

Supporting Information

Selective hydride interstitials induced in a high-entropy lanthanide oxyhydride

Yuvraj Vaishnav,^{a,b} Rohit K. Rai,^{a,c} Walid Al Maksoud,^{a,c} Fumitaka Takeiri,^{d,e} Shusaku Hayama,^f Hiroshi Yaguchi^d, Samy Ould-Chikh,^a Marcell Toth,^{a,b} Raza Ullah Shah Bacha,^{a,c} Bambar Davaasuren,^g Maxim Avdeev^{h,i} Genki Kobayashi,^d Yoji Kobayashi^{*a,b,c}

[a] KAUST Catalysis Center (KCC), Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia

[b] Chemistry Program, Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia

[c] Center for Renewable Energy and Storage Technologies (CREST), Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia

[d] Solid State Chemistry Laboratory, Cluster for Pioneering Research (CPR), RIKEN, Wako 351-0198, Japan

[e] Department of Chemistry, Kindai University, Osaka 577-8502, Japan

[f] Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom

[g] Core Labs, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia

[h] Australian Nuclear Science and Technology Organisation, New Illawarra Rd, Lucas Heights, NSW 2234, Australia

[i] School of Chemistry, The University of Sydney, Sydney 2006, Australia

HAADF-STEM image and EDX spectrum

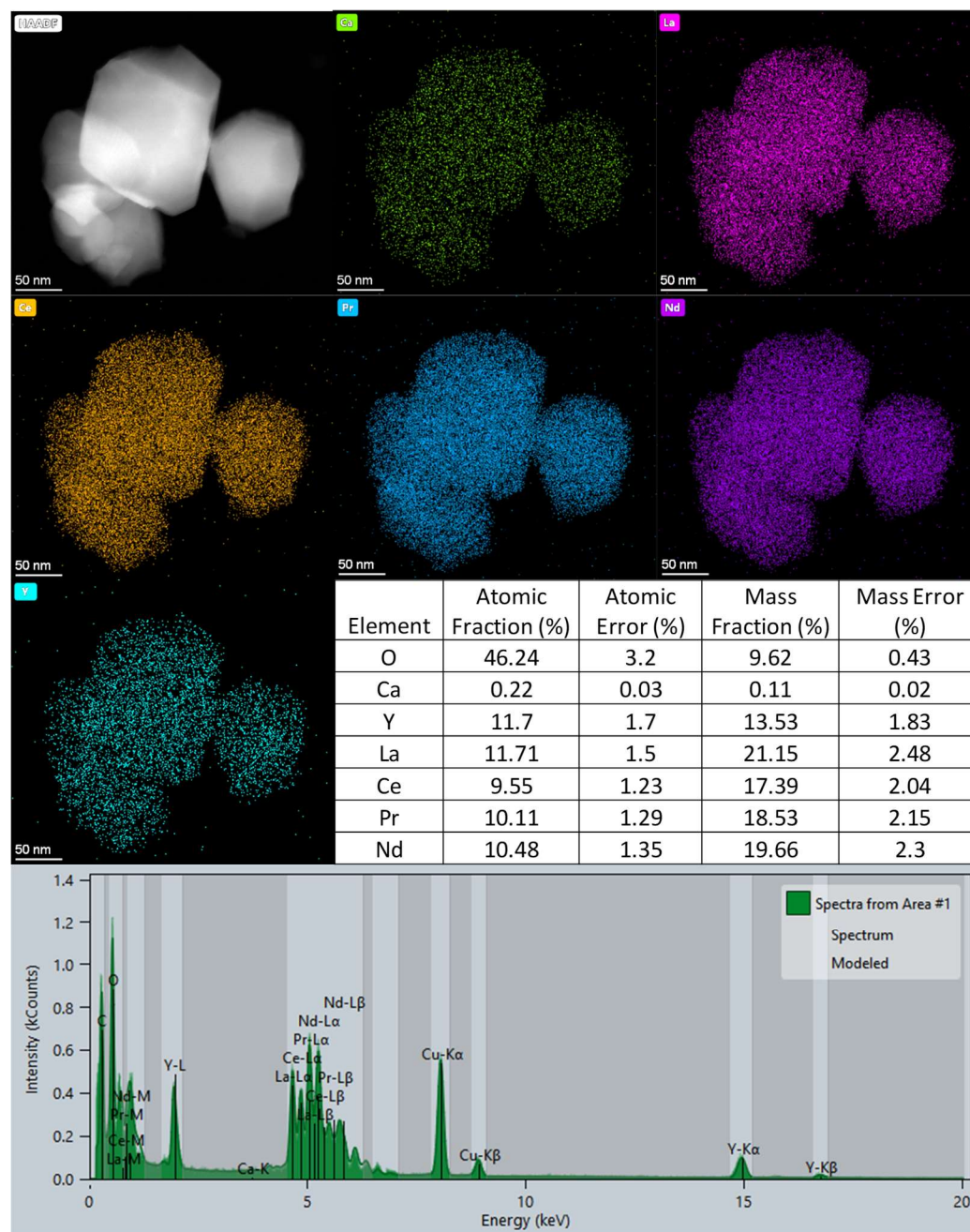


Fig. S1. HAADF-STEM images along with corresponding EDX spectrum of the $(\text{La,Ce,Pr,Nd,Y})\text{H}_{3-2x}\text{O}_x$.

