Tuning Luminescence in Gold(I)-Phosphane Complexes: Structural, Photophysical, and Theoretical Insights

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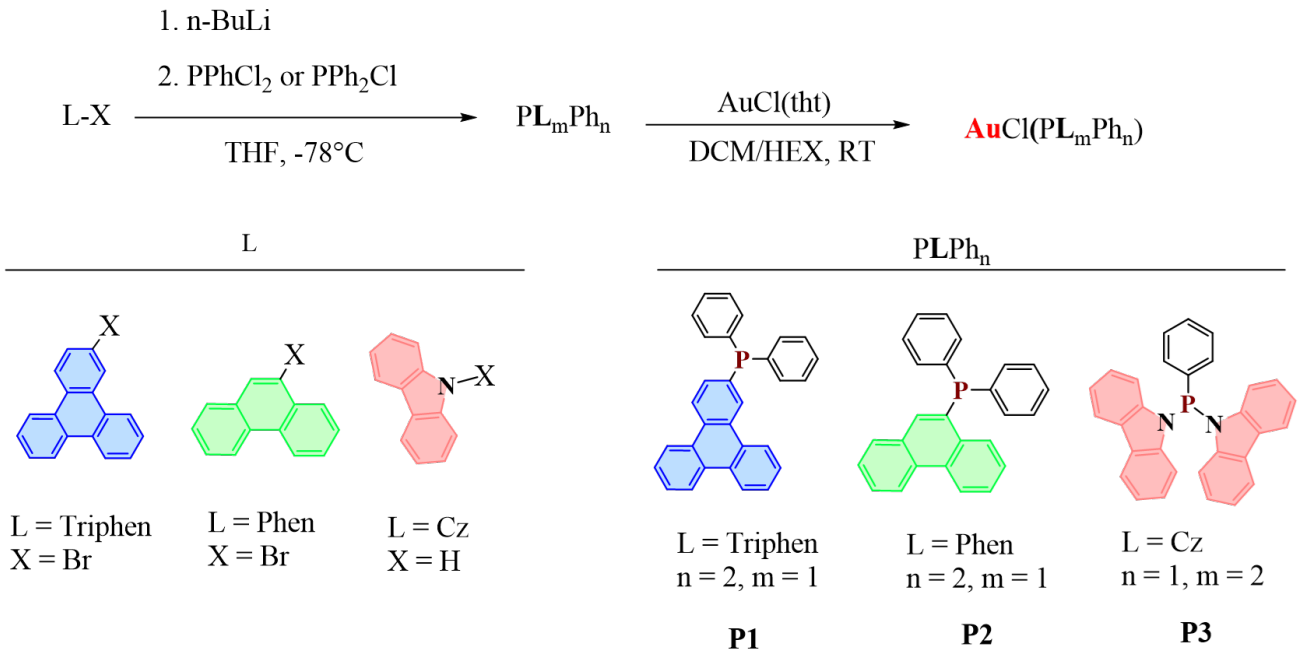
Supporting Information



Scheme S1. Synthesis of phosphane ligands and their corresponding AuCl precursors

