

Supplementary material for:

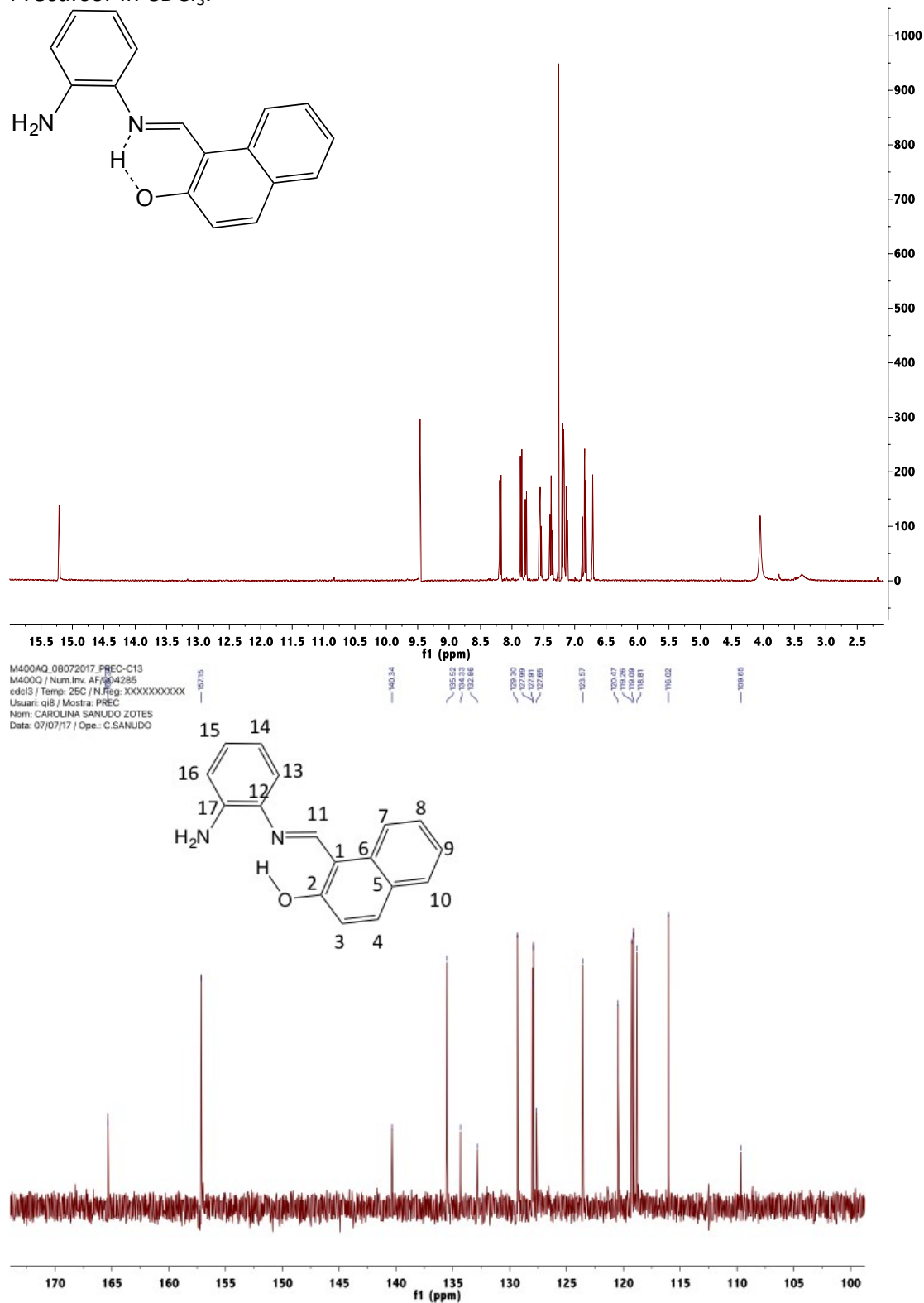
Double decker luminescent Ytterbium and
Erbium SMMs with symmetric and asymmetric
Schiff base ligands

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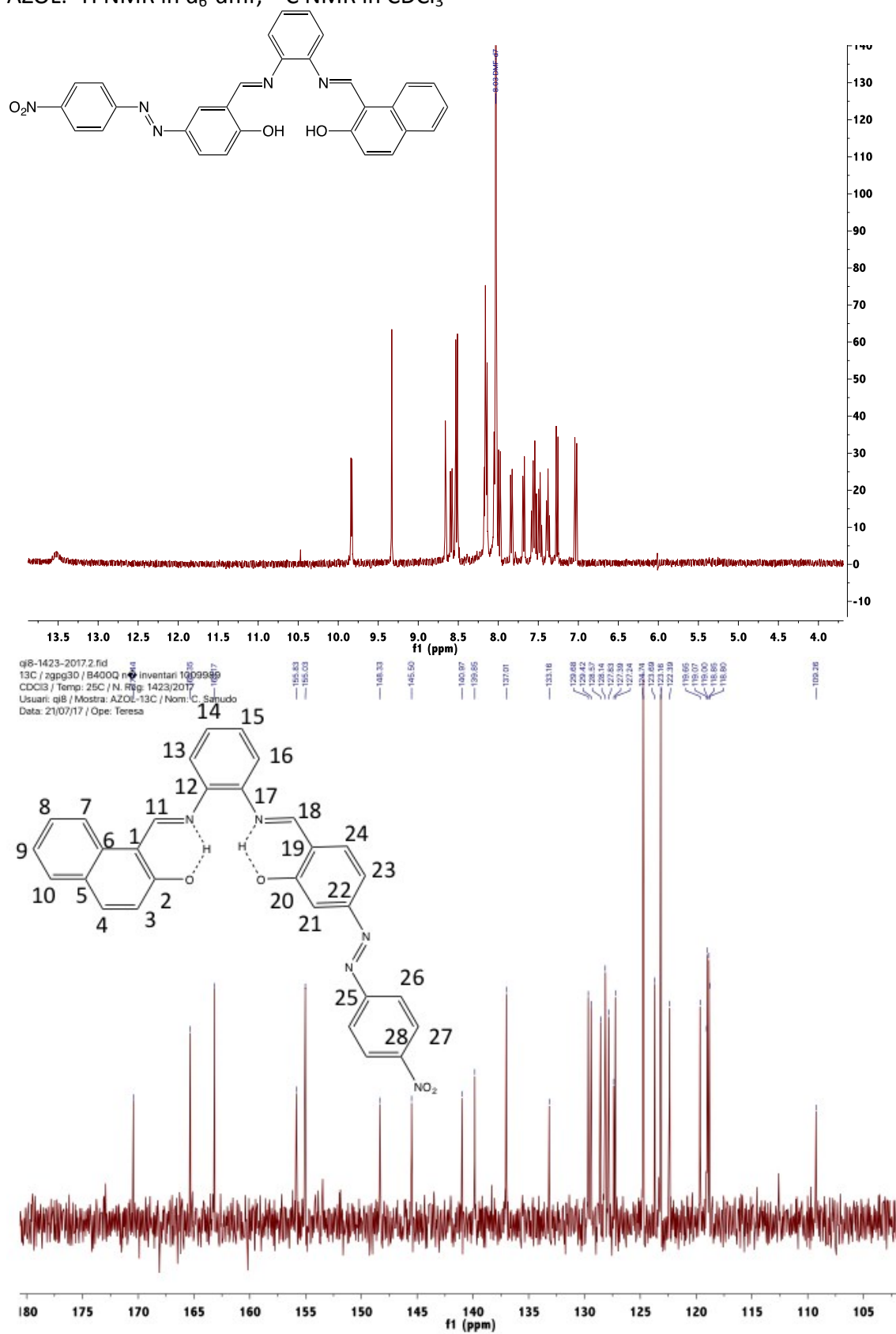
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Proton and ^{13}C NMR spectra of the new ligands AZOL, SYML and the precursor of AZOL. Due to the limited solubility of these compounds at least 2000 acquisitions were necessary in order to obtain ^{13}C NMR.

