Electronic Supplementary Information (ESI)

Tuning the Fluorescence Emission in Mononuclear Heteroleptic Trigonal Silver(I) Complexes

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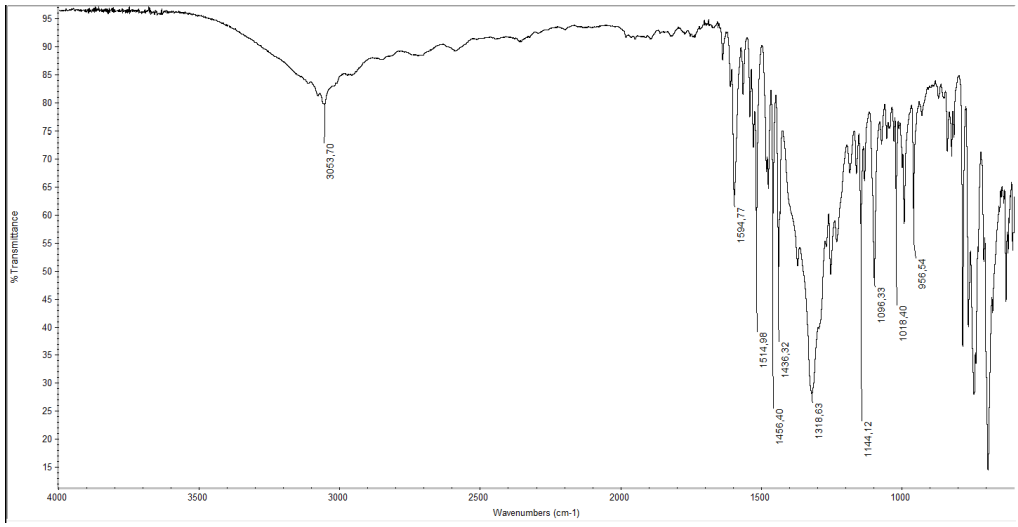


Figure S1. Infrared spectrum (ATR) of [Ag(N∩N)(PPh_3)](NO_3) (**1**).

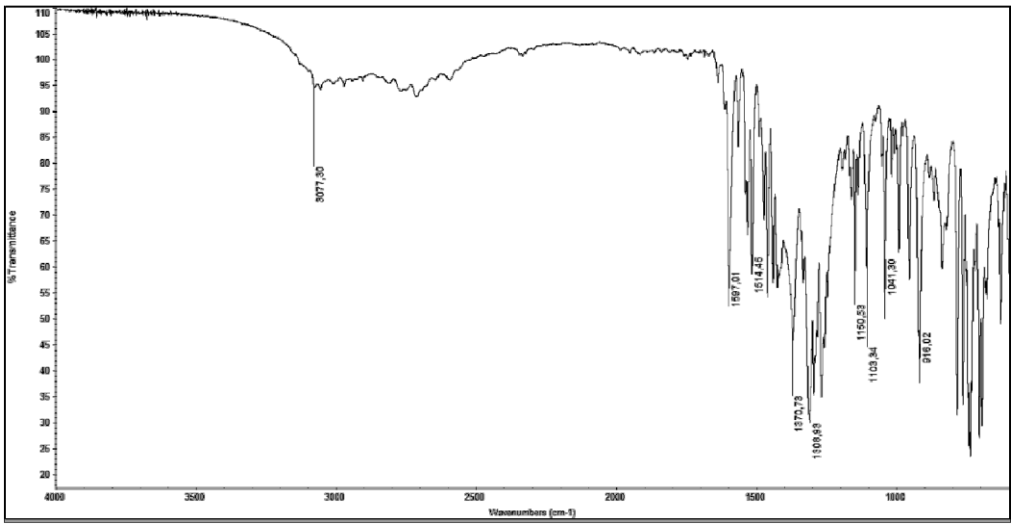


Figure S2. Infrared spectrum (ATR) of [Ag(N∩N)(PMe_2Ph)](NO_3) (**2**).

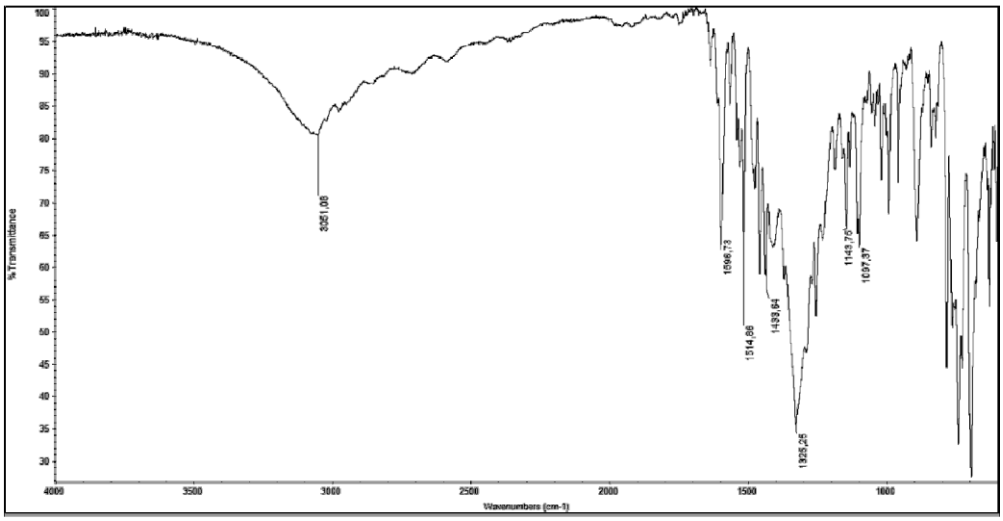


Figure S3. Infrared spectrum (ATR) of [Ag(N∩N)($PMePh_2$)](NO_3) (**3**).

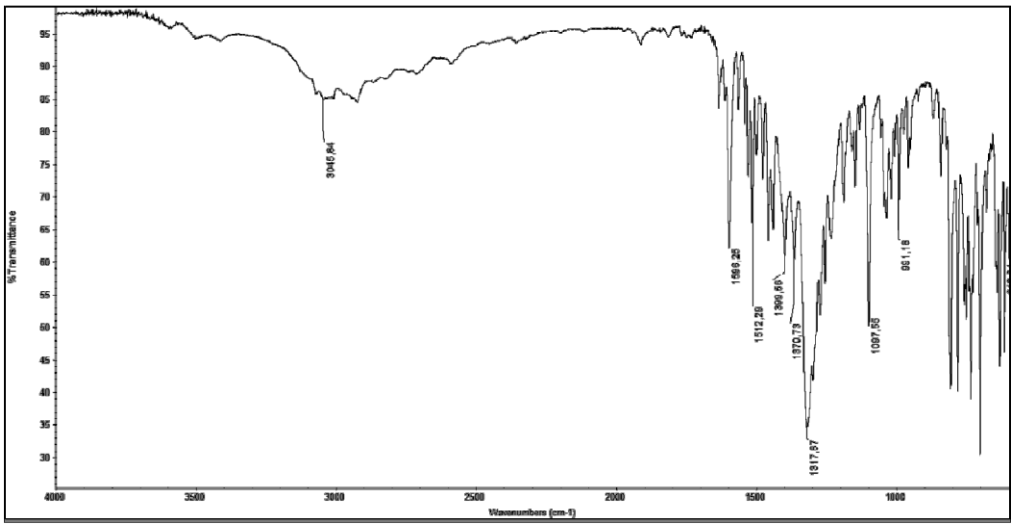


Figure S4. Infrared spectrum (ATR) of [Ag(N∩N)(P(*p*-tolyl)$_3$)](NO$_3$) (**4**).

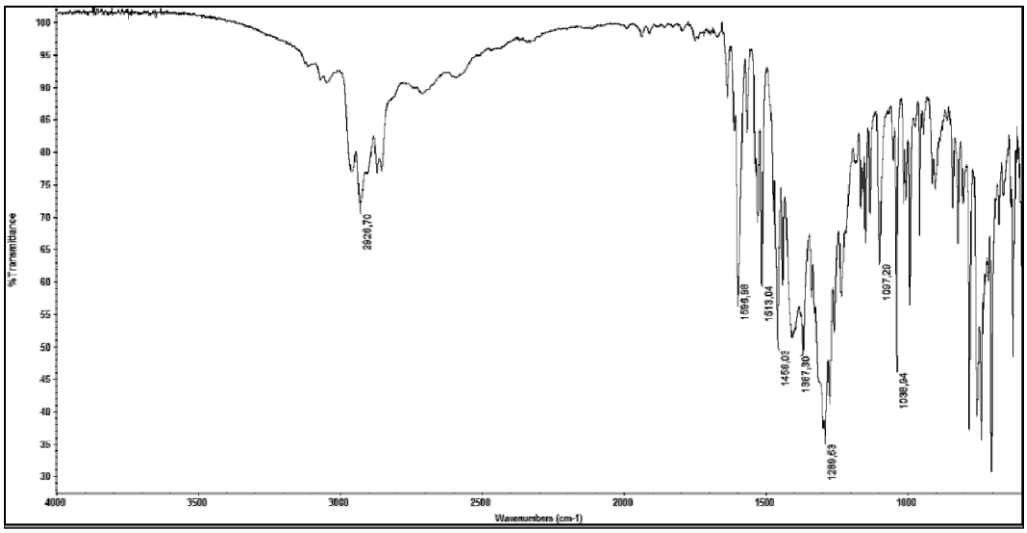


Figure S5. Infrared spectrum (ATR) of [Ag(N∩N)(PBu$_3$)](NO$_3$) (**5**).

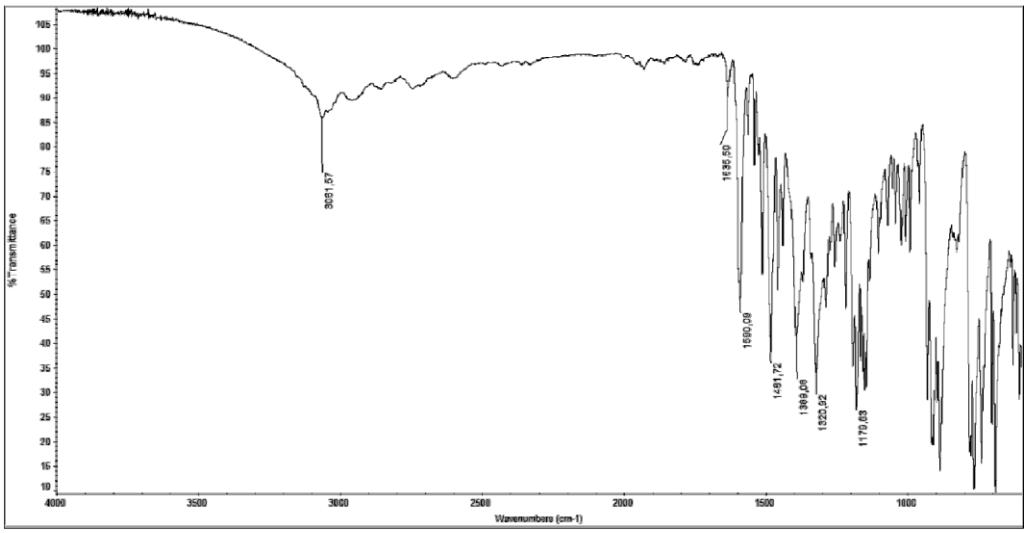


Figure S6. Infrared spectrum (ATR) of [Ag(N∩N)(P(OPh)$_3$)](NO$_3$) (**6**).

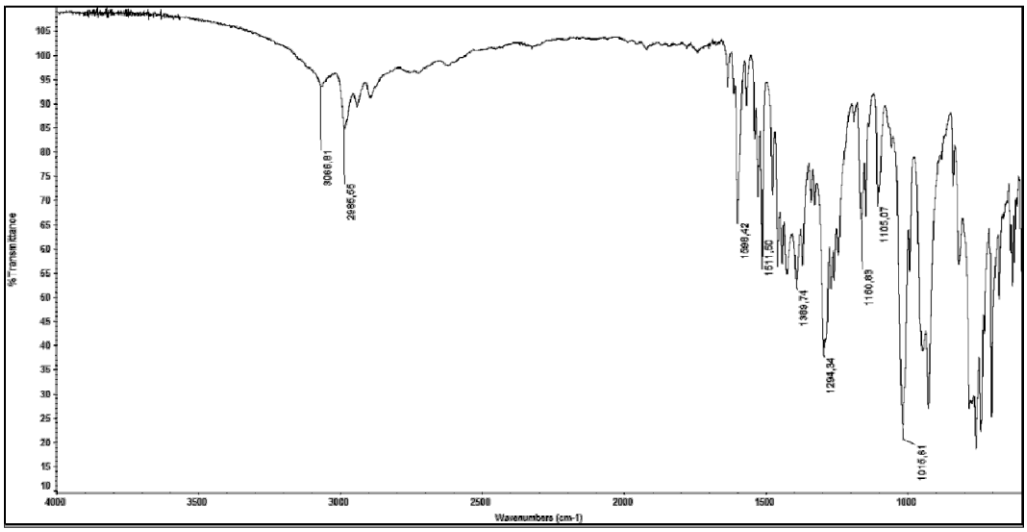
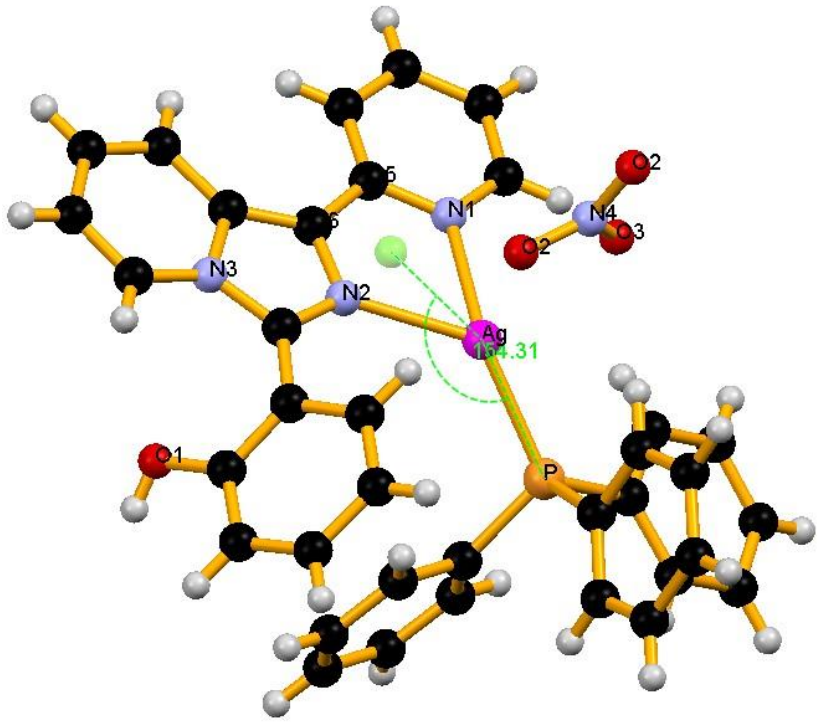
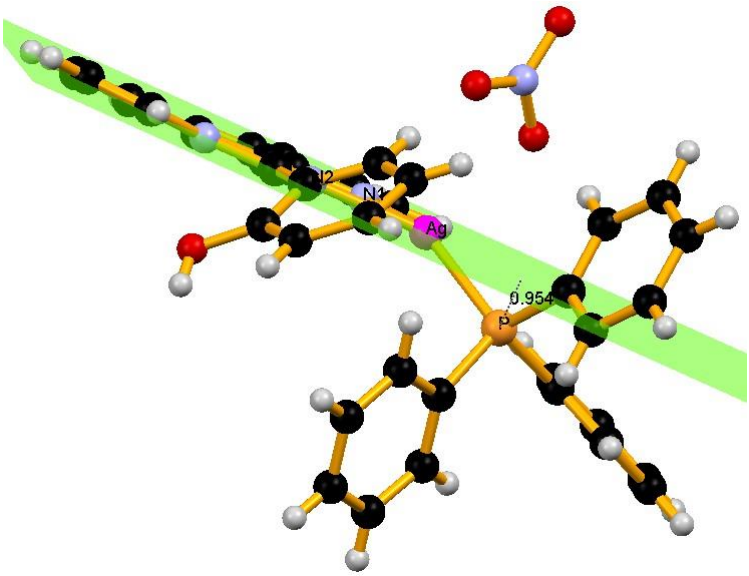


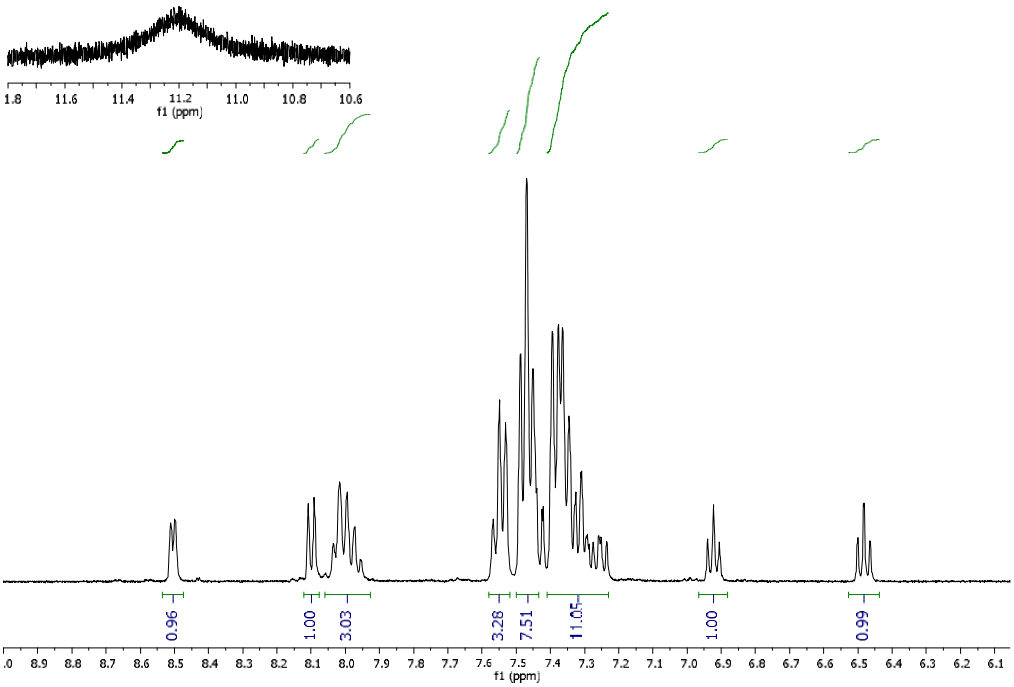
Figure S7. Infrared spectrum (ATR) of [Ag(N∩N)(P(OEt)$_3$)](NO$_3$) (**7**).



