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Supporting information for article:

Ce-exchange capacity of zeolite L in different cationic forms: a structural investigation

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Table S1 XRF and LOI/TG analyses of K-LTL, Na-LTL and Na-LTL-80°C.

	LOI/TG	Na ₂ O	MgO	Al ₂ O ₃	SiO ₂	K ₂ O	TiO ₂	MnO	Fe ₂ O ₃
K-LTL	10.92	0.45	0	16.49	57.01	15.06	0.01	0.00	0.05
Na-LTL	12.51	3.28	0	17.33	56.89	10.09	0.02	0.00	0.03
Na-LTL-80°C	12.46	3.20	0.13	16.69	56.57	9.93	0.02	0.00	0.03

Table S2 EDS analysis recalculated on the basis of H₂O and NH₄ contents obtained by TG and elemental analysis, respectively.

	SiO ₂	K ₂ O	Al ₂ O ₃	Ce ₂ O ₃	Na ₂ O	H ₂ O	(NH ₄) ₂ O	SiO ₂ esd	K ₂ O esd	Al ₂ O ₃ esd	Ce ₂ O ₃ esd	Na ₂ O esd
NH ₄ -LTL	60.49	3.97	17.33	/	/	11.46	6.67	0.06	0.08	0.07	/	/
K-Ce-LTL	55.29	8.57	16.74	6.58	0.23	12.60	/	0.16	0.06	0.06	0.14	0.02
Na-Ce-LTL	57.82	8.49	16.74	7.09	0.16	12.70	/	0.17	0.06	0.06	0.02	0.02
NH ₄ -Ce-LTL	57.02	3.03	16.28	6.77	/	13.29	3.60	0.10	0.06	0.08	0.19	/
NH ₄ -Ce-LTL-rev	74.42	4.03	20.77	0.71	/	11.63	6.62	0.09	0.02	0.03	0.05	/

Table S3 Nitrogen (%) content from elemental analysis, and calculated NH₄⁺ amount (%).

Name	N %	NH ₄ %
NH ₄ -LTL	3.59	4.62
NH ₄ -Ce-LTL	1.99	2.56
NH ₄ -Ce-LTL-rev	3.56	4.58

Table S4 H₂O amount from L.O.I. or TG (measured at 290 °C) in the LTL samples.

Sample	Technique	Water amount (%)
<i>K-LTL</i>	TG	10.92
<i>Na-LTL</i>	TG	12.51
<i>Na-LTL-80°C</i>	L.O.I.	12.46
<i>NH₄-LTL</i>	TG	11.46
<i>K-Ce-LTL</i>	TG	12.60
<i>Na-Ce-LTL</i>	TG	12.70
<i>NH₄-Ce-LTL</i>	TG	13.29
<i>NH₄-Ce-LTL-rev</i>	TG	11.63

Table S5 Structural refinement parameters of the LTL samples.

	<i>K-LTL</i>	<i>Na-LTL</i>	<i>NH₄-LTL</i>	<i>K-Ce-LTL</i>	<i>Na-Ce-LTL</i>	<i>NH₄-Ce-LTL</i>
R _{wp} (%)	7.76	8.94	7.78	7.92	7.69	7.46
R _p (%)	5.62	6.53	5.70	5.66	5.51	5.34
R _f ² (%)	7.66	8.73	9.31	8.91	8.90	9.08
N _{obs}	1641	1680	1651	1632	1631	1646
N _{var}	67	67	67	67	67	67

Table S6 Atomic coordinates, occupancy factors and isotropic thermal parameters of sample *K-LTL*.

Site		<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	Occupancy factor	<i>U</i> _{iso}
Si1	Si ⁴⁺	0.0932(1)	0.3570(1)	1/2	1	0.0125(2)
Si2	Si ⁴⁺	0.1655(1)	0.4980(1)	0.2118(2)	1	0.0125(2)
O1	O ²⁻	0	0.2711(3)	1/2	1	0.0254(5)
O2	O ²⁻	0.1639(2)	0.3277(3)	1/2	1	0.0254(5)
O3	O ²⁻	0.2628(1)	0.5257(2)	0.2573(5)	1	0.0254(5)
O4	O ²⁻	0.1026(2)	0.4138(1)	0.3291(3)	1	0.0254(5)
O5	O ²⁻	0.4246(1)	0.8493(2)	0.2766(5)	1	0.0254(5)
O6	O ²⁻	0.1437(2)	0.4762(2)	0	1	0.0254(5)
KB	K ⁺	1/3	2/3	1/2	1	0.026(1)
KC	K ⁺	0	1/2	1/2	0.954(4)	0.027(1)
KD	K ⁺	0	0.2999(2)	0	0.826(3)	0.073(1)
W1	O	0.0595(7)	0.119(1)	1/2	0.333	0.13
W2	O	0	0.127(3)	1/2	0.166	0.13
W3	O	0	-0.1430(2)	0.2019(6)	0.5	0.13
W4	O	0	0	0.210(4)	0.58(1)	0.13
W5	O	0.1261(2)	0.2523(4)	0	1	0.13
W6	O	0	0.0946(6)	0	0.307(5)	0.13

