581051753959	-3.34930163923773	1.09730887180361	
H	7.13379512818748	-6.49011173407486	0.08594323326390	
H	12.20983812253295	4.88737907085350	-7.56671586556538	
H	11.26399059887193	2.12326481198197	-9.16153380214521	
H	9.71794355017136	3.03014805571318	-6.35335339754256	
H	16.75643684316939	3.26372318450091	-7.36415820439960	
H	17.41585270598848	0.31858755374633	-5.93551840366204	
H	15.90182426926113	0.43213068063085	-8.89841257336878	
H	13.70142411059784	2.40719057056288	-3.94761251703162	
H	14.50432849146765	6.11193995750085	0.59086837176210	
H	12.24394385272991	-4.36100330368985	1.66219562225481	
H	10.23951605110907	-0.63457633713800	4.85595540959898	
H	-2.27470571959086	3.85141601044228	-2.11847983251446	
H	-2.35822880317397	7.72228859440076	0.40438129805027	
H	1.60214140943235	9.24161131954890	2.42755591280618	
H	5.52566908811659	6.67507091405408	1.92266723382755	
H	-1.96124387345028	0.69960799377929	-4.15459851217704	
H	-1.44177114967704	-3.25910371390608	-6.50918339833582	
H	2.83552455619406	-5.32858109710980	-6.59528017536801	
H	6.36766014127495	-3.24823992426560	-4.31210752335387	
H	12.09933357667359	-2.18156501164522	-9.15507295677995	
H	10.60158899156506	-6.49428010776872	-8.33763656859501	
H	10.17600986650895	-8.06623793700032	-3.98939980273386	
H	7.37338291929415	4.45087047723601	8.90815778641343	
H	8.07553432263134	8.98525695593887	8.17982241136938	
H	10.77512323087272	10.42459092975037	4.70830494858656	
H	16.69812939489038	-1.51844624339647	0.01885904645916	
H	16.12819475077707	2.11267902233871	3.75878966583646	

P	-4.07255237791635	12.04736455546673	-2.48336742240672	*
F	-4.37333819544691	9.14775745148421	-3.21954235959881	*
F	-1.07822275193695	11.70510680840514	-2.54715701746959	*
F	-4.13338077214193	11.30503667001287	0.43801877516212	*
F	-7.08158029369308	12.36809643224272	-2.40996857000013	*
F	-4.02558323508877	12.79742708994870	-5.38877409586573	*
F	-3.76302468733327	14.93691264728789	-1.72804578011992	*
P	4.07255237791635	-12.04736455546673	2.48336742240672	*
F	4.37333819544691	-9.14775745148421	3.21954235959881	*
F	1.07822275193695	-11.70510680840514	2.54715701746959	*
F	4.13338077214193	-11.30503667001287	-0.43801877516212	*
F	7.08158029369308	-12.36809643224272	2.40996857000013	*
F	4.02558323508877	-12.79742708994870	5.38877409586573	*
F	3.76302468733327	-14.93691264728789	1.72804578011992	*

T_{1B} ($1\ ^3A_g$)