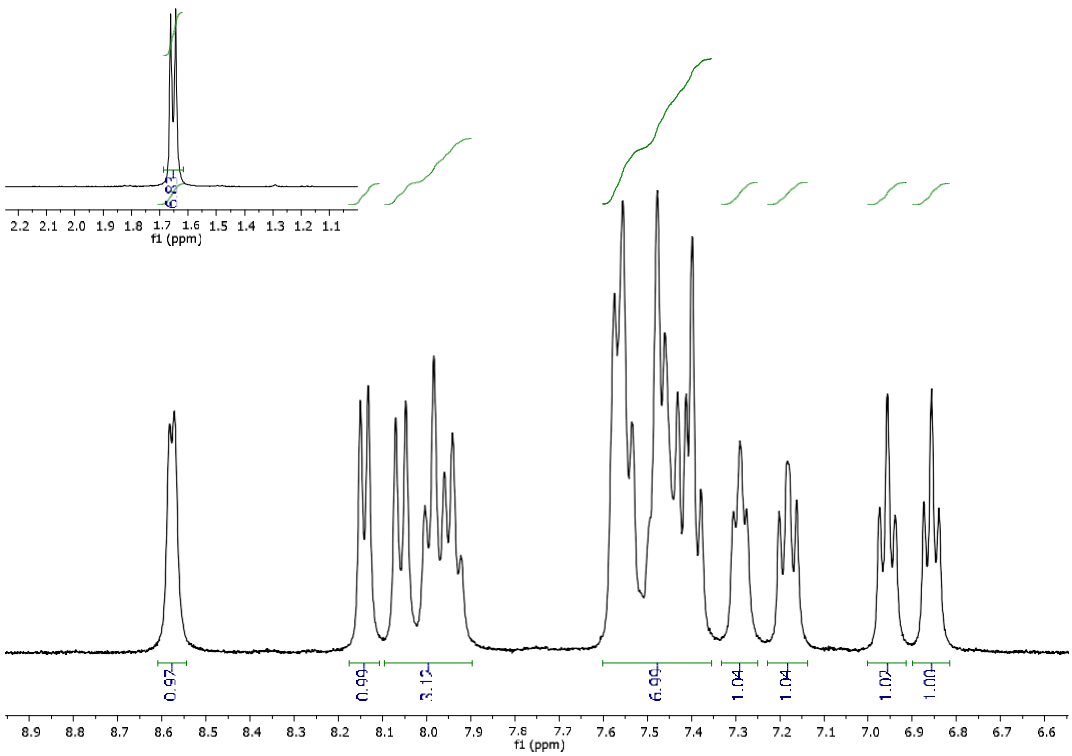
 # Figure S8. Angle formed between P and the centroid of the Ag-N(1)-C(5)-C(6)-N(2) fragment (here complex **1** is taken as example). Angle between P and the centroid (green dot): 154.31°.



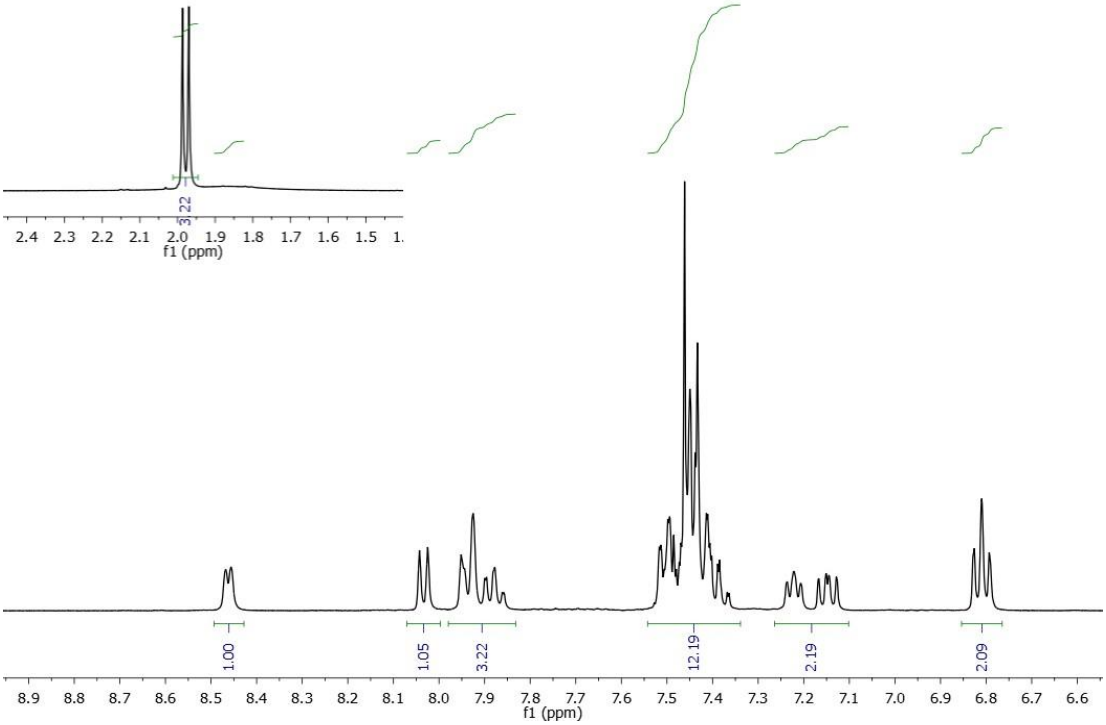
 # Figure S9. Distance (= 0.954Å) between P and the plane defined by atoms Ag-N(1)-N(2) in complex **1**.



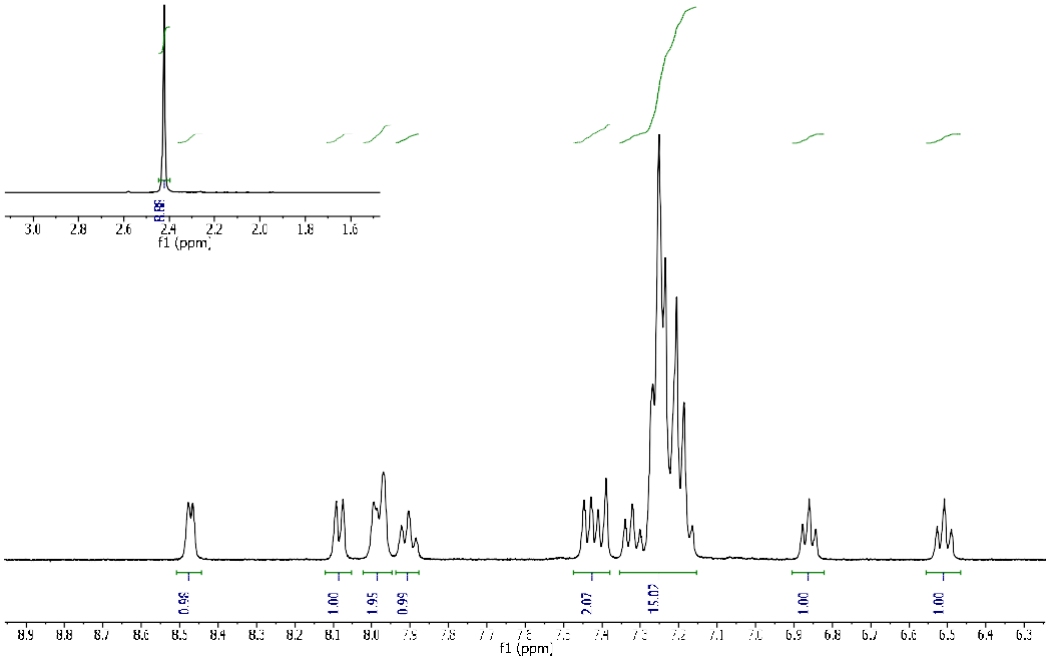
 # Figure S10. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)(PPh_3)](NO_3) (**1**).



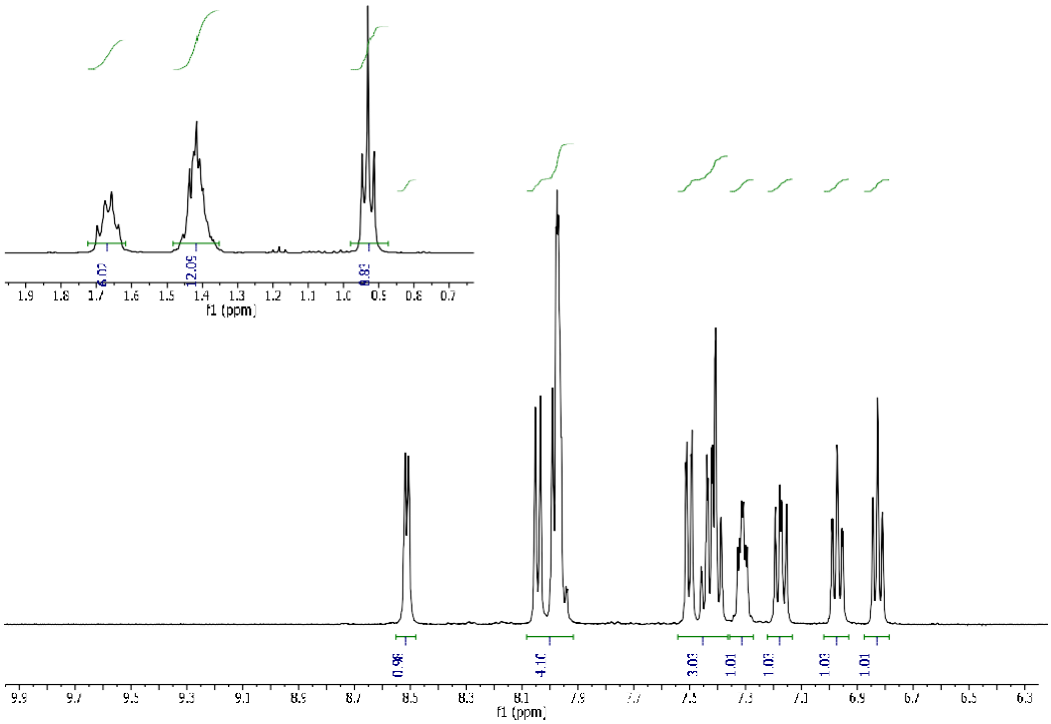
 # Figure S11. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)(PMe_2Ph)](NO_3) (**2**).



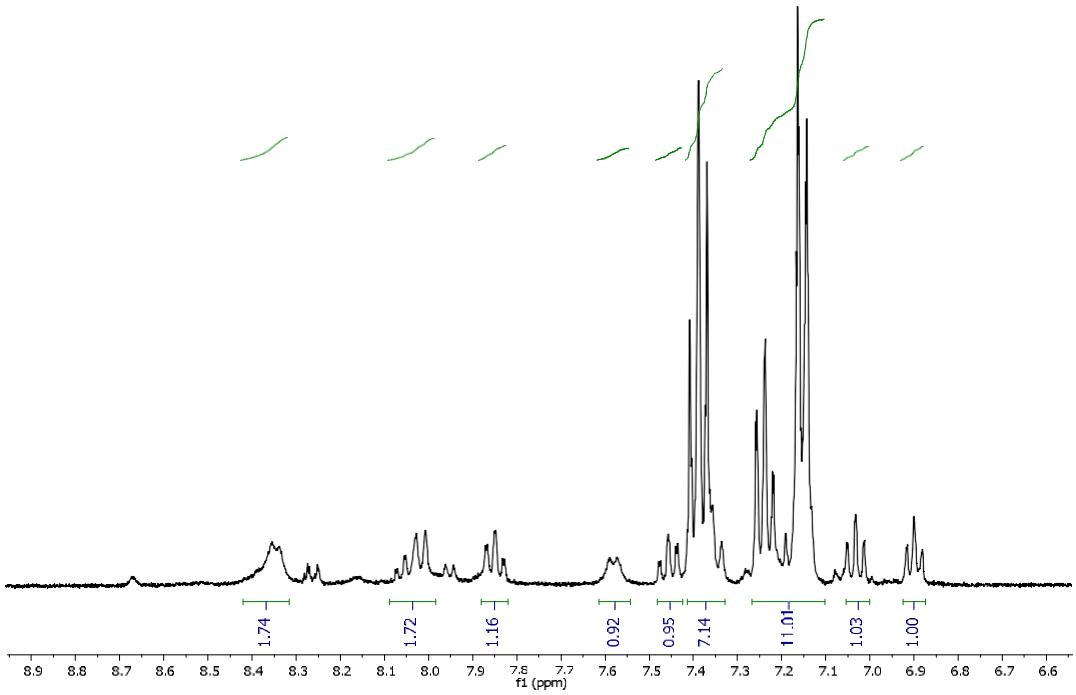
 # Figure S12. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)($PMePh_2$)](NO_3) (**3**).



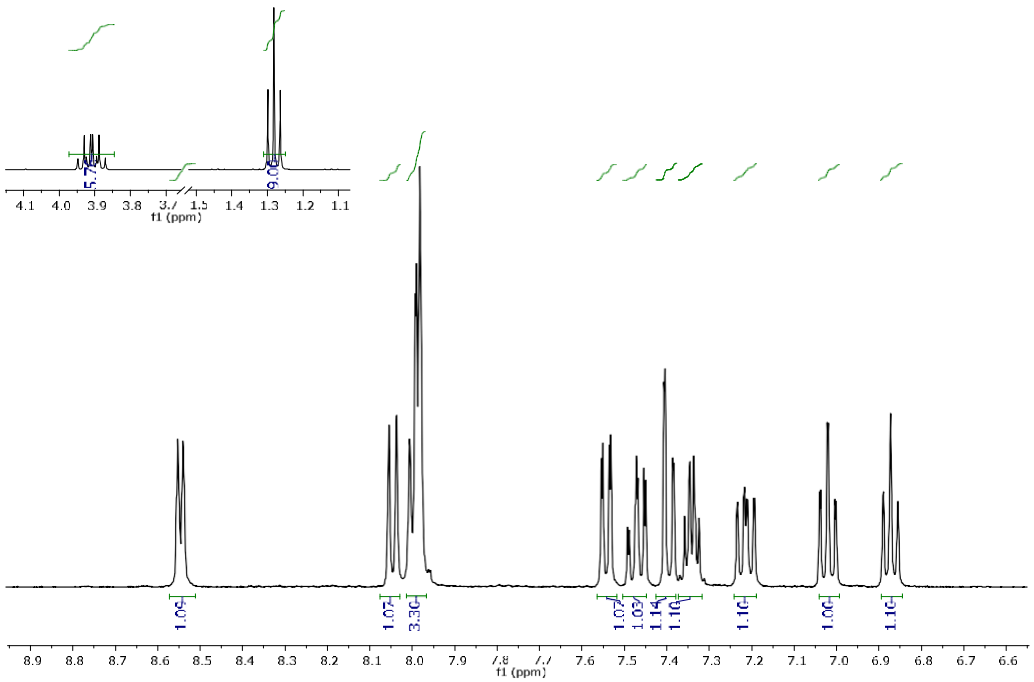
 # Figure S13. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)(P(*p*-tolyl)$_3$)](NO_3) (**4**).



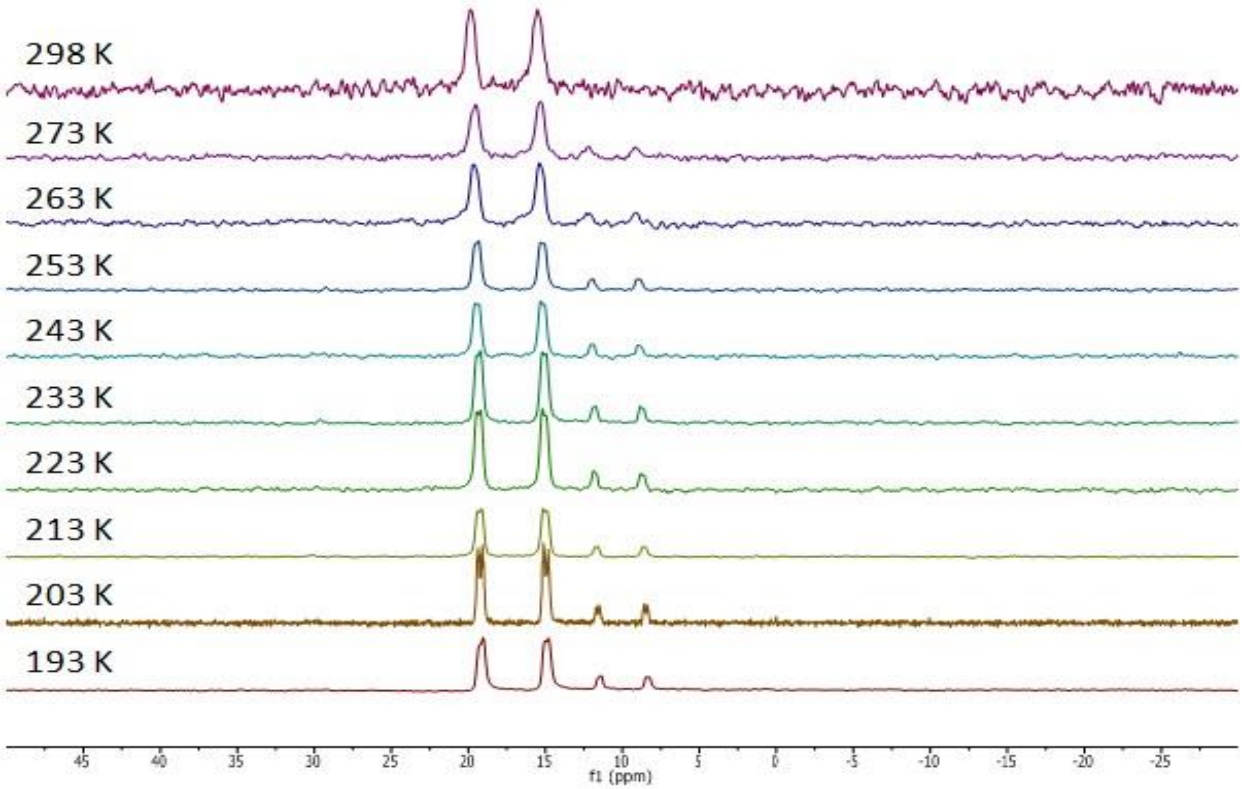
 # Figure S14. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)(PBu_3)](NO_3) (**5**).



