Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Luminescent Isomeric Pr-Ag Coordination Polymers Immobilized with Organic Sensitizer and Ag-S Clusters

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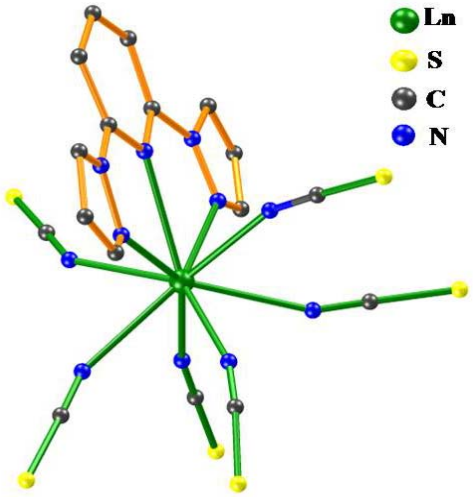


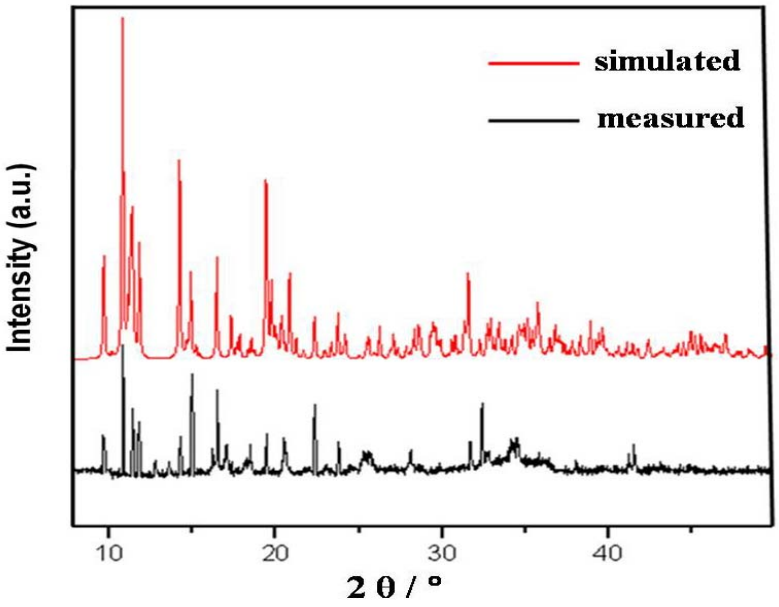
Fig. S1 Anionic coordination unit of $[PrL(SCN)_6]^{3-}$ showing all N atoms bonded to Pr^{III} ion exclusively in **1** and **2**.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for 1-2