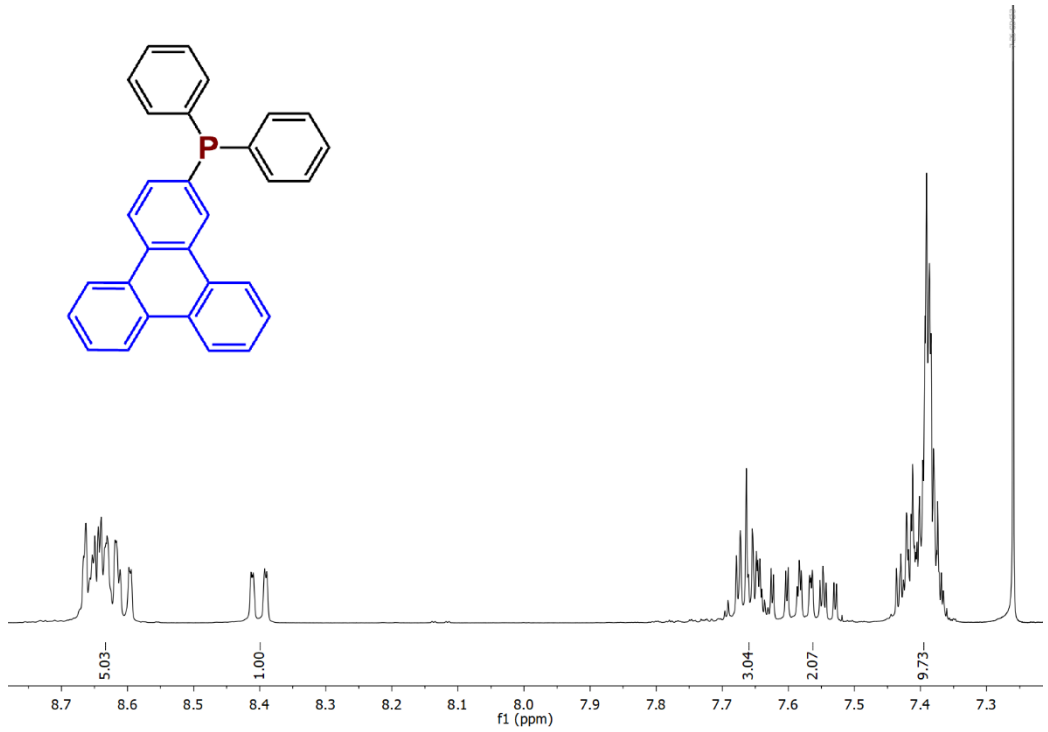


Figure S1. ^{1}H-NMR spectra of **P1** in $CDCl_3$

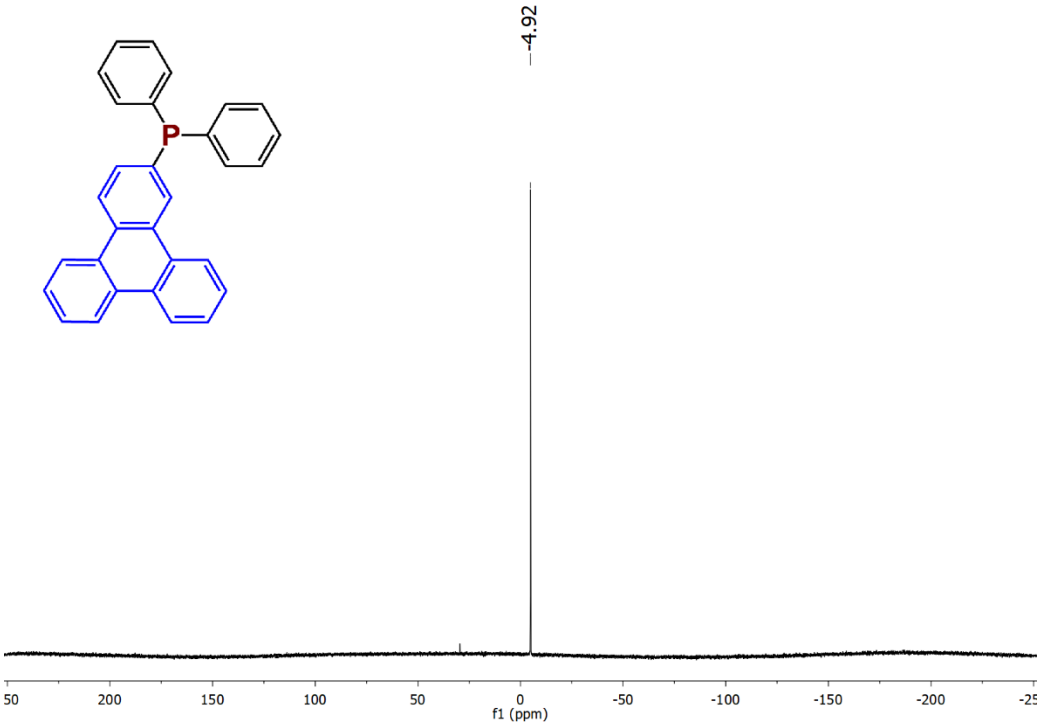


Figure S2. ^{31}P-NMR spectra of **P1** in $CDCl_3$

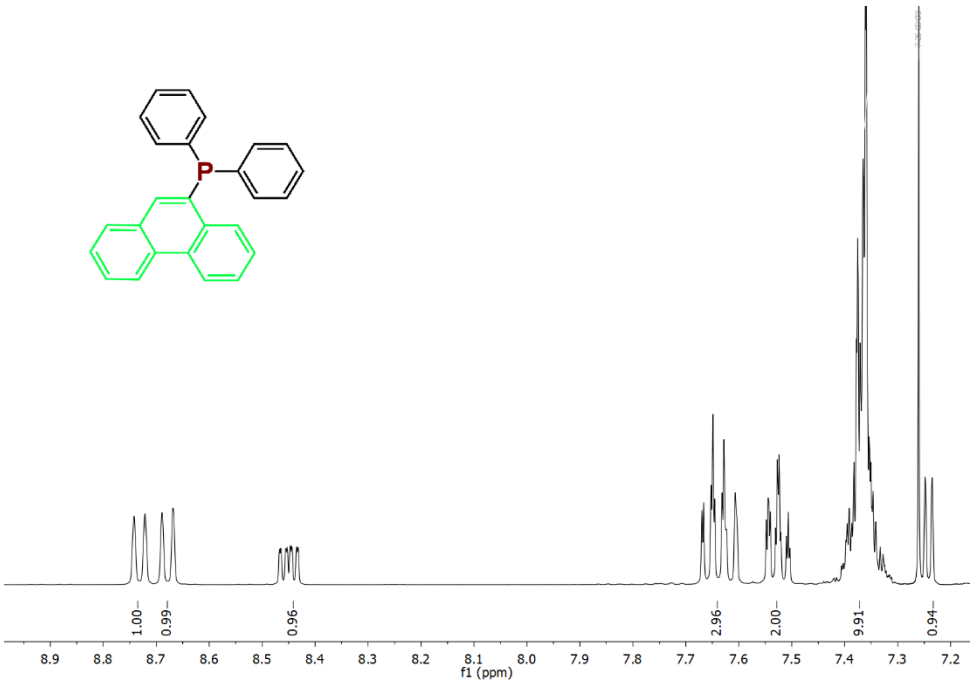


Figure S3. ^{1}H-NMR spectra of **P2** in $CDCl_3$

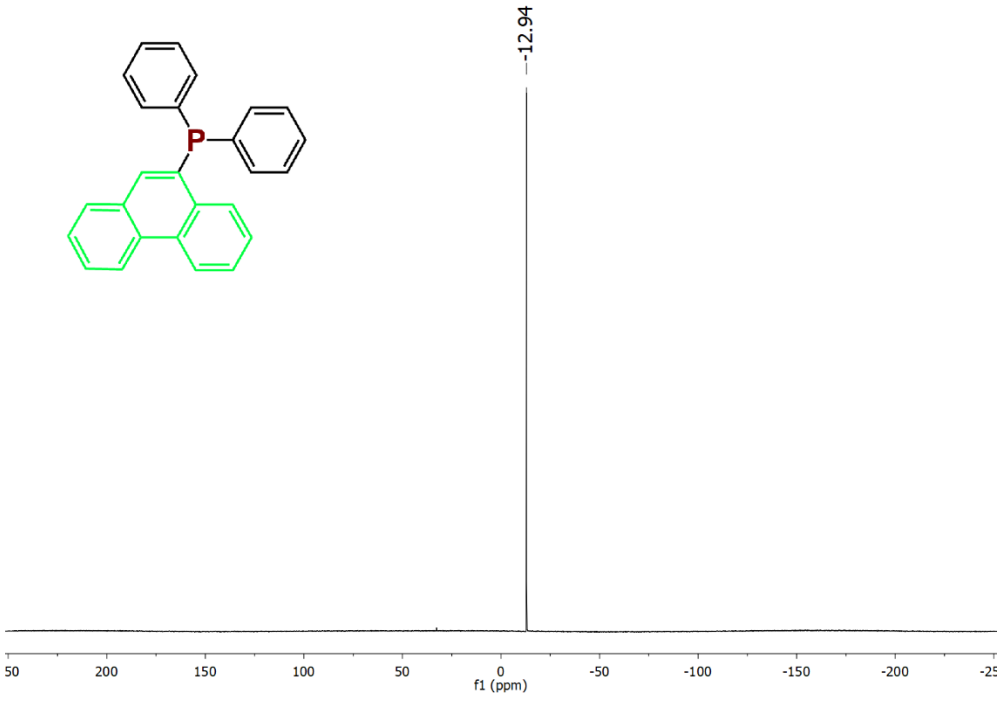


Figure S4. ^{31}P-NMR spectra of **P2** in $CDCl_3$

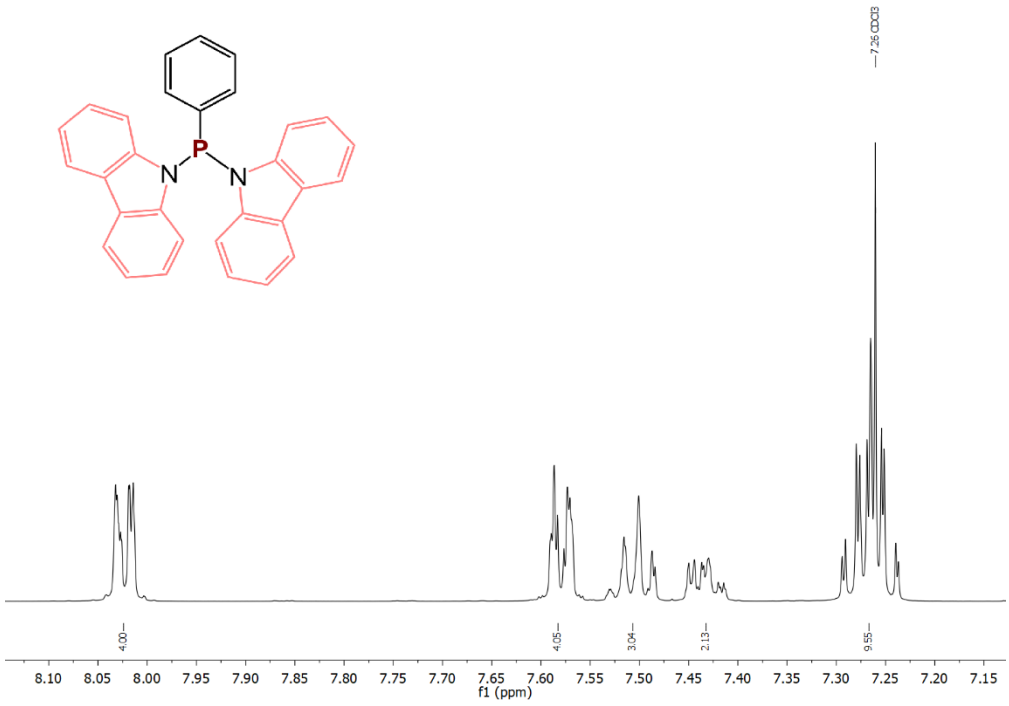


Figure S5. ^{1}H-NMR spectra of **P3** in $CDCl_3$

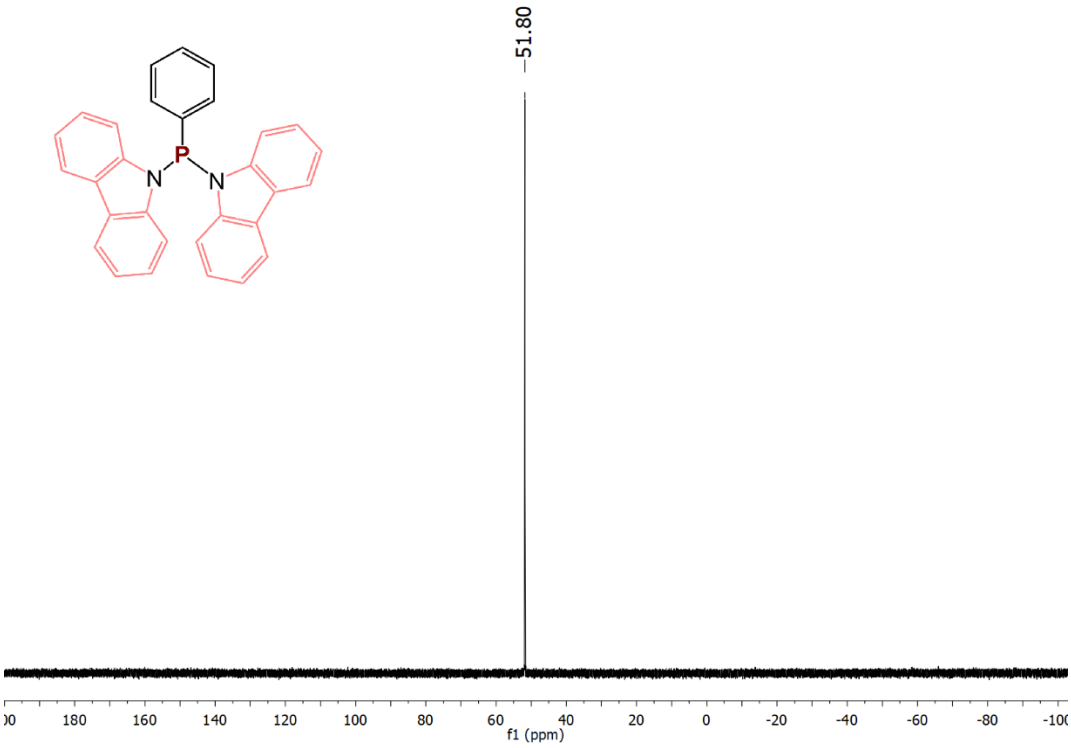


Figure S6. ^{31}P-NMR spectra of **P3** in $CDCl_3$

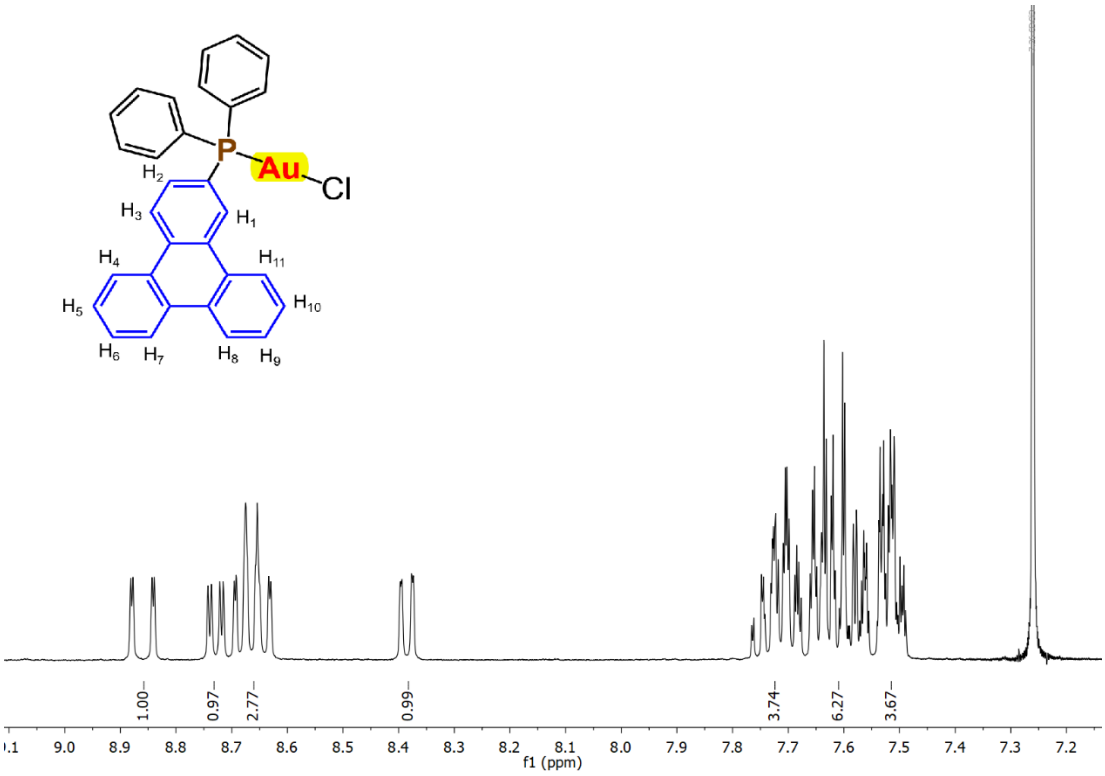


Figure S7. ^{1}H-NMR spectra of **[AuCl(P1)]** in $CDCl_3$

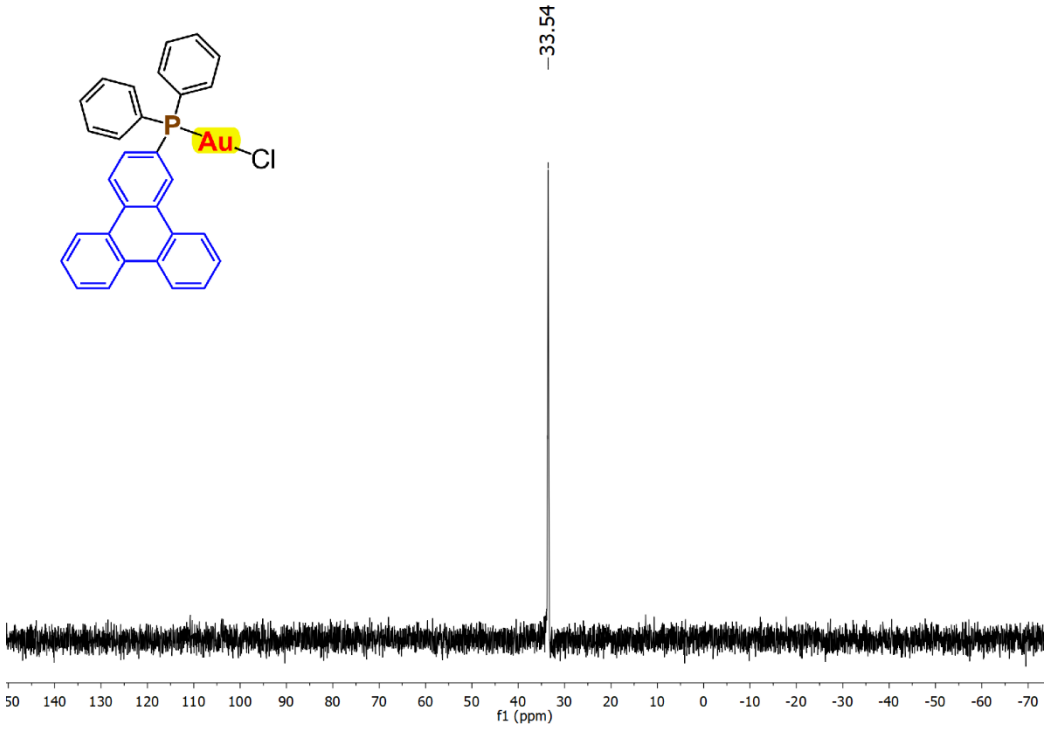


Figure S8. ^{31}P-NMR spectra of **[AuCl(P1)]** in $CDCl_3$

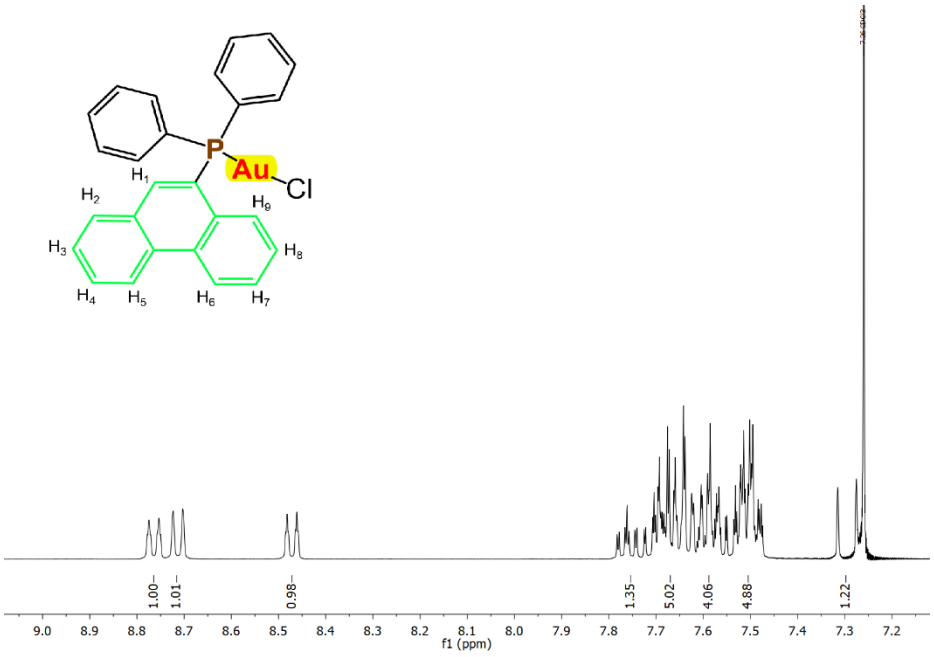


Figure S9. ^{1}H-NMR spectra of **[AuCl(P2)]** in $CDCl_3$

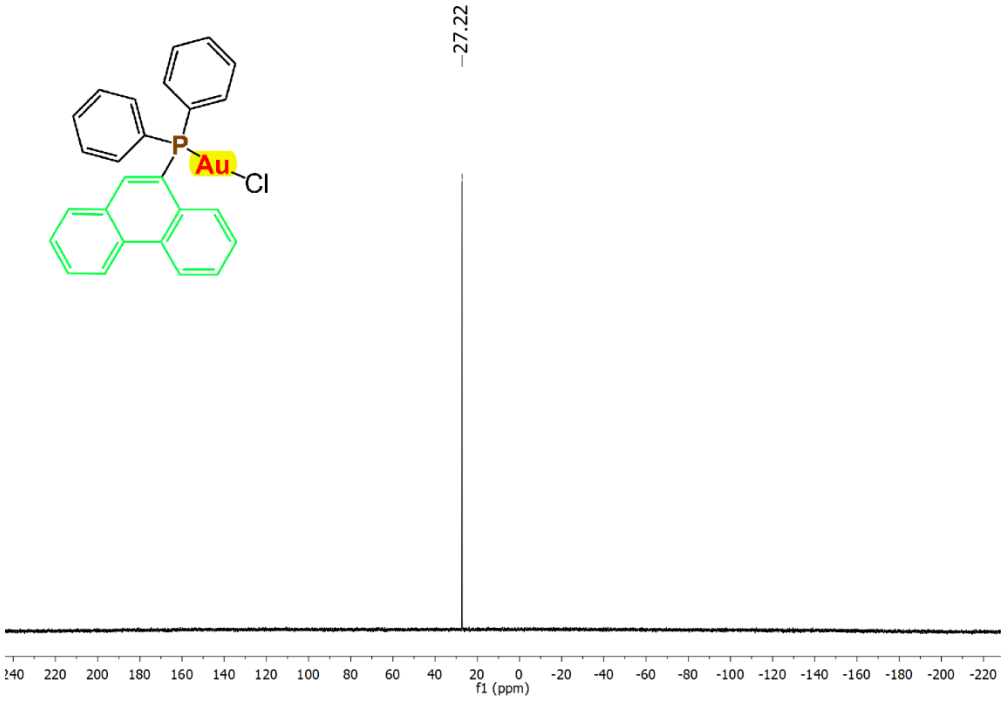


Figure S10. ^{31}P-NMR spectra of **[AuCl(P2)]** in $CDCl_3$

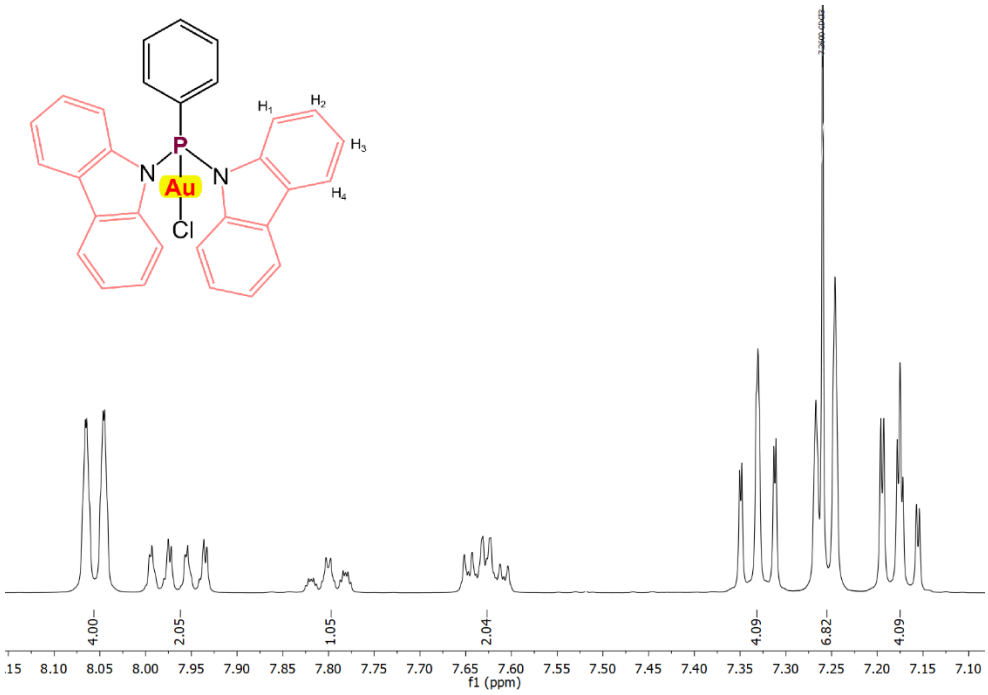


Figure S11. ^{1}H-NMR spectra of **[AuCl(P3)]** in $CDCl_3$

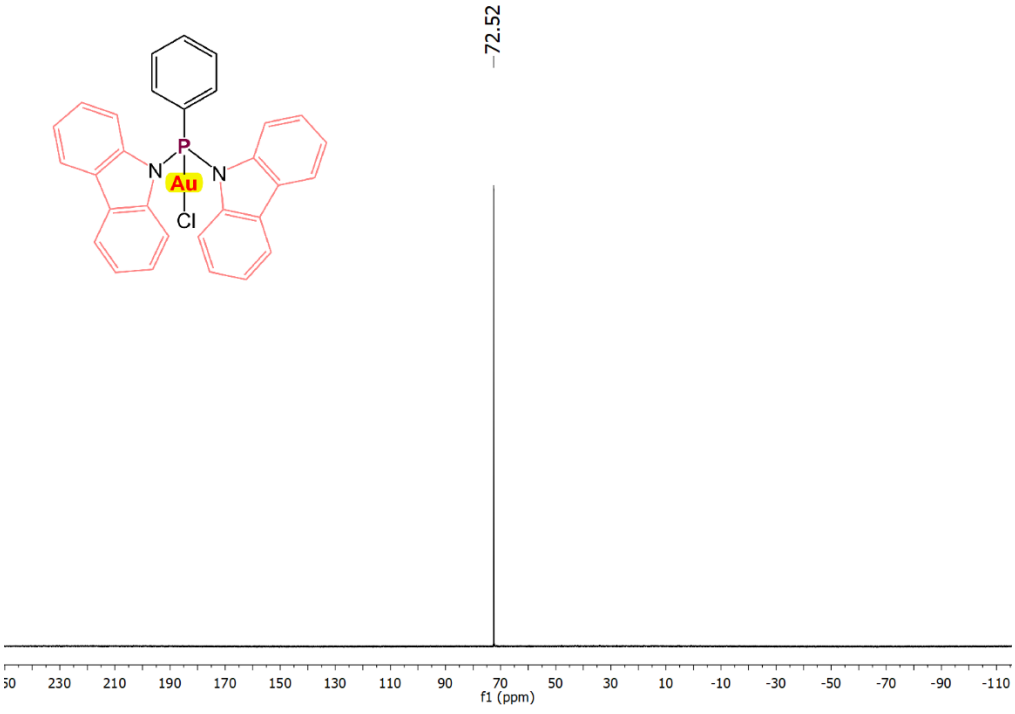


Figure S12. ^{31}P-NMR spectra of **[AuCl(P3)]** in $CDCl_3$

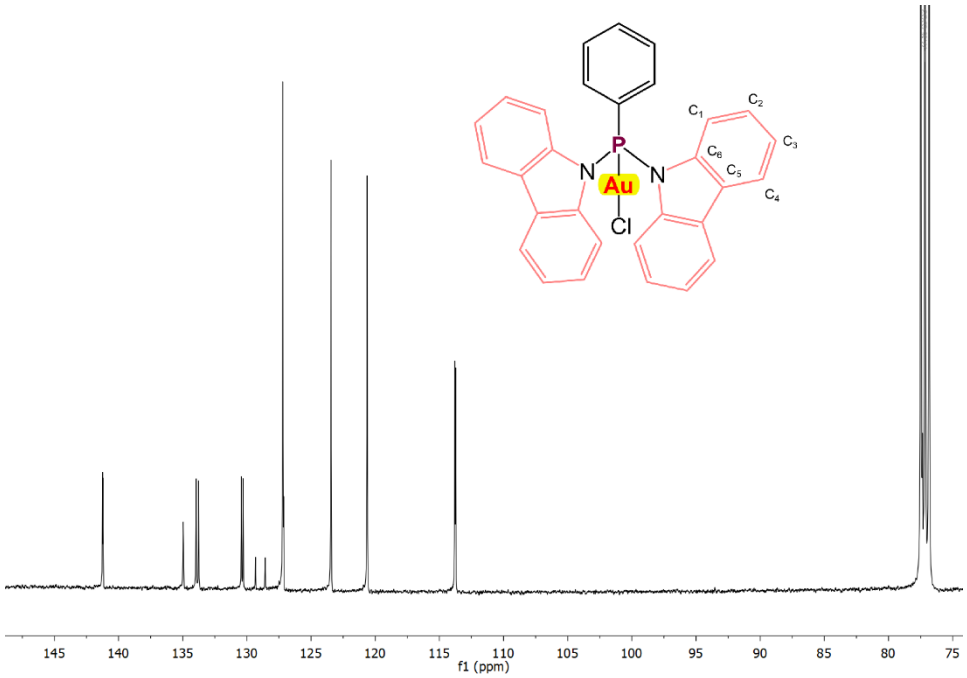


Figure S13. $^{13}C\{^{1}H\}$ NMR of **[AuCl(P3)]**

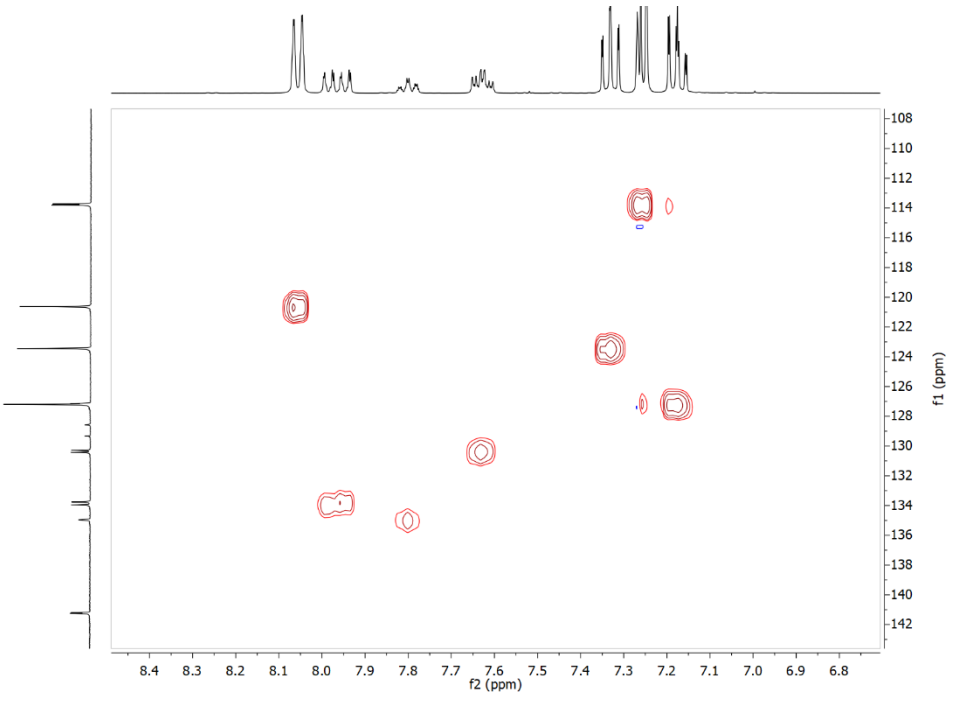


Figure S14. HSQC NMR spectrum of **[AuCl(P3)]**

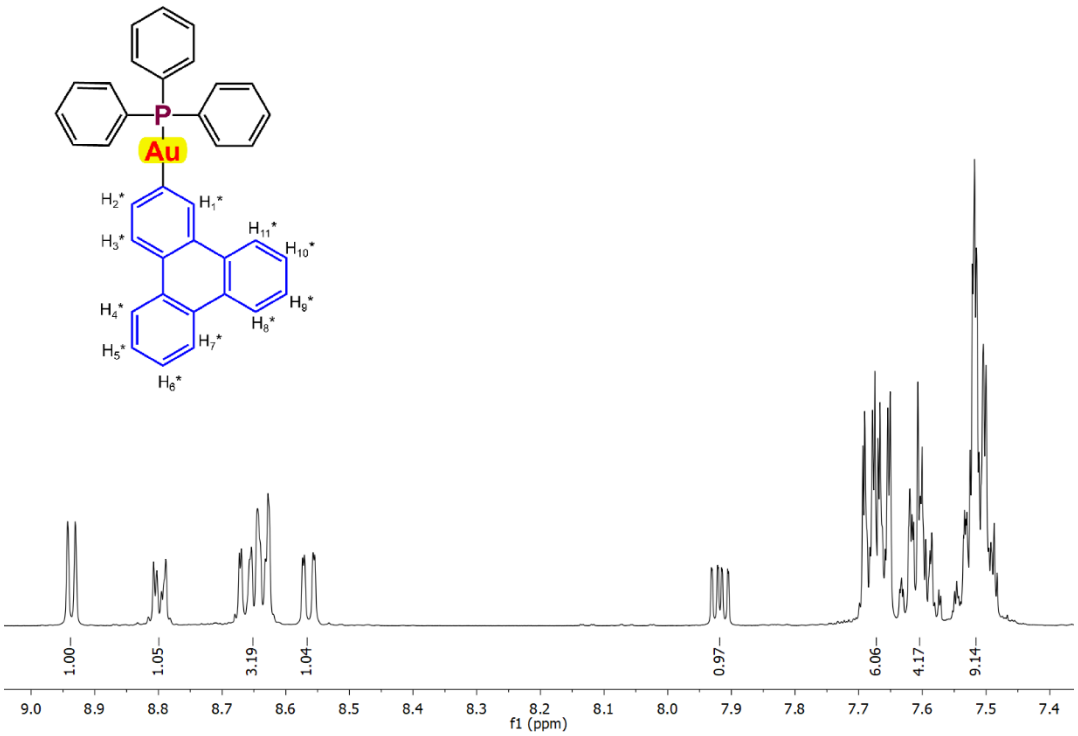


Figure S15. ^{1}H-NMR spectra of **1a** in $CDCl_3$

Figure S16. ^{31}P-NMR spectra of **1a** in $CDCl_3$

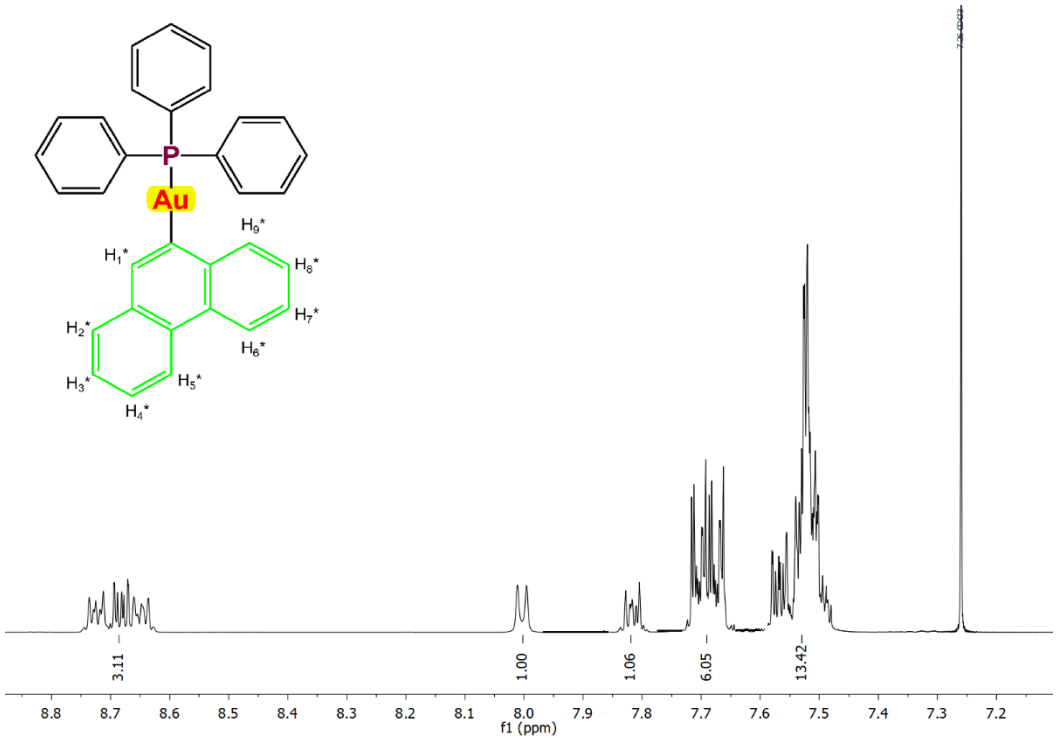


Figure S17. ^{1}H-NMR spectra of **2a** in $CDCl_3$

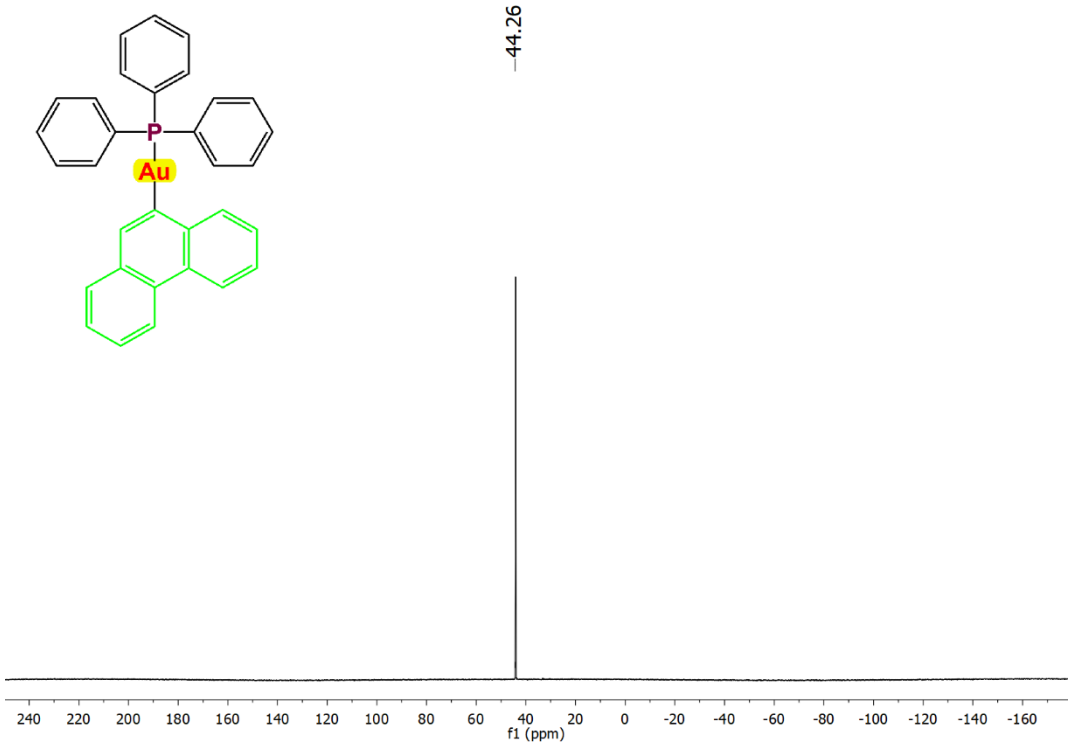


Figure S18. ^{31}P-NMR spectra of **2a** in $CDCl_3$

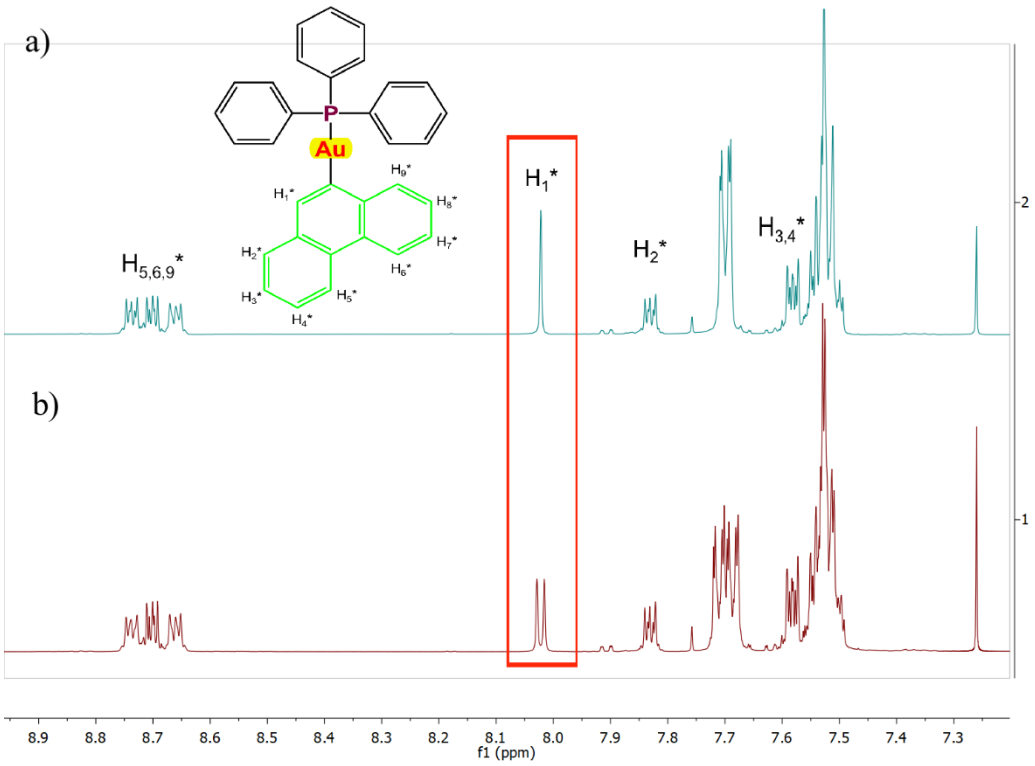


Figure S19. a) ^{1}H-NMR spectra of **2a** in $CDCl_3$ b) ^{1}H decoupled NMR spectra of **2a** in $CDCl_3$

