Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and characterisation of a series of fluorescent aminophosphines and their coordination to gold(I)

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Additional X-ray information for [AuCl(L3)]

Table S1. π-π. interactions between phenyl rings (P) and anthraquinones (A_N (ring with N bonded) ,A_O (ring with O bonded), A_E (end ring))

π-π interaction type	Angle between planes / °	centroid- centroid distances / Å	shift distance / Å
A_{O1} - A_{O1}	0.00(11)	3.559(2)	1.486(4)
A_{O31} - A_{O31}	0.02(9)	3.702(2)	1.151(3)
A_{E31} - A_{E31}	0.03(12)	3.615(2)	1.258(4)
P_{51} – P_{51}	0.03(13)	3.823(2)	0.961(5)
A_{N31} - A_{O31}	0.67(10)	3.819(2)	1.484(3)
A_{N31} - A_{E31}	3.11(11)	3.767(2)	1.109(3)
A_{N1} - A_{O1}	3.66(11)	3.939(2)	2.263(4)
A_{N1}- A_{E1}	7.99(12)	3.743(2)	1.360(4)

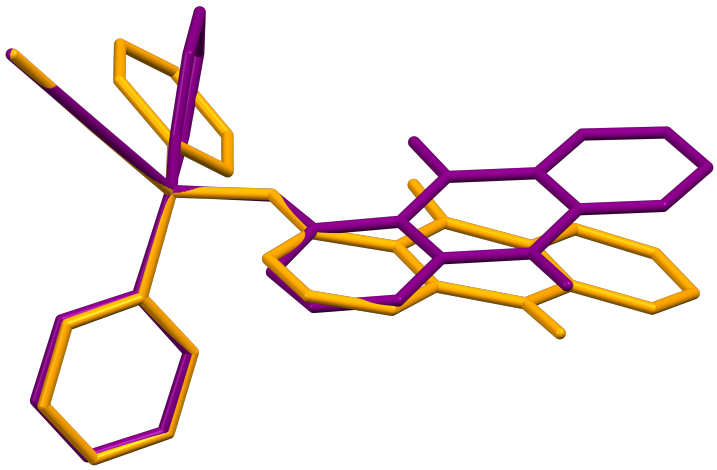

Figure S1. Superimposed structures of the two forms of [AuCl(L3)] obtained from the crystal structure.

DFT parameters

Table S2 Optimised coordinates for **L3** (acetonitrile)

P	2.33040	-0.38695	-1.08249
O	-1.08969	1.46702	0.55186
O	-5.09337	-1.90324	-0.75752
N	0.69891	-0.16147	-0.52529
H	0.43449	0.69037	-0.01922
C	-0.36792	-0.96991	-0.81190
C	-1.69998	-0.59502	-0.46510
C	-1.97596	0.67018	0.22571
C	-3.38923	1.00415	0.55022
C	-3.66451	2.20898	1.20096
H	-2.83144	2.86835	1.45151
C	-4.97427	2.55057	1.51723
H	-5.18213	3.49484	2.02579
C	-6.02391	1.69054	1.18681
H	-7.05230	1.96144	1.43641
C	-5.75826	0.48971	0.54058
H	-6.55958	-0.20167	0.27175
C	-4.44451	0.14162	0.22008
C	-4.18107	-1.14266	-0.46674
C	-2.76507	-1.47371	-0.79202
C	-2.53255	-2.68051	-1.43267
H	-3.38174	-3.32443	-1.66491
C	-1.22341	-3.04689	-1.75602
H	-1.02912	-4.00151	-2.25059
C	-0.16503	-2.21750	-1.44681
H	0.85528	-2.52446	-1.69400

C	3.10241	-1.22593	0.36399
C	2.37649	-1.70877	1.45600
H	1.29525	-1.54600	1.50599
C	3.02654	-2.38774	2.48705
H	2.45016	-2.75906	3.33873
C	4.40362	-2.58888	2.43616
H	4.91069	-3.11971	3.24594
C	5.13427	-2.11367	1.34608
H	6.21525	-2.27000	1.29990
C	4.48571	-1.44485	0.31325
H	5.06275	-1.07992	-0.54503
C	2.91294	1.33333	-0.80961
C	2.92398	1.93996	0.45421
H	2.59698	1.37516	1.33435
C	3.35337	3.25520	0.59731
H	3.35619	3.72300	1.58517
C	3.78739	3.97388	-0.51802
H	4.13020	5.00529	-0.40221
C	3.78758	3.37732	-1.77599
H	4.12960	3.93756	-2.64980
C	3.34965	2.06128	-1.92087
H	3.34602	1.59093	-2.90947

