Electronic Supplementary Information for Dalton Transactions

Tuning the Self-assembly of Lanthanide Triple Stranded Heterobimetallic Helicates by Ligand Design

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Electronic Supplementary Information

(11 pages)

Table S1 ^{1}H NMR of L^{AB4} in $CDCl_3$.

	1 or 3	2	23	8 and 10		3 or 1	15 and 17		20	6, 12, 21, 22	7 and 11	
δ / ppm	8.38	7.93	7.86	7.73	7.71	7.54	7.46	7.45	7.45	7.28 – 7.38	7.25	7.22
	dd 1H	t 1H	dd 1H	s 1H	s 1H	dd 1H	d 1H	d 1H	dd 1H	m 4H	dd 1H	dd 1H
J / Hz	8.1; 1.2	7.9	6.8; 2.2			7.8; 1.1	2.4	2.4	6.5; 1.3		8.3; 1.8	8.3; 1.8

	4, 13, 18	9	24 or 26	28	26 or 24	5	14 and 19		25 or 27	29	27 or 25
δ / ppm	4.68 – 4.79	4.30	3.61	3.54	3.36	1.45	1.34	1.32	1.29	1.26	1.08
	m 6H	s 2H	q 2H	q 4H	q 2H	t 3H	t 3H	t 3H	t 3H	t 6H	t 3H
J / Hz			7.1	7.1	7.1	7.2	7.1	7.1	7.0	7.2	7.1

Table S2 ^{1}H NMR of L^{AB5} in $CDCl_3$.

	15 and 17		1 or 3	2	23	8 and 10		3 or 1	20	6, 12, 21, 22	7 or 11
δ / ppm	8.39	8.38	8.38	7.93	7.87	7.74	7.70	7.54	7.49	7.33 – 7.41	7.27
	d 1H	d 1H	dd 1H	t 1H	dd 1H	d 1H	d 1H	dd 1H	dd 1H	m 4H	dd 1H
J / Hz	1.9	1.9	8.2; 1.1	7.9	7.3; 2.0	1.3	1.3	7.7; 1.1	7.4; 1.8		8.6; 1.5

	11 or 7	18	13	4	9	24 and 26		5	19	14	25 and 27	
δ / ppm	7.25	4.81	4.77	4.75	4.31	3.61	3.36	1.45	1.38	1.29	1.29	1.08
	dd 1H	q 2H	q 2H	q 2H	s 2H	q 2H	q 2H	t 3H	t 3H	t 3H	t 3H	t 3H
J / Hz	8.0; 1.5	7.2	7.2	7.1		7.1	7.1	7.1	7.2	7.2	7.1	7.1

Table S3 Definition of least squares planes.

	L^1	L^2	L^3
bpb moiety			
terminal benzimidazole	*1*: C1-7; N1-2	*2*: C48-54; N11-12	*3*: C95-101; N21-22
imidazole only	*1i*: C1,6-7; N1-2	*2i*: C48,53-54; N11-12	*3i*: C95,100-101; N21-22
pyridine	*4*: C8-12; N3	*5*: C55-59; N13	*6*: C102-106; N23
bridging benzimidazole	*7*: C13-19; N4-5	*8*: C60-66; N14-15	*9*: C107-113; N24-25
imidazole only	*7i*: C13-14,19; N4-5	*8i*: C60-61,66; N14-15	*9i*: C107-108, 113; N24-25
bpa moiety			
bridging benzimidazole	*10*: C21-27; N6-7	*11*: C68-74; N16-17	*12*: C115-121; N26-27
pyridine	*13*: C28-32; N8	*14*: C75-79; N18	*15*: C122-126; N28

Table S4 Angles and distances between least squares planes.