Table S7 Selected framework and extraframework distances of sample *K-LTL*.

Si1_O1	1.649(3)	Si1_O2	1.635(2)	Si1_O4 x2	1.611(2)	Si2_O3	1.633(2)
Si2_O4	1.649(2)	Si2_O5	1.648(2)	Si2_O6	1.644(1)		
KB_O3 x6	2.894(4)						
KC_O4 x8	3.270(2)	KC_O5 x4	2.929(3)				
KD_O4 x4	3.181(3)	KD_O6 x2	2.985(4)	KD_W3 x2	3.257(5)	KD_W5 x2	2.857(3)
W1_W2 x2	3.00(4)	W1_W3 x4	2.628(3)	W1_W4 x2	2.89(3)		
W2_O1	2.65(6)	W2_W1 x2	3.00(4)	W2_W4 x2	3.19(5)		
W3_KD	3.257(5)	W3_W1 x2	2.628(3)	W3_W3 x2	2.628(3)	W3_W4	2.629(4)
W3_W5 x2	2.656(5)	W3_W6 x2	2.769(4)				
W4_W1 x6	2.89(3)	W4_W2 x6	3.19(5)	W4_W3 x6	2.629(4)	W4_W4	3.16(6)
W5_KD x2	2.857(3)	W5_W3 x4	2.656(5)	W5_W6 x2	2.655(4)		
W6_W3 x4	2.769(4)	W6_W5 x2	2.655(4)	W6_W6 x2	3.01(2)		

Table S8 Atomic coordinates, occupancy factors and isotropic thermal parameters of sample *Na-LTL*.

Site		<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	Occupancy factor	<i>U</i> _{ISO}
Si1	Si ⁴⁺	0.0929(1)	0.3560(1)	1/2	1	0.019(1)
Si2	Si ⁴⁺	0.1661(1)	0.4986(1)	0.2123(2)	1	0.019(1)
O1	O ²⁻	0	0.2671(3)	1/2	1	0.0245(6)
O2	O ²⁻	0.1616(2)	0.3233(4)	1/2	1	0.0245(6)
O3	O ²⁻	0.2627(1)	0.5255(3)	0.2579(5)	1	0.0245(6)
O4	O ²⁻	0.1032(2)	0.4138(2)	0.3280(3)	1	0.0245(6)
O5	O ²⁻	0.4243(1)	0.8486(2)	0.2811(6)	1	0.0245(6)
O6	O ²⁻	0.1429(3)	0.4743(3)	0	1	0.0245(6)
KB	K ⁺	1/3	2/3	1/2	1	0.021(1)
KC	K ⁺	0	1/2	1/2	0.939(4)	0.018(1)
KD	K ⁺	0	0.2966(4)	0	0.639(4)	0.107(2)
W1	O	0.066(1)	0.132(2)	1/2	0.333	0.13
W2	O	0	0.125(4)	1/2	0.1666	0.13
W3	O	0	-0.1373(3)	0.1947(4)	0.5	0.13
W4	O	0	0	0.3026(23)	0.170(1)	0.13
W5	O	0.1214(1)	0.2427(3)	0	1	0.13
W6	O	0	0.0833(2)	0	0.422(6)	0.13

Table S9 Selected framework and extraframework distances of sample *Na-LTL*.