Table S3 Optimised coordinates for **L3** (chloroform)

P	2.32817	-0.38831	-1.08018
O	-1.08868	1.45814	0.57235
O	-5.09677	-1.89440	-0.76565
N	0.69828	-0.16273	-0.51878
H	0.43453	0.68876	-0.01118
C	-0.36986	-0.96775	-0.81206
C	-1.70164	-0.59346	-0.46395
C	-1.97572	0.66739	0.23624
C	-3.38948	1.00306	0.55840
C	-3.66290	2.20552	1.21433
H	-2.82727	2.86019	1.46890
C	-4.97242	2.54835	1.52897
H	-5.17953	3.49088	2.04137
C	-6.02329	1.69212	1.19223
H	-7.05170	1.96443	1.44090
C	-5.75936	0.49384	0.54107
H	-6.56008	-0.19599	0.26627
C	-4.44564	0.14481	0.22182
C	-4.18398	-1.13729	-0.47118
C	-2.76773	-1.46810	-0.79722
C	-2.53713	-2.67130	-1.44525
H	-3.38866	-3.31080	-1.68129
C	-1.22845	-3.03713	-1.76960
H	-1.03493	-3.98893	-2.27020
C	-0.16873	-2.21143	-1.45457

H	0.85148	-2.51754	-1.70331
C	3.10257	-1.22599	0.36571
C	2.37406	-1.73347	1.44450
H	1.28998	-1.58819	1.48545
C	3.02450	-2.41501	2.47336
H	2.44564	-2.80575	3.31465
C	4.40463	-2.59427	2.43369
H	4.91211	-3.12720	3.24187
C	5.13808	-2.09412	1.35700
H	6.22190	-2.23248	1.31986
C	4.48939	-1.42267	0.32645
H	5.06884	-1.03699	-0.52103
C	2.91439	1.33106	-0.81114
C	2.94257	1.93509	0.45326
H	2.62708	1.36809	1.33604
C	3.37427	3.24967	0.59303
H	3.39003	3.71558	1.58168
C	3.79359	3.97019	-0.52630
H	4.13816	5.00137	-0.41311
C	3.77667	3.37631	-1.78520
H	4.10700	3.93836	-2.66242
C	3.33654	2.06094	-1.92659
H	3.31897	1.59184	-2.91569

Table S4 Optimised coordinates for [AuCl(**L3**)] (acetonitrile)

Au	2.25425	-1.23428	-0.92629
Cl	3.15357	-3.07033	-2.09680
P	1.37371	0.55936	0.20530
O	-2.50267	1.76476	-0.52249
O	-5.50480	-2.48655	0.88299
N	-0.32086	0.57860	0.32966
H	-0.83300	1.36153	-0.10051
C	-1.14318	-0.48052	0.66675
C	-2.54234	-0.41598	0.42570
C	-3.15758	0.77284	-0.18940
C	-4.62569	0.77260	-0.41278
C	-5.21882	1.89534	-0.99456
H	-4.58364	2.73944	-1.26923
C	-6.59105	1.92585	-1.21420
H	-7.04912	2.80670	-1.66969
C	-7.38418	0.83446	-0.85405
H	-8.46223	0.86125	-1.02765
C	-6.80141	-0.28606	-0.27444
H	-7.39913	-1.15228	0.01634
C	-5.42396	-0.32285	-0.05154
C	-4.82106	-1.52482	0.56633
C	-3.34662	-1.52237	0.78882
C	-2.79151	-2.65604	1.36643
H	-3.44851	-3.48613	1.62907

C	-1.41953	-2.70570	1.60563
H	-0.97447	-3.58831	2.07005
C	-0.60913	-1.63506	1.27005
H	0.46106	-1.68487	1.48949
C	1.98861	0.72029	1.90627
C	1.14737	1.09124	2.95981
H	0.08274	1.26423	2.77541
C	1.66861	1.23514	4.24338
H	1.00970	1.52030	5.06687
C	3.02465	1.01477	4.47605
H	3.42998	1.12718	5.48454
C	3.86511	0.64418	3.42653
H	4.92743	0.46693	3.60954
C	3.34855	0.48932	2.14424
H	4.00507	0.18563	1.32117
C	1.67294	2.16443	-0.57829
C	1.33605	3.34935	0.09020
H	0.91153	3.31437	1.09858
C	1.54821	4.57651	-0.52764
H	1.28417	5.49933	-0.00613
C	2.10269	4.62766	-1.80702
H	2.27288	5.59426	-2.28736
C	2.44362	3.45260	-2.47169
H	2.87984	3.49304	-3.47226
C	2.22879	2.21962	-1.86011
H	2.49452	1.29358	-2.38021

