Table S1. Crystallographic data for the chelates of DOTMA with the light lanthanides. The crystallographic parameters for GdDOTMA have been published previously [Aime *et al. Inorg. Chem.* (2011), 7955].

	CeDOTMA	PrDOTMA	NdDOTMA	SmDOTMA	EuDOTMA
Empirical formula	$C_{40}H_{86}Ce_2Cl_2N_8Na_4O_{30}$	$C_{40}H_{82}ClN_8O_{45}Pr_3$	$C_{40}H_{82}ClN_8Nd_3O_{25}$	$C_{40}H_{82}ClN_8O_{25}Sm_3$	$C_{40}H_{100}ClEu_2N_8Na_3O_{34}$
Formula weight	1602.27	1835.14	1543.31	1561.64	1645.62
Temperature (K)	173(2)	103(2)	173(2)	173(2)	101(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	P 2	C 222_1	C 222_1	C 222_1	C 222_1
a (Å)	9.7484(7)	13.0332(3)	13.1080(4)	13.0375(5)	13.2556(7)
b (Å)	9.6633(7)	14.3742(4)	14.3674(4)	14.3825(5)	13.7374(7)
c (Å)	18.8976(14)	39.0639(9)	39.0837(11)	39.0608(11)	37.126(2)
α	90°	90°	90°	90°	90°
β	98.384(1)°	90°	90°	90°	90°
γ	90°	90°	90°	90°	90°
Volume ($Å^3$)	1761.2(2)	7318.3(3)	7360.6(4)	7324.4(5)	6760.6(6)
Z	1	4	4	4	8
Density (calculated) (Mg/m^3)	1.511	1.666	1.393	1.416	1.617
Absorption coefficient (mm^{-1})	1.457	2.104	2.188	2.477	1.989
F(000)	816	3655	3100	3124	3375
Crystal color, morphology	colourless, block	colourless, irregular	colourless, block	colourless, block	pale pink, prism
Crystal size (mm^3)	0.50 × 0.30 × 0.20	0.30 × 0.20 × 0.10	0.50 × 0.25 × 0.20	0.50 × 0.50 × 0.35	0.30 × 0.20 × 0.20
Theta range for data collection	2.11 to 27.49°	2.1 to 27.0°	2.08 to 25.03°	2.09 to 25.05°	3.786 to 28.485°
Index ranges	-12 ≤*h* ≤ 12 -12 ≤*k* ≤ 12 0 ≤*l* ≤ 24	-17 ≤ h ≤ 17 -19 ≤ k ≤19 -52≤ l ≤52	-15 ≤*h* ≤ 15 -16 ≤*k* ≤ 17 -46 ≤*l* ≤ 46	-15 ≤*h* ≤ 15 -17 ≤*k* ≤ 17 -46 ≤*l* ≤ 46	-16 ≤ h ≤17 - 18≤ k ≤15 - 50≤ l ≤50
Reflections collected	20692	64287	33120	32642	29906
Independent reflections	7915 [R(int) = 0.0279]	9228 [R(int) = 0.0455]	6507 [R(int) = 0.0439]	6482 [R(int) = 0.0391]	7919 [R(int) = 0.0618]
Observed reflections	7645	9213	6051	6306	7189
Completeness to theta = 25.05°	99.4%	99.7%	99.9%	99.8%	92.8%
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.75 and 0.60	1.0 and 0.8089	0.6687 and 0.4076	0.4777 and 0.3706	0.83 and 0.742
Refinement method	Full-matrix least-squares on F^2	Full-matix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7915 / 1 / 395	9228 / 6 / 407	6507 / 0 / 340	6482 / 0 / 353	7919 / 0 / 404
Goodness-of-fit on F^2	1.088	1.333	1.042	1.066	1.152
Final *R* indices [$I>2\sigma(I)$]	*R*1 = 0.0309 *wR*2 = 0.0825	*R*1 = 0.0722 *wR*2 = 0.1518	*R*1 = 0.0409 *wR*2 = 0.0952	*R*1 = 0.0330 *wR*2 = 0.0904	*R*1 = 0.0724 *wR*2 = 0.1909
R indices (all data)	*R*1 = 0.0322 *wR*2 = 0.0835	*R*1 = 0.0723 *wR*2 = 0.1518	*R*1 = 0.0452 *wR*2 = 0.0969	*R*1 = 0.0340 *wR*2 = 0.0909	*R*1 = 0.0796 *wR*2 = 0.1959
Absolute structure parameter	0.022(12)	0.018(5)	0.08(2)	0.070(18)	0.12(3)
Largest diff. peak and hole	1.453 and -0.833 e.$Å^{-3}$	1.820 and -4.231 e.$Å^{-3}$	1.305 and -1.081 e.$Å^{-3}$	0.721 and -0.857 e.$Å^{-3}$	1.816 and -2.515 e.$Å^{-3}$

Table S2. Crystallographic data for the chelates of DOTMA with the heavy lanthanides. The crystallographic parameters for HoDOTMA have been published previously [Payne *et al. Chem Commun.* (2013), 2320].