Si1_O1	1.672(3)	Si1_O2	1.648(3)	Si1_O4 x2	1.624(2)	Si2_O3	1.623(2)
Si2_O4	1.649(3)	Si2_O5	1.653(2)	Si2_O6	1.656(2)		
KB_O3 x6	2.893(4)						
KC_O4 x8	3.284(3)	KC_O5 x4	2.918(4)				
KD_O4 x4	3.200(4)	KD_O6 x2	2.996(6)	KD_W3 x2	3.273(8)	KD_W5 x2	2.856(5)
W1_W2 x2	3.11(4)	W1_W3 x4	2.623(3)	W1_W4 x2	2.57(3)		
W2_O1	2.61(7)	W2_W1 x2	3.11(4)	W2_W4 x2	2.73(6)		
W3_KD	3.273(8)	W3_W1 x2	2.623(3)	W3_W3 x2	2.523(5)	W3_W4	2.650(5)
W3_W5 x2	2.559(4)	W3_W6 x2	2.644(3)				
W4_W1 x6	2.57(3)	W4_W2 x6	2.73(6)	W4_W3 x6	2.650(5)	W4_W4	2.97(4)
W4_W6 x6	2.75(1)						
W5_KD x2	2.856(5)	W5_W3 x4	2.559(4)	W5_W6 x2	2.648(4)		
W6_W3 x4	2.644(3)	W6_W4 x2	2.75(1)	W6_W5 x2	2.648(4)	W6_W6 x2	2.652(7)
W6_W6	3.062(8)						

Table S10 Atomic coordinates, occupancy factors and isotropic thermal parameters of sample *NH₄-LTL*.

Site		x/a	y/b	z/c	Occupancy factor	U _{ISO}
Si1	Si ⁴⁺	0.0938(1)	0.3579(1)	1/2	1	0.0145(2)
Si2	Si ⁴⁺	0.1661(1)	0.4987(1)	0.2116(2)	1	0.0145(2)
O1	O ²⁻	0	0.2743(3)	1/2	1	0.0262(5)
O2	O ²⁻	0.1649(17)	0.3298(3)	1/2	1	0.0262(5)
O3	O ²⁻	0.2635(1)	0.5270(2)	0.2539(5)	1	0.0262(5)
O4	O ²⁻	0.1039(2)	0.4148(2)	0.3267(3)	1	0.0262(5)
O5	O ²⁻	0.4249(1)	0.8498(2)	0.2809(5)	1	0.0262(5)
O6	O ²⁻	0.1451(2)	0.4766(2)	0	1	0.0262(5)
KB	K ⁺	1/3	2/3	1/2	1	0.034(1)
KC	K ⁺	0	1/2	1/2	0.515(4)	0.058(3)
KD	K ⁺	0	0.2905(4)	0	0.533(3)	0.125(3)
W1	O	0.0611(9)	0.122(2)	1/2	0.333	0.13
W2	O	0	0.122(3)	1/2	0.166	0.13
W3	O	0	-0.1375(2)	0.1939(5)	0.5	0.13
W4	O	0	0	0.291(3)	0.31(1)	0.13
W5	O	0.1210(1)	0.2420(2)	0	0.950(7)	0.13
W6	O	0	0.0830(2)	0	0.260(5)	0.13

Table S11 Selected framework and extraframework distances for the structural refinement of sample *NH₄-LTL*.

Si1_O1	1.642(2)	Si1_O2	1.630(2)	Si1_O4 x2	1.627(2)	Si2_O3	1.630(2)
Si2_O4	1.639(2)	Si2_O5	1.659(2)	Si2_O6	1.645(1)		
KB_O3 x6	2.901(4)						
KC_O4 x8	3.292(2)	KC_O5 x4	2.910(4)				
KD_O4 x4	3.254(4)	KD_O6 x2	3.119(6)	KD_W3 x2	3.175(8)	KD_W5 x2	2.786(5)
W1_W2 x2	2.97(3)	W1_W3 x4	2.644(3)	W1_W4 x2	2.51(3)		
W2_O1	2.81(6)	W2_W1 x2	2.97(3)	W2_W4 x2	2.74(5)		
W3_KD	3.175(8)	W3_W1 x2	2.644(3)	W3_W3 x2	2.534(4)	W3_W4	2.638(4)
W3_W5 x2	2.554(4)	W3_W6 x2	2.650(3)				
W4_W1 x6	2.51(3)	W4_W2 x6	2.74(5)	W4_W3 x6	2.638(4)	W4_W4	3.15(4)
W4_W6 x6	2.68(2)						
W5_KD x2	2.786(5)	W5_W3 x4	2.554(4)	W5_W6 x2	2.649(3)		
W6_W3 x4	2.650(3)	W6_W4 x2	2.68(2)	W6_W5 x2	2.649(3)	W6_W6 x2	2.648(5)

W6 W6 3.058(6)

Table S12 Atomic coordinates, occupancy factors and isotropic thermal parameters of sample *K-Ce-LTL*.

