Supporting Information

Chirality transfer between hexaazamacrocycles in heterodinuclear rare earth complexes

Przemysław Starynowicz and Jerzy Lisowski*

Contents:

- 1. Scheme S1 page 2.
- 2. Spectra pages 3-7.
- 3. Crystallographic data and figure pages 8-10.



mixture of homochiral homodinuclear and homochiral heterodinuclear complexes

Scheme S1.



Figure S1. ¹H NMR spectra of $[Eu_2(L1^R)_2(\mu-OH)_2(NO_3)(H_2O)](NO_3)_3\cdot 7H_2O$ (top) and $[Nd_2(L1^S)_2(\mu-OH)_2(NO_3)_2](NO_3)_2\cdot 5H_2O$ (bottom) complexes.



Figure S2. ¹H NMR spectra of $[Tb_2(L1^5)_2(\mu-OH)_2(NO_3)(H_2O)](NO_3)_3 \cdot 4H_2O$ (top) and $[Yb_2(L1^5)_2(\mu-OH)_2(H_2O)_2][Na(NO_3)_3(H_2O)_2](NO_3)_2 \cdot H_2O \cdot 2CH_3OH$ (bottom) complexes.



Figure S3. UV region of the CD spectrum of water solution of the mixture of $[Y(L1^{s})(NO_{3})_{2}](NO_{3})$ and $[Nd(L2)(NO_{3})_{2}](NO_{3})$ complexes (green), the same mixture after addition of 1 equivalent of NaOH (blue).



Figure S4. ¹H NMR spectra of the dinuclear species generated by the addition of 1 equivalent of NaOH to the D₂O solution of $[Nd(L2)(NO_3)_2](NO_3)$ complex (green), $[Y(L1^5)(NO_3)_2](NO_3)$ complex (red) or to the mixture of $[Y(L1^5)(NO_3)_2](NO_3)$ and $[Nd(L2)(NO_3)_2](NO_3)$ complexes (dark blue).



Figure S5 . CD spectra of water solution of the mixture of $[Pr(L1^R)(NO_3)_2](NO_3)$ and $[Nd(L2)(NO_3)_2](NO_3)$ complexes (green), the same mixture after addition of 0.5 equivalents of NaOH (light blue), 1 equivalent of NaOH (orange) and after addition of 2 equivalents of NaOH (violet). Label Pr dentotes f-f transitions of the praseodymium(III) cation bound by L1 macrocyle and the label Nd dentotes f-f transitions of neodymium(III) bound by the L2 macrocyle.

Crystallographic data



Figure. S6. The basic lanthanide-Schiff base unit together with atom labelling pattern. For the macrocyle connected with the other lanthanide (see text) the numbers of the carbon atoms are increased by 30 (e.g. $C1\rightarrow C31$ etc.) and those of N atoms - by 6.