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C	-11.44385563011843	-8.07207440764481	1.13130360835596	*
Ag	-7.33937254119731	-1.56882427550032	0.68818440938002	
N	-12.80615787863992	0.51464947579435	0.69014036553132	*
N	-12.37777586344851	-2.29818140454536	-2.17135663169588	*
N	-4.21983548726703	0.42428249771410	2.99597163088516	
N	-3.73012235814967	-3.79830244911283	0.17038006325406	
C	-11.09520551458212	-1.12118249535732	-0.29992116623037	*
C	-12.25007951030304	2.16642128680724	2.78511531373107	*
C	-15.11398779806527	0.35965791850480	-0.53804933464671	*
C	-11.24034026040563	-4.13363837432412	-3.84316142935593	*
C	-14.83304032539103	-1.41273511104296	-2.36020641196036	*
C	-9.71192221190381	-3.24550489027251	-5.81460687051502	*
C	-1.91626660027975	-0.73341300026159	2.96000410916074	
C	-8.56962245381615	-5.05764641912564	-7.36664460584854	*
C	-12.51779701037878	1.21800175992782	5.23426273220818	*
C	-2.64941176232952	3.55799553154229	5.82818604995922	
C	-11.67451428616903	-6.69773405350997	-3.37518965185361	*
C	-1.64221358673019	-2.96589818548354	1.44216741785189	
C	-11.10212947110275	5.55752347909145	-0.43407849299592	*
C	-11.43514456768880	4.63036337111406	2.25616585363932	*
C	-9.22190299970548	-0.45300557330764	-6.27201885843294	*
C	-8.96765168799383	-7.60916219149985	-6.95873966294357	*
C	-0.28074078254398	2.40892279403728	5.82507411822811	
C	0.77238735202629	-6.47323272779511	-0.18345176987782	
C	0.65795563285782	-4.31513035210982	1.24394382735637	
C	-1.39308530567158	-7.30844908279514	-1.41702228458660	
C	-10.50183340117576	-8.42259858129727	-4.99868738058985	*
C	0.09201697158154	0.27384538394228	4.40980281359928	
C	-3.59535987377566	-5.87847649432030	-1.18594601511380	
C	-13.19895068172626	-7.61556458361008	-1.12083331257680	*
C	-4.55963156365477	2.46573013311148	4.36645572398125	
C	-12.00515399701642	8.27784659645235	-0.78741948377845	*
C	-11.91237600320180	2.84108185919051	7.22998170543808	*
C	-13.45846299096887	-1.44218082351687	5.74702290859026	*
C	-10.83555903478467	6.16095460465919	4.31703124528957	*
C	-10.14801430968370	0.38698146854076	-8.86816807214469	*
C	-6.40897385360728	0.16979335531139	-5.99603569628809	*
C	-11.07002680369761	5.26801932652491	6.76970111326299	*
C	-16.03724751132143	-1.35598285606820	7.06161466663843	*

C	-8.34615478067465	5.29980074048886	-1.24861848285012	*
C	-11.54781381869124	-2.95459856092149	7.29818570072808	*
H	-16.00020970122257	-10.38051277280603	-0.09203239717689	
H	-13.60181820476141	-11.61590081565924	-2.01630397497181	
H	-15.96650323832177	-9.68141224637455	-3.35394712932626	
H	-10.38429188458672	-6.37404966391022	1.61621108616440	
H	-10.08675424723117	-9.56522551981767	0.70709811440311	
H	-12.52715498228762	-8.64931271419014	2.78691641292816	
H	-14.50452365366135	-6.11204608185708	-0.59095011499118	
H	-9.84261512149414	2.40958481493583	-9.11091020890010	
H	-9.13723912751814	-0.58806783887122	-10.37650493630173	
H	-12.15871260032467	0.00888791419833	-9.11325494910854	
H	-6.10558005553403	2.19883900270861	-6.17885216271408	
H	-5.71355837072964	-0.43689190558288	-4.15476821557451	
H	-5.29875523710374	-0.77859332640782	-7.44986370471579	
H	-10.23975051270394	0.63486886160349	-4.85631669200766	
H	-11.95881663998800	8.77360837553728	-2.78469270135357	
H	-13.92917661392247	8.53087272484139	-0.09315488340215	
H	-10.77186791899837	9.62618740536958	0.15958513637012	
H	-8.09414039970492	5.94234828133752	-3.18682111137889	
H	-7.13531725028257	6.49067496342631	-0.08530720145930	
H	-7.69390474902244	3.35034192906731	-1.09670553019816	
H	-12.24402474144693	4.36094384461568	-1.66205367267084	
H	-16.75638206737638	-3.26374253776342	7.36405487768162	
H	-15.90185479290885	-0.43223591956283	8.89847660606645	
H	-17.41590206678628	-0.31858015812144	5.93557277774092	
H	-12.21003879517301	-4.88726507470945	7.56687631625098	
H	-9.71828860045199	-3.03045993683995	6.35286238863463	
H	-11.26378767486369	-2.12306634179573	9.16140536453016	
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H	-10.17587833521866	8.06623089368841	3.98935753536795	
H	-10.60185205859488	6.49432208420021	8.33768449433493	
H	-12.09924303217713	2.18154688148232	9.15504508001200	
H	-6.42525462341360	3.30381478694712	4.31561183710493	
H	-3.02743585872249	5.25410285304410	6.89714326472283	
H	1.25655732970129	3.19497612343142	6.91728816790375	
H	1.90361767171904	-0.64345155111935	4.40566032674633	
H	2.32283110386869	-3.69549689570733	2.24067839672954	
H	2.49308338575816	-7.55377184266031	-0.29951688769117	
H	-1.38689274711111	-9.04527629228112	-2.48741994362668	
H	-5.31369337038491	-6.45340845713985	-2.14041434415269	
H	-7.37338802524451	-4.45088129699498	-8.90812084797846	
H	-8.07545922941236	-8.98529383577004	-8.17973295178298	
H	-10.77447820549920	-10.42458009508813	-4.70781591176454	
H	-16.12871337611942	-2.11401897629333	-3.75763857717251	
H	-16.69845646305406	1.51753282493881	-0.01781447893673	
C	14.77741424770508	9.95536766148294	1.69423778420757	*
C	11.44385563011843	8.07207440764481	-1.13130360835596	*
Ag	7.33937254119731	1.56882427550032	-0.68818440938002	
N	12.80615787863992	-0.51464947579435	-0.69014036553132	*
N	12.37777586344851	2.29818140454536	2.17135663169588	*
N	4.21983548726703	-0.42428249771410	-2.99597163088516	
N	3.73012235814967	3.79830244911283	-0.17038006325406	
C	11.09520551458212	1.12118249535732	0.29992116623037	*
C	12.25007951030304	-2.16642128680724	-2.78511531373107	*
C	15.11398779806527	-0.35965791850480	0.53804933464671	*
C	11.24034026040563	4.13363837432412	3.84316142935593	*
C	14.83304032539103	1.41273511104296	2.36020641196036	*
C	9.71192221190381	3.24550489027251	5.81460687051502	*

