Electronic Supplementary Information for Dalton Transactions

Heteroleptic ytterbium(II) complexes supported by a bulky β-diketiminato ligand

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Supplementary Information:

The results of the ^{1}H pulsed gradient spin-echo (PGSE) NMR diffusion measurements of complexes **5** and **8** (experimental details were described in: I. Fernández, E. Martínez-Viviente and P. S. Pregosin, *Inorg. Chem.,* 2005, **44**, 5509)

Table 1S Diffusion coefficients D ($\times 10^{10}$ m^2 s^{-1}) and r_H (Å) values[a] of [Yb(L^1)(NHAr*)(thf)]·PhMe (**5**) in toluene-d_8 at 299 K

Nucleus	D [b]	r_H [c]	r [d]
^{1}H (L^1)	6.26	6.2	
^{1}H (C_4H_8O)	6.33	6.2	2.0
^{1}H (NHAr*)	6.26	6.2	
^{1}H (C_7H_8)	19.9	2.0	2.4

[a] All at 54 mM.

[b] Experimental error is *ca.* ± 2%.

[c] Standard deviation is *ca.* ± 0.1 Å; η (toluene, 299 K) = 0.5601×10^{-3} Kg s^{-1} m^{-1}.

[d] Estimated using Chem3D by averaging the distances between the centroid and the outer hydrogen.

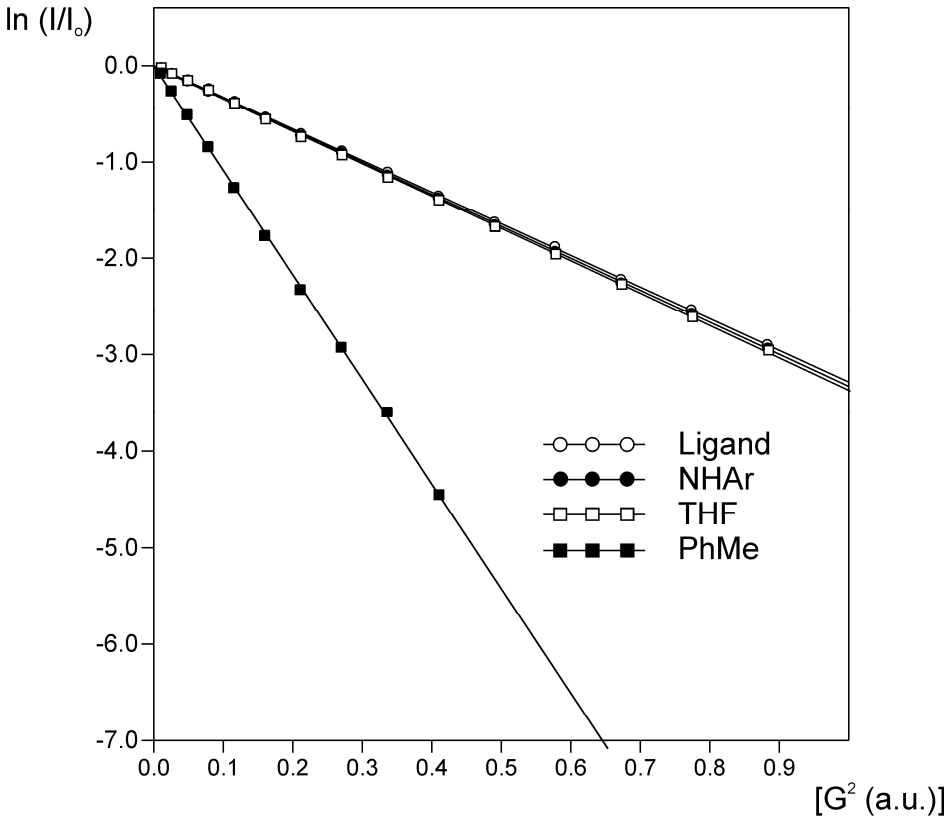

Fig. 1S Plot of the ln (I/I_o) vs. arbitrary units proportional to the square of the gradient amplitude for ^{1}H PGSE diffusion measurements on a 54 mM sample of **5** in toluene-d_8 at 299 K. ^{1}H (δ = 2 ms; Δ = 68 ms). [Ligand = {N($C_6H_3Pr^i_2$-2,6)C(Me)}$_2$CH]