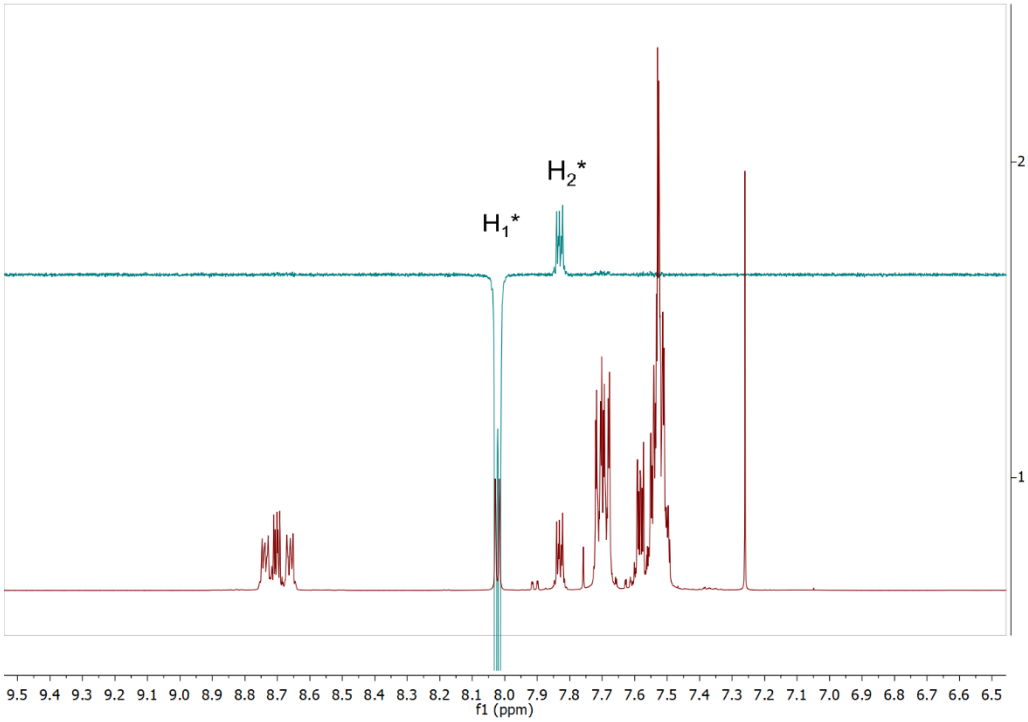


Figure S20. NOESY spectra of **2a** in $CDCl_3$

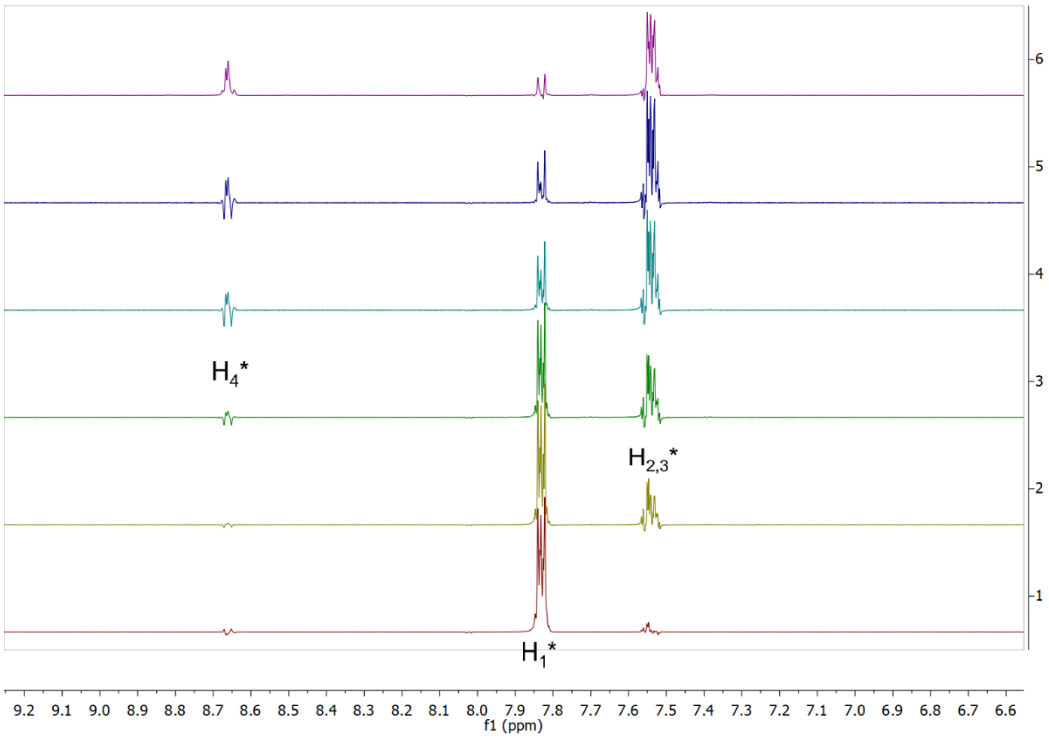


Figure S21. TOCSY spectra of **2a** in $CDCl_3$

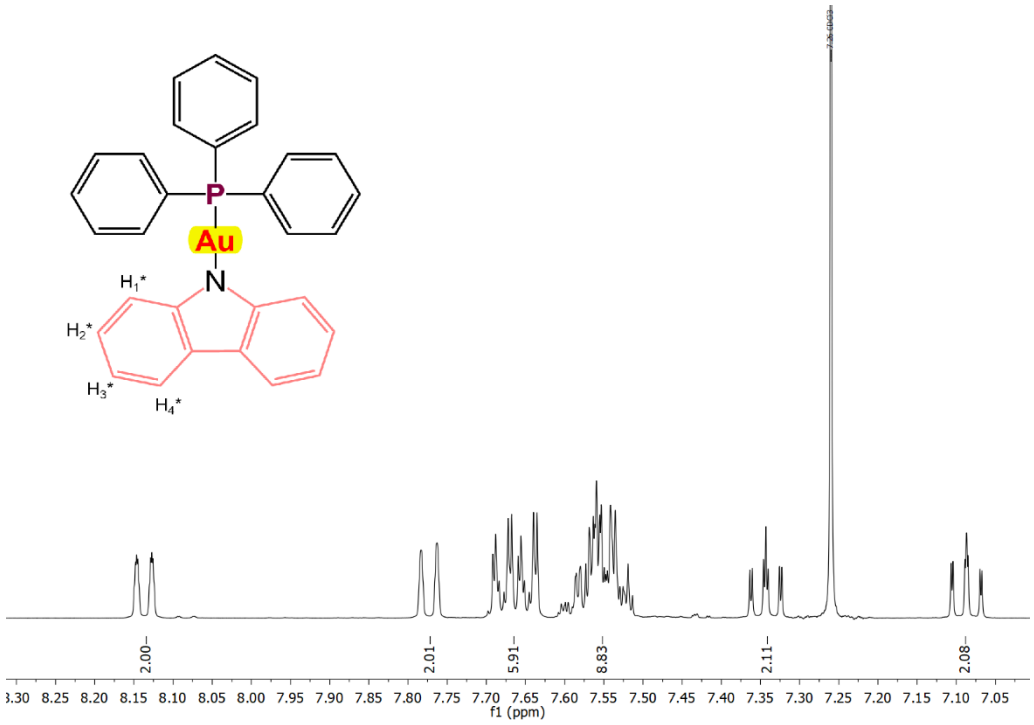


Figure S22. ^{1}H-NMR spectra of **3a** in $CDCl_3$

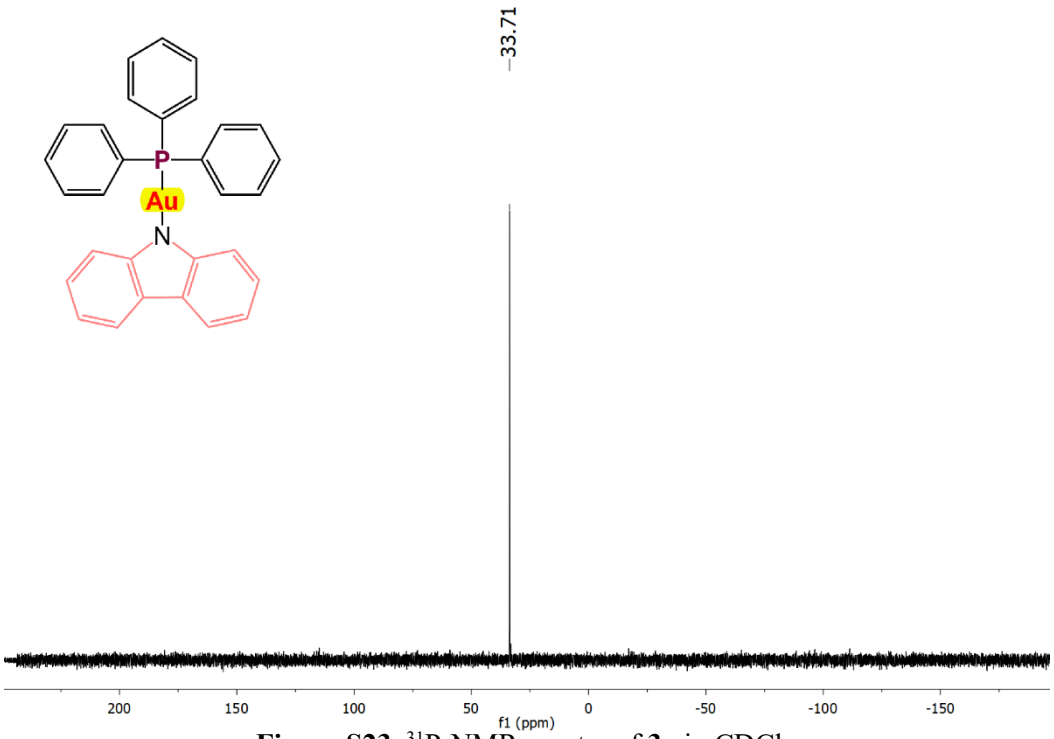


Figure S23. ^{31}P-NMR spectra of **3a** in $CDCl_3$

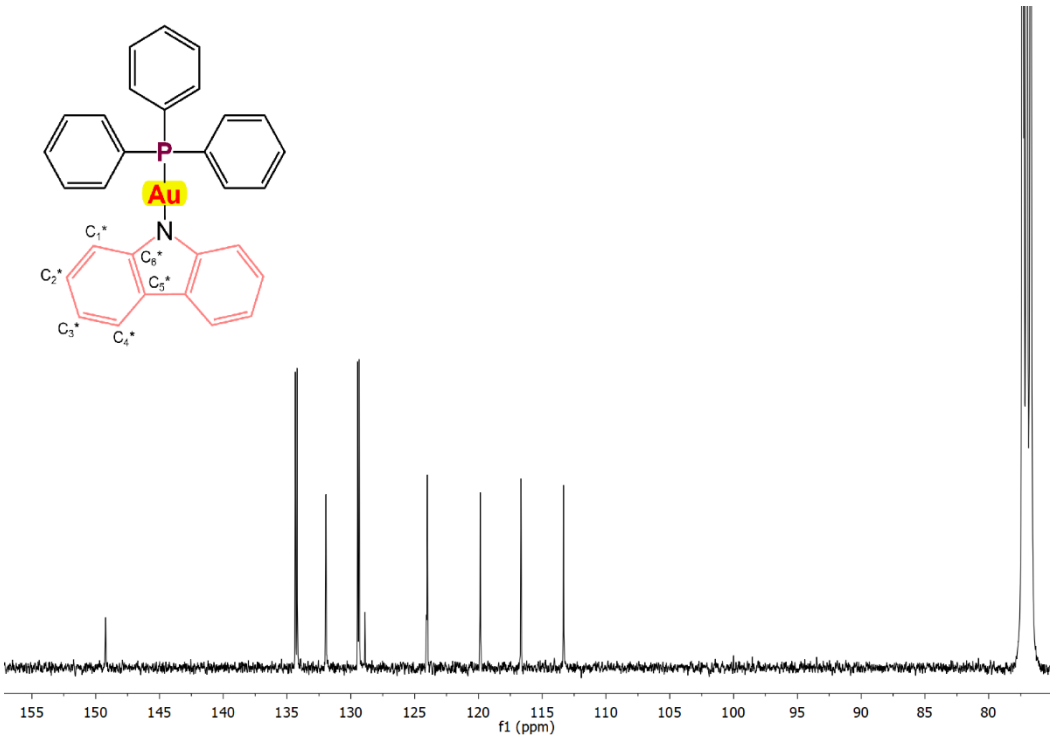


Figure S24. $^{13}C\{^{1}H\}$ NMR of **3a**

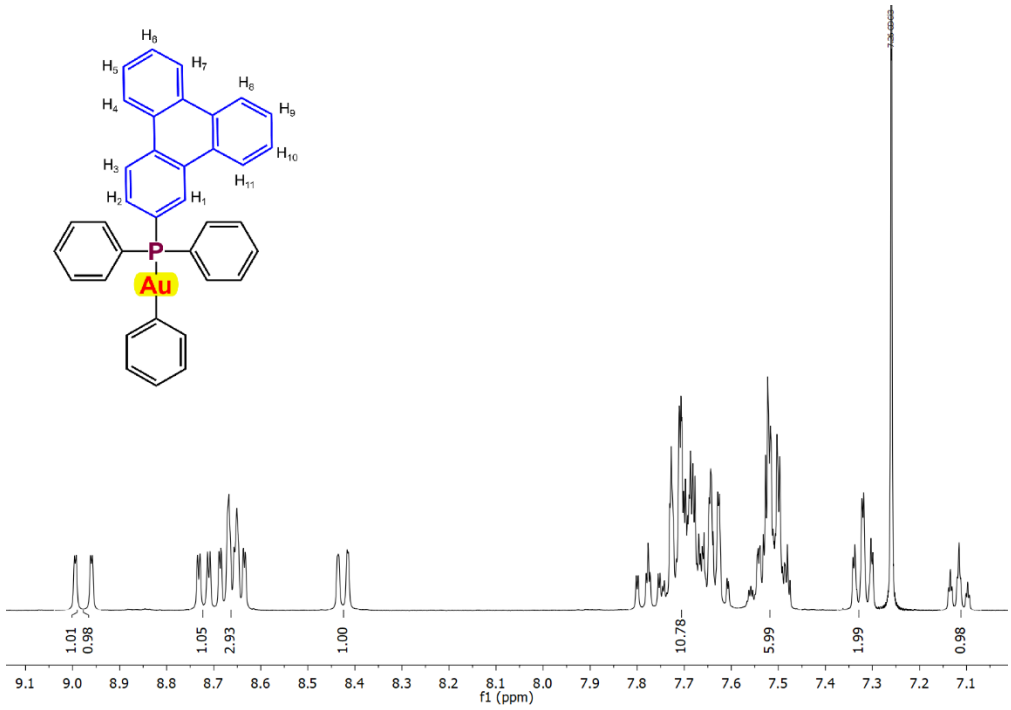


Figure S25. ^{1}H-NMR spectra of **1b** in $CDCl_3$

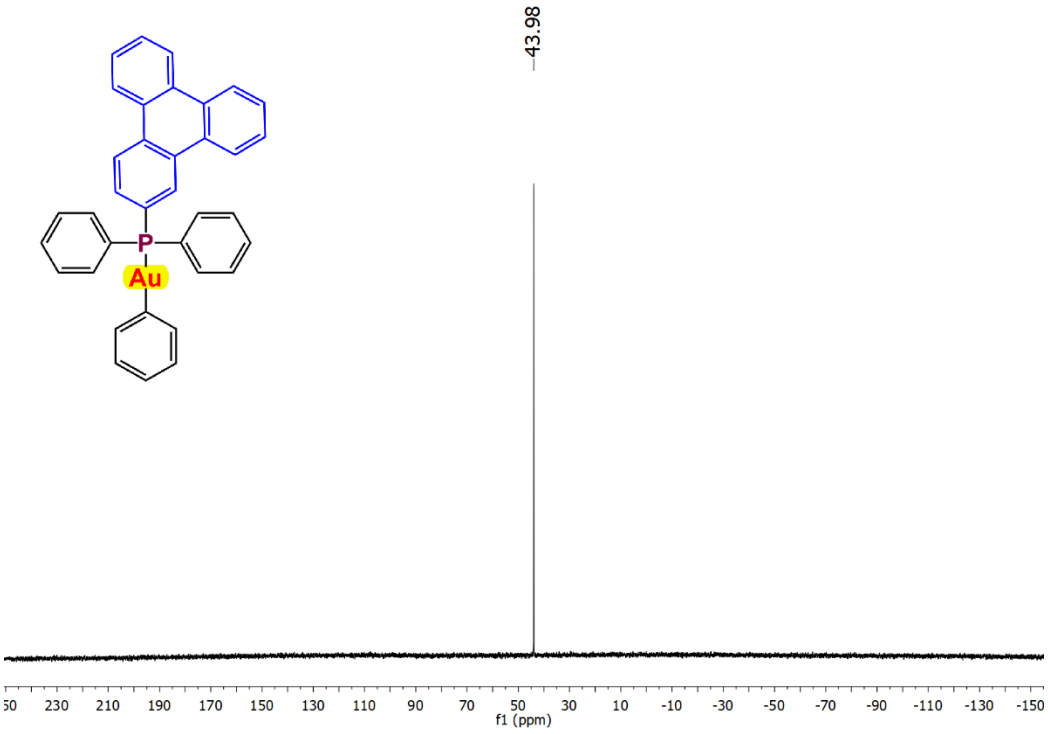


Figure S26. ^{31}P-NMR spectra of **1b** in $CDCl_3$

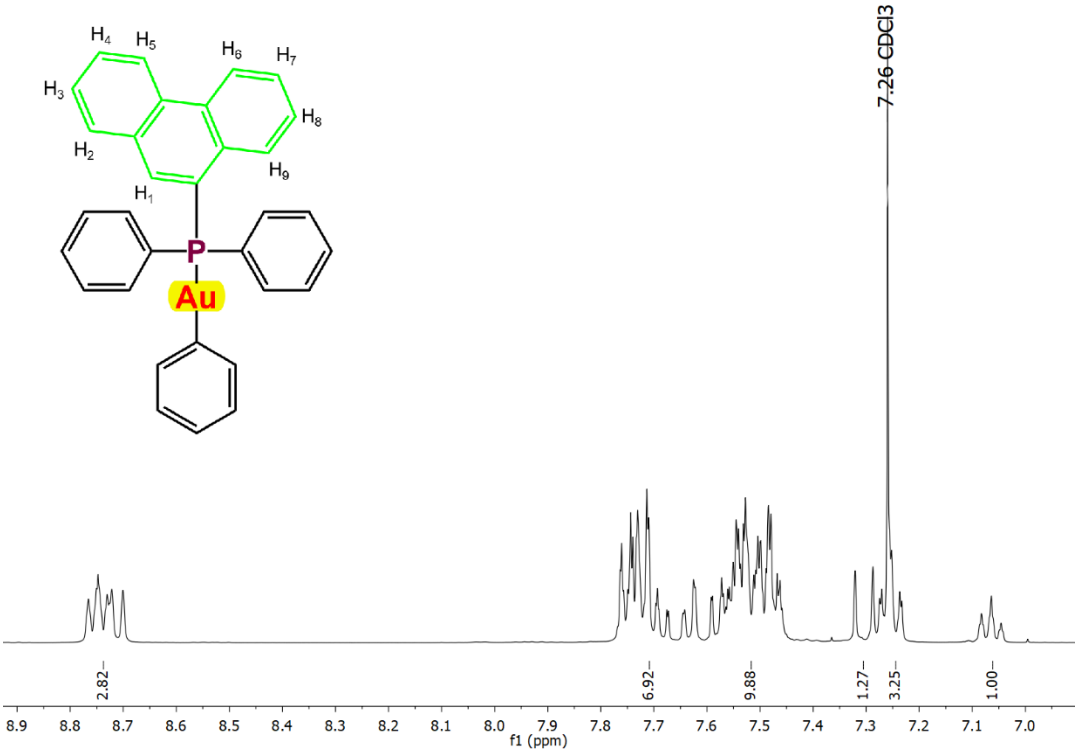


Figure S27. ^{1}H-NMR spectra of **2b** in $CDCl_3$

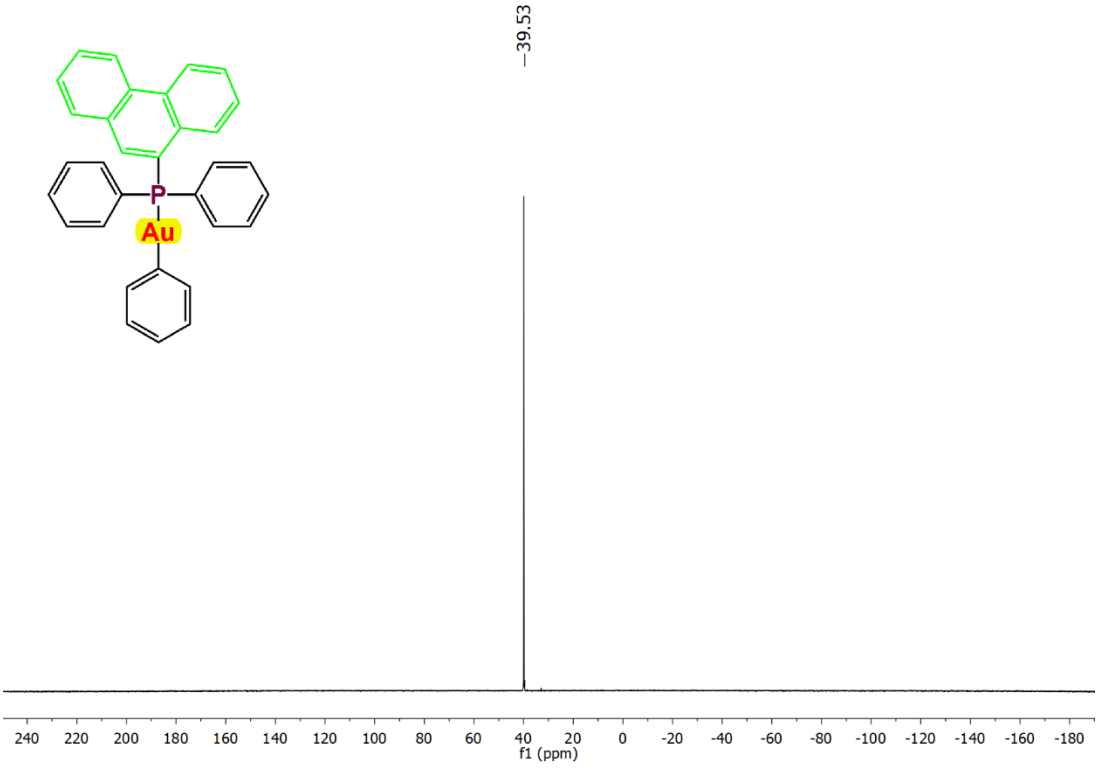


Figure S28. ^{31}P-NMR spectra of **2b** in $CDCl_3$

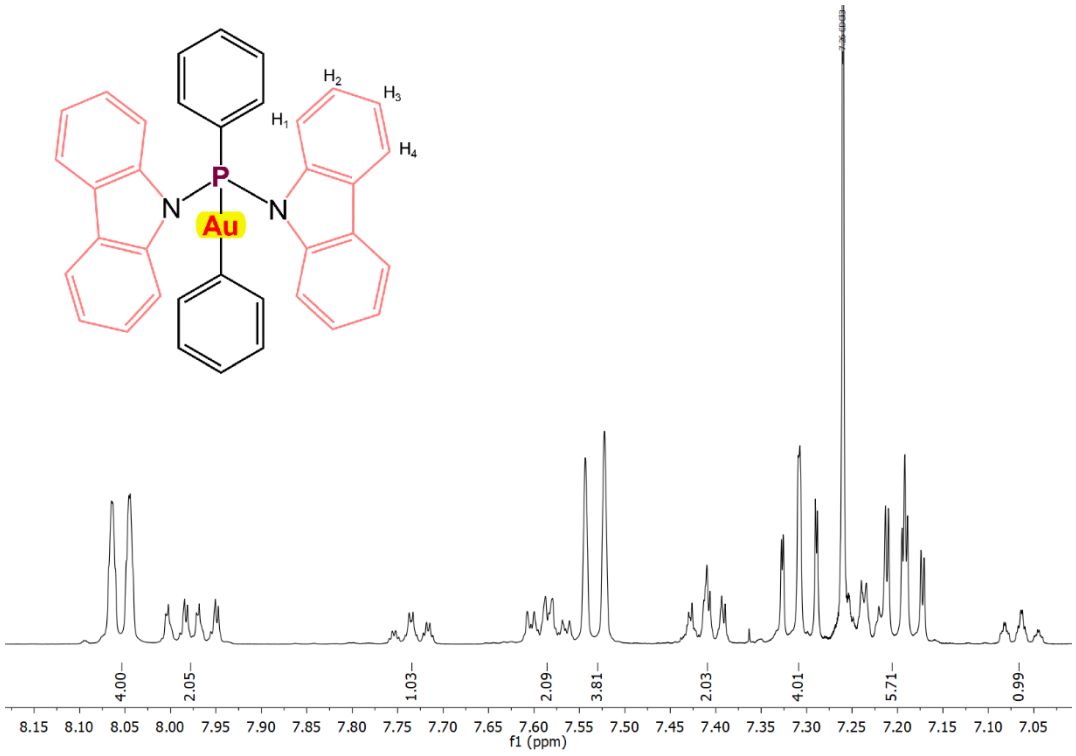


Figure S29. ^{1}H-NMR spectra of **3b** in $CDCl_3$

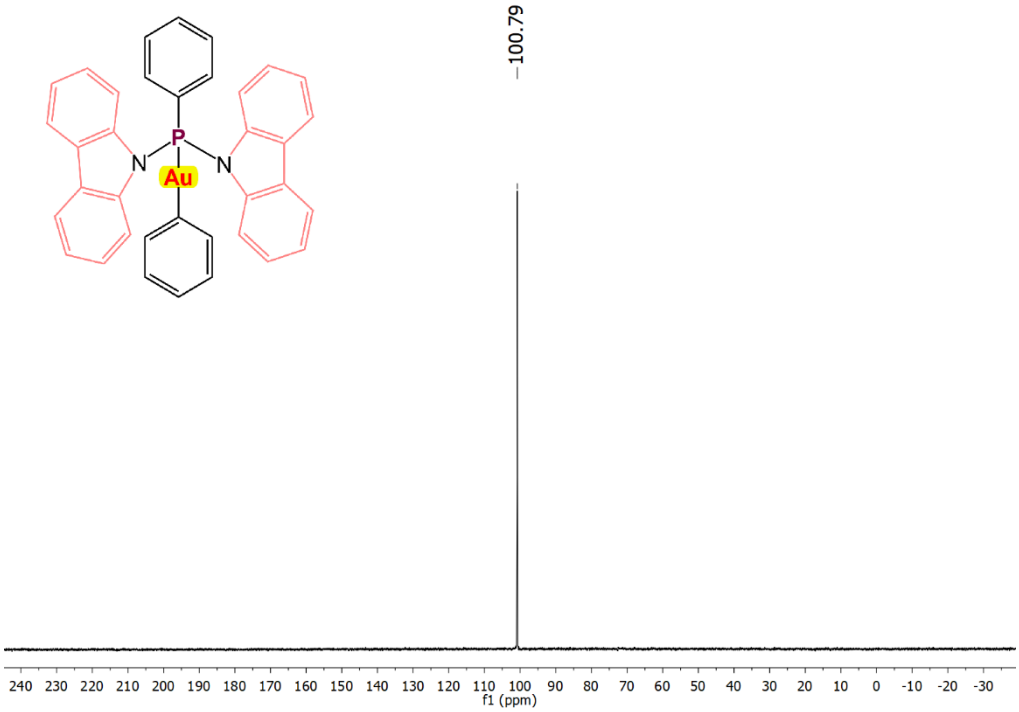


Figure S30. ^{31}P-NMR spectra of **3b** in $CDCl_3$

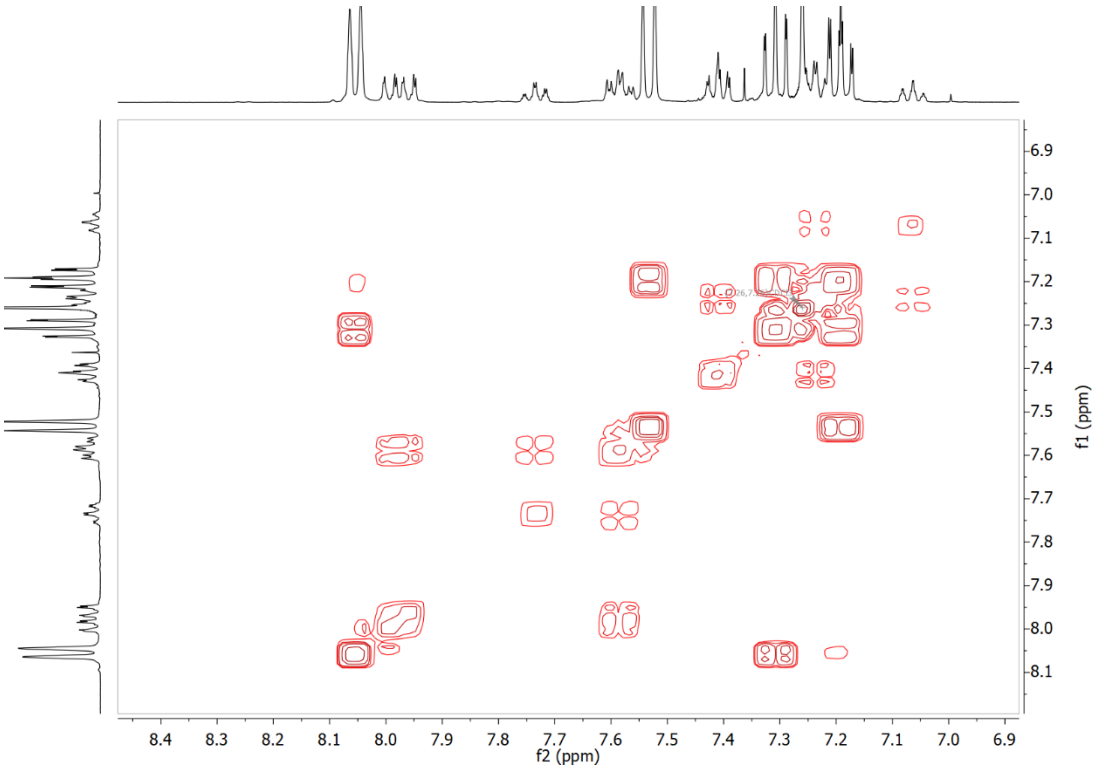


Figure S31. Partial ^{1}H-^{1}H COSY NMR spectrum of **3b**