	TbDOTMA	DyDOTMA	ErDOTMA	TmDOTMA	YbDOTMA
Empirical formula	$C_{80}H_{160}Cl_4N_{16}Na_2O_{64}Tb_6$	$C_{80}H_{128}Cl_2Dy_6N_{16}NaO_{67}$	$C_{40}H_{86}ClEr_2N_8Na_3O_{27}$	$C_{40}H_{84}ClN_8Na_3O_{26}Tm_2$	$C_{40}H_{86}ClN_8Na_3O_{27}Yb_2$
Formula weight	3535.01	3454.87	1550.10	1535.42	1561.67
Temperature (K)	297(2)	296(2)	297(2)	298(2)	173(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Triclinic
Space group	P 2_1	P 2_1	P 2	C 222_1	P 1
a (Å)	13.4186(2)	13.4034(4)	13.1684(2)	13.063(2)	9.393(2)
b (Å)	37.0201(7)	36.9704(16)	19.0482(3)	13.840(2)	9.405(2)
c (Å)	13.6498(3)	13.6578(4)	13.1654(2)	37.274(5)	19.293(5)
α	90°	90°	90°	90°	81.712(4)°
β	90.293(2)°	90.236(3)°	90.0550(10)°	90°	88.039(3)°
γ	90°	90°	90°	90°	84.747(2)°
Volume ($Å^3$)	6780.6(2)	6767.8(4)	3302.33(9)	6739.1(17)	1679.1(7)
Z	2	2	4	4	1
Density (calculated) (Mg/m^3)	1.731	1.695	1.559	1.513	1.544
Absorption coefficient (mm^{-1})	3.227	3.409	2.663	2.751	2.905
F(000)	3559	3394	1568	3104	788
Crystal color, morphology	colourless, prism	pale pink, prism	pink, prism	pink, prism	colourless, block
Crystal size (mm^3)	0.78 × 0.58 × 0.16	0.40 × 0.20 × 0.20	0.25 × 0.25 × 0.20	0.30 × 0.30 × 0.30	0.50 x 0.20 x 0.20
Theta range for data collection	3 to 28°	2.1 to 27.5°	3.447 to 32.216°	3.503 to 23.964°	2.13 to 26.42°
Index ranges	-18 ≤ h ≤19 - 51≤ k ≤53 - 20≤ l ≤19	-19 ≤ h ≤14 - 29≤ k ≤54 - 15≤ l ≤ 20	-19≤ h ≤ 18 -28 ≤ k ≤23 -18 ≤ l ≤19	- 16≤ h ≤16 - 12≤ k ≤17 - 45≤ l ≤45	-11 ≤ *h* ≤ 11 -11 ≤ *k* ≤ 11 -24 ≤ *l* ≤ 24
Reflections collected	46091	29993	43429	14851	18344
Independent reflections	35954[R(int) = 0.0284]	22913 [R(int) = 0.0359]	17447 [R(int) = 0.0232]	6421 [R(int) = 0.1358]	13282 [R(int) = 0.0215]
Observed reflections	32762	22046	15451	5812	12673
Completeness to theta = 25.05°	92.2%	89.8%	93.5%	99.3%	99.4%
Absorption correction	Analytical, 8 faces	Multi-scan	Analytical, 8 faces	Multi-scan	Multi-scan
Max. and min. transmission	0.586 and 0.158	1.0 and 0.468	0.359 and 0.260	1.0 and 0.481	0.5942 and 0.3245
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	35954 / 1 / 1517	22911 1 / 1479	17447 / 1 / 428	6421 / 241 / 378	13282 / 4 / 741
Goodness-of-fit on F^2	1.053	1.173	1.066	1.679	1.033
Final *R* indices [$I>2\sigma(I)$]	R1 = 0.0660 wR2 = 0.1508	R1 = 0.0769 wR2 = 0.1833	R1 = 0.0360 wR2 = 0.0919	R1 = 0.1705 wR2 = 0.4116	R1 = 0.0360 wR2 = 0.0919
R indices (all data)	R1 = 0.0722 wR2 = 0.1548	R1 = 0.0790 wR2 = 0.1848	R1 = 0.0360 wR2 = 0.0919	R1 = 0.1633 wR2 = 0.4072	R1 = 0.0382 wR2 = 0.0938
Absolute structure parameter	0.080(12)	0.061(11)	0.006(10)	0.21(6)	0.071(9)
Largest diff. peak and hole	2.274 and -2.930 e.Å-3	2.653 and -3.544e.Å-3	1.873 and -1.725 e.Å-3	3.313 and -3.572 e.Å-3	1.946 and -1.169 e.Å-3