Site		<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	Occupancy factor	<i>U</i> _{ISO}
Si1	Si ⁴⁺	0.0929(1)	0.3560(1)	1/2	1	0.0100(2)
Si2	Si ⁴⁺	0.1645(1)	0.4970(1)	0.2105(2)	1	0.0100(2)
O1	O ²⁻	0	0.2693(3)	1/2	1	0.0138(5)
O2	O ²⁻	0.1626(2)	0.3252(4)	1/2	1	0.0138(5)
O3	O ²⁻	0.2624(1)	0.5248(2)	0.2536(5)	1	0.0138(5)
O4	O ²⁻	0.1034(2)	0.4126(2)	0.3286(3)	1	0.0138(5)
O5	O ²⁻	0.4240(1)	0.8479(2)	0.2729(5)	1	0.0138(5)
O6	O ²⁻	0.1464(3)	0.4777(2)	0	1	0.0138(5)
KB	K ⁺	1/3	2/3	1/2	1	0.028(1)
KC	K ⁺	0	1/2	1/2	0.929(4)	0.014(1)
KD	Ce ³⁺	0	0.2907(3)	0	0.231(1)	0.163(3)
Ce	Ce ³⁺	0	0	1/2	0.882(2)	0.07(1)
W2	O	0	0.126(1)	1/2	0.5	0.13
W3	O	0	-0.1050(6)	0.282(1)	0.5	0.13
W5	O	0.1129(2)	0.2257(4)	0	1	0.13
W6	O	0	0.0652(6)	0	0.1666	0.13

Table S13 Selected framework and extraframework distances for the structural refinement of sample *K-Ce-LTL*.

Si1_O1	1.651(3)	Si1_O2	1.636(3)	Si1_O4 x2	1.605(2)	Si2_O3	1.636(2)
Si2_O4	1.646(3)	Si2_O5	1.645(2)	Si2_O6	1.621(2)		
KB_O3 x6	2.920(4)						
KC_O4 x8	3.299(3)	K2_O5 x4	2.960(4)				
KD_O4 x4	3.236(4)	KD_O6 x2	3.127(5)	KD_W5 x2	2.859(5)		
Ce_W2 x6	2.30(2)	Ce_W3 x12	2.53(1)				
W2_O1	2.64(2)	W2_Ce	2.30(2)	W2_W3 x4	2.695(8)		
W3_W2 x2	2.695(8)	W3_Ce	2.53(1)	W3_W3 x2	3.28(2)	W3_W5 x2	3.019(9)
W3_W6 x2	2.711(9)						
W5_KD	2.859(5)	W5_W3 x4	3.019(9)	W5_W6 x2	2.619(6)		
W6_W3 x4	2.711(9)	W6_W5 x2	2.619(6)				

Table S14 Atomic coordinates, occupancy factors and isotropic thermal parameters of sample *Na-Ce-LTL*.

Site		<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	Occupancy factor	<i>U</i> _{ISO}
Si1	Si ⁴⁺	0.0927(1)	0.3556(1)	1/2	1	0.0106(2)
Si2	Si ⁴⁺	0.1645(1)	0.4973(1)	0.2106(2)	1	0.0106(2)
O1	O ²⁻	0	0.2689(3)	1/2	1	0.0155(4)
O2	O ²⁻	0.1628(2)	0.3256(4)	1/2	1	0.0155(4)
O3	O ²⁻	0.2622(2)	0.5243(2)	0.2553(5)	1	0.0155(4)
O4	O ²⁻	0.1040(2)	0.4133(2)	0.3287(3)	1	0.0155(4)
O5	O ²⁻	0.4238(1)	0.8476(2)	0.2742(5)	1	0.0155(4)
O6	O ²⁻	0.1463(3)	0.4768(2)	0	1	0.0155(4)
KB	K ⁺	1/3	2/3	1/2	1	0.022(1)
KC	K ⁺	0	1/2	1/2	0.935(4)	0.015(1)
KD	Ce ³⁺	0	0.2922(3)	0	0.225(1)	0.181(2)
Ce	Ce ³⁺	0	0	1/2	0.979(2)	0.089(1)
W2	O	0	0.1259(4)	1/2	0.5	0.13
W3	O	0	-0.1023(5)	0.261(1)	0.5	0.13
W5	O	0.1098(2)	0.2197(4)	0	1	0.13
W6	O	0	0.0564(7)	0	0.1666	0.13

Table S15 Selected framework and extraframework distances for the structural refinement of sample *Na-Ce-LTL*.