C	1.91626660027975	0.73341300026159	-2.96000410916074	
C	8.56962245381615	5.05764641912564	7.36664460584854	*
C	12.51779701037878	-1.21800175992782	-5.23426273220818	*
C	2.64941176232952	-3.55799553154229	-5.82818604995922	
C	11.67451428616903	6.69773405350997	3.37518965185361	*
C	1.64221358673019	2.96589818548354	-1.44216741785189	
C	11.10212947110275	-5.55752347909145	0.43407849299592	*
C	11.43514456768880	-4.63036337111406	-2.25616585363932	*
C	9.22190299970548	0.45300557330764	6.27201885843294	*
C	8.96765168799383	7.60916219149985	6.95873966294357	*
C	0.28074078254398	-2.40892279403728	-5.82507411822811	
C	-0.77238735202629	6.47323272779511	0.18345176987782	
C	-0.65795563285782	4.31513035210982	-1.24394382735637	
C	1.39308530567158	7.30844908279514	1.41702228458660	
C	10.50183340117576	8.42259858129727	4.99868738058985	*
C	-0.09201697158154	-0.27384538394228	-4.40980281359928	
C	3.59535987377566	5.87847649432030	1.18594601511380	
C	13.19895068172626	7.61556458361008	1.12083331257680	*
C	4.55963156365477	-2.46573013311148	-4.36645572398125	
C	12.00515399701642	-8.27784659645235	0.78741948377845	*
C	11.91237600320180	-2.84108185919051	-7.22998170543808	*
C	13.45846299096887	1.44218082351687	-5.74702290859026	*
C	10.83555903478467	-6.16095460465919	-4.31703124528957	*
C	10.14801430968370	-0.38698146854076	8.86816807214469	*
C	6.40897385360728	-0.16979335531139	5.99603569628809	*
C	11.07002680369761	-5.26801932652491	-6.76970111326299	*
C	16.03724751132143	1.35598285606820	-7.06161466663843	*
C	8.34615478067465	-5.29980074048886	1.24861848285012	*
C	11.54781381869124	2.95459856092149	-7.29818570072808	*
H	16.00020970122257	10.38051277280603	0.09203239717689	
H	15.96650323832177	9.68141224637455	3.35394712932626	
H	13.60181820476141	11.61590081565924	2.01630397497181	
H	12.52715498228762	8.64931271419014	-2.78691641292816	
H	10.08675424723117	9.56522551981767	-0.70709811440311	
H	10.38429188458672	6.37404966391022	-1.61621108616440	
H	9.84261512149414	-2.40958481493583	9.11091020890010	
H	12.15871260032467	-0.00888791419833	9.11325494910854	
H	9.13723912751814	0.58806783887122	10.37650493630173	
H	6.10558005553403	-2.19883900270861	6.17885216271408	
H	5.29875523710374	0.77859332640782	7.44986370471579	
H	5.71355837072964	0.43689190558288	4.15476821557451	
H	11.95881663998800	-8.77360837553728	2.78469270135357	
H	10.77186791899837	-9.62618740536958	-0.15958513637012	
H	13.92917661392247	-8.53087272484139	0.09315488340215	
H	8.09414039970492	-5.94234828133752	3.18682111137889	
H	7.69390474902244	-3.35034192906731	1.09670553019816	
H	7.13531725028257	-6.49067496342631	0.08530720145930	
H	12.21003879517301	4.88726507470945	-7.56687631625098	
H	11.26378767486369	2.12306634179573	-9.16140536453016	
H	9.71828860045199	3.03045993683995	-6.35286238863463	
H	16.75638206737638	3.26374253776342	-7.36405487768162	
H	17.41590206678628	0.31858015812144	-5.93557277774092	
H	15.90185479290885	0.43223591956283	-8.89847660606645	
H	13.70137756244711	2.40729249279464	-3.94766348529170	
H	14.50452365366135	6.11204608185708	0.59095011499118	
H	12.24402474144693	-4.36094384461568	1.66205367267084	
H	10.23975051270394	-0.63486886160349	4.85631669200766	
H	-2.32283110386869	3.69549689570733	-2.24067839672954	
H	-2.49308338575816	7.55377184266031	0.29951688769117	