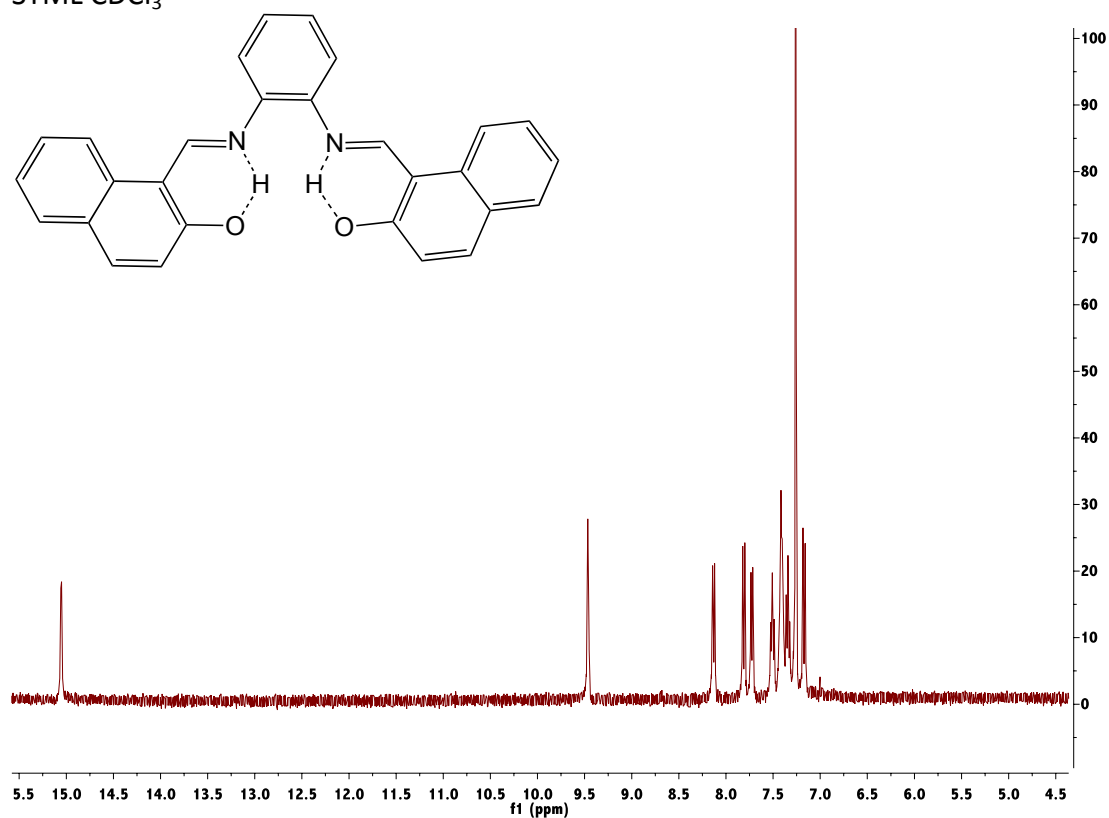
Precursor in CDCl_3 .



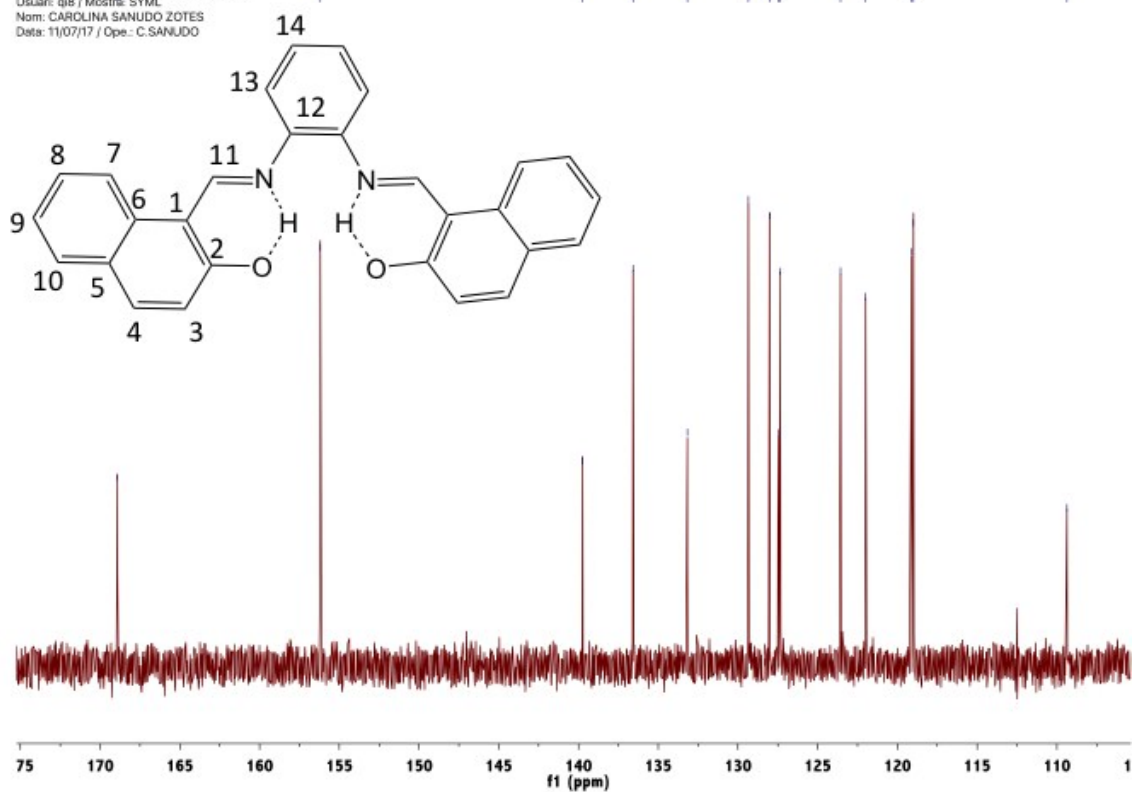
AZOL: ^1H NMR in $\text{d}_6\text{-dmf}$, ^{13}C NMR in CDCl_3



