Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary material

First Light-Emitting Electrochemical Cell with [Ag(I)(N^N)(P^P)] type Complex**

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Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb,M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.;Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada,M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.;Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.;Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.;Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.;Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.;Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2010.

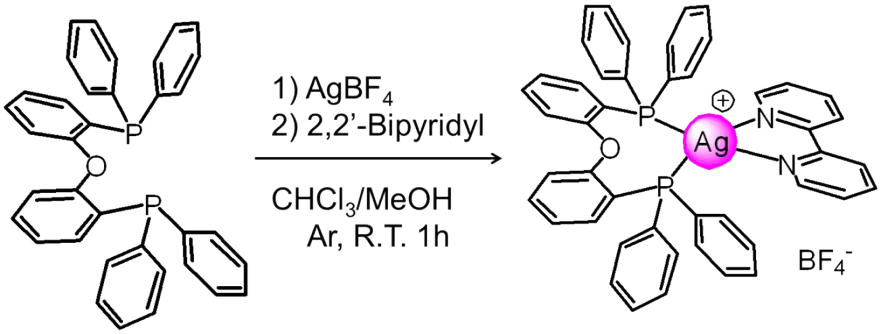

Figure S1a. Synthesis of [Ag(Bipy)(POP)]BF_4 complex.

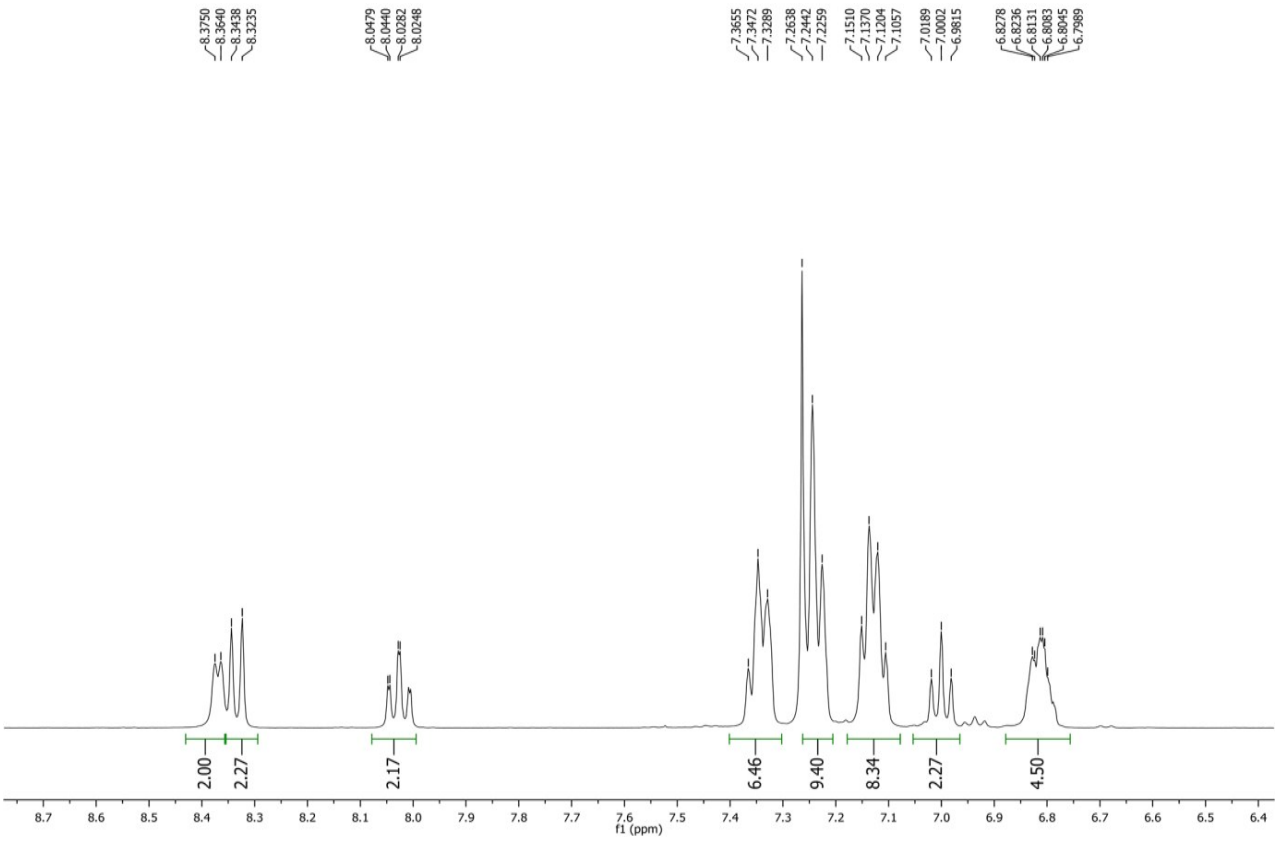

Figure S1b. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of [Ag(Bipy)(POP)]BF_4

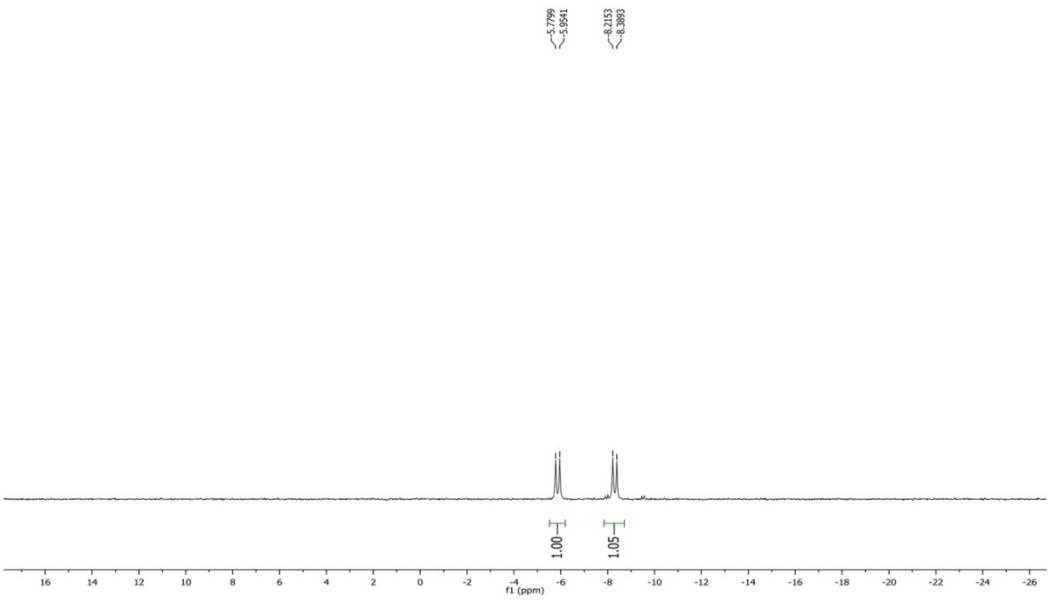

Figure S1b. ^{31}P $\{^{1}H\}$ NMR spectrum (162 MHz, $CDCl_3$, 298 K) of $[Ag(Bipy)(POP)]BF_4$