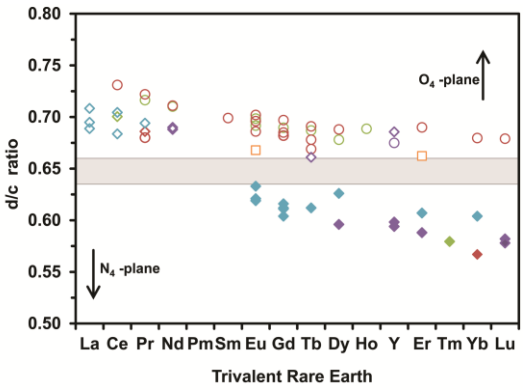

Figure S1. The position of the Ln^{3+} ion relative to the N_4 and O_4 planes (the d/c ratio) in the crystal structures of various of DOTA-type chelates. Open symbols represents chelates in which a coordinated water molecule was identified, the closed symbols chelates in which no coordinated water molecule was identified.

Circles: SAP	Diamonds: TSAP
Acetates	Green
Amides	Red
Pyridyls	Orange
Phosphinates	Blue
Phosphonates	Purple

Table S3. Selected parameters from the crystal structures of the LnDOTMA chelates.

Ln Ion	Space Group	Metal Ion Label	q	Ln-OH_2	d (Å)	c (Å)	d/c	O4 Area ($Å^2$)	O-Ln-O °		Ave
Ce	P2	1	1	2.565	1.719	2.477	0.69	10.91	144.20	143.99	144.10
Pr	C2221	1	1	2.598	1.662	2.479	0.67	10.49	141.67	139.75	140.71
Nd	C2221	1	1	2.563	1.651	2.478	0.67	10.44	141.01	139.35	140.18
Pm											
Sm	C2221	1	1	2.511	1.633	2.470	0.66	10.10	140.06	138.23	139.15
Eu	C2221	1	1	2.584	1.624	2.449	0.66	9.93	139.15	139.59	139.37
Gd	P2	1	1	2.500	1.663	2.457	0.68	9.99	140.86	140.87	140.87
Tb	P21	1	1	2.592	1.618	2.483	0.65	9.50	136.55	136.76	136.66
		2	1	2.617	1.599	2.480	0.64	9.44	135.85	135.62	135.74
		3	1	2.569	1.618	2.469	0.66	9.66	137.78	137.60	137.69
		4	1	2.628	1.569	2.494	0.63	9.24	133.15	133.70	133.43
Dy	P21	2	1	2.550	1.601	2.453	0.65	9.68	137.45	137.89	137.67
		3	1	2.606	1.602	2.482	0.65	9.36	136.47	134.89	135.68
		5	0	-	1.514	2.501	0.61	8.78	129.81	129.33	129.57
		6	1	2.659	1.568	2.482	0.63	9.13	133.44	133.65	133.55
Ho	C222	1	1	2.662	1.581	2.460	0.64	9.14	135.25	135.38	135.32
		2	0	-	1.469	2.493	0.59	8.51	127.16	127.30	127.23
Er	P2	1	0	(2.902)	1.556	2.479	0.63	8.88	132.64	132.76	132.70
		2	0	-	1.456	2.493	0.58	8.44	126.22	126.22	126.22
		3	0	-	1.453	2.501	0.58	8.38	126.22	125.69	125.96
		4	1	2.732	1.551	2.465	0.63	8.95	133.37	133.14	133.26
Tm	C2221	1	0	-	1.413	2.453	0.58	8.00	122.05	128.39	125.22
Yb	P1	1	0	-	1.439	2.515	0.57	7.90	124.92	122.65	123.79
		2	0	-	1.425	2.494	0.57	7.91	122.39	124.57	123.48

Table S4. Selected parameters from the crystal structures of the LnDOTMA chelates.