SYML CDCl₃



M400AQ_11072017_SYML-C13
M400Q / Num. Ineg: AF/004285
cdcl3 / Temp: 25C / N.Reg: XXXXXXXXXX
Usuari: qib / Mostria: SYML
Nom: CAROLINA SANUDO ZOTES
Data: 11/07/17 / Ope.: C.SANUDO



13C NMR (101 MHz, CDCl ₃) δ (ppm)					
C	Precursor	C	SYML	C	AZOL
2	165.34	2	168.91	2	170.44
11	157.15	11	156.19	20	165.35
6	140.34	6	139.74	18	163.17
4	135.52	4	136.58	22	155.83
17	134.33	5	133.17	3	155.03
12	132.86	9	129.35	25	148.33
15	129.30	8	128.02	28	145.50
8	127.99	12	127.48	13	140.97
10	127.91	10	127.35	6	139.85
5	127.65	7	123.57	4	137.01
7	123.57	3	121.99	5	133.16
3	120.47	14	119.15	9	129.68
14	119.26	13	118.99	24	129.42
9	119.09	1	109.37	16	128.57
13	118.81			8	128.14
16	116.02			27	127.83
1	109.65			12	127.39
				10	127.24
				14	124.74
				7	123.69
				15	123.16
				3	122.39
				18	119.65
				23	119.07
				21	119.00
				12	118.85
				17	118.80
				1	109.26

Figure S01. Crystal packing and crystal structure of SYML-Er2. The three different ligands of the complex are colored in pink, blue and green.

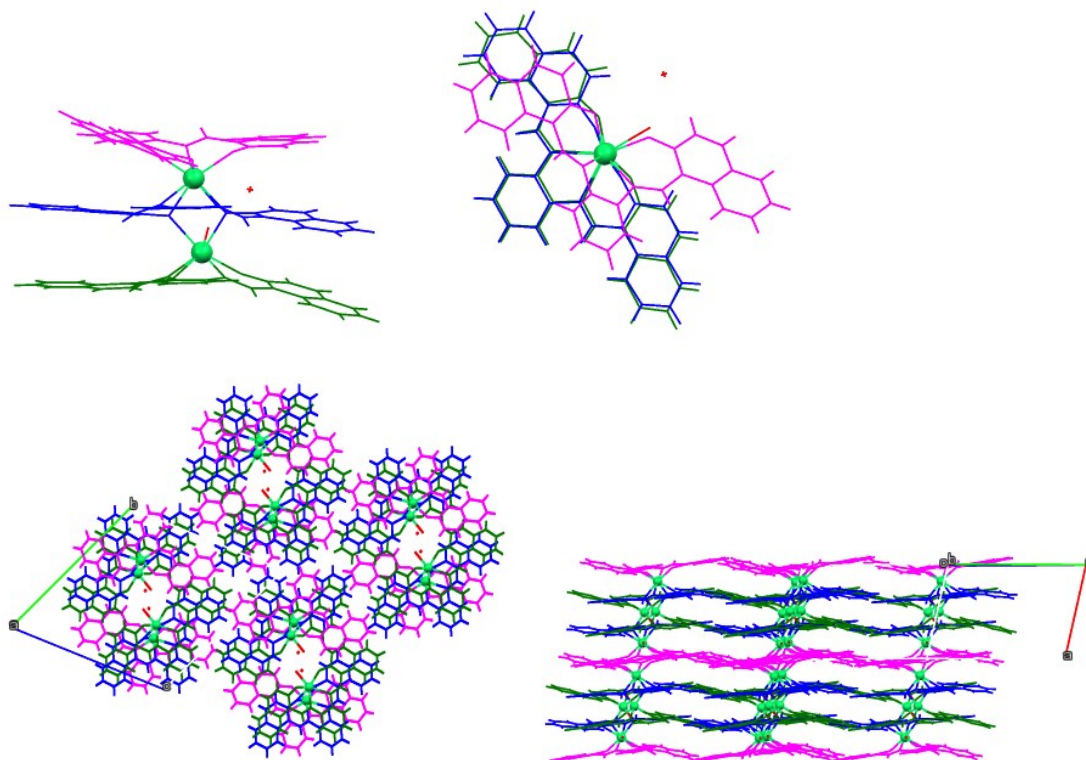
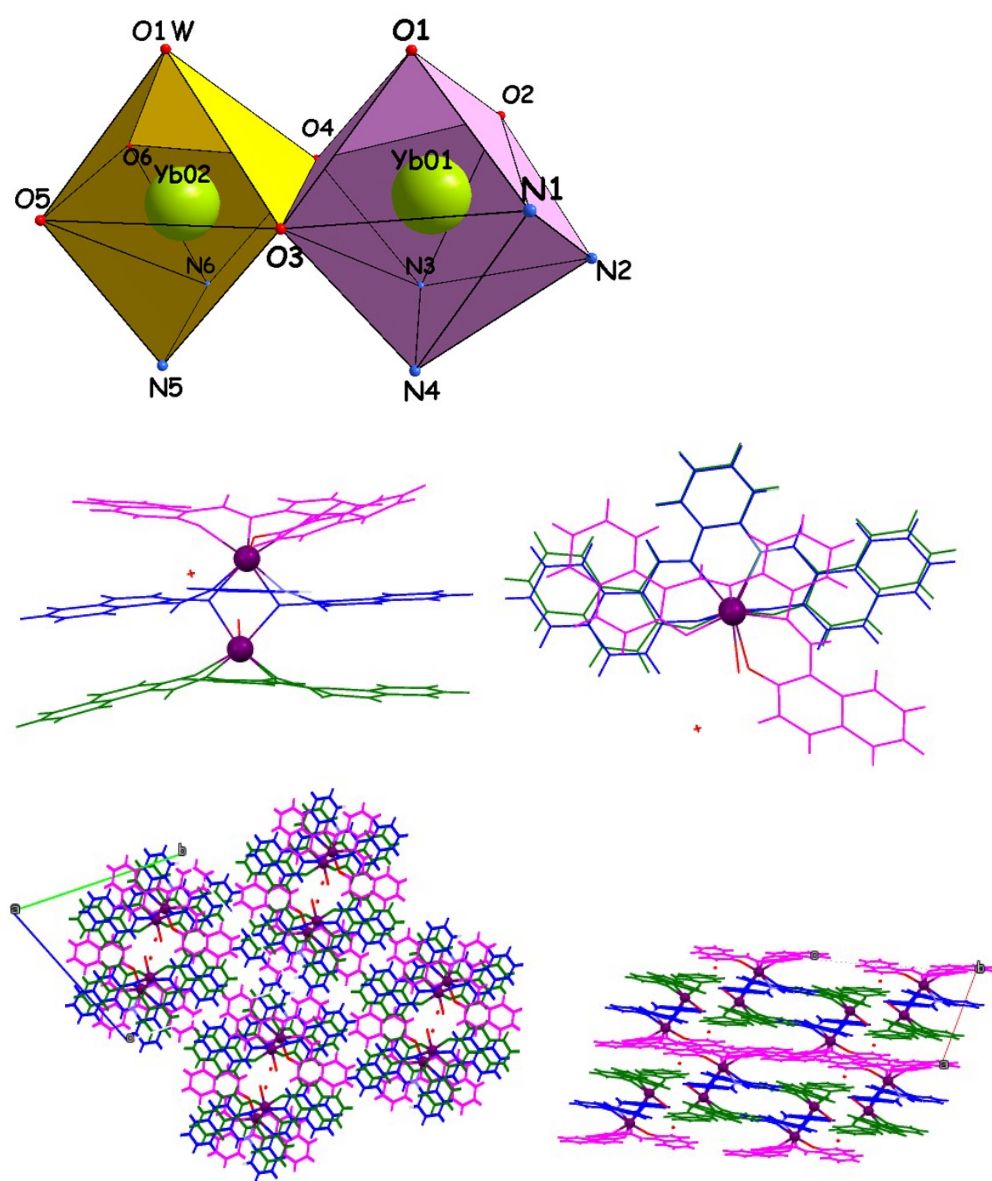


Figure S02. Crystal packing. polyhedral representation around Yb and crystal structure of SYML-Yb2. The three different ligands of the complex are colored in pink, blue and green.



