Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A Coupling between a photo-excited cyclic π system and the 4f electronic system in a lanthanide single molecule magnet

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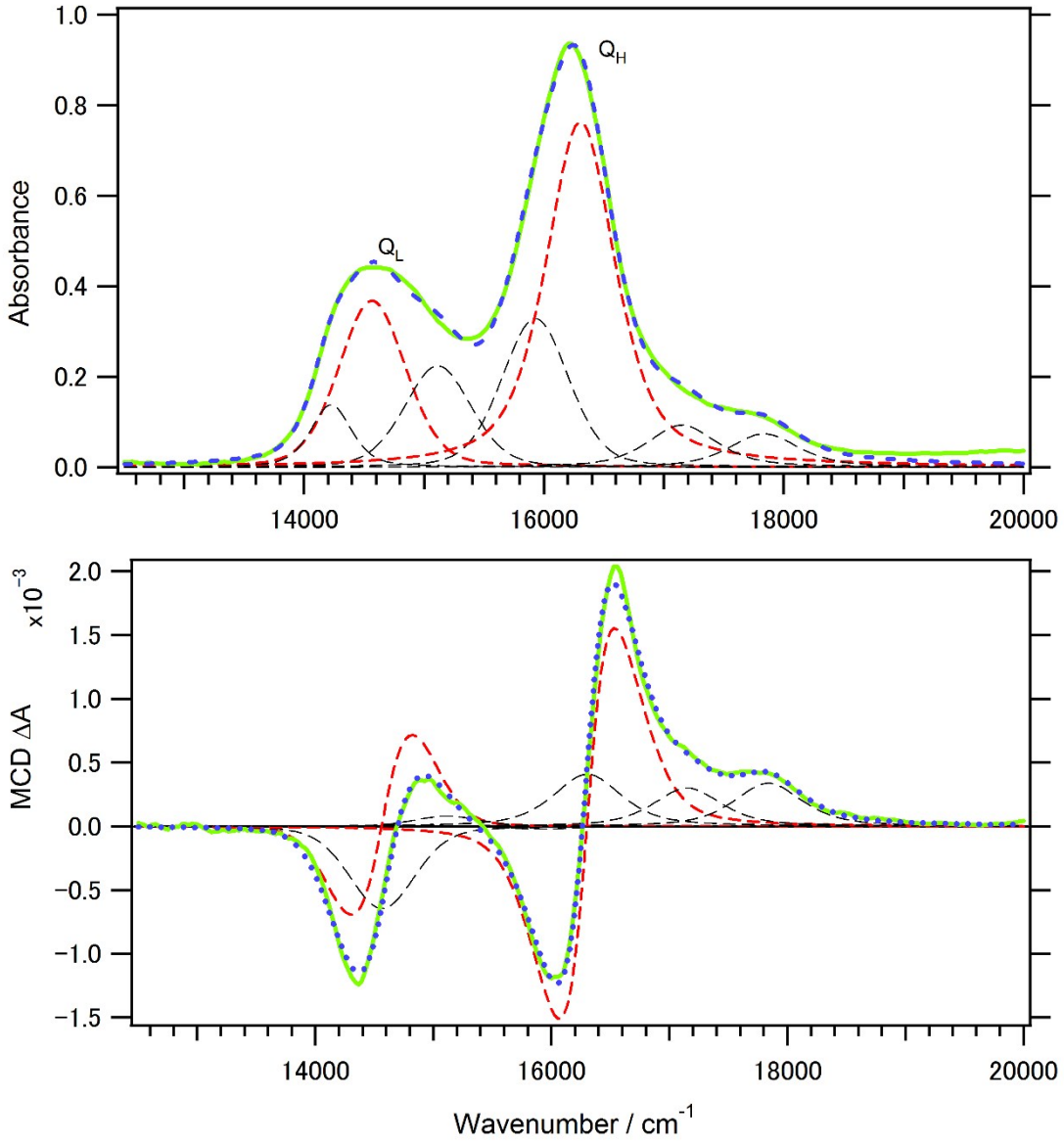

Figure S1 Results of band deconvolution of absorption (top) and MCD (bottom) spectra of Pc_2Y^- doped in PMMA measured at 1.5K under a magnetic field of 1T. Observed spectra are shown in solid lines (green). A-term components are shown in thick broken lines (red) and B-term components in thin broken lines (black). The Sum of these components are shown in dotted lines (blue).