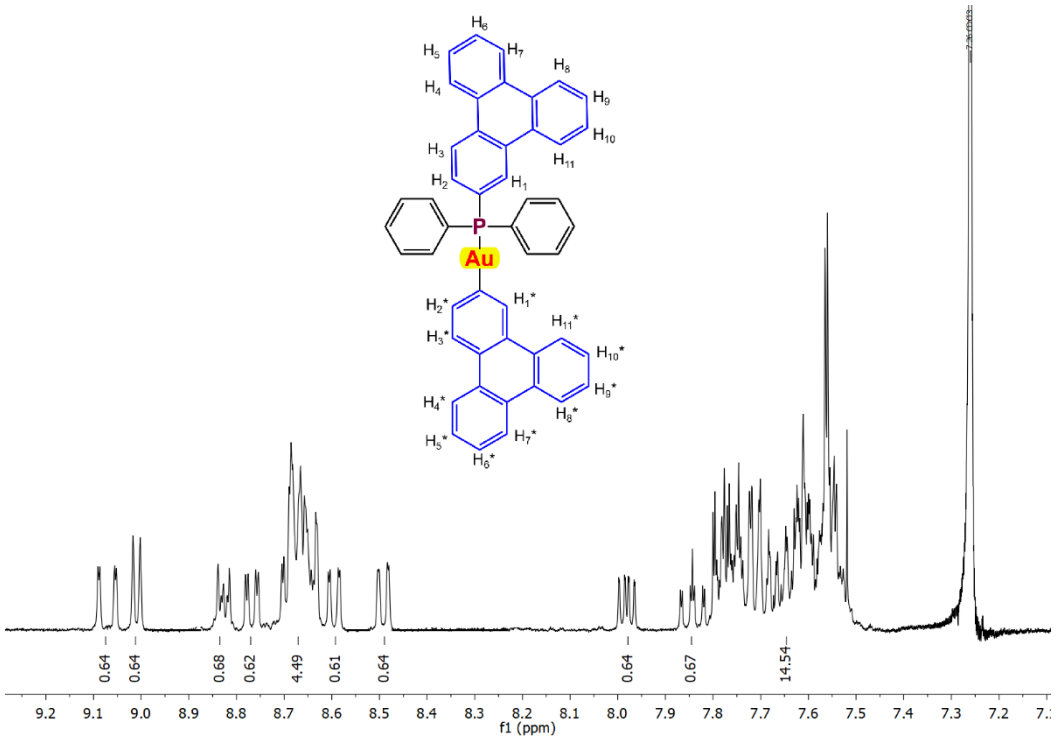


Figure S32. ^{1}H-NMR spectra of **1c** in $CDCl_3$

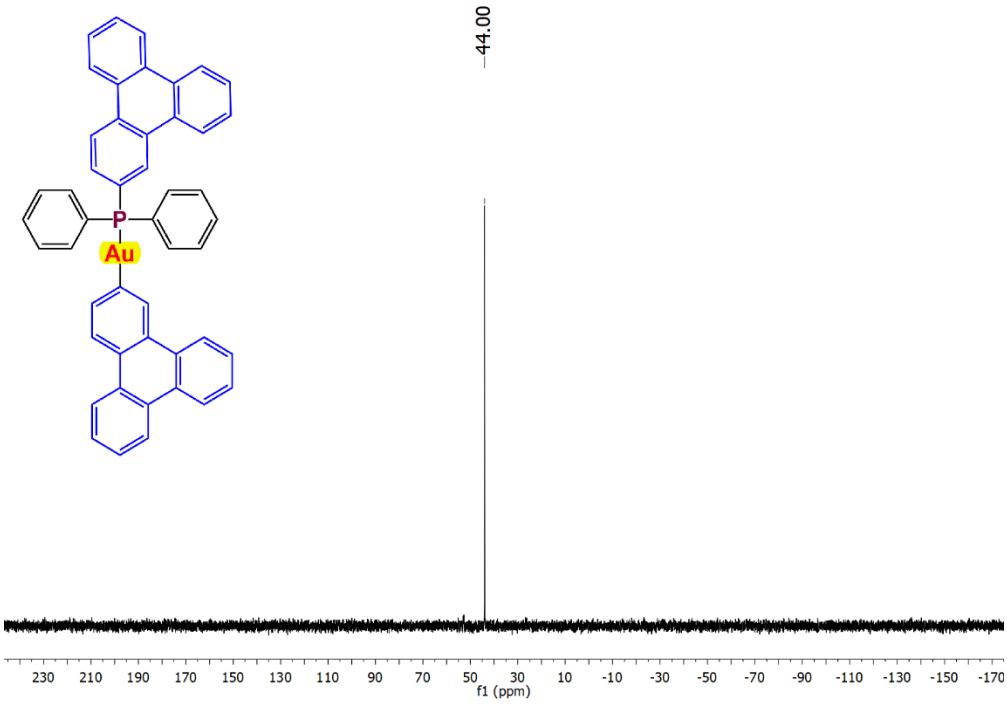


Figure S33. ^{31}P-NMR spectra of **1c** in $CDCl_3$

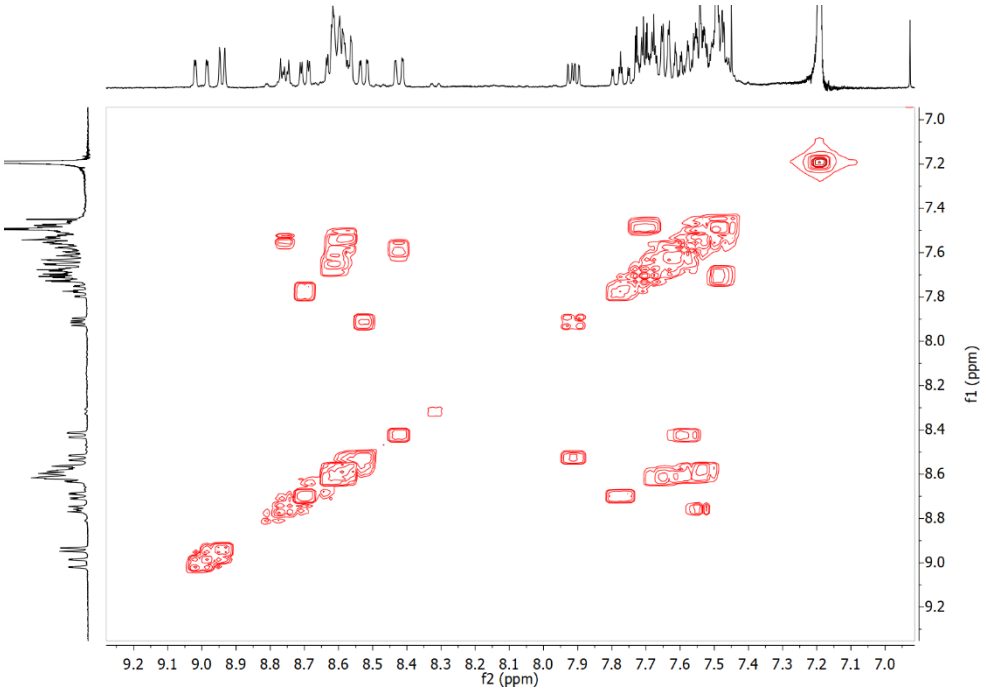


Figure S34. Partial ^{1}H-^{1}H COSY NMR spectrum of **1c**

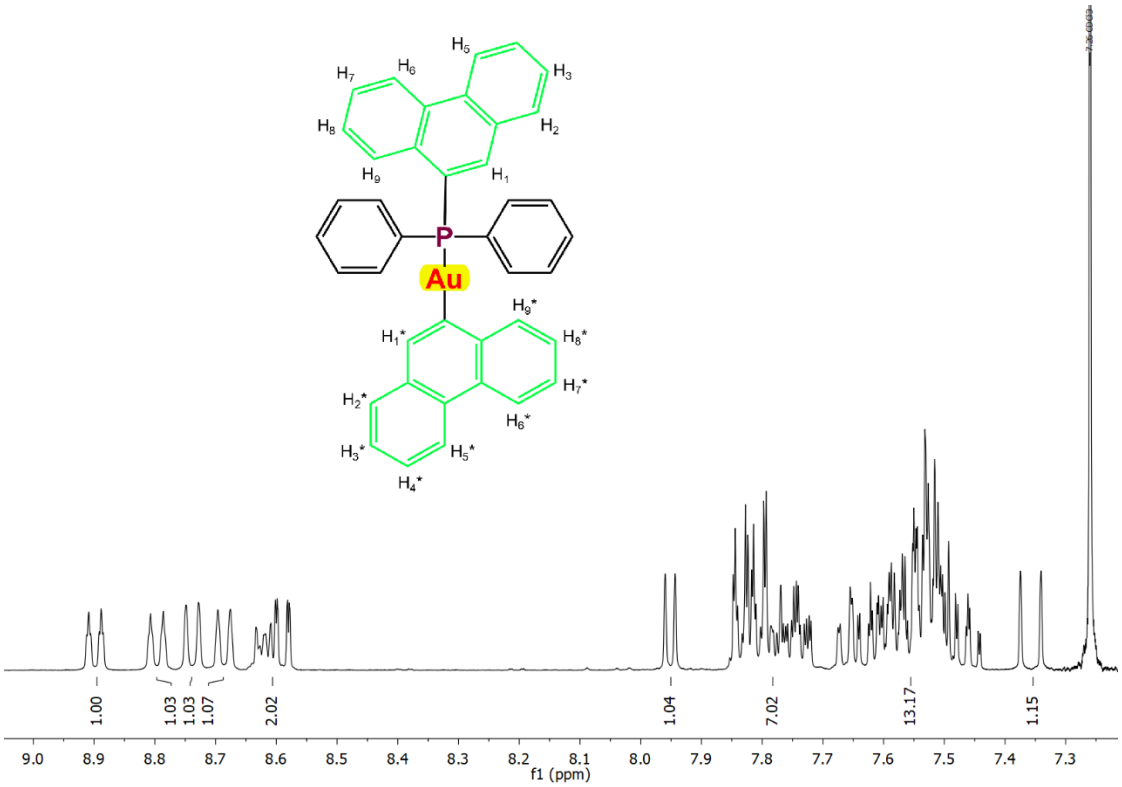


Figure S35. ^{1}H-NMR spectra of **2c** in $CDCl_3$

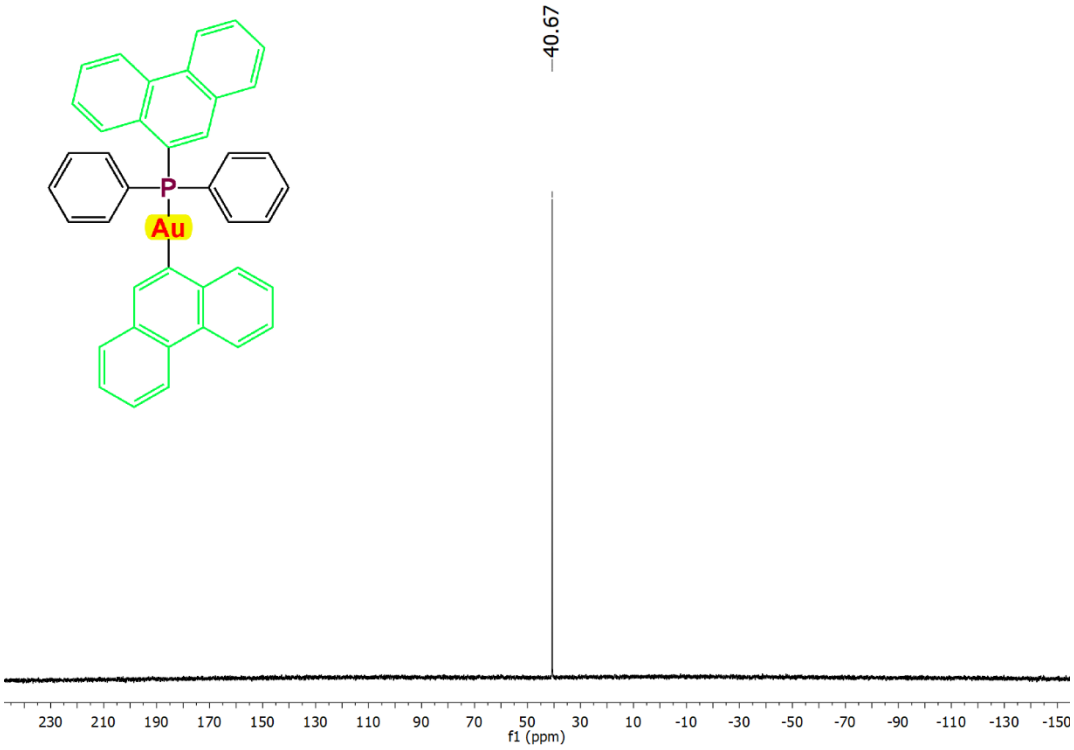


Figure S36. ^{31}P-NMR spectra of **2c** in $CDCl_3$

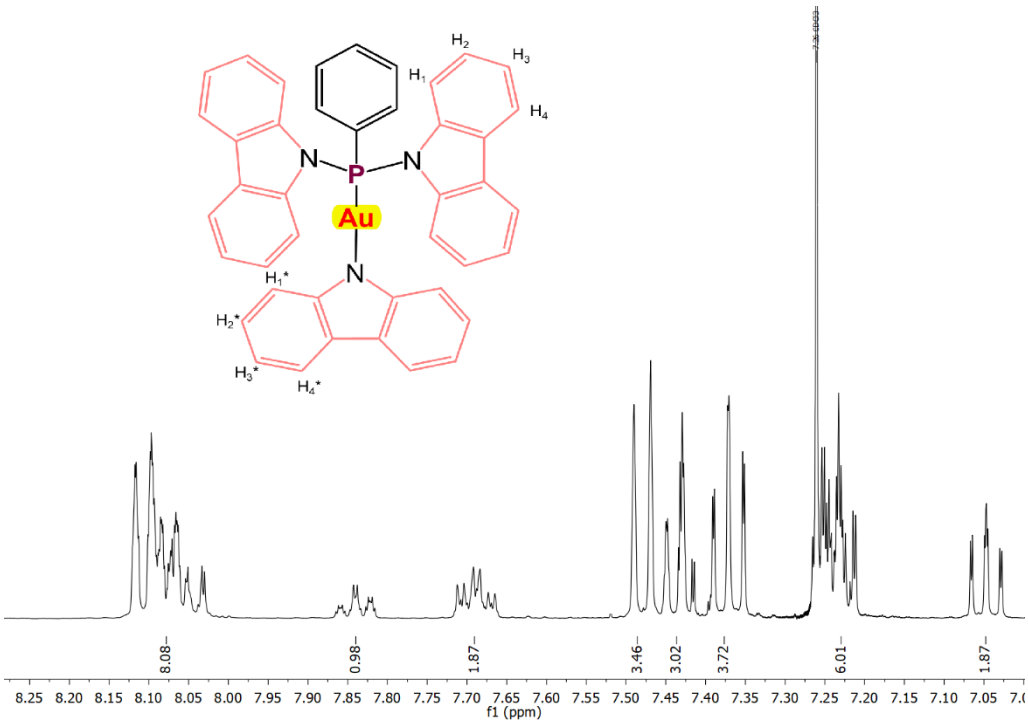


Figure S37. ^{1}H-NMR spectra of **3c** in $CDCl_3$

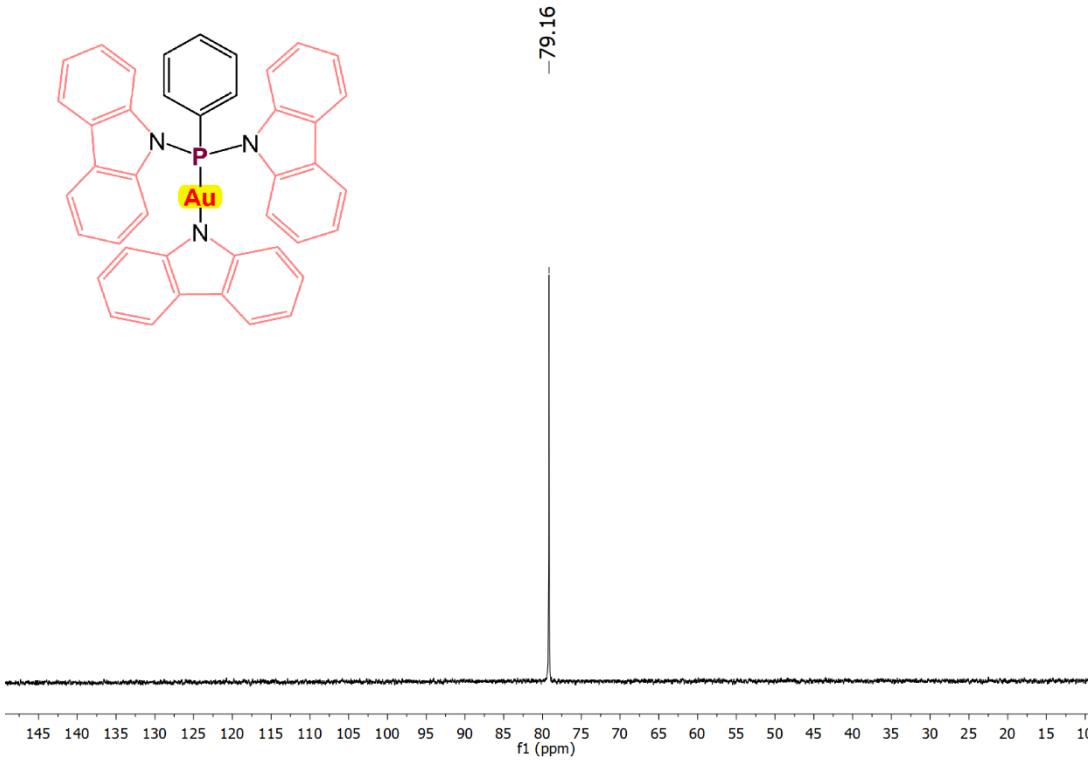


Figure S38. ^{31}P-NMR spectra of **3c** in $CDCl_3$

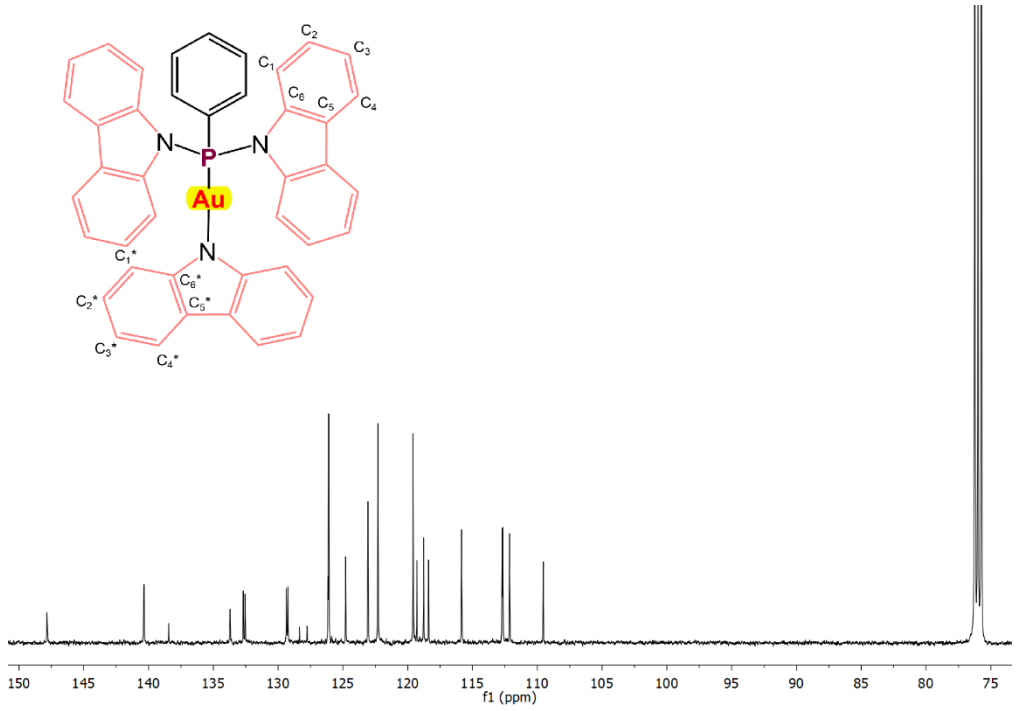


Figure S39. $^{13}C\{^{1}H\}$ NMR of **3c**

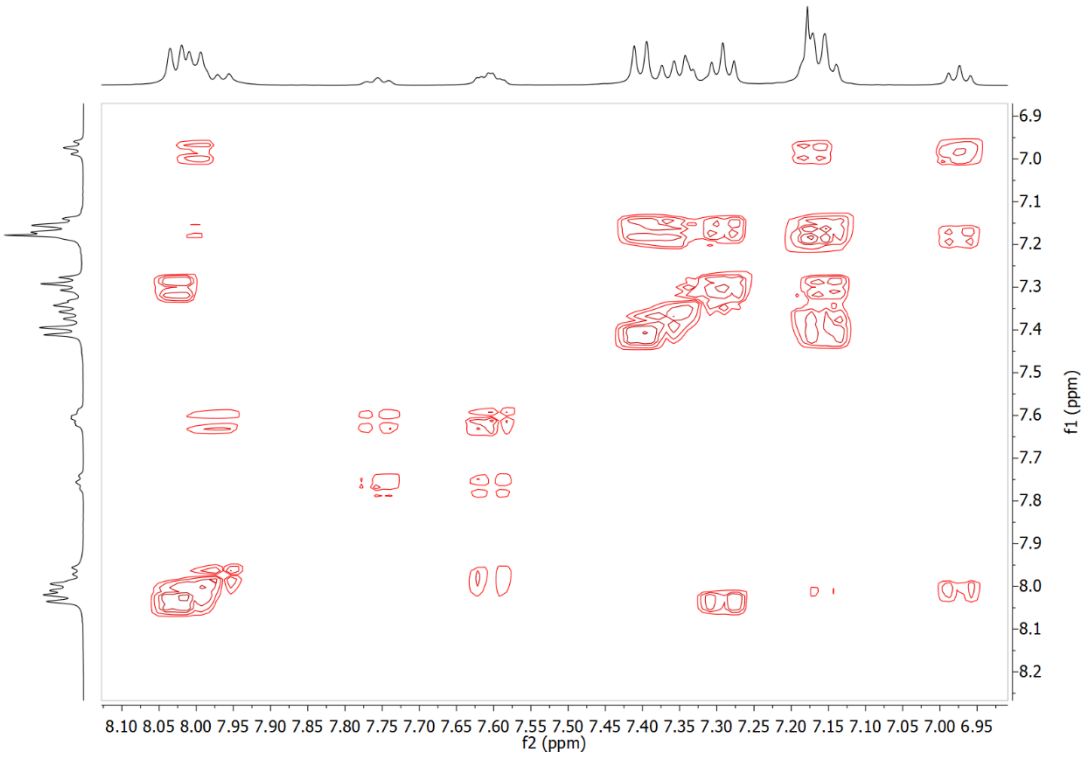


Figure S40. Partial ^{1}H-^{1}H COSY NMR spectrum of **3c**

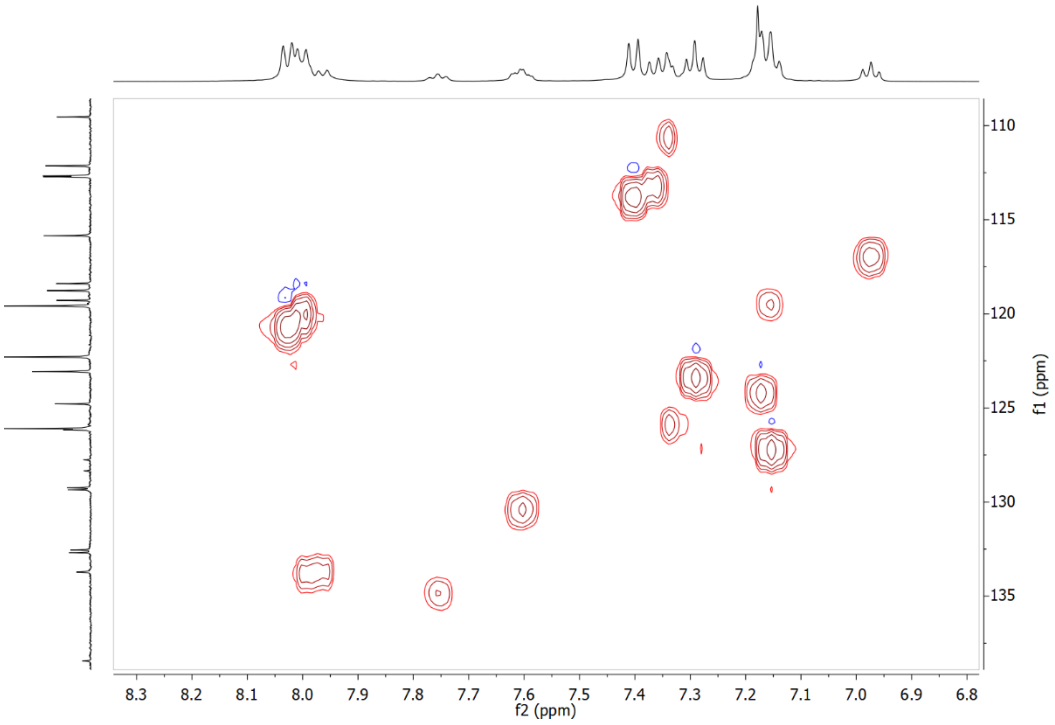


Figure S41. HSQC NMR spectrum of **3c**

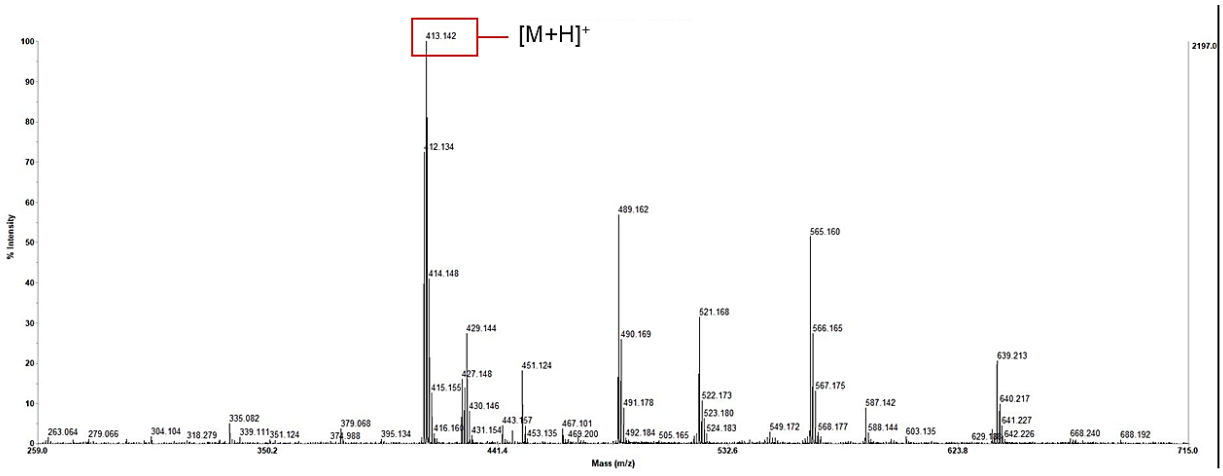


Figure S42. Mass spectra of **P1**

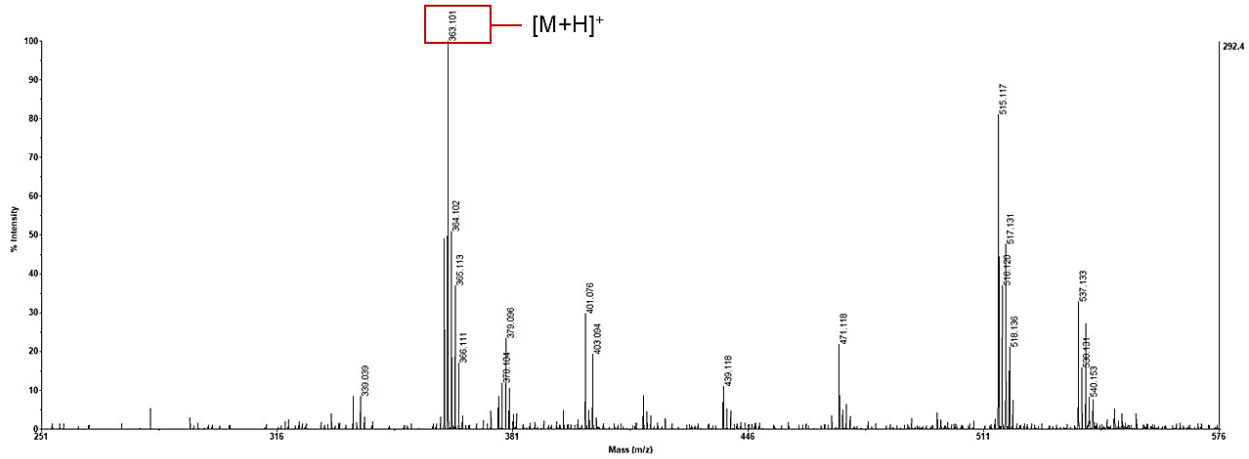