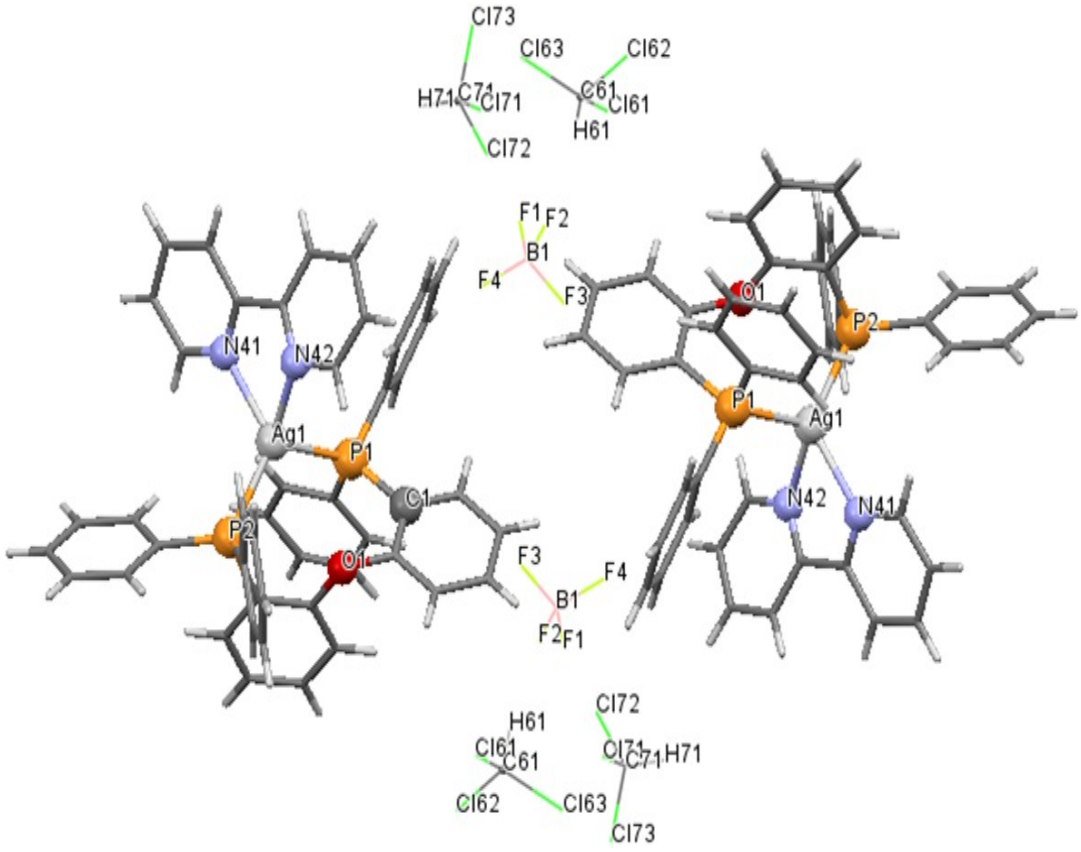

Figure S2. Mercury view of the cationic part of two adjacent moieties of $[Ag(I)(Bipy)(POP)]^{+}$.

Table S1. Crystal data and structure refinement.

Empirical formula	$C_{48}H_{38}AgBCl_6F_4N_2OP_2$	
Formula weight	1128.12	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 9.5560(7) Å	α = 109.126(6)°
	b = 13.9607(10) Å	β = 91.419(5)°
	c = 19.4900(14) Å	γ = 95.515(5)°
Volume	2440.9(3) Å^3	
Z	2	
Density (calculated)	1.535 Mg / m^3	
Absorption coefficient	0.861 mm^{-1}	
F(000)	1136	
Crystal	Block; Colourless	
Crystal size	0.180 × 0.150 × 0.080 mm^3	
θ range for data collection	2.933 – 27.485°	
Index ranges	$-12 \le h \le 12$, $-18 \le k \le 17$, $-25 \le l \le 24$	
Reflections collected	38260	
Independent reflections	11101 [R_{int} = 0.0740]	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.610	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11101 / 0 / 586	
Goodness-of-fit on F^2	1.021	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0503, *wR2* = 0.1334	
R indices (all data)	*R1* = 0.0553, *wR2* = 0.1388	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.927 and –0.834 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100μm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27* (Rigaku, 2013). **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 3.1 b27* (Rigaku, 2012). **Structure solution**: *SUPERFLIP* (Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst. 40, 786-790.) **Structure refinement**: *SHELXL-2013* (G Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565

Table S2. Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [$Å^2$ × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
Ag1	455(1)	6876(1)	3106(1)	24(1)	1
C1	3420(3)	5459(2)	3357(2)	24(1)	1
C2	2939(3)	4689(2)	2711(2)	26(1)	1
C3	3287(3)	3694(2)	2554(2)	30(1)	1
C4	4181(3)	3473(2)	3043(2)	33(1)	1
C5	4708(3)	4232(2)	3683(2)	33(1)	1
C6	4319(3)	5211(2)	3840(2)	29(1)	1
C7	1783(3)	5842(2)	1421(1)	24(1)	1
C8	2636(3)	5295(2)	1711(1)	26(1)	1
C9	3997(3)	5151(2)	1493(2)	29(1)	1
C10	4511(3)	5560(2)	981(2)	35(1)	1
C11	3689(3)	6106(2)	683(2)	34(1)	1
C12	2334(3)	6244(2)	904(2)	30(1)	1
C13	3238(3)	7305(2)	4528(2)	27(1)	1
C14	2235(3)	7060(2)	4968(2)	29(1)	1
C15	2435(3)	7454(2)	5728(2)	34(1)	1
C16	3628(3)	8108(3)	6044(2)	38(1)	1
C17	4616(3)	8370(3)	5607(2)	43(1)	1
C18	4428(3)	7967(2)	4851(2)	36(1)	1
C19	4251(3)	7377(2)	3154(2)	26(1)	1
C20	3943(3)	8238(2)	2992(2)	36(1)	1
C21	4938(4)	8753(3)	2692(2)	42(1)	1
C22	6240(3)	8402(2)	2542(2)	37(1)	1
C23	6563(3)	7550(2)	2704(2)	31(1)	1
C24	5578(3)	7044(2)	3015(2)	29(1)	1
C25	–983(3)	4858(2)	1487(1)	25(1)	1
C26	–639(3)	4062(2)	887(2)	28(1)	1
C27	–1481(3)	3131(2)	660(2)	33(1)	1
C28	–2667(3)	2988(2)	1025(2)	34(1)	1
C29	–3010(3)	3772(2)	1624(2)	36(1)	1
C30	–2173(3)	4714(2)	1862(2)	30(1)	1
C31	–672(3)	6811(2)	1271(1)	24(1)	1
C32	–1682(3)	6372(2)	696(2)	27(1)	1
C33	–2253(3)	6965(2)	331(2)	33(1)	1
C34	–1807(3)	8008(2)	535(2)	34(1)	1
C35	–788(3)	8447(2)	1104(2)	35(1)	1
C36	–238(3)	7865(2)	1474(2)	31(1)	1
O1	2036(2)	4900(1)	2218(1)	26(1)	1
P1	2883(1)	6744(1)	3542(1)	23(1)	1
P2	70(1)	6097(1)	1799(1)	23(1)	1

C41	–287(3)	9239(2)	3576(2)	27(1)	1
C42	–911(3)	10108(2)	3944(2)	31(1)	1
C43	–1711(3)	10100(2)	4525(2)	32(1)	1
C44	–1870(3)	9222(2)	4715(2)	29(1)	1
C45	–1222(3)	8372(2)	4318(1)	24(1)	1
C46	–1394(3)	7399(2)	4483(1)	24(1)	1
C47	–1748(3)	7387(2)	5170(2)	31(1)	1
C48	–1900(3)	6458(2)	5298(2)	36(1)	1
C49	–1717(3)	5575(2)	4736(2)	36(1)	1
C50	–1343(3)	5656(2)	4073(2)	33(1)	1
N41	–429(2)	8387(2)	3757(1)	24(1)	1
N42	–1160(2)	6548(2)	3943(1)	26(1)	1
B1	2415(3)	770(2)	2906(2)	28(1)	1
F1	3721(2)	921(1)	2641(1)	34(1)	1
F2	1507(2)	74(1)	2351(1)	35(1)	1
F3	1830(2)	1698(1)	3156(1)	36(1)	1
F4	2546(2)	388(1)	3482(1)	32(1)	1
C61	3285(3)	78(2)	928(2)	35(1)	1
Cl61	4159(1)	1295(1)	1036(1)	51(1)	1
Cl62	2167(1)	–351(1)	128(1)	39(1)	1
Cl63	4512(1)	–790(1)	904(1)	70(1)	1
C71	9386(3)	1715(2)	2172(2)	36(1)	1
Cl71	7621(1)	1159(1)	1996(1)	47(1)	1
Cl72	9491(1)	3038(1)	2639(1)	45(1)	1
Cl73	10253(1)	1478(1)	1351(1)	40(1)	1

Table S3. Bond lengths [Å] and angles [°].