HAADF-STEM image and EDX spectrum

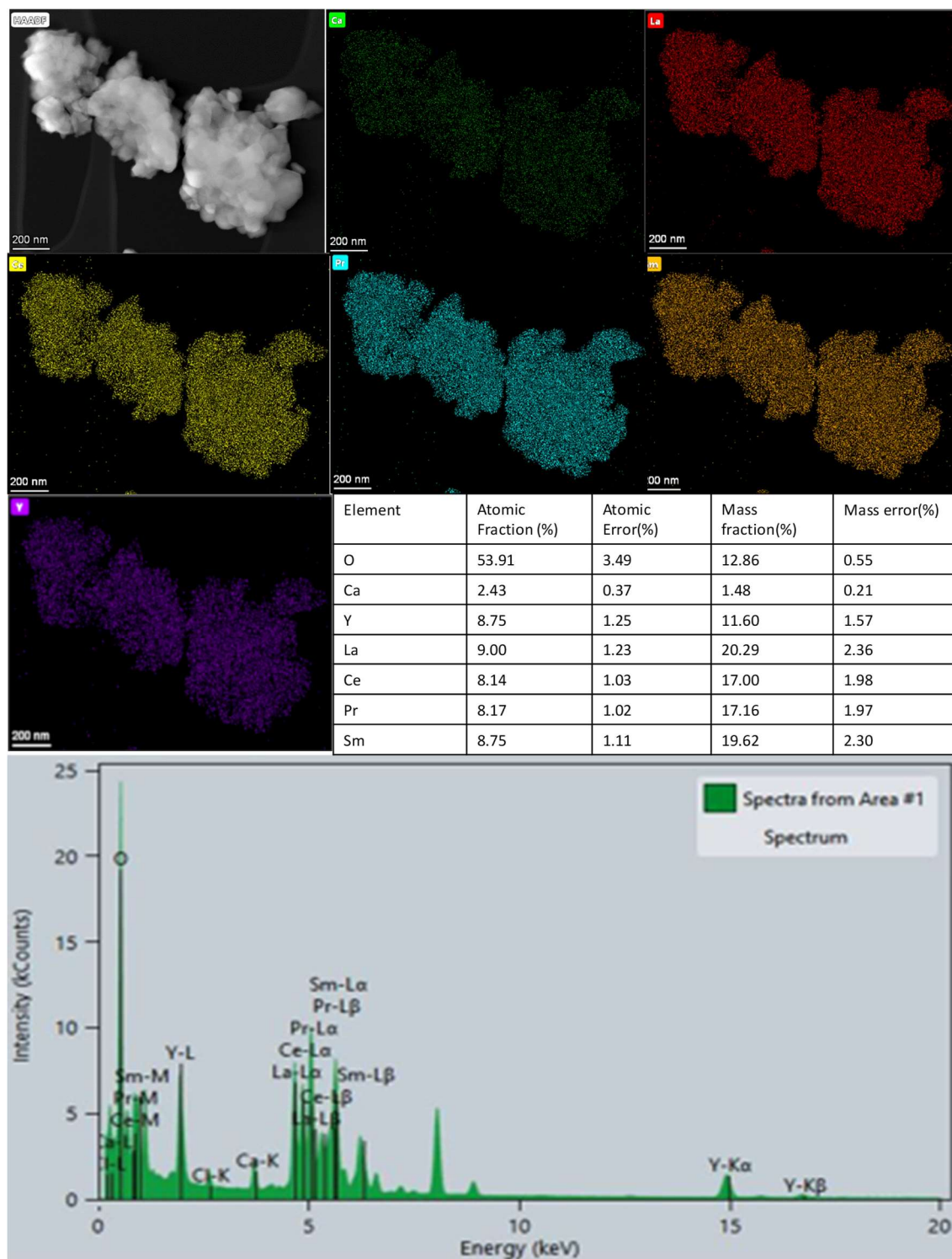


Fig. S2. HAADF-STEM images along with corresponding EDX spectrum of the $(\text{La,Ce,Pr,Sm,Y})\text{H}_{3-2x}\text{O}_x$.

Refinements:

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray-Neutron combined refinement:

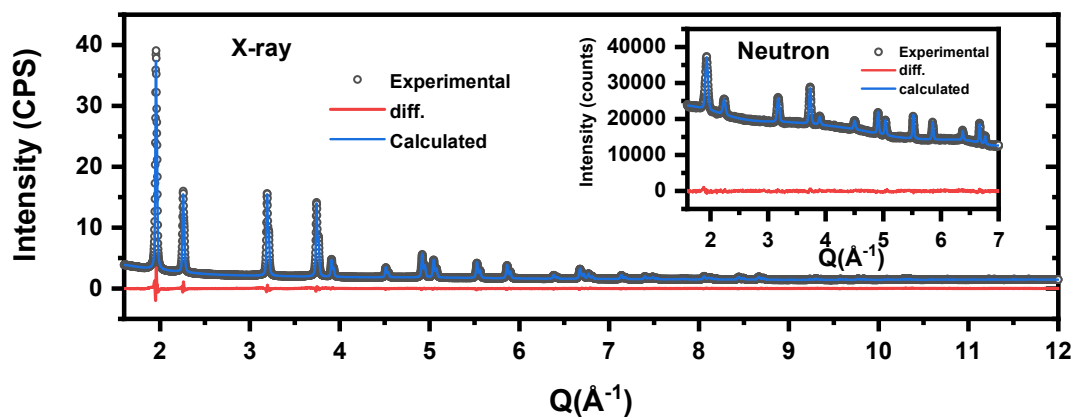


Figure S-3 Combined refinement of x-ray and neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x.

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La	0.00	0.00	0.00	0.01233(11)	0.2000
2	Ce	0.00	0.00	0.00	0.01233(11)	0.2000
3	Pr	0.00	0.00	0.00	0.01233(11)	0.2000
4	Nd	0.00	0.00	0.00	0.01233(11)	0.2000
5	Y	0.00	0.00	0.00	0.01233(11)	0.2000
6	O1	0.250	0.250	0.250	0.005	0.3757(16)
7	H1	0.250	0.250	0.250	0.005	0.37(8)
8	H2	0.500	0.0925(6)	0.0925(6)	0.0280(23)	0.0327(6)
9	H3	0.713(7)	0.713(7)	0.713(7)	0.0103(31)	0.046(19)

X-ray $R_{wp} = 2.04\%$ R_F , $R_F^2 = 5.46\%$, 5.95% ; Neutron $R_{wp} = 1.09\%$ R_F , $R_F^2 = 3.56\%$, 9.07% . *

All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁺) fixed to be equal. **

ICP shows equimolar cation so ** constrain similar occupancy.

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray powder diffraction:

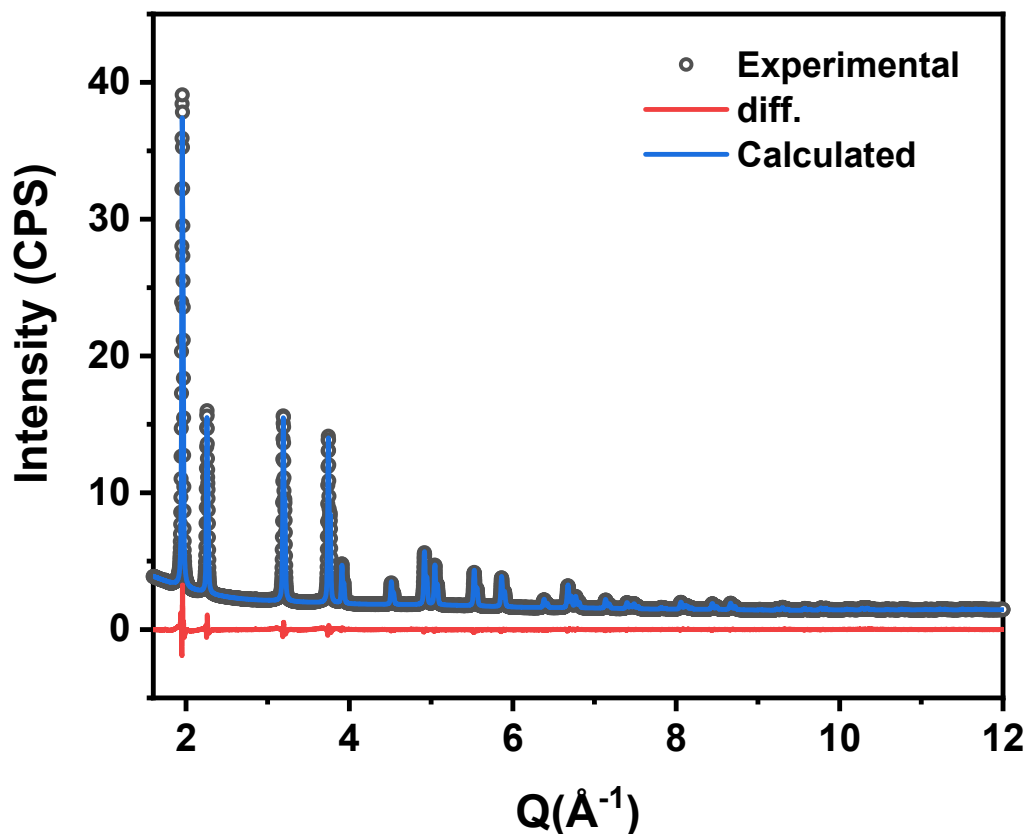


Figure S-4 Refinement of X-ray powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x.

S.No.	Atom	x	y	Z	*U _{iso}	**Occ.
1	La	0.000	0.000	0.000	0.01914(11)	0.2000
2	Ce	0.000	0.000	0.000	0.01914(11)	0.2000
3	Pr	0.000	0.000	0.000	0.01914(11)	0.2000
4	Nd	0.000	0.000	0.000	0.01914(11)	0.2000
5	Y	0.000	0.000	0.000	0.01914(11)	0.2000
6	O1	0.250	0.250	0.250	0.0465(31)	0.510(8)
7	H1	0.250	0.250	0.250	0.0465(31)	0.490(8)

R_{wp} = 2.93% R_F, R_F² = 9.59%, 8.84%*

All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁻) sets to similar. ** ICP shows equimolar cation so ** constrain similar occupancy.