H	1.38689274711111	9.04527629228112	2.48741994362668	
H	5.31369337038491	6.45340845713985	2.14041434415269	
H	-1.90361767171904	0.64345155111935	-4.40566032674633	
H	-1.25655732970129	-3.19497612343142	-6.91728816790375	
H	3.02743585872249	-5.25410285304410	-6.89714326472283	
H	6.42525462341360	-3.30381478694712	-4.31561183710493	
H	12.09924303217713	-2.18154688148232	-9.15504508001200	
H	10.60185205859488	-6.49432208420021	-8.33768449433493	
H	10.17587833521866	-8.06623089368841	-3.98935753536795	
H	7.37338802524451	4.45088129699498	8.90812084797846	
H	8.07545922941236	8.98529383577004	8.17973295178298	
H	10.77447820549920	10.42458009508813	4.70781591176454	
H	16.69845646305406	-1.51753282493881	0.01781447893673	
H	16.12871337611942	2.11401897629333	3.75763857717251	
P	-4.07255237791635	12.04736455546673	-2.48336742240672	*
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F	-1.07822275193695	11.70510680840514	-2.54715701746959	*
F	-4.13338077214193	11.30503667001287	0.43801877516212	*
F	-7.08158029369308	12.36809643224272	-2.40996857000013	*
F	-4.02558323508877	12.79742708994870	-5.38877409586573	*
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P	4.07255237791635	-12.04736455546673	2.48336742240672	*
F	4.37333819544691	-9.14775745148421	3.21954235959881	*
F	1.07822275193695	-11.70510680840514	2.54715701746959	*
F	4.13338077214193	-11.30503667001287	-0.43801877516212	*
F	7.08158029369308	-12.36809643224272	2.40996857000013	*
F	4.02558323508877	-12.79742708994870	5.38877409586573	*
F	3.76302468733327	-14.93691264728789	1.72804578011992	*

Electrochemical Impedance Spectroscopy

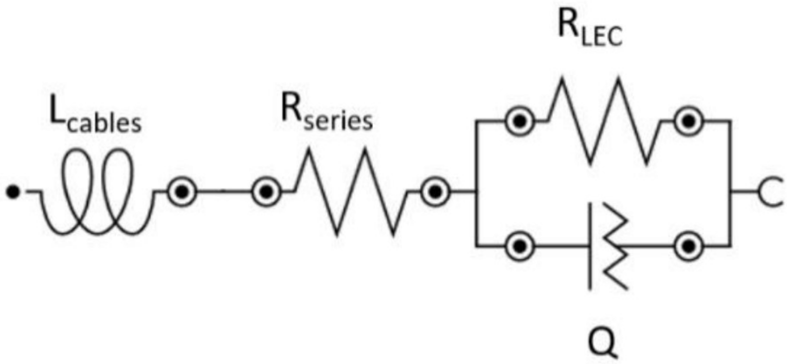

Figure S7. Simplified circuit model with electrical resistance (R_{LEC}) and Constant Phase Element (Q) used for static EIS assays. A series resistor (R_{series}) and inductor elements for the cables (L_{cables}) were also included.[2,3]