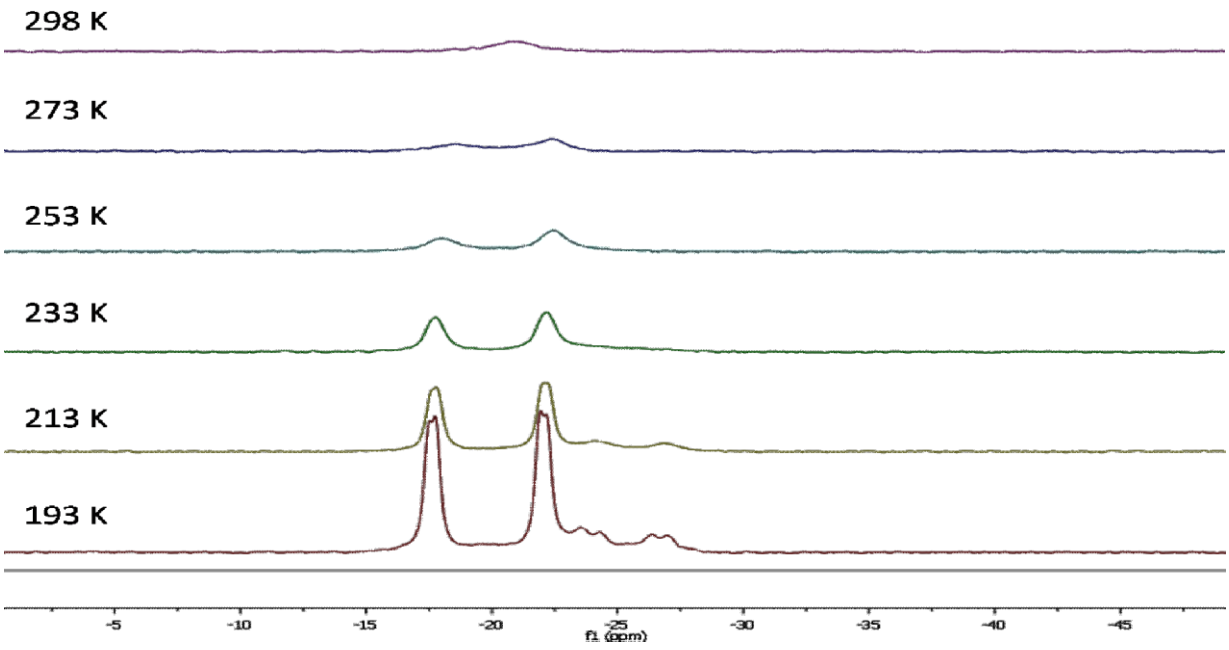
 # Figure S15. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)($P(OPh)_3$)](NO_3) (**6**).



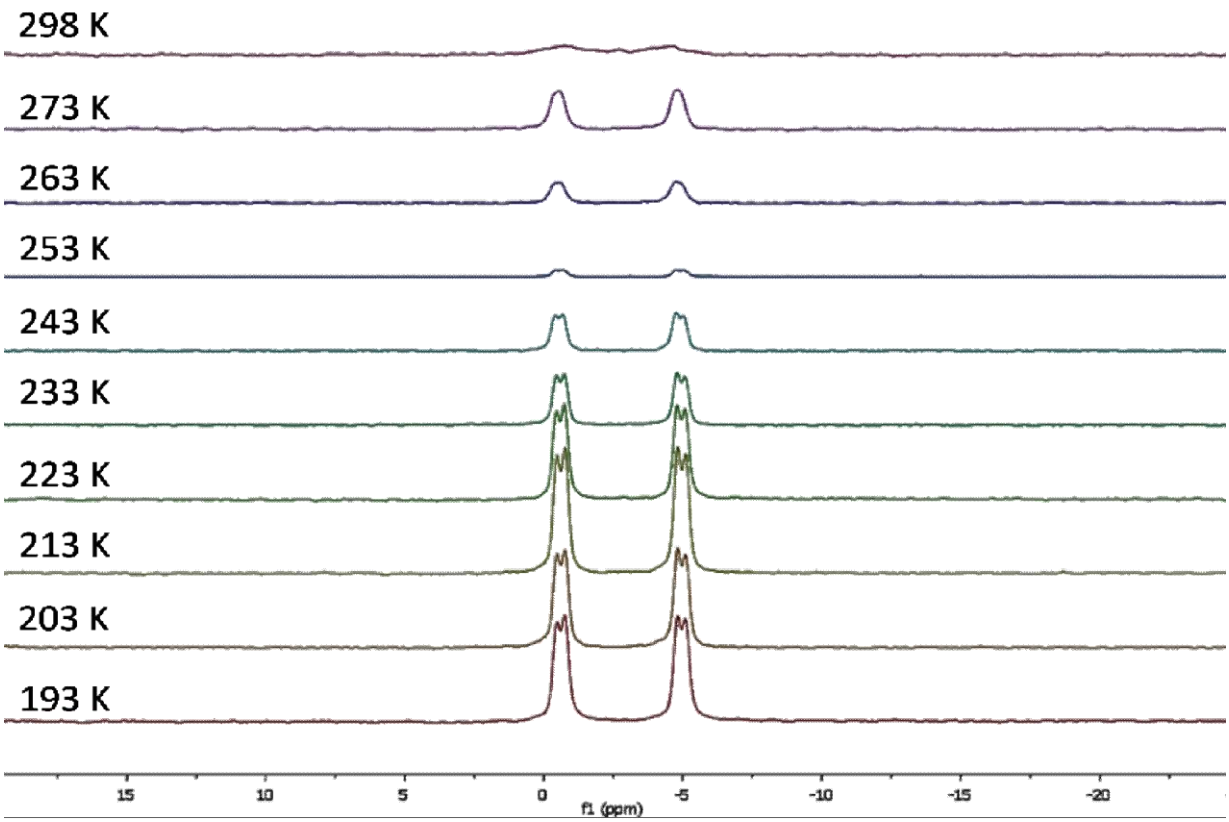
 # Figure S16. ^{1}H NMR spectrum (CD_2Cl_2, 25°C) of [Ag(N∩N)($P(OEt)_3$)](NO_3) (**7**).



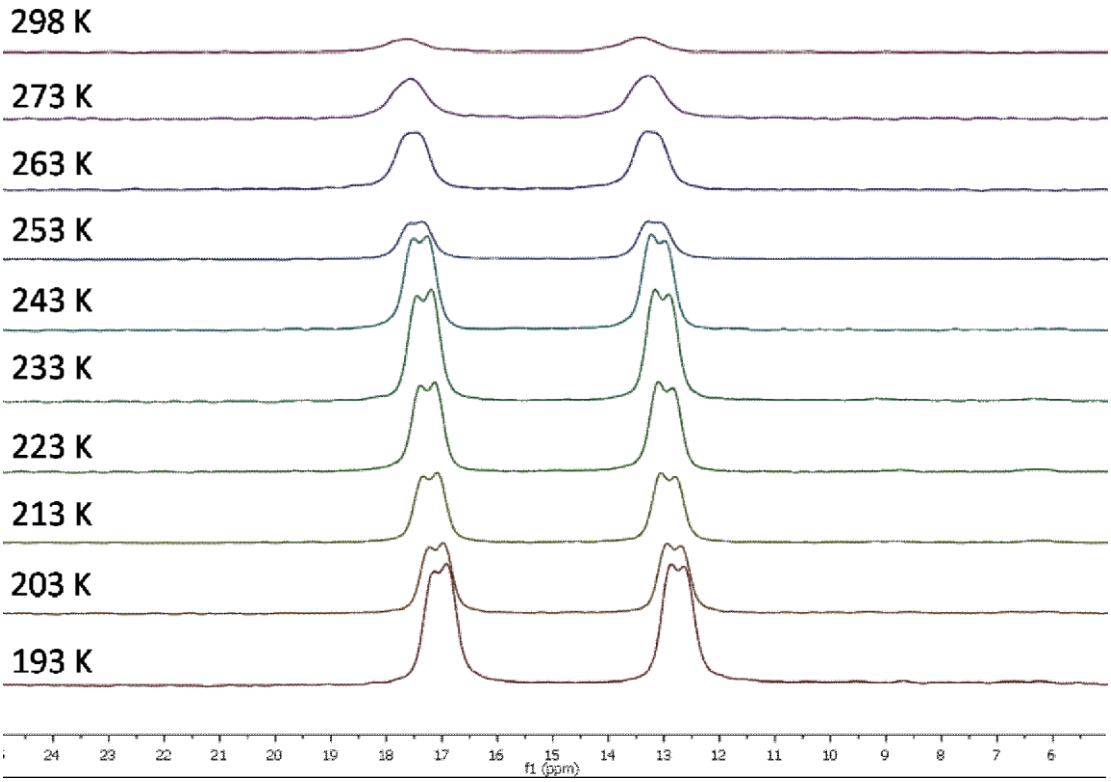
 # Figure S17. Variable temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)(PPh_3)](NO_3) (**1**).



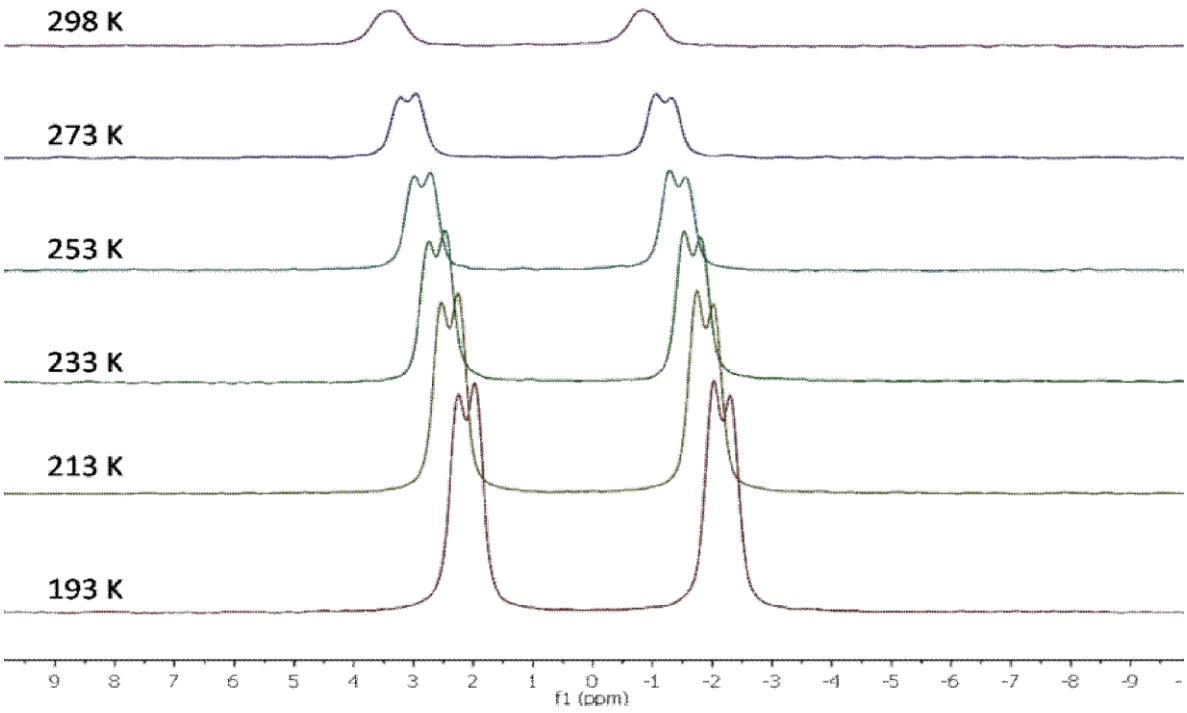
 # Figure S18. Variable temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)(PMe_2Ph)](NO_3) (**2**).



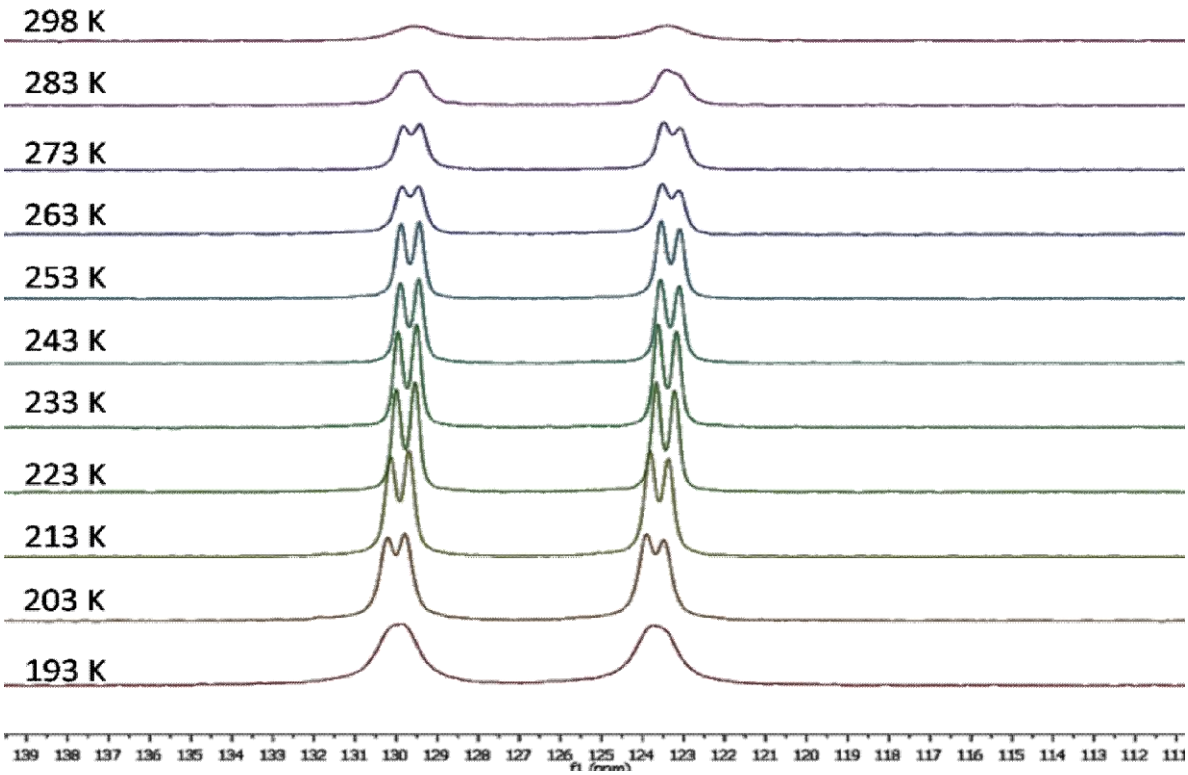
 # Figure S19. Variable temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)($PMePh_2$)](NO_3) (**3**).



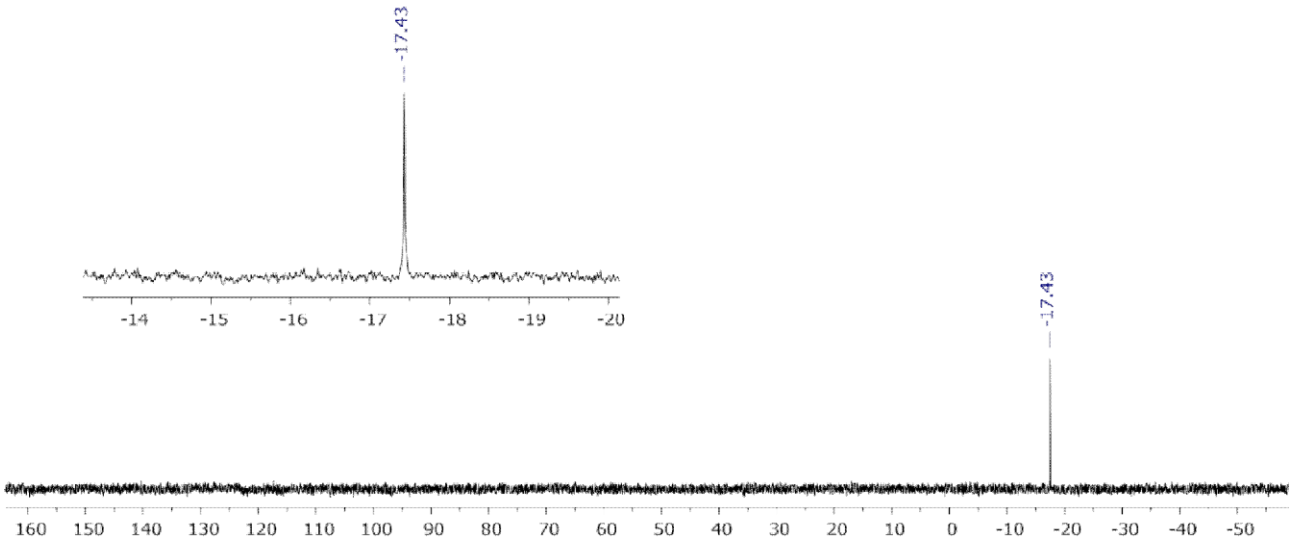
 # Figure S20. Variable temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)(P(*p*-tolyl)$_3$)](NO_3) (**4**).