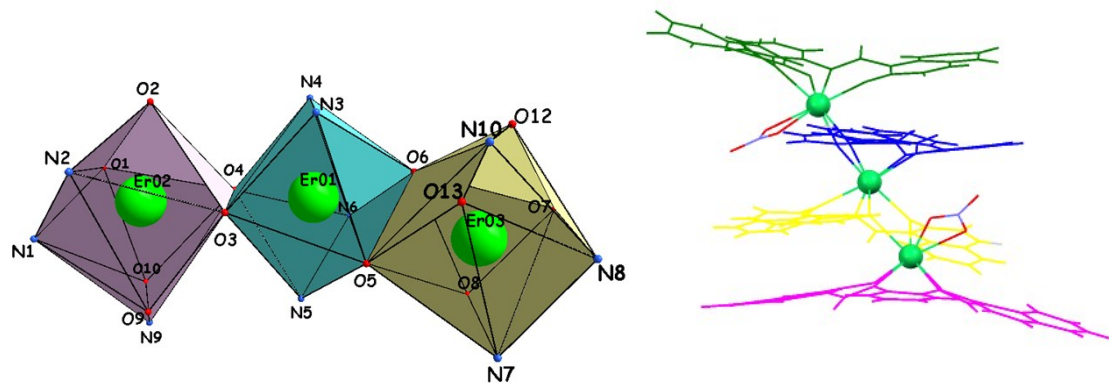
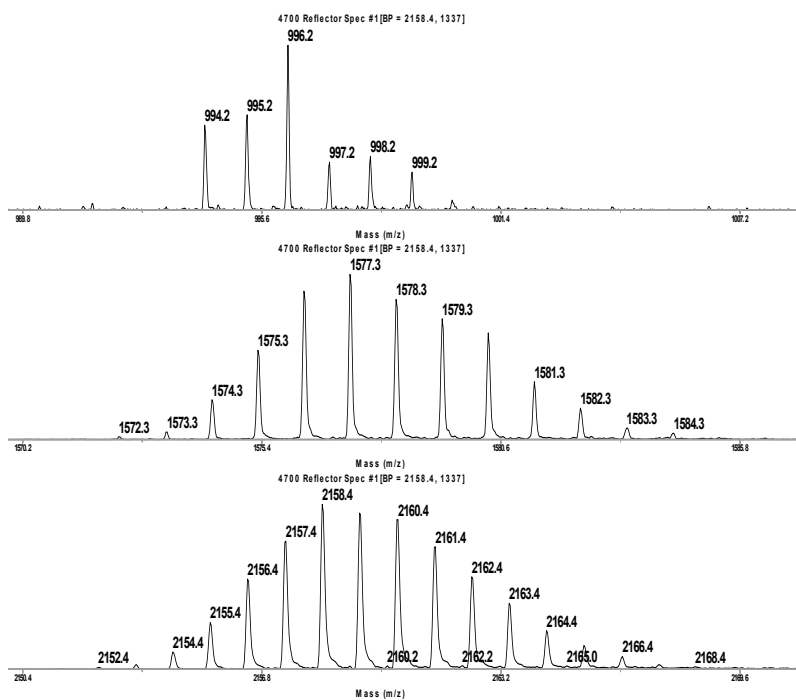


Figure S04. MALDI-TOF spectra for the Yb and Er complexes of SYML and AZOL.

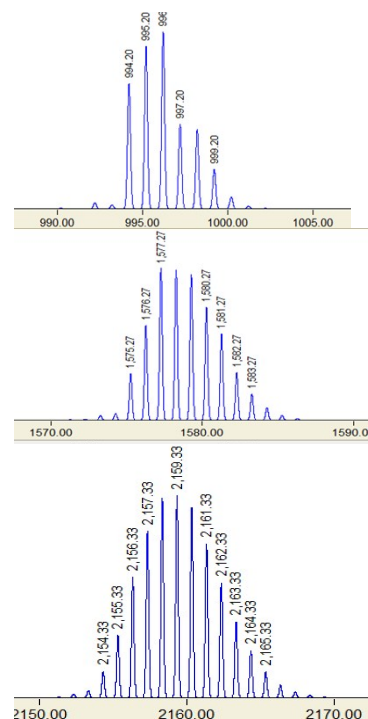
The spectra for an aliquot of the reaction mixture shows the species Ligand:Ln 2:1, 3:2 and 4:3.

