Supplementary materials :

R	Pyr gas	PyrH$^+$ gas	Pyr PCM	PyrH$^+$ PCM	Me$_4$BTP gas	Me$_4$BTPH$^+$ gas	Me$_4$BTP PCM	Me$_4$BTPH$^+$ PCM
Cl	-707.8868	-708.2556	-707.8951	-708.3551	-1423.4547	-1423.8673	-1423.4556	-1423.9119
F	-347.5251	-347.8951	-347.5334	-347.9956	-1063.0932	-1063.5072	-1063.0971	-1063.5552
H	-248.2926	-248.6681	-248.3037	-248.7666	-963.8608	-964.2791	-963.8666	-964.3277
Me	-287.6146	-287.9972	-287.6228	-288.0898	-1003.1827	-1003.6057		-1003.6465
^{t}But	-405.5604	-405.9469	-405.5682	-406.0350	-1121.1286	-1121.5538	-1121.1303	-1121.5926
Ph			-479.3690	-479.8357			-1194.9261	-1195.3901
OMe	-362.8209	-363.2094	-362.8308	-363.2998	-1078.3888	-1078.8160	-1078.3939	-1078.8587
NH$_2$	-303.6550	-304.0537	-303.6718	-304.1437	-1019.2238	-1019.6584	-1019.2375	-1019.7122
NMe$_2$	-382.2714	-382.6765	-382.2818	-382.7588	-1097.8395	-1098.2792	-1097.8450	-1098.3180

Table S1: Total energies (in a.u.) of neutral and protonated pyridines and Me$_4$BTPs in the gas phase and in PCM – water. B3LYP/6-31G(d,p) calculations.

R	Yb(L)$_3$$^{3+}$	Eu(L)$_3$$^{3+}$	Eu(L)$_3$$^{3+}$ PCM	La(L)$_3$$^{3+}$	Eu(NO$_3$)$_3$(L)	La(NO$_3$)$_3$(L)
Cl	-4309.3189	-4305.2255	-4305.5723	-4301.4986	-2299.9692	-2296.2397
F	-3228.2443	-3224.1509		-3220.4241	-1939.6113	-1935.8819
H	-2930.5654	-2926.4718		-2922.7448	-1840.3815	-1836.6521
Me	-3048.5427	-3044.4491		-3040.7221	-1879.7042	-1875.9747
^{t}But	-3402.3827	-3398,2891		-3394.5620	-1997.6485	-1993.9191
C$_6$H$_6$	/	/		/	-2071.4419	-2067.7125
OMe	-3274.1683	-3270.0747		-3266.3476	-1954.9102	-1951.1807
NH$_2$	-3096.6946	-3092.6040		-3088.8738	-1895.7482	-1892.0187
NMe$_2$	-3332.5534	-3328.4597	-3328.7672	-3324.7324	-1974.3644	-1970.6348

Table S2: Total Energies (in a.u.) of the 1:3 and 1:1 complexes. L= R-substituted Me$_4$BTP. B3LYP/6-31G(d,p) calculations.

	Eu-N$_1$	Eu-N$_2$	qN$_1$	qN$_2$	qEu	La-N$_1$	La-N$_2$	qN$_1$	qN$_2$	qLa
Cl	2.68	2.63	-0.55	-0.38	1.38	2.82	2.71	-0.55	-0.38	1.48
F	2.68	2.63	-0.55	-0.38	1.38	2.82	2.71	-0.56	-0.38	1.48
H	2.69	2.62	-0.55	-0.38	1.37	2.82	2.71	-0.55	-0.39	1.48
Me	2.67	2.62	-0.56	-0.38	1.37	2.81	2.71	-0.57	-0.39	1.48
^{t}But	2.66	2.62	-0.57	-0.38	1.37	2.80	2.71	-0.56	-0.39	1.48
C$_6$H$_6$	2.67	2.62	-0.56	-0.38	1.37	2.81	2.71	-0.56	-0.39	1.48
OMe	2.66	2.62	-0.58	-0.38	1.37	2.80	2.71	-0.57	-0.39	1.48
NH$_2$	2.65	2.62	-0.59	-0.38	1.37	2.78	2.71	-0.59	-0.39	1.48

NMe$_2$	2.64	2.62	-0.60	-0.38	1.37	2.78	2.70	-0.60	-0.39	1.48

Table S3: Optimized Ln(NO$_3$)$_3$(R-BTP) complexes (Ln = Eu; La). Distances (Å) and Mulliken charges q (in e).