Table S5 Optimised coordinates for [AuCl(**L3**)] (chloroform)

Au	2.27156	-1.22533	-0.92550
Cl	3.20905	-3.03158	-2.08887
P	1.36746	0.55531	0.20568
O	-2.51235	1.76602	-0.50420
O	-5.51072	-2.49851	0.86764
N	-0.32795	0.57088	0.32547
H	-0.84159	1.35511	-0.10104
C	-1.14876	-0.49260	0.65463
C	-2.54848	-0.42634	0.41727
C	-3.16493	0.76810	-0.18546
C	-4.63248	0.76620	-0.41357
C	-5.22543	1.89141	-0.99086
H	-4.58910	2.73692	-1.25869
C	-6.59680	1.92044	-1.21435
H	-7.05519	2.80277	-1.66697
C	-7.38911	0.82579	-0.86219
H	-8.46678	0.85171	-1.03914
C	-6.80657	-0.29679	-0.28680
H	-7.40174	-1.16665	-0.00151
C	-5.42974	-0.33230	-0.06070
C	-4.82692	-1.53745	0.55280

C	-3.35170	-1.53614	0.77206
C	-2.79525	-2.67489	1.33789
H	-3.45303	-3.50679	1.59299
C	-1.42267	-2.72642	1.57228
H	-0.97549	-3.61422	2.02475
C	-0.61308	-1.65244	1.24545
H	0.45827	-1.70546	1.45862
C	1.97261	0.71634	1.91115
C	1.12390	1.07608	2.96237
H	0.05887	1.24111	2.77252
C	1.63708	1.21733	4.24931
H	0.97175	1.49308	5.07098
C	2.99321	1.00520	4.48812
H	3.39244	1.11498	5.49939
C	3.84126	0.64525	3.44136
H	4.90367	0.47332	3.62898
C	3.33246	0.49303	2.15579
H	3.99503	0.19606	1.33507
C	1.66274	2.16576	-0.56954
C	1.32215	3.34746	0.10223
H	0.89815	3.30712	1.11067
C	1.53079	4.57714	-0.51126
H	1.26383	5.49761	0.01304
C	2.08550	4.63413	-1.79011
H	2.25283	5.60285	-2.26733
C	2.43032	3.46247	-2.45822
H	2.86688	3.50712	-3.45848
C	2.21906	2.22701	-1.85073
H	2.48799	1.30317	-2.37324

Table S6 TD-DFT data for **L3**

#	State	Transition energy (nm)	Participating MO	Transition character
1	Singlet	465 (0.1397)[a]	HOMO → LUMO (0.70)[b]	π→π*, n→π*
2	Singlet	403 (0.0153)	HOMO-5 → LUMO (0.49); HOMO-1 → LUMO (0.41)	π→π*, n→π*
3	Singlet	376 (0.0177)	HOMO-1 → LUMO (0.45); HOMO-8 → LUMO (0.38)	π→π*, n→π*
4	Singlet	347 (0.0086)	HOMO-8 → LUMO (0.39); HOMO-1 → LUMO (0.34); HOMO-10 → LUMO (0.33)	π→π*, n→π*
5	Singlet	335 (0.0019)	HOMO-6 → LUMO (0.66)	π→π*
6	Singlet	314 (0.0425)	HOMO-7 → LUMO (0.66)	π→π*
7	Singlet	310 (0.2202)	HOMO → LUMO+1 (0.64)	π→π*, n→π*
8	Singlet	308 (0.0004)	HOMO-2 → LUMO (0.68)	π→π*
9	Singlet	301 (0.0005)	HOMO-3 → LUMO (0.65)	π→π*
10	Singlet	297 (0.0007)	HOMO-4 → LUMO (0.67)	π→π*
11	Singlet	281 (0.0273)	HOMO → LUMO+2 (0.65)	π→π*, n→π*
12	Singlet	272 (0.1444)	HOMO-9 → LUMO (0.57); HOMO-10 → LUMO (0.30)	π→π*, n→π*
13	Singlet	271 (0.0111)	HOMO-1 → LUMO+1 (0.39) ; HOMO-10 → LUMO (-0.36); HOMO-8 → LUMO (0.32)	π→π*, n→π*
14	Singlet	270 (0.0561)	HOMO-1 → LUMO+1 (0.63); HOMO-9 → LUMO (-	π→π*, n→π*

