Supporting Information for:

Kinetic Control of Anion Stoichiometry in Hexagonal $BaTiO_3$

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Table S5. List of descriptors of structural parameters.

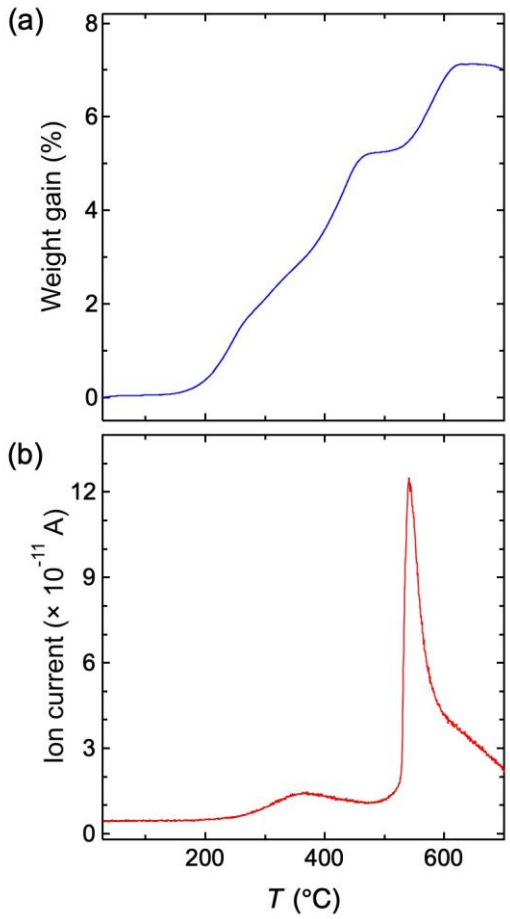

Figure S1. Results of (a) thermogravimetric analysis which was performed in oxygen flow at a rate of 300 ml/min, and (b) quadruple mass spectrometry of H_2, the sample was heated in flowing O_2 at a rate of 300 ml/min. The specimen of BTOH-L2 prepared by hydride reduction of BTO-L with CaH_2 at 520 ℃ for 120 hours was selected in the experiment.

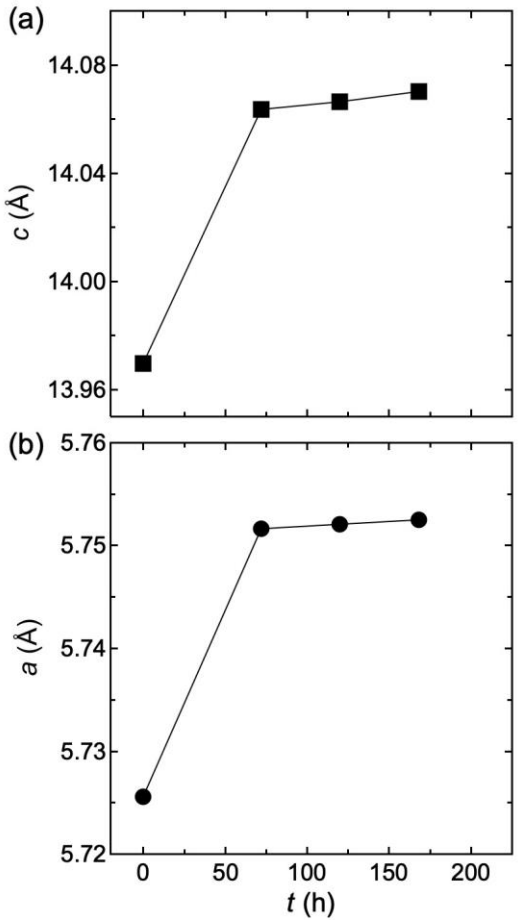

Figure S2. The relationship between lattice parameters (a) *c*, (b) *a* and reaction time for the h-$BaTiO_{3-x}H_x$ reduced by H_2 at 1450 °C for 1 hour and hydrogenated with CaH_2 at 520 °C.