nd				
Nd1-02	2.336 (4)	Nd2-01	2.341 (4)	
Nd1-01	2.341 (4)	Nd2—02	2.345 (4)	
Nd1-011	2.629 (5)	Nd2—022	2.616 (5)	
Nd1—012	2.640 (5)	Nd2—N11	2.628 (6)	
Nd1—N2	2.662 (6)	Nd2—N10	2.643 (6)	
Nd1—N1	2.665 (6)	Nd2—N7	2.692 (6)	
Nd1—N5	2.676 (6)	Nd2—N8	2.693 (6)	
Nd1—N4	2.690 (6)	Nd2—021	2.702 (5)	
Nd1—N3	2.731 (5)	Nd2—N12	2.714 (5)	
Nd1—N6	2.740 (6)	Nd2—N9	2.715 (6)	
Nd1—Nd2	3.9258 (7)			
eu				
Eu1—01	2.319 (4)	Eu2—02	2.266 (4)	
Eu1—02	2.332 (4)	Eu2—01	2.276 (4)	
Fu1_011	2,593 (5)	Fu2_0W1	2 111 (5)	
		202 0001	2.441 (3)	
Eu1-012	2.600 (5)	Eu2—N11	2.441 (3) 2.638 (6)	
Eu1-011 Eu1-N5	2.600 (5) 2.624 (6)	Eu2—N11 Eu2—N8	2.638 (6) 2.647 (6)	
Eu1—011 Eu1—N5 Eu1—N2	2.600 (5) 2.624 (6) 2.634 (5)	Eu2—N11 Eu2—N8 Eu2—N7	2.638 (6) 2.647 (6) 2.660 (6)	
Eu1—011 Eu1—N5 Eu1—N2 Eu1—N4	2.600 (5) 2.624 (6) 2.634 (5) 2.646 (6)	Eu2—N11 Eu2—N8 Eu2—N7 Eu2—N10	2.638 (6) 2.647 (6) 2.660 (6) 2.668 (6)	
Eu1—011 Eu1—N5 Eu1—N2 Eu1—N4 Eu1—N1	2.600 (5) 2.624 (6) 2.634 (5) 2.646 (6) 2.680 (6)	Eu2—N11 Eu2—N8 Eu2—N7 Eu2—N10 Eu2—N9	2.638 (6) 2.647 (6) 2.660 (6) 2.668 (6) 2.700 (6)	
Eu1—012 Eu1—N5 Eu1—N2 Eu1—N4 Eu1—N1 Eu1—N3	2.600 (5) 2.624 (6) 2.634 (5) 2.646 (6) 2.680 (6) 2.691 (6)	Eu2—N11 Eu2—N8 Eu2—N7 Eu2—N10 Eu2—N9 Eu2—N12	2.638 (6) 2.647 (6) 2.660 (6) 2.668 (6) 2.700 (6) 2.721 (5)	
Eu1—011 Eu1—N5 Eu1—N2 Eu1—N4 Eu1—N1 Eu1—N3 Eu1—N6	2.600 (5) 2.624 (6) 2.634 (5) 2.646 (6) 2.680 (6) 2.691 (6) 2.725 (5)	Eu2—N11 Eu2—N8 Eu2—N7 Eu2—N10 Eu2—N9 Eu2—N12	2.638 (6) 2.647 (6) 2.660 (6) 2.668 (6) 2.700 (6) 2.721 (5)	
Eu1—012 Eu1—N5 Eu1—N2 Eu1—N4 Eu1—N1 Eu1—N3 Eu1—N6 Eu1—Eu2	2.600 (5) 2.624 (6) 2.634 (5) 2.646 (6) 2.680 (6) 2.691 (6) 2.725 (5) 3.8281 (6)	Eu2—N11 Eu2—N8 Eu2—N7 Eu2—N10 Eu2—N9 Eu2—N12	2.638 (6) 2.647 (6) 2.660 (6) 2.668 (6) 2.700 (6) 2.721 (5)	
Eu1-011 Eu1-012 Eu1-N5 Eu1-N2 Eu1-N4 Eu1-N1 Eu1-N3 Eu1-N6 Eu1-Eu2 yb	2.600 (5) 2.624 (6) 2.634 (5) 2.646 (6) 2.680 (6) 2.691 (6) 2.725 (5) 3.8281 (6)	Eu2—N11 Eu2—N8 Eu2—N7 Eu2—N10 Eu2—N9 Eu2—N12	2.641 (3) 2.638 (6) 2.667 (6) 2.668 (6) 2.700 (6) 2.721 (5)	

Table S1. Selected distances (Å) involving Ln cations in $[Nd_2(L1^{S})_2(\mu-OH)_2(NO_3)_2](NO_3)_2$, $[Eu_2(L1^{R})_2(\mu-OH)_2(NO_3)(H_2O)_2](NO_3)_3$ and $[Yb_2(L1^{S})_2(\mu-OH)_2(H_2O)_2][Na(NO_3)_3(H_2O)_2](NO_3)_2$.^{*)}

Yb1-02	2.207 (4)	Yb2—01	2.214 (4)
Yb1—OW1	2.275 (4)	Yb2—OW2	2.269 (4)
Yb1—N6	2.592 (5)	Yb2—N9	2.598 (5)
Yb1—N4	2.614 (5)	Yb2—N12	2.606 (5)
Yb1—N3	2.619 (5)	Yb2—N10	2.614 (5)
Yb1—N1	2.639 (5)	Yb2—N7	2.630 (5)
Yb1—N5	2.706 (5)	Yb2—N8	2.710 (5)
Yb1—N2	2.727 (5)	Yb2—N11	2.717 (5)
Yb1—Yb2	3.6498 (10)		

^{*)} Key to oxygen atom labels: O1, O2 - bridging hydroxyl; O11, O12, O21, O22, O31, O32 - nitrate, OW1, OW2 - water