Ln Ion	Metal Ion Label	Chelate Torsion Angle (°)				Ave	N-C-C-O Torsion (°)				Ave
Ce	1	-25.17	-25.26	-25.88	-25.20	-25.38	-14.69	-14.53	-15.59	-35.40	-20.05
Pr	1	-25.62	-26.78	-25.20	-25.38	-25.75	-28.43	-9.74	-19.57	-34.11	-22.96
Nd	1	-25.45	-25.85	-25.56	-26.63	-25.87	-17.21	-11.94	-29.32	-26.44	-21.23
Pm											
Sm	1	-24.70	-25.20	-24.28	-26.14	-25.08	-28.08	-12.60	-19.94	-26.14	-21.69
Eu	1	-27.89	-25.98	-27.59	-27.35	-27.20	-23.45	-14.62	-12.86	-13.19	-16.03
Gd	1	-25.10	-27.14	-26.71	-25.41	-26.09	-16.66	-13.63	-16.14	-28.68	-18.78
Tb	1	-25.47	-26.74	-25.78	-24.70	-25.67	-15.10	-22.99	-27.47	-17.64	-20.80
	2	-27.61	-25.52	-24.66	-23.20	-25.25	-24.44	-11.82	-27.52	-19.63	-20.85
	3	-25.91	-25.55	-25.84	-25.67	-25.74	-34.58	-25.63	-19.75	-14.14	-23.53
	4	-24.95	-26.35	-25.75	-25.86	-25.73	-16.74	-19.46	-26.37	-33.42	-24.00
Dy	2	-26.77	-25.32	-25.99	-25.13	-25.80	-24.82	-21.66	-15.80	-35.24	-24.38
	3	-25.98	-26.88	-25.40	-25.53	-25.95	-14.19	-27.20	-23.37	-13.54	-19.58
	5	-25.91	-25.98	-25.52	-25.75	-25.79	-20.28	-24.45	-25.58	-32.39	-25.68
	6	-26.30	-27.11	-24.43	-24.18	-25.51	-23.55	-17.98	-30.61	-32.57	-26.18
Ho	1	-24.75	-25.26	-25.11	-24.87	-25.00	-19.18	-21.30	-21.30	-19.18	-20.24
	2	-25.32	-25.32	-25.45	-25.46	-25.39	-23.41	-23.22	-23.41	-23.22	-23.32
Er	1	-25.64	-25.69	-25.64	-25.59	-25.64	-26.24	-26.27	-26.24	-26.15	-26.23
	2	-25.26	-25.49	-25.26	-25.49	-25.38	-23.90	-23.97	-23.9	-23.97	-23.94
	3	-25.50	-25.38	-25.50	-25.38	-25.44	-23.99	-24.43	-23.99	-24.43	-24.21
	4	-26.26	-26.03	-26.01	-26.23	-26.13	-20.83	-19.71	-20.83	-19.71	-20.27
Tm	1	-30.38	-32.77	-29.23	-33.01	-31.35	-8.83	-7.37	-9.28	-19.98	-11.37
Yb	1	-26.34	-25.43	-24.99	-24.28	-25.26	-25.66	-22.87	-14.66	-23.54	-21.68
	2	-24.95	-26.66	-24.57	-24.65	-25.21	-19.30	-6.31	-24.27	-25.52	-18.85

Table S5. Selected parameters from the crystal structures of the LnDOTMA chelates.