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x Neutron powder diffraction:

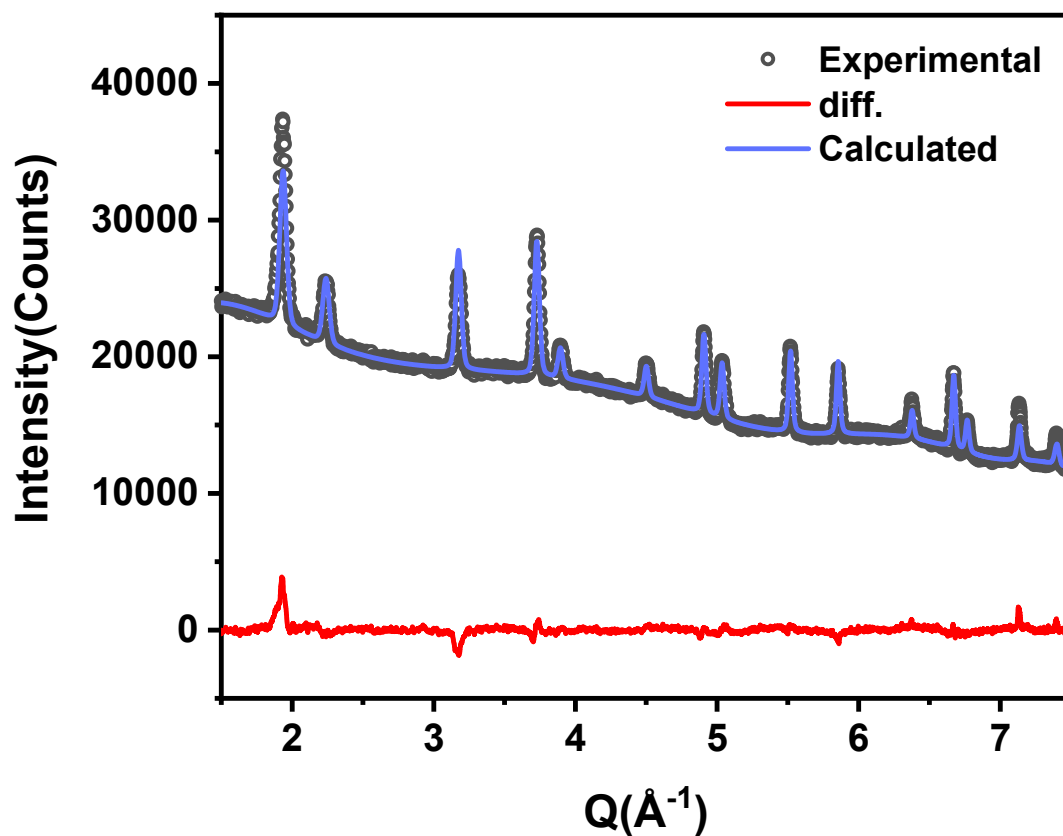


Figure S-5 Refinement of Neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x.

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La	0.000	0.000	0.000	0.01411(29)	0.2000
2	Ce	0.000	0.000	0.000	0.01411(29)	0.2000
3	Pr	0.000	0.000	0.000	0.01411(29)	0.2000
4	Nd	0.000	0.000	0.000	0.01411(29)	0.2000
5	Y	0.000	0.000	0.000	0.01411(29)	0.2000
6	O1	0.250	0.250	0.250	0.01411(29)	0.5603(20)
7	H1	0.250	0.250	0.250	0.01411(29)	0.4800(20)

R_{wp} = 1.69% R_F, R_F² = 8.64%, 23.96%* All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H) sets to similar. ** ICP shows equimolar cation so ** constrain similar occupancy

(La,Ce,Pr,Sm,Y)H_{3-2x}O_x X-ray powder diffraction:

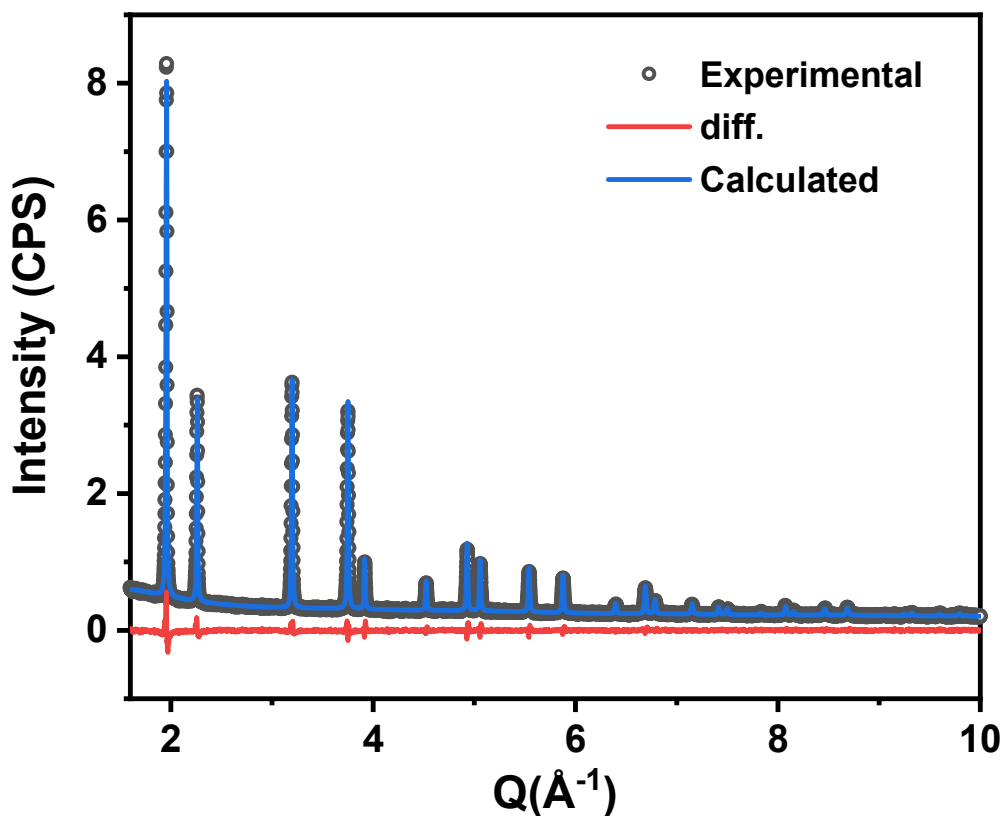


Figure S-6 Refinement of X-ray powder diffraction data of (La,Ce,Pr,Sm,Y)H_{3-2x}O_x.

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La	0.000	0.000	0.000	0.01962(13)	0.2000
2	Ce	0.000	0.000	0.000	0.01962(13)	0.2000
3	Pr	0.000	0.000	0.000	0.01962(13)	0.2000
4	Sm	0.000	0.000	0.000	0.01962(13)	0.2000
5	Y	0.000	0.000	0.000	0.01962(13)	0.2000
6	O1	0.250	0.250	0.250	0.0340(31)	0.498(10)
7	H1	0.250	0.250	0.250	0.0340(31)	0.502(10)

R_{wp} = 4.57%; R_F, R_F² = 14.26%, 10.63% %* All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H-) sets to similar. ** ICP shows equimolar cation so ** constrain similar occupancy.

$^{154}\text{SmH}_{3-2x}\text{O}_x$ Neutron powder diffraction:

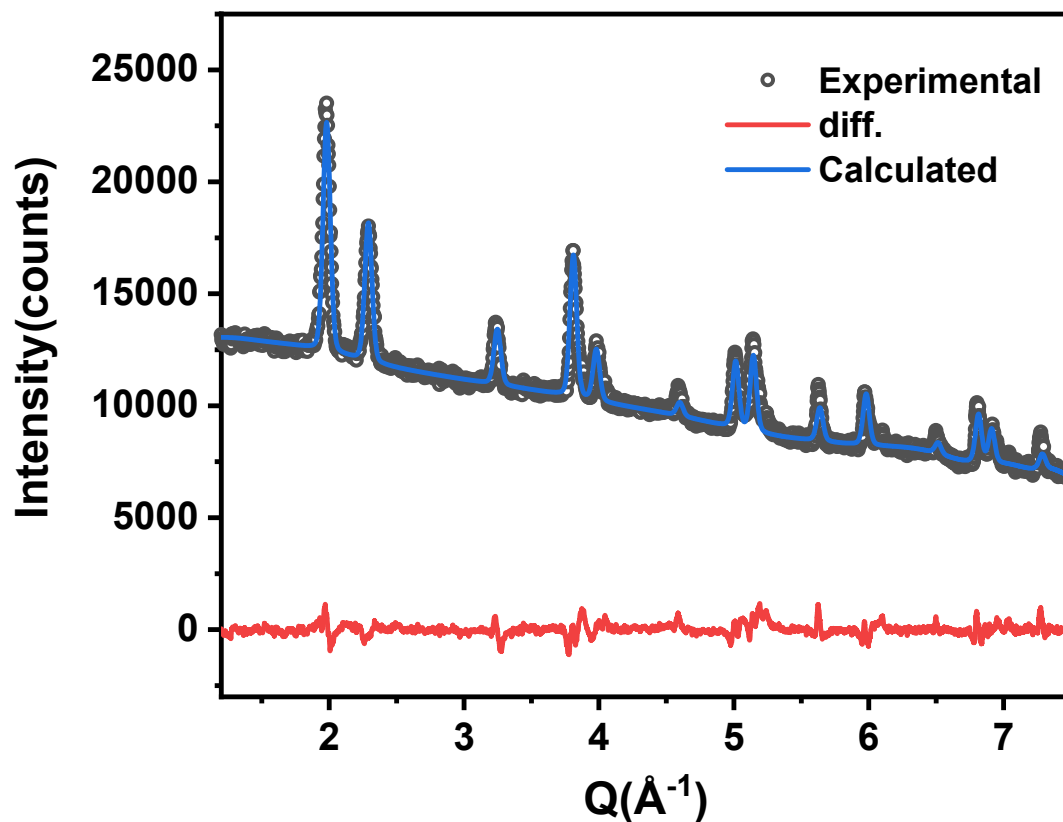


Figure S-7 Refinement of Neutron powder diffraction data of $^{154}\text{SmH}_{3-2x}\text{O}_x$.

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	Sm	0.000	0.000	0.000	0.0165(4)	1
2	O1	0.250	0.250	0.250	0.073(5)	0.258(8)
3	H1	0.250	0.250	0.250	0.073(5)	0.756(8)
4	H2	0.500	0.0940(19)	0.0940(19)	0.008(6)	0.0378(23)

$R_{wp} = 2.45\%$; $R_F, R_F^2 = 6.42\%, 16.03\%$. *U_{iso} (O²⁻/H⁻) sets to similar. Sm occupancy sets to 1.

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray-Neutron combined refinement with P4/nmm model

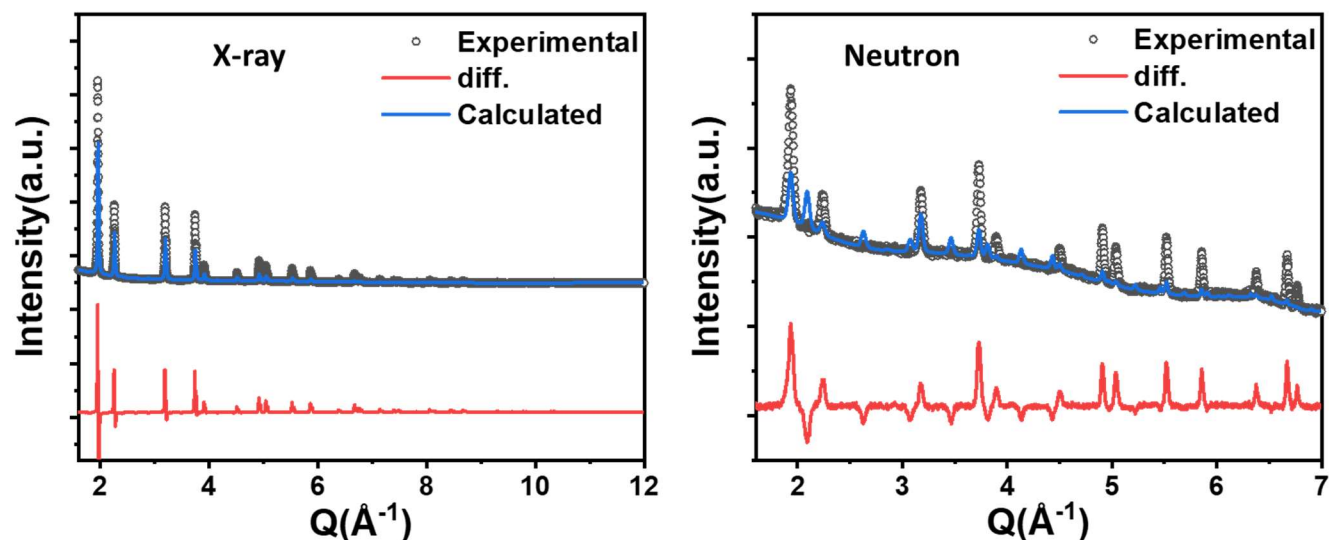


Figure S-8 Combined refinement of x-ray and neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x with P4/nmm space group model

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La1	0.7500	0.2500	0.0000	0.05	0.2000
2	La2	0.2500	0.2500	0.9590	0.05	0.2000
3	La3	0.0000	0.0000	0.5000	0.05	0.2000
4	Ce1	0.7500	0.2500	0.0000	0.05	0.2000
5	Ce2	0.2500	0.2500	0.9590	0.05	0.2000
6	Ce3	0.0000	0.0000	0.5000	0.05	0.2000
7	Pr1	0.7500	0.2500	0.0000	0.05	0.2000
8	Pr2	0.2500	0.2500	0.9590	0.05	0.2000
9	Pr3	0.0000	0.0000	0.5000	0.05	0.2000
10	Nd1	0.7500	0.2500	0.0000	0.05	0.2000
11	Nd2	0.2500	0.2500	0.9590	0.05	0.2000
12	Nd3	0.0000	0.0000	0.5000	0.05	0.2000
13	Y1	0.7500	0.2500	0.0000	0.05	0.2000
14	Y2	0.2500	0.2500	0.9590	0.05	0.2000
15	Y3	0.0000	0.0000	0.5000	0.05	0.2000
16	O1	0.2500	0.5010	0.7470	0.053	1.0000
17	H1	0.2500	0.5050	0.2680	0.053	1.0000

X-ray R_{wp} = 16.013% R_F, R_F² = 66.66%, 46.79%; Neutron R_{wp} = 5.79% R_F, R_F² = 50.33%, 73.94%. * All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁺) fixed to be equal. **

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray-Neutron combined refinement without interstitial model

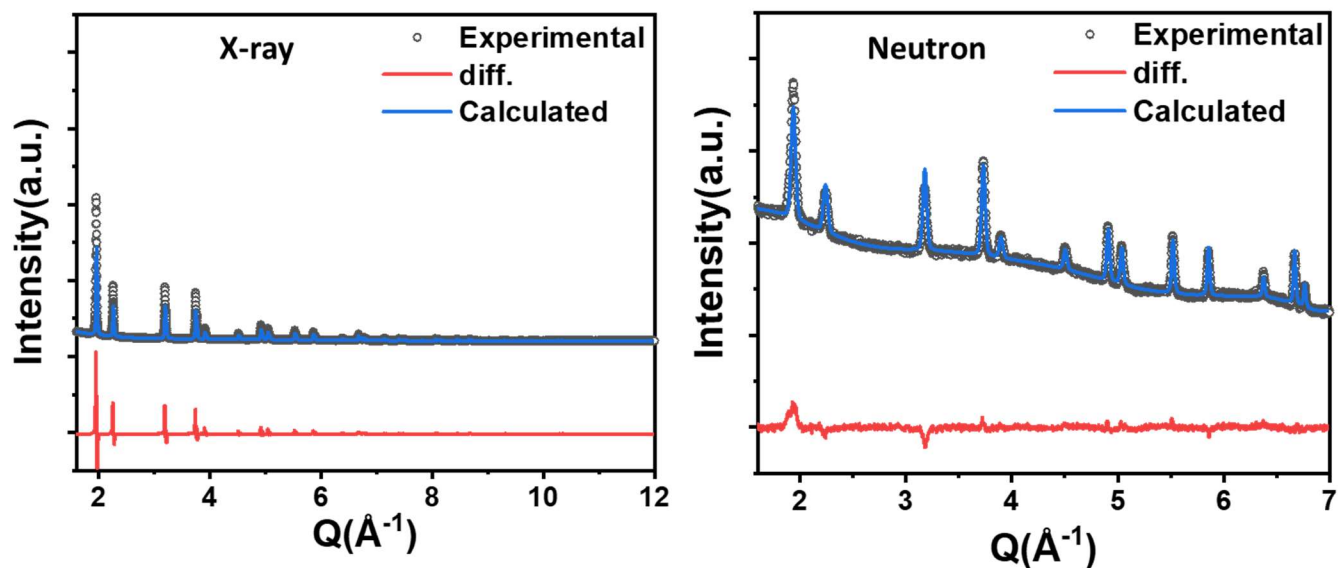


Figure S-9 Combined refinement of x-ray and neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x without interstitial model