	$[Pr_2(L^{AB4})_3](ClO_4)_6$		$[Nd_2(L^{AB4})_3](ClO_4)_6$		$[Sm_2(L^{AB4})_3](ClO_4)_6$	
Planes	Angle	*d*	Angle	*d*	Angle	*d*
1 - 6	19.4 º	3.474 Å	20.3 º	3.492 Å	20.8 º	3.479 Å
2 - 4	43.4 º	4.247 Å	43.0 º	4.269 Å	44.0 º	4.231 Å
3 - 5	32.6 º	3.969 Å	31.7 º	3.953 Å	32.0 º	3.887 Å
1i - 9i	21.2 º	4.290 Å	22.6 º	4.295 Å	20.3 º	4.291 Å
2i - 7i	10.9 º	3.510 Å	10.9 º	3.505 Å	12.9 º	3.489 Å
3i - 8i	41.1 º	4.141 Å	42.1 º	4.123 Å	43.0 º	4.087 Å
4 - 9	38.5 º	3.909 Å	39.0 º	3.905 Å	36.8 º	3.785 Å
5 - 7	40.4 º	4.169 Å	39.5 º	4.172 Å	40.9 º	4.145 Å
6 - 8	80.1 º	4.962 Å	79.8 º	4.939 Å	79.5 º	4.896 Å
7 - 12	25.7 º	4.191 Å	26.1 º	4.225 Å	26.6 º	4.240 Å
8 - 10	19.3 º	4.204 Å	19.9 º	4.259 Å	20.2 º	4.277 Å
9 - 11	27.9 º	4.416 Å	28.7 º	4.449 Å	27.2 º	4.476 Å
10 - 15	27.9 º	3.945 Å	29.8 º	3.938 Å	28.8 º	3.867 Å
11 - 13	73.3 º	4.836 Å	72.0 º	4.832 Å	74.8 º	4.797 Å
12 - 14	87.9 º	5.182 Å	87.7 º	5.202 Å	88.3 º	5.159 Å

Table S5 Pitch and Ln^1-Ln^2 distances in L^{AB4} complexes.

	Pr_2	Nd_2	Sm_2
Pitch (Å)	13.4(2)	13.4(2)	13.3(3)
$d(Ln^1\text{-}Ln^2)$ (Å)	9.093(2)	9.148(3)	9.156(2)

Table S6 Angles (º) and distances (Å) in the coordination polyhedra of L^{AB4} complexes.

benzimidazole-pyridine-carboxamide moiety	Φ	θ(P1) θ(P3)	ω (P1-P3) interstrand ω(P1-P2) intrastrand	α P1-P2 P1-P3 P2-P3	β P1 P2 P3	Distances P1 - P2 P2 - P3	Distances Ln – P1 Ln – P2 Ln – P3
Pr_2	175.2	49(2) 54(4)	15(3) 56(2)	6.3 3.1 6.6	12.2 6.1 11.6	1.402 1.783	1.605 0.210 1.561
Nd_2	175.7	48(1) 53(4)	15(3) 56(2)	4.7 3.9 5.3	11.5 6.8 10.6	1.434 1.790	1.622 0.194 1.586
Sm_2	175.4	47(2) 53(5)	14(3) 56(3)	5.5 3.8 6.4	11.6 6.4 11.0	1.446 1.754	1.619 0.180 1.560
Regular trigonal tricapped prism	180	θ(P1) = θ(P3)	0 60	0 0 0	0 0 0	d(P1-P2)= d(P2-P3)	0
benzimidazole-pyridine-benzimidazole moiety	Φ	θ(P4) θ(P6)	ω (P4-P6) interstrand ω(P4-P5) intrastrand	α P4-P5 P4-P6 P5-P6	β P4 P5 P6	Distances P4 – P5 P5 – P6	Distances Ln – P4 Ln – P5 Ln – P6
Pr_2	178.2	51(3) 50(2)	14(2) 53(2)	4.4 7.5 3.5	4.6 8.9 11.6	1.655 1.738	1.681 0.036 1.695
Nd_2	178.4	51(3) 51(3)	13(2) 53(2)	4.1 7.1 3.0	4.9 8.9 11.7	1.651 1.722	1.674 0.030 1.686
Sm_2	178.1	50(3) 50(3)	12(1) 55(2)	4.7 8.2 3.5	3.5 7.9 11.4	1.646 1.693	1.658 0.022 1.663
Regular trigonal tricapped prism	180	θ(P4) = θ(P6)	0 60	0 0 0	0 0 0	d(P4-P5) = d(P5-P6)	0

Table S7 Assignment of ^{1}H NMR spectra of homobimetallic HHH-$[Ln_2(L^{ABX})_3]^{6+}$ complexes in CD_3CN.