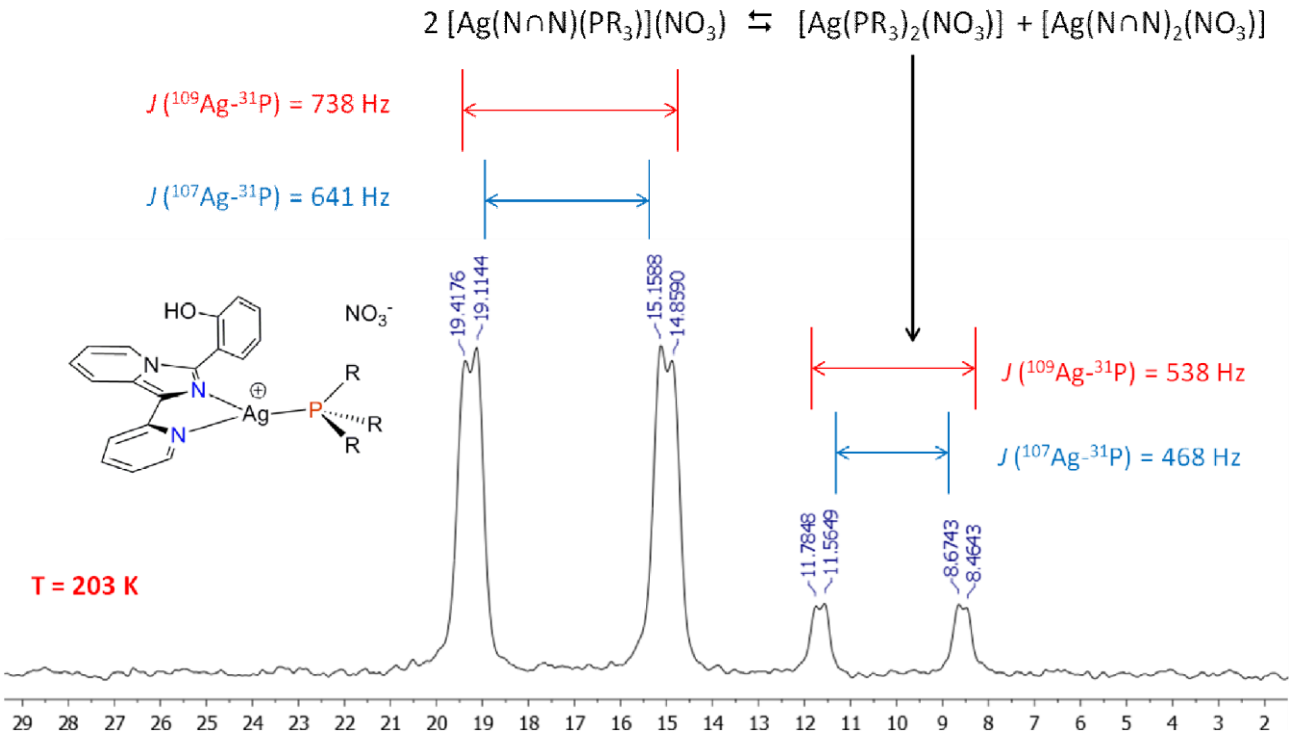
 # Figure S21. Variable temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)(PBu_3)](NO_3) (**5**).



 # Figure S22. Variable temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)($P(OEt)_3$)](NO_3) (**7**).



 # Figure S23. Room temperature ^{31}P NMR spectrum (CD_2Cl_2) of [Ag(N∩N)(P(OPh)$_3$)](NO$_3$) (**6**). Variable temperature spectra missing due to poor solubility of **6** at low temperatures.



 # Figure S24. Determination of J(^{109}Ag-^{31}P) and J(^{107}Ag-^{31}P) for complex [Ag(N∩N)(PPh$_3$)](NO$_3$) (**1**).

Table T1. Electronic transitions in complexes **1**-**7**.

Complex 1 [Ag(N∩N)(PPh_3)](NO_3)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	363.7	0.4602	HOMO -> LUMO (91%)	
2	321.4	0.0278	HOMO -> L+2 (48%)	HOMO -> L+1 (7%)
3	319.0	0.0103	H-1 -> LUMO (97%)	
4	314.1	0.0184	HOMO -> L+1 (28%)	HOMO -> L+2 (5%), HOMO -> L+4 (3%)
5	311.7	0.0094	HOMO -> L+3 (35%)	HOMO -> L+4 (8%)
6	306.7	0.0467	H-2 -> LUMO (87%)	
7	295.7	0.0019	H-3 -> LUMO (96%)	
8	292.7	0.3397	HOMO -> L+4 (20%),	HOMO -> L+5 (2%), HOMO -> L+3 (10%)
9	291.2	0.0031	HOMO -> L+6 (81%)	
10	281.0	0.1546	HOMO -> L+5 (59%)	
11	278.5	0.0023	HOMO -> L+7 (100%)	
12	273.2	0.0055	H-1 -> L+1 (97%)	
13	266.8	0.0018	HOMO -> L+8 (95%)	
14	263.7	0.0152	H-2 -> L+1 (80%)	
15	261.4	0.0590	H-1 -> L+2 (73%)	
16	261.0	0.0022	H-4 -> LUMO (69%)	
17	259.0	0.0100	HOMO -> L+9 (60%)	
18	258.7	0.0061	H-1 -> L+3 (23%)	H-1->L+4 (7%)
19	258.6	0.0093	H-5 -> LUMO (85%)	
20	256.4	0.0056	H-3 -> L+1 (66%)	

Complex 2 [Ag(N∩N)(PMe_2Ph)](NO_3)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	345.9	0.4901	HOMO->LUMO (90%)	
2	306.4	0.0077	HOMO->L+1 (82%)	

3	299.6	0.0402	H-1->LUMO (87%)	
4	298.5	0.0002	HOMO->L+3 (96%)	
5	290.9	0.0105	H-2->LUMO (94%)	
6	286.9	0.2344	HOMO->L+2 (55%)	HOMO->L+4 (4%)
7	276.7	0.0033	H-3->LUMO (94%)	
8	276.4	0.1849	HOMO->L+4 (56%)	HOMO->L+2 (3%)
9	269.6	0.0010	HOMO->L+5 (100%)	
10	259.1	0.0157	H-1->L+1 (88%)	
11	253.0	0.0010	H-2->L+1 (93%)	
12	249.0	0.0355	HOMO->L+6 (79%)	
13	248.8	0.0003	H-4->LUMO (98%)	
14	246.2	0.0001	H-5->LUMO (100%)	
15	245.1	0.0005	H-1->L+3 (97%)	
16	243.4	0.0070	H-1->L+2 (12%)	H-2->L+2 (9%), H-1->L+4 (3%), H-3->L+1 (2%)
17	242.5	0.0131	H-3->L+1 (32%)	H-1->L+2 (3%), H-1->L+4 (2%)
18	241.5	0.0100	H-2->L+2 (30%)	H-3->L+1 (8%)
19	239.5	0.0125	H-2->L+3 (95%)	
20	238.5	0.0112	H-6->LUMO (77%)	

Complex 3 [Ag(N∩N)($PMePh_2$)](NO_3)

No.	**Wavelength (nm)**	**Osc. Strength**	**Major contribs**	**Minor contribs**
1	358.9	0.4886	HOMO->LUMO (90%)	
2	319.0	0.0043	H-1->LUMO (97%)	
3	315.8	0.1033	HOMO->L+1 (36%)	HOMO->L+2 (5%), HOMO->L+3 (2%)
4	311.3	0.0054	HOMO->L+2 (39%)	HOMO->L+1 (8%)
5	301.8	0.0324	H-2->LUMO (91%)	
6	296.6	0.0112	H-3->LUMO (95%)	
7	293.0	0.0412	HOMO->L+5 (30%)	HOMO->L+3 (8%)
8	290.4	0.1337	HOMO->L+5 (19%)	HOMO->L+3 (6%), HOMO->L+4 (3%)
9	281.0	0.0759	HOMO->L+6 (44%)	HOMO->L+3 (3%)
10	279.1	0.1588	HOMO->L+4 (37%)	HOMO->L+6 (6%)

11	275.0	0.0008	H-1->L+1 (99%)	
12	264.8	0.0209	H-1->L+2 (93%)	
13	260.0	0.0160	H-2->L+1 (42%)	H-3->L+1 (5%)
14	259.4	0.0067	HOMO->L+7 (91%)	
15	258.1	0.0085	H-3->L+1 (50%)	H-2->L+2 (2%)
16	256.6	0.0051	H-4->LUMO (95%)	
17	253.0	0.0203	H-1->L+3 (62%)	H-3->L+2 (3%)
18	250.7	0.0057	H-2->L+2 (17%)	HOMO->L+8 (6%)
19	250.0	0.0061	H-5->LUMO (73%)	
20	249.1	0.0330	HOMO->L+8 (12%)	H-3->L+2 (8%), H-1->L+4 (7%)

Complex 4 [Ag(N∩N)(P(*p*-tolyl)$_3$)](NO$_3$)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	364.5	0.4666	HOMO->LUMO (90%)	
2	337.3	0.0095	H-1->LUMO (99%)	
3	316.6	0.0168	HOMO->L+1 (69%)	
4	309.5	0.0393	H-2->LUMO (80%)	
5	305.5	0.0252	HOMO->L+3 (87%)	
6	303.0	0.0097	HOMO->L+4 (86%)	
7	301.1	0.0023	H-3->LUMO (98%)	
8	295.0	0.2432	HOMO->L+2 (50%)	
9	287.3	0.0978	HOMO->L+6 (75%)	
10	286.2	0.0050	H-1->L+1 (98%)	
11	282.2	0.1494	HOMO->L+5 (64%)	
12	274.1	0.0245	H-4->LUMO (78%)	
13	273.6	0.0035	H-5->LUMO (82%)	
14	270.9	0.0054	H-1->L+2 (96%)	
15	269.9	0.0060	HOMO->L+7 (95%)	
16	265.2	0.0159	H-2->L+1 (81%)	
17	262.5	0.0036	HOMO->L+8 (95%)	
18	261.0	0.0057	H-3->L+1 (87%)	

19	259.9	0.0480	H-1->L+3 (25%), H-1->L+5 (14%)	
20	257.9	0.0118	HOMO->L+9 (86%)	

Complex 5 [Ag(N∩N)(P(^{n}Bu)$_3$)](NO$_3$)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	358.6	0.5114	HOMO->LUMO (91%)	
2	327.5	0.0060	H-1->LUMO (98%)	
3	313.5	0.0434	HOMO->L+1 (75%)	
4	300.0	0.0401	H-2->LUMO (74%)	
5	299.4	0.2775	HOMO->L+2 (55%)	
6	288.4	0.0260	H-3->LUMO (92%)	
7	282.7	0.0012	H-1->L+1 (95%)	
8	280.2	0.1539	HOMO->L+3 (79%)	
9	269.6	0.0104	H-1->L+2 (98%)	
10	260.3	0.0061	H-2->L+1 (39%), HOMO->L+4 (10%)	
11	257.1	0.0439	HOMO->L+4 (36%)	H-2->L+1 (5%)
12	255.6	0.0007	H-1->L+3 (98%)	
13	252.8	0.0171	H-3->L+1 (50%)	H-2->L+2 (7%)
14	245.6	0.0223	H-2->L+2 (16%), H-3->L+2 (14%)	
15	243.6	0.0267	H-4->LUMO (80%)	
16	239.5	0.0095	H-2->L+3 (23%), H-3->L+2 (12%)	
17	235.9	0.0190	H-2->L+3 (13%), HOMO->L+5 (11%)	
18	232.3	0.0614	HOMO->L+5 (17%), H-3->L+3 (15%)	
19	230.9	0.0091	H-1->L+4 (88%)	
20	229.5	0.0449	H-3->L+3 (20%)	

Complex 6 [Ag(N∩N)(P(OPh)$_3$)](NO$_3$)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	364.4	0.4340	HOMO->LUMO (88%)	
2	314.1	0.0533	HOMO->L+1 (69%)	
3	301.3	0.2366	HOMO->L+2 (43%)	HOMO->L+3 (2%)
4	299.7	0.0484	H-1->LUMO (75%)	

5	295.8	0.0157	H-2->LUMO (84%)	
6	293.2	0.0720	HOMO->L+3 (36%)	HOMO->L+4 (7%)
7	284.7	0.0076	H-3->LUMO (95%)	
8	277.7	0.0935	HOMO->L+4 (30%)	HOMO->L+5 (3%), HOMO->L+3 (2%)
9	275.8	0.0740	HOMO->L+5 (60%)	HOMO->L+4 (2%)
10	271.7	0.0023	H-4->LUMO (96%)	
11	265.6	0.0084	H-5->LUMO (96%)	
12	265.1	0.0119	HOMO->L+6 (78%)	
13	262.5	0.0120	HOMO->L+7 (62%)	
14	262.1	0.0151	H-6->LUMO (96%)	
15	260.6	0.0053	HOMO->L+8 (83%)	
16	259.3	0.0072	H-1->L+1 (80%)	
17	258.5	0.0018	H-7->LUMO (97%)	
18	255.7	0.0185	H-2->L+1 (32%), H-8->LUMO (10%)	
19	255.6	0.0012	H-8->LUMO (43%)	H-2->L+1 (6%)
20	253.3	0.0141	HOMO->L+9 (34%), HOMO->L+11 (10%)	

Complex 7 [Ag(N∩N)(P(OEt)$_3$)](NO$_3$)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	359.4	0.5069	HOMO->LUMO (91%)	
2	310.5	0.0264	HOMO->L+1 (77%)	
3	300.8	0.0277	H-1->LUMO (91%)	
4	295.0	0.2902	HOMO->L+2 (68%)	
5	291.0	0.0071	H-2->LUMO (97%)	
6	277.9	0.1778	HOMO->L+3 (76%)	
7	273.1	0.0186	H-3->LUMO (99%)	
8	259.5	0.0198	HOMO->L+4 (63%)	H-1->L+1 (3%)
9	256.4	0.0314	H-1->L+1 (48%)	HOMO->L+4 (2%)
10	252.5	0.0080	H-2->L+1 (87%)	
11	245.2	0.0124	HOMO->L+5 (63%)	H-1->L+2 (3%)
12	242.2	0.0153	H-2->L+2 (50%)	H-1->L+2 (2%)

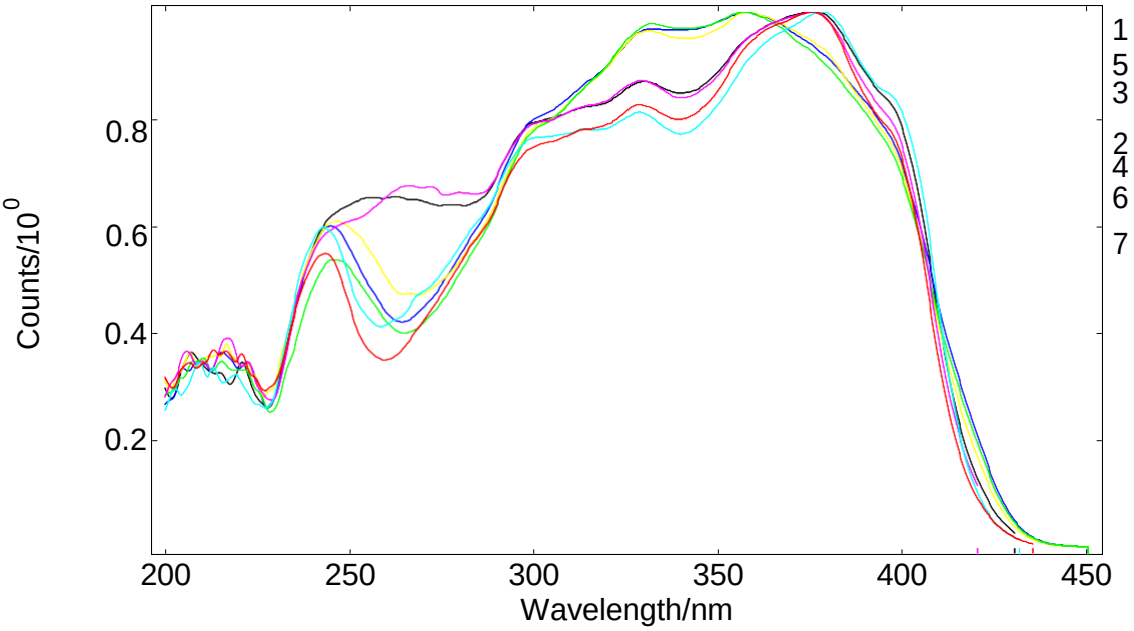
13	239.5	0.0686	H-1->L+3 (11%)	H-1->L+2 (5%), H-2->L+2 (2%)
14	238.0	0.0075	H-3->L+1 (64%)	H-4->LUMO (2%)
15	237.1	0.0011	H-4->LUMO (44%)	
16	232.6	0.0507	H-2->L+3 (43%)	H-1->L+3 (3%)
17	230.6	0.0466	H-2->L+3 (10%)	H-1->L+3 (6%), H-3->L+2 (2%)
18	229.8	0.0037	H-5->LUMO (98%)	
19	228.1	0.0156	H-3->L+2 (68%)	
20	225.1	0.0008	HOMO->L+6 (95%)	

Complex [Ag(phen)(PPh_3)](NO_3)

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	354.7	0.0029	HOMO->LUMO (96%)	
2	333.8	0.0000	HOMO->L+1 (98%)	
3	325.4	0.0009	H-1->LUMO (95%)	
4	309.0	0.0001	H-1->L+1 (99%)	
5	283.4	0.0345	H-2->LUMO (82%)	
6	280.7	0.0002	H-3->LUMO (96%)	
7	280.2	0.0000	H-4->LUMO (97%)	
8	268.4	0.0002	H-6->LUMO (100%)	
9	266.1	0.0005	H-3->L+1 (98%)	
10	265.6	0.0004	H-4->L+1 (98%)	
11	263.4	0.0008	H-7->LUMO (100%)	
12	261.2	0.0043	H-8->LUMO (91%)	
13	260.9	0.0536	H-2->L+1 (44%)	H-5->LUMO (6%)
14	258.4	0.0537	HOMO->L+2 (55%)	HOMO->L+3 (4%)
15	256.7	0.0736	HOMO->L+3 (56%)	HOMO->L+2 (4%)
16	254.9	0.0001	H-6->L+1 (100%)	
17	250.4	0.0002	H-7->L+1 (99%)	
18	249.2	0.0014	H-9->LUMO (99%)	
19	248.2	0.0025	H-8->L+1 (96%)	
20	245.5	0.0108	HOMO->L+4 (66%)	HOMO->L+5 (2%)