Figure S43. Mass spectra of **P2**

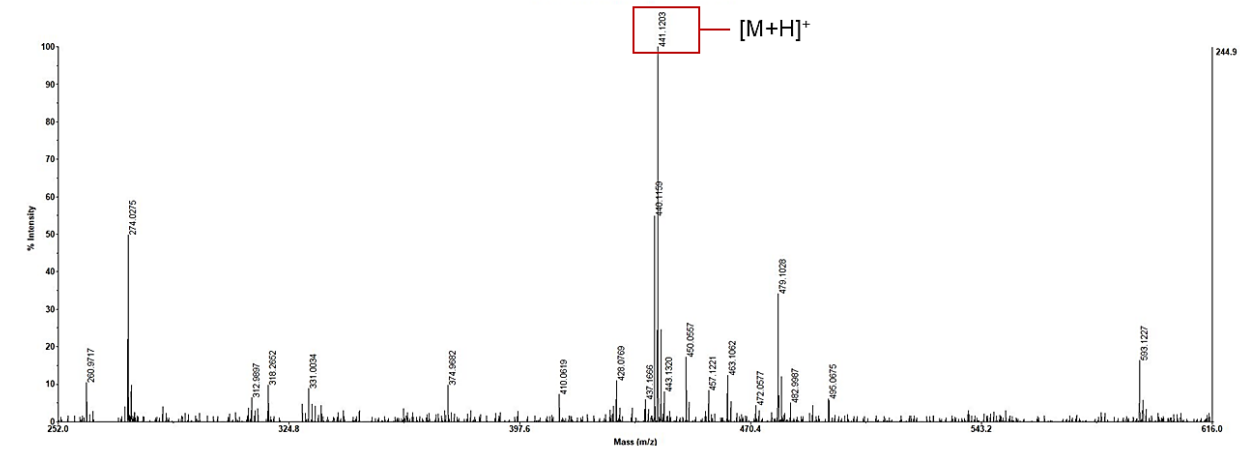


Figure S44. Mass spectra of **P3**

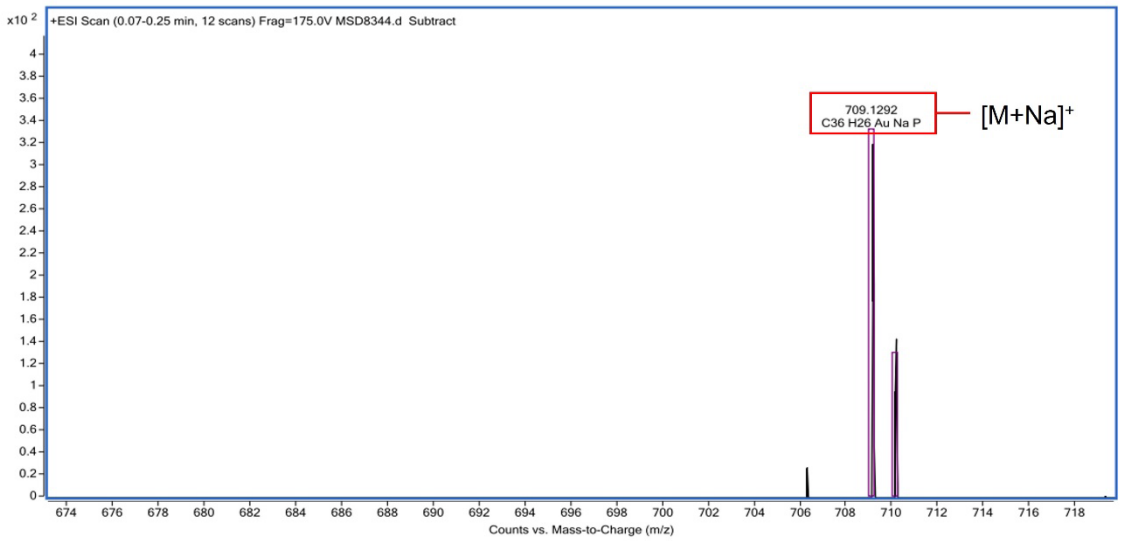


Figure S45. Mass spectra of **1a**

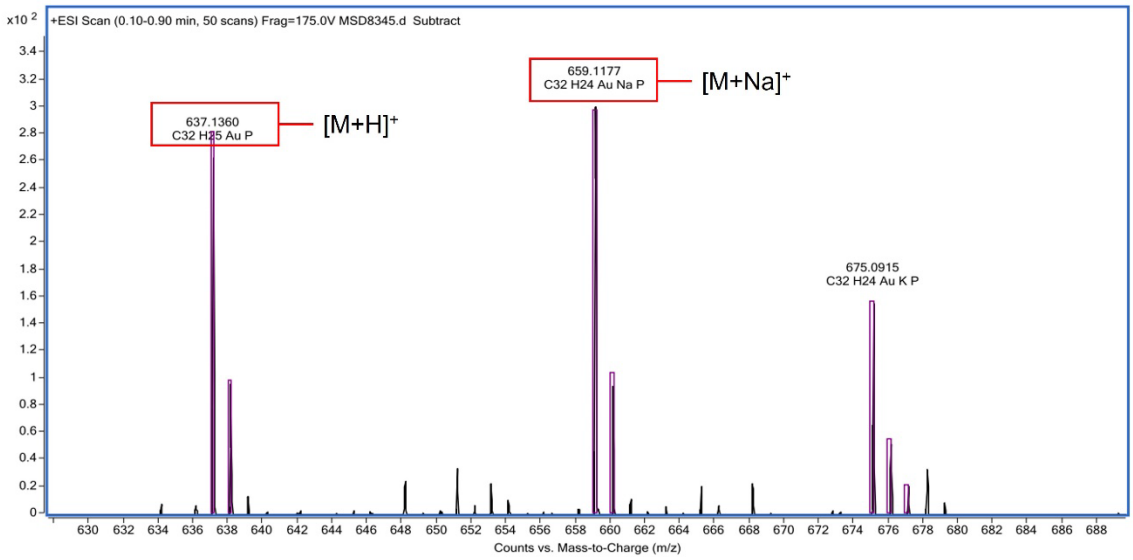


Figure S46. Mass spectra of **2a**

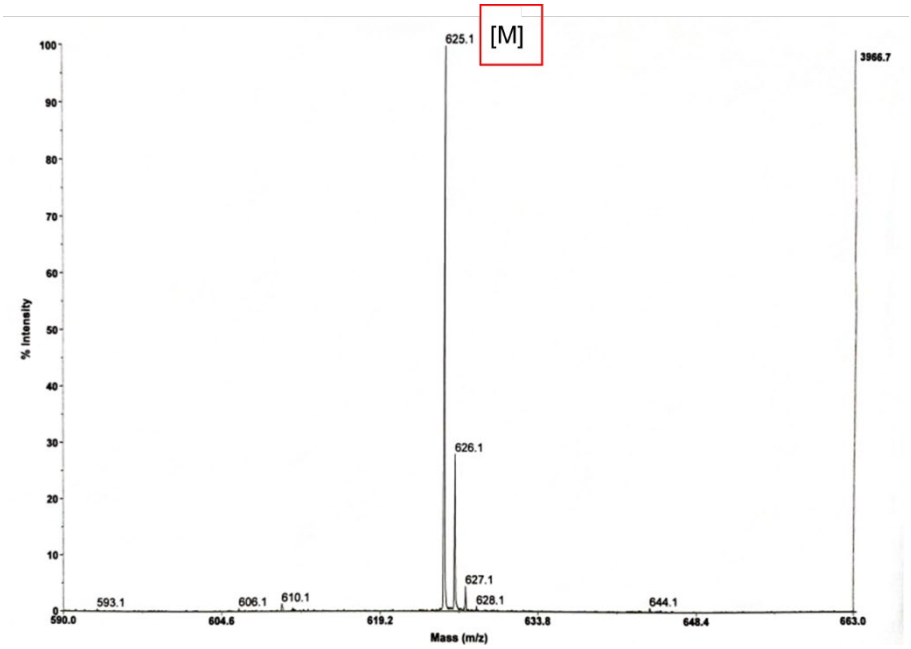


Figure S47. Mass spectra of **3a**

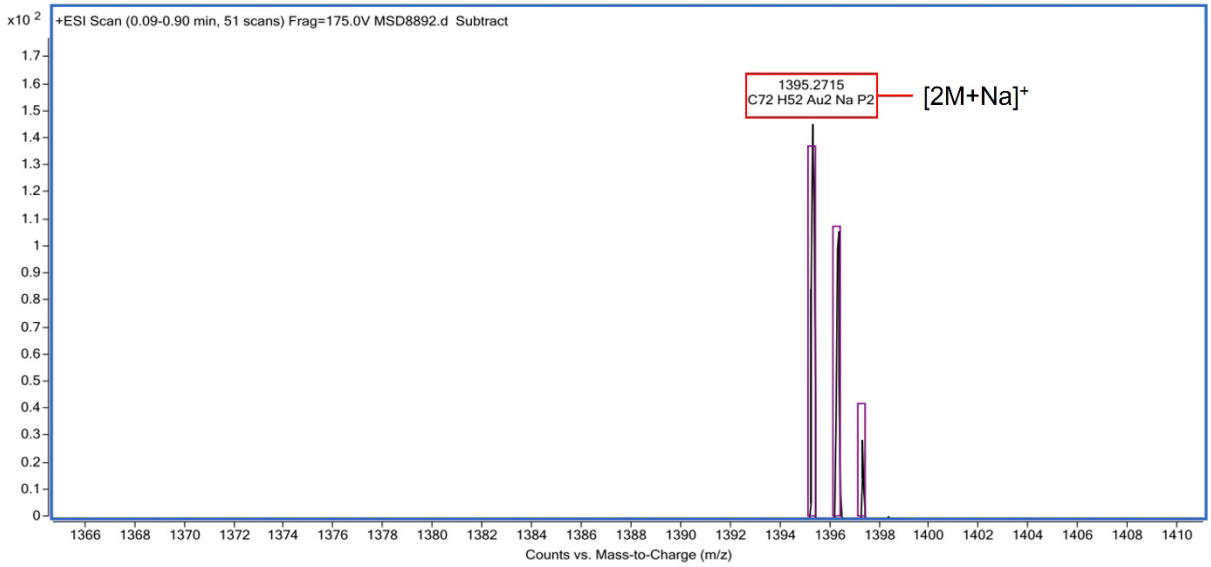


Figure S48. Mass spectra of **1b**

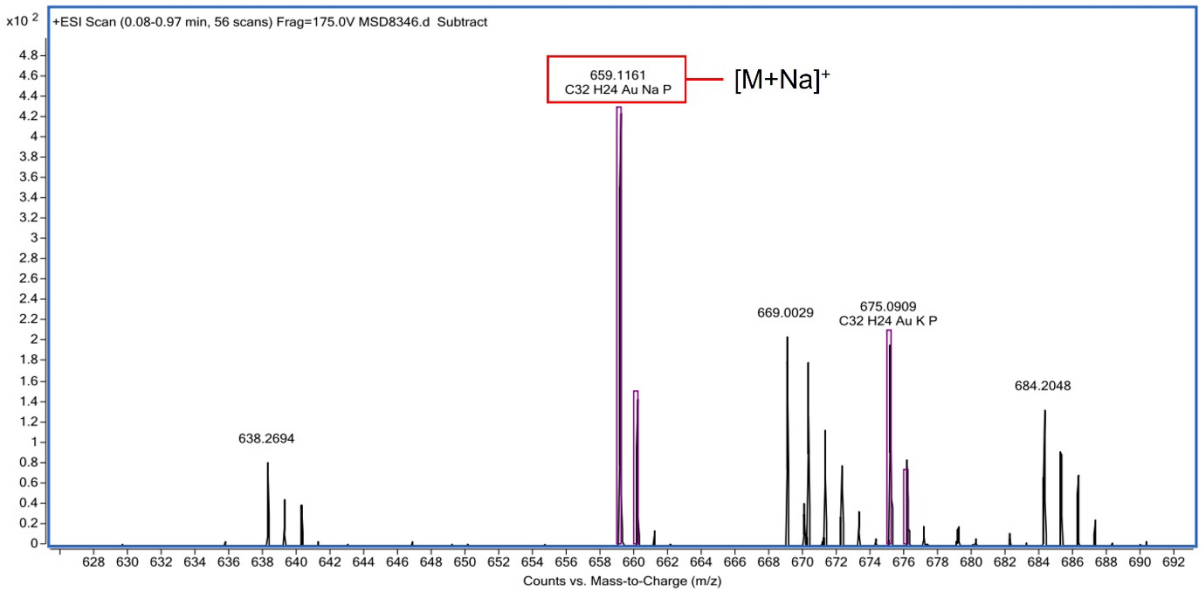


Figure S49. Mass spectra of **2b**

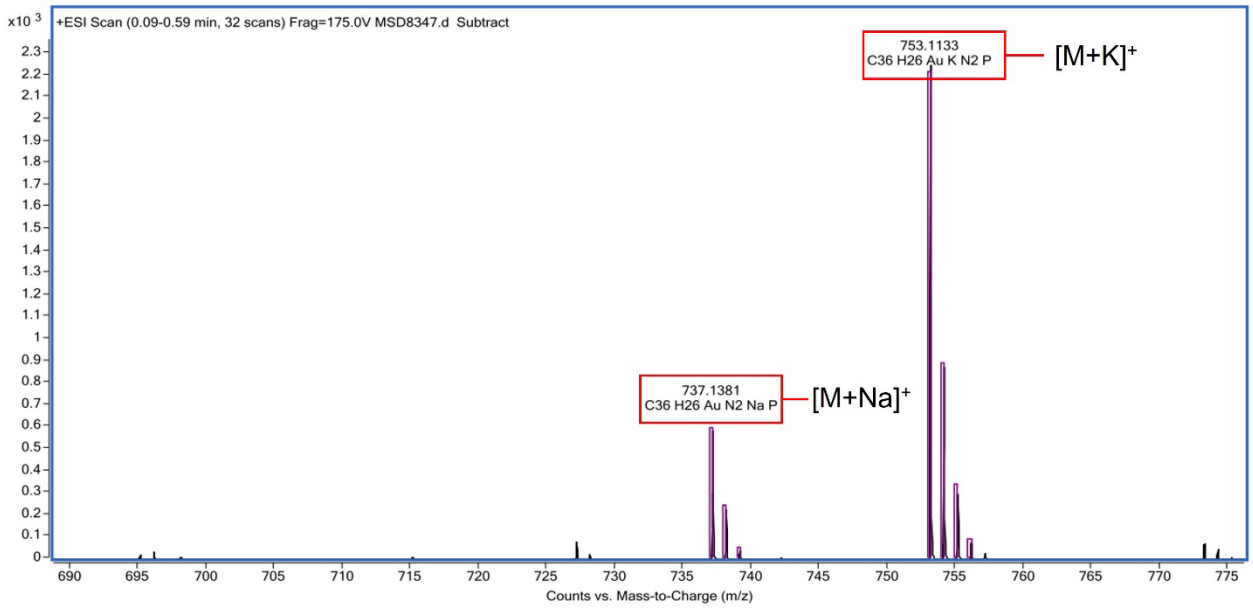


Figure S50. Mass spectra of **3b**

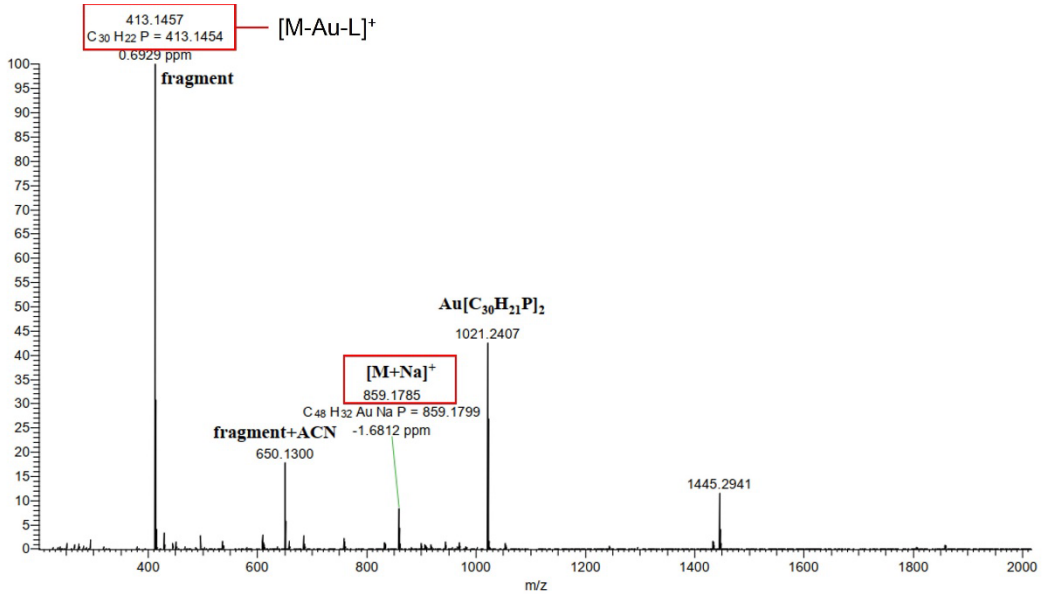


Figure S51. Mass spectra of **1c**

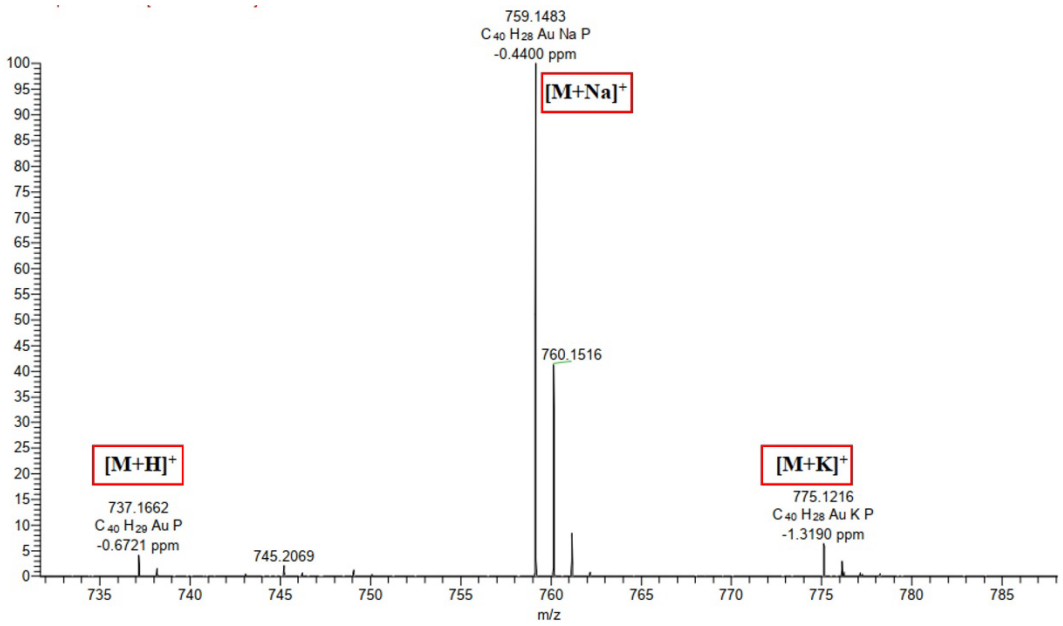


Figure S52. Mass spectra of **2c**

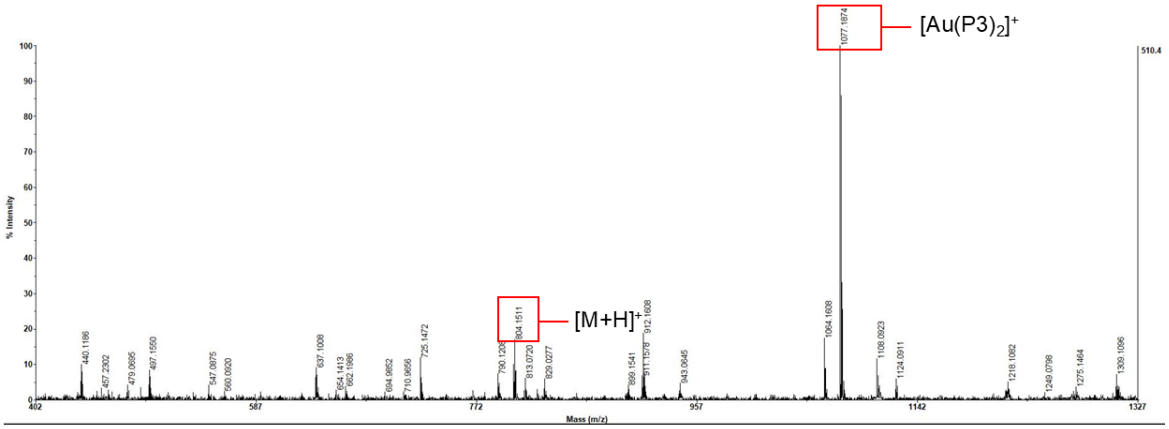


Figure S53. Mass spectra of **3c**

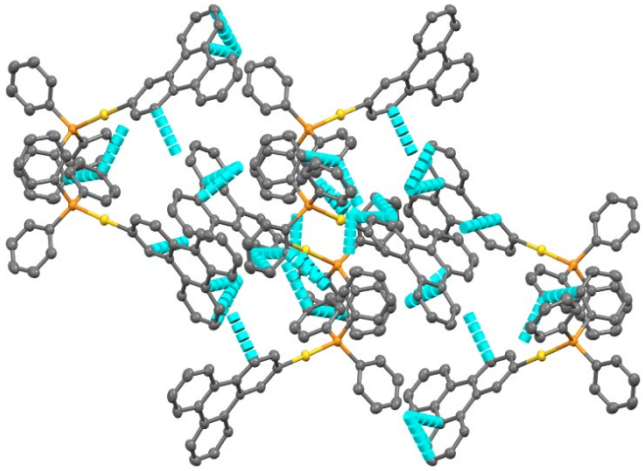


Figure S54. View of the molecular packing of compound **1a** along the crystallographic *b*-axis. Weak C H···π (ring) interactions between hydrogen atoms of the phosphane phenyl ring and the triphenylene of adjacent molecules are indicated in blue color.