	Yb		Eu		La	
	Yb-N$_1$	Yb-N$_2$	Eu-N$_1$	Eu-N$_2$	La-N$_1$	La-N$_2$
Cl	2.54	2.56	2.62	2.63	2.73	2.71
F	2.54	2.56	2.62	2.63	2.73	2.71
H	2.54	2.56	2.62	2.62	2.74	2.71
Me	2.53	2.56	2.62	2.63	2.73	2.71
^{t}But	2.53	2.56	2.61	2.62	2.73	2.71
OMe	2.53	2.65	2.61	2.63	2.72	2.71
NH$_2$	2.52	2.57	2.60	2.63	2.71	2.72
NMe$_2$	2.51	2.56	2.59	2.63	2.70	2.72

Table S4: QM optimized Ln(R-BTP)$_3$$^{3+}$ complexes. Distances (Å).

	Yb			Eu			La		
	N$_1$	N$_2$	Yb	N$_1$	N$_2$	Eu	N$_1$	N$_2$	La
Cl	-0.59	-0.40	1.55	-0.59	-0.41	1.57	-0.60	-0.42	1.67
F	-0.59	-0.40	1.55	-0.60	-0.41	1.57	-0.61	-0.42	1.67
H	-0.58	-0.40	1.54	-0.59	-0.41	1.57	-0.59	-0.42	1.67
Me	-0.59	-0.40	1.54	-0.60	-0.41	1.57	-0.61	-0.42	1.67
^{t}But	-0.60	-0.40	1.54	-0.61	-0.41	1.57	-0.61	-0.42	1.66
OMe	-0.61	-0.39	1.55	-0.62	-0.40	1.57	-0.63	-0.42	1.67
NH$_2$	-0.62	-0.39	1.55	-0.63	-0.40	1.57	-0.64	-0.42	1.66
NMe$_2$	-0.64	-0.39	1.54	-0.64	-0.40	1.56	-0.65	-0.42	1.66

Table S5: QM optimized Ln (R-BTP)$_3$$^{3+}$ complexes. Mulliken charges (e).
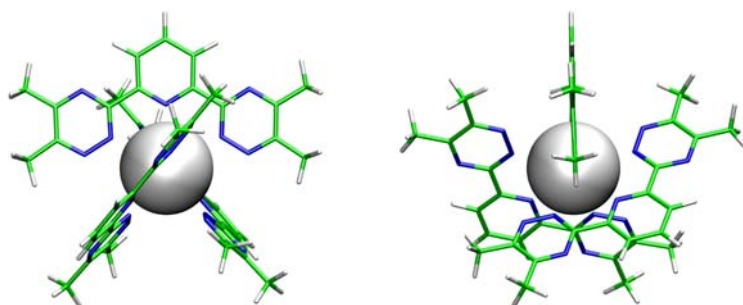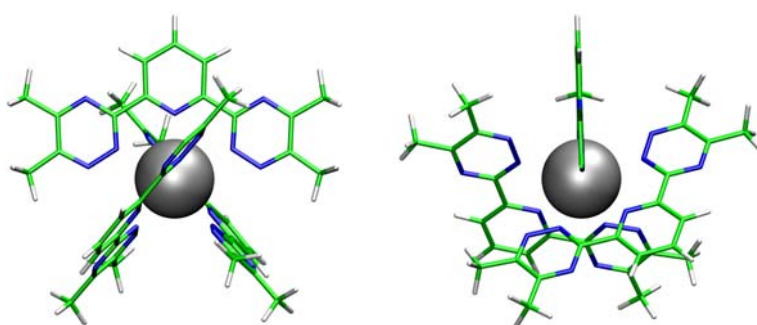
La(H-BTP)$_3$$^{3+}$

Eu(H-BTP)$_3$$^{3+}$
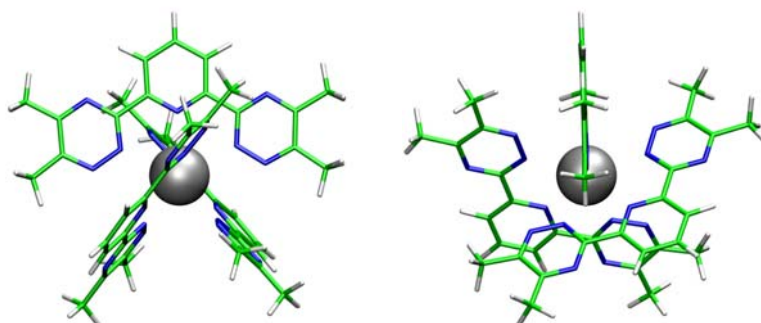
Yb(H-BTP)$_3$$^{3+}$

Figure S1: Optimized Ln(H-BTP)$_3$$^{3+}$ complexes (orthogonal views).