 # Table T2. HOMO/LUMO energies gap calculated for complexes **1-7**.

Compd	**1**	**2**	**3**	**4**	**5**	**6**	**7**
PR_3	PPh_3	PMe_2Ph	$PMePh_2$	P(*p*-tolyl)$_3$	P(^{n}Bu)$_3$	$P(OPh)_3$	$P(OEt)_3$
HOMO (eV)	-5.61	-5.65	-5.62	-5.58	-5.61	-5.67	-5.66
LUMO (eV)	-3.16	-3.19	-3.15	-3.14	-3.14	-3.23	-3.20
ΔE (eV)	2.45	2.46	2.47	2.44	2.47	2.44	2.46



 # Figure S25. Normalized excitation spectra (CH_2Cl_2, 10^{-5} M) for complexes **1-7**.

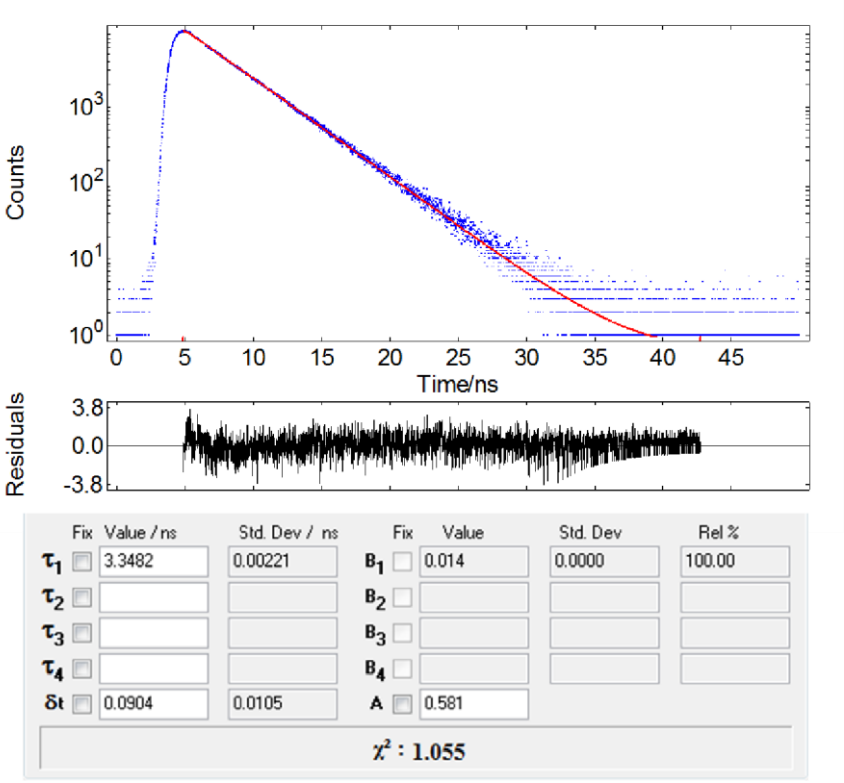


Figure S26. Monoexponential fitting of the lifetime decay of ligand N∩N (CH_2Cl_2 solution, 10^{-5} M).

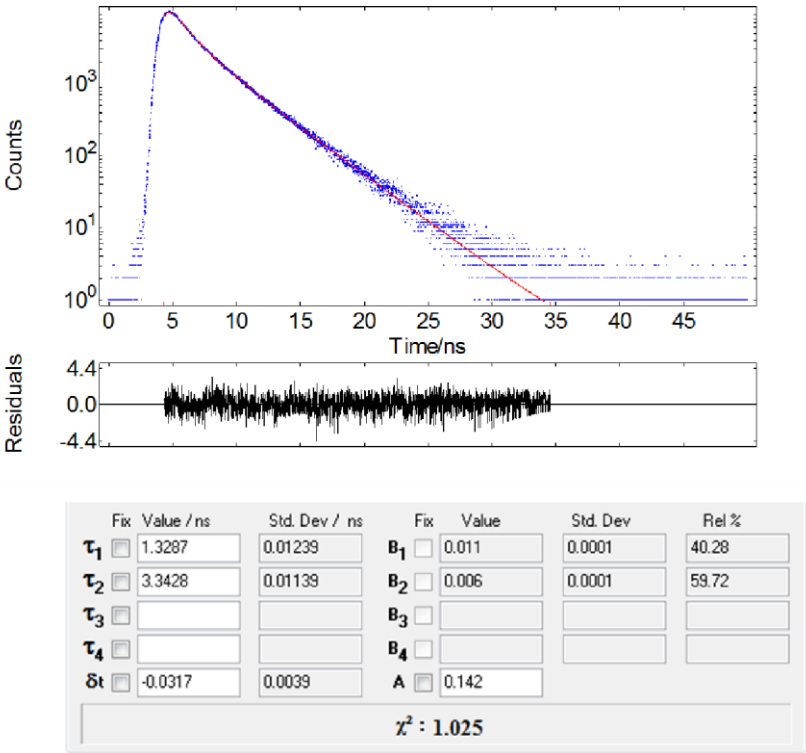
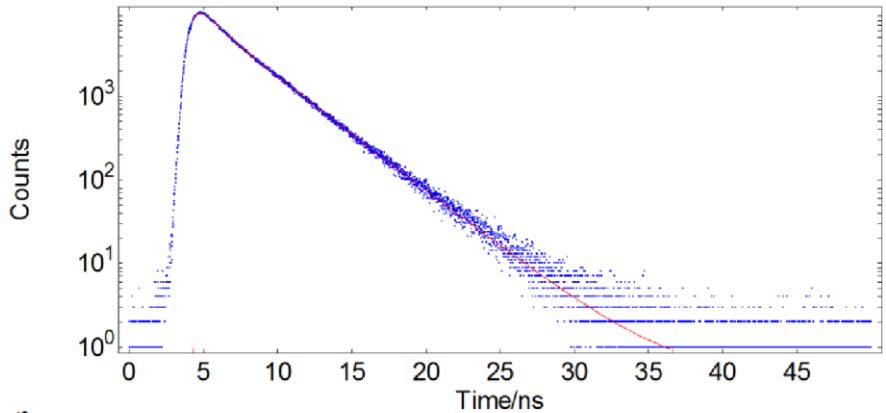


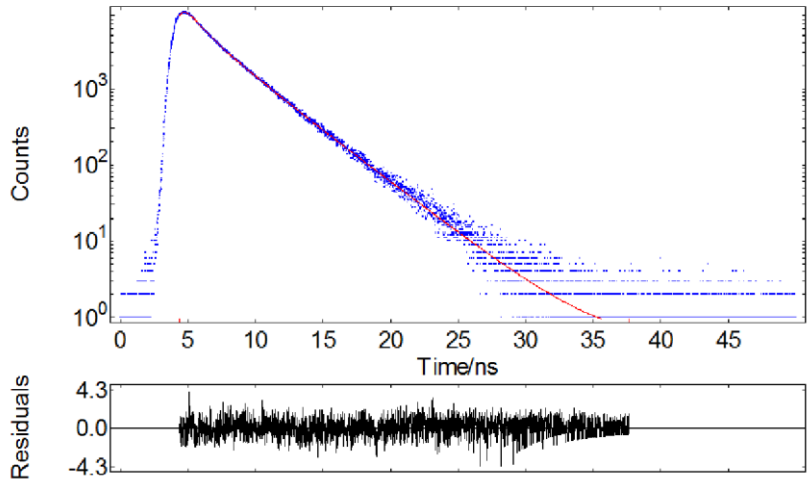
Figure S27. (b) Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(PPh_3)](NO_3) (**1**) (CH_2Cl_2 solution, 10^{-5} M).



	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	1.4093	0.02777	B_1	☐	0.006	0.0001	20.21
τ_2	☐	3.2494	0.00942	B_2	☐	0.010	0.0001	79.79
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
δt	☐	0.0072	0.0037	A	☐	0.480		

χ^2 : 1.060

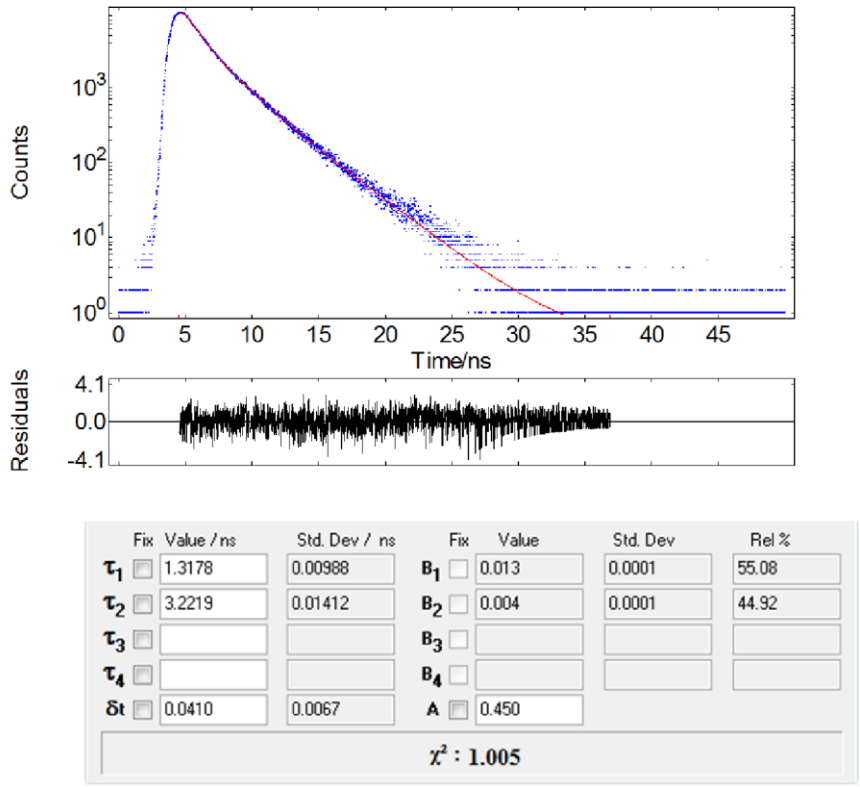
 # Figure S28. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(PMe_2Ph)](NO_3) (**2**) (CH_2Cl_2 solution, 10^{-5} M).



	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	1.4080	0.01932	B_1	☐	0.008	0.0001	30.36
τ_2	☐	3.2350	0.01055	B_2	☐	0.008	0.0001	69.64
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
δt	☐	0.0325	0.0050	A	☐	0.472		

χ^2 : 1.045

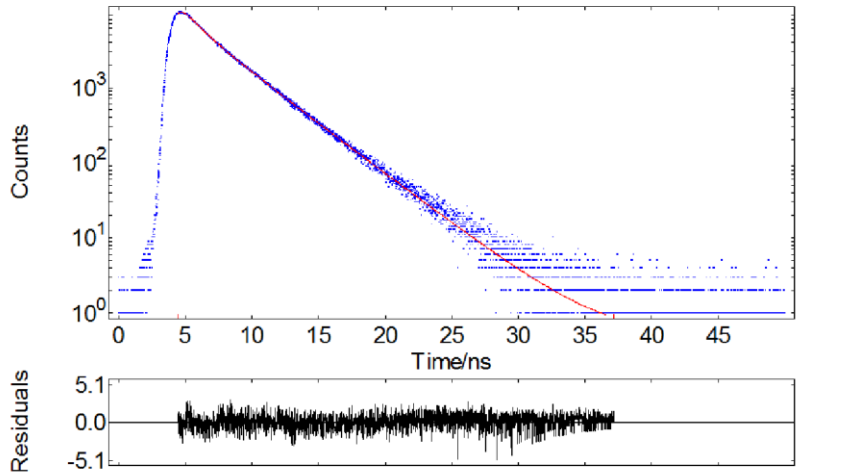
 # Figure S29. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)($PMePh_2$)](NO_3) (**3**) (CH_2Cl_2 solution, 10^{-5} M).



	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	1.3178	0.00988	B_1	☐	0.013	0.0001	55.08
τ_2	☐	3.2219	0.01412	B_2	☐	0.004	0.0001	44.92
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
δt	☐	0.0410	0.0067	A	☐	0.450		

χ^2 : 1.005

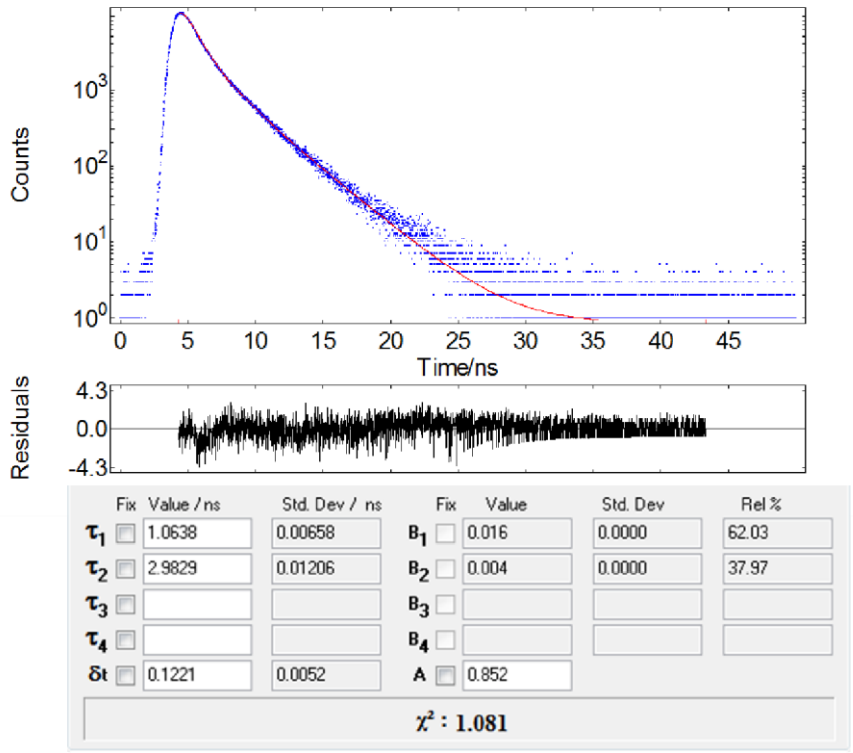
 # Figure S30. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(*p*-tolyl)$_3$)](NO$_3$) (**4**) (CH_2Cl_2 solution, 10^{-5} M).



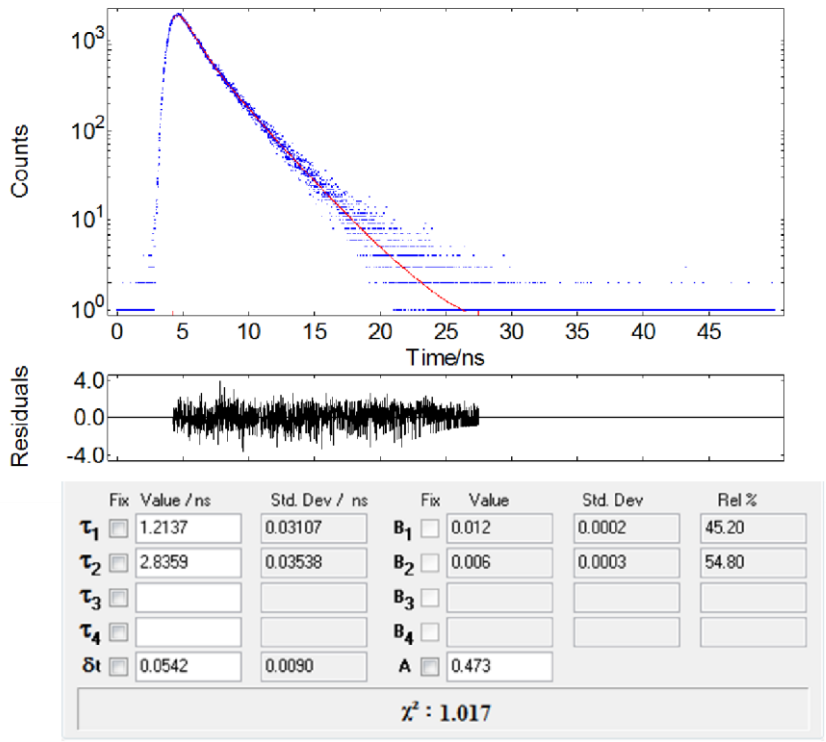
	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	1.4094	0.02535	B_1	☐	0.007	0.0001	23.54
τ_2	☐	3.2809	0.00987	B_2	☐	0.009	0.0001	76.46
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
δt	☐	0.0640	0.0066	A	☐	0.488		

χ^2 : 1.076

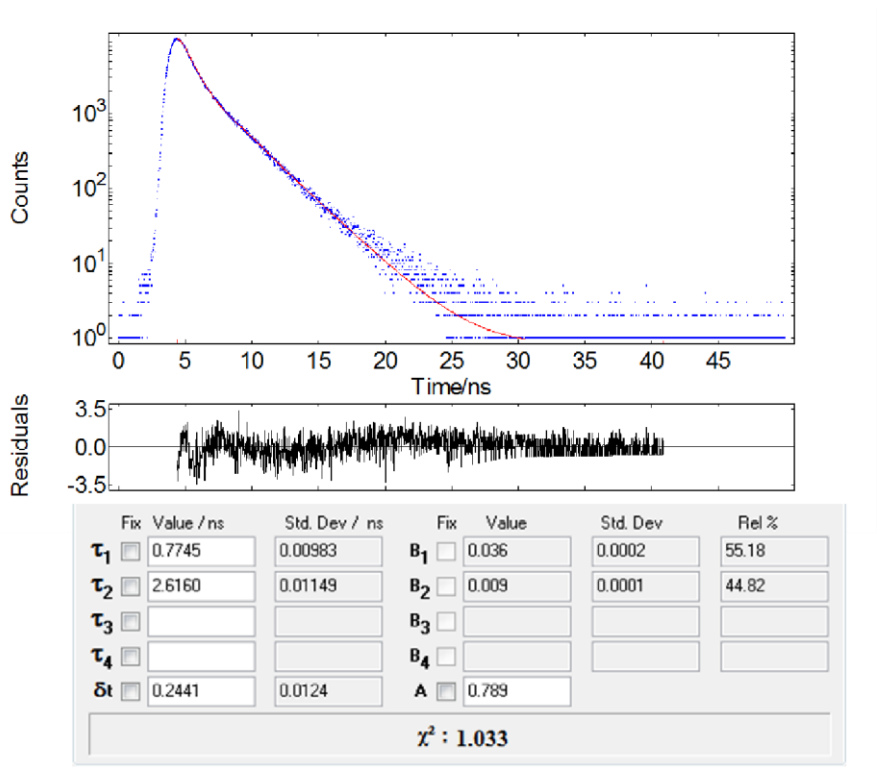
 # Figure S31. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(^{n}Bu)$_3$)](NO$_3$) (**5**) (CH_2Cl_2 solution, 10^{-5} M).