Ag1–N41	2.328(2)	C19–P1	1.824(3)
Ag1–N42	2.394(2)	C20–C21	1.391(4)
Ag1–P2	2.4227(7)	C20–H20	0.9500
Ag1–P1	2.4961(7)	C21–C22	1.384(5)
C1–C2	1.393(4)	C21–H21	0.9500
C1–C6	1.405(4)	C22–C23	1.386(4)
C1–P1	1.837(3)	C22–H22	0.9500
C2–C3	1.395(4)	C23–C24	1.391(4)
C2–O1	1.395(3)	C23–H23	0.9500
C3–C4	1.390(4)	C24–H24	0.9500
C3–H3	0.9500	C25–C26	1.395(4)
C4–C5	1.390(4)	C25–C30	1.400(4)
C4–H4	0.9500	C25–P2	1.822(3)
C5–C6	1.389(4)	C26–C27	1.392(4)
C5–H5	0.9500	C26–H26	0.9500
C6–H6	0.9500	C27–C28	1.386(4)
C7–C8	1.395(4)	C27–H27	0.9500
C7–C12	1.397(4)	C28–C29	1.385(5)
C7–P2	1.830(3)	C28–H28	0.9500
C8–O1	1.390(3)	C29–C30	1.403(4)
C8–C9	1.391(4)	C29–H29	0.9500
C9–C10	1.380(4)	C30–H30	0.9500
C9–H9	0.9500	C31–C32	1.395(4)
C10–C11	1.384(5)	C31–C36	1.410(4)
C10–H10	0.9500	C31–P2	1.823(3)
C11–C12	1.386(4)	C32–C33	1.394(4)
C11–H11	0.9500	C32–H32	0.9500
C12–H12	0.9500	C33–C34	1.397(4)
C13–C18	1.387(4)	C33–H33	0.9500
C13–C14	1.393(4)	C34–C35	1.393(4)
C13–P1	1.830(3)	C34–H34	0.9500
C14–C15	1.401(4)	C35–C36	1.379(4)
C14–H14	0.9500	C35–H35	0.9500
C15–C16	1.382(5)	C36–H36	0.9500
C15–H15	0.9500	C41–N41	1.343(3)
C16–C17	1.388(5)	C41–C42	1.390(4)
C16–H16	0.9500	C41–H41	0.9500
C17–C18	1.395(4)	C42–C43	1.385(4)
C17–H17	0.9500	C42–H42	0.9500
C18–H18	0.9500	C43–C44	1.388(4)
C19–C20	1.393(4)	C43–H43	0.9500
C19–C24	1.394(4)	C44–C45	1.398(4)

C44–H44	0.9500	B1–F1	1.386(4)
C45–N41	1.351(3)	B1–F4	1.399(4)
C45–C46	1.489(4)	B1–F3	1.401(4)
C46–N42	1.346(3)	B1–F2	1.404(3)
C46–C47	1.394(4)	C61–Cl63	1.757(3)
C47–C48	1.395(4)	C61–Cl62	1.765(3)
C47–H47	0.9500	C61–Cl61	1.766(3)
C48–C49	1.384(4)	C61–H61	1.0000
C48–H48	0.9500	C71–Cl72	1.763(3)
C49–C50	1.387(4)	C71–Cl71	1.764(3)
C49–H49	0.9500	C71–Cl73	1.769(3)
C50–N42	1.346(4)	C71–H71	1.0000
C50–H50	0.9500		

N41–Ag1–N42	70.84(8)
N41–Ag1–P2	122.86(6)
N42–Ag1–P2	122.93(6)
N41–Ag1–P1	113.52(6)
N42–Ag1–P1	108.23(6)
P2–Ag1–P1	112.17(2)
C2–C1–C6	117.7(2)
C2–C1–P1	119.7(2)
C6–C1–P1	122.7(2)
C1–C2–C3	121.8(3)
C1–C2–O1	119.5(2)
C3–C2–O1	118.7(2)
C4–C3–C2	119.2(3)
C4–C3–H3	120.4
C2–C3–H3	120.4
C5–C4–C3	120.4(3)
C5–C4–H4	119.8
C3–C4–H4	119.8
C6–C5–C4	119.7(3)
C6–C5–H5	120.1
C4–C5–H5	120.1
C5–C6–C1	121.3(3)
C5–C6–H6	119.4
C1–C6–H6	119.4
C8–C7–C12	118.1(2)
C8–C7–P2	118.4(2)
C12–C7–P2	123.2(2)
O1–C8–C9	122.8(2)
O1–C8–C7	116.0(2)
C9–C8–C7	121.1(3)
C10–C9–C8	119.3(3)
C10–C9–H9	120.3
C8–C9–H9	120.3
C9–C10–C11	120.8(3)
C9–C10–H10	119.6
C11–C10–H10	119.6
C10–C11–C12	119.4(3)
C10–C11–H11	120.3
C12–C11–H11	120.3
C11–C12–C7	121.1(3)
C11–C12–H12	119.4
C7–C12–H12	119.4
C18–C13–C14	119.1(3)
C18–C13–P1	123.5(2)
C14–C13–P1	117.4(2)
C13–C14–C15	120.8(3)

C13–C14–H14	119.6
C15–C14–H14	119.6
C16–C15–C14	119.6(3)
C16–C15–H15	120.2
C14–C15–H15	120.2
C15–C16–C17	119.8(3)
C15–C16–H16	120.1
C17–C16–H16	120.1
C16–C17–C18	120.6(3)
C16–C17–H17	119.7
C18–C17–H17	119.7
C13–C18–C17	120.1(3)
C13–C18–H18	120.0
C17–C18–H18	120.0
C20–C19–C24	119.0(3)
C20–C19–P1	117.7(2)
C24–C19–P1	123.3(2)
C21–C20–C19	120.6(3)
C21–C20–H20	119.7
C19–C20–H20	119.7
C22–C21–C20	119.9(3)
C22–C21–H21	120.1
C20–C21–H21	120.1
C21–C22–C23	120.1(3)
C21–C22–H22	120.0
C23–C22–H22	120.0
C22–C23–C24	120.1(3)
C22–C23–H23	120.0
C24–C23–H23	120.0
C23–C24–C19	120.4(3)
C23–C24–H24	119.8
C19–C24–H24	119.8
C26–C25–C30	119.8(2)
C26–C25–P2	121.8(2)
C30–C25–P2	118.4(2)
C27–C26–C25	120.1(3)
C27–C26–H26	120.0
C25–C26–H26	120.0
C28–C27–C26	120.4(3)
C28–C27–H27	119.8
C26–C27–H27	119.8
C29–C28–C27	119.9(3)
C29–C28–H28	120.0
C27–C28–H28	120.0
C28–C29–C30	120.5(3)
C28–C29–H29	119.7

C30–C29–H29	119.7
C25–C30–C29	119.3(3)
C25–C30–H30	120.3
C29–C30–H30	120.3
C32–C31–C36	118.6(3)
C32–C31–P2	123.2(2)
C36–C31–P2	118.2(2)
C33–C32–C31	120.6(3)
C33–C32–H32	119.7
C31–C32–H32	119.7
C32–C33–C34	120.1(3)
C32–C33–H33	119.9
C34–C33–H33	119.9
C35–C34–C33	119.4(3)
C35–C34–H34	120.3
C33–C34–H34	120.3
C36–C35–C34	120.6(3)
C36–C35–H35	119.7
C34–C35–H35	119.7
C35–C36–C31	120.6(3)
C35–C36–H36	119.7
C31–C36–H36	119.7
C8–O1–C2	117.9(2)
C19–P1–C13	105.00(12)
C19–P1–C1	103.42(12)
C13–P1–C1	102.14(12)
C19–P1–Ag1	112.98(9)
C13–P1–Ag1	114.40(9)
C1–P1–Ag1	117.39(9)
C25–P2–C31	104.43(12)
C25–P2–C7	104.36(12)
C31–P2–C7	103.74(12)
C25–P2–Ag1	115.55(9)
C31–P2–Ag1	119.41(9)
C7–P2–Ag1	107.78(8)
N41–C41–C42	122.9(3)
N41–C41–H41	118.5
C42–C41–H41	118.5
C43–C42–C41	118.7(3)
C43–C42–H42	120.6
C41–C42–H42	120.6
C42–C43–C44	118.8(3)
C42–C43–H43	120.6
C44–C43–H43	120.6
C43–C44–C45	119.5(3)
C43–C44–H44	120.3

C45–C44–H44	120.3
N41–C45–C44	121.5(2)
N41–C45–C46	116.7(2)
C44–C45–C46	121.8(2)
N42–C46–C47	122.3(3)
N42–C46–C45	116.7(2)
C47–C46–C45	121.0(2)
C46–C47–C48	119.0(3)
C46–C47–H47	120.5
C48–C47–H47	120.5
C49–C48–C47	118.9(3)
C49–C48–H48	120.5
C47–C48–H48	120.5
C48–C49–C50	118.5(3)
C48–C49–H49	120.8
C50–C49–H49	120.8
N42–C50–C49	123.4(3)
N42–C50–H50	118.3
C49–C50–H50	118.3
C41–N41–C45	118.5(2)
C41–N41–Ag1	124.14(18)
C45–N41–Ag1	117.14(17)
C50–N42–C46	117.8(2)
C50–N42–Ag1	123.51(19)
C46–N42–Ag1	112.89(17)
F1–B1–F4	110.4(2)
F1–B1–F3	109.8(2)
F4–B1–F3	108.9(2)
F1–B1–F2	109.8(2)
F4–B1–F2	109.1(2)
F3–B1–F2	108.8(2)
Cl63–C61–Cl62	110.68(17)
Cl63–C61–Cl61	110.37(18)
Cl62–C61–Cl61	110.03(17)
Cl63–C61–H61	108.6
Cl62–C61–H61	108.6
Cl61–C61–H61	108.6
Cl72–C71–Cl71	111.28(17)
Cl72–C71–Cl73	110.18(18)
Cl71–C71–Cl73	110.36(17)
Cl72–C71–H71	108.3
Cl71–C71–H71	108.3
Cl73–C71–H71	108.3

