Electronic Supplementary Material (ESI) for Dalton Transactions.

Structural, optical and sensing properties of novel Eu(III) complexes with furan- and pyridine-based ligands.

Electronic Supplementary Information

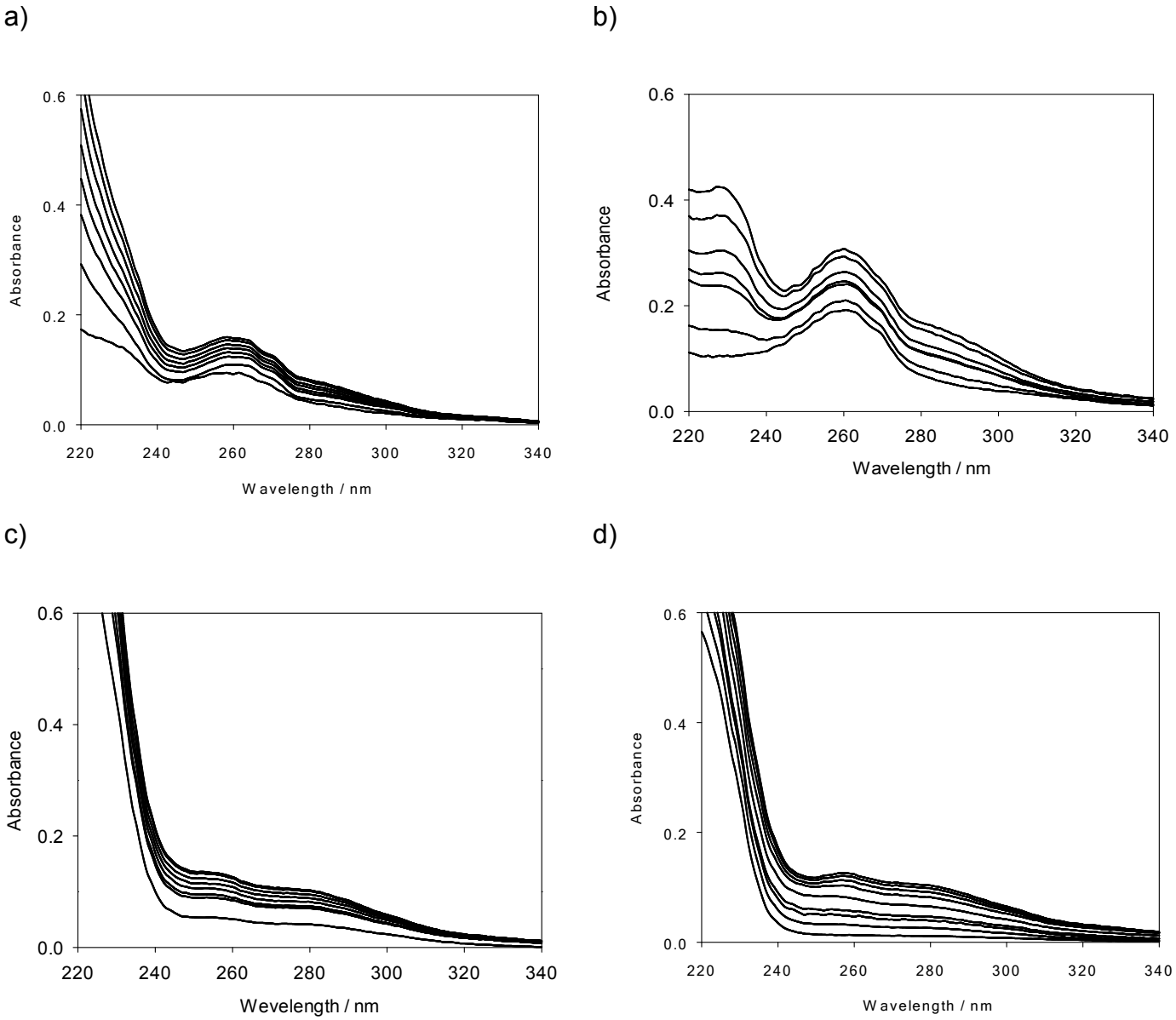

Figure S1. Electronic spectra of (a) **L3** (C_{L3} = 0.0104 mmol dm^{-3}) titrated with $Eu(NO_3)_3$; (b) **L3** (C_{L3} = 0.023 mmol dm^{-3}) titrated with $Eu(OTf)_3$; (c) **L4** (C_{L4} = 0.0425 mmol dm^{-3}) titrated with $Eu(NO_3)_3$; (d) **L4** (C_{L4} = 0.0388 mmol dm^{-3}) titrated with $Eu(OTf)_3$.