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La	0.00	0.00	0.00	0.01476(14)	0.2000
2	Ce	0.00	0.00	0.00	0.01476(14)	0.2000
3	Pr	0.00	0.00	0.00	0.01476(14)	0.2000
4	Nd	0.00	0.00	0.00	0.01476(14)	0.2000
5	Y	0.00	0.00	0.00	0.01476(14)	0.2000
6	O1	0.250	0.250	0.250	0.01	0.4385(6)
7	H1	0.250	0.250	0.250	0.01	0.5615(6)

X-ray $R_{wp} = 14.60\%$ R_F , $R_F^2 = 18.36, 22.82\%$; Neutron $R_{wp} = 1.527\%$ R_F , $R_F^2 = 7.88\%, 20.28\%$.

* All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁻) fixed to be equal. **

ICP shows equimolar cation so ** constrain similar occupancy.

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray-Neutron combined refinement with 48i interstitial model

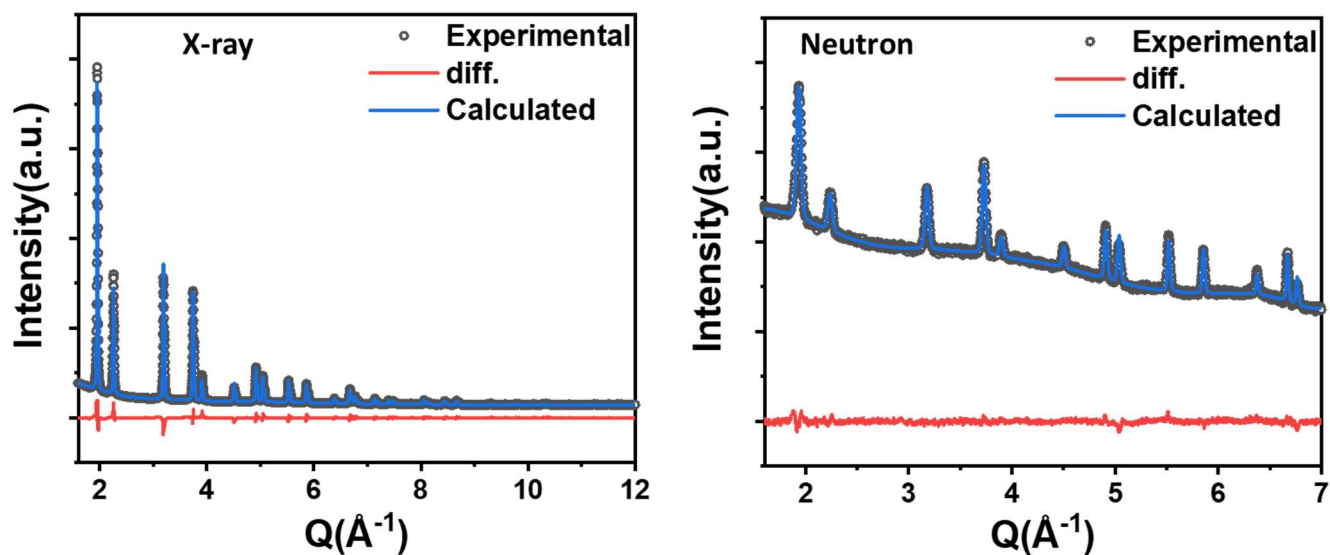


Figure S-10 Combined refinement of x-ray and neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x with 48i interstitial model

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La	0.00	0.00	0.00	0.01450(17)	0.2000
2	Ce	0.00	0.00	0.00	0.01450(17)	0.2000
3	Pr	0.00	0.00	0.00	0.01450(17)	0.2000
4	Nd	0.00	0.00	0.00	0.01450(17)	0.2000
5	Y	0.00	0.00	0.00	0.01450(17)	0.2000
6	O1	0.250	0.250	0.250	0.01	0.4039(8)
7	H1	0.250	0.250	0.250	0.01	0.5031(14)
8	H2	0.500	0.0959(5)	0.0959(5)	0.01	0.0315(4)

X-ray $R_{wp} = 2.87\%$ R_F , $R_F^2 = 8.55\%$, 7.09% ; Neutron $R_{wp} = 1.192\%$ R_F , $R_F^2 = 6.78\%$, 14.76% . *

All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁻) fixed to be equal. **

ICP shows equimolar cation so ** constrain similar occupancy.

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray-Neutron combined refinement with 32*f* interstitial model

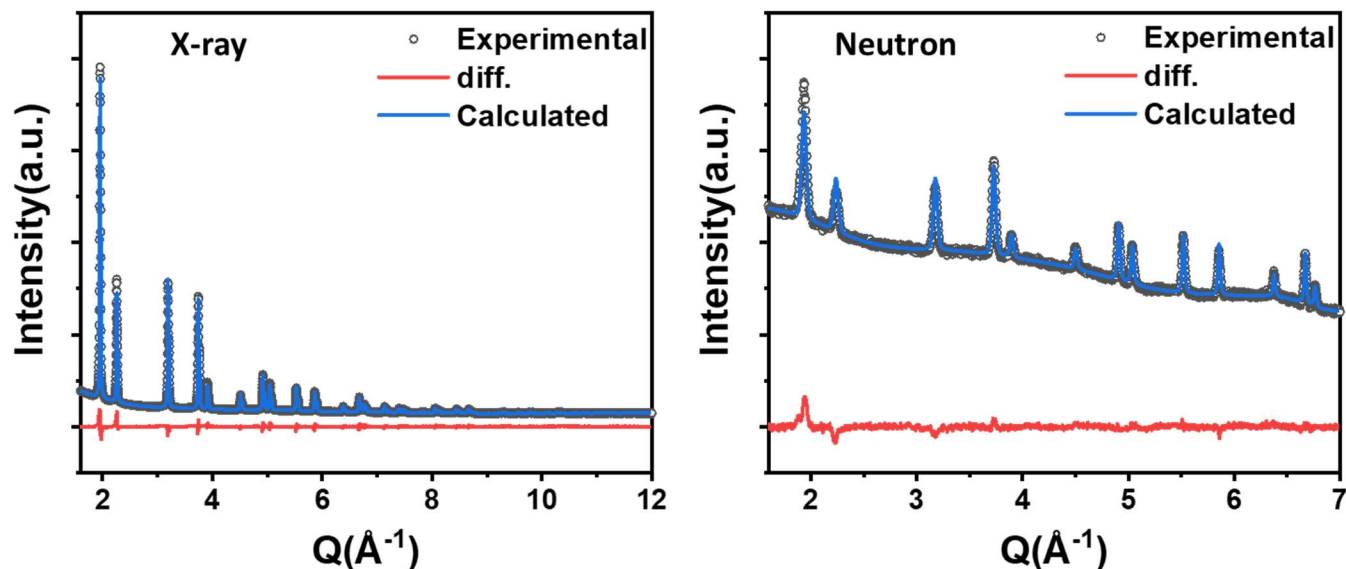


Figure S-11 Combined refinement of x-ray and neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x with 32*f* interstitial model

S.No.	Atom	x	Y	z	*U _{iso}	**Occ.
1	La	0.00	0.00	0.00	0.01405(13)	0.2000
2	Ce	0.00	0.00	0.00	0.01405(13)	0.2000
3	Pr	0.00	0.00	0.00	0.01405(13)	0.2000
4	Nd	0.00	0.00	0.00	0.01405(13)	0.2000
5	Y	0.00	0.00	0.00	0.01405(13)	0.2000
6	O1	0.250	0.250	0.250	0.01	0.474(3)
7	H1	0.250	0.250	0.250	0.01	0.526(3)
8	H2	0.7126(26)	0.7126(26)	0.7126(26)	0.01	0.0437(20)

X-ray $R_{wp} = 3.10\%$ R_F , $R_F^2 = 8.28\%$, 7.78% ; Neutron $R_{wp} = 1.429\%$ R_F , $R_F^2 = 6.98\%$, 17.54% . * All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁻) fixed to be equal. ** ICP shows equimolar cation so ** constrain similar occupancy.