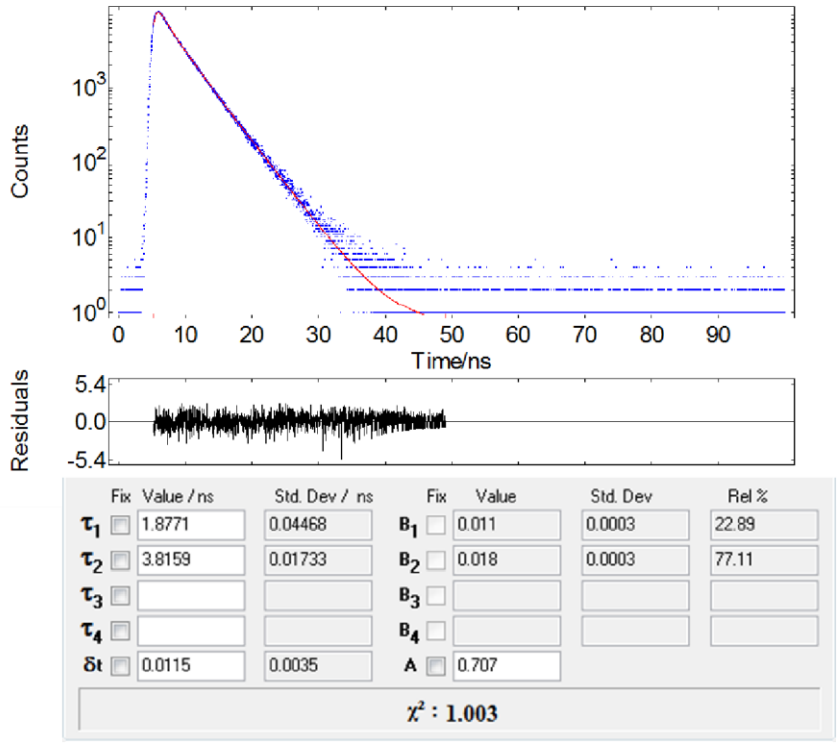
 # Figure S32. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(OPh)$_3$)](NO$_3$) (**6**) (CH_2Cl_2 solution, 10^{-5} M).



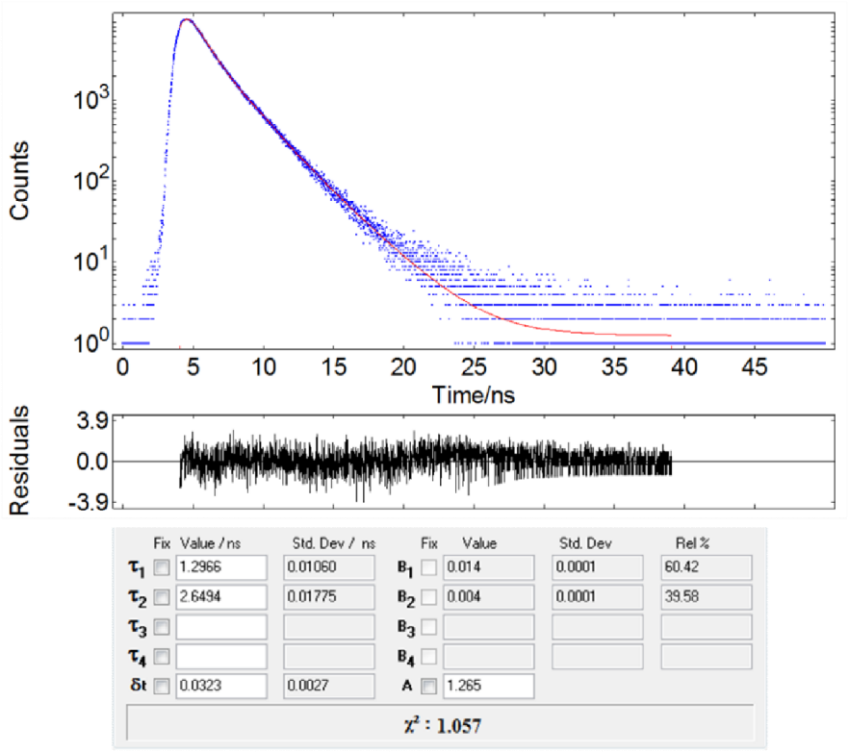
 # Figure S33. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(OEt)$_3$)](NO$_3$) (**7**) (CH_2Cl_2 solution, 10^{-5} M).



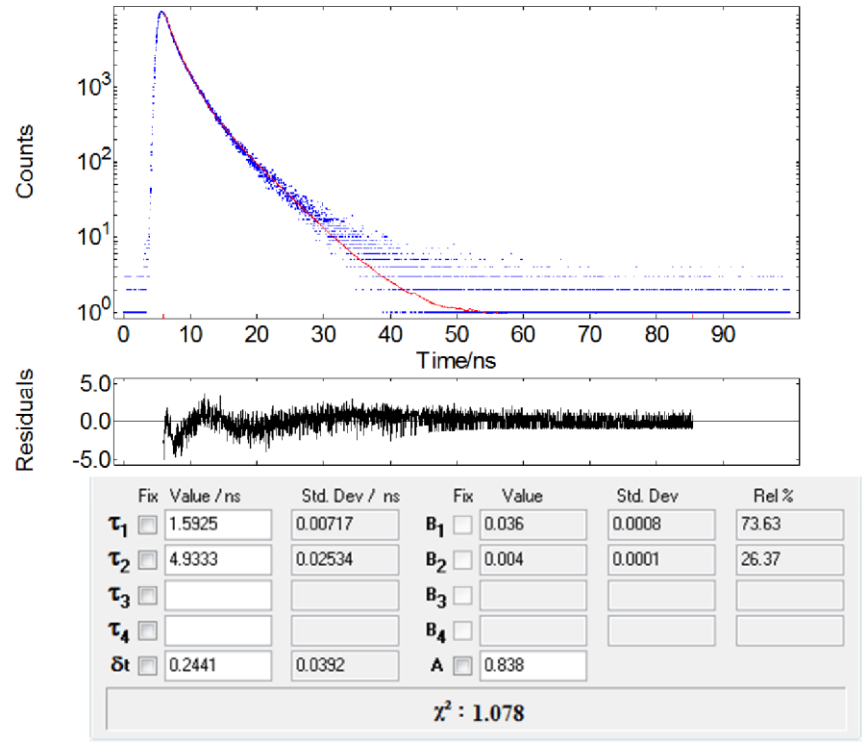
 # Figure S34. Biexponential fitting of the lifetime decay of ligand N∩N in the solid state.



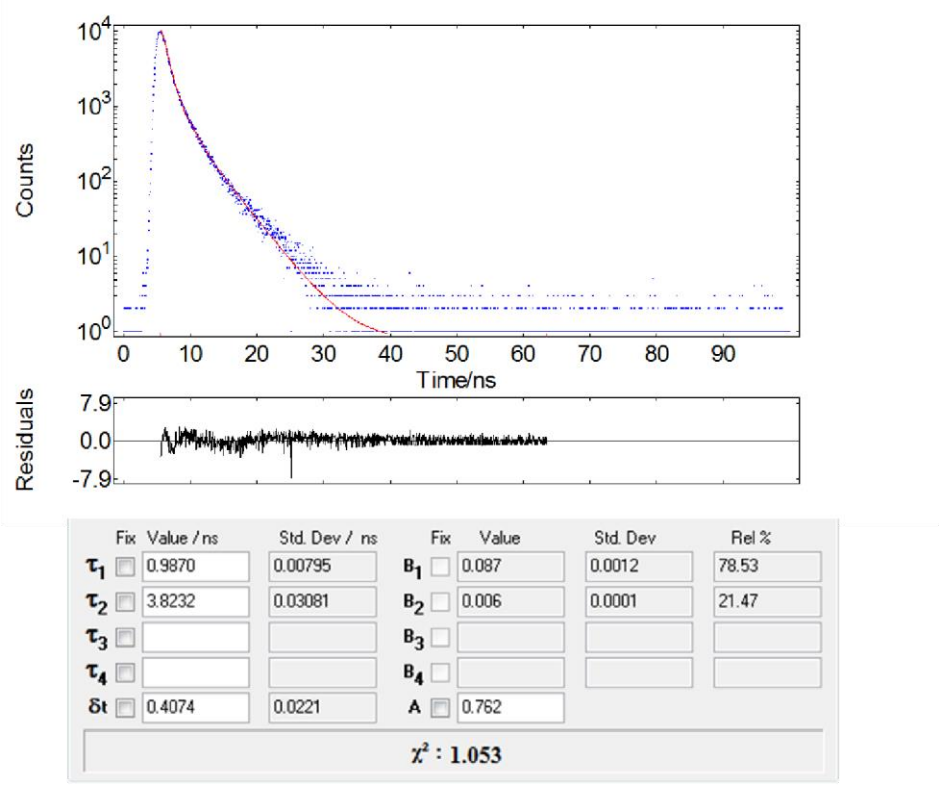
 # Figure S35. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(PPh_3)](NO_3) (**1**) in the solid state.



 # Figure S36. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(PMe_2Ph)](NO_3) (**2**) in the solid state.



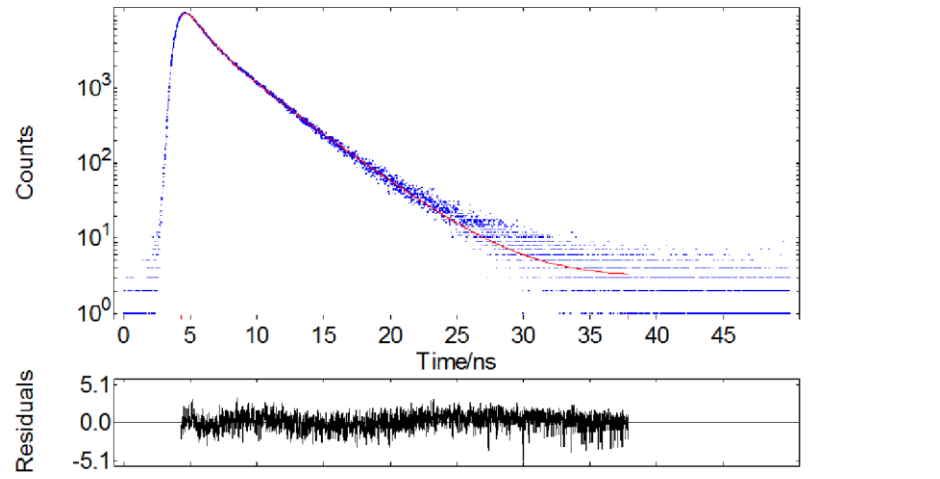
 # Figure S37. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)($PMePh_2$)](NO_3) (**3**) in the solid state.



	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	0.9870	0.00795	B_1	☐	0.087	0.0012	78.53
τ_2	☐	3.8232	0.03081	B_2	☐	0.006	0.0001	21.47
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
δt	☐	0.4074	0.0221	A	☐	0.762		

χ^2 : 1.053

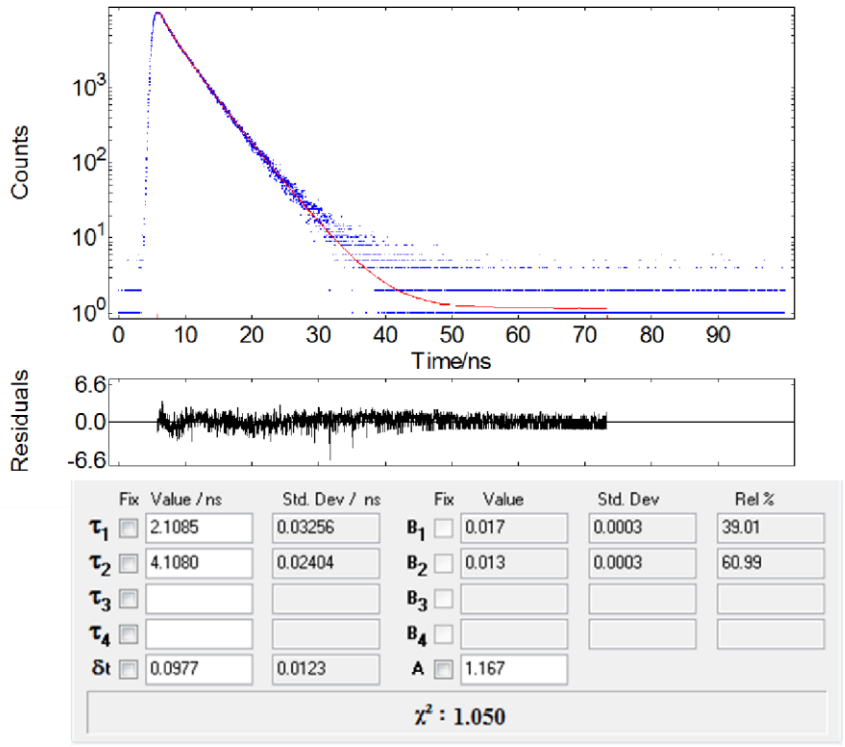
 # Figure S38. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(*p*-tolyl)$_3$)](NO$_3$) (**4**) in the solid state.



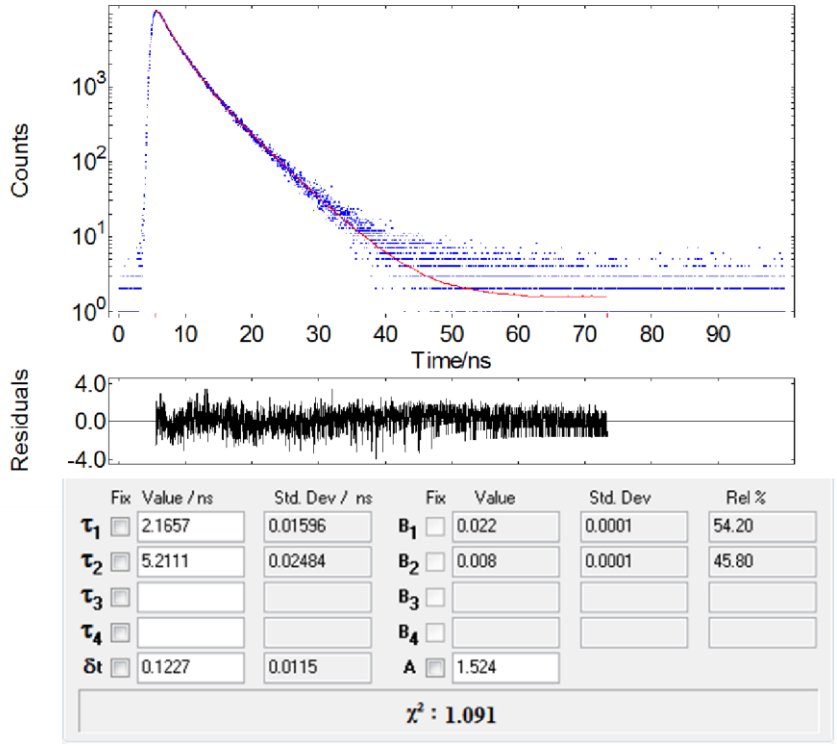
	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	1.4688	0.02132	B_1	☐	0.052	0.0010	53.58
τ_2	☐	3.6326	0.02662	B_2	☐	0.018	0.0005	46.42
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
δt	☐	0.1886	0.0349	A	☐	1.303		

χ^2 : 1.086

 # Figure S39. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(^{n}Bu)$_3$)](NO$_3$) (**5**) in the solid state.



 # Figure S40. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(OPh)$_3$)](NO$_3$) (**6**) in the solid state.



 # Figure S41. Biexponential fitting of the lifetime decay of complex [Ag(N∩N)(P(OEt)$_3$)](NO$_3$) (**7**) in the solid state.

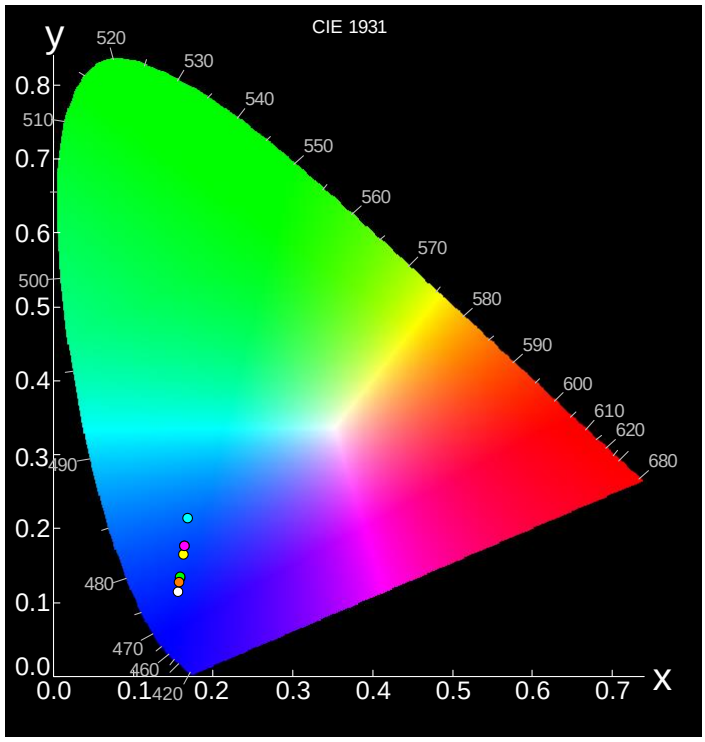


Figure S42. Chromaticity plot (CIE 1931) for complexes **1**-**7** and ligand N∩N in solution.