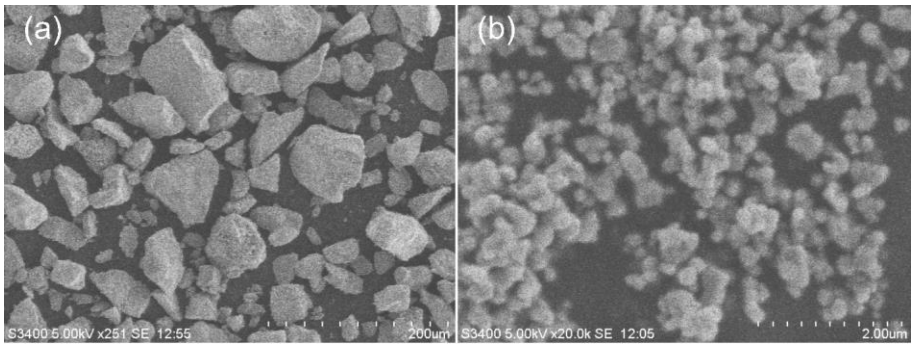

Figure S3. SEM images of 6H $BaTiO_{3-x}$. (a) Specimen prepared by H_2 reduction at 1450 °C for 1 hour (BTO-L). (b) Specimen prepared by Mg reduction twice at 1000 °C for 10 hours (BTO-S).

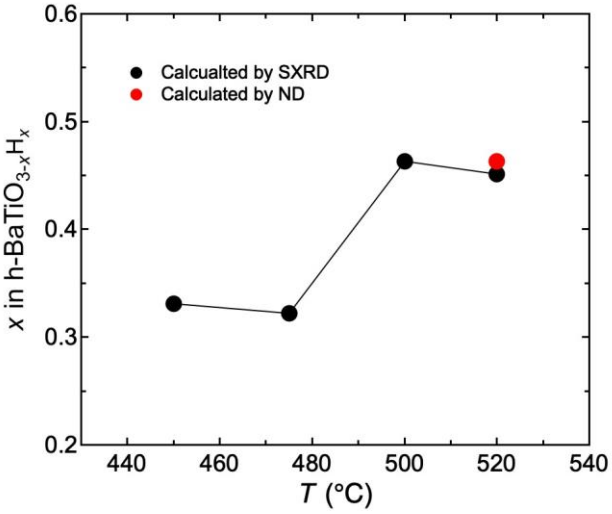

Figure S4. Variation of hydrogen content in h-$BaTiO_{3-x}H_x$ as a function of hydrogenation temperature by CaH_2 reduction. The hydrogen content is assumed to be equivalent to oxygen deficiency in SXRD analysis, whereas it was directly refined for the NPD data (Table S3).

Regression analysis of energy calculations

Formation energies for each structure parameters were analyzed with linear regression method as to the hexagonal $BaTiO_{3-x}H_x$ structures in order to analyze the most important structural parameter for the formation energies. The 1496 independent configurations shown in Table S2 were constructed and have been calculated. Then, the formation energies were standardized for each composition in order to remove too large influence of hydrogen amounts. The structural parameters used in regression analysis are shown in Table S5. The database was standardized before the analysis. Linear regression analysis was performed using least absolute shrinkage and selection operator (LASSO) [35], which is one of the least squared methods with the regularization term. The magnitude of the absolute value of the coefficients corresponds to the importance of the parameters, and the sign of the coefficients corresponds to positive or negative correlation between the formation energies and the parameters.

Figure S6 shows the relationship between predicted values from LASSO regression and calculated values. The obtained coefficients with the regression were presented in Figure S7. The coefficients of N_*face* and N_*trans* have large negative value, which implies that H^- anion energetically prefers the face-sharing site and *trans*-coordination. These results support the site selectivity of H^- in the hexagonal $BaTiO_{3-x}H_x$ structures discussed in the text.