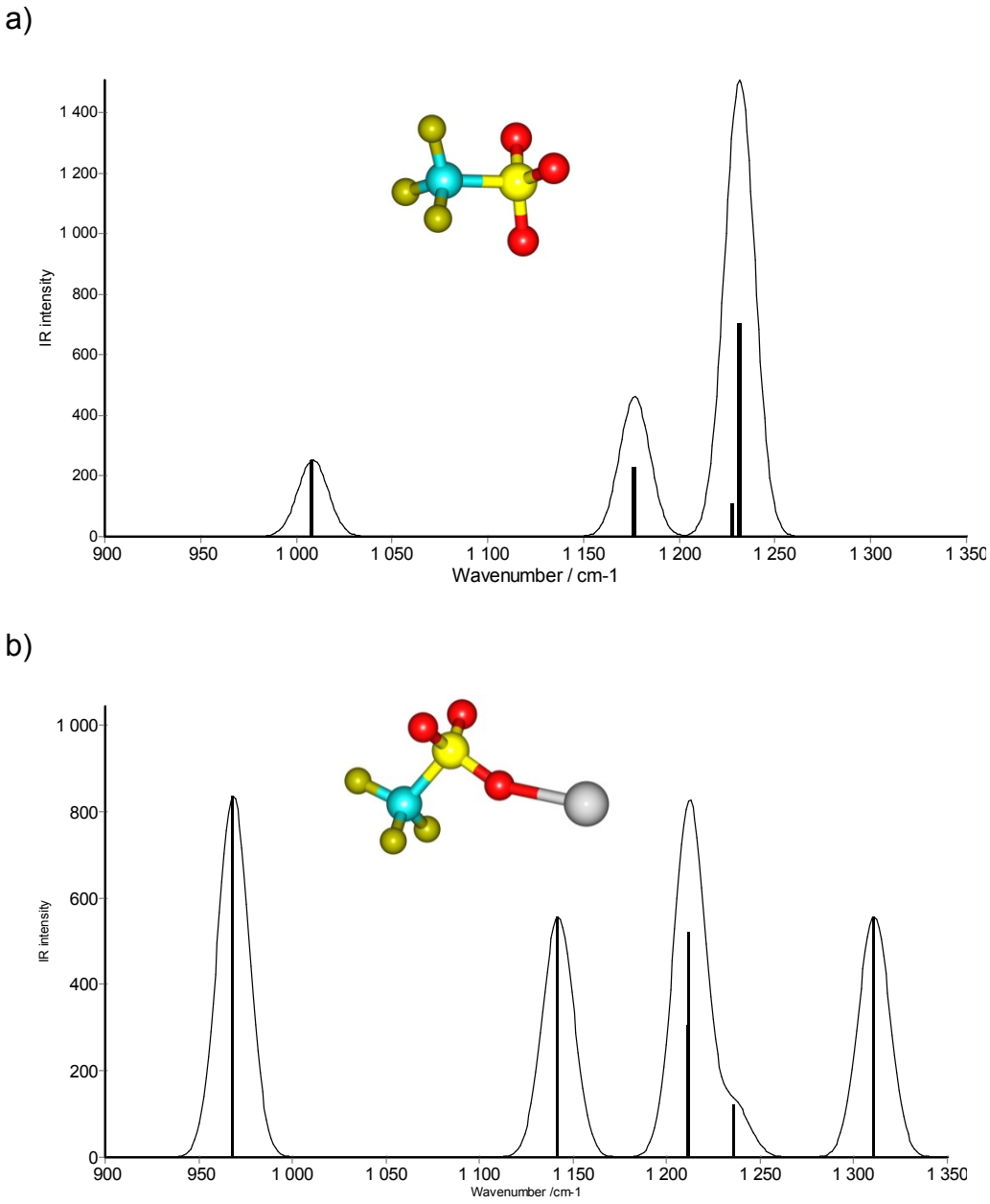

Figure S2. Theoretical vibrational spectra of $CF_3SO_3^-$ anion and of $La(OTf)^{2+}$ in acetonitrile (PCM). Line broadening applied with 19 cm^{-1} half height bandwidth. $CF_3SO_3^-$ frequencies (cm^{-1}): 1231 (SO_3 asymm. str.), 1227 (SO_3+CS+CF_3 str.), 1176(CF_3 asymm. str.), 1008(SO_3+CF_3 str.). $La(OTf)^{2+}$ frequencies (cm^{-1}): 1310 (SO_3 asymm. str.), 1236 (CS+CF_3 str.), 1212 (CF_3 asymm. str.), 1142 (SO_3 +CF_3 str.) 968 (SO_3+CF_3 str.).