Mass spectra of an aliquot of the SYML reaction with Er(III) in MeCN

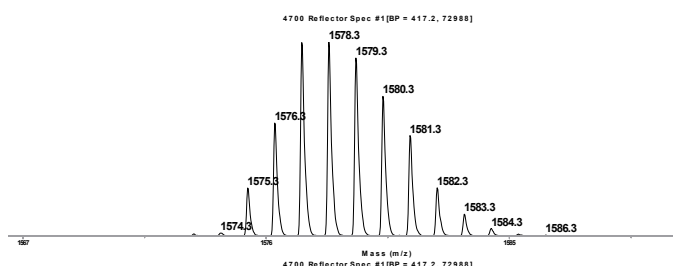
Experimental



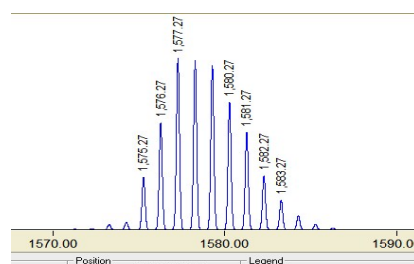
Calculated



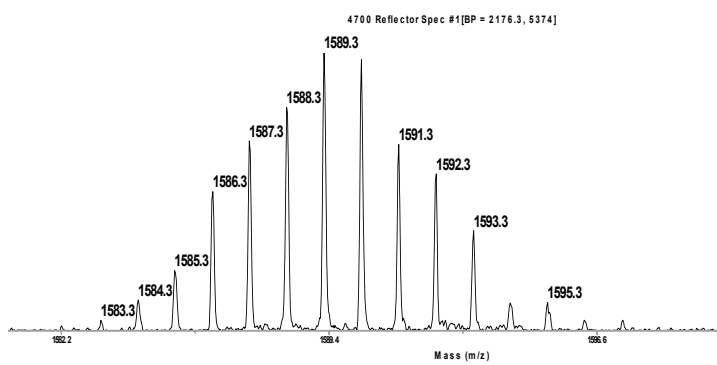
SYML-Er2 crystals: experimental



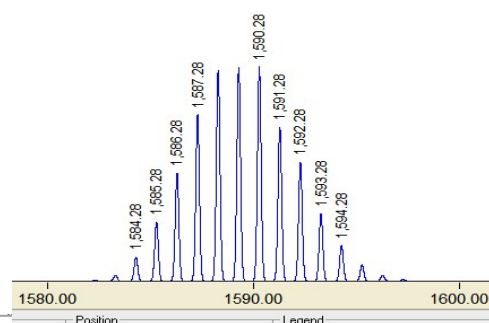
Calculated



SYML-Yb2 crystals: experimental

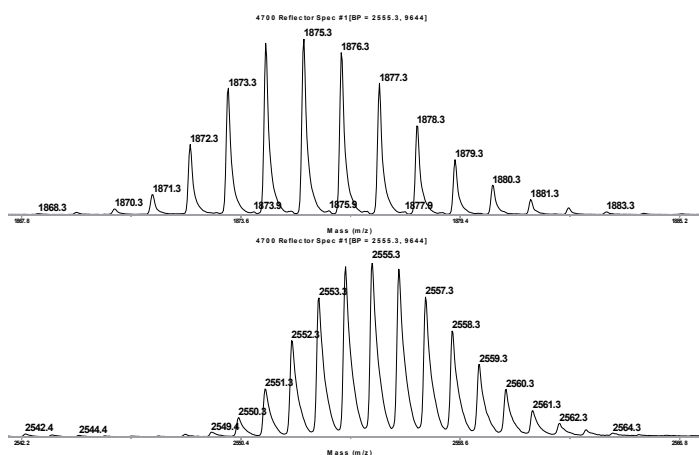


Calculated

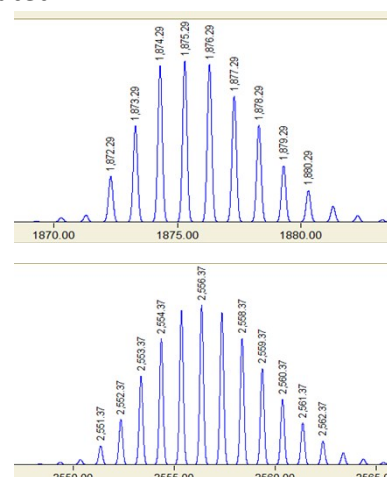


The spectra for the AZOL-Ln3 species show the molecular peak for the Ligand:Ln 4:3 species and the fragmentation into the Ligand:Ln species 3:2.

AZOL-Er3 powder MS Experimental

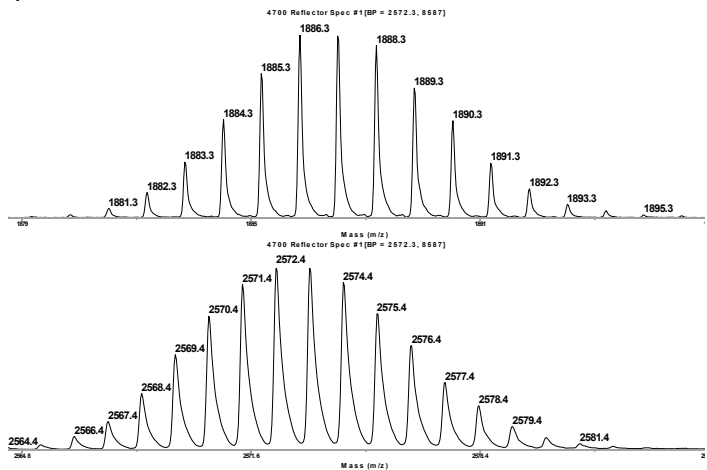


Calculated



AZOL-Yb3 powder

Experimental



Calculated

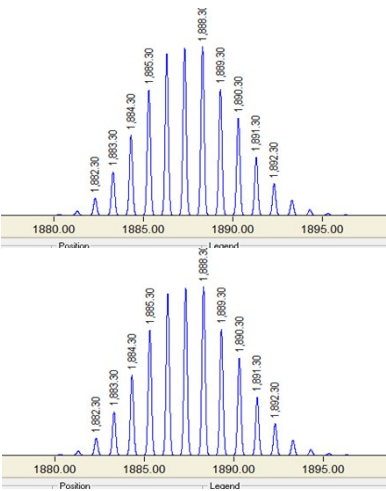


Figure S05. Electronic spectra of CH₃CN solutions at room temperature of AZOL and AZOL-Ln₃ complexes (Ln = Er, Yb) before and after irradiation with a Xenon lamp for 1 hour (360 nm).