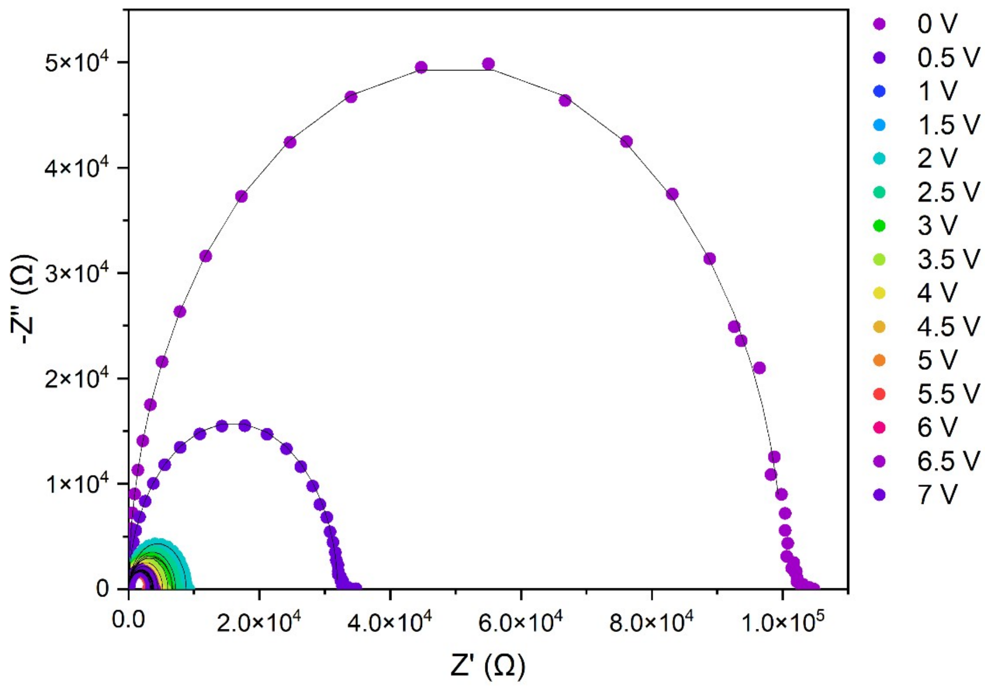

Figure S8. Nyquist plot of $[Ag(IPr)(bpy)][PF_6]$ fresh device

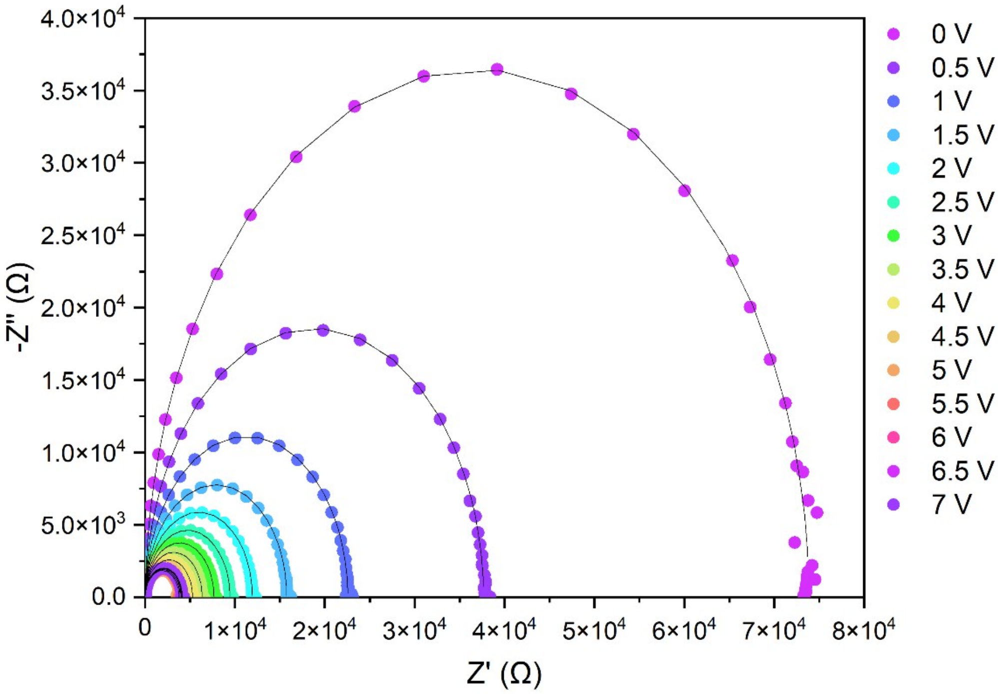

Figure S9. Nyquist plot of [Ag(IPr)(bpy)][PF_6] used device

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