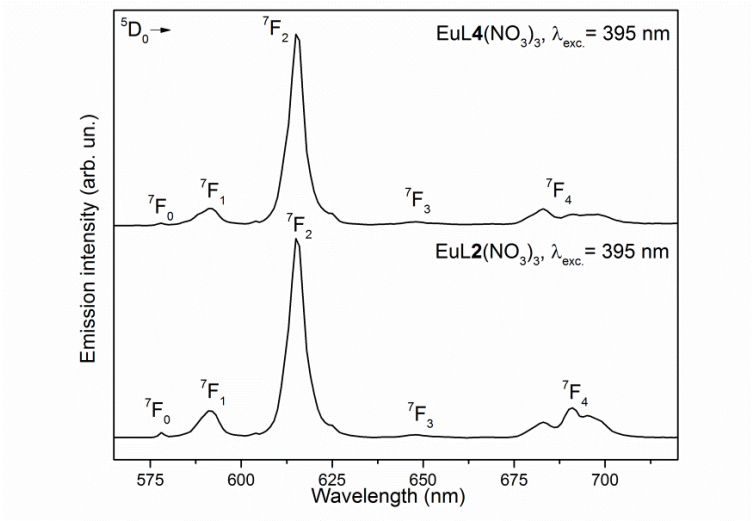

Figure S3. Luminescence emission spectra of Eu**L**$(NO_3)_3$ in AN solution (Eu(III) concentration of 1 mmol dm^{-3}) for furan-based complexes (Eu**L2**$(NO_3)_3$ and Eu**L4**$(NO_3)_3$).

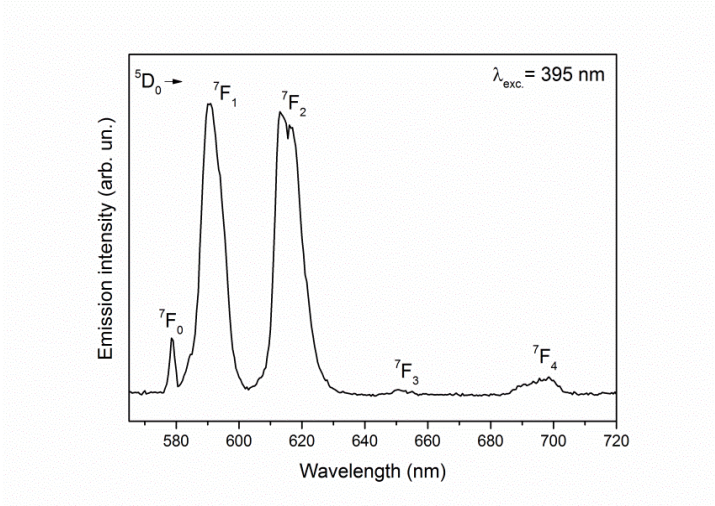

Figure S4. Luminescence emission spectra of $Eu(OTf)_3$ in AN (1 mmol dm^{-3}).

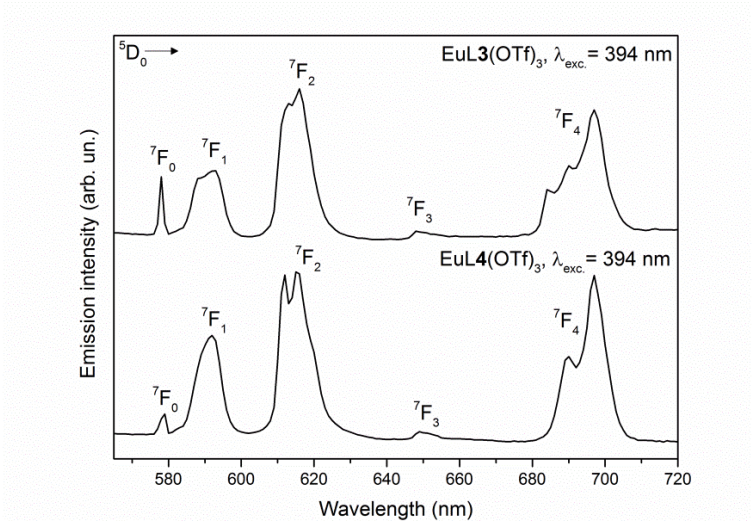

Figure S5. Luminescence emission spectra of EuL triflates in AN solution (Eu(III) concentration of 1 mmol dm^{-3}; R_c = 0.5) for amine-based complexes (Eu**L3**$(OTf)_3$ and Eu**L4**$(OTf)_3$).

	L1	**L2**	**L3**	**L4**
ΔE_{isom}	-5.4	0.2	-1.6	-0.3
E_{reorg} (*cis*)	+2.9	+3.8	+7.6	+6.0
E_{reorg} (*trans*)	+8.3	+3.6	+9.3	+6.3

Table S1. Difference in energy (ΔE_{isom}) between the minimum energy *cis* and *trans* isomers with respect to the intra-annular X-C-C-N dihedral angle (X = N, O in the heteroaromatic ring) and reorganization energy E_{reorg} (all values in kcal mol^{-1}).

Triflate	**L1**		**L2**		**L3**		**L4**	
complex	R_c = 1	R_c = 2	R_c = 1	R_c = 2	R_c = 0.5	R_c = 2	R_c = 0.5	R_c = 3
%EuL	75	---	96.5	5	35.8	---	41	1.3
%EuL_2	12.5	>99	1.7	95	7.1	>99	4.3	98.5

Table S2. Speciation in 1 mmol dm^{-3} $Eu(OTf)_3$ acetonitrile solution as calculated from the formation constants reported in table 1.