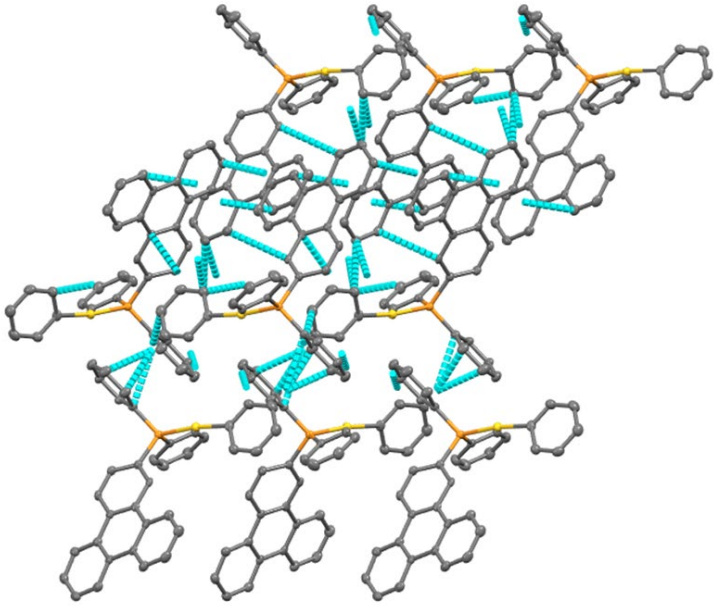


Figure S55. View of the molecular packing of compound **1b** along the crystallographic *b*-axis. Weak C H···π (ring) interactions between hydrogen atoms of the phosphane phenyl rings of adjacent molecules are indicated in blue color.

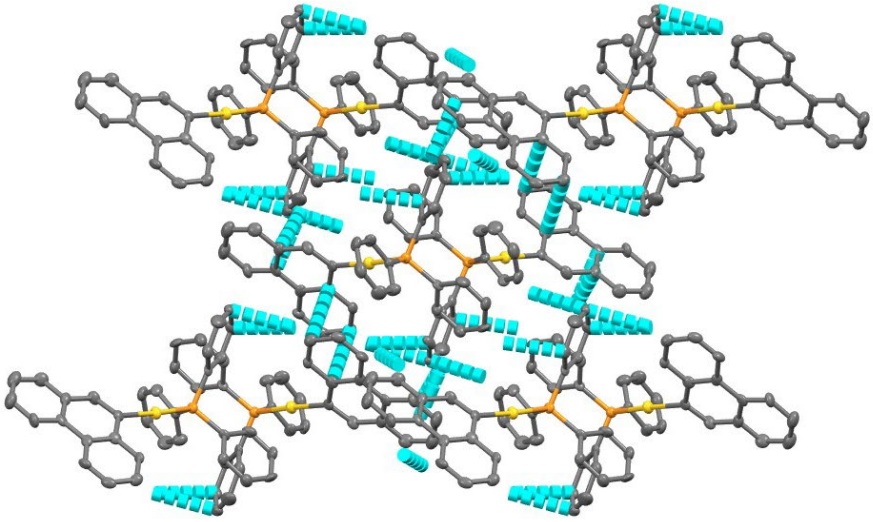


Figure S56. View of the molecular packing of compound **2a** along the crystallographic *b*-axis. Weak C H···π (ring) interactions between hydrogen atoms of the phosphane phenyl rings of adjacent molecules are indicated in blue color.

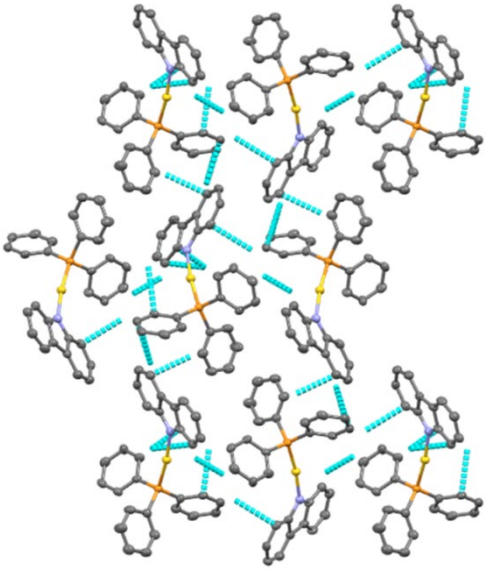


Figure S57. View of the molecular packing of compound **3a** along the crystallographic *a*-axis. Weak C H···π (ring) interactions between hydrogen atoms of the phosphane phenyl ring and the carbazole ring of adjacent molecules are indicated in blue colour.

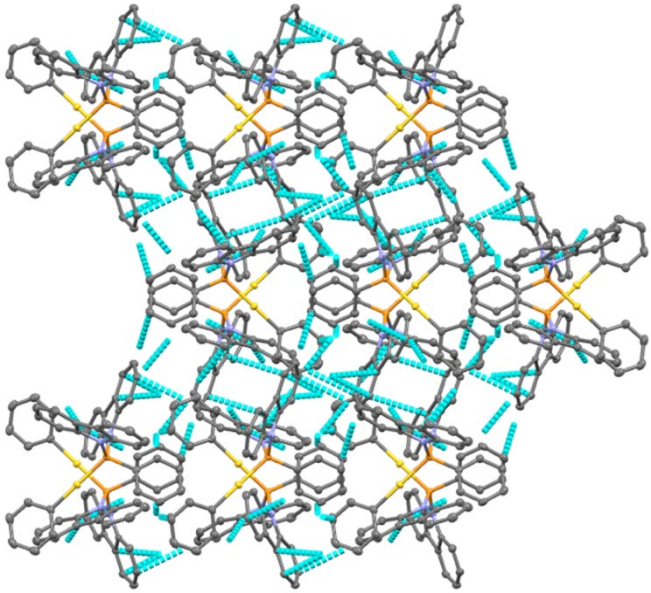


Figure S58. View of the molecular packing of compound **3b** along the crystallographic *c*-axis. Weak C H···π (ring) interactions between hydrogen atoms of the phosphane phenyl ring and the carbazole ring of adjacent molecules are indicated in blue color.

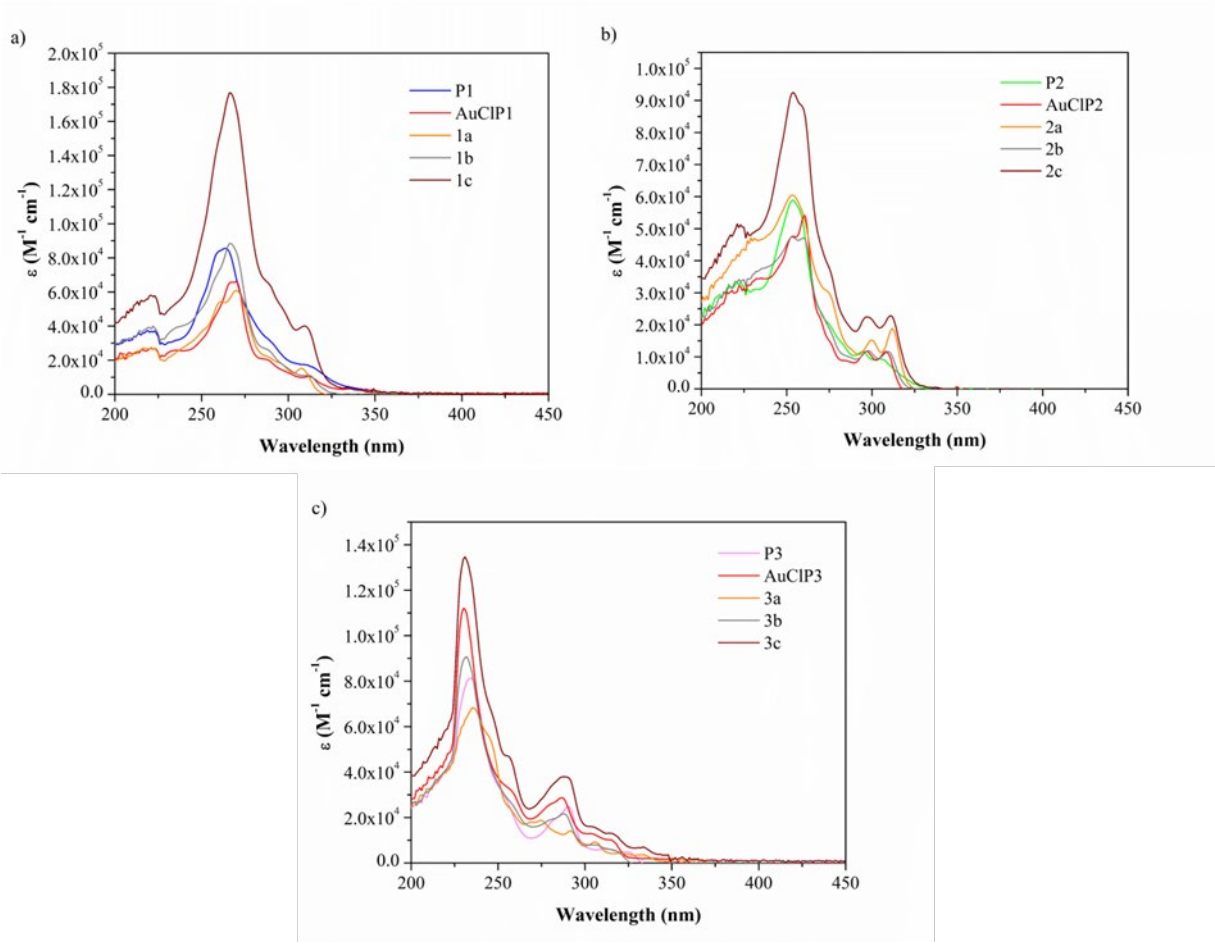


Figure S59. Absorption spectra of 1.0 x10^{-5} M dichloromethane solutions solutions of a) series **1** b) series **2** c) series **3** complexes at 298 K

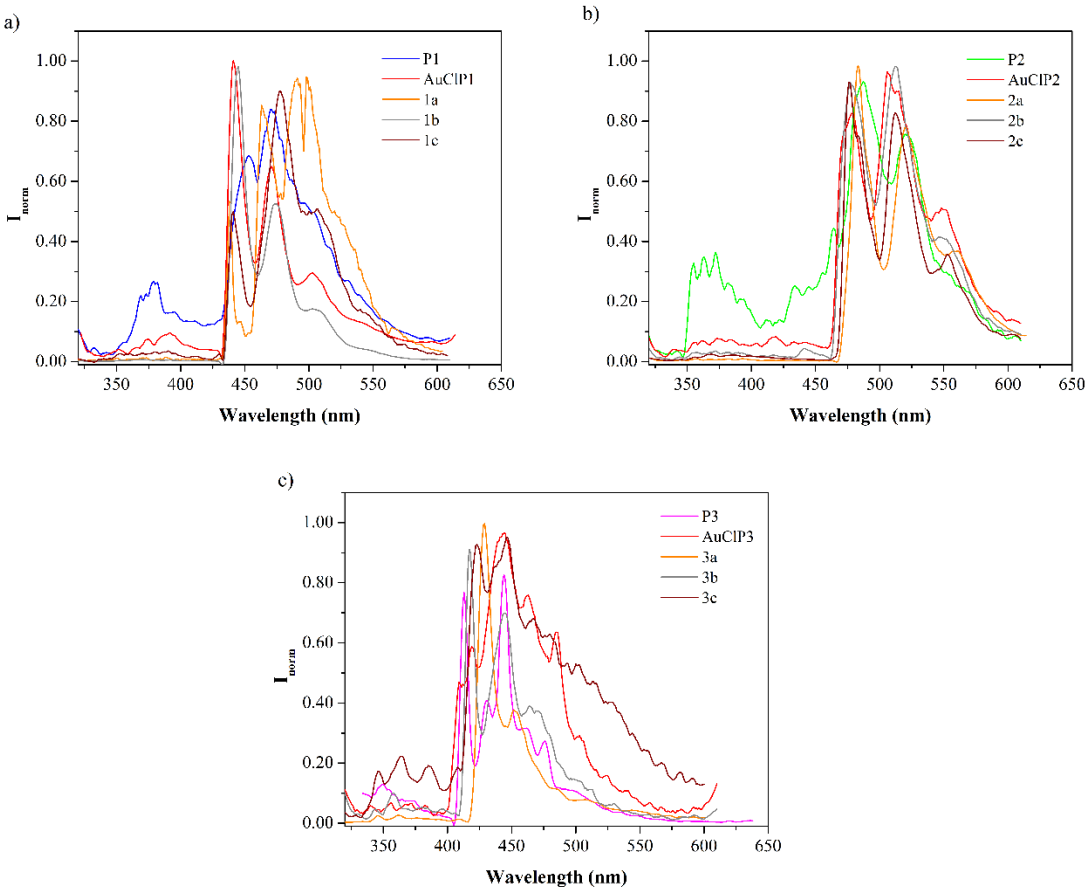


Figure S60. Emission spectra of 1.0 x10^{-5} M dichloromethane solutions at 77 K of a) series **1** b) series **2** c) series **3** complexes.

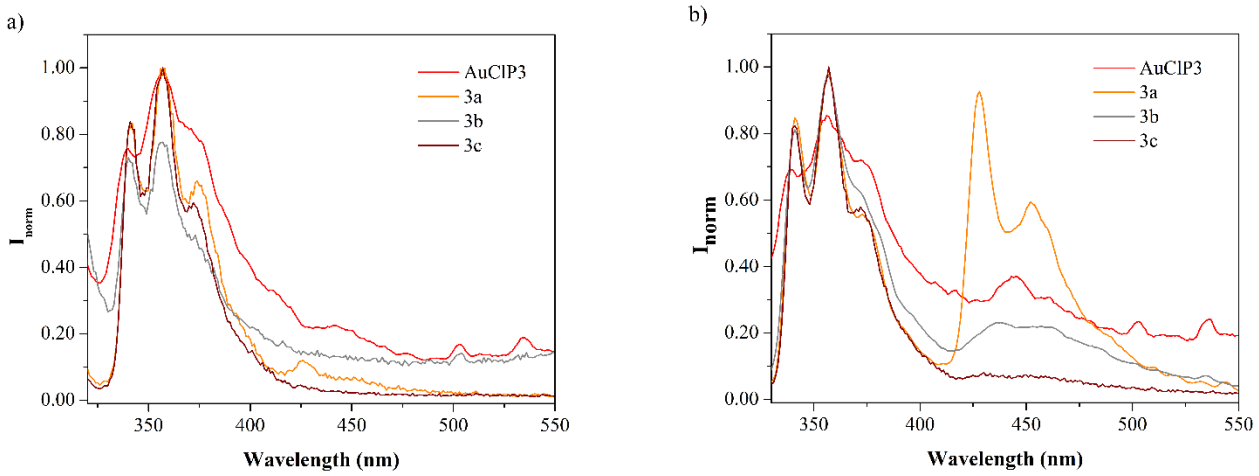


Figure S61. Normalized emission spectra of a) series 3 air-equilibrated conditions b) series 3 N_2-saturated conditions of PS matrixes.

Table S1. Crystal data and structure refinement for **1a**.

Compound	**1a**
Formula	$C_{36}H_{26}AuP$
Crystal size, mm	0.028 x 0.044 x 0.120
Fw	686.50
Temperature, K	120.0(1)
Wavelength, Å	1.54184
Crystal system	orthorhombic
Space group	*Pbca*
a, Å	14.26560(10)
b, Å	15.26220(10)
c, Å	24.83410(10)
α, °	90
β, °	90
γ, °	90
Volume, Å^3	5406.99(6)
Z	8
$D_{calc.}$, mg m^{-3}	1.687
Absorption coefficient, mm^{-1}	10.954
F(000)	2688
θ range for data collection, °	3.560 to 74.501
Reflections collected/independent	84597/5526
Data/restraint/parameters	5526/0/343
GooF on F^2	1.039
Final *R* index ($I > 2\sigma(I)$)	R_1 = 0.0332, wR_2 = 0.0879
R index (all data)	R_1 = 0.0383, wR_2 = 0.0913
Peak and hole, e Å^{-3}	2.123 and -1.172
CCDC number	2409503

Table S2. Crystal data and structure refinement for **1b**.

Compound	**1b**
Formula	$C_{36}H_{26}AuP$
Crystal size, mm	0.159 x 0.210 x 0.368
Fw	686.50
Temperature, K	120.0(1)
Wavelength, Å	1.54184
Crystal system	monoclinic
Space group	$P2_1/c$
a, Å	18.0178(2)
b, Å	10.80640(10)
c, Å	14.3298(2)
α, °	90
β, °	109.9380(10)
γ, °	90
Volume, Å^3	2622.89(5)
Z	4
$D_{calc.}$, mg m^{-3}	1.738
Absorption coefficient, mm^{-1}	11.290
F(000)	1344
θ range for data collection, °	2.609 to 74.482
Reflections collected/independent	32904/5380
Data/restraint/parameters	5380/0/343
GooF on F^2	1.114
Final *R* index ($I > 2\sigma(I)$)	$R_1 = 0.0327$, $wR_2 = 0.0834$
R index (all data)	$R_1 = 0.033$, $wR_2 = 0.0863$
Peak and hole, e Å^{-3}	1.511 and -1.876
CCDC number	2409504

Table S3. Crystal data and structure refinement for **3a**.

Compound	**3a**
Formula	$C_{30}H_{23}AuNP$
Crystal size, mm	0.044 x 0.073 x 0.262
Fw	625.43
Temperature, K	120.0(1)
Wavelength, Å	1.54184
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a, Å	7.13710(10)
b, Å	15.3778(3)
c, Å	21.5667(3)
α, °	90
β, °	90
γ, °	90
Volume, Å^3	2367.01(7)
Z	4
$D_{calc.}$, mg m^{-3}	1.755
Absorption coefficient, mm^{-1}	12.449
F(000)	1216
θ range for data collection, °	3.530 to 77.296
Reflections collected/independent	28858/4922
Data/restraint/parameters	4922/0/298
GooF on F^2	1.102
Final *R* index ($I > 2\sigma(I)$)	R_1 = 0.0410, wR_2 = 0.1077
R index (all data)	R_1 = 0.0426, wR_2 = 0.1091
Peak and hole, e Å^{-3}	2.678 and -1.007
CCDC number	2409505

Table S4. Crystal data and structure refinement for **3b**.

Compound	**3b**
Formula	$C_{36}H_{26}AuN_2P$
Crystal size, mm	0.042 x 0.230 x 0.274
Fw	714.52
Temperature, K	120.0(1)
Wavelength, Å	1.54184
Crystal system	orthorhombic
Space group	*Pbca*
a, Å	17.85940(10)
b, Å	19.73910(10)
c, Å	15.67780(10)
α, °	90
β, °	90
γ, °	90
Volume, $Å^3$	5526.87(5)
Z	8
$D_{calc.}$, mg m^{-3}	1.717
Absorption coefficient, mm^{-1}	10.766
F(000)	2800
θ range for data collection, °	4.370 to 74.498
Reflections collected/independent	67074/5661
Data/restraint/parameters	5661/0/361
GooF on F^2	1.029
Final *R* index ($I > 2\sigma(I)$)	R_1 = 0.0238, wR_2 = 0.0585
R index (all data)	R_1 = 0.0257, wR_2 = 0.0606
Peak and hole, e $Å^{-3}$	0.489 and -1.060
CCDC number	2409506

Table S5. HOMO-LUMO gaps for compounds **1a**, **1b**, **3a**, **3b** in eV in their monomeric (gap_{mon}) and dimeric (gap_{dim}) forms at the CAM-B3LYP(solvent = CH_2Cl_2)/def2-TZVP//RI-BP86-D4/def2-TZVP level of theory.

Compound	**gap_{mon}**	**gap_{dim}**	**gap_{mon}–gap_{dim}**
1a	6.83	6.53	0.30
1b	6.91	6.48	0.43
2a	6.66	6.37	0.29
3a	6.26	5.81	0.45
3b	6.91	6.73	0.28

Table S6. Luminescence lifetimes in solution.

Compound	Air-equilibrated samples		N_2-saturated samples	
	τ_{Fl} (ns)	τ_{Ph}	τ_{Fl} (ns)	τ_{Ph} (μs)
P1	7.4	-	17.5	0
AuClP1	5.6	-	5.6	131
1a	5.1	-	5.1	78
1b	5.9	-	5.9	183
1c	5.4	-	5.4	133
P2	13.4	-	21.4	0
AuClP2	11.1	-	11.1	582
2a	7.41	-	7.41	173
2b	11.2	-	11.2	362
2c	11.9	-	11.9	240
P3		-		-
AuCl(P3)	9.5	-	129	-
3a	6.1	-	8.1	-
3b	6.1	-	113	-
3c	7.4	-	8.0	-

Table S7. Emission data of the different series of gold (I) phosphane complexes in PS organic matrix and ratio of phosphorescence and fluorescence intensities (I_P/I_F)

Compound	Fluorescence emission λ_{max} (nm)	Phosphorescence emission λ_{max} (nm)	I_P/I_F (air-equilibrated)	I_P/I_F (N_2-saturated)
AuClP1	374	464	0.71	38.14
1a	370	459	5.23	112.83
1b	371	460	0.81	44.33
1c	373	459	1.61	52.50
AuClP2	376	497	0.22	22.81
2a	375	502	5.39	86.42
2b	371	500	0.16	19.78
2c	375	502	0.34	10.64
AuClP3	355	-	-	-
3a	358	-	440	0.88
3b	350	-	446	0.23
3c	356	-	-	-

XYZ Coordinates of the optimized monomer 1a

P	-0.0255616	1.3568112	-0.1303625
Au	0.7218749	2.4394991	-2.0330773
C	1.3949541	3.4145637	-3.7026211
C	0.8133464	3.2089985	-4.9540662
C	2.4704041	4.3305251	-3.6432191
C	1.2459949	3.8625384	-6.1301573
H	-0.0160679	2.5080038	-5.0259862
C	2.9189204	4.9862307	-4.7769360
H	2.9650867	4.5325711	-2.6913927
C	2.3301535	4.7767831	-6.0425872
C	0.6046562	3.6185713	-7.4209433
H	3.7510394	5.6816640	-4.6742666
C	2.8067584	5.4668962	-7.2369069
C	1.0665123	4.2919972	-8.5866490
C	2.1849301	5.2276118	-8.4940506
C	3.8846740	6.3791715	-7.1828322
C	2.6737645	5.9111114	-9.6297113
C	4.3444357	7.0370335	-8.3106674
H	4.3745374	6.5770735	-6.2313858
C	3.7319649	6.8003204	-9.5497388
H	2.2143782	5.7419852	-10.6018239
H	5.1790041	7.7349634	-8.2319711
H	4.0839908	7.3113477	-10.4467235
C	-0.4795847	2.7214764	-7.5500138
C	0.4208835	4.0341826	-9.8165939
C	-1.0948022	2.4856934	-8.7674692
H	-1.9298292	1.7865351	-8.8295968
C	-0.6396786	3.1499769	-9.9153645
H	-0.8501582	2.1961434	-6.6721621
H	0.7569814	4.5405212	-10.7194274
H	-1.1155101	2.9743153	-10.8809662
C	-1.8401419	1.2606752	0.0157402
C	-2.5123564	1.4520313	1.2296279
C	-2.5725955	0.9659218	-1.1443404
C	-3.9031471	1.3387368	1.2832141
H	-1.9497765	1.6954579	2.1313602
C	-3.9598424	0.8452465	-1.0850588
H	-2.0489764	0.8410678	-2.0940788
C	-4.6270535	1.0316486	0.1292021
H	-4.4221026	1.4934633	2.2301485
H	-4.5230889	0.6167335	-1.9905178
H	-5.7134600	0.9461098	0.1731334
C	0.5298651	-0.3715330	0.0320857
C	-0.2668721	-1.3662946	0.6146949
C	1.8161595	-0.6919551	-0.4272629
C	0.2248747	-2.6660164	0.7469649
H	-1.2732130	-1.1253372	0.9584361
C	2.3064311	-1.9895706	-0.2861719
H	2.4241615	0.0789152	-0.9048297

C	1.5116398	-2.9776609	0.3015595
H	-0.4004011	-3.4378081	1.1975495
H	3.3067916	-2.2329749	-0.6458620
H	1.8926850	-3.9945157	0.4038698
C	0.5119333	2.1576957	1.4165892
C	0.9162084	1.4322708	2.5445486
C	0.4976651	3.5604137	1.4610551
C	1.2924397	2.1049094	3.7089550
H	0.9426042	0.3428788	2.5112024
C	0.8650206	4.2275978	2.6284235
H	0.2055018	4.1238154	0.5728065
C	1.2632933	3.5003967	3.7539650
H	1.6110809	1.5355959	4.5830862
H	0.8508728	5.3176576	2.6566495
H	1.5594343	4.0232640	4.6642299

XYZ Coordinates of the optimized dimer 1a

Au	0.9818665	0.8536034	-0.4818661
P	0.1629119	-0.4894302	-2.1813252
C	1.4301563	1.9923749	1.1583503
C	0.5609635	3.0486021	1.5183778
H	-0.2944102	3.2870856	0.8834738
C	0.7600100	3.7855708	2.6714334
H	0.0523520	4.5734252	2.9152205
C	1.8484184	3.5402005	3.5310438
C	2.1159001	4.3939613	4.6791741
C	1.3507446	5.5560487	4.9231721
H	0.5269406	5.8101356	4.2600692
C	1.6394164	6.4105924	5.9729097
H	1.0343015	7.3049701	6.1261380
C	2.7149265	6.1237385	6.8269849
H	2.9538095	6.7896390	7.6572578
C	3.4793021	4.9893244	6.6074686
H	4.3178094	4.7940822	7.2733019
C	3.2099939	4.1047869	5.5395232
C	4.0524734	2.9424732	5.2738747
C	5.1361014	2.6108074	6.1165644
H	5.3265404	3.2045426	7.0086449
C	5.9718869	1.5399275	5.8474193
H	6.8001186	1.3119174	6.5194078
C	5.7377784	0.7490306	4.7128245
H	6.3820902	-0.1032877	4.4927884
C	4.6759337	1.0477950	3.8761325
H	4.5038650	0.4156160	3.0078947
C	3.8153656	2.1407199	4.1220016
C	2.7124770	2.4591554	3.2210206
C	2.4805557	1.7232547	2.0362370
H	3.1545421	0.9038078	1.7940023
C	1.3518255	-1.2709024	-3.3235859
C	2.6648040	-0.7846328	-3.3639083