Si1_O1	1.649(3)	Si1_O2	1.633(3)	Si1_O4 x2	1.615(2)	Si2_O3	1.637(2)
Si2_O4	1.639(3)	Si2_O5	1.641(2)	Si2_O6	1.625(2)		
KB_O3 x6	2.917(4)						
KC_O4 x8	3.296(3)	K2_O5 x4	2.959(4)				
KD_O4 x4	3.233(4)	KD_O6 x2	3.096(5)	KD_W5 x2	2.918(5)		
Ce_W2 x6	2.309(8)	Ce_W3 x12	2.60(1)				
W2_O1	2.624(7)	W2_Ce	2.309(8)	W2_W3 x4	2.786(7)		
W3_W2 x2	2.786(7)	W3_Ce	2.60(1)	W3_W3 x2	3.25(2)	W3_W5 x2	2.865(8)
W3_W6 x2	2.550(9)						
W5_KD x2	2.918(5)	W5_W3 x4	2.865(8)	W5_W6 x2	2.645(7)		
W6_W3 x4	2.550(9)	W6_W5 x2	2.645(7)				

Table S16 Atomic coordinates, occupancy factors and isotropic thermal parameters of sample *NH₄-Ce-LTL*.

Site		<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	Occupancy factor	<i>U</i> _{ISO}
Si1	Si ⁴⁺	0.0926(1)	0.3561(1)	1/2	1	0.010(2)
Si2	Si ⁴⁺	0.1651(1)	0.4975(1)	0.2096(2)	1	0.010(2)
O1	O ²⁻	0	0.2701(3)	1/2	1	0.0152(3)
O2	O ²⁻	0.1625(2)	0.3251(3)	1/2	1	0.0152(3)
O3	O ²⁻	0.2625(1)	0.5250(2)	0.2559(6)	1	0.0152(3)
O4	O ²⁻	0.1046(2)	0.4142(2)	0.3283(3)	1	0.0152(3)
O5	O ²⁻	0.4239(1)	0.8477(2)	0.2710(5)	1	0.0152(3)
O6	O ²⁻	0.1474(3)	0.4766(2)	0	1	0.0152(3)
KB	K ⁺	1/3	2/3	1/2	0.973(5)	0.019(1)
KC	K ⁺	0	1/2	1/2	0.532(5)	0.036(3)
KD	Ce ³⁺	0	0.2875(4)	0	0.200(1)	0.198(3)
Ce	Ce ³⁺	0	0	1/2	0.961(2)	0.107(1)
W2	O	0	0.1270(4)	1/2	0.5	0.13
W3	O	0	-0.1013(5)	0.2572(14)	0.5	0.13
W5	O	0.1086(2)	0.2171(4)	0	1	0.13
W6	O	0	0.0536(6)	0	0.1666	0.13

Table S17 Selected framework and extraframework distances for the structural refinement of sample *NH₄-Ce-LTL*.

Si1_O1	1.645(3)	Si1_O2	1.647(3)	Si1_O4 x2	1.623(2)	Si2_O3	1.637(2)
Si2_O4	1.637(3)	Si2_O5	1.643(2)	Si2_O6	1.621(1)		
KB_O3 x6	2.913(4)						
KC_O4 x8	3.301(3)	K2_O5 x4	2.977(4)				
KD_O4 x4	3.283(4)	KD_O6 x2	3.163(6)	KD_W5 x2	2.871(6)		
Ce_W2 x6	2.336(8)	Ce_W3 x12	2.61(1)				
W2_O1	2.631(6)	W2_Ce	2.336(8)	W2_W3 x4	2.816(7)		
W3_W2 x2	2.816(7)	W3_Ce	2.61(1)	W3_W3 x2	3.23(2)	W3_W5 x2	2.834(9)
W3_W6 x2	2.523(9)						
W5_KD x2	2.871(6)	W5_W3 x4	2.834(9)	W5_W6 x2	2.649(6)		
W6_W3 x4	2.523(9)	W6_W5 x2	2.649(6)				