(La,Ce,Pr,Nd,Y)H_{3-2x}O_x X-ray-Neutron combined refinement with both interstitials model

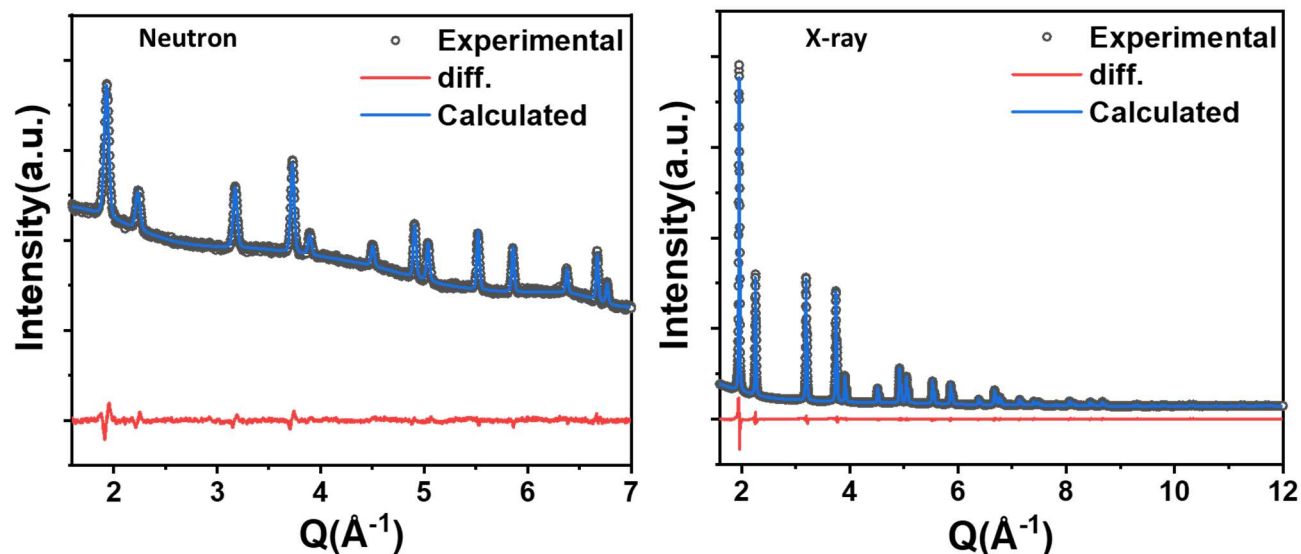


Figure S-12 Combined refinement of x-ray and neutron powder diffraction data of (La,Ce,Pr,Nd,Y)H_{3-2x}O_x with both interstitials.

S.No.	Atom	x	y	z	*U _{iso}	**Occ.
1	La	0.00	0.00	0.00	0.01329(17)	0.2000
2	Ce	0.00	0.00	0.00	0.01329(17)	0.2000
3	Pr	0.00	0.00	0.00	0.01329(17)	0.2000
4	Nd	0.00	0.00	0.00	0.01329(17)	0.2000
5	Y	0.00	0.00	0.00	0.01329(17)	0.2000
6	O1	0.250	0.250	0.250	0.01	0.3757(18)
7	H1	0.250	0.250	0.250	0.01	0.336(19)
8	H2	0.500	0.0925(7)	0.0925(7)	0.0289(25)	0.0325(6)
9	H3	0.7155(22)	0.7155(22)	0.7155(22)	0.0151(27)	0.054(4)

X-ray $R_{wp} = 2.57\%$ R_F , $R_F^2 = 6.34\%$, 6.17% ; Neutron $R_{wp} = 1.181\%$ R_F , $R_F^2 = 4.74\%$, 11.89% . *

All the cations are at similar position so *U_{iso} of cations and *U_{iso} (O²⁻/H⁻) fixed to be equal. **

ICP shows equimolar cation so ** constrain similar occupancy.

XANES Fitted data:

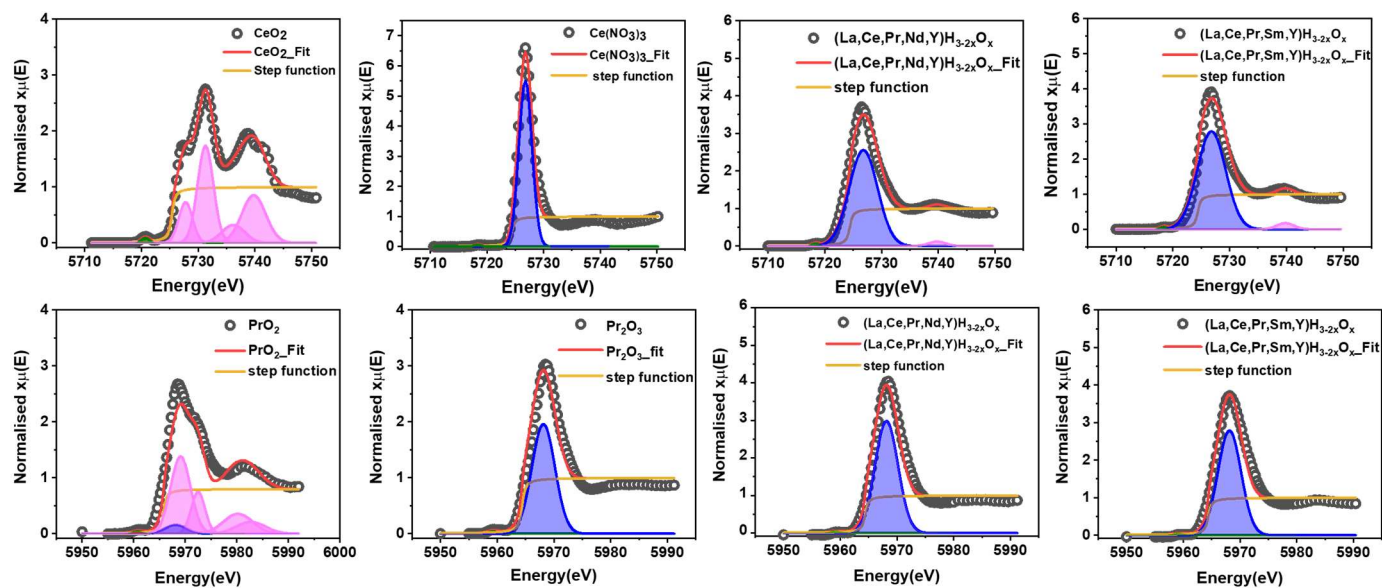


Figure S-13 XANES fitted diagrams of Ce-L₃-edge and Pr-L₃ edge.