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag1	24(1)	26(1)	19(1)	4(1)	4(1)	7(1)
C1	22(1)	24(1)	27(1)	8(1)	6(1)	5(1)
C2	21(1)	27(1)	29(1)	9(1)	5(1)	5(1)
C3	27(1)	26(1)	36(2)	5(1)	6(1)	4(1)
C4	30(1)	27(1)	44(2)	12(1)	10(1)	7(1)
C5	31(1)	34(1)	38(2)	17(1)	5(1)	8(1)
C6	28(1)	31(1)	29(1)	10(1)	5(1)	6(1)
C7	23(1)	26(1)	19(1)	1(1)	2(1)	3(1)
C8	27(1)	24(1)	20(1)	1(1)	2(1)	2(1)
C9	24(1)	34(1)	27(1)	3(1)	3(1)	7(1)
C10	23(1)	45(2)	32(2)	7(1)	8(1)	4(1)
C11	32(2)	43(2)	26(1)	9(1)	8(1)	2(1)
C12	29(1)	33(1)	24(1)	5(1)	2(1)	3(1)
C13	27(1)	28(1)	24(1)	5(1)	–1(1)	10(1)
C14	34(2)	28(1)	26(1)	8(1)	1(1)	6(1)
C15	45(2)	35(2)	25(1)	11(1)	5(1)	13(1)
C16	40(2)	47(2)	24(1)	3(1)	0(1)	17(1)
C17	30(2)	55(2)	32(2)	–3(1)	–6(1)	8(1)
C18	25(1)	44(2)	31(2)	2(1)	3(1)	7(1)
C19	27(1)	26(1)	23(1)	3(1)	0(1)	5(1)
C20	28(1)	35(2)	49(2)	18(1)	7(1)	11(1)
C21	39(2)	40(2)	58(2)	27(2)	8(2)	12(1)
C22	35(2)	38(2)	37(2)	13(1)	5(1)	0(1)
C23	24(1)	34(1)	29(1)	4(1)	4(1)	4(1)
C24	27(1)	28(1)	29(1)	6(1)	2(1)	6(1)
C25	23(1)	26(1)	24(1)	8(1)	1(1)	4(1)
C26	31(1)	29(1)	22(1)	7(1)	5(1)	2(1)
C27	39(2)	27(1)	28(1)	5(1)	–2(1)	1(1)
C28	30(1)	30(1)	44(2)	16(1)	–4(1)	–1(1)
C29	24(1)	35(2)	55(2)	21(1)	8(1)	5(1)
C30	27(1)	30(1)	36(2)	12(1)	9(1)	10(1)
C31	24(1)	26(1)	22(1)	6(1)	6(1)	6(1)
C32	26(1)	29(1)	24(1)	6(1)	6(1)	6(1)
C33	30(1)	38(2)	29(2)	10(1)	0(1)	5(1)
C34	37(2)	37(2)	34(2)	16(1)	5(1)	10(1)
C35	43(2)	28(1)	33(2)	11(1)	6(1)	6(1)
C36	34(2)	30(1)	26(1)	6(1)	2(1)	3(1)
O1	22(1)	27(1)	25(1)	5(1)	4(1)	5(1)
P1	24(1)	23(1)	22(1)	4(1)	2(1)	6(1)
P2	22(1)	24(1)	19(1)	4(1)	3(1)	5(1)
C41	27(1)	27(1)	26(1)	7(1)	3(1)	3(1)
C42	33(1)	24(1)	35(2)	7(1)	3(1)	5(1)
C43	34(2)	27(1)	31(2)	3(1)	4(1)	10(1)
C44	26(1)	30(1)	27(1)	4(1)	6(1)	5(1)

C45	23(1)	25(1)	22(1)	4(1)	2(1)	5(1)
C46	22(1)	27(1)	22(1)	6(1)	5(1)	4(1)
C47	32(1)	32(1)	27(1)	6(1)	10(1)	7(1)
C48	37(2)	42(2)	33(2)	16(1)	10(1)	3(1)
C49	38(2)	31(1)	40(2)	15(1)	6(1)	2(1)
C50	35(2)	28(1)	35(2)	9(1)	6(1)	4(1)
N41	24(1)	24(1)	22(1)	4(1)	3(1)	3(1)
N42	28(1)	24(1)	24(1)	5(1)	5(1)	5(1)
B1	30(2)	29(2)	24(2)	7(1)	2(1)	2(1)
F1	32(1)	35(1)	33(1)	10(1)	7(1)	1(1)
F2	40(1)	35(1)	25(1)	6(1)	–4(1)	–5(1)
F3	41(1)	35(1)	31(1)	7(1)	2(1)	11(1)
F4	35(1)	35(1)	27(1)	12(1)	–1(1)	0(1)
C61	40(2)	37(2)	26(1)	7(1)	5(1)	7(1)
Cl61	47(1)	55(1)	42(1)	12(1)	2(1)	–15(1)
Cl62	50(1)	33(1)	29(1)	5(1)	–1(1)	2(1)
Cl63	89(1)	80(1)	44(1)	12(1)	4(1)	51(1)
C71	36(2)	38(2)	33(2)	10(1)	3(1)	9(1)
Cl71	39(1)	55(1)	49(1)	20(1)	2(1)	1(1)
Cl72	46(1)	40(1)	43(1)	6(1)	3(1)	12(1)
Cl73	39(1)	48(1)	34(1)	11(1)	5(1)	13(1)

Table S5. Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H3	2917	3174	2119	36	1
H4	4433	2801	2938	39	1
H5	5331	4081	4011	39	1
H6	4667	5723	4283	35	1
H9	4567	4776	1694	35	1
H10	5441	5465	831	42	1
H11	4052	6384	331	41	1
H12	1770	6619	700	36	1
H14	1406	6621	4750	35	1
H15	1754	7272	6024	41	1
H16	3772	8377	6558	46	1
H17	5428	8828	5826	52	1
H18	5115	8145	4557	43	1
H20	3045	8474	3087	43	1
H21	4724	9346	2591	50	1
H22	6913	8745	2328	44	1
H23	7459	7312	2603	37	1
H24	5809	6467	3133	34	1
H26	170	4156	633	33	1
H27	–1241	2591	253	39	1
H28	–3245	2354	864	41	1
H29	–3819	3670	1876	43	1
H30	–2410	5250	2273	36	1
H32	–1984	5663	552	32	1
H33	–2947	6660	–57	39	1
H34	–2195	8414	287	41	1
H35	–469	9153	1238	41	1
H36	439	8178	1868	37	1
H41	265	9248	3179	32	1
H42	–791	10696	3799	37	1
H43	–2143	10685	4790	38	1
H44	–2414	9199	5112	35	1
H47	–1883	8002	5544	37	1
H48	–2126	6431	5764	44	1
H49	–1844	4929	4804	43	1
H50	–1208	5049	3689	39	1
H61	2696	133	1354	42	1
H71	9876	1393	2486	43	1

Table S6. Torsion angles [°].