	L^{AB4}							L^{AB5}							
	La_2	Ce_2	Pr_2	Nd_2	Sm_2	Eu_2	Lu_2	La_2	Ce_2	Pr_2	Nd_2	Sm_2	Eu_2	Y_2	Lu_2
H1	7.67	8.77	9.53	9.05	7.81	5.57	7.73	7.71	8.97	9.79	9.19	7.88	5.39	7.75	7.75
H2	8.24	9.76	10.56	9.58	8.42	6.57	8.23	8.28	9.99	10.88	9.75	8.50	6.36	8.27	8.26
H3	8.24	10.20	11.65	10.48	8.52	4.93	8.33	8.28	10.61	12.25	10.82	8.65	4.53	8.36	8.37
H4	4.46	4.82	5.07	4.71	4.56	4.17	4.60	4.47	4.99	5.32	4.88	4.70	4.08	4.61	4.67
H4'	4.64	5.34	5.91	5.17	4.81	4.25	4.73	4.68	5.63	6.28	5.38	4.93	3.96	4.76	4.78
H5	1.49	2.46	3.05	2.18	1.67	0.71	1.51	1.51	2.66	3.34	2.33	1.72	0.47	1.52	1.51
H6	7.14	7.01	7.04	7.39	7.03	6.42	7.21	7.16	7.20	7.30	7.57	7.12	6.24	7.22	7.25
H7	6.80	6.21	5.75	6.21	6.66	7.52	6.81	6.93	6.38	5.93	6.39	6.81	7.57	6.91	6.92
H8	6.02	-3.16	-9.95	-1.91	3.94	14.17	5.52	5.97	-1.54	-7.75	-0.74	4.13	12.34	5.51	5.41
H9	3.41	2.75	2.10	2.74	3.29	4.26	3.39	3.47	2.85	2.33	2.83	3.39	4.36	3.49	3.49
H9'	3.69	2.86	2.27	2.78	3.49	4.85	3.63	3.72	3.17	2.57	3.01	3.60	4.51	3.67	3.66
H10	6.12	-5.26	-14.68	-5.39	3.38	18.65	5.60	5.91	-1.85	-8.81	-2.38	4.17	13.57	5.52	5.41
H11	7.26	6.97	6.68	6.95	7.19	7.65	7.21	7.38	7.13	6.88	7.14	7.35	7.73	7.38	7.35
H12	7.54	8.01	8.64	8.61	7.63	5.93	7.55	7.67	7.88	8.39	8.58	7.72	6.33	7.71	7.70
H13	4.26	5.93	7.56	6.48	4.26	1.43	4.36	4.26	4.94	6.18	5.73	4.70	3.05	4.49	4.51
H13'	3.66	5.59	7.56	6.04	4.68	1.02	3.96	3.94	4.68	5.81	5.33	4.48	2.95	4.24	4.29
H14	1.64	2.61	3.51	2.75	1.86	0.34	1.58	1.31	2.02	2.86	2.38	1.55	0.54	1.44	1.44
H15	6.22	8.57	11.25	9.97	6.65	0.84	6.21	7.56	8.21	9.81	9.66	7.62	4.61	7.52	7.51
H17	6.44	8.63	11.12	9.97	6.80	1.14	6.33	7.54	8.32	9.95	9.76	7.61	4.32	7.48	7.47
H18	3.88	6.02	7.79	6.39	4.52	1.12	4.08	4.28	4.94	6.12	5.35	4.31	2.95	4.35	4.37
H18'	4.38	6.05	8.08	6.68	4.81	1.51	4.47	4.52	5.12	6.24	5.87	4.58	3.24	4.57	4.58
H19	1.53	2.27	2.93	2.37	1.70	0.64	1.52	1.49	1.83	2.30	2.02	1.57	1.02	1.48	1.47
H20	7.65	8.40	9.23	8.95	7.74	5.70	7.61	7.69	8.02	8.61	8.70	7.72	6.15	7.72	7.70
H21	7.29	7.25	7.23	7.25	7.28	7.42	7.26	7.38	7.17	7.03	7.20	7.35	7.63	7.34	7.35
H22	6.82	5.93	5.07	5.87	6.58	7.97	6.76	6.88	6.15	5.41	6.02	6.68	7.66	6.82	6.80
H23	6.98	0.12	-6.03	-0.52	5.11	15.44	6.48	6.61	2.60	-2.24	1.32	5.47	11.46	6.31	6.19
H24	3.35	3.53	3.95	3.66	3.46	2.83	3.33	3.37	3.77	4.28	3.82	3.45	2.60	3.33	3.35
H24'	3.25	2.86	2.81	3.17	3.22	3.24	3.33	3.27	3.08	3.11	3.33	3.28	3.04	3.33	3.35
H25	0.92	1.04	1.26	1.11	0.99	0.77	1.05	0.87	1.20	1.51	1.23	1.01	0.57	1.02	1.06
H26	2.81	1.33	0.47	1.72	2.49	4.03	2.59	2.77	1.58	0.87	1.93	2.53	3.72	2.63	2.60
H26'	2.88	2.33	2.05	2.44	2.64	3.26	2.72	2.84	2.60	2.45	2.65	2.69	2.95	2.70	2.72
H27	0.71	-2.33	-4.57	-1.91	0.06	3.64	0.62	0.72	-2.15	-4.31	-1.75	0.10	3.49	0.64	0.63
H28	3.51	4.12	4.79	4.15	3.56	2.75	3.40								
H28'	3.42	4.12	4.79	4.15	3.63	2.53	3.40								
H29	1.18	1.73	2.34	1.87	1.28	0.27	1.10								