Thermogravimetric analysis:

The TG experiments were performed using a Bruker AXS TG-DTA 2000S instrument. The samples, weighing approximately 20 mg, were heated at a rate of 10 K per minute in a flowing stream of highly pure O₂/Argon gas (7:3) up to a temperature of 1073 K. The experiment was carried out after a blank run in TG which helps in baseline correction. The weight gain was observed quantitatively which helped to convert it to amount of hydrogen in HEH_{3-2x}O_x. HE=(La,Ce,Pr,Nd,Y)

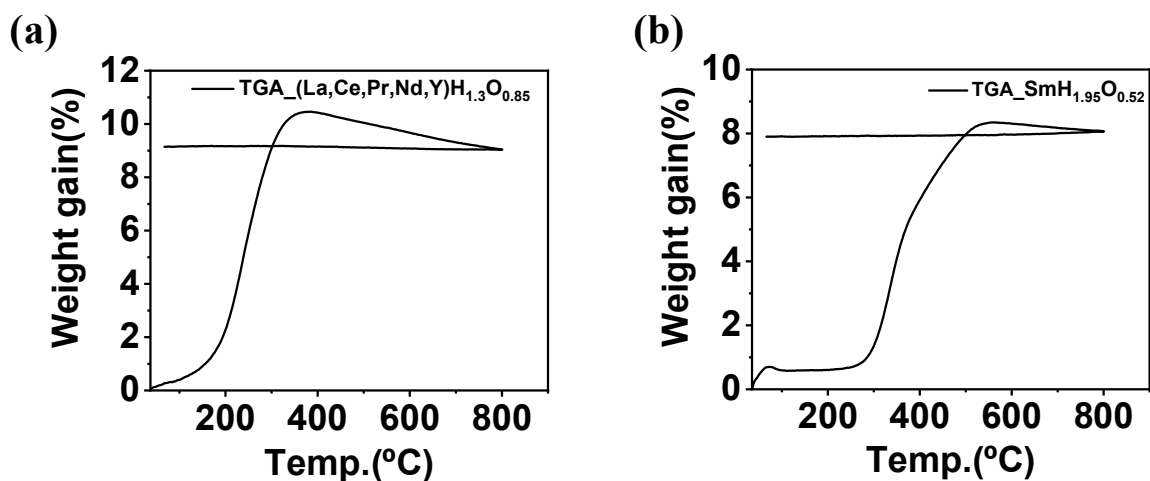


Figure S-14 TGA weight gain profile v/s temp. of (a) (La,Ce,Pr,Nd,Y)H_{3-2x}O_x. (b) ¹⁵⁴SmH_{3-2x}O_x

H-D exchange:

H-D exchange measurements were carried out using fully automated AutoChem 2950 (Micromeritics Instrument Co.) equipped with a mass spectrometer coupled to the outlet of the chemisorption instrument. For H-D exchange measurements, sample (40 mg) tube was prepared in an argon filled dry glovebox. Subsequently, the sample was heated in a mixture of 5% D₂/Ar (total flow 50 mL.min⁻¹) from room temperature to 900 °C with a ramp rate of 5°/min. The mass signal of H₂(m/z=2), HD(m/z=3) and D₂(m/z=4) was monitored using a mass spectrometer coupled to the outlet of the chemisorption instrument.

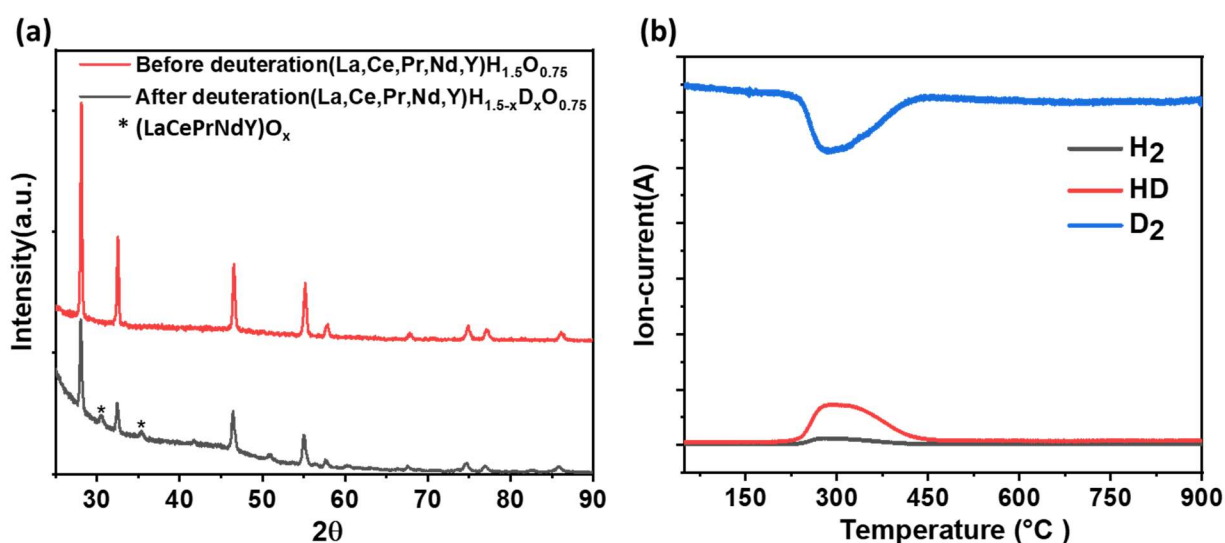


Figure S-15 (a) XRD (Cu-K α , $\lambda=1.54\text{\AA}$) pattern of before and after deuteration of (La,Ce,Pr,Nd,Y)H_{1.5}O_{0.75}. (b) H-D exchange in ¹⁵⁴SmH_{3-2x}O_x. *Trace of High entropy oxide (LaCePrNdY)O_{1.5-x}. It could be originated from remaining oxygen in instrument lines which oxidize the material.

Kramers- Kronig transformations:

Kramers-Kronig transforms were applied to data to check the stability of the system during measurement. These transforms are mathematical tools used to ensure that the data adheres to the principles of Linear Systems Theory, such as causality, linearity, and stability. Zsimpwin software was used to perform the transformations. In Figure S-16, experimental results were fitted with a polynomial before integrating the data. Both figures demonstrate that the fitted values closely match the measured values, indicating that the system remained stable during the measurement.

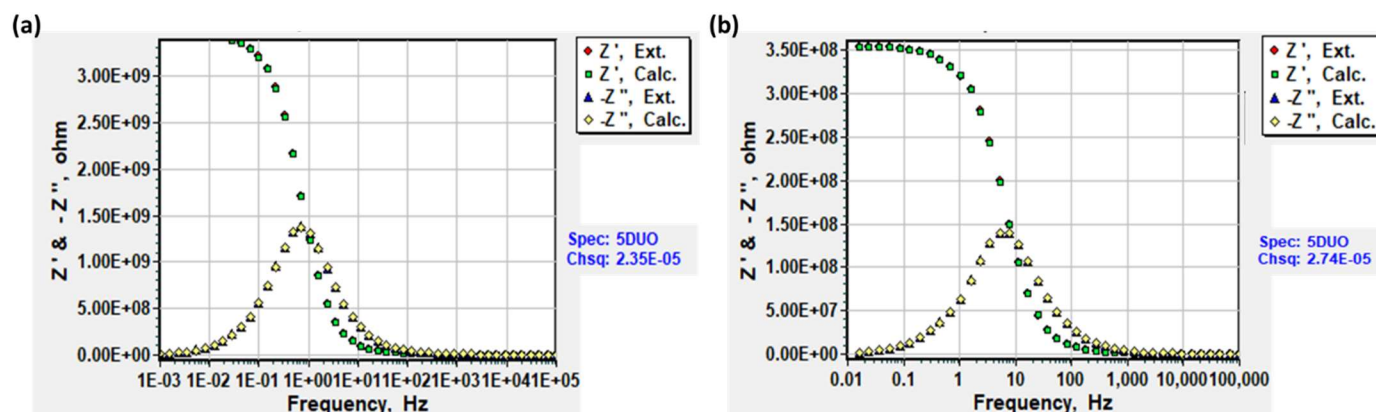


Figure S-16 Fitting and extrapolation of data with Kramers-Kronig transformation (a) 50°C and (b) 100°C.