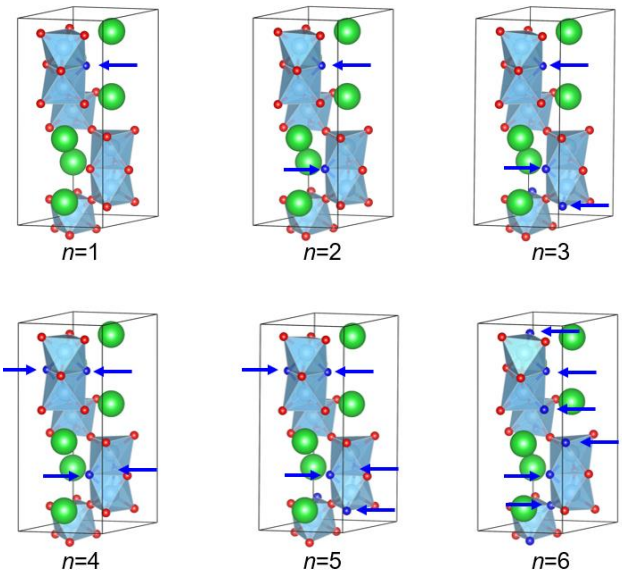

Figure S5. Most stable structures in 6H-type system for $Ba_6Ti_6O_{18-n}H_n$ for n = 1 ~ 6. Green, light blue, red, and blue balls represent Ba, Ti, O, and H atoms, respectively.

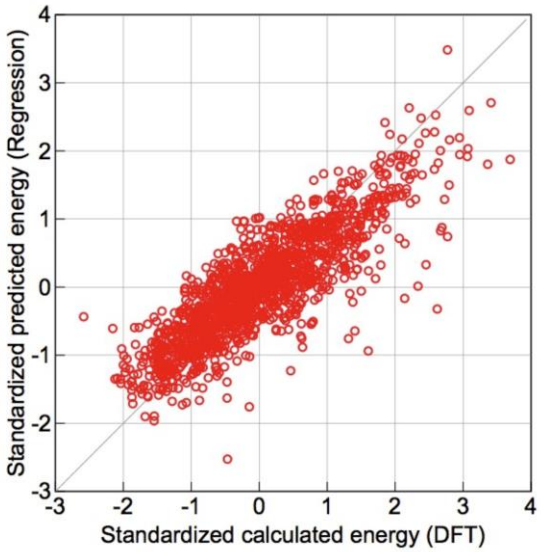

Figure S6. Relationship between predicted energies from LASSO regression and DFT calculations for $Ba_6Ti_6O_{18-n}H_n$.

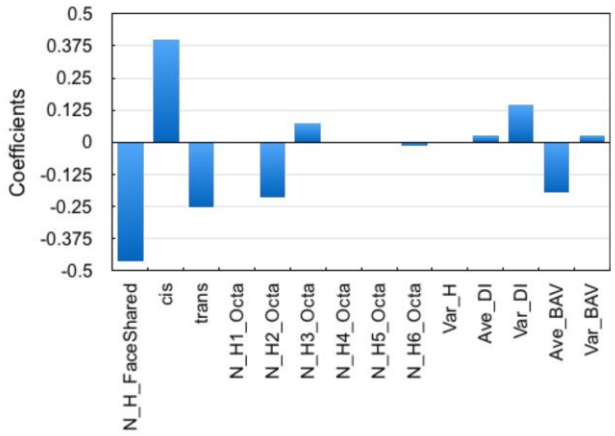

Figure S7. Obtained coefficients from LASSO regression. In h-$BaTiO_{3-x}H_x$, hydride anions are more likely to occupy the face-sharing site and have weaker *cis*/*trans* preference.

Table S1. Sample lists. (a) $BaTiO_3$ (BT03, Sakai) was reduced in H_2 atmosphere and hydrided by CaH_2. (b), (c), (d) and (e) $BaTiO_3$ (BT01, Sakai) were prepared by Mg reduction method and hydrided by CaH_2.

(a)	$BaTiO_{3-x}$		$BaTiO_{3-x}H_x$	
	H_2 reduction	⇒	CaH_2 Hydrogenation	
Specimen	L-1		L-1-1	L-1-2	L-1-3
Condition	1450 ℃/1 h		520 ℃/72 h	520 ℃/120 h	520 ℃/168 h

(b)	$BaTiO_{3-x}$		$BaTiO_{3-x}H_x$	
	Mg reduction	⇒	CaH_2 Hydrogenation	
Specimen	S-1		S-1-1	S-1-2	S-1-3
Condition	1) 950 ℃/10 h 2) 1000 ℃/10 h		450 ℃/120 h	475 ℃/120 h	500 ℃/120 h