Table 2S Diffusion coefficients D ($\times 10^{10}$ m^2 s^{-1}) and r_H (Å) values[a] of [Yb(L^1){η^5-C$_6$H$_5$CPh$_2$}(thf)] (**8**) in toluene-d_8 at 299 K

Nucleus	D [b]	r_H [c]	r [d]
^{1}H (L^1)	5.35	7.3	
^{1}H (C$_4$H$_8$O)	5.32	7.3	2.0
^{1}H (Ph$_3$C$^-$)	5.33	7.3	
^{1}H (C$_7$H$_8$)	19.08	2.0	2.4

[a] All at 0.1 M.

[b] Experimental error is *ca.* ± 2%.

[c] Standard deviation is *ca.* ± 0.1 Å; η (toluene, 299 K) = 0.5601 × 10^{-3} Kg s^{-1} m^{-1}.

[d] Estimated using Chem3D by averaging the distances between the centroid and the outer hydrogen.

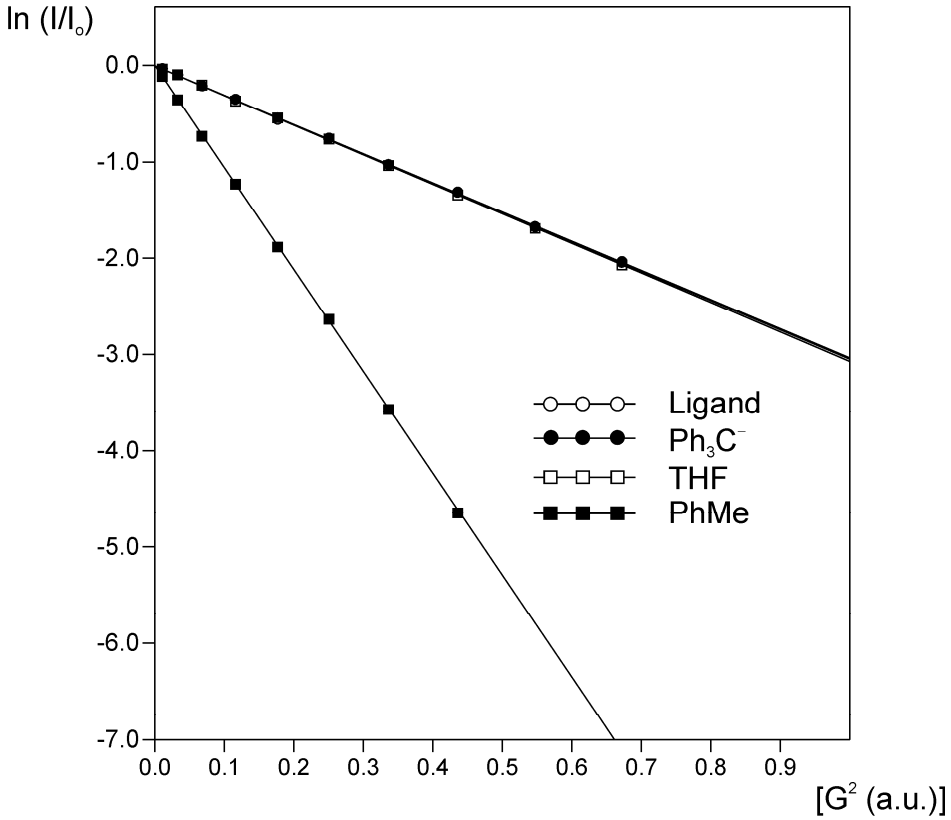

Fig. 2S Plot of the ln (I/I_o) vs. arbitrary units proportional to the square of the gradient amplitude for ^{1}H PGSE diffusion measurements on a 0.1 M sample of **8** in toluene-d_8 at 299 K. ^{1}H (δ = 2 ms; Δ = 68 ms). [Ligand = {N(C$_6$H$_3$Pr$^i_2$-2,6)C(Me)}$_2$CH]