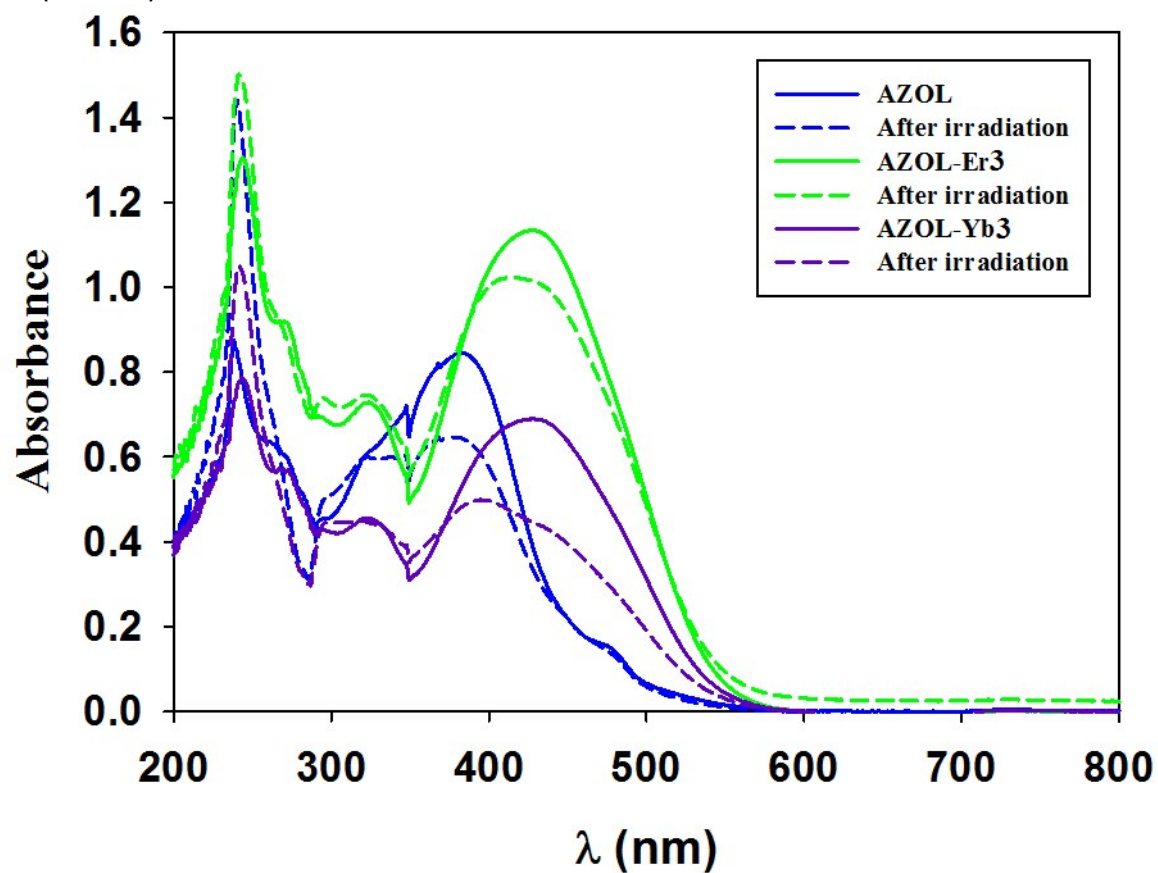


Figure S06. Electronic and emission spectra of CH₃CN solutions at room temperature of SYML and SYML-Ln₂ complexes (Ln = Er, Yb). Excitation wavelength 440 nm.

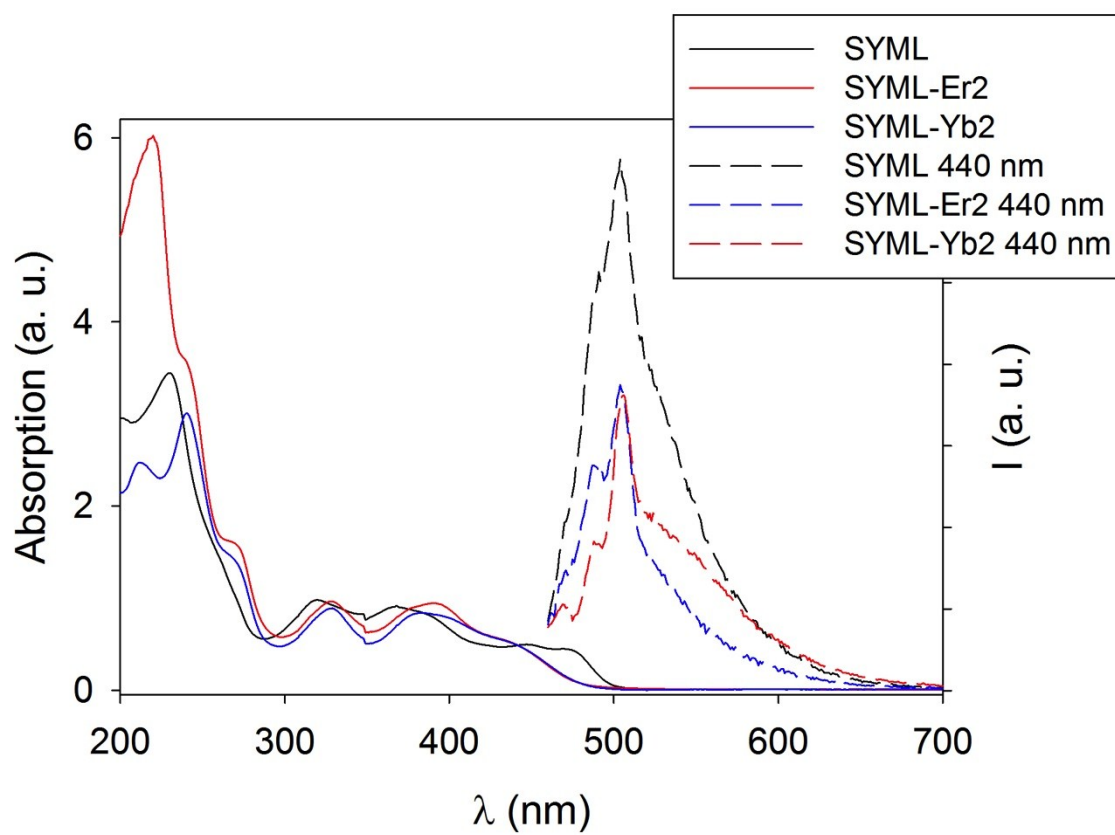


Figure S07. Solid state NIR emission of AZOL-Er3 and SYML-Er2 upon excitation by 590 nm light.

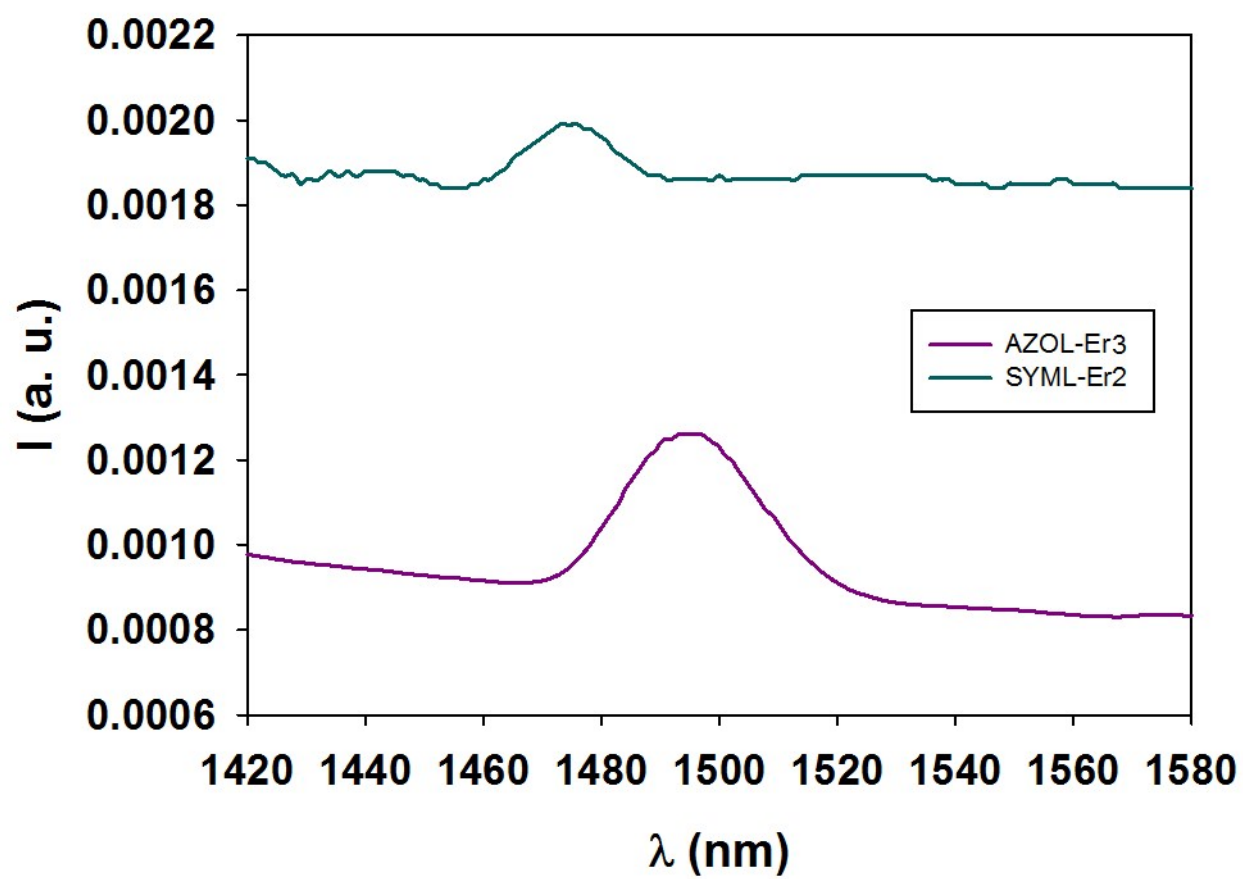


Figure S08. Magnetization vs field plot for SYML-Er2 and SYML-Yb2 at 2 K.