(c)	$BaTiO_{3-x}$		$BaTiO_{3-x}H_x$	
	Mg reduction	⇒	CaH_2 Hydrogenation	
Specimen	S-2		S-2-1	S-2-2	
Condition	1) 1000 ℃/10 h 2) 1000 ℃/10 h		475 ℃/120 h	520 ℃/120 h	

(d)	$BaTiO_{3-x}$		$BaTiO_{3-x}H_x$	
	Mg reduction	⇒	CaH_2 Hydrogenation	
Specimen	S-3		S-3-1		
Condition	1) 1025 ℃/10 h 2) 950 ℃/10 h		475 ℃/120 h		

(e)	$BaTiO_{3-x}$		$BaTiO_{3-x}H_x$	
	Mg reduction	⇒	CaH_2 Hydrogenation	
Specimen	S-4		S-4-1		
Condition	1) 1025 ℃/10 h 2) 1000 ℃/10 h		475 ℃/120 h		

Table S2. Number of symmetrically independent O/H configurations of a hexagonal unit cell with the composition of $Ba_6Ti_6O_{18-n}H_n$ ($n = 1 \sim 6$).

n in $Ba_6Ti_6O_{18-n}H_n$	Number of symmetrically independent O/H configurations
1	2
2	14
3	46
4	164
5	400
6	870
Total	1496

Table S3-1. Crystallographic parameters for the hexagonal $BaTiO_{2.72}$ (S-1) from SXRD refinement[a]

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.45(1)
Ba2	4*f*	1	0.333333	0.666667	0.09291(5)	0.57(1)
Ti1	2*a*	1	0	0	0	0.37(3)
Ti2	4*f*	1	0.333333	0.666667	0.8503(1)	0.53(3)
O1	6*h*	0.72(1)	0.5260(6)	0.052	0.25	0.6(1)
O2	12*k*	1	0.8294(4)	0.6588	0.0835(2)	0.43(5)

[a]Space group: $P6_3/mmc$; $Z = 6$; $a = 5.7476$ (1) Å, and $c = 14.0608(1)$ Å; $R_p = 6.16\%$, $R_{wp} = 8.17\%$, $R_B = 5.69\%$, $R_F = 11.50\%$, and GOF = 1.42 for SXRD. g^b represents the occupancy factor of each site.

Table S3-2. Crystallographic parameters for the hexagonal $BaTiO_{2.72}$ (S-2) from SXRD refinement[a]

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.503(7)
Ba2	4*f*	1	0.333333	0.666667	0.08857(5)	0.589(5)
Ti1	2*a*	1	0	0	0	0.52(2)
Ti2	4*f*	1	0.333333	0.666667	0.8498(1)	0.48(2)
O1	6*h*	0.72(1)	0.527(2)	0.054	0.25	1.20(1)
O2	12*k*	1	0.8299(9)	0.6599	0.0842(2)	0.47(4)

[a]Space group: $P6_3/mmc$; $Z = 6$; $a = 5.7526(1)$ Å, and $c = 14.0852(1)$ Å; $R_p = 5.49\%$, $R_{wp} = 8.53\%$, $R_B = 3.47\%$, $R_F = 3.17\%$, and GOF = 5.50 for SXRD. g^b represents the occupancy factor of each site.

Table S3-3. Crystallographic parameters for the hexagonal $BaTiO_{2.76}$ (S-3) from SXRD refinement[a]

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.40(1)
Ba2	4*f*	1	0.333333	0.666667	0.09360(5)	0.46(1)
Ti1	2*a*	1	0	0	0	0.21(3)
Ti2	4*f*	1	0.333333	0.666667	0.8497(1)	0.57(3)
O1	6*h*	0.76(1)	0.5242(5)	0.0485	0.25	0.4(1)
O2	12*k*	1	0.8308(4)	0.6615	0.0826(3)	0.33(4)

[a]Space group: $P6_3/mmc$; $Z = 6$; $a = 5.7426(1)$ Å, and $c = 14.0337(1)$ Å; $R_p = 6.24\%$, $R_{wp} = 9.16\%$, $R_B = 5.42\%$, $R_F = 3.12\%$, and GOF = 2.89 for SXRD. g^b represents the occupancy factor of each site.