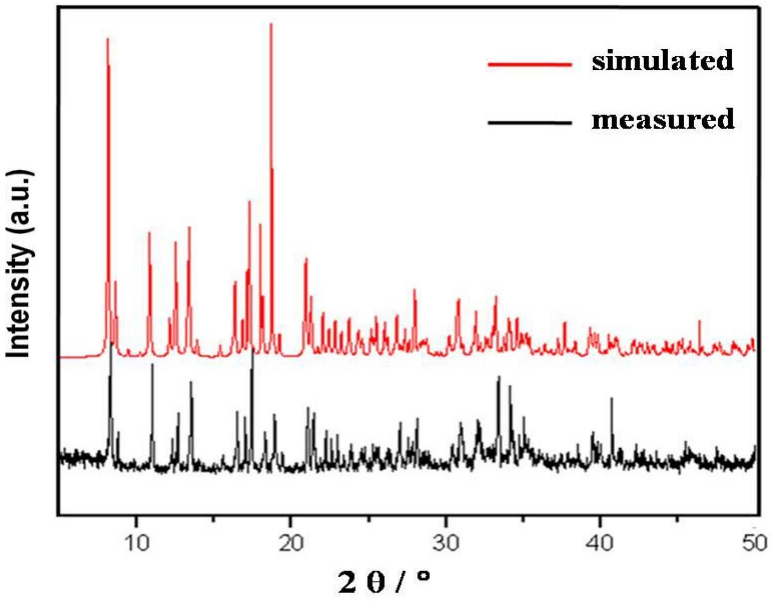
1		2	
Pr(1)-N(9)	2.532(4)	Pr(1)-N(10)	2.531(5)
Pr(1)-N(11)	2.569(4)	Pr(1)-N(11)#1	2.536(4)
Pr(1)-N(8)	2.572(4)	Pr(1)-N(1)	2.561(4)
Pr(1)-N(6)	2.586(4)	Pr(1)-N(6)#2	2.575(4)
Pr(1)-N(5)	2.597(4)	Pr(1)-N(5)	2.604(4)
Pr(1)-N(1)	2.605(3)	Pr(1)-N(9)	2.611(5)
Pr(1)-N(7)	2.606(4)	Pr(1)-N(8)	2.624(4)
Pr(1)-N(10)	2.619(4)	Pr(1)-N(7)#2	2.625(4)
Pr(1)-N(3)	2.710(3)	Pr(1)-N(3)	2.714(4)
Ag(1)-Ag(1)#3	3.0138(8)	Ag(1)-Ag(2)	3.4992(3)
Ag(1)-Ag(3)	3.1730(6)	Ag(1)-Ag(3)	4.3630(6)
Ag(2)-Ag(3)#5	2.9444(6)	Ag(2)-Ag(3)	3.5398(2)
Ag(1)-S(4)#1	2.5329(12)	Ag(1)-S(2)	2.5721(15)
Ag(1)-S(1)	2.5549(12)	Ag(1)-S(4)#3	2.5786(16)
Ag(1)-S(2)	2.5795(11)	Ag(1)-S(1)	2.6268(15)
Ag(1)-S(4)#2	2.7926(12)	Ag(1)-S(3)	2.6453(16)
Ag(2)-S(6)#4	2.5401(14)	Ag(2)-S(3)#4	2.5086(17)
Ag(2)-S(1)#5	2.6384(12)	Ag(2)-S(1)	2.5269(15)
Ag(2)-S(3)	2.6755(13)	Ag(2)-S(5)	2.6086(15)
Ag(2)-S(5)	2.7463(13)	Ag(3)-S(6)	2.5350(15)
Ag(3)-S(2)	2.5770(11)	Ag(3)-S(5)	2.5684(14)
Ag(3)-S(3)#6	2.6131(12)	Ag(3)-S(4)	2.6599(17)
Ag(3)-S(5)#6	2.6615(12)	Ag(3)-S(2)	2.6933(16)
Ag(3)-S(2)#7	2.7275(11)		
N(9)-Pr(1)-N(11)	74.54(13)	N(10)-Pr(1)-N(11)#1	99.25(17)
N(9)-Pr(1)-N(8)	96.44(14)	N(10)-Pr(1)-N(1)	144.07(15)
N(11)-Pr(1)-N(8)	139.91(12)	N(11)#1-Pr(1)-N(1)	77.74(15)
N(9)-Pr(1)-N(6)	138.81(13)	N(10)-Pr(1)-N(6)#2	141.82(15)
N(11)-Pr(1)-N(6)	135.60(12)	N(11)#1-Pr(1)-N(6)#2	75.05(15)
N(8)-Pr(1)-N(6)	75.82(13)	N(1)-Pr(1)-N(6)#2	72.72(15)
N(9)-Pr(1)-N(5)	150.38(13)	N(10)-Pr(1)-N(5)	84.07(16)
N(11)-Pr(1)-N(5)	89.11(12)	N(11)#1-Pr(1)-N(5)	142.09(14)
N(8)-Pr(1)-N(5)	80.16(13)	N(1)-Pr(1)-N(5)	120.36(14)
N(6)-Pr(1)-N(5)	69.26(12)	N(6)#2-Pr(1)-N(5)	79.35(15)
N(9)-Pr(1)-N(1)	78.99(13)	N(10)-Pr(1)-N(9)	72.56(16)
N(11)-Pr(1)-N(1)	72.40(12)	N(11)#1-Pr(1)-N(9)	73.41(15)
N(8)-Pr(1)-N(1)	145.39(12)	N(1)-Pr(1)-N(9)	72.32(14)
N(6)-Pr(1)-N(1)	85.24(13)	N(6)#2-Pr(1)-N(9)	136.80(15)
N(5)-Pr(1)-N(1)	119.93(11)	N(5)-Pr(1)-N(9)	141.37(14)
N(9)-Pr(1)-N(7)	70.80(13)	N(10)-Pr(1)-N(8)	71.54(15)