C6–C1–C2–C3	2.3(4)
P1–C1–C2–C3	–178.2(2)
C6–C1–C2–O1	179.5(2)
P1–C1–C2–O1	–1.1(3)
C1–C2–C3–C4	–2.5(4)
O1–C2–C3–C4	–179.7(2)
C2–C3–C4–C5	0.8(4)
C3–C4–C5–C6	1.1(4)
C4–C5–C6–C1	–1.3(4)
C2–C1–C6–C5	–0.4(4)
P1–C1–C6–C5	–179.8(2)
C12–C7–C8–O1	–179.3(2)
P2–C7–C8–O1	6.3(3)
C12–C7–C8–C9	–0.1(4)
P2–C7–C8–C9	–174.4(2)
O1–C8–C9–C10	179.3(2)
C7–C8–C9–C10	0.1(4)
C8–C9–C10–C11	–0.1(4)
C9–C10–C11–C12	0.0(4)
C10–C11–C12–C7	0.0(4)
C8–C7–C12–C11	0.0(4)
P2–C7–C12–C11	174.0(2)
C18–C13–C14–C15	–1.5(4)
P1–C13–C14–C15	179.5(2)
C13–C14–C15–C16	1.2(4)
C14–C15–C16–C17	0.1(5)
C15–C16–C17–C18	–1.0(5)
C14–C13–C18–C17	0.6(5)
P1–C13–C18–C17	179.4(2)
C16–C17–C18–C13	0.7(5)
C24–C19–C20–C21	0.4(5)
P1–C19–C20–C21	–179.8(3)
C19–C20–C21–C22	1.0(5)
C20–C21–C22–C23	–1.3(5)
C21–C22–C23–C24	0.3(5)
C22–C23–C24–C19	1.1(4)
C20–C19–C24–C23	–1.5(4)
P1–C19–C24–C23	178.7(2)
C30–C25–C26–C27	0.3(4)
P2–C25–C26–C27	–179.2(2)
C25–C26–C27–C28	0.3(4)
C26–C27–C28–C29	–0.7(5)
C27–C28–C29–C30	0.6(5)
C26–C25–C30–C29	–0.5(4)

P2–C25–C30–C29	179.0(2)
C28–C29–C30–C25	0.0(4)
C36–C31–C32–C33	–0.2(4)
P2–C31–C32–C33	177.4(2)
C31–C32–C33–C34	0.6(4)
C32–C33–C34–C35	0.1(5)
C33–C34–C35–C36	–1.1(5)
C34–C35–C36–C31	1.6(5)
C32–C31–C36–C35	–0.9(4)
P2–C31–C36–C35	–178.6(2)
C9–C8–O1–C2	23.9(3)
C7–C8–O1–C2	–156.8(2)
C1–C2–O1–C8	86.6(3)
C3–C2–O1–C8	–96.2(3)
C20–C19–P1–C13	–93.5(2)
C24–C19–P1–C13	86.3(2)
C20–C19–P1–C1	159.8(2)
C24–C19–P1–C1	–20.4(3)
C20–C19–P1–Ag1	31.8(3)
C24–C19–P1–Ag1	–148.3(2)
C18–C13–P1–C19	–7.3(3)
C14–C13–P1–C19	171.5(2)
C18–C13–P1–C1	100.3(3)
C14–C13–P1–C1	–80.8(2)
C18–C13–P1–Ag1	–131.8(2)
C14–C13–P1–Ag1	47.1(2)
C2–C1–P1–C19	–90.0(2)
C6–C1–P1–C19	89.4(2)
C2–C1–P1–C13	161.1(2)
C6–C1–P1–C13	–19.5(3)
C2–C1–P1–Ag1	35.1(2)
C6–C1–P1–Ag1	–145.46(19)
C26–C25–P2–C31	87.7(2)
C30–C25–P2–C31	–91.8(2)
C26–C25–P2–C7	–20.9(3)
C30–C25–P2–C7	159.6(2)
C26–C25–P2–Ag1	–139.1(2)
C30–C25–P2–Ag1	41.4(2)
C32–C31–P2–C25	–8.1(3)
C36–C31–P2–C25	169.5(2)
C32–C31–P2–C7	101.0(2)
C36–C31–P2–C7	–81.5(2)
C32–C31–P2–Ag1	–139.1(2)
C36–C31–P2–Ag1	38.4(2)
C8–C7–P2–C25	–70.8(2)
C12–C7–P2–C25	115.2(2)

C8–C7–P2–C31	–179.9(2)
C12–C7–P2–C31	6.1(2)
C8–C7–P2–Ag1	52.6(2)
C12–C7–P2–Ag1	–121.5(2)
N41–C41–C42–C43	0.3(4)
C41–C42–C43–C44	–0.6(4)
C42–C43–C44–C45	0.0(4)
C43–C44–C45–N41	0.8(4)
C43–C44–C45–C46	–178.1(3)
N41–C45–C46–N42	–21.0(3)
C44–C45–C46–N42	157.9(3)
N41–C45–C46–C47	157.6(3)
C44–C45–C46–C47	–23.5(4)
N42–C46–C47–C48	–1.6(4)
C45–C46–C47–C48	179.8(3)
C46–C47–C48–C49	–1.0(5)
C47–C48–C49–C50	2.1(5)
C48–C49–C50–N42	–0.6(5)
C42–C41–N41–C45	0.5(4)
C42–C41–N41–Ag1	175.2(2)
C44–C45–N41–C41	–1.1(4)
C46–C45–N41–C41	177.9(2)
C44–C45–N41–Ag1	–176.1(2)
C46–C45–N41–Ag1	2.8(3)
C49–C50–N42–C46	–1.9(4)
C49–C50–N42–Ag1	149.4(2)
C47–C46–N42–C50	3.0(4)
C45–C46–N42–C50	–178.4(2)
C47–C46–N42–Ag1	–151.2(2)
C45–C46–N42–Ag1	27.4(3)

Symmetry transformations used to generate equivalent atoms:

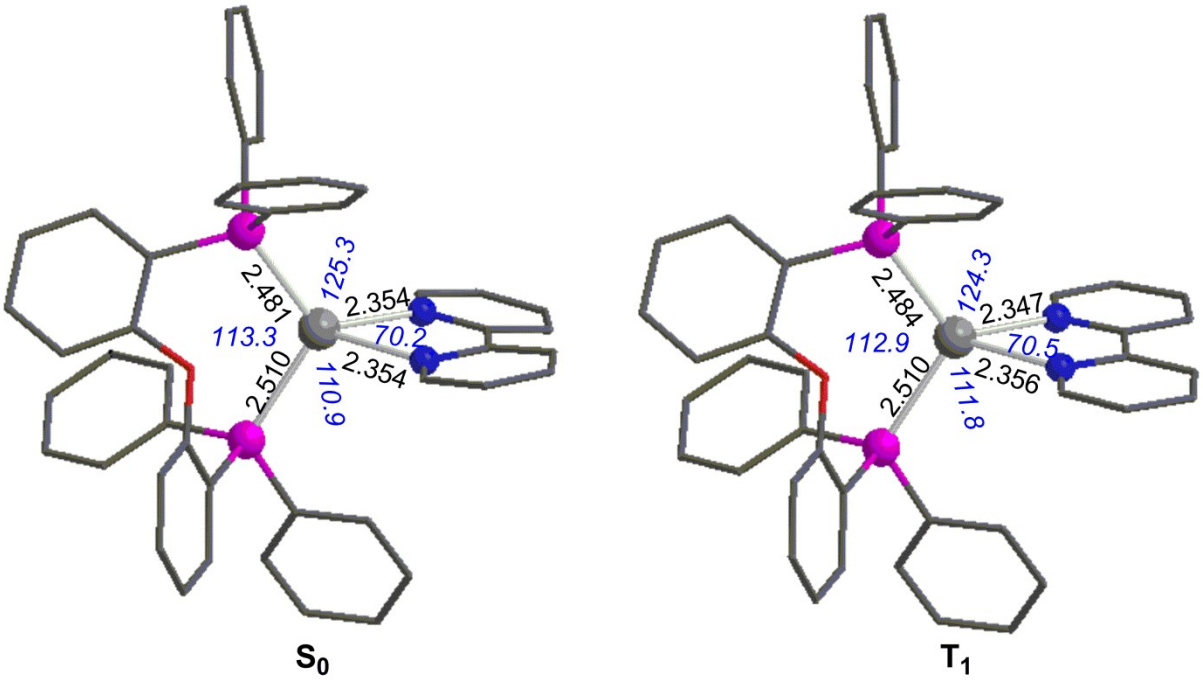

Figure S3. The molecular structure of the cationic $[Ag(Bipy)(POP)]^+$ complex in S_0 (left) and T_1 (right) states along with relevant structural parameters, optimized at the PBE0/TZP(Ag)∪6-31G(d,p)(E) level in $CHCl_3$ solution.