Table S8 Percentages of HHH isomer in $[Ln_2(L^{ABX})_3]^{6+}$ complexes in CD_3CN solution at room temperature. Table S3 Percentages of HHH isomer in $[Ln_2(L^{ABX})_3]^{6+}$ complexes in CD_3CN solution at room temperature.

Ln	L^{AB1}	L^{AB2}	L^{AB3}	L^{AB4}	L^{AB5}
La	73	20	79	96	60
Ce	69	13	79	95	53
Pr	67	12	87	93	53
Nd	69	15	87	95	55
Sm	65	11	85	95	56
Eu	69	8	85	96	54
Y	63	8	82		61
Lu	68	6	86	94	60

Table S9 Assignment of ^{1}H NMR spectra of heterobimetallic HHH-$[Ln^{1}Ln^{2}(L^{AB4})_{3}]^{6+}$ complexes in CD_3CN solution.

	LaCe	LaPr	LaNd	LaEu	LaLu	CeLu	PrLu	NdLu	EuLu
H1	9.20	10.33	9.51	5.01	7.73	7.31	6.94	7.28	8.26
H2	10.13	11.25	9.99	6.07	8.24	7.87	7.55	7.84	8.71
H3	10.80	12.74	11.12	4.16	8.36	7.78	7.27	7.73	9.08
H4	5.59	6.06	5.28	3.49	4.52	3.98	3.50	3.96	5.27
H4'	5.80	6.90	5.77	3.49	4.72	4.16	3.66	4.12	5.45
H5	2.60	3.75	2.58	0.15	1.46	1.09	0.76	1.07	1.96
H6	7.46	7.94	7.88	5.68	7.05	6.54	6.08	6.53	7.83
H7	6.47	6.31	6.52	7.05	6.72	6.39	6.08	6.36	7.23
H8	-0.15	-3.95	1.45	10.61	5.64	2.72	0.16	2.47	9.22
H9	2.87	2.54	2.99	3.91	3.38	3.19	3.01	3.11	3.79
H9'	3.53	3.44	3.53	3.91	3.67	2.96	2.34	2.88	4.58
H10	3.19	1.25	3.80	8.69	6.03	-2.56	-10.41	-3.17	16.17
H11	7.04	6.81	7.06	7.53	7.27	7.18	7.12	7.15	7.41
H12	7.19	6.92	7.26	7.97	7.60	8.39	9.27	8.90	5.58
H13	3.85	3.60	3.95	4.68	4.31	6.21	8.18	6.76	1.07
H13'	3.19	2.88	3.28	4.08	3.67	6.04	8.18	6.36	0.62
H14	1.39	1.23	1.46	1.92	1.69	2.84	3.86	2.94	0.12
H15	5.71	5.39	5.82	6.67	6.21	9.01	11.96	10.29	0.39
H17	6.06	5.83	6.15	6.78	6.44	8.95	11.62	10.17	0.84
H18	3.50	3.30	3.59	4.25	3.89	6.36	8.26	6.63	0.74
H18'	4.08	3.87	4.15	4.73	4.30	6.36	8.61	6.90	1.18
H19	1.30	1.14	1.35	1.77	1.54	2.52	3.31	2.55	0.41
H20	7.40	7.24	7.46	7.89	7.66	8.65	9.65	9.14	5.45
H21	7.07	6.93	7.12	7.49	7.29	7.49	7.62	7.44	7.21
H22	6.54	6.37	6.61	7.06	6.82	6.25	5.67	6.12	7.72
H23	6.53	6.24	6.61	7.37	6.99	0.76	-4.91	0.02	15.03
H24	3.93	4.70	4.08	2.34	3.33	2.96	2.62	2.94	3.82
H24'	3.24	3.53	3.52	2.77	3.33	2.96	2.64	2.94	3.82
H25	1.35	1.87	1.45	0.34	1.06	0.76	0.49	0.73	1.44
H26	1.70	1.20	2.16	3.57	2.57	2.11	1.71	2.08	3.18
H26'	2.77	2.90	2.94	2.77	2.71	2.33	2.00	2.30	3.18
H27	-1.98	-3.87	-1.53	3.25	0.61	0.24	-0.08	0.22	1.10
H28	3.25	3.30	3.32	3.67	3.49	4.27	5.05	4.27	2.58
H28'	3.25	3.15	3.23	3.58	3.42	4.27	5.05	4.27	2.37
H29	1.02	0.92	1.05	1.32	1.18	1.89	2.57	1.98	0.12