Table S3-4. Crystallographic parameters for the hexagonal $BaTiO_{2.74}$ (S-4) from SXRD refinement[a]

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.494(6)
Ba2	4*f*	1	0.333333	0.666667	0.09297(3)	0.602(4)
Ti1	2*a*	1	0	0	0	0.52(2)
Ti2	4*f*	1	0.333333	0.666667	0.84990(8)	0.52(2)
O1	6*h*	0.74(1)	0.5256(12)	0.0513	0.25	0.83(9)
O2	12*k*	1	0.8308(7)	0.6615	0.0834(2)	0.52(4)

[a]Space group: $P6_3/mmc$; $Z = 6$; $a = 5.7476(1)$ Å, and $c = 14.0585(1)$ Å; $R_p = 5.00\%$, $R_{wp} = 7.85\%$, $R_B = 3.00\%$, $R_F = 3.21\%$, and GOF = 5.12 for SXRD. g^b represents the occupancy factor of each site.

Table S3-5. Summary of the lattice parameters for the hexagonal $BaTiO_{3-x}$ from SXRD refinement[a]

Sample	x	a (Å)	c (Å)	V (Å ^{3})
S-1	0.28(1)	5.7476(1)	14.0608(1)	402.268
S-2	0.28(1)	5.7526(1)	14.0852(1)	403.664
S-3	0.24(1)	5.7426(1)	14.0337(1)	400.786
S-4	0.26(1)	5.7476(1)	14.0585(1)	402.206

[a]Space group: $P6_3/mmc$; $Z = 6$.

Table S4-1. Crystallographic parameters for the hexagonal $BaTiO_{2.67}H_{0.33}$ (S-1-1) from SXRD refinement[a]. H^- content is estimated from the occupancy (g) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.569(8)
Ba2	4*f*	1	0.333333	0.666667	0.09134(5)	0.733(6)
Ti1	2*a*	1	0	0	0	0.52(2)
Ti2	4*f*	1	0.333333	0.666667	0.8500(1)	0.57(2)
O1	6*h*	0.67(1)	0.528(2)	0.0566	0.25	1.20(2)
O2	12*k*	1	0.83(1)	0.6615	0.0841(2)	0.62(5)

[a]Space group: $P6_3/mmc$; $Z = 6$; $a = 5.7567(1)$ Å, and $c = 14.0905(1)$ Å; $R_p = 6.49\%$, $R_{wp} = 9.21\%$, $R_B = 4.60\%$, $R_F = 10.67\%$, and GOF = 2.74 for SXRD. $Ti^{3+}/Ti^{4+} = 0.33/0.67$. g^b represents the occupancy factor of each site.

Table S4-2. Crystallographic parameters for the hexagonal $BaTiO_{2.68}H_{0.32}$ (S-1-2) from SXRD refinement[a]. H^- content is estimated from the occupancy (g) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.560(9)
Ba2	4*f*	1	0.333333	0.666667	0.09054(6)	0.719(7)
Ti1	2*a*	1	0	0	0	0.36(3)
Ti2	4*f*	1	0.333333	0.666667	0.8499(2)	0.60(4)
O1	6*h*	0.68(1)	0.526(2)	0.0511	0.25	0.92(5)
O2	12*k*	1	0.8274(5)	0.6548	0.0843(2)	0.47(6)

[a]Space group: $P6_3/mmc$; $Z = 6$; $a = 5.7589(1)$ Å, and $c = 14.0892(1)$ Å; $R_p = 7.51\%$, $R_{wp} = 10.54\%$, $R_B = 5.19\%$, $R_F = 10.23\%$, and GOF = 3.76 for SXRD. $Ti^{3+}/Ti^{4+} = 0.32/0.68$. g^b represents the occupancy factor of each site.