Table 2S Diffusion coefficients D ($\times 10^{10}$ m^2 s^{-1}) and r_H (Å) values[a] of [Yb(L^1){η^5-C$_6$H$_5$CPh$_2$}(thf)] (**8**) in thf-d_8 at 299 K

Nucleus	D [b]	r_H [c]	r [d]
^{1}H (L^1)	7.86	6.0	
^{1}H (C$_4$H$_8$O)	23.4	2.0	2.0
^{1}H (Ph$_3$C$^-$)	7.44	6.4	

[a] All at 0.1 M.

[b] Experimental error is *ca.* ± 2%.

[c] Standard deviation is *ca.* ± 0.1 Å; η (thf, 299 K) = 0.461 × 10^{-3} Kg s^{-1} m^{-1}.

[d] Estimated using Chem3D by averaging the distances between the centroid and the outer hydrogen.

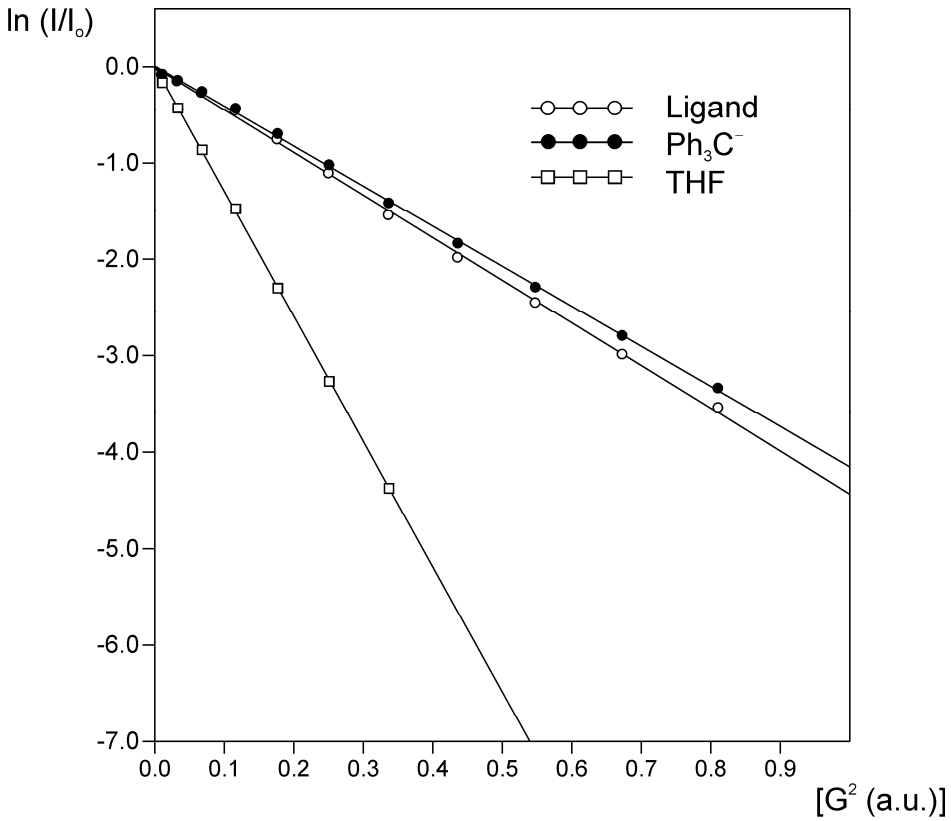

Fig. 3S Plot of the ln (I/I_o) vs. arbitrary units proportional to the square of the gradient amplitude for ^{1}H PGSE diffusion measurements on a 0.1 M sample of **8** in thf-d_8 at 299 K. ^{1}H (δ = 2 ms; Δ = 68 ms). [Ligand = {N(C$_6$H$_3$Pr$^i_2$-2,6)C(Me)}$_2$CH]