Table S10 Assignment of ^{1}H NMR spectra of heterobimetallic HHH-$[Ln^{1}Ln^{2}(L^{AB5})_{3}]^{6+}$ complexes in CD_3CN solution.

	LaCe	LaPr	LaNd	LaEu	LaLu	CeLu	PrLu	NdLu	SmLu	EuLu
H1	9.19	10.26	9.49	5.13	7.76	7.54	7.27	7.46	7.70	8.03
H2	10.21	11.35	10.05	6.09	8.27	8.10	7.85	8.00	8.22	8.50
H3	11.00	13.04	11.29	4.08	8.38	8.10	7.74	8.01	8.31	8.75
H4	5.25	5.87	5.21	3.58	4.51	4.23	3.89	4.17	4.51	4.98
H4'	5.94	6.89	5.76	3.58	4.76	4.47	4.12	4.38	4.70	5.16
H5	2.90	3.80	2.61	0.17	1.47	1.27	1.04	1.22	1.44	1.75
H6	7.42	7.83	7.85	5.74	7.06	6.79	6.45	6.74	7.09	7.60
H7	6.53	6.31	6.60	7.24	6.84	6.62	6.35	6.57	6.83	7.21
H8	-0.33	-4.31	1.30	10.44	5.55	4.02	2.25	3.58	5.15	7.34
H9	2.92	2.57	3.03	3.97	3.45	3.31	3.14	3.21	3.46	3.87
H9'	3.56	3.42	3.54	3.97	3.70	3.31	2.84	3.14	3.59	4.20
H10	2.70	1.01	3.57	8.62	5.91	1.36	-4.05	-0.12	4.64	10.91
H11	7.15	6.93	7.18	7.65	7.40	7.36	7.33	7.34	7.39	7.47
H12	7.31	7.03	7.38	8.07	7.70	8.25	9.02	8.87	7.77	5.97
H13	3.85	3.55	3.94	4.67	4.29	5.32	6.78	6.02	4.64	2.63
H13'	3.49	3.17	3.54	4.30	3.88	5.06	6.50	5.61	4.37	2.68
H14	1.03	0.86	1.13	1.65	1.43	2.31	3.25	2.57	1.64	0.36
H15	7.00	6.66	7.11	7.99	7.50	8.66	10.55	9.97	7.68	4.16
H17	7.14	6.90	7.23	7.88	7.53	8.65	10.46	9.97	7.67	4.06
H18	3.96	3.72	3.99	4.60	4.25	5.26	6.66	5.71	4.52	2.65
H18'	4.23	4.03	4.30	4.82	4.53	5.44	6.71	6.08	4.64	2.90
H19	1.24	1.09	1.30	1.73	1.51	2.09	2.71	2.21	1.60	0.80
H20	7.47	7.31	7.53	7.94	7.72	8.30	9.06	8.90	7.77	5.92
H21	7.17	7.02	7.21	7.58	7.39	7.42	7.45	7.39	7.39	7.42
H22	6.61	6.42	6.66	7.13	6.88	6.48	5.95	6.28	6.74	7.42
H23	6.16	5.87	6.27	7.04	6.68	3.22	-1.21	1.87	5.60	11.00
H24	4.02	4.82	4.15	2.31	3.33	3.11	2.89	3.06	3.29	3.58
H24’	3.28	3.59	3.60	2.77	3.38	3.16	2.92	3.09	3.32	3.62
H25	1.38	1.96	1.47	0.26	1.05	0.90	0.70	0.84	1.02	1.26
H26	1.83	1.40	2.20	3.42	2.55	2.30	2.04	2.26	2.52	2.85
H26'	2.87	3.06	2.95	2.63	2.70	2.51	2.28	2.44	2.67	2.95
H27	-1.95	-3.86	-1.52	3.24	0.62	0.43	0.20	0.36	0.58	0.86