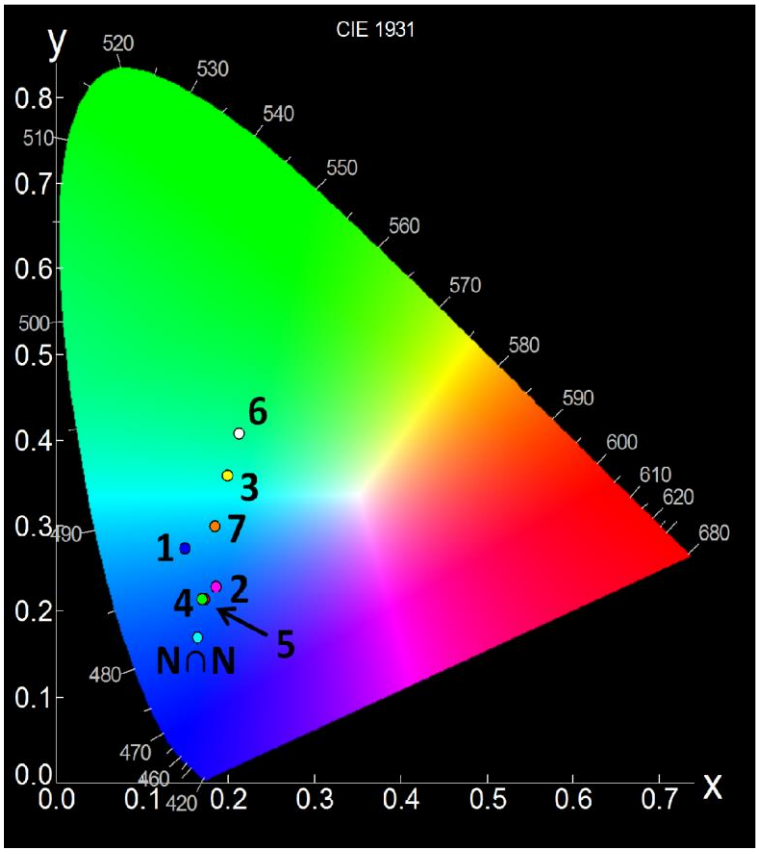


Figure S43. Chromaticity plot (CIE 1931) for complexes **1**-**7** and ligand N∩N in the solid state.

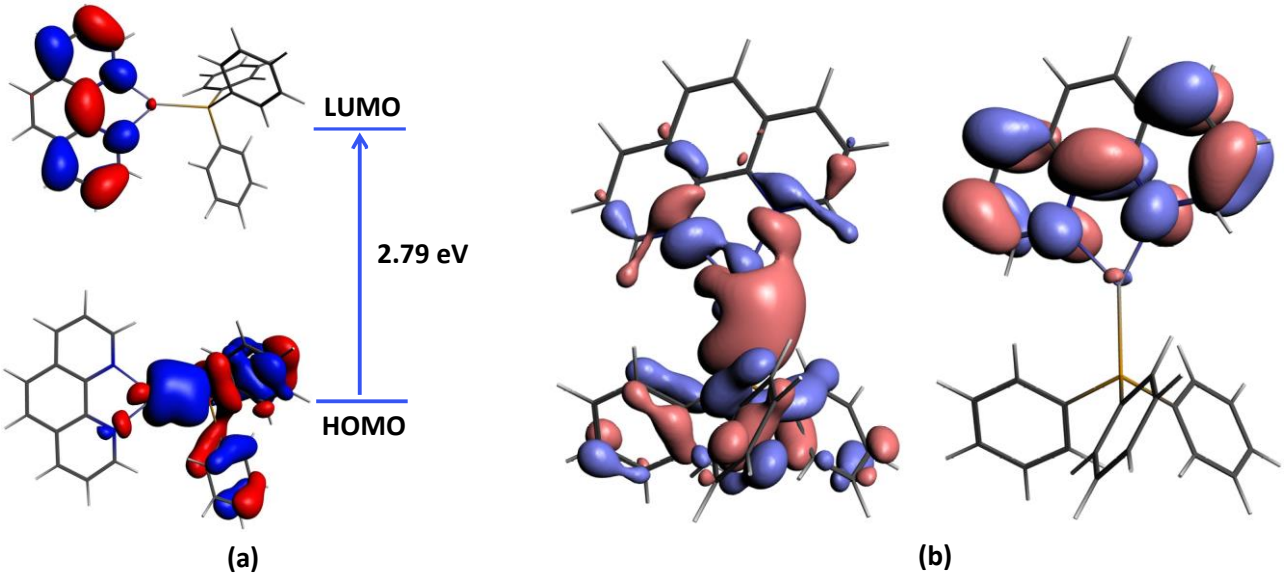


Figure S44. (a) Frontier molecular orbitals for [Ag(phen)(PPh_3)](NO_3) (phen = 1,10-phenanthroline) with the corresponding energy gap; (b) The dominant (Natural Transition Orbitals) NTO pair of the $S_0 \rightarrow S_1$ excitation of complex [Ag(phen)(PPh_3)](NO_3), which accounts for >99% of the transition density. The donor orbital (left-hand side) has a significant metal-based d-orbital character, whereas the acceptor state (right-hand side) is a phenanthroline localized π^* orbital.

Table T3. Crystallographic and structure refinement parameters for complexes **1**, **2**, **5** and **6**.

	1	**2**	**5**	**6**
Chemical formula	$C_{36}H_{28}AgN_4O_4P$	$C_{26}H_{24}AgN_4O_4P$	$C_{30}H_{40}AgN_4O_4P$	$C_{36}H_{28}AgN_4O_7P$
Formula weight	719.46	595.33	659.50	767.46
Crystal system	Monoclinic	triclinic	Monoclinic	Monoclinic
Space group	*C* 2/*c* (no. 15)	*P* -1 (no. 2)	*P* 2_1/*c* (no. 14)	*P* 2_1/*c* (no. 14)
Crystal colour and shape	yellow block	yellow block	yellow block	yellow block
Crystal size	0.21 x 0.18 x 0.17	0.19 x 0.16 x 0.15	0.24 x 0.21 x 0.18	0.21 x 0.20 x 0.17
a (Å)	30.9447(16)	8.3612(7)	19.5618(5)	9.3609(4)
b (Å)	9.9074(3)	10.4096(9)	8.2302(11)	13.7302(7)
c (Å)	21.4664(11)	14.7569(11)	20.9709(11)	26.0386(10)
□ (°)	90	95.769(7)	90	90
□ (°)	108.445(4)	97.078(6)	112.52(4)	100.3550(10)
γ (°)	90	94.544(7)	90	90
V (Å^3)	6243.1(5)	1262.68(18)	3118.9(5)	3292.2(3)
Z	8	2	4	4
T (K)	203(2)	203(2)	203(2)	203(2)
D_c (g.cm^{-3})	1.531	1.566	1.405	1.548
μ (mm^{-1})	0.744	0.902	0.737	0.718
Scan range (°)	2.00 < θ < 26.00	1.98 < θ < 29.23	1.97 < θ < 29.22	1.59 < θ < 25.63
Unique reflections	6130	6829	8428	6211
Reflections used [I>2σ(I)]	4828	5046	6029	5283
R_{int}	0.0355	0.0700	0.0643	0.0270
Final R indices [I>2σ(I)]*	0.0260, *w*R_2 0.0411	0.0281, *w*R_2 0.0549	0.0408, *w*R_2 0.0922	0.0216, *w*R_2 0.0543
R indices (all data)	0.0509, *w*R_2 0.0533	0.0465, *w*R_2 0.0572	0.0623, *w*R_2 0.0977	0.0276, *w*R_2 0.0554
Goodness-of-fit	0.928	0.816	0.906	1.004
Max, Min Δρ (e Å^{-3})	0.461, -0.329	0.534, -0.853	0.803, -0.981	0.355, -0.452

* Structures were refined on F_0^2: $wR_2 = [\Sigma[w (F_0^2 - F_c^2)^2] / \Sigma w (F_0^2)^2]^{1/2}$, where $w^{-1} = [\Sigma(F_0^2) + (aP)^2 + bP]$ and $P = [\max(F_0^2, 0) + 2F_c^2]/3$

Full list of authors for Reference 41c:

E.J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, J.W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, H. van Schoot, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev

 # Coordinates of the optimized structures of complexes 1-7.

Complex 1 [Ag(N∩N)(PPh3)](NO3)

1	C	0.000050	-0.000076	0.000013
2	H	0.000003	0.000019	0.000006
3	C	-0.000026	0.000024	-0.000003
4	H	-0.000001	0.000007	0.000002
5	C	-0.000002	-0.000009	-0.000020
6	H	0.000004	-0.000004	0.000001
7	C	-0.000021	-0.000020	-0.000018
8	H	-0.000019	0.000024	0.000001
9	C	-0.000057	-0.000007	0.000023
10	C	-0.000029	0.000058	-0.000045
11	C	0.000038	0.000064	-0.000024
12	C	-0.000007	-0.000024	0.000006
13	H	0.000026	-0.000003	0.000000
14	C	0.000008	0.000026	-0.000026
15	H	-0.000010	0.000005	0.000004
16	C	-0.000042	-0.000062	-0.000004
17	H	-0.000008	-0.000003	-0.000008
18	C	0.000036	0.000045	0.000034
19	H	0.000017	-0.000008	0.000032
20	C	0.000123	0.000069	0.000009
21	C	-0.000076	0.000020	-0.000006
22	C	-0.000015	0.000014	0.000045
23	H	0.000005	0.000032	-0.000012
24	C	0.000097	-0.000032	0.000030
25	H	0.000030	0.000044	-0.000018
26	C	-0.000007	0.000069	0.000073
27	H	-0.000090	-0.000066	-0.000026
28	C	0.000024	-0.000046	-0.000058
29	H	0.000020	-0.000018	0.000027
30	C	0.000027	-0.000014	-0.000086
31	H	-0.000017	-0.000041	-0.000004
32	N	0.000053	0.000085	-0.000015
33	N	-0.000044	-0.000141	0.000078
34	N	-0.000071	-0.000053	-0.000065
35	H	-0.000035	-0.000027	0.000021
36	O	-0.000041	0.000007	0.000161
37	H	0.000015	0.000030	-0.000087
38	P	0.000031	-0.000070	0.000041
39	C	0.000006	0.000023	0.000008
40	C	0.000017	-0.000001	0.000034
41	H	0.000000	0.000005	-0.000018
42	C	-0.000008	0.000025	0.000001
43	H	-0.000010	-0.000018	0.000006
44	C	0.000000	0.000024	0.000014
45	H	0.000003	0.000000	-0.000003
46	C	-0.000004	-0.000015	0.000005
47	H	0.000004	-0.000021	0.000007
48	C	-0.000028	0.000030	-0.000050
49	H	0.000016	-0.000012	0.000003
50	Ag	-0.000035	-0.000011	-0.000091
51	C	0.000009	0.000023	-0.000005
52	C	0.000109	0.000035	-0.000038
53	C	-0.000041	-0.000047	0.000010
54	C	0.000009	0.000027	-0.000011
55	C	-0.000001	-0.000042	0.000004
56	C	-0.000013	-0.000006	0.000021
57	H	-0.000054	-0.000023	0.000012
58	H	0.000013	0.000009	0.000004
59	H	-0.000002	0.000000	0.000003
60	H	-0.000008	0.000016	0.000000
61	C	-0.000007	0.000047	0.000027
62	C	-0.000006	-0.000081	-0.000042
63	C	0.000045	0.000078	0.000014
64	C	0.000000	0.000025	0.000003
65	C	-0.000030	-0.000036	-0.000022
66	C	0.000057	0.000013	-0.000027
67	H	0.000013	0.000028	0.000036
68	H	-0.000041	-0.000028	-0.000014
69	H	-0.000011	0.000003	-0.000005
70	H	0.000012	0.000013	0.000031

Complex 6 [Ag(N∩N)(POPh3)](NO3)

1	C	-0.000015	-0.000021	-0.000041
2	H	-0.000012	0.000014	0.000019
3	C	0.000005	-0.000018	0.000034
4	H	-0.000001	0.000006	-0.000008
5	C	0.000002	0.000022	-0.000012
6	H	0.000000	-0.000006	0.000001
7	C	-0.000016	-0.000017	-0.000001
8	H	-0.000011	0.000001	-0.000002
9	C	0.000070	-0.000009	0.000002
10	C	-0.000023	0.000024	0.000030
11	C	0.000035	-0.000066	0.000018
12	C	-0.000008	-0.000022	-0.000009
13	H	0.000004	0.000006	0.000020
14	C	0.000016	0.000007	-0.000007
15	H	0.000002	0.000008	-0.000004
16	C	0.000001	0.000000	-0.000014

17	H	-0.000001	0.000001	-0.000001
18	C	-0.000020	0.000012	0.000020
19	H	0.000005	-0.000012	0.000014
20	C	-0.000151	0.000045	0.000019
21	C	0.000024	0.000085	0.000010
22	C	-0.000042	0.000049	0.000138
23	H	0.000023	0.000000	0.000019
24	C	-0.000025	0.000041	0.000113
25	H	-0.000036	-0.000014	-0.000006
26	C	-0.000113	-0.000029	0.000119
27	H	0.000008	0.000004	0.000008
28	C	-0.000004	0.000015	0.000081
29	H	0.000001	-0.000003	0.000002
30	C	0.000004	0.000045	-0.000089
31	O	-0.000017	0.000151	-0.000348
32	N	-0.000049	0.000008	0.000075
33	N	0.000022	-0.000010	-0.000040
34	N	0.000021	0.000050	0.000001
35	O	-0.000062	-0.000123	-0.000090
36	O	-0.000004	-0.000043	0.000057
37	H	-0.000022	-0.000012	-0.000012
38	P	-0.000091	0.000045	0.000192
39	O	0.000016	-0.000145	-0.000050
40	Ag	-0.000135	-0.000170	-0.000089
41	H	0.000018	-0.000034	0.000000
42	H	-0.000016	-0.000009	-0.000005
43	H	0.000003	-0.000003	0.000009
44	C	0.000128	0.000060	0.000062
45	C	-0.000034	0.000004	-0.000034
46	C	-0.000013	-0.000015	-0.000009
47	C	-0.000021	0.000035	0.000006
48	C	0.000028	-0.000019	-0.000011
49	C	-0.000035	0.000001	-0.000024
50	H	-0.000006	0.000000	0.000014
51	H	-0.000005	0.000000	-0.000002
52	H	0.000008	-0.000003	-0.000007
53	H	-0.000003	0.000002	0.000009
54	C	0.000119	-0.000006	0.000007
55	C	0.000011	-0.000024	-0.000054
56	C	-0.000004	0.000011	0.000002
57	C	-0.000029	-0.000016	0.000031
58	C	0.000018	0.000019	-0.000018
59	C	-0.000011	0.000005	0.000060
60	H	0.000003	-0.000001	0.000024
61	H	0.000001	0.000007	-0.000001
62	H	0.000000	-0.000005	-0.000003
63	H	-0.000001	-0.000001	0.000001
64	C	-0.000002	0.000110	-0.000009
65	C	0.000180	-0.000086	-0.000116
66	C	0.000061	-0.000028	-0.000064
67	C	0.000023	0.000006	0.000037
68	C	-0.000012	-0.000026	0.000003
69	C	-0.000018	0.000053	-0.000006
70	H	0.000134	0.000029	-0.000019
71	H	0.000069	0.000006	-0.000038
72	H	0.000001	-0.000002	-0.000008
73	H	0.000005	0.000013	-0.000006

Complex 2 [Ag(N∩N)(PMe2Ph)](NO3)

1	C	0.000050	-0.000080	-0.000002
2	H	-0.000019	0.000037	0.000012
3	C	-0.000020	-0.000068	-0.000003
4	H	0.000016	0.000040	-0.000008
5	C	-0.000068	0.000064	-0.000080
6	H	0.000024	-0.000010	0.000017
7	C	0.000021	-0.000066	0.000029
8	H	-0.000054	-0.000049	0.000000
9	C	-0.000154	-0.000018	-0.000151
10	C	0.000126	0.000211	0.000094
11	C	0.000012	-0.000111	-0.000136
12	C	0.000007	-0.000054	0.000202
13	H	0.000156	0.000155	-0.000019
14	C	-0.000053	-0.000021	-0.000191
15	H	-0.000044	-0.000024	0.000042
16	C	-0.000002	0.000014	0.000022
17	H	0.000020	-0.000008	0.000035
18	C	0.000047	-0.000117	0.000007
19	H	-0.000010	-0.000024	-0.000126
20	C	0.000238	0.000007	-0.000108
21	C	-0.000446	0.000187	-0.000087
22	C	0.000232	0.000127	0.000129
23	H	0.000005	0.000037	0.000027
24	C	-0.000150	-0.000115	-0.000180
25	H	0.000021	0.000059	-0.000013
26	C	0.000060	0.000063	0.000159
27	H	-0.000020	-0.000007	-0.000037
28	C	0.000034	0.000041	-0.000057
29	H	-0.000040	-0.000063	-0.000023
30	C	0.000094	-0.000257	0.000074
31	C	-0.000278	0.000003	-0.000071
32	H	0.000076	-0.000023	-0.000029
33	H	0.000041	0.000027	0.000020
34	H	-0.000033	-0.000041	0.000060
35	C	0.000014	0.000229	-0.000143
36	H	0.000058	-0.000082	0.000002
37	H	0.000022	0.000027	0.000071
38	H	-0.000030	0.000032	0.000009
39	C	0.000399	-0.000274	-0.000209
40	C	-0.000041	0.000111	0.000005
41	H	-0.000073	0.000075	-0.000024
42	C	0.000079	-0.000081	-0.000012
43	H	-0.000021	0.000014	-0.000023
44	C	-0.000053	0.000056	0.000110
45	H	0.000025	-0.000013	-0.000021
46	C	0.000005	-0.000035	-0.000127
47	H	0.000024	-0.000004	0.000044
48	C	-0.000183	0.000141	0.000116
49	H	0.000057	-0.000047	-0.000022
50	Ag	-0.000343	0.000094	-0.000757
51	N	0.000292	0.000193	0.000450
52	N	-0.000053	-0.000339	0.000022
53	N	-0.000113	0.000144	0.000147
54	O	0.000088	0.000097	0.000090
55	H	-0.000035	0.000037	0.000029
56	P	-0.000006	-0.000294	0.000632