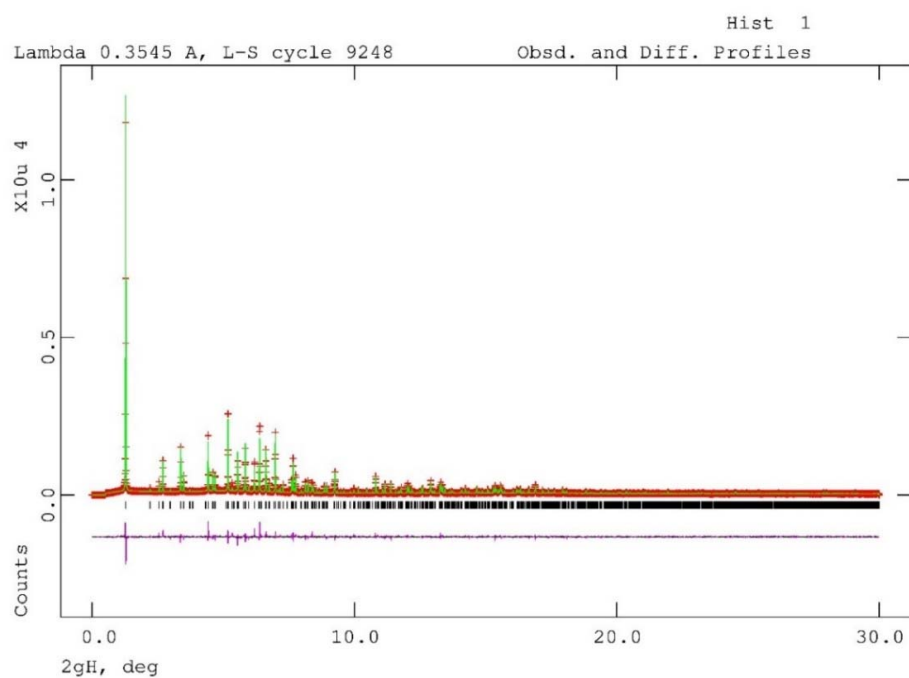


Figure S1 Observed (red dash marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinement of *K-LTL*

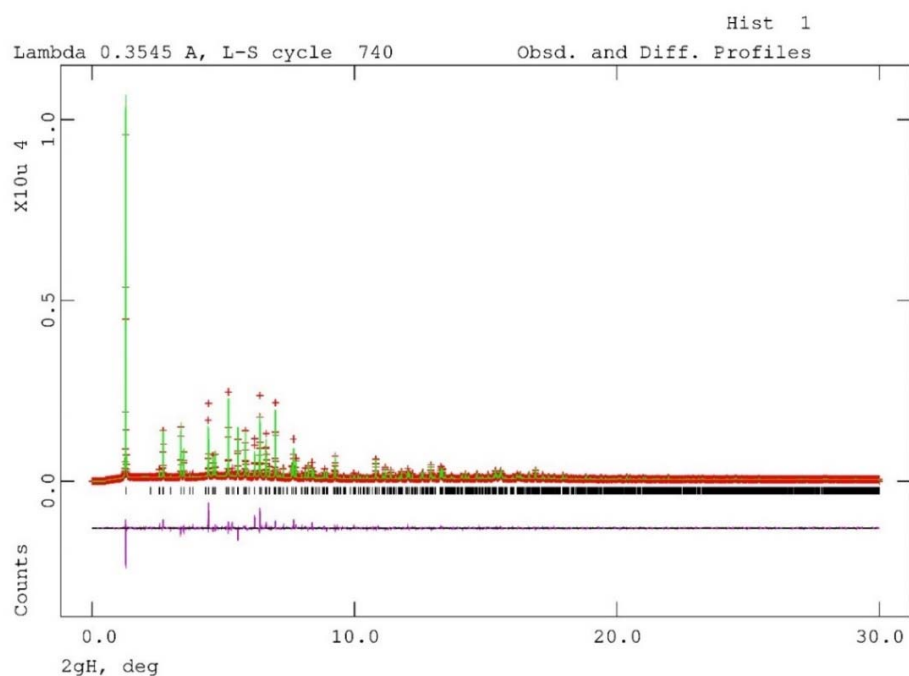


Figure S2 Observed (red dash marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinement of *Na-LTL*.