After ammonia synthesis: (Le Bail Refinement):

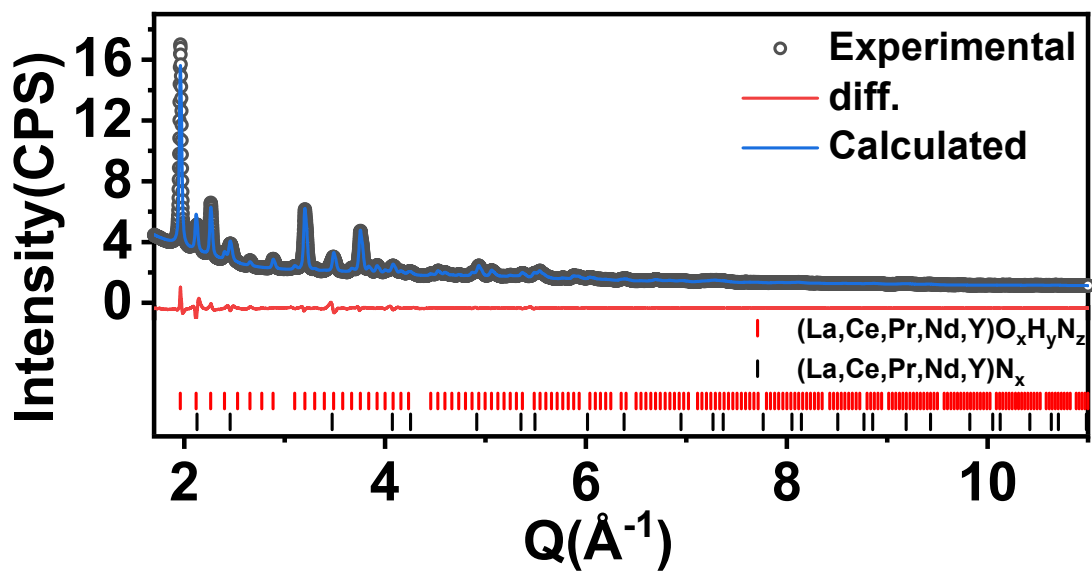


Figure S-17 Le-bail refinement on XRD pattern of $\text{Ru}/(\text{La,Ce,Pr,Nd,Y})\text{H}_{3-2x}\text{O}_x$ after catalytic test.

ICP-OES

Table S1:

Elements	ICP(wt%)	Stoichiometry
La	20.9	0.22
Ce	23.2	0.23
Pr	20.1	0.20
Nd	20.6	0.20
Y	13.7	0.22
Ca	0.9	--

HERFD-XANES fitted data

Table S2:

Ce-L₃ edge fitted data:

	Position (eV)	Width(eV)	Amplitude (Ce (NO ₃) ₃)	Amplitude (La,Ce,Pr,Nd,Y)H _{3-2x} O _x	Amplitude (La,Ce,Pr,Sm,Y)H _{3-2x} O _x
Arctan step	5724.40	0.400	1.000	1.000	1.000
Pre-edge	5718.40	0.600	0.100	0.100	0.100
Peak ₊₃	5726.80	2.503	16.112±0.217	16.025±0.204	16.288±0.193
Peak ₊₄	5739.8	1.498	-	0.435±0.181	0.661±0.189

Pr-L₃ edge fitted data:

	Position (eV)	Width(eV)	Amplitude (Pr ₂ O ₃)	Amplitude (La,Ce,Pr,Nd,Y)H _{3-2x} O _x	Amplitude (La,Ce,Pr,Sm,Y)H _{3-2x} O _x
Arctan step	5764.40	0.400	1.000	1.000	1.000
Pre-edge	5959.30	1.000	0.100	0.100	0.100
Peak ₊₃	5968.15	2.035	10.269±0.230	15.212±0.268	14.222±0.239

CHNS- analysis

The hydride content in $\text{HEH}_{3-2x}\text{O}_x$ was determined using combustion elemental analysis. A calibration curve was established by heating different quantities of TiH_2 in an argon environment up to 1073 K. The peak area corresponding to the release of H_2 was measured and integrated, resulting in a calibration curve that exhibited a high level of linearity (R-squared = 0.9895). Subsequently, $\text{HEH}_{3-2x}\text{O}_x$ was subjected to the same experimental conditions as TiH_2 . By utilizing the calibration curve, the hydride content of $\text{HEH}_{3-2x}\text{O}_x$ was estimated to be approximately 1.50. $\text{HE}=(\text{La,Ce,Pr,Nd/Sm,Y})$

Table S3:

Material	Weight(mg)	mmol of compound	n(H) in mmol	Weight percentage of H	Peak area(V*sec)	stoichiometry
TiH_2	3.175	0.063	0.126	4.009	1.731	2
TiH_2	6.467	0.129	0.258	4.009	3.541	2
TiH_2	9.553	0.191	0.382	4.009	5.242	2
TiH_2	12.897	0.240	0.480	4.009	7.035	2
TiH_2	17.614	0.353	0.706	4.009	9.588	2
$(\text{La,Ce,Pr,Nd,Y})\text{H}_{3-2x}\text{O}_x$	15.94	0.110	0.165	1.04	2.253	1.5
$(\text{La,Ce,Pr,Sm,Y})\text{H}_{3-2x}\text{O}_x$	16.86	0.115	0.172	1.10	2.483	1.60
$^{154}\text{SmH}_{3-2x}\text{O}_x$	16.30	0.102	0.225	1.38	3.018	2.2

Fitting data for equivalent circuit:

Table S4: The values of resistance are taken by fitting on the data shown in Figure 5b.

<i>Impedence data on (LaCePrNdY) H_{1.5}O_{0.75} at 50°C data</i>	<i>Impedence data on (LaCePrNdY) H_{1.5}O_{0.75} at 100°C data</i>
$R_c = 9.547 \times 10^{-12} \text{ Ohm}$	$R_c = 1.475 \times 10^{-10} \text{ Ohm}$
$Q_{\text{ion}}(\text{CPE}) = 77.08 \times 10^{-12} \text{ F}$	$Q_{\text{ion}}(\text{CPE}) = 1.069 \times 10^{-10} \text{ F}$
$a(\text{CPE}) = 0.8917$	$a(\text{CPE}) = 0.8804$
$R_{\text{ion}} = 3.373 \times 10^{-9} \text{ Ohm}$	$R_{\text{ion}} = 3.422 \times 10^{-10} \text{ Ohm}$

Comparison of Ammonia synthesis activity with different catalysts.

Table S5:

Catalyst	Ru wt% (Nominal)	Ru wt% (Actual)	Rate (mmol g ⁻¹ h ⁻¹)	(Temp., Pressure)	Ref.
Ru/(La,Ce,Pr,Sm,Y)H _{1.6} O _{0.70}	2	1.9	41	400°C,5Mpa	
Ru/(La,Ce,Pr,Nd,Y)H _{1.5} O _{0.75}	2	1.8	31	400°C,5Mpa	
Ru/SmH _{2.0} O _{0.5}	2	1.6	18	400°C,5Mpa	
TiH ₂			2.8	400°C,5Mpa	1
*4 %Cs/Ru/BaCeO ₃	1.25	1.25	28	450°C,3Mpa	2
**Ru/CeO ₂ -NaOH	2.5	2.5	16.5	450°C, 3Mpa	3
***Ru/BaTiO ₃		3.63	15.67	400°C,5Mpa	4
***Ru/MgO		3.74	7.39	400°C,5Mpa	4
***Ru/Al ₂ O ₃		3.79	0.39	400°C,5Mpa	4
Ru/BaTiO ₃	1	0.89	4.1	400°C,5Mpa	5
Ru/BaTiO _{2.51} H _{0.49}	1	0.86	28.8	400°C,5Mpa	5
Ru/BaTiO _{2.7} H _{0.3}	1	0.81	30.3	400°C,5Mpa	5
Ru/SrTiO _{2.6} H _{0.4}	1	0.75	15.74	400°C,5Mpa	5
Ru/CaTiO _{2.77} H _{0.23}	1	0.71	5.37	400°C,5Mpa	5
Ru/CaTiO ₃	1	0.73	0.77	400°C,5Mpa	5
Ru/SrTiO ₃	1	0.66	2.03	400°C,5Mpa	5
#10-Cs-FePc700			27.7	400°C,7Mpa	6

Catalyst=0.1 g, N₂:H₂: Ar=22.5 : 67.5 : 10, Total flow=110 ml/min.

*Catalyst=0.1 g, H₂/N₂=3; Total flow 60 ml/min **Catalyst=150 mg, WHSV=24000 h⁻¹.

***Catalyst= 2ml with particle size of 12-16 mesh, GHSV = 10000 h⁻¹ H₂/N₂=3.

#Catalyst = 200 mg, Total flow = 40 ml/min.

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