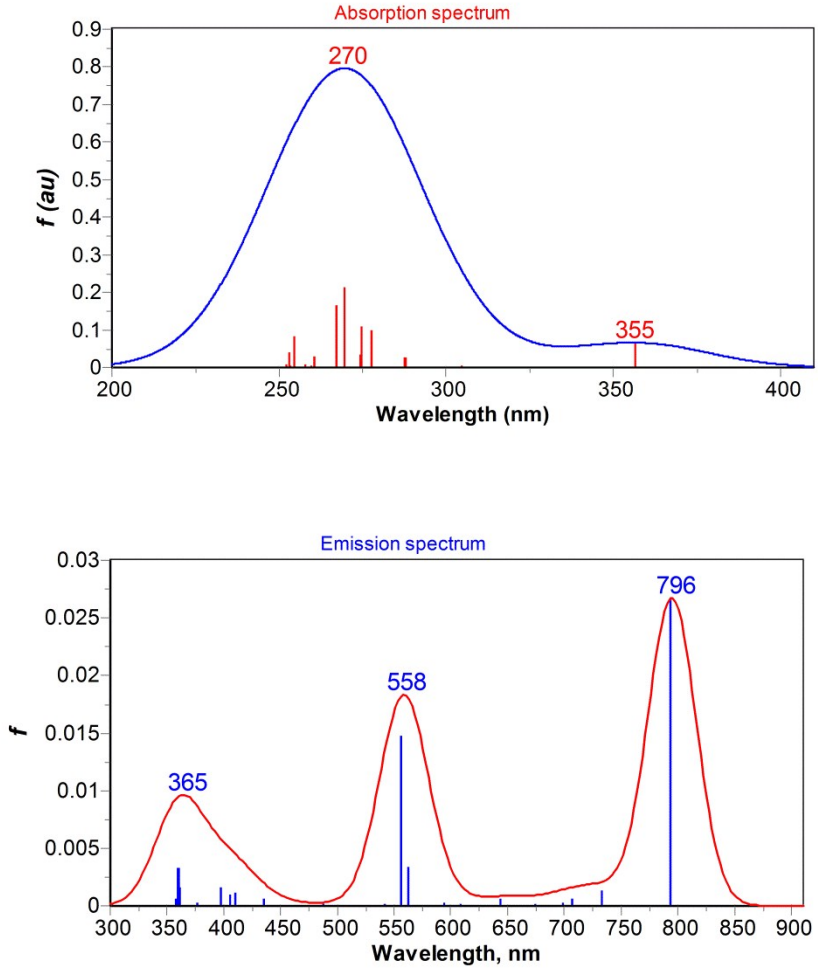

Figure S4. Simulated absorption (top) and emission (bottom) spectra (FWHM=50) of the cationic $[Ag(Bipy)(POP)]^+$ complex, calculated in $CHCl_3$ solution at the TD-DFT/PBE0/TZP(Ag)∪6-31G(d,p)(E) level.

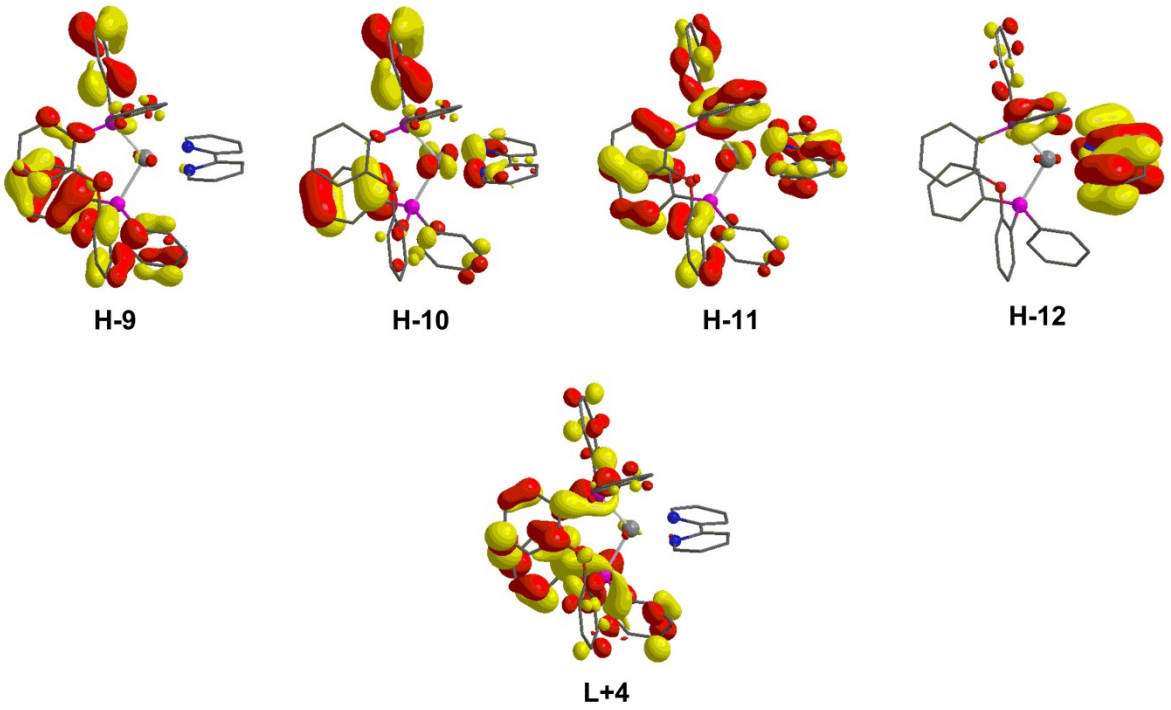

Figure S5. 3-D contour plots of the MOs involved in the most important electronic transitions in the absorption spectrum of the cationic $[Ag(Bipy)(POP)]^+$ complex.

Table S7. Cartesian coordinates and energetic data.

$[Ag(Bipy)(POP)]^+$ (S_0) (Gas Phase)

Ag	-0.056075000	-0.752582000	-0.371660000
C	-1.977712000	1.414766000	1.736983000
C	-0.769561000	1.657718000	2.408225000
C	-0.742351000	2.018951000	3.750059000
H	0.217415000	2.178259000	4.231729000
C	-1.938788000	2.162288000	4.446875000
H	-1.920982000	2.446924000	5.494424000
C	-3.150463000	1.933063000	3.801544000
H	-4.085667000	2.039216000	4.342386000
C	-3.166943000	1.556434000	2.461397000
H	-4.114493000	1.356124000	1.969711000
C	1.994890000	2.078676000	0.119514000
C	1.038042000	2.467841000	1.071145000
C	0.761809000	3.808556000	1.312636000
H	0.012613000	4.085557000	2.046470000
C	1.455186000	4.783364000	0.600818000
H	1.239552000	5.830814000	0.788937000
C	2.416143000	4.424833000	-0.338548000
H	2.957225000	5.187727000	-0.888827000
C	2.679407000	3.079140000	-0.575958000
H	3.418062000	2.796699000	-1.319771000
C	-3.623075000	0.205120000	-0.282917000
C	-3.872023000	-1.104841000	0.149852000
H	-3.073602000	-1.677044000	0.617325000
C	-5.130627000	-1.672161000	-0.013239000
H	-5.316913000	-2.684186000	0.334267000
C	-6.147855000	-0.946624000	-0.630956000
H	-7.128925000	-1.392184000	-0.766150000
C	-5.902257000	0.347425000	-1.080396000
H	-6.690478000	0.913098000	-1.568441000
C	-4.646592000	0.925555000	-0.905889000
H	-4.463933000	1.935388000	-1.260522000
C	-1.863436000	2.418164000	-0.966028000
C	-1.141980000	2.424395000	-2.163659000
H	-0.617758000	1.523811000	-2.474926000
C	-1.079320000	3.575599000	-2.942990000
H	-0.514748000	3.571991000	-3.870559000
C	-1.731437000	4.732577000	-2.525978000
H	-1.680149000	5.632931000	-3.131036000
C	-2.443358000	4.738954000	-1.327890000
H	-2.946784000	5.643274000	-0.998751000
C	-2.508837000	3.588622000	-0.548395000