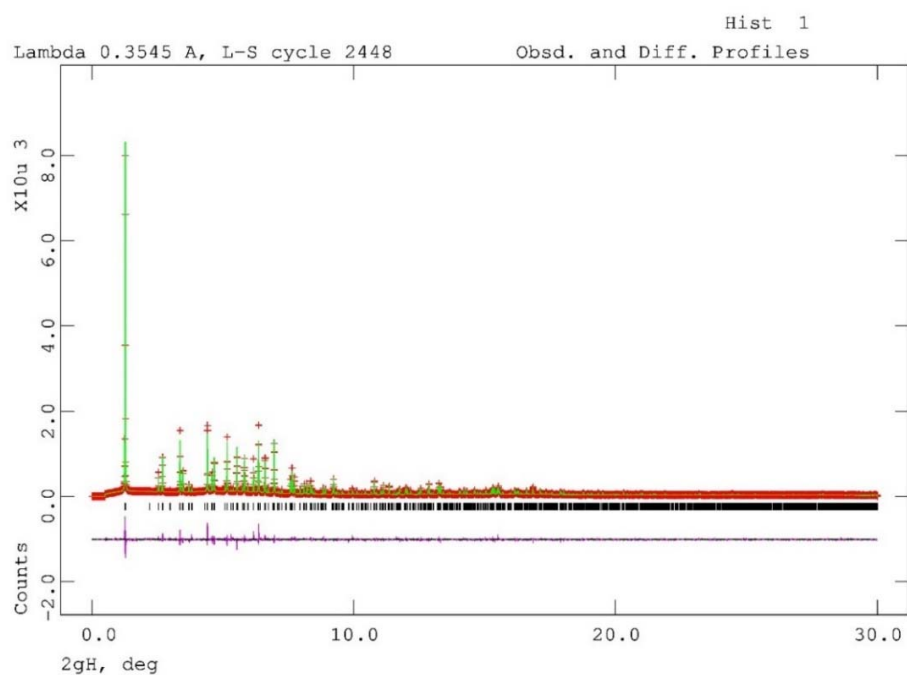


Figure S3 Observed (red dash marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinement of *NH₄-LTL*.

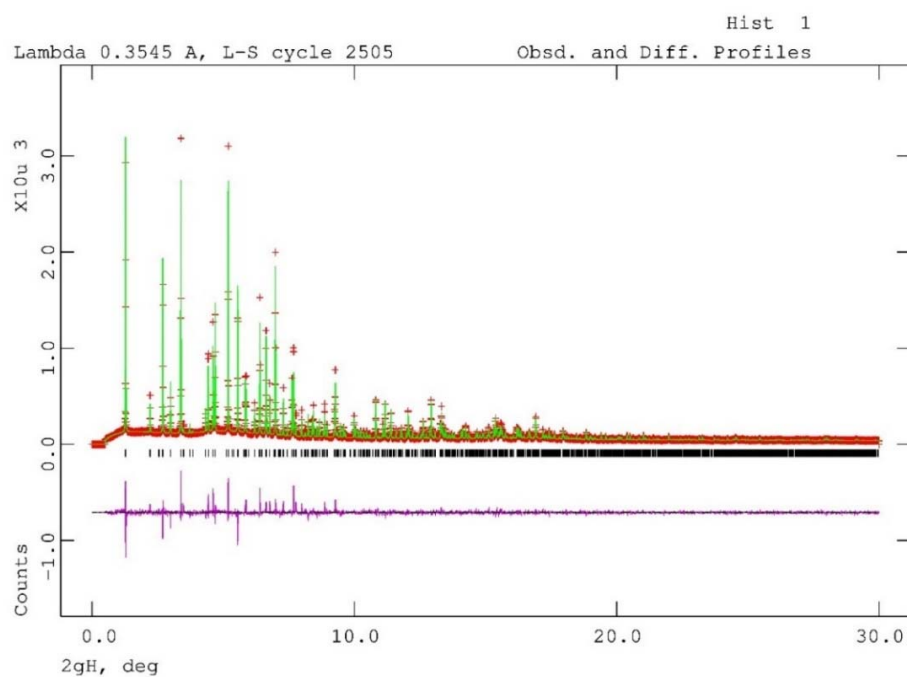


Figure S4 Observed (red dash marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinement of *K-Ce-LTL*.