N(11)-Pr(1)-N(7)	133.87(13)	N(11)#1-Pr(1)-N(8)	145.93(15)
N(8)-Pr(1)-N(7)	74.23(13)	N(1)-Pr(1)-N(8)	90.86(15)
N(6)-Pr(1)-N(7)	68.16(12)	N(6)#2-Pr(1)-N(8)	132.29(14)
N(5)-Pr(1)-N(7)	134.33(13)	N(5)-Pr(1)-N(8)	71.05(14)
N(1)-Pr(1)-N(7)	71.89(12)	N(9)-Pr(1)-N(8)	72.54(15)
N(9)-Pr(1)-N(10)	79.04(13)	N(10)-Pr(1)-N(7)#2	72.78(15)
N(11)-Pr(1)-N(10)	72.14(12)	N(11)#1-Pr(1)-N(7)#2	74.83(15)
N(8)-Pr(1)-N(10)	67.79(12)	N(1)-Pr(1)-N(7)#2	137.54(14)
N(6)-Pr(1)-N(10)	130.55(13)	N(6)#2-Pr(1)-N(7)#2	69.29(14)
N(5)-Pr(1)-N(10)	72.41(12)	N(5)-Pr(1)-N(7)#2	70.17(14)
N(1)-Pr(1)-N(10)	142.07(12)	N(9)-Pr(1)-N(7)#2	127.61(15)
N(7)-Pr(1)-N(10)	127.70(13)	N(8)-Pr(1)-N(7)#2	129.05(15)
N(9)-Pr(1)-N(3)	129.91(12)	N(10)-Pr(1)-N(3)	132.74(15)
N(11)-Pr(1)-N(3)	66.62(11)	N(11)#1-Pr(1)-N(3)	128.00(14)
N(8)-Pr(1)-N(3)	133.66(12)	N(1)-Pr(1)-N(3)	60.24(13)
N(6)-Pr(1)-N(3)	68.99(11)	N(6)#2-Pr(1)-N(3)	64.70(13)
N(5)-Pr(1)-N(3)	59.92(11)	N(5)-Pr(1)-N(3)	60.26(14)
N(1)-Pr(1)-N(3)	60.25(11)	N(9)-Pr(1)-N(3)	116.07(14)
N(7)-Pr(1)-N(3)	116.72(11)	N(8)-Pr(1)-N(3)	68.25(13)
N(10)-Pr(1)-N(3)	115.46(11)	N(7)#2-Pr(1)-N(3)	116.31(13)
S(4)#1-Ag(1)-S(1)	109.30(4)	S(2)-Ag(1)-S(4)#3	127.93(6)
S(4)#1-Ag(1)-S(2)	116.49(4)	S(2)-Ag(1)-S(1)	112.34(5)
S(1)-Ag(1)-S(2)	124.49(4)	S(4)#3-Ag(1)-S(1)	106.49(5)
S(4)#1-Ag(1)-S(4)#2	111.27(3)	S(2)-Ag(1)-S(3)	98.26(5)
S(1)-Ag(1)-S(4)#2	95.20(4)	S(4)#3-Ag(1)-S(3)	106.85(6)
S(2)-Ag(1)-S(4)#2	95.90(3)	S(1)-Ag(1)-S(3)	101.26(6)
S(6)#4-Ag(2)-S(1)#5	100.42(4)	S(3)#4-Ag(2)-S(1)	136.15(5)
S(6)#4-Ag(2)-S(3)	122.82(5)	S(3)#4-Ag(2)-S(5)	109.72(6)
S(1)#5-Ag(2)-S(3)	116.56(4)	S(1)-Ag(2)-S(5)	105.12(4)
S(6)#4-Ag(2)-S(5)	112.38(5)	S(6)-Ag(3)-S(5)	101.32(5)
S(1)#5-Ag(2)-S(5)	103.24(4)	S(6)-Ag(3)-S(4)	114.68(6)
S(3)-Ag(2)-S(5)	100.24(4)	S(5)-Ag(3)-S(4)	127.18(5)
S(2)-Ag(3)-S(3)#6	123.64(4)	S(6)-Ag(3)-S(2)	127.12(5)
S(2)-Ag(3)-S(5)#6	121.90(4)	S(5)-Ag(3)-S(2)	92.76(4)
S(3)#6-Ag(3)-S(5)#6	104.15(4)	S(4)-Ag(3)-S(2)	94.62(5)
S(2)-Ag(3)-S(2)#7	100.06(3)		
S(3)#6-Ag(3)-S(2)#7	104.30(4)		
S(5)#6-Ag(3)-S(2)#7	97.72(4)		