Magnetization vs. field plots for AZOL-Er3 and AZOL-Yb3 at 2 K.

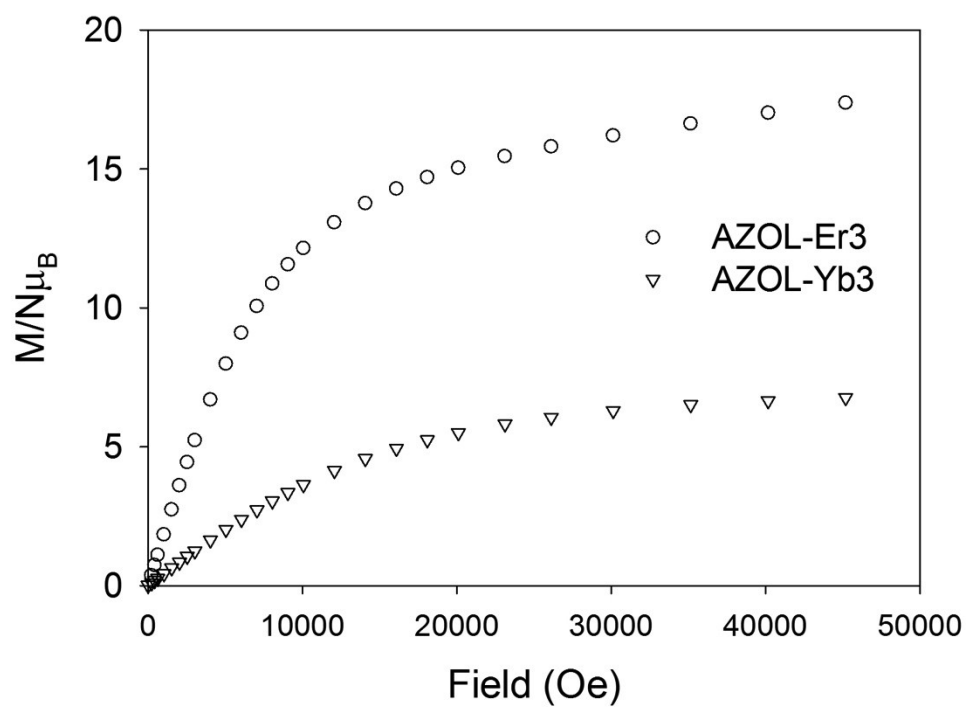
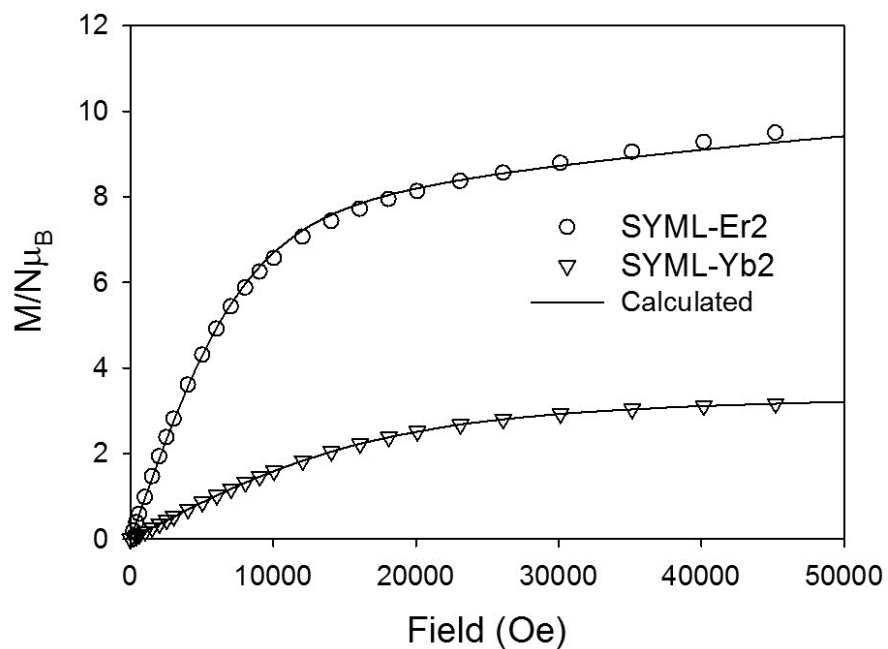


Figure S09. TGA for AZOL-Yb3 and AZOL-Er3 under N₂. in the 15 to 500°C temperature range. For AZOL-Er3 a loss of uncoordinated solvent + 3 NO₃⁻ represents 11 % weight loss. For AZOL-Yb the loss of uncoordinated solvents + 3 NO₃⁻ represents 10.8 % weight loss.

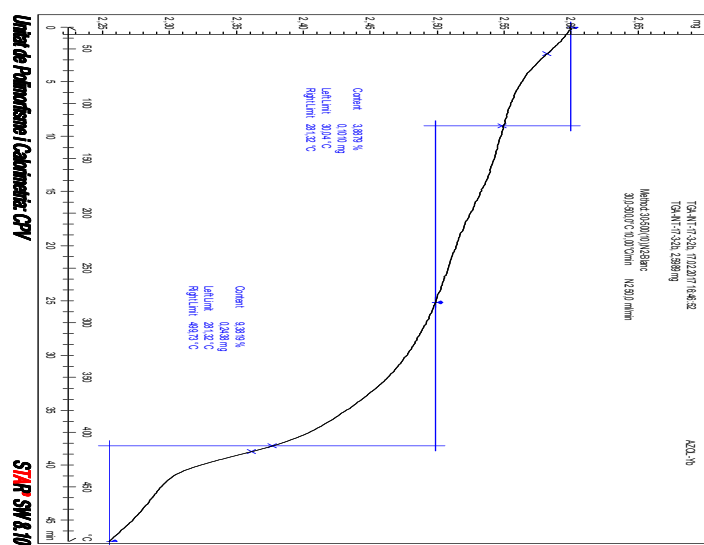
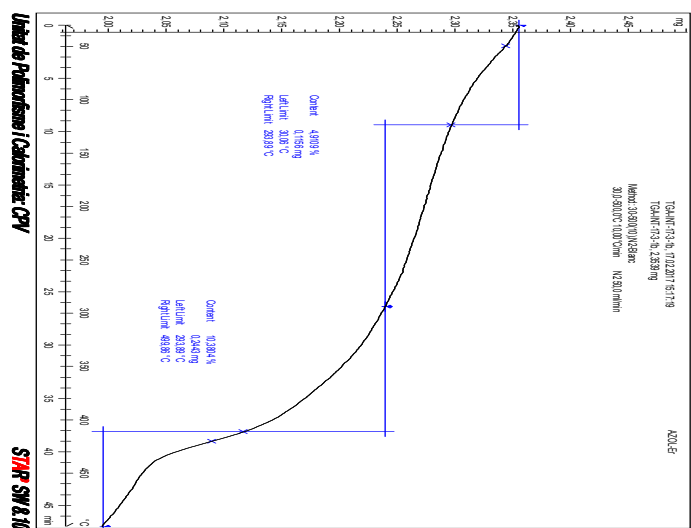


Table S01. Fitting parameters for SYML-Yb2 using a Debye model.