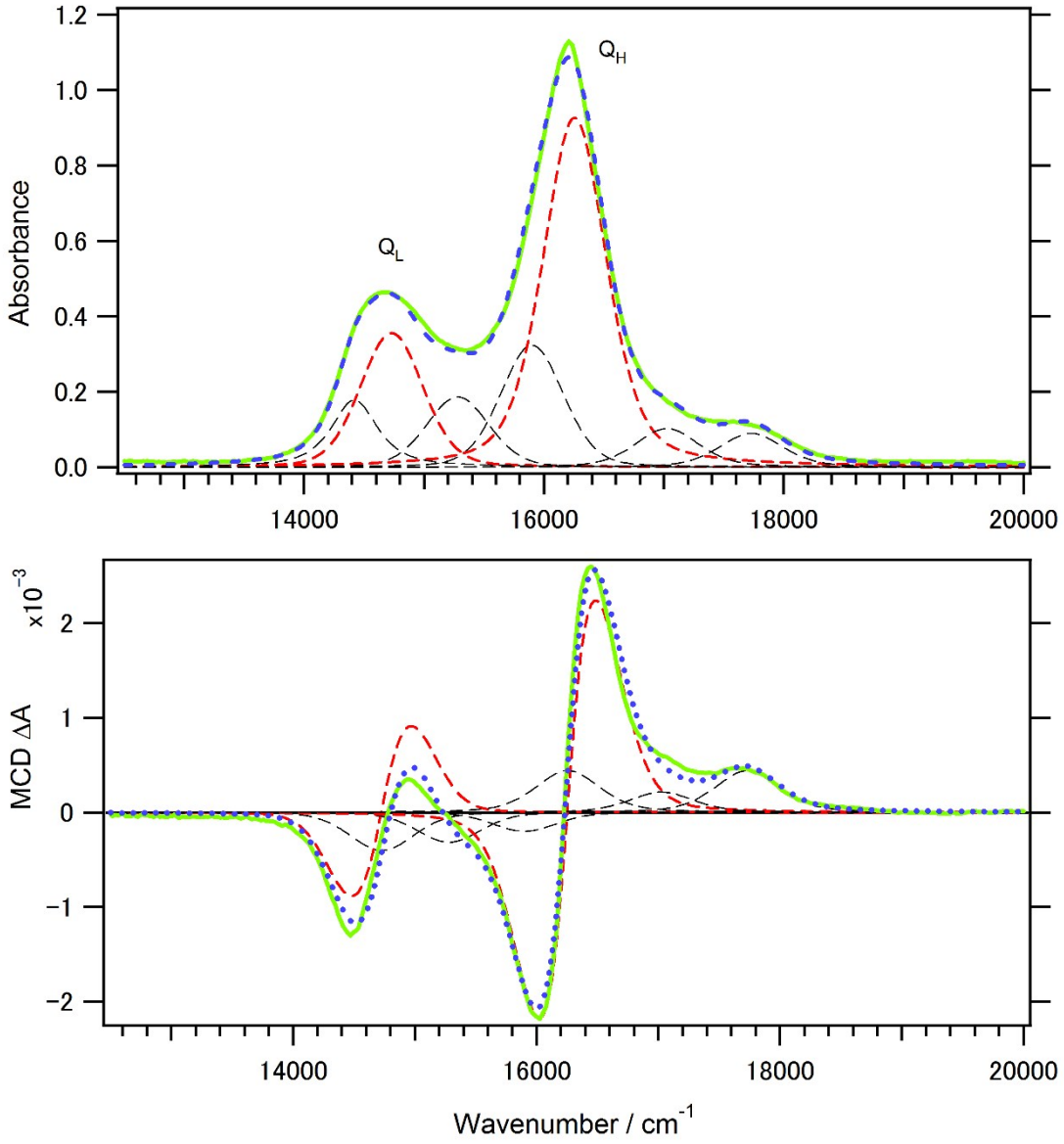

Figure S2 Results of band deconvolution of absorption (top) and MCD (bottom) spectra of Pc_2Tb^- doped in PMMA measured at 100K under a magnetic field of 1T. Observed spectra are shown in solid lines (green). A-term components are shown in thick broken lines (red) and B-term components in thin broken lines (black). The Sum of these components are shown in dotted lines (blue).