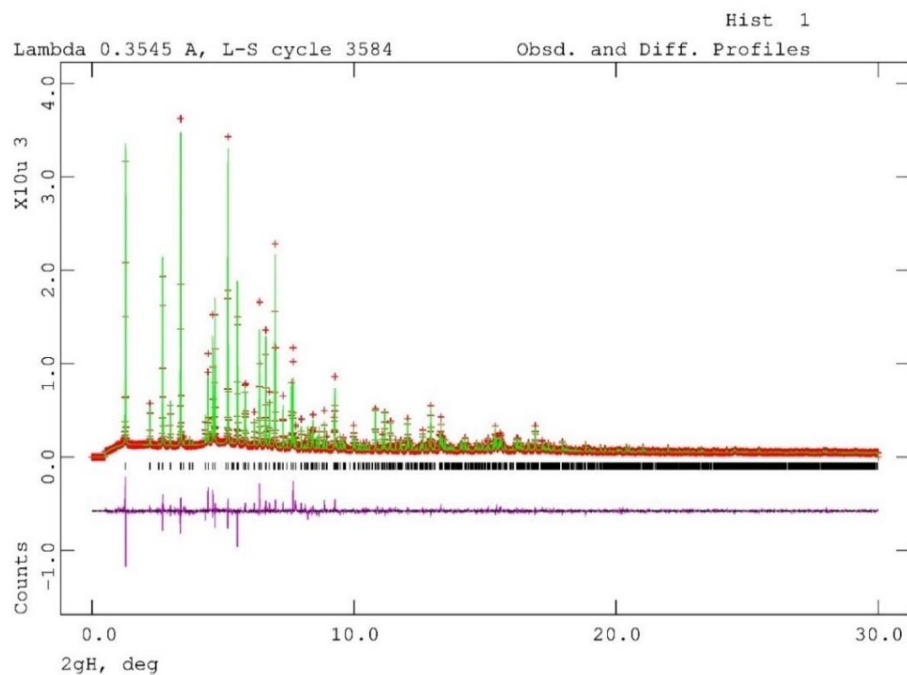


Figure S5 Observed (red dash marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinement of *Na-Ce-LTL*.

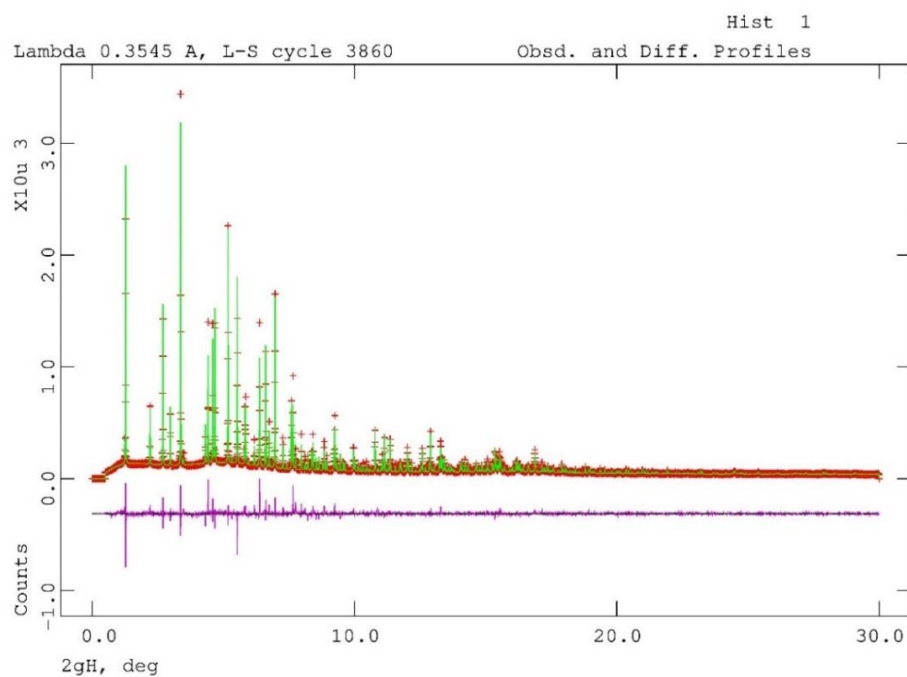


Figure S6 Observed (red dash marks) and calculated (green line) diffraction patterns and final difference curve (purple line) from Rietveld refinement of *NH₄-Ce-LTL*.