T (K)	α	τ (s ⁻¹)
1.8	0.34	1.93e-4
1.9	0.35	1.64e-4
2.0	0.37	1.26e-4
2.1	0.38	1.05e-4
2.3	0.35	9.94e-5
2.5	0.34	8.06e-5
2.7	0.30	8.09e-5
3.0	0.25	7.88e-5
3.5	0.16	6.43e-5
4.0	0.094	4.86e-5
4.5	0.023	5.04e-5
5.0	0.009	1.30e-6

Figure S10. Arrhenius plot for SYML-Yb2 using the data obtained from the Argand plot.

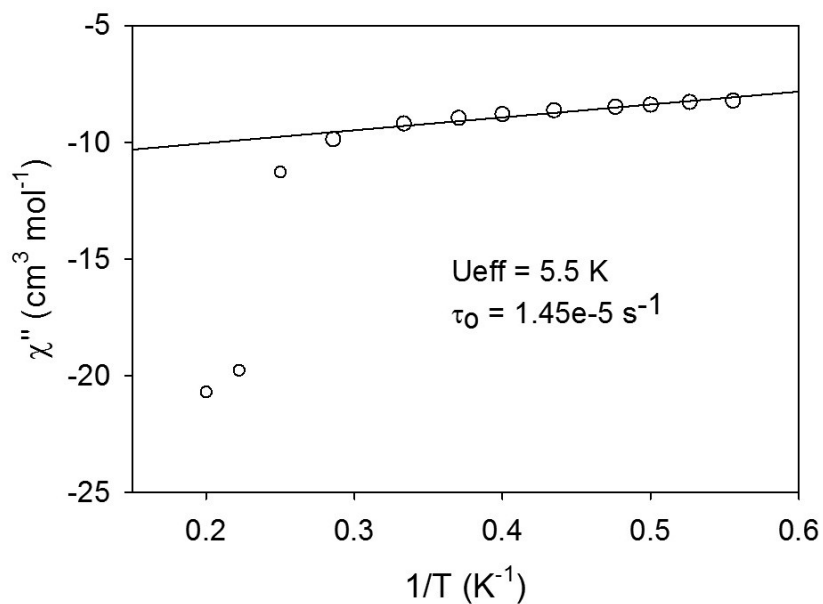


Figure S11. AC magnetic susceptibility and Argand plot for SYML-Er2 at an applied dc field of 0.2 T and temperatures between 1.8 K and 4.5 K.

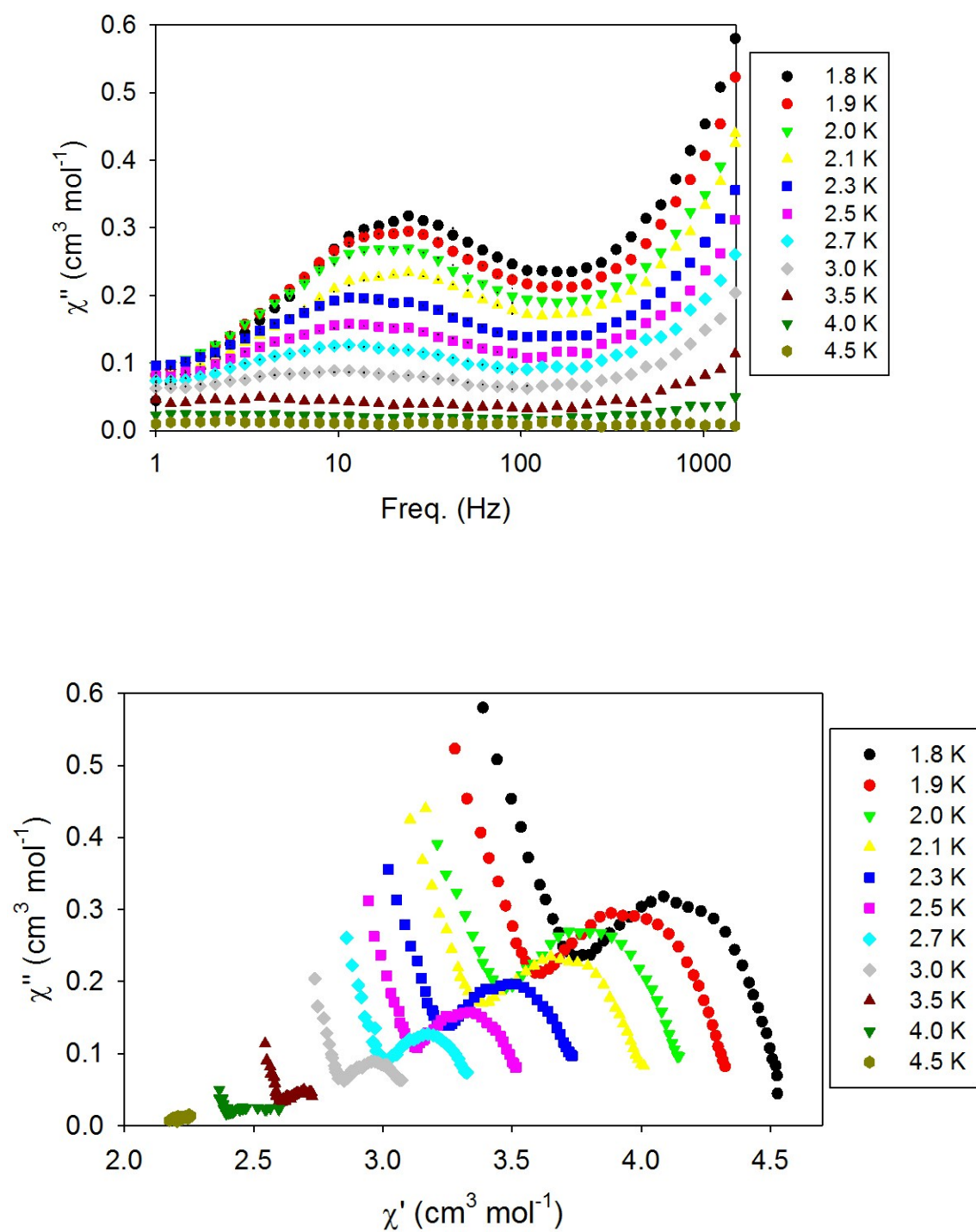


Figure S12. Out-of-phase AC magnetic susceptibility vs. frequency plot for AZOL-Er3 at different applied dc fields.