Ln Ion	Metal Ion Label	N-C-C-N Torsion (°)				Ave	Ln-Cl Distance (Å)
Ce	1	-60.23	-61.33	-59.18	-60.51	-60.31	5.979
Pr	1	-61.85	-60.02	-58.18	-59.39	-59.86	5.933
Nd	1	-60.85	-60.34	-59.74	-61.44	-60.59	5.933
Pm							
Sm	1	-60.14	-59.72	-61.77	-61.43	-60.77	5.921
Eu	1	-62.20	-61.40	-56.69	-59.99	-60.07	5.880
Gd	1	-59.73	-60.56	-59.31	-59.23	-59.71	5.935
Tb	1	-60.33	-59.93	-63.79	-59.88	-60.98	5.938
	2	-55.89	-56.58	-60.17	-60.27	-58.23	5.911
	3	-60.86	-58.35	-62.60	-58.82	-60.16	5.934
	4	-58.98	-58.77	-58.47	-57.82	-58.51	5.860
Dy	2	-56.11	-57.36	-61.97	-56.45	-57.97	5.926
	3	-57.21	-60.69	-65.77	-60.69	-61.09	5.948
	5	-61.41	-59.10	-54.24	-59.39	-58.54	5.807
	6	-58.88	-59.81	-60.45	-57.19	-59.08	5.880
Ho	1	-58.94	-59.22	-58.94	-59.22	-59.08	5.868
	2	-58.63	-59.30	-58.63	-59.30	-58.97	5.705
Er	1	-57.83	-59.14	-57.83	-59.14	-58.49	5.849
	2	-59.05	-59.72	-59.05	-59.72	-59.39	5.731
	3	-59.11	-56.75	-59.11	-56.75	-57.93	5.702
	4	-58.27	-57.63	-58.27	-57.63	-57.95	5.826
Tm	1	-57.71	-52.67	-54.93	-44.17	-52.37	5.701
Yb	1	-57.92	-59.43	-58.53	-57.91	-58.45	5.710
	2	-57.39	-54.06	-56.43	-59.91	-56.95	5.750

Table S6. Selected parameters from the crystal structures of the LnDOTMA chelates.

Ln Ion	Metal Ion Label	Calc'd IR (Å)	Calc'd CN	N-Ln Distance (Å)				Ave	O-Ln Distance (Å)				Ave
Ce	1	1.176	8.63	2.726	2.716	2.765	2.740	2.737	2.454	2.437	2.454	2.477	2.456
Pr	1	1.147	8.39	2.706	2.681	2.683	2.732	2.701	2.462	2.428	2.449	2.393	2.433
Nd	1	1.141	8.58	2.703	2.690	2.673	2.696	2.691	2.436	2.416	2.463	2.407	2.431
Pm													
Sm	1	1.115	8.69	2.687	2.673	2.661	2.668	2.672	2.411	2.361	2.426	2.396	2.399
Eu	1	1.091	8.47	2.659	2.652	2.670	2.603	2.646	2.402	2.360	2.390	2.355	2.377
Gd	1	1.107	9.00	2.674	2.659	2.704	2.686	2.681	2.391	2.369	2.373	2.358	2.373
Tb	1	1.079	8.70	2.651	2.653	2.646	2.656	2.652	2.349	2.353	2.323	2.357	2.346
	2	1.071	8.55	2.592	2.672	2.639	2.636	2.635	2.364	2.329	2.358	2.334	2.346
	3	1.085	8.82	2.662	2.660	2.628	2.663	2.653	2.367	2.349	2.359	2.352	2.357
	4	1.062	8.40	2.609	2.606	2.640	2.640	2.624	2.366	2.305	2.322	2.369	2.341
Dy	2	1.080	8.94	2.607	2.644	2.630	2.679	2.640	2.334	2.359	2.369	2.377	2.360
	3	1.069	8.76	2.642	2.644	2.622	2.663	2.643	2.348	2.342	2.334	2.320	2.336
	5	1.032	8.08	2.586	2.569	2.601	2.592	2.587	2.315	2.320	2.334	2.297	2.317
	6	1.055	8.49	2.639	2.613	2.609	2.635	2.624	2.304	2.332	2.331	2.333	2.325
Ho	1	1.043	8.49	2.616	2.612	2.616	2.612	2.614	2.314	2.309	2.309	2.314	2.312
	2	1.006	7.84	2.547	2.552	2.547	2.552	2.550	2.300	2.305	2.300	2.305	2.303
Er	1	1.030	8.45	2.603	2.596	2.596	2.603	2.600	2.302	2.299	2.302	2.299	2.301
	2	1.000	7.93	2.546	2.548	2.546	2.548	2.547	2.297	2.288	2.297	2.288	2.293
	3	1.005	8.02	2.543	2.544	2.543	2.544	2.544	2.300	2.313	2.300	2.313	2.307
	4	1.031	8.46	2.595	2.600	2.595	2.600	2.598	2.301	2.307	2.301	2.307	2.304
Tm	1	0.969	7.56	2.518	2.499	2.507	2.532	2.514	2.268	2.273	2.315	2.197	2.263
Yb	1	0.983	7.97	2.525	2.539	2.504	2.518	2.522	2.286	2.293	2.286	2.275	2.285
	2	0.964	7.63	2.505	2.501	2.512	2.524	2.511	2.244	2.245	2.285	2.255	2.257

Table S7. Selected parameters from the crystal structures of the LnDOTMA chelates: Ln-*ax*^{S} and Ln-ac are the distance between the Ln^{3+} ion and the axial proton on the side carbon and the acetate proton, respectively.