Symmetry codes:		Symmetry codes:	
#1 x+1, y-1, z	#2 -x+1, -y+2, -z	#1 -x-1/2, y-1/2, -z+3/2	#2 x+1/2, -y+1/2, z-1/2
#3 -x+2, -y+1, -z	#4 x+1, y, z	#3 x+1/2, -y+1/2, z+1/2	#4 -x, -y+1, -z+2
#5 x, y+1, z	#6 x, y-1, z	#5 x-1/2, -y+1/2, z+1/2	#6 -x-1/2, y+1/2, -z+3/2
#7 -x+1, -y+1, -z		#7 x-1/2, -y+1/2, z-1/2	



(a)



(b)

Fig. S2 X-ray Powder diffraction patterns of **1** (a) and **2** (b).

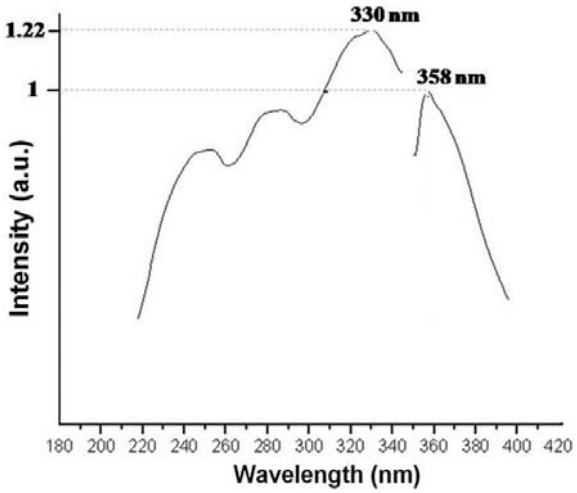


Fig. S3 Excitation and emission spectra of **L** in the solid state.

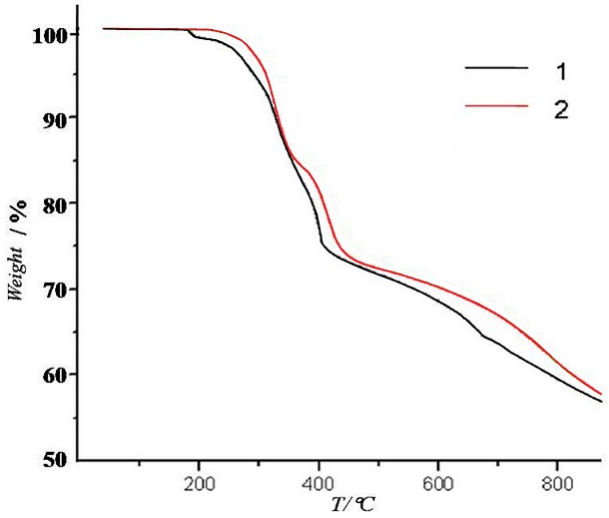


Fig. S4 TGA plots of **1-2**