Electronic supplementary information (ESI)

DERIVATION OF NOVEL EQUATIONS FOR MODEL-FREE ANALYSIS OF LANTHANIDE INDUCED SHIFTS

Given: $\Delta\delta_k = \langle S_Z \rangle_{\mathrm{Ln}} \cdot F_k + D_{\mathrm{Ln}} \cdot A_2^0 \cdot G_k$

Division of both sides by D_{Ln} produces

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_k + A_2^0 \cdot G_k$$

Expression of A_2^0 for atoms *k* and *l* from eqn. (esi2) produces

$$\begin{cases} A_2^0 = \dfrac{1}{G_k} \cdot \left(\dfrac{\Delta\delta_k}{D_{\mathrm{Ln}}} - \dfrac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_k \right) \\ A_2^0 = \dfrac{1}{G_l} \cdot \left(\dfrac{\Delta\delta_l}{D_{\mathrm{Ln}}} - \dfrac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_l \right) \end{cases}$$

Setting right sides of expressions equal produces

$$\frac{1}{G_k} \cdot \left(\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} - \frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_k \right) = \frac{1}{G_l} \cdot \left(\frac{\Delta\delta_l}{D_{\mathrm{Ln}}} - \frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_l \right)$$

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot \left(F_k - F_l \cdot R_{kl} \right) + \frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot R_{kl}, \quad R_{kl} = \frac{G_k}{G_l}$$

eqn. (8) from original manuscript

Expression of $\frac{\langle S_Z \rangle_{Ln}}{D_{\mathrm{Ln}}}$ from $\frac{\Delta\delta_l}{D_{\mathrm{Ln}}} = \frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_l + A_2^0 \cdot G_l$ produces

$$\frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} = \frac{1}{F_l}\left(\frac{\Delta\delta_l}{D_{\mathrm{Ln}}} - A_2^0 \cdot G_l\right)$$

Substitution of $\frac{\langle S_Z \rangle_{Ln}}{D_{\mathrm{Ln}}}$ in $\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\langle S_Z \rangle_{\mathrm{Ln}}}{D_{\mathrm{Ln}}} \cdot F_k + A_2^0 \cdot G_k$ produces

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{F_k}{F_l}\left(\frac{\Delta\delta_l}{D_{\mathrm{Ln}}} - A_2^0 \cdot G_l\right) + A_2^0 \cdot G_k$$

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot \frac{F_k}{F_l} + A_2^0 \cdot \left(G_k - G_l \cdot \frac{F_k}{F_l}\right)$$

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot \Phi_{kl} + A_2^0 \cdot \Gamma_{kl}, \quad \Phi_{kl} = \frac{F_k}{F_l}, \quad \Gamma_{kl} = \left(G_k - G_l \cdot \frac{F_k}{F_l}\right)$$

eqns. (9)-(11) from original manuscript

Expression of A_2^0 for pairs of atoms *kl* and *lm* from eqn.(9) produces

$$\begin{cases} A_2^0 = \frac{1}{\Gamma_{kl}}\left(\frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot \Phi_{kl} - \frac{\Delta\delta_k}{D_{\mathrm{Ln}}}\right) \\ A_2^0 = \frac{1}{\Gamma_{lm}}\left(\frac{\Delta\delta_m}{D_{\mathrm{Ln}}} \cdot \Phi_{kl} - \frac{\Delta\delta_l}{D_{\mathrm{Ln}}}\right) \end{cases}$$

Setting right sides of expressions equal and subsequent rearrangements produce

$$\frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot \Phi_{kl} - \frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\Gamma_{kl}}{\Gamma_{lm}}\left(\frac{\Delta\delta_m}{D_{\mathrm{Ln}}} \cdot \Phi_{kl} - \frac{\Delta\delta_l}{D_{\mathrm{Ln}}}\right)$$

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot \Phi_{kl} + \frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot \frac{\Gamma_{kl}}{\Gamma_{lm}} - \frac{\Delta\delta_m}{D_{\mathrm{Ln}}} \cdot \frac{\Gamma_{kl}}{\Gamma_{lm}} \cdot \Phi_{kl}$$

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\Delta\delta_l}{D_{\mathrm{Ln}}}\left(\Phi_{kl} + \frac{\Gamma_{kl}}{\Gamma_{lm}}\right) - \frac{\Delta\delta_m}{D_{\mathrm{Ln}}}\left(\frac{\Gamma_{kl}}{\Gamma_{lm}} \cdot \Phi_{kl}\right)$$

$$\frac{\Delta\delta_k}{D_{\mathrm{Ln}}} = \frac{\Delta\delta_l}{D_{\mathrm{Ln}}} \cdot S_{klm} - \frac{\Delta\delta_m}{D_{\mathrm{Ln}}} \cdot M_{klm}, \quad S_{klm} = \left(\Phi_{kl} + \frac{\Gamma_{kl}}{\Gamma_{lm}}\right), \quad M_{klm} = \left(\frac{\Gamma_{kl}}{\Gamma_{lm}} \cdot \Phi_{kl}\right)$$

eqns. (12)-(14) from original manuscript

Table S1 Values of S_{klm} and M_{klm} for (Nd-Eu) and (Tb-Yb) subfamilies of (Pc)M[(15C5)$_4$Pc]M(Pc) in $CDCl_3$ at 298K

klm	S_{klm}	M_{klm}	S_{klm}	M_{klm}
	(Nd-Eu)		(Tb-Yb)	
123	3.875	-1.368	2.336	0.665
124	-5.364	6.568	2.356	0.328
125	1.907	1.588	2.308	0.661
126	1.849	2.565	1.364	3.165
127	2.244	2.054	1.349	3.542
134	-0.827	2.771	0.914	1.794
135	1.43	3.04	0.871	3.263
136	1.261	4.892	0.697	5.272
137	2.049	4.622	0.661	5.895
145	1.76	1.107	0.503	3.17
146	1.755	1.714	0.417	5.12
147	1.947	1.418	0.421	5.655
156	-4.334	13.178	-6.281	15.942
157	8.626	-8.046	-2.165	10.635
167	9.703	-3.803	1.97	4.762
234	0.155	0.707	0.105	0.769
235	0.731	0.777	0.108	1.378
236	0.679	1.261	0.035	2.226
237	0.898	1.167	0.026	2.48
245	0.897	-0.208	0.09	1.317
246	0.899	-0.323	0.059	2.114
247	0.862	-0.266	0.067	2.315
256	-4.869	9.622	1.006	0.728
257	3.972	-4.735	1.884	-0.691
267	4.54	-2.867	10.596	-9.211
345	1.228	-1.348	0.495	0.043
346	1.324	-2.335	0.478	0.113
347	0.952	-1.571	0.468	0.156
356	-7.107	12.214	-13.399	22.062
357	4.259	-6.273	-7.796	14.877
367	4.81	-4.201	-12.953	15.928
456	-4.638	9.867	-16.278	27.823
457	4.556	-5.09	-6.883	14.791
467	5.184	-2.919	7.333	-5.062
567	1.167	0.442	3.147	-1.779