Ln Ion	Metal Ion Label	q	Ln-OH_2	Ln-*ax*^{S} Distance (Å)				Ave	Ln-*ac* Distance (Å)				Ave
Ce	1	1	2.565	3.848	3.784	3.824	3.808	3.816	3.346	3.539	3.522	3.564	3.493
Pr	1	1	2.598	3.781	3.872	3.753	3.697	3.776	3.440	3.640	3.579	3.466	3.531
Nd	1	1	2.563	3.780	3.750	3.715	3.714	3.740	3.553	3.532	3.356	3.461	3.476
Pm													
Sm	1	1	2.511	3.717	3.723	3.759	3.683	3.721	3.545	3.399	3.355	3.436	3.434
Eu	1	1	2.584	3.714	3.764	3.687	3.718	3.721	3.480	3.436	3.531	3.331	3.445
Gd	1	1	2.500	3.762	3.784	3.755	3.793	3.774	3.460	3.478	3.295	3.500	3.433
Tb	1	1	2.592	3.735	3.654	3.705	3.667	3.690	3.486	3.419	3.321	3.465	3.423
	2	1	2.617	3.648	3.727	3.736	3.739	3.713	3.372	3.322	3.541	3.378	3.403
	3	1	2.569	3.736	3.682	3.666	3.719	3.701	3.334	3.398	3.425	3.497	3.414
	4	1	2.628	3.660	3.707	3.655	3.709	3.683	3.365	3.388	3.458	3.285	3.374
Dy	2	1	2.550	3.725	3.751	3.667	3.652	3.699	3.365	3.411	3.309	3.375	3.365
	3	1	2.606	3.707	3.671	3.684	3.659	3.680	3.485	3.450	3.348	3.426	3.427
	5	0	-	3.644	3.675	3.660	3.628	3.652	3.340	3.359	3.463	3.298	3.365
	6	1	2.659	3.658	3.749	3.640	3.707	3.689	3.381	3.380	3.537	3.351	3.412
Ho	1	1	2.662	3.695	3.685	3.695	3.685	3.690	3.399	3.410	3.399	3.410	3.405
	2	0	-	3.621	3.596	3.596	3.621	3.609	3.333	3.324	3.333	3.324	3.329
Er	1	0	(2.902)	3.664	3.668	3.664	3.668	3.666	3.402	3.385	3.402	3.385	3.394
	2	0	-	3.604	3.605	3.605	3.604	3.605	3.346	3.328	3.346	3.328	3.337
	3	0	-	3.615	3.601	3.615	3.601	3.608	3.343	3.329	3.343	3.329	3.336
	4	1	2.732	3.650	3.658	3.650	3.658	3.654	3.398	3.398	3.398	3.398	3.398
Tm	1	0	-	3.528	3.704	3.613	3.551	3.599	3.312	3.256	3.443	3.392	3.351
Yb	1	0	-	3.557	3.571	3.603	3.620	3.588	3.341	3.407	3.391	3.309	3.362
	2	0	-	3.626	3.583	3.561	3.569	3.585	3.344	3.467	3.360	3.268	3.360

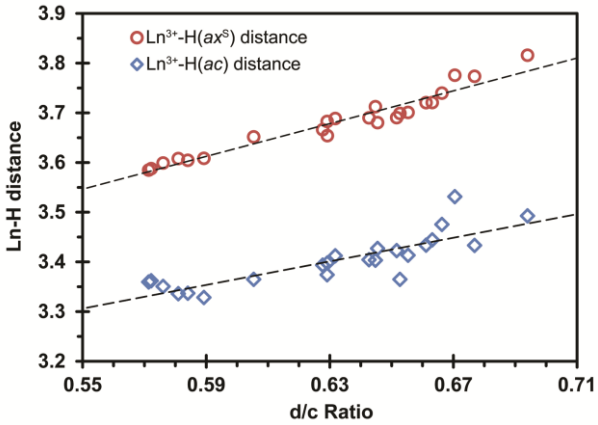

Figure S2. The variation of in the Ln^{3+}-H distance with d/c ratio (chelates hydration) is different for the axial proton on the side carbon (ax^S) and the acetate proton (*ac*), consistent with previous solution state observations (Webber *et al. Dalton Trans.* (2014) 251).