H	2.9445598	0.0385006	-2.7048477
C	3.5990776	-1.3489915	-4.2335564
H	4.6183900	-0.9620039	-4.2607443
C	3.2282923	-2.4096071	-5.0634337
H	3.9573153	-2.8495017	-5.7451680
C	1.9288805	-2.9206892	-5.0046180
H	1.6426050	-3.7629287	-5.6356267
C	0.9968745	-2.3608279	-4.1322844
H	-0.0036325	-2.7890227	-4.0626864
C	-0.6846054	-1.9493094	-1.4740013
C	0.0911773	-2.8660926	-0.7469361
H	1.1646656	-2.7014061	-0.6377990
C	-0.5031773	-3.9827013	-0.1648092
H	0.1079001	-4.6913286	0.3956676
C	-1.8809862	-4.1892323	-0.2911641
H	-2.3467385	-5.0616767	0.1687049
C	-2.6575098	-3.2732818	-1.0012517
H	-3.7330822	-3.4266597	-1.0988188
C	-2.0633360	-2.1550382	-1.5925364
H	-2.6739771	-1.4434991	-2.1476418
C	-1.1285015	0.3265095	-3.1669243
C	-1.7533457	1.4436787	-2.5940501
H	-1.3705823	1.8468930	-1.6552856
C	-2.8404511	2.0412768	-3.2305403
H	-3.3100783	2.9193181	-2.7867002
C	-3.3052877	1.5357706	-4.4449684
H	-4.1397657	2.0179639	-4.9546089
C	-2.6757919	0.4323711	-5.0265471
H	-3.0159211	0.0517903	-5.9893256
C	-1.5907510	-0.1703207	-4.3935807
H	-1.0954694	-1.0138636	-4.8708060
Au	1.3734298	5.0215493	-1.3699558
P	2.1918834	6.3640762	0.3300784
C	0.9252895	3.8829379	-3.0103389
C	1.7940995	2.8262649	-3.3700185
H	2.6492863	2.5875242	-2.7349381
C	1.5949663	2.0891658	-4.5229821
H	2.3023295	1.3009707	-4.7665138
C	0.5066855	2.3346595	-5.3827268
C	0.2391658	1.4808367	-6.5307962
C	1.0043476	0.3187788	-6.7747509
H	1.8283348	0.0648599	-6.1117675
C	0.7155866	-0.5356928	-7.8245163
H	1.3207356	-1.4299955	-7.9777704
C	-0.3601254	-0.2490474	-8.6784062
H	-0.5991286	-0.9149982	-9.5085944
C	-1.1244196	0.8854258	-8.4590104
H	-1.9630654	1.0805788	-9.1246968
C	-0.8549780	1.7699769	-7.3911183
C	-1.6973999	2.9323404	-7.1254955

C	-2.7811118	3.2640092	-7.9680954
H	-2.9715059	2.6703529	-8.8602217
C	-3.6169866	4.3348155	-7.6988881
H	-4.4453614	4.5626670	-8.3707615
C	-3.3830751	5.1255722	-6.5641609
H	-4.0276609	5.9776674	-6.3439346
C	-2.3211032	4.8268480	-5.7276034
H	-2.1492412	5.4589404	-4.8592734
C	-1.4602292	3.7341899	-5.9737112
C	-0.3570978	3.4160088	-5.0729310
C	-0.1247725	4.1524102	-3.8885239
H	-0.7982044	4.9724503	-3.6466819
C	1.0029640	7.1456243	1.4722722
C	-0.3100530	6.6594537	1.5125530
H	-0.5898528	5.8362795	0.8535991
C	-1.2442351	7.2239148	2.3822163
H	-2.2635899	6.8370829	2.4093741
C	-0.8733556	8.2845911	3.2119692
H	-1.6023304	8.7245968	3.8936378
C	0.4260922	8.7955489	3.1531854
H	0.7124719	9.6377984	3.7841347
C	1.3580443	8.2355533	2.2809101
H	2.3585879	8.6636150	2.2112797
C	3.0395127	7.8238710	-0.3773232
C	2.2636856	8.7406821	-1.1043706
H	1.1901557	8.5760881	-1.2135799
C	2.8580920	9.8571934	-1.6867068
H	2.2471270	10.5658562	-2.2473301
C	4.2359534	10.0636693	-1.5604310
H	4.7018525	10.9360234	-2.0203962
C	5.0124872	9.1477697	-0.8502311
H	6.0881176	9.3009796	-0.7527284
C	4.4182788	8.0295807	-0.2587875
H	5.0288204	7.3179794	0.2963970
C	3.4832717	5.5480426	1.3155714
C	4.1080214	4.4308101	0.7426939
H	3.7253092	4.0276664	-0.1961569
C	5.1948467	3.8329386	1.3794125
H	5.6642783	2.9547254	0.9356669
C	5.6595024	4.3382408	2.5940016
H	6.4937055	3.8557461	3.1038482
C	5.0302612	5.4418931	3.1754184
H	5.3701692	5.8222428	4.1383664
C	3.9454569	6.0448373	2.5422784
H	3.4502076	6.8884020	3.0195360

XYZ Coordinates of the optimized monomer 1b

P	0.0045518	1.3798848	-0.1812025
Au	0.7531014	2.4251511	-2.1037598
C	1.4446126	3.3754477	-3.7822839

C	0.8713689	3.1540411	-5.0498810
C	2.5201540	4.2832349	-3.7121675
C	1.3477182	3.8053424	-6.1918518
H	0.0354832	2.4594885	-5.1547173
C	3.0009938	4.9375589	-4.8503632
H	2.9960263	4.4870365	-2.7508368
C	2.4158894	4.7003969	-6.0963417
H	3.8363802	5.6357467	-4.7633237
C	-1.8072091	1.3435081	0.0205620
C	-2.4281549	1.4969413	1.2672906
C	-2.5905173	1.1310459	-1.1237467
C	-3.8187359	1.4250532	1.3684238
H	-1.8244323	1.6786844	2.1570172
C	-3.9783532	1.0530223	-1.0176336
H	-2.1051935	1.0386516	-2.0972596
C	-4.5939333	1.1989360	0.2287430
H	-4.2977205	1.5484601	2.3407165
H	-4.5819761	0.8890272	-1.9109751
H	-5.6803131	1.1454289	0.3101801
C	0.5160416	-0.3610227	0.0027053
C	-0.2717571	-1.3112276	0.6663982
C	1.7722751	-0.7300634	-0.5006332
C	0.2006091	-2.6138209	0.8367156
H	-1.2546747	-1.0327673	1.0472389
C	2.2430075	-2.0308340	-0.3236312
H	2.3730878	0.0069385	-1.0372672
C	1.4587483	-2.9733885	0.3469671
H	-0.4174978	-3.3503340	1.3517673
H	3.2201271	-2.3117736	-0.7179527
H	1.8245228	-3.9923780	0.4792837
C	0.6042992	2.1721428	1.3439681
C	1.0831741	1.4441001	2.4222688
C	0.5713428	3.5780243	1.4233831
C	1.5291572	2.0669429	3.6062250
H	1.1126312	0.3605522	2.3408823
C	0.9879442	4.2073902	2.5795469
H	0.2234385	4.1642682	0.5713288
C	1.4687377	3.4837426	3.6952132
C	2.0432754	1.2806246	4.7231596
H	0.9501962	5.2940775	2.6135113
C	1.8993299	4.1554515	4.9164513
C	2.4641519	1.9350314	5.9134772
C	2.3850283	3.3905001	6.0135460
C	1.8402209	5.5611185	5.0442024
C	2.7857540	4.0730946	7.1832895
C	2.2409678	6.2053426	6.2014502
H	1.4697139	6.1647639	4.2181466
C	2.7190553	5.4521439	7.2833230
H	3.1590222	3.5108274	8.0369305
H	2.1829173	7.2921304	6.2682125

H	3.0377665	5.9471900	8.2012716
C	2.9562945	1.1456316	6.9764819
C	2.1406720	-0.1269110	4.6508417
C	3.0386512	-0.2329970	6.8835393
H	3.4246044	-0.8128465	7.7226409
C	2.6283678	-0.8764810	5.7070529
H	2.6944358	-1.9614375	5.6200690
H	3.2865543	1.6219982	7.8973859
H	1.8347164	-0.6480071	3.7454903
H	2.7896229	5.2092906	-6.9865536
H	0.8824521	3.6126609	-7.1610234

XYZ Coordinates of the optimized dimer 1b

Au	-0.3173153	0.9351932	0.0714612
P	-1.2302636	-0.5146605	1.6373720
C	0.2778678	2.1824082	-1.4413278
C	-0.4496966	3.3528955	-1.7340358
H	-1.2845628	3.6479239	-1.0944011
C	-0.1336193	4.1569841	-2.8323736
H	-0.7157885	5.0595749	-3.0307206
C	0.9261852	3.8104968	-3.6744015
H	1.1750327	4.4359259	-4.5334446
C	1.6675324	2.6585674	-3.4022020
H	2.5024406	2.3816494	-4.0497158
C	1.3463687	1.8594844	-2.3000851
H	1.9441267	0.9653208	-2.1108901
C	-2.9154906	0.0063383	2.0713209
C	-3.5198084	0.9470843	1.2488966
H	-2.9264287	1.3639867	0.4356801
C	-4.8546940	1.3515710	1.4288116
C	-5.4445750	2.3879830	0.5929370
C	-4.6868685	3.0682212	-0.3843353
H	-3.6450694	2.8022612	-0.5530147
C	-5.2427260	4.0738689	-1.1547979
H	-4.6357367	4.5753359	-1.9088346
C	-6.5827326	4.4377226	-0.9617478
H	-7.0303900	5.2336356	-1.5571419
C	-7.3457775	3.7842700	-0.0105678
H	-8.3802278	4.0895473	0.1245995
C	-6.8078555	2.7435720	0.7753984
C	-7.6275619	2.0090177	1.7309432
C	-9.0195271	2.2237928	1.8194546
H	-9.4916872	2.9653575	1.1804129
C	-9.8164768	1.4929166	2.6828927
H	-10.8930010	1.6548910	2.7040109
C	-9.2385661	0.5111089	3.5004644
H	-9.8661889	-0.0870480	4.1609269
C	-7.8736641	0.2900324	3.4420132
H	-7.4461188	-0.4952823	4.0631040
C	-7.0405129	1.0192957	2.5656171

C	-5.6190786	0.7296536	2.4506035
C	-4.9696891	-0.1795508	3.3164283
H	-5.5193098	-0.6151469	4.1488618
C	-3.6442652	-0.5297260	3.1501940
H	-3.1691092	-1.2093480	3.8580316
C	-0.3918219	-0.7338660	3.2389113
C	-0.4938827	0.2901649	4.1933852
H	-1.1204574	1.1602328	3.9912267
C	0.1977612	0.1953082	5.3992503
H	0.1085650	0.9933448	6.1372116
C	1.0042661	-0.9164170	5.6603770
H	1.5453853	-0.9886611	6.6045324
C	1.1170113	-1.9320437	4.7091421
H	1.7466214	-2.8004300	4.9072843
C	0.4230741	-1.8428839	3.5009847
H	0.5129070	-2.6403952	2.7628489
C	-1.4213232	-2.2089312	0.9756459
C	-0.8960967	-2.4926395	-0.2920577
H	-0.3478999	-1.7126778	-0.8251795
C	-1.0867439	-3.7491708	-0.8706777
H	-0.6834373	-3.9558205	-1.8624563
C	-1.7992703	-4.7320126	-0.1829806
H	-1.9582311	-5.7105919	-0.6375202
C	-2.3104895	-4.4618107	1.0905673
H	-2.8630224	-5.2308648	1.6318155
C	-2.1230064	-3.2077877	1.6675766
H	-2.5349148	-3.0027285	2.6553722
Au	-11.9468178	1.0168545	-0.2666452
P	-11.0338629	2.4666252	-1.8324577
C	-12.5419401	-0.2303238	1.2461705
C	-11.8144409	-1.4008417	1.5388779
H	-10.9795611	-1.6959266	0.8992951
C	-12.1304315	-2.2048458	2.6372963
H	-11.5482208	-3.1074037	2.8356936
C	-13.1901753	-1.8582829	3.4793626
H	-13.4390051	-2.4837137	4.3383964
C	-13.9315670	-0.7064130	3.2071100
H	-14.7663935	-0.4293895	3.8546893
C	-13.6104393	0.0925809	2.1049309
H	-14.2081980	0.9867272	1.9157756
C	-9.3486359	1.9456161	-2.2664530
C	-8.7443425	1.0048079	-1.4440473
H	-9.3378136	0.5877685	-0.6309653
C	-7.4093820	0.6004716	-1.6238388
C	-6.8194767	-0.4359346	-0.7879534
C	-7.5771770	-1.1161983	0.1892891
H	-8.6190081	-0.8503689	0.3578873
C	-7.0213312	-2.1218149	0.9597823
H	-7.6283386	-2.6233168	1.7137578
C	-5.6813483	-2.4856712	0.7667487

H	-5.2336564	-3.2815265	1.3621558
C	-4.9183349	-1.8322444	-0.1844376
H	-3.8839341	-2.1375685	-0.3196494
C	-5.4562199	-0.7915484	-0.9703925
C	-4.6365078	-0.0569956	-1.9259154
C	-3.2445686	-0.2719042	-2.0145004
H	-2.7724320	-1.0135249	-1.3755055
C	-2.4475582	0.4588956	-2.8779599
H	-1.3710223	0.2968400	-2.8991057
C	-3.0254620	1.4406763	-3.6955762
H	-2.3978027	2.0387296	-4.3561193
C	-4.3903556	1.6619148	-3.6370507
H	-4.8178344	2.4472502	-4.2581883
C	-5.2235359	0.9327764	-2.7605536
C	-6.6449942	1.2224013	-2.6456261
C	-7.2943687	2.1315921	-3.5114863
H	-6.7447384	2.5670932	-4.3439762
C	-8.6197944	2.4817714	-3.3452543
H	-9.0948964	3.1614306	-4.0530885
C	-11.8725466	2.6858181	-3.4339026
C	-11.7704269	1.6619047	-4.3884756
H	-11.1440773	0.7917244	-4.1862104
C	-12.4619377	1.7568556	-5.5944056
H	-12.3726281	0.9589464	-6.3324902
C	-13.2684543	2.8685286	-5.8555746
H	-13.8093881	2.9408000	-6.7998342
C	-13.3811031	3.8841763	-4.9043556
H	-14.0105306	4.7526640	-5.1025983
C	-12.6874357	3.7948050	-3.6960543
H	-12.7772965	4.5923173	-2.9579537
C	-10.8426994	4.1609155	-1.1708094
C	-11.3679894	4.4446552	0.0968431
H	-11.9160367	3.6646593	0.6300237
C	-11.1773569	5.7011628	0.6754897
H	-11.5805656	5.9078097	1.6672770
C	-10.4647496	6.6840205	-0.0120411
H	-10.3057429	7.6625489	0.4425976
C	-9.9536354	6.4138504	-1.2856053
H	-9.4012549	7.1829710	-1.8268727
C	-10.1410782	5.1598493	-1.8626731
H	-9.7292356	4.9549231	-2.8505058

XYZ Coordinates of the optimized monomer 1c

P	-0.0037189	1.3686995	-0.1406840
Au	0.7378462	2.4203372	-2.0610361
C	1.4146357	3.3825411	-3.7362686
C	0.8270888	3.1848043	-4.9861521
C	2.5010707	4.2856541	-3.6789862
C	1.2637195	3.8349514	-6.1626909
H	-0.0111310	2.4941467	-5.0563164

C	2.9528071	4.9385737	-4.8128705
H	3.0009909	4.4801121	-2.7283304
C	2.3568217	4.7386967	-6.0766024
C	0.6182210	3.5976315	-7.4526444
H	3.7927484	5.6246942	-4.7119643
C	2.8331599	5.4309079	-7.2697637
C	1.0805879	4.2723378	-8.6174037
C	2.2025297	5.2036006	-8.5246484
C	3.9178105	6.3352890	-7.2164279
C	2.6868945	5.8934998	-9.6583165
C	4.3743411	6.9981419	-8.3426759
H	4.4152964	6.5229723	-6.2668610
C	3.7510404	6.7755707	-9.5789774
H	2.2186736	5.7359467	-10.6281382
H	5.2146006	7.6893139	-8.2651204
H	4.0993569	7.2920145	-10.4743085
C	-0.4693446	2.7045423	-7.5823036
C	0.4330922	4.0188624	-9.8471826
C	-1.0871030	2.4737521	-8.7994698
H	-1.9245447	1.7774713	-8.8624364
C	-0.6306332	3.1386030	-9.9465137
H	-0.8396360	2.1771311	-6.7055992
H	0.7715553	4.5242916	-10.7496484
H	-1.1073949	2.9661078	-10.9121596
C	-1.8153310	1.3324215	0.0543978
C	-2.4413572	1.4933818	1.2974334
C	-2.5931488	1.1120035	-1.0920685
C	-3.8324352	1.4228548	1.3923972
H	-1.8414305	1.6802020	2.1886256
C	-3.9812794	1.0350354	-0.9919603
H	-2.1033379	1.0123644	-2.0625857
C	-4.6023752	1.1901352	0.2505389
H	-4.3157234	1.5528992	2.3615517
H	-4.5807322	0.8654123	-1.8869604
H	-5.6891636	1.1388142	0.3267229
C	0.5077230	-0.3721967	0.0377863
C	-0.2732203	-1.3192427	0.7142633
C	1.7531265	-0.7466139	-0.4877715
C	0.1948848	-2.6246613	0.8732702
H	-1.2481079	-1.0365965	1.1123602
C	2.2197668	-2.0503941	-0.3219345
H	2.3479728	-0.0117092	-1.0339475
C	1.4418720	-2.9901937	0.3597313
H	-0.4179269	-3.3591131	1.3974236
H	3.1881446	-2.3358406	-0.7341509
H	1.8034949	-4.0120167	0.4814655
C	0.5943434	2.1639538	1.3824423
C	1.0910405	1.4379140	2.4536819
C	0.5424764	3.5690400	1.4679756
C	1.5372158	2.0618518	3.6369179

H	1.1337982	0.3551622	2.3678598
C	0.9614986	4.1993384	2.6226671
H	0.1774530	4.1543135	0.6225011
C	1.4628960	3.4777527	3.7307418
C	2.0600762	1.2764584	4.7503171
H	0.9071311	5.2851730	2.6619922
C	1.9021611	4.1506062	4.9482567
C	2.4774937	1.9309780	5.9416801
C	2.3979000	3.3864171	6.0414392
C	1.8458949	5.5565473	5.0748462
C	2.8104925	4.0699292	7.2064614
C	2.2578234	6.2015935	6.2277510
H	1.4717791	6.1599551	4.2502285
C	2.7450344	5.4490255	7.3059084
H	3.1951459	3.5086947	8.0556724
H	2.2040396	7.2886675	6.2934663
H	3.0737663	5.9448559	8.2198289
C	2.9668794	1.1417276	7.0060217
C	2.1629279	-0.1306062	4.6762340
C	3.0534751	-0.2365341	6.9118458
H	3.4365338	-0.8164713	7.7521756
C	2.6501846	-0.8798186	5.7328511
H	2.7187778	-1.9645377	5.6451327
H	3.2882123	1.6178408	7.9301611
H	1.8596544	-0.6518788	3.7700821

XYZ Coordinates of the optimized monomer 2a

P	-0.0262625	1.3432323	-0.1371930
Au	0.6985341	2.3727171	-2.0750033
C	-1.8398767	1.2468301	0.0175682
C	-2.5058132	1.4318671	1.2359453
C	-2.5781453	0.9572678	-1.1400002
C	-3.8960909	1.3165734	1.2962194
H	-1.9385746	1.6725621	2.1355831
C	-3.9649630	0.8352119	-1.0742655
H	-2.0601214	0.8407432	-2.0936510
C	-4.6257595	1.0143443	0.1443998
H	-4.4105711	1.4665188	2.2463536
H	-4.5323603	0.6116475	-1.9782562
H	-5.7118546	0.9274321	0.1937665
C	0.5348046	-0.3801885	0.0551216
C	-0.2625294	-1.3710790	0.6431987
C	1.8237328	-0.7023501	-0.3959833
C	0.2305824	-2.6690349	0.7878428
H	-1.2708128	-1.1291942	0.9803203
C	2.3151146	-1.9980622	-0.2429160
H	2.4327385	0.0652462	-0.8775298
C	1.5190373	-2.9827376	0.3490123
H	-0.3955332	-3.4379454	1.2421734
H	3.3168810	-2.2430255	-0.5976531

H	1.9003101	-3.9987028	0.4591221
C	1.3570421	3.3265690	-3.7705604
C	2.2319177	4.3799349	-3.6639425
C	0.9171373	2.9355720	-5.0923408
C	2.7192070	5.1070441	-4.7966330
H	2.5903189	4.7034565	-2.6831130
C	1.3726564	3.6321567	-6.2582824
C	0.0246796	1.8496574	-5.2645462
C	3.6193914	6.1864301	-4.6305820
C	2.2933548	4.7445119	-6.1088651
C	0.9061505	3.2057740	-7.5234789
H	-0.3061979	1.3227293	-4.3659723
C	-0.4145655	1.4525497	-6.5130743
C	4.0929071	6.8971737	-5.7174468
H	3.9348038	6.4482181	-3.6180918
C	2.7941722	5.4896602	-7.2006294
C	0.0314842	2.1416811	-7.6556796
H	1.2400828	3.7221499	-8.4229168
H	-1.1013376	0.6106622	-6.6134291
C	3.6740143	6.5429879	-7.0143925
H	4.7863381	7.7270359	-5.5737459
H	2.4882014	5.2380241	-8.2155501
H	-0.3084320	1.8376714	-8.6468081
H	4.0431172	7.0993078	-7.8771506
C	0.5181594	2.1788569	1.3884557
C	0.9148603	1.4786365	2.5349568
C	0.5197327	3.5823088	1.3961701
C	1.2998432	2.1772775	3.6810313
H	0.9296434	0.3884706	2.5296184
C	0.8963093	4.2757551	2.5451682
H	0.2336688	4.1252447	0.4932414
C	1.2873555	3.5737398	3.6891052
H	1.6129840	1.6277903	4.5697122
H	0.8957418	5.3662699	2.5443834
H	1.5911299	4.1165909	4.5850286

XYZ Coordinates of the optimized monomer 2b

P	-0.1167433	1.3546544	-0.0345195
Au	0.7196989	2.3861157	-1.9371628
C	1.4550146	3.2688655	-3.6325521
C	0.7266751	4.2613186	-4.3179009
C	2.7108117	2.9100087	-4.1610101
C	1.2265839	4.8660637	-5.4755161
H	-0.2515461	4.5712570	-3.9451443
C	3.2160283	3.5119756	-5.3175854
H	3.3099440	2.1448677	-3.6634335
C	2.4749043	4.4935846	-5.9798806
H	4.1931749	3.2126672	-5.7028818
C	-1.9360220	1.2653160	-0.0398032
C	-2.7275933	1.6550562	1.0480186

C	-2.5556298	0.8508275	-1.2308405
C	-4.1196262	1.6044312	0.9541223
H	-2.2610161	2.0046319	1.9679344
C	-3.9455955	0.7886042	-1.3154087
H	-1.9432190	0.5967321	-2.0980734
C	-4.7304469	1.1635624	-0.2213363
H	-4.7282460	1.9133974	1.8048658
H	-4.4168274	0.4632848	-2.2435394
H	-5.8181957	1.1253683	-0.2909259
C	0.4765331	-0.3705093	0.0819618
C	-0.3400210	-1.4821392	-0.1561803
C	1.8364203	-0.5595857	0.3699055
C	0.1969423	-2.7696137	-0.0961744
H	-1.3990943	-1.3460160	-0.3767195
C	2.3659235	-1.8462803	0.4372325
H	2.4791014	0.3044443	0.5475765
C	1.5474728	-2.9552475	0.2034812
H	-0.4460408	-3.6308307	-0.2824585
H	3.4226682	-1.9844509	0.6693211
H	1.9638623	-3.9620105	0.2524667
H	2.8674079	4.9645557	-6.8827960
H	0.6384988	5.6321300	-5.9856862
C	0.3890998	2.1402592	1.5324482
C	0.9937473	3.3634526	1.3932528
C	0.2251418	1.5600306	2.8483321
C	1.4719814	4.1098055	2.5093747
H	1.1280499	3.7809134	0.3915631
C	0.7101182	2.2738167	3.9912243
C	-0.4064074	0.3100695	3.0462560
C	2.0824665	5.3708004	2.3159118
C	1.3416638	3.5714728	3.8227618
C	0.5479166	1.6866120	5.2666741
H	-0.7847311	-0.2372974	2.1868256
C	-0.5507097	-0.2358531	4.3073499
C	2.5565119	6.0972972	3.3911786
H	2.1715053	5.7566621	1.2989631
C	1.8385435	4.3379383	4.9007009
C	-0.0651484	0.4574920	5.4285985
H	0.9107569	2.2105274	6.1494412
H	-1.0396262	-1.2029599	4.4276664
C	2.4312378	5.5721034	4.6913842
H	3.0255959	7.0692929	3.2366187
H	1.7604500	3.9628862	5.9199870
H	-0.1729935	0.0310834	6.4265454
H	2.8051296	6.1409426	5.5436360

XYZ Coordinates of the optimized monomer 2c

P	-0.1425769	1.3261975	-0.0402626
Au	0.6738037	2.3412640	-1.9583129
C	-1.9634498	1.3099861	-0.0101582