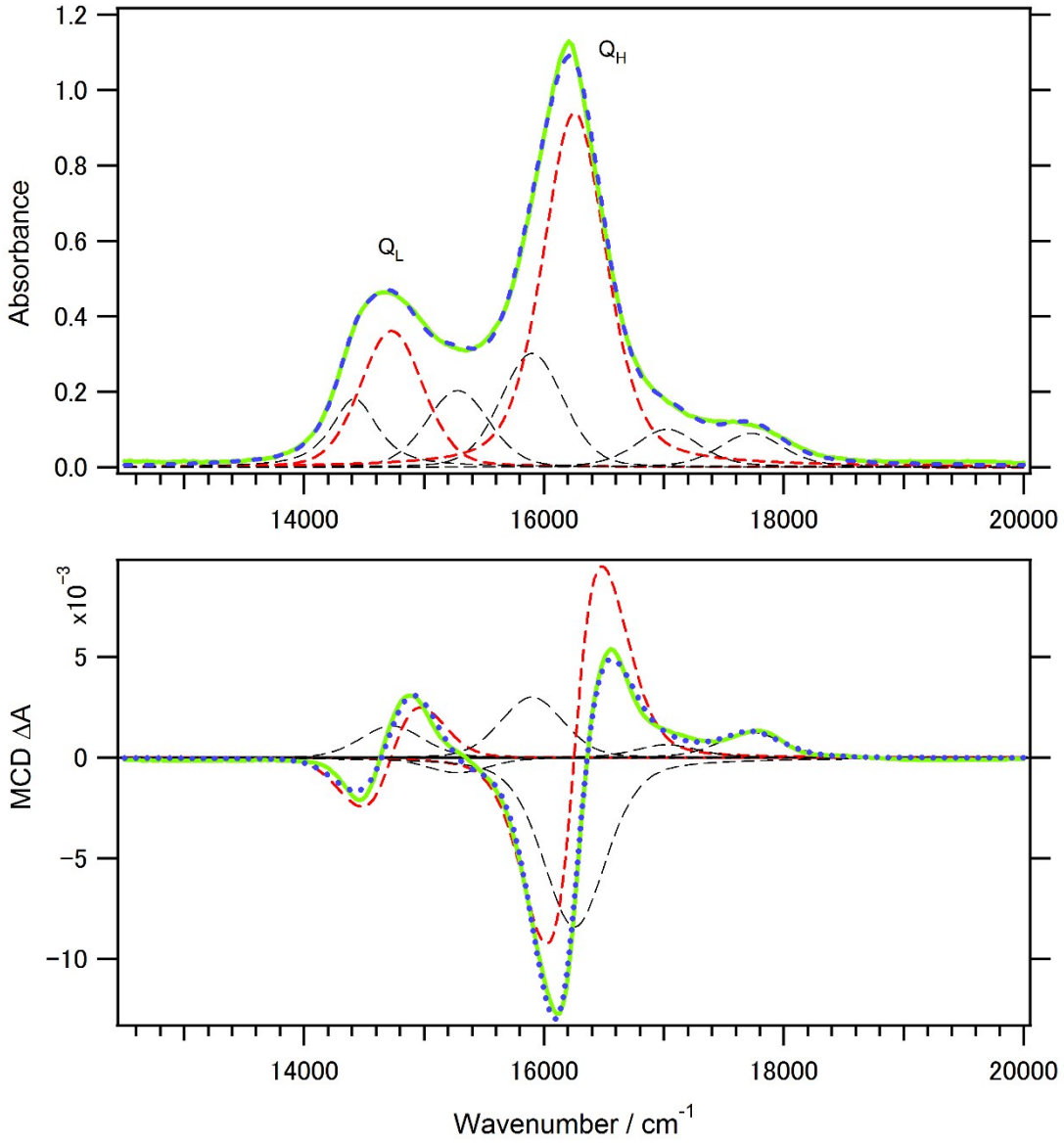

Figure S3 Results of band deconvolution of absorption (top) and MCD (bottom) spectra of Pc_2Tb^- doped in PMMA measured at 1.5K under a magnetic field of 1T. Observed spectra are shown in solid lines (green). A-term components are shown in thick broken lines (red) and B-term components in thin broken lines (black). The Sum of these components are shown in dotted lines (blue).

Table S1 Parameters determined by the band deconvolution of absorption and MCD spectra of Pc_2Y^- doped in PMMA measured at 1.5K.

E_0 (cm^{-1})[a]	Γ(cm^{-1})[a]	η[a]	D_0	A_1/D_0	B_0/D_0
14221	402	0.576	1.8		0.0
14560	656	0.315	7.1	2.0	-0.0037
15108	656	0.315	4.1		0.00070
15922	656	0.315	5.8		-0.00019
16299	685	0.683	15.8	2.2	0.0011
17146	685	0.683	1.8		0.0078
17831	685	0.683	1.4		0.0095

a) E_0, Γ, η are the parameters defining the normalized pseudo-Voight function,

$f(E) = (1-\eta)f_G(E;E_0,\gamma_G) + \eta f_L(E;E_0,\gamma_L)$

where $f_G(E;E_0,\gamma_G)$ and $f_L(E;E_0,\gamma_L)$ are the normalized Gaussian and Lorentzian function,

$$f_G(E;E_0,\gamma_G) = \left(\frac{1}{\sqrt{\pi}\gamma_G}\right)\exp\left(-\frac{(E-E_0)^2}{\gamma_G^2}\right)$$

$$f_L(E;E_0,\gamma_L) = \left(\frac{1}{\gamma_L}\right)\left(1+\frac{(E-E_0)^2}{\gamma_L^2}\right)^{-1}$$

with $\Gamma = 2\sqrt{ln2}\gamma_G = 2\gamma_L$

Table S2 Parameters determined by the band deconvolution of absorption and MCD spectra of Pc_2Tb^- doped in PMMA measured at 100K and 1.5K.

E_0 (cm^{-1})[a]	Γ(cm^{-1})[a]	η[a]	D_0	A_1/D_0		B_0/D_0	
				100K	1.5k	100K	1.5K
14416	458	0.83	3.4			0.0	0.0
14723	614	0.27	7.1	2.4	6.5	-0.0024	0.0094
15275	614	0.27	3.8			-0.0035	-0.0084
15894	614	0.27	5.5			-0.00096	0.019
16250	624	0.50	18.6	2.4	10.0	0.00091	-0.019
17021	624	0.50	1.9			0.0049	0.013
17723	624	0.50	1.6			0.010	0.030