H	-3.055754000	3.601900000	0.390676000
C	3.211700000	-0.347691000	1.135697000
C	3.822326000	0.481911000	2.080704000
H	3.689002000	1.558450000	2.022881000
C	4.605213000	-0.068249000	3.093296000
H	5.077176000	0.583688000	3.822624000
C	4.790219000	-1.446012000	3.166077000
H	5.405930000	-1.871199000	3.953198000
C	4.185139000	-2.278604000	2.226251000
H	4.328409000	-3.354021000	2.277969000
C	3.393523000	-1.733908000	1.221100000
H	2.916561000	-2.386573000	0.493529000
C	3.299786000	0.238651000	-1.682690000
C	4.688232000	0.379366000	-1.570989000
H	5.142673000	0.511488000	-0.592956000
C	5.487947000	0.340111000	-2.709060000
H	6.564574000	0.446922000	-2.615118000
C	4.911269000	0.161229000	-3.964928000
H	5.539011000	0.128980000	-4.850481000
C	3.531676000	0.014186000	-4.083639000
H	3.081624000	-0.134915000	-5.060705000
C	2.730782000	0.045910000	-2.946137000
H	1.654499000	-0.087457000	-3.031829000
O	0.427115000	1.442372000	1.753930000
P	-1.936803000	0.861535000	-0.013910000
P	2.186176000	0.296137000	-0.235979000
C	-1.062712000	-2.629636000	-2.859011000
H	-0.908174000	-1.683770000	-3.370965000
C	-1.616878000	-3.713448000	-3.528123000
H	-1.897481000	-3.627350000	-4.572071000
C	-1.807011000	-4.891866000	-2.816768000
H	-2.251013000	-5.761729000	-3.290782000
C	-1.428499000	-4.940070000	-1.481864000
H	-1.595308000	-5.843517000	-0.907205000
C	-0.859987000	-3.810117000	-0.887102000
C	-0.428793000	-3.808632000	0.536653000
C	-0.264712000	-4.991058000	1.263546000
H	-0.410356000	-5.957363000	0.795049000
C	0.116704000	-4.920308000	2.597614000
H	0.249098000	-5.829854000	3.175499000
C	0.333188000	-3.674433000	3.173935000
H	0.631973000	-3.572001000	4.211356000
C	0.171370000	-2.547478000	2.376487000
H	0.349566000	-1.551232000	2.771845000
N	-0.692566000	-2.669731000	-1.577689000
N	-0.198933000	-2.610436000	1.096634000

Sum of electronic and zero-point Energies= -7836.879848
Sum of electronic and thermal Energies= -7836.834271
Sum of electronic and thermal Enthalpies= -7836.833326
Sum of electronic and thermal Free Energies= -7836.967448

[Ag(Bipy)(POP)]$^{+}$ (T_1) (Gas Phase)

Ag	0.054790000	0.740748000	-0.406040000
C	2.030490000	-1.401524000	1.670619000
C	0.842979000	-1.626590000	2.383888000
C	0.856320000	-1.961155000	3.732896000
H	-0.088512000	-2.108416000	4.246936000
C	2.073354000	-2.094469000	4.395310000
H	2.087233000	-2.358875000	5.448222000
C	3.264975000	-1.881077000	3.708597000
H	4.216209000	-1.979014000	4.222387000
C	3.240970000	-1.531444000	2.361173000
H	4.173394000	-1.344324000	1.836479000
C	-1.997079000	-2.079170000	0.194845000
C	-1.013357000	-2.454143000	1.124512000
C	-0.740704000	-3.790997000	1.389716000
H	0.029241000	-4.057038000	2.105928000
C	-1.464460000	-4.776433000	0.724197000
H	-1.251497000	-5.820968000	0.930680000
C	-2.452211000	-4.431848000	-0.192243000
H	-3.017118000	-5.202792000	-0.706169000
C	-2.712039000	-3.089867000	-0.453527000
H	-3.472393000	-2.818605000	-1.179444000
C	3.616481000	-0.247715000	-0.431452000
C	3.868297000	1.092934000	-0.109730000
H	3.071696000	1.702392000	0.311215000
C	5.125676000	1.644860000	-0.328286000
H	5.313783000	2.682416000	-0.067999000
C	6.138365000	0.870810000	-0.891485000
H	7.118073000	1.303638000	-1.070815000
C	5.889812000	-0.455830000	-1.232041000
H	6.674291000	-1.059276000	-1.679164000
C	4.635701000	-1.016903000	-1.001883000
H	4.449718000	-2.051434000	-1.274363000
C	1.816722000	-2.457675000	-1.004573000
C	1.080715000	-2.472713000	-2.193369000
H	0.571956000	-1.567473000	-2.516540000
C	0.985314000	-3.637328000	-2.948908000
H	0.410104000	-3.640196000	-3.869942000
C	1.618475000	-4.799340000	-2.516661000
H	1.541495000	-5.710085000	-3.103151000

C	2.344157000	-4.796889000	-1.327022000
H	2.832726000	-5.704844000	-0.985675000
C	2.442651000	-3.632913000	-0.571362000
H	2.999994000	-3.639307000	0.361659000
C	-3.143731000	0.381983000	1.203255000
C	-3.735546000	-0.419792000	2.183635000
H	-3.631025000	-1.500003000	2.135123000
C	-4.462227000	0.162441000	3.220063000
H	-4.920049000	-0.468369000	3.976504000
C	-4.609458000	1.545270000	3.282347000
H	-5.181310000	1.995606000	4.088351000
C	-4.023300000	2.350626000	2.307336000
H	-4.138493000	3.429852000	2.350166000
C	-3.287570000	1.773487000	1.277748000
H	-2.823499000	2.404268000	0.523231000
C	-3.361432000	-0.273186000	-1.595323000
C	-4.746302000	-0.378220000	-1.419683000
H	-5.160657000	-0.465349000	-0.419114000
C	-5.593604000	-0.361670000	-2.523446000
H	-6.667179000	-0.440372000	-2.379847000
C	-5.068277000	-0.242212000	-3.808472000
H	-5.732936000	-0.228103000	-4.667157000
C	-3.692149000	-0.131998000	-3.991082000
H	-3.281661000	-0.030425000	-4.991413000
C	-2.843576000	-0.140191000	-2.888318000
H	-1.769264000	-0.036799000	-3.025014000
O	-0.372762000	-1.418098000	1.763243000
P	1.934847000	-0.881741000	-0.088624000
P	-2.186017000	-0.303884000	-0.197379000
C	0.872768000	2.721934000	-2.877270000
H	0.783041000	1.778813000	-3.413335000
C	1.230136000	3.892531000	-3.598691000
H	1.413183000	3.836640000	-4.665191000
C	1.326402000	5.102757000	-2.887646000
H	1.582526000	6.024310000	-3.400315000
C	1.090908000	5.102596000	-1.540442000
H	1.157771000	6.029004000	-0.984804000
C	0.749789000	3.863636000	-0.851194000
C	0.536212000	3.804930000	0.518905000
C	0.618831000	4.977960000	1.386582000
H	0.886229000	5.941681000	0.972675000
C	0.353955000	4.864117000	2.723311000
H	0.410320000	5.734764000	3.368877000
C	0.008505000	3.605501000	3.251566000
H	-0.214672000	3.465337000	4.302530000
C	-0.030317000	2.494188000	2.361631000

H	-0.283078000	1.508451000	2.748228000
N	0.635877000	2.679126000	-1.593510000
N	0.220574000	2.562774000	1.083528000

Sum of electronic and zero-point Energies= -7836.775347
Sum of electronic and thermal Energies= -7836.728926
Sum of electronic and thermal Enthalpies= -7836.727982
Sum of electronic and thermal Free Energies= -7836.865228

[Ag(Bipy)(POP)]$^{+}$ (S_0) ($CHCl_3$ Solution)

Ag	-0.049458000	-0.775364000	-0.269408000
C	-1.942425000	1.657299000	1.648159000
C	-0.728499000	1.970930000	2.278705000
C	-0.688866000	2.497666000	3.564424000
H	0.274779000	2.705602000	4.018757000
C	-1.879556000	2.739641000	4.243522000
H	-1.852041000	3.152613000	5.247145000
C	-3.097571000	2.443203000	3.637922000
H	-4.028656000	2.625336000	4.165417000
C	-3.125709000	1.901425000	2.355707000
H	-4.078928000	1.654333000	1.898024000
C	2.056243000	2.081127000	-0.019916000
C	1.101182000	2.595004000	0.872904000
C	0.857924000	3.960832000	0.965542000
H	0.110595000	4.335352000	1.656699000
C	1.584503000	4.835374000	0.161601000
H	1.394775000	5.902184000	0.233224000
C	2.544265000	4.353029000	-0.722646000
H	3.110089000	5.037860000	-1.346045000
C	2.773698000	2.982524000	-0.810788000
H	3.512148000	2.603297000	-1.510418000
C	-3.610812000	0.200449000	-0.184040000
C	-3.818907000	-1.112661000	0.258525000
H	-2.985079000	-1.679534000	0.666305000
C	-5.081383000	-1.691530000	0.174829000
H	-5.233843000	-2.708178000	0.525273000
C	-6.143455000	-0.971924000	-0.369622000
H	-7.127120000	-1.426299000	-0.443567000
C	-5.940194000	0.328117000	-0.826718000
H	-6.764294000	0.889028000	-1.257847000
C	-4.680426000	0.915355000	-0.733980000
H	-4.529763000	1.928385000	-1.095436000
C	-1.875018000	2.295820000	-1.172078000
C	-1.338578000	2.074801000	-2.445667000
H	-0.936009000	1.095415000	-2.694333000