C	-2.7164488	1.7108705	1.1006230
C	-2.6233179	0.9402111	-1.1940871
C	-4.1109732	1.7178479	1.0344947
H	-2.2176845	2.0254909	2.0163369
C	-4.0157372	0.9361949	-1.2517893
H	-2.0399867	0.6741642	-2.0773768
C	-4.7625290	1.3237838	-0.1356903
H	-4.6893875	2.0359080	1.9027596
H	-4.5178995	0.6474180	-2.1757242
H	-5.8520020	1.3321136	-0.1839088
C	0.3794383	-0.4219023	0.0640723
C	-0.4967356	-1.4960062	-0.1316170
C	1.7390170	-0.6714650	0.3031702
C	-0.0187987	-2.8068305	-0.0759506
H	-1.5556723	-1.3117990	-0.3147107
C	2.2091448	-1.9811925	0.3686187
H	2.4282048	0.1631146	0.4432119
C	1.3313092	-3.0525683	0.1788387
H	-0.7076727	-3.6386421	-0.2290476
H	3.2659448	-2.1671868	0.5637794
H	1.7016737	-4.0771948	0.2262746
C	0.4232632	2.1030322	1.5097257
C	1.0407907	3.3174613	1.3506198
C	0.2848400	1.5306278	2.8319013
C	1.5618645	4.0596167	2.4498566
H	1.1499318	3.7321105	0.3447790
C	0.8168308	2.2383262	3.9578197
C	-0.3698253	0.2965563	3.0533829
C	2.1810529	5.3130404	2.2360867
C	1.4661270	3.5240066	3.7672881
C	0.6787905	1.6591662	5.2397415
H	-0.7861618	-0.2446049	2.2079327
C	-0.4904384	-0.2410668	4.3205364
C	2.7001341	6.0332432	3.2945363
H	2.2390233	5.6995084	1.2171248
C	2.0111865	4.2825954	4.8274306
C	0.0436486	0.4445577	5.4243177
H	1.0764552	2.1789478	6.1098513
H	-0.9985935	-1.1957289	4.4590516
C	2.6137223	5.5083597	4.5980221
H	3.1745703	6.9999934	3.1244403
H	1.9635804	3.9076906	5.8486090
H	-0.0448599	0.0243012	6.4267557
H	3.0252526	6.0711856	5.4367547
C	1.3789225	3.2572533	-3.6559283
C	2.2846873	4.2845223	-3.5560510
C	0.9271406	2.8720148	-4.9753271
C	2.7928926	4.9905931	-4.6929794
H	2.6538442	4.6033358	-2.5775918
C	1.4002419	3.5499732	-6.1452774

C	0.0038343	1.8113376	-5.1410679
C	3.7250843	6.0435646	-4.5341337
C	2.3541840	4.6348069	-6.0028064
C	0.9172509	3.1331220	-7.4074669
H	-0.3390582	1.2977888	-4.2392667
C	-0.4499949	1.4221511	-6.3867555
C	4.2175305	6.7348508	-5.6252049
H	4.0505024	6.3009311	-3.5236435
C	2.8752090	5.3592245	-7.0990737
C	0.0117002	2.0943745	-7.5332149
H	1.2625868	3.6369353	-8.3097299
H	-1.1605286	0.5996524	-6.4820475
C	3.7862327	6.3869059	-6.9197430
H	4.9358999	7.5441514	-5.4867577
H	2.5603736	5.1112594	-8.1121727
H	-0.3408521	1.7974749	-8.5221221
H	4.1704008	6.9275958	-7.7858525

XYZ Coordinates of the optimized monomer 3a

P	0.0011236	1.3651130	-0.2276506
Au	0.7416646	2.3926914	-2.0856960
C	-1.8125175	1.2721428	-0.1030999
C	-2.4853488	1.4513874	1.1123119
C	-2.5407814	0.9831575	-1.2667898
C	-3.8755715	1.3325912	1.1629043
H	-1.9247424	1.6916183	2.0161411
C	-3.9276627	0.8585536	-1.2100726
H	-2.0171465	0.8680473	-2.2175018
C	-4.5963726	1.0327386	0.0051049
H	-4.3966296	1.4788091	2.1098175
H	-4.4889155	0.6363960	-2.1181337
H	-5.6825344	0.9440126	0.0468129
C	0.5694504	-0.3534720	-0.0299694
C	-0.2340687	-1.3395741	0.5576728
C	1.8665832	-0.6739075	-0.4568665
C	0.2624819	-2.6333864	0.7256530
H	-1.2484770	-1.0981861	0.8760270
C	2.3604013	-1.9654865	-0.2807317
H	2.4809455	0.0906130	-0.9363042
C	1.5589870	-2.9460755	0.3108598
H	-0.3676176	-3.3998352	1.1783833
H	3.3686570	-2.2102194	-0.6161521
H	1.9429834	-3.9586899	0.4398455
C	0.5382311	2.2196932	1.2875085
C	0.9185373	1.5236294	2.4420273
C	0.5439526	3.6230825	1.2853578
C	1.2927395	2.2280558	3.5879360
H	0.9298439	0.4334698	2.4434131
C	0.9124516	4.3215112	2.4336879
H	0.2664743	4.1629904	0.3780838

C	1.2872715	3.6245240	3.5860687
H	1.5934154	1.6828840	4.4833851
H	0.9175129	5.4117965	2.4254535
H	1.5841228	4.1719096	4.4814470
N	1.4212182	3.3623370	-3.7278637
C	1.0493635	3.1359470	-5.0433189
C	2.3069148	4.4285239	-3.7291807
C	0.1749221	2.1687323	-5.5538887
C	1.7013183	4.0654716	-5.9107181
C	2.9585954	5.0278572	-2.6438670
C	2.5138365	4.9010106	-5.0613500
C	-0.0447450	2.1361002	-6.9288026
H	-0.3162100	1.4571444	-4.8866084
C	1.4637312	4.0118668	-7.2899438
C	3.8123910	6.0990882	-2.8961451
H	2.8012602	4.6580533	-1.6282179
C	3.3776637	5.9800156	-5.2884869
C	0.5916935	3.0486116	-7.7930234
H	-0.7225356	1.3889124	-7.3449831
H	1.9556106	4.7161745	-7.9635246
C	4.0225287	6.5745958	-4.2056335
H	4.3296914	6.5784857	-2.0634249
H	3.5441004	6.3517580	-6.3012740
H	0.3981584	2.9973720	-8.8650979
H	4.6974986	7.4153512	-4.3698116

XYZ Coordinates of the optimized dimer 3a

Au	0.0319442	0.6012727	0.1439079
P	1.7265048	0.2171628	1.5837900
N	-1.3676430	0.9474799	-1.3008442
C	-1.4611872	0.2469957	-2.4912828
C	-0.6691991	-0.8170841	-2.9448071
H	0.1576892	-1.1924165	-2.3383205
C	-0.9613821	-1.3730526	-4.1894067
H	-0.3564377	-2.2034998	-4.5585036
C	-2.0234823	-0.8863160	-4.9774152
H	-2.2403790	-1.3567600	-5.9372207
C	-2.8147759	0.1698823	-4.5306242
H	-3.6560275	0.5199866	-5.1309873
C	-2.5405643	0.7466503	-3.2853647
C	-3.1276484	1.8195790	-2.5233984
C	-4.1939227	2.7000913	-2.7413574
H	-4.7925345	2.6331628	-3.6512427
C	-4.5042186	3.6403755	-1.7611964
H	-5.3503838	4.3117249	-1.9058790
C	-3.7576666	3.7078683	-0.5677850
H	-4.0281072	4.4434913	0.1913562
C	-2.6853917	2.8498096	-0.3311074
H	-2.1135095	2.9006781	0.5959644
C	-2.3717844	1.9009211	-1.3113908

C	2.8959268	-1.0083769	0.9242676
C	3.1422335	-1.0212310	-0.4574153
H	2.6097900	-0.3270377	-1.1104462
C	4.0639889	-1.9197005	-0.9936713
H	4.2517769	-1.9271243	-2.0679341
C	4.7374598	-2.8142553	-0.1551801
H	5.4529012	-3.5218122	-0.5762843
C	4.4900430	-2.8072693	1.2203061
H	5.0120534	-3.5061387	1.8750183
C	3.5718155	-1.9057539	1.7626503
H	3.3806711	-1.9070983	2.8359068
C	2.6975856	1.7174523	1.9155147
C	4.0711502	1.6554266	2.1884422
H	4.5952978	0.6996235	2.1590699
C	4.7719721	2.8233702	2.4944309
H	5.8416182	2.7732243	2.7011043
C	4.1052330	4.0516843	2.5348266
H	4.6558317	4.9621744	2.7744407
C	2.7354863	4.1163677	2.2596503
H	2.2153055	5.0746868	2.2834611
C	2.0329849	2.9530637	1.9434136
H	0.9674950	3.0012643	1.7124165
C	1.2579359	-0.4151016	3.2224476
C	1.6617538	0.2129660	4.4071829
H	2.2917269	1.1014967	4.3719892
C	1.2494844	-0.2970862	5.6409574
H	1.5613482	0.1992337	6.5605902
C	0.4428320	-1.4354873	5.6946301
H	0.1198235	-1.8308517	6.6584389
C	0.0463999	-2.0684347	4.5119386
H	-0.5840532	-2.9564632	4.5518833
C	0.4458822	-1.5580172	3.2789491
H	0.1221520	-2.0458968	2.3580384
Au	-5.3462413	0.0098854	-0.2580694
P	-4.2758143	-0.4630569	1.6660105
N	-6.3379024	0.3237517	-2.0135687
C	-6.1172855	-0.3915757	-3.1753860
C	-5.3711006	-1.5650898	-3.3496573
H	-4.8412892	-2.0148096	-2.5077354
C	-5.3025631	-2.1207411	-4.6232620
H	-4.7133612	-3.0252060	-4.7802649
C	-5.9542834	-1.5213670	-5.7211397
H	-5.8725112	-1.9773980	-6.7089938
C	-6.6970939	-0.3525160	-5.5557370
H	-7.2004876	0.1062291	-6.4097364
C	-6.7911771	0.2205342	-4.2789830
C	-7.4654491	1.3742994	-3.7365484
C	-8.2790204	2.3792526	-4.2791851
H	-8.5217461	2.3834399	-5.3441725
C	-8.7755631	3.3769365	-3.4406663

H	-9.4100247	4.1648880	-3.8495389
C	-8.4660192	3.3779713	-2.0637467
H	-8.8636851	4.1710458	-1.4276153
C	-7.6585571	2.3923500	-1.5019491
H	-7.4042582	2.4067087	-0.4406232
C	-7.1554338	1.3871053	-2.3390329
C	-3.0756647	-1.8114211	1.4304386
C	-2.3901309	-1.8853362	0.2081749
H	-2.5743559	-1.1398981	-0.5645495
C	-1.4838091	-2.9203204	-0.0229644
H	-0.9549961	-2.9690763	-0.9749447
C	-1.2757665	-3.8999275	0.9525105
H	-0.5799402	-4.7184827	0.7640044
C	-1.9712715	-3.8386525	2.1638519
H	-1.8204007	-4.6093796	2.9204947
C	-2.8625701	-2.7920147	2.4092031
H	-3.4018881	-2.7518803	3.3558605
C	-3.3898021	0.9344336	2.4081401
C	-2.0589504	0.8332731	2.8217587
H	-1.5210505	-0.1058870	2.7093344
C	-1.4239809	1.9377244	3.3959410
H	-0.3882398	1.8534271	3.7225374
C	-2.1178090	3.1369149	3.5635982
H	-1.6198387	3.9975971	4.0122495
C	-3.4544405	3.2350419	3.1586550
H	-3.9986447	4.1711742	3.2871141
C	-4.0870527	2.1405961	2.5737389
H	-5.1207288	2.2256191	2.2346010
C	-5.3861878	-1.0461859	2.9860048
C	-5.1166435	-0.7853135	4.3369902
H	-4.2516794	-0.1844476	4.6183714
C	-5.9624578	-1.2918563	5.3262210
H	-5.7514526	-1.0842919	6.3759535
C	-7.0756136	-2.0596620	4.9717789
H	-7.7370318	-2.4504325	5.7461570
C	-7.3464711	-2.3210192	3.6244182
H	-8.2178792	-2.9143719	3.3451898
C	-6.5067744	-1.8130596	2.6328438
H	-6.7222935	-2.0052446	1.5800058

XYZ Coordinates of the optimized monomer 3b

P	-0.2887370	1.2139917	-0.1511104
Au	0.1747949	2.3392179	-2.1039983
C	-2.0516543	1.0981047	0.2155955
C	-2.8648020	2.1635025	-0.2026364
C	-2.6230596	-0.0204135	0.8359439
C	-4.2346263	2.1324471	0.0503184
H	-2.4172321	3.0113283	-0.7247542
C	-3.9959757	-0.0482737	1.0792674
H	-1.9993875	-0.8646566	1.1259385

C	-4.7992198	1.0303603	0.6989797
H	-4.8637389	2.9638880	-0.2682626
H	-4.4403181	-0.9163865	1.5670732
H	-5.8720357	1.0044203	0.8934365
N	0.4270611	2.0187866	1.1911935
C	1.8393751	2.0859341	1.2477410
C	-0.0784800	2.5029587	2.4204863
C	2.7751566	1.6926174	0.2899061
C	2.2296171	2.6021835	2.5037593
C	-1.3920563	2.6467903	2.8750843
C	1.0199731	2.8713598	3.2438120
C	4.1241866	1.8365751	0.6113588
H	2.4816898	1.2952466	-0.6813498
C	3.5891215	2.7368761	2.8047939
C	-1.5884790	3.1504682	4.1621912
H	-2.2492353	2.3857961	2.2645310
C	0.7959363	3.3776880	4.5276258
C	4.5301580	2.3509889	1.8534052
H	4.8749825	1.5402529	-0.1213135
H	3.9058314	3.1323473	3.7707161
C	-0.5119820	3.5125837	4.9850836
H	-2.6090577	3.2672223	4.5281406
H	1.6383574	3.6614825	5.1597540
H	5.5937799	2.4464978	2.0731866
H	-0.7026129	3.9051333	5.9841512
N	0.3166475	-0.3910010	0.0410704
C	0.7390093	-0.9633895	1.2678973
C	1.0144255	-1.0622680	-0.9960799
C	0.3239059	-0.6755554	2.5679342
C	1.7150104	-1.9558451	1.0060277
C	0.9068146	-0.9005304	-2.3762319
C	1.8870418	-2.0200198	-0.4276755
C	0.9272495	-1.3765294	3.6126415
H	-0.4377512	0.0687708	2.7860247
C	2.2996494	-2.6524743	2.0680547
C	1.7266909	-1.6856643	-3.1880137
H	0.2116866	-0.1844023	-2.8152241
C	2.6907825	-2.8062196	-1.2597847
C	1.9070966	-2.3511314	3.3704022
H	0.6238522	-1.1583461	4.6367854
H	3.0527631	-3.4178705	1.8775989
C	2.6120229	-2.6265407	-2.6391654
H	1.6671255	-1.5680135	-4.2701161
H	3.3669666	-3.5488143	-0.8342255
H	2.3582955	-2.8807168	4.2097452
H	3.2342658	-3.2293018	-3.3011313
C	0.5189323	3.4735643	-3.7704601
C	1.0137517	4.7882552	-3.6699627
C	0.2846300	2.9653761	-5.0629874
C	1.2647766	5.5602231	-4.8080381

H	1.2101818	5.2214682	-2.6874538
C	0.5347514	3.7332860	-6.2041068
H	-0.1006292	1.9513969	-5.1884137
C	1.0262462	5.0347997	-6.0801380
H	1.6492026	6.5766497	-4.7006853
H	0.3450567	3.3131390	-7.1940405
H	1.2223676	5.6358529	-6.9695996

XYZ Coordinates of the optimized dimer 3b

Au	-0.2551942	0.6122959	-0.2824286
P	1.3173198	2.2317187	0.1977895
N	0.8944386	3.0464244	1.6605757
N	1.5983979	3.4962961	-0.9204651
C	-1.6120074	-0.8934908	-0.5385270
C	-1.2975102	-2.0651929	-1.2530849
H	-0.3024498	-2.1890725	-1.6844285
C	-2.2381011	-3.0849125	-1.4264336
H	-1.9676120	-3.9833889	-1.9849370
C	-3.5199788	-2.9578483	-0.8862372
H	-4.2545882	-3.7536332	-1.0201129
C	-3.8529164	-1.8044591	-0.1721431
H	-4.8518103	-1.6963893	0.2557299
C	-2.9097012	-0.7869101	-0.0015537
H	-3.1933322	0.1034492	0.5631369
C	1.6397008	3.4396739	2.8001187
C	2.9354013	3.1045384	3.2066869
H	3.5684966	2.4359382	2.6342362
C	3.4175712	3.6635157	4.3911410
H	4.4273764	3.4095019	4.7145063
C	2.6390415	4.5332333	5.1688733
H	3.0482645	4.9502088	6.0891169
C	1.3459266	4.8583874	4.7702449
H	0.7296945	5.5285507	5.3710887
C	0.8413904	4.3123252	3.5857459
C	-0.4334170	4.4487840	2.9252869
C	-1.5957939	5.1652661	3.2298716
H	-1.6400510	5.7934362	4.1203064
C	-2.6940098	5.0621634	2.3801992
H	-3.6057437	5.6170892	2.6005469
C	-2.6381401	4.2473589	1.2392224
H	-3.5093397	4.1728023	0.5883345
C	-1.4830350	3.5386385	0.9079950
H	-1.4552787	2.9062666	0.0191121
C	-0.3834150	3.6493788	1.7600383
C	1.0356329	3.5654160	-2.2268094
C	0.3250287	2.6068730	-2.9480207
H	0.0984730	1.6240869	-2.5297219
C	-0.0966839	2.9416607	-4.2350585
H	-0.6596163	2.2058421	-4.8100753
C	0.1886116	4.1944781	-4.7996233

H	-0.1600305	4.4292766	-5.8049601
C	0.9107108	5.1414363	-4.0827279
H	1.1432758	6.1117529	-4.5177199
C	1.3414519	4.8263248	-2.7898353
C	2.1131568	5.5584154	-1.8159716
C	2.6782388	6.8362224	-1.8234153
H	2.5381606	7.4848281	-2.6842730
C	3.4013181	7.2627524	-0.7145662
H	3.8348153	8.2627193	-0.7015663
C	3.5704151	6.4163447	0.3909302
H	4.1459920	6.7580670	1.2516459
C	3.0110908	5.1385330	0.4213645
H	3.1691287	4.5074308	1.2899102
C	2.2713626	4.7236889	-0.6846664
C	2.9301001	1.4838075	0.5175770
C	2.9530872	0.3270763	1.3143288
H	2.0240092	-0.0594274	1.7372601
C	4.1605411	-0.3195390	1.5645345
H	4.1774583	-1.2121335	2.1903393
C	5.3443478	0.1700361	1.0034321
H	6.2892619	-0.3388588	1.1970942
C	5.3155875	1.2979114	0.1803254
H	6.2356653	1.6700881	-0.2712383
C	4.1102355	1.9556988	-0.0690528
H	4.0906730	2.8360759	-0.7092533
Au	0.8331594	11.4751770	-3.7952195
P	-0.7399219	9.8563803	-4.2752887
N	-0.3173173	9.0412959	-5.7381003
N	-1.0224736	8.5921547	-3.1568851
C	2.1893792	12.9816362	-3.5395852
C	1.8748484	14.1525783	-2.8237837
H	0.8801212	14.2755569	-2.3913504
C	2.8147457	15.1730510	-2.6509676
H	2.5441708	16.0711955	-2.0919153
C	4.0962864	15.0470231	-3.1922686
H	4.8305225	15.8431678	-3.0585881
C	4.4294081	13.8942889	-3.9073846
H	5.4280277	13.7871473	-4.3361147
C	3.4866267	12.8763186	-4.0779484
H	3.7704324	11.9865114	-4.6434718
C	-1.0628314	8.6483127	-6.8776644
C	-2.3592463	8.9822026	-7.2830985
H	-2.9927888	9.6495053	-6.7095738
C	-2.8418226	8.4230907	-8.4673218
H	-3.8523089	8.6758544	-8.7895781
C	-2.0628371	7.5548006	-9.2461774
H	-2.4722343	7.1379511	-10.1663843
C	-0.7690209	7.2309858	-8.8488312
H	-0.1525866	6.5619872	-9.4507772
C	-0.2643383	7.7766558	-7.6641906

C	1.0105549	7.6399883	-7.0040392
C	2.1724546	6.9229618	-7.3090337
H	2.2163124	6.2955092	-8.1999622
C	3.2705557	7.0243637	-6.4590630
H	4.1819237	6.4688800	-6.6795287
C	3.2151024	7.8385326	-5.3176467
H	4.0863200	7.9121271	-4.6666591
C	2.0606025	8.5482673	-4.9862620
H	2.0335041	9.1805300	-4.0972218
C	0.9607656	8.4386170	-5.8382291
C	-0.4601990	8.5217993	-1.8504227
C	0.2513683	9.4792635	-1.1287687
H	0.4792268	10.4618543	-1.5469545
C	0.6722070	9.1434526	0.1583138
H	1.2363226	9.8781552	0.7336215
C	0.3850305	7.8908164	0.7223884
H	0.7331082	7.6551812	1.7276866
C	-0.3381597	6.9450047	0.0050844
H	-0.5724653	5.9749178	0.4396124
C	-0.7677703	7.2609921	-1.2879327
C	-1.5394985	6.5299703	-2.2626124
C	-2.1045515	5.2521264	-2.2571160
H	-1.9639722	4.6018608	-1.3976691
C	-2.8275565	4.8270913	-3.3665879
H	-3.2604101	3.8269049	-3.3814201
C	-2.9969881	5.6750993	-4.4707644
H	-3.5730727	5.3349388	-5.3317557
C	-2.4372131	6.9526936	-4.4995307
H	-2.5952538	7.5851528	-5.3670897
C	-1.6968816	7.3657273	-3.3932723
C	-2.3529842	10.6039383	-4.5946121
C	-2.3780158	11.7588683	-5.3939031
H	-1.4497336	12.1459276	-5.8181067
C	-3.5867318	12.4025805	-5.6455859
H	-3.6056163	13.2930327	-6.2743726
C	-4.7695849	11.9122873	-5.0830275
H	-5.7157892	12.4176845	-5.2794651
C	-4.7384922	10.7874801	-4.2558244
H	-5.6575350	10.4151412	-3.8022599
C	-3.5319743	10.1323117	-4.0053851
H	-3.5105534	9.2536217	-3.3628929

XYZ Coordinates of the optimized monomer 3c

P	-0.2367896	1.1063494	-0.1225654
Au	0.3111735	2.2581137	-1.9569645
C	-1.9958776	0.9897959	0.2344220
C	-2.7926397	2.1051874	-0.0658299
C	-2.5736975	-0.1706746	0.7660321
C	-4.1579122	2.0739076	0.2089444

H	-2.3372991	2.9923089	-0.5096942
C	-3.9424513	-0.1966021	1.0322508
H	-1.9572052	-1.0446693	0.9721855
C	-4.7310911	0.9258999	0.7637062
H	-4.7766638	2.9423823	-0.0171043
H	-4.3950214	-1.0968816	1.4487868
H	-5.8006794	0.9005259	0.9749284
N	0.8721076	3.3988374	-3.5196565
C	0.3588334	3.3815824	-4.8065743
C	1.9505898	4.2727606	-3.5151668
C	-0.7267725	2.6534487	-5.3073982
C	1.1115813	4.2547590	-5.6500181
C	2.7887559	4.6211850	-2.4491161
C	2.1395770	4.8292659	-4.8157634
C	-1.0547912	2.8005008	-6.6533790
H	-1.3023287	1.9931297	-4.6547428
C	0.7606994	4.3856893	-6.9994076
C	3.8197954	5.5249720	-2.6934126
H	2.6391977	4.1935892	-1.4560499
C	3.1830811	5.7379015	-5.0342194
C	-0.3196920	3.6578910	-7.4949878
H	-1.8983757	2.2427639	-7.0632150
H	1.3259301	5.0496459	-7.6561522
C	4.0184735	6.0805410	-3.9727122
H	4.4845206	5.8086431	-1.8759455
H	3.3417736	6.1715540	-6.0233267
H	-0.6022193	3.7515505	-8.5441537
H	4.8347624	6.7863608	-4.1310865
N	0.4978773	1.8514594	1.2348809
C	1.8664060	2.2024683	1.1450853
C	-0.0451051	2.5110573	2.3633905
C	2.8237955	1.7593718	0.2314517
C	2.1807008	3.1114997	2.1794002
C	-1.3168049	2.4345122	2.9363225
C	0.9759997	3.3021902	2.9546270
C	4.1114714	2.2849394	0.3466064
H	2.5982355	1.0309448	-0.5460865
C	3.4803455	3.6187909	2.2802544
C	-1.5616111	3.1871154	4.0868122
H	-2.1040438	1.8123118	2.5237592
C	0.7050180	4.0467341	4.1063615
C	4.4364922	3.2072066	1.3537252
H	4.8759082	1.9685980	-0.3624970
H	3.7395133	4.3256242	3.0691604
C	-0.5693123	3.9913695	4.6653533
H	-2.5501359	3.1382361	4.5445108
H	1.4865506	4.6552788	4.5626453
H	5.4525066	3.5973956	1.4145281
H	-0.7952263	4.5662348	5.5635696
N	0.3626176	-0.4962161	-0.0193875

C	0.7862933	-1.1389281	1.1720676
C	0.9587996	-1.1836141	-1.1094682
C	0.4413338	-0.8688468	2.4964887
C	1.6677141	-2.1951005	0.8354677
C	0.8020848	-0.9754853	-2.4790676
C	1.7785965	-2.2212375	-0.6061058
C	1.0159413	-1.6631710	3.4897806
H	-0.2471114	-0.0736254	2.7709462
C	2.2266363	-2.9814953	1.8480448
C	1.5250853	-1.7946854	-3.3470777
H	0.1391065	-0.2056441	-2.8726583
C	2.4850215	-3.0392998	-1.4944114
C	1.9009851	-2.7054663	3.1740356
H	0.7656648	-1.4653228	4.5322802
H	2.9053490	-3.7985079	1.6009715
C	2.3614270	-2.8126589	-2.8632685
H	1.4259585	-1.6408223	-4.4215720
H	3.1201640	-3.8427972	-1.1194805
H	2.3309073	-3.3071306	3.9750151
H	2.9087061	-3.4386779	-3.5682692