			0.33); HOMO-10 → LUMO (0.31)	
15	Singlet	266 (0.0286)	HOMO → LUMO+3 (0.63)	π→π*, n→π*
16	Singlet	259 (0.0724)	HOMO → LUMO+4 (0.66)	π→π*, n→π*
17	Singlet	254 (0.0071)	HOMO-1 → LUMO+2 (0.52); HOMO-5 → LUMO+1 (0.30)	π→π*, n→π*
18	Singlet	252 (0.0008)	HOMO → LUMO+5 (0.55)	π→π*, n→π*
19	Singlet	250 (0.0148)	HOMO-5 → LUMO+1 (0.43); HOMO-1 → LUMO+2 (0.39)	π→π*, n→π*
20	Singlet	243 (0.0091)	HOMO → LUMO+6 (0.48)	π→π*, n→π*

[a] Oscillator strength; [b] expansion coefficient

Table S7 TD-DFT data for [AuCl(**L3**)]

#	State	Transition energy (nm)	Participating MO	Transition character
1	Singlet	417 (0.1857)[a]	HOMO → LUMO (0.69)[b]	π→π*, n→π*, σ_{AuP}→π* [c]
2	Singlet	397 (0.0018)	HOMO-7 → LUMO (0.41); HOMO-3 → LUMO (0.30)	π→π*, n→π*, MLCT
3	Singlet	357 (0.0006)	HOMO-11 → LUMO (0.60)	n→π*, ILCT
4	Singlet	340 (0.0068)	HOMO-8 → LUMO (0.31); HOMO-7 → LUMO (0.32); HOMO-2 → LUMO (0.31); HOMO-1 → LUMO (-0.31)	π→π*, n→π*, MLCT, σ_{AuP}→π*
5	Singlet	320 (0.0785)	HOMO-6 → LUMO (0.61)	π→π*
6	Singlet	318 (0.0052)	HOMO-1 → LUMO (0.59)	π→π*, σ_{AuP}→π*
7	Singlet	297 (0.0031)	HOMO-2 → LUMO (0.47); HOMO-3 → LUMO (-0.44)	π→π*, n→π*, MLCT
8	Singlet	295 (0.0006)	HOMO-5 → LUMO (0.47); HOMO-4 → LUMO (-0.46)	π→π*, n→π*, MLCT
9	Singlet	294 (0.0026)	HOMO-3 → LUMO (0.40)	π→π*, n→π*, MLCT
10	Singlet	293 (0.0094)	HOMO-7 → LUMO (0.32); HOMO-5 → LUMO (0.30); HOMO-4 → LUMO (0.37)	π→π*, n→π*, MLCT
11	Singlet	292 (0.1602)	HOMO → LUMO+1 (0.64)	π→π*, n→π*, σ_{AuP}→π*
12	Singlet	285 (0.0027)	HOMO-9 → LUMO (0.65)	π→π*, n→π*, MLCT
13	Singlet	275 (0.0259)	HOMO → LUMO+2 (0.67)	π→π*, n→π*, σ_{AuP}→π*
14	Singlet	274 (0.0359)	HOMO-10 → LUMO (0.67)	π→π*, n→π*, MLCT

15	Singlet	271 (0.1979)	HOMO-1 → LUMO (0.65)	π→π*, σ_{AuP}→π*
16	Singlet	261 (0.0408)	HOMO → LUMO+3 (0.68)	π→π*, n→π*, σ_{AuP}→π*
17	Singlet	255 (0.0092)	HOMO-7 → LUMO+1 (0.32); HOMO-3 → LUMO+1 (0.28)	π→π*, n→π*, MLCT
18	Singlet	252 (0.0298)	HOMO-1 → LUMO+1 (0.43); HOMO-1 → LUMO+2 (0.31)	π→π*, σ_{AuP}→π*
19	Singlet	250 (0.0544)	HOMO-1 → LUMO+2 (0.32); HOMO-1 → LUMO+4 (0.31); HOMO-1 → LUMO+5 (0.38)	π→π*, n→π*, σ_{AuP}→π*
20	Singlet	245 (0.1161)	HOMO-13 → LUMO (0.42)	π→π*, n→π*, σ_{AuP}→π*, MLCT

[a] Oscillator strength; [b] expansion coefficient; [c] occupied orbital contains electron density associated with the Au–P bond, derived from the P lone pair in the free ligand