C	-1.312115000	3.099234000	-3.387090000
H	-0.894405000	2.917883000	-4.372955000
C	-1.810524000	4.358019000	-3.058633000
H	-1.783727000	5.160639000	-3.789753000
C	-2.336272000	4.589476000	-1.789180000
H	-2.720330000	5.571727000	-1.529695000
C	-2.370328000	3.564083000	-0.848006000
H	-2.776729000	3.752693000	0.141869000
C	3.185384000	-0.239397000	1.291202000
C	3.898939000	0.671168000	2.077073000
H	3.871961000	1.730720000	1.838519000
C	4.643331000	0.223316000	3.166300000
H	5.193045000	0.937592000	3.772434000
C	4.685964000	-1.134112000	3.475405000
H	5.267899000	-1.480414000	4.324532000
C	3.977436000	-2.046929000	2.695941000
H	4.003920000	-3.105981000	2.935539000
C	3.224917000	-1.601657000	1.613713000
H	2.661569000	-2.313740000	1.015534000
C	3.341674000	0.026097000	-1.576989000
C	4.732964000	0.121176000	-1.454121000
H	5.179322000	0.332969000	-0.486508000
C	5.547198000	-0.062413000	-2.568252000
H	6.625913000	0.009891000	-2.464849000
C	4.981715000	-0.339796000	-3.811695000
H	5.620254000	-0.484065000	-4.678299000
C	3.598334000	-0.439904000	-3.941050000
H	3.155166000	-0.663393000	-4.907051000
C	2.782854000	-0.264757000	-2.826641000
H	1.703327000	-0.357719000	-2.919850000
O	0.460013000	1.662025000	1.649198000
P	-1.919085000	0.880240000	-0.016203000
P	2.201457000	0.264225000	-0.167587000
C	-0.843681000	-2.665449000	-2.825007000
H	-0.629745000	-1.726775000	-3.328563000
C	-1.337012000	-3.752040000	-3.536139000
H	-1.511180000	-3.673609000	-4.603433000
C	-1.605234000	-4.922519000	-2.836684000
H	-2.005629000	-5.794212000	-3.344457000
C	-1.360717000	-4.961572000	-1.470393000
H	-1.587095000	-5.860446000	-0.909823000
C	-0.846717000	-3.829391000	-0.831860000
C	-0.557960000	-3.818417000	0.627610000
C	-0.507350000	-4.994340000	1.381768000
H	-0.640479000	-5.962655000	0.914516000
C	-0.259449000	-4.915760000	2.746333000

H	-0.216091000	-5.820415000	3.344577000
C	-0.063107000	-3.668603000	3.328070000
H	0.129953000	-3.559885000	4.389497000
C	-0.107953000	-2.549552000	2.505305000
H	0.055303000	-1.553862000	2.908096000
N	-0.604650000	-2.695975000	-1.512196000
N	-0.345676000	-2.619459000	1.193932000

Sum of electronic and zero-point Energies= -7836.919731
Sum of electronic and thermal Energies= -7836.874327
Sum of electronic and thermal Enthalpies= -7836.873383
Sum of electronic and thermal Free Energies= -7837.005556

[Ag(Bipy)(POP)]$^+$ (T_1) ($CHCl_3$ Solution)

symmetry C_1

Ag	0.048059000	0.777077000	-0.237483000
C	1.994899000	-1.716233000	1.562370000
C	0.799425000	-2.052390000	2.216208000
C	0.796140000	-2.618868000	3.485570000
H	-0.154034000	-2.843079000	3.960147000
C	2.005759000	-2.878906000	4.123430000
H	2.006865000	-3.323165000	5.113985000
C	3.205982000	-2.560348000	3.494004000
H	4.151661000	-2.756422000	3.989598000
C	3.197713000	-1.978814000	2.228975000
H	4.137500000	-1.715288000	1.753076000
C	-2.057263000	-2.097652000	0.004249000
C	-1.075966000	-2.636930000	0.852547000
C	-0.836704000	-4.005582000	0.904874000
H	-0.068146000	-4.399547000	1.561108000
C	-1.595163000	-4.857769000	0.106331000
H	-1.408806000	-5.926820000	0.146648000
C	-2.582284000	-4.350537000	-0.732731000
H	-3.173377000	-5.018113000	-1.351427000
C	-2.806615000	-2.977165000	-0.781609000
H	-3.566480000	-2.577997000	-1.446394000
C	3.608866000	-0.210274000	-0.281005000
C	3.832221000	1.098513000	0.166698000
H	3.010437000	1.664736000	0.598993000
C	5.093637000	1.675209000	0.054830000
H	5.257606000	2.688767000	0.409036000
C	6.139272000	0.957628000	-0.522848000
H	7.121827000	1.410299000	-0.618837000
C	5.920667000	-0.338067000	-0.985451000
H	6.731658000	-0.897188000	-1.442973000

C	4.662182000	-0.922774000	-0.864902000
H	4.499300000	-1.931964000	-1.231849000
C	1.830284000	-2.267850000	-1.270585000
C	1.249630000	-2.009812000	-2.517707000
H	0.840228000	-1.023444000	-2.725062000
C	1.187407000	-3.007263000	-3.486107000
H	0.735514000	-2.797503000	-4.451072000
C	1.693774000	-4.275768000	-3.211684000
H	1.638937000	-5.057074000	-3.964012000
C	2.263416000	-4.544132000	-1.968791000
H	2.653727000	-5.533961000	-1.750828000
C	2.333090000	-3.545847000	-1.000812000
H	2.773497000	-3.763278000	-0.031567000
C	-3.130210000	0.195674000	1.404948000
C	-3.845524000	-0.726179000	2.176087000
H	-3.850880000	-1.776503000	1.898312000
C	-4.549500000	-0.301615000	3.300891000
H	-5.100823000	-1.024548000	3.895195000
C	-4.549656000	1.043987000	3.660770000
H	-5.100142000	1.372246000	4.537607000
C	-3.839077000	1.967959000	2.896477000
H	-3.833501000	3.017691000	3.175426000
C	-3.126583000	1.545478000	1.778379000
H	-2.559351000	2.264407000	1.192275000
C	-3.380015000	-0.003897000	-1.464490000
C	-4.768421000	-0.060170000	-1.295827000
H	-5.188416000	-0.263165000	-0.314681000
C	-5.613890000	0.150911000	-2.381700000
H	-6.690171000	0.108851000	-2.242251000
C	-5.082832000	0.416517000	-3.642591000
H	-5.745544000	0.581837000	-4.487008000
C	-3.702078000	0.477673000	-3.817751000
H	-3.285078000	0.691489000	-4.797539000
C	-2.855320000	0.276091000	-2.731637000
H	-1.777207000	0.338814000	-2.860945000
O	-0.404984000	-1.725015000	1.628331000
P	1.919734000	-0.886983000	-0.075133000
P	-2.196761000	-0.276733000	-0.096871000
C	0.646562000	2.734067000	-2.793657000
H	0.501710000	1.789380000	-3.314262000
C	0.939453000	3.899072000	-3.553411000
H	1.018254000	3.834983000	-4.631951000
C	1.109083000	5.113552000	-2.862456000
H	1.324919000	6.029396000	-3.402776000
C	0.998174000	5.124687000	-1.499711000
H	1.128883000	6.052999000	-0.959218000

C	0.713524000	3.891293000	-0.772900000
C	0.625994000	3.843316000	0.611022000
C	0.791414000	5.022983000	1.454985000
H	0.971670000	5.990582000	1.005271000
C	0.716247000	4.911803000	2.816100000
H	0.839620000	5.787773000	3.444545000
C	0.474844000	3.649205000	3.390492000
H	0.407011000	3.508749000	4.462559000
C	0.309595000	2.538956000	2.517656000
H	0.109789000	1.556215000	2.940487000
N	0.530159000	2.701069000	-1.493079000
N	0.373401000	2.603885000	1.214554000

Sum of electronic and zero-point Energies= -7836.815064
Sum of electronic and thermal Energies= -7836.768957
Sum of electronic and thermal Enthalpies= -7836.768013
Sum of electronic and thermal Free Energies= -7836.902181