Complex 5 [Ag(N∩N)(PBu3)](NO3)

1	C	0.000078	-0.000110	0.000046
2	H	0.000002	0.000000	0.000020
3	C	-0.000042	0.000026	-0.000077
4	H	0.000001	0.000018	0.000006
5	C	0.000023	0.000005	0.000022
6	H	-0.000012	-0.000002	-0.000010
7	C	-0.000023	0.000039	0.000029
8	H	-0.000012	-0.000043	-0.000029
9	C	0.000019	0.000045	-0.000016
10	C	-0.000152	0.000065	-0.000025
11	C	0.000023	-0.000125	0.000004
12	C	-0.000061	-0.000074	0.000010
13	H	0.000017	0.000042	-0.000046
14	C	-0.000069	0.000063	-0.000066
15	H	0.000000	0.000008	0.000007
16	C	0.000077	0.000045	-0.000050
17	H	-0.000013	0.000008	-0.000012
18	C	0.000039	-0.000032	0.000109
19	H	-0.000018	-0.000028	-0.000002
20	C	0.000078	-0.000047	0.000123
21	C	0.000002	-0.000009	-0.000122

22	C	-0.000105	0.000100	0.000188
23	H	0.000006	-0.000038	-0.000054
24	C	-0.000094	-0.000059	-0.000166
25	H	-0.000009	0.000055	0.000074
26	C	0.000161	-0.000055	0.000027
27	H	-0.000098	0.000197	-0.000054
28	C	-0.000084	0.000141	0.000141
29	H	0.000213	-0.000077	-0.000035
30	C	0.000112	-0.000374	0.000101
31	H	0.000023	-0.000004	-0.000024
32	C	0.000021	0.000031	-0.000005
33	H	-0.000019	-0.000017	-0.000011
34	H	-0.000006	-0.000013	0.000012
35	H	-0.000006	0.000011	-0.000015
36	C	-0.000022	0.000010	0.000034
37	H	0.000005	-0.000002	-0.000022
38	H	-0.000006	0.000007	-0.000008
39	H	0.000017	-0.000028	-0.000004
40	O	-0.000082	0.000268	-0.000085
41	H	-0.000037	-0.000074	0.000041
42	P	0.000138	-0.000097	-0.000058
43	Ag	-0.000230	0.000026	0.000198
44	N	0.000126	-0.000033	0.000045
45	N	0.000060	0.000102	-0.000202
46	N	-0.000005	0.000074	-0.000004
47	C	-0.000072	0.000111	-0.000017
48	H	-0.000045	0.000021	0.000012
49	H	0.000032	-0.000003	0.000015
50	C	0.000016	-0.000010	-0.000021
51	H	-0.000022	-0.000021	0.000022
52	H	0.000002	-0.000016	-0.000001
53	C	-0.000050	-0.000019	0.000112
54	H	0.000030	-0.000050	-0.000043
55	H	0.000001	-0.000008	0.000000
56	C	0.000019	0.000061	-0.000001
57	H	0.000013	0.000000	-0.000014
58	H	-0.000006	-0.000010	-0.000014
59	C	-0.000015	-0.000009	-0.000024
60	H	0.000008	-0.000012	-0.000003
61	H	-0.000008	0.000014	0.000011
62	C	-0.000003	-0.000003	0.000032
63	H	-0.000001	-0.000008	-0.000001
64	H	0.000000	-0.000007	0.000000
65	C	0.000131	-0.000007	-0.000047
66	H	-0.000014	-0.000018	0.000003
67	H	-0.000013	-0.000005	-0.000039
68	C	-0.000120	-0.000032	0.000024
69	H	0.000045	-0.000017	0.000009
70	H	0.000002	0.000033	-0.000028
71	C	0.000041	-0.000028	0.000008
72	H	-0.000010	0.000009	0.000012
73	H	0.000006	0.000013	-0.000034
74	C	-0.000016	-0.000021	-0.000026
75	H	0.000004	0.000001	-0.000003
76	H	0.000009	-0.000004	0.000023

Complex 7 [Ag(NΩN)(P(OEt)3)](NO3)

1	C	0.000002	0.000022	0.000013
2	H	0.000003	-0.000004	0.000001
3	C	0.000003	0.000004	-0.000005
4	H	0.000001	-0.000003	0.000002
5	C	-0.000017	0.000004	-0.000008
6	H	0.000001	0.000003	0.000001
7	C	0.000006	0.000021	0.000037
8	H	0.000049	-0.000032	-0.000017
9	C	-0.000056	0.000001	0.000012
10	C	0.000092	-0.000019	-0.000032
11	C	0.000000	-0.000106	-0.000109
12	C	-0.000002	0.000027	0.000014
13	H	-0.000051	0.000028	0.000018
14	C	-0.000018	-0.000014	-0.000006
15	H	0.000010	-0.000008	-0.000009
16	C	0.000021	-0.000014	0.000030
17	H	-0.000002	-0.000003	-0.000003
18	C	0.000060	0.000102	-0.000071
19	H	0.000003	-0.000003	0.000040
20	C	0.000207	-0.000059	0.000054
21	C	0.000065	0.000057	0.000054
22	C	-0.000037	-0.000054	0.000018
23	H	0.000000	-0.000051	0.000026
24	C	0.000033	-0.000043	-0.000039
25	H	0.000002	-0.000003	-0.000001
26	C	-0.000022	0.000072	-0.000040
27	H	-0.000001	-0.000003	0.000014
28	C	0.000082	-0.000016	0.000013
29	H	-0.000002	-0.000064	-0.000136
30	C	-0.000232	0.000170	-0.000031
31	O	0.000017	-0.000007	-0.000044
32	H	0.000023	0.000050	0.000192
33	P	0.000028	0.000163	-0.000017
34	Ag	-0.000015	0.000042	0.000153
35	O	0.000021	-0.000085	0.000001
36	N	0.000045	-0.000040	-0.000054
37	N	-0.000098	-0.000064	-0.000076
38	N	-0.000222	0.000103	0.000100
39	O	-0.000057	-0.000124	-0.000072
40	O	0.000107	-0.000163	-0.000062
41	H	0.000032	-0.000033	0.000017
42	H	-0.000031	0.000009	0.000020
43	H	0.000028	-0.000020	0.000044
44	C	-0.000073	0.000051	-0.000036
45	H	0.000013	-0.000012	0.000006
46	H	0.000007	0.000030	-0.000020
47	C	-0.000008	0.000044	-0.000024
48	H	0.000010	-0.000023	0.000028
49	H	-0.000015	-0.000013	0.000025
50	C	0.000022	0.000014	0.000073
51	H	0.000015	0.000011	-0.000008
52	H	-0.000050	0.000031	-0.000037
53	C	-0.000012	0.000010	-0.000035
54	H	0.000015	-0.000027	-0.000006
55	H	-0.000003	0.000001	0.000000
56	C	0.000034	0.000035	0.000016
57	H	0.000016	-0.000017	0.000014
58	H	0.000008	0.000007	0.000000
59	C	-0.000031	0.000022	-0.000011
60	H	-0.000007	0.000013	0.000009
61	H	-0.000022	-0.000022	-0.000034

Complex 4 [Ag(NΩN)(P(p-tolyl)3)](NO3)

1	C	0.000020	0.000066	-0.000010
2	H	0.000018	-0.000027	-0.000014
3	C	0.000007	0.000012	-0.000014
4	H	0.000002	-0.000003	-0.000003
5	C	-0.000002	-0.000006	0.000016
6	H	0.000005	-0.000010	-0.000006
7	C	-0.000001	0.000020	0.000035
8	H	-0.000017	0.000036	0.000000
9	C	0.000006	-0.000141	-0.000030
10	C	-0.000037	0.000032	0.000012
11	C	0.000020	-0.000042	-0.000068
12	C	-0.000023	0.000066	0.000032
13	H	0.000010	-0.000020	-0.000032
14	C	-0.000004	-0.000023	0.000017
15	H	-0.000007	-0.000007	-0.000002
16	C	-0.000007	-0.000009	0.000036
17	H	0.000002	-0.000011	-0.000002
18	C	-0.000009	0.000041	-0.000066

19	H	-0.000002	-0.000004	0.000010
20	C	0.000066	-0.000031	0.000069
21	C	0.000139	0.000045	0.000014
22	C	-0.000144	-0.000062	0.000060
23	H	0.000078	-0.000044	0.000023
24	C	0.000010	-0.000007	-0.000051
25	H	-0.000013	0.000037	-0.000011
26	C	-0.000034	-0.000002	-0.000027
27	H	-0.000001	0.000000	0.000007
28	C	-0.000005	0.000022	0.000010
29	H	-0.000067	-0.000017	-0.000019
30	C	0.000063	-0.000043	0.000004
31	H	0.000000	-0.000011	0.000002
32	N	-0.000116	0.000027	-0.000074
33	N	0.000003	-0.000025	-0.000021
34	N	-0.000043	0.000025	-0.000031
35	H	0.000045	-0.000034	-0.000046
36	O	0.000002	0.000082	0.000037
37	H	0.000036	0.000008	0.000003
38	P	0.000029	-0.000056	-0.000101
39	C	-0.000003	0.000039	-0.000040
40	C	-0.000017	-0.000038	0.000024
41	H	0.000014	0.000001	-0.000002
42	C	-0.000005	0.000004	0.000009
43	H	-0.000004	0.000006	0.000002
44	C	-0.000011	-0.000028	-0.000002
45	H	-0.000002	-0.000001	-0.000004
46	C	-0.000001	0.000054	0.000025
47	H	-0.000001	0.000001	-0.000008
48	C	0.000011	-0.000046	0.000032
49	H	0.000001	0.000012	-0.000005
50	Ag	0.000041	0.000037	0.000152
51	C	-0.000023	-0.000050	0.000097
52	C	-0.000019	-0.000036	0.000024
53	C	0.000042	0.000030	0.000010
54	C	-0.000029	0.000011	0.000001
55	C	-0.000009	0.000026	0.000059
56	C	-0.000017	0.000109	-0.000110
57	H	0.000004	-0.000004	-0.000004
58	H	-0.000007	-0.000006	0.000007
59	H	-0.000004	0.000002	-0.000004
60	H	-0.000009	-0.000006	-0.000016
61	C	0.000020	-0.000001	0.000008
62	C	0.000053	0.000053	-0.000027
63	C	-0.000053	0.000001	-0.000051
64	C	0.000009	-0.000032	0.000013
65	C	-0.000059	-0.000033	-0.000002
66	C	0.000036	0.000040	0.000034
67	H	-0.000052	-0.000030	-0.000005
68	H	0.000034	0.000024	0.000025
69	H	-0.000001	-0.000007	-0.000019
70	H	0.000021	-0.000009	-0.000020
71	C	0.000002	-0.000003	0.000022
72	H	-0.000002	0.000013	0.000019
73	H	-0.000005	0.000005	-0.000010
74	C	-0.000025	-0.000020	0.000002
75	H	0.000020	-0.000004	-0.000004
76	H	0.000012	0.000002	0.000023
77	C	-0.000004	0.000020	-0.000019
78	H	0.000002	-0.000014	-0.000002
79	H	0.000010	-0.000006	0.000011

Complex 3 [Ag(N∩N)(PMePh2)](NO3)

1	Ag	-0.000139	0.000436	-0.000082
2	P	-0.000171	-0.000214	0.000149
3	H	0.000012	0.000009	0.000011
4	N	0.000172	-0.000245	-0.000227
5	N	0.000137	-0.000183	0.000259
6	C	0.000096	-0.000019	0.000028
7	C	-0.000071	-0.000031	-0.000032
8	C	-0.000017	0.000001	0.000026
9	C	-0.000015	-0.000016	-0.000009
10	C	0.000043	0.000054	-0.000005
11	C	-0.000005	-0.000029	-0.000036
12	C	-0.000076	0.000032	-0.000099
13	C	0.000105	-0.000016	0.000059
14	C	0.000084	0.000072	0.000025
15	C	-0.000119	0.000000	-0.000023
16	C	0.000071	-0.000011	0.000081
17	C	-0.000064	0.000057	-0.000059
18	C	-0.000051	-0.000094	0.000022
19	C	0.000039	-0.000052	-0.000086
20	C	0.000011	0.000056	0.000060
21	C	-0.000003	0.000033	0.000010
22	H	0.000048	-0.000056	0.000003
23	C	0.000020	0.000026	0.000024
24	C	-0.000052	0.000027	-0.000041
25	C	-0.000024	0.000165	0.000319
26	C	0.000067	-0.000002	-0.000083
27	C	-0.000094	0.000031	0.000006
28	C	0.000067	0.000005	0.000015
29	C	0.000032	-0.000061	-0.000016
30	C	-0.000132	0.000046	-0.000012
31	C	-0.000041	0.000021	0.000021
32	C	0.000072	0.000076	-0.000003
33	C	0.000009	0.000067	0.000029
34	C	-0.000031	-0.000079	-0.000027
35	C	0.000015	0.000034	-0.000045
36	C	0.000086	-0.000030	-0.000004
37	N	-0.000047	-0.000011	-0.000042
38	C	-0.000033	0.000027	-0.000146
39	H	-0.000043	0.000018	0.000061
40	H	0.000008	0.000027	0.000016
41	H	0.000047	0.000045	-0.000023
42	H	0.000001	0.000001	0.000015
43	H	0.000005	0.000010	-0.000007
44	H	-0.000028	-0.000024	0.000025
45	H	0.000013	0.000001	-0.000005
46	H	-0.000023	0.000004	-0.000010
47	H	-0.000010	-0.000025	-0.000013
48	H	0.000015	-0.000001	0.000000
49	H	0.000006	-0.000003	0.000016
50	H	0.000058	-0.000009	-0.000010
51	H	-0.000007	0.000002	0.000021
52	H	-0.000022	0.000017	-0.000017
53	H	-0.000013	-0.000029	-0.000082
54	H	-0.000010	-0.000035	-0.000045
55	H	0.000002	-0.000001	0.000044
56	H	-0.000018	-0.000027	0.000006
57	H	0.000004	0.000000	0.000007
58	H	0.000008	-0.000004	0.000003
59	H	-0.000013	-0.000015	-0.000005
60	H	-0.000010	-0.000009	0.000002
61	H	-0.000021	-0.000045	-0.000027
62	O	0.000013	-0.000069	-0.000046
63	H	0.000036	0.000045	0.000006

Complex [Ag(phen)(PPh3)](NO3)

1	H	0.000016	0.000002	-0.000007
2	H	-0.000026	0.000022	0.000001
3	P	0.000206	-0.000156	0.000100
4	H	-0.000006	0.000069	0.000020
5	H	0.000030	0.000001	-0.000010
6	C	0.000065	0.000036	0.000036
7	C	-0.000097	0.000035	0.000036
8	C	-0.000002	0.000012	0.000011
9	C	0.000013	-0.000029	-0.000017

10	C	-0.000067	-0.000007	0.000005
11	N	0.000006	-0.000062	0.000058
12	C	0.000042	0.000014	0.000009
13	H	0.000008	-0.000008	-0.000005
14	H	-0.000004	0.000005	0.000004
15	H	0.000023	-0.000017	-0.000012
16	C	0.000216	-0.000046	-0.000021
17	C	-0.000052	-0.000012	0.000013
18	C	-0.000022	0.000025	-0.000013
19	C	0.000074	-0.000026	0.000001
20	C	-0.000203	-0.000023	0.000042
21	N	0.000101	0.000136	-0.000088
22	C	-0.000014	-0.000007	-0.000005
23	H	0.000012	0.000004	0.000002
24	H	0.000003	-0.000004	-0.000006
25	H	-0.000048	0.000020	-0.000006
26	Ag	-0.000139	-0.000006	-0.000070
27	H	-0.000022	-0.000013	0.000000
28	C	-0.000036	-0.000014	-0.000075
29	C	-0.000040	0.000051	-0.000028
30	C	-0.000033	-0.000009	0.000031
31	C	0.000040	0.000003	-0.000019
32	C	0.000023	-0.000017	-0.000038
33	C	0.000003	0.000025	0.000043
34	H	-0.000003	0.000007	0.000031
35	H	0.000004	0.000002	0.000020
36	H	-0.000009	0.000007	-0.000014
37	H	-0.000016	0.000004	-0.000010
38	C	-0.000020	0.000052	-0.000017
39	C	0.000025	-0.000031	-0.000024
40	C	-0.000058	-0.000013	0.000023
41	C	0.000004	0.000025	-0.000025
42	C	0.000051	0.000044	0.000009
43	C	-0.000039	-0.000072	0.000039
44	H	-0.000017	-0.000030	-0.000002
45	H	0.000014	0.000014	-0.000017
46	H	-0.000005	-0.000003	0.000009
47	H	-0.000011	-0.000011	-0.000008
48	C	-0.000024	-0.000013	0.000021
49	C	-0.000019	0.000006	0.000004
50	C	0.000009	0.000004	-0.000046
51	C	-0.000001	-0.000019	0.000013
52	C	0.000005	0.000008	0.000010
53	C	0.000048	-0.000016	-0.000007
54	H	-0.000017	0.000018	-0.000009
55	H	0.000002	0.000008	0.000002
56	H	0.000005	0.000003	0.000001
57	H	0.000004	0.000000	0.000001