Table S4-3. Crystallographic parameters for the hexagonal $BaTiO_{2.54}H_{0.46}$ (S-1-3) from SXRD refinement[a]. H^- content is estimated from the occupancy (g) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.603(13)
Ba2	4*f*	1	0.333333	0.666667	0.08970(7)	0.732(9)
Ti1	2*a*	1	0	0	0	0.51(4)
Ti2	4*f*	1	0.333333	0.666667	0.8493(2)	0.57(4)
O1	6*h*	0.54(1)	0.5322(2)	0.0643	0.25	0.46(6)
O2	12*k*	1	0.8294(6)	0.6608	0.0802(3)	0.46(6)

[a]Space group: *P*63/*mmc*; $Z = 6$; $a = 5.7604(1)$ Å, and $c = 14.0830(1)$ Å; $R_p = 7.32\%$, $R_{wp} = 9.88\%$, $R_B = 8.77\%$, $R_F = 13.81\%$, and GOF = 5.76 for SXRD. $Ti^{3+}/Ti^{4+} = 0.46/0.54$. g^b represents the occupancy factor of each site.

Table S4-4. Crystallographic parameters for the hexagonal $BaTiO_{2.66}H_{0.34}$ (S-2-1) from SXRD refinement[a]. H^- content is estimated from the occupancy (g) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.452(7)
Ba2	4*f*	1	0.333333	0.666667	0.09118(3)	0.579(5)
Ti1	2*a*	1	0	0	0	0.36(2)
Ti2	4*f*	1	0.333333	0.666667	0.85019(8)	0.47(2)
O1	6*h*	0.66(1)	0.5259(5)	0.05176687	0.25	1.4(1)
O2	12*k*	1	0.8295(3)	0.659	0.0845(1)	0.44(3)

[a]Space group: *P*63/*mmc*; $Z = 6$; $a = 5.7572(2)$ Å, and $c = 14.0876(1)$ Å; $R_p = 4.92\%$, $R_{wp} = 6.86\%$, $R_B = 2.70\%$, $R_F = 2.30\%$, and GOF = 4.22 for SXRD. $Ti^{3+}/Ti^{4+} = 0.34/0.66$. g^b represents the occupancy factor of each site.

Table S4-5. Crystallographic parameters for the hexagonal $BaTiO_{2.55}H_{0.45}$ (S-2-2) from SXRD (upper) and those of h-$BaTiO_{2.4}H_{0.6}$ (S-2-2) from Time-of-Flight NPD (lower) refinement[a]. H^- content is estimated from the occupancy (g) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_{x}Ti^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	x	y	z	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.574(19)
						0.258(4)
Ba2	4*f*	1	0.333333	0.666667	0.08857(9)	0.568(10)
					0.0948(2)	0.258(4)
Ti1	2*a*	1	0	0	0	0.53(5)
						0.48(5)
Ti2	4*f*	1	0.333333	0.666667	0.8485(2)	0.49(4)
					0.8644(3)	0.48(5)
O1	6*h*	0.55(1)	0.533(1)	0.0652	0.25	0.89(3)
		0.54(1)	0.5312(5)	0.0625	0.25	1.10(2)
H1	6*h*					
		0.46(1)	0.5312(5)	0.0625	0.25	1.10(2)
O2	12*k*	1	0.8331(7)	0.6662	0.0865(4)	0.66(9)
		1	0.8284(2)	0.6573	0.08920(1)	0.42(2)
H2	12*k*					

[a]Space group: *P*63/*mmc*; $Z = 6$; $a = 5.7664(1)$ Å, and $c = 14.0713(1)$ Å for SXRD and $a = 5.76499(6)$ Å and $c = 14.0792(3)$ Å for NPD. $R_p = 8.93\%$, $R_{wp} = 12.85\%$, $R_B = 10.94\%$, $R_F = 9.77\%$, and GOF = 2.23 for SXRD and $R_p = 1.57\%$, $R_{wp} = 2.07\%$, $R_B = 16.97\%$, $R_F = 15.15\%$, and GOF = 3.96 for NPD. $Ti^{3+}/Ti^{4+} = 0.45/0.55$ for SXRD and $Ti^{3+}/Ti^{4+} = 0.46/0.54$ for ND. g^b represents the occupancy factor of each site.