Table S11 Composition in % of L^{AB4} complexes in solution. For hetero pairs, the first mentioned Ln is in the bpb cavity.

			Ln^1Ln^2		Ln^2Ln^1			$Ln^1{}_2$		$Ln^2{}_2$	
Ln^1	Ln^2	$\Delta r(Ln^1\text{-}Ln^2)$ / pm	*HHH*	*HHT*	*HHT*	*HHH*	Total hetero	*HHH*	*HHT*	*HHH*	*HHT*
La	Ce	2	34			14	48	10		41	
La	Pr	3.7	41			13	54	24		23	
La	Nd	5.3	54			7	61	16		23	
Eu	Lu	8.8	62				62	14		24	
La	Eu	9.6	75				75	14		12	
Nd	Lu	13.1	68				68	16		16	
Pr	Lu	14.7	82				82	13		5	
Ce	Lu	16.4	76				76	14		11	
La	Lu	18.4	79				79	11		9	

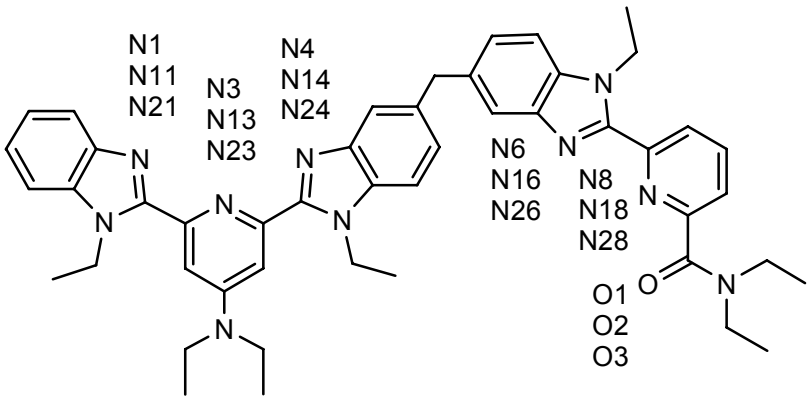
Table S12 Composition in % of L^{AB5} complexes in solution. For hetero pairs, the first mentioned Ln is in the bpb cavity.

			Ln^1Ln^2		Ln^2Ln^1			$Ln^1{}_2$		$Ln^2{}_2$	
Ln^1	Ln^2	$\Delta r(Ln^1\text{-}Ln^2)$ / pm	*HHH*	*HHT*	*HHT*	*HHH*	Total hetero	*HHH*	*HHT*	*HHH*	*HHT*
La	Ce	2	24	12		9	45	15	12	16	12
La	Pr	3.7	29	9		7	45	17	13	13	12
La	Nd	5.3	39	9		4	52	14	10	13	12
La	Sm	8.4	47	9			56	14	11	9	10
Eu	Lu	8.8	39	13			52	15	11	11	11
La	Eu	9.6	48	9			57	10	9	10	15
Sm	Lu	10	57	9			66	10	8	7	9
Nd	Lu	13.1	71	9			80	6	6	5	4
Pr	Lu	14.7	63	7			70	9	9	8	5
Ce	Lu	16.4	79	13			92	4	1	2	1
La	Lu	18.4	77	15			92	3	1	1	1

Table S13 Total percentages of heterobimetallic $[Ln^1Ln^2(L^{ABX})_3]^{6+}$ helicates in CD_3CN.