Table S4-6. Crystallographic parameters for the hexagonal $BaTiO_{2.69}H_{0.31}$ (S-3-1) from SXRD refinement[a]. H^- content is estimated from the occupancy (*g*) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	*x*	*y*	*z*	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.46(3)
Ba2	4*f*	1	0.333333	0.666667	0.09177(5)	0.48(3)
Ti1	2*a*	1	0	0	0	0.46(3)
Ti2	4*f*	1	0.333333	0.666667	0.8504(1)	0.49(3)
O1	6*h*	0.69(1)	0.5239(6)	0.048	0.25	0.9(1)
O2	12*k*	1	0.8297(4)	0.6595	0.0843(2)	0.52(4)

[a]Space group: *P*63/*mmc*; $Z = 6$; $a = 5.7540(1)$ Å, and $c = 14.0826(1)$ Å; $R_p = 5.26\%$, $R_{wp} = 7.65\%$, $R_B = 3.80\%$, $R_F = 2.30\%$, and GOF = 6.01 for SXRD. $Ti^{3+}/Ti^{4+} = 0.31/0.69$. g^b represents the occupancy factor of each site.

Table S4-7. Crystallographic parameters for the hexagonal $BaTiO_{2.73}H_{0.27}$ (S-4-1) from SXRD refinement[a]. H^- content is estimated from the occupancy (*g*) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

atom	site	g^b	*x*	*y*	*z*	B_{iso} (Å^2)
Ba1	2*b*	1	0	0	0.25	0.51(2)
Ba2	4*f*	1	0.333333	0.666667	0.09261(6)	0.59(1)
Ti1	2*a*	1	0	0	0	0.40(3)
Ti2	4*f*	1	0.333333	0.666667	0.8510(1)	0.54(4)
O1	6*h*	0.73(1)	0.5271(8)	0.05413413	0.25	1.5(2)
O2	12*k*	1	0.8308(5)	0.6615	0.0835(3)	0.61(6)

[a]Space group: *P*6$_3$/*mmc*; $Z = 6$; $a = 5.7481(1)$ Å, and $c = 14.0671(1)$ Å; $R_p = 6.75\%$, $R_{wp} = 10.74\%$, $R_B = 6.34\%$, $R_F = 5.50\%$, and GOF = 9.84 for SXRD. $Ti^{3+}/Ti^{4+} = 0.27/0.73$. g^b represents the occupancy factor of each site.

Table S4-8. Summary of lattice parameters and Ti^{3+}/Ti^{4+} ratio for the hexagonal $BaTiO_{3-x}H_x$ from SXRD refinement[a] and NPD refinement[a] (S-2-2, lower). H^- content is estimated from the occupancy (*g*) of oxygen assuming oxygen deficits are filled with H^- anions. Ti^{3+}/Ti^{4+} ratios were estimated with the formula of $BaTi^{3+}_xTi^{4+}_{1-x}O_{3-x}H_x$.

Sample	*x*	*a* (Å)	*c* (Å)	*V* (Å ^{3})	Ti^{3+}/Ti^{4+}
S-1-1	0.33(1)	5.7567(1)	14.0905(1)	404.392	0.33/0.67
S-1-2	0.32(1)	5.7589(1)	14.0892(1)	404.661	0.32/0.68
S-1-3	0.46(1)	5.7604(1)	14.0830(1)	404.699	0.46/0.54
S-2-1	0.34(1)	5.7572(2)	4.0876(1)	404.381	0.34/0.66
S-2-2	0.45(1)	5.7664(1)	14.0713(1)	405.198	0.45/0.55
	0.46(1)	5.76499(6)	14.0792(3)	405.233	0.46/0.54
S-3-1	0.31(1)	5.7540(1)	14.0826(1)	403.791	0.31/0.69
S-4-1	0.27(1)	5.7481(1)	14.0671(1)	402.522	0.27/0.73

Table S5. List of descriptors of structural parameters.

Descriptor	Brief description
cis	Number of *cis*-configurations in the structure
trans	Number of *trans*-configurations in the structure
N_H_FaceShared	Number of hydrogen atoms at face-shared sites in the structure
N_H*n*-Octa (*n* = 1 ~ 6)	Number of octahedra with *n* hydrogen atoms
Var_H	Variance of hydrogen atoms in octahedra
Av_DI	Average of Baur's distortion index of octahedra
Var_DI	Variance of Baur's distortion index of octahedra
Av_BAV	Average of bond angel variance of octahedra
Var_BAV	Variance of bond angel variance of octahedra