Ln^1Ln^2	$\Delta r(Ln^1\text{-}Ln^2)$ / pm	L^{AB1}	L^{AB2}	L^{AB3}	L^{AB4}	L^{AB5}
LaCe	2	42		49	48	45
LaPr	3.7	41		48	54	45
LaNd	5.3	51		57	61	52
LaSm	8.4					56
EuLu	8.8	73	21	75	62	52
LaEu	9.6	64		63	75	57
SmLu	10	84		65		66
NdLu	13.1	90	27	70	68	80
PrLu	14.7	95	51	88	82	70
CeLu	16.4	92	60	80	76	92
LaLu	18.4	96	65	87	79	92

Chart S1 Numbering of ligating atoms in L^{AB4}.



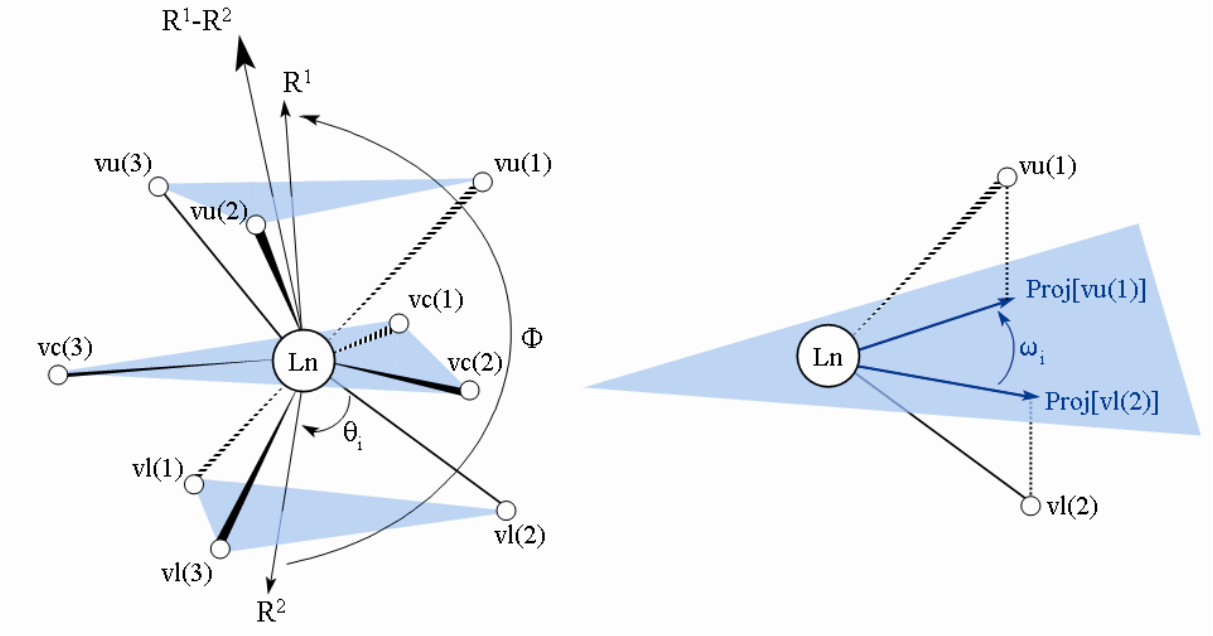


Figure S1 Definition of angles in the coordination polyhedron. The vectors vu(*n*), vc(*n*) and vl(*n*) are defined by the Ln atom and the coordinating atoms of ligand *n* (=1, 2 or 3) in the upper, capping and lower positions of the tricapped trigonal prism. The angles between them are denoted θ_i. The vectors R^1 and R^2 go through the midpoints of the triangles defined by the upper and lower coordinating atoms, respectively. Φ is the angle between them. The projection vectors Proj[v*m*(*n*)] are the projections of vectors v*m*(*n*) onto a plane perpendicular to R^1-R^2. The angles between these vectors are denoted ω_i. Planes in the coordination polydra are defined as follows: P1: O1, O2, O3; P2: N8, N18, N28; P3: N6, N16, N26; P4: N4, N14, N24; P5: N3, N13, N23; P6: N1, N11, N21. The angles α and β are the angles between planes and the angles between a plane and a plane normal to the molecular (Ln-Ln) axis, respectively.