

# Extreme Sensitivity of a Topochemical Reaction to Cation Substitution: $\text{SrVO}_2\text{H}$ vs $\text{SrV}_{1-x}\text{Ti}_x\text{O}_{1.5}\text{H}_{1.5}$ .

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## Supporting Information

### 1. X-ray powder diffraction data from samples of composition $\text{SrV}_{0.5}\text{Ti}_{0.5}\text{O}_3$ prepared by ceramic and arc-melt routes

**Figure S1.** X-ray powder diffraction data collected from samples of nominal composition  $\text{SrV}_{0.5}\text{Ti}_{0.5}\text{O}_3$  prepared by ceramic and arc-melt routes.

### 2. Manganometric titrations of ceramic and arc-melted samples of $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$

**Table S1.** Parameters from the manganometric titration of  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via ceramic route.

**Table S2.** Parameters from the manganometric titration of  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via arc-melt route.

### 3. Structural characterization of reduced ‘ceramic’ $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$

**Figure S2.** Observed, calculated and difference plot from the refinement of reduced ceramic  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  against synchrotron X-ray powder diffraction data. Lower tick marks (black) indicate peak positions of the majority  $\text{SrVO}_2\text{H}$  phase, middle tick marks (red)  $\text{SrVO}_3$ , middle tick marks (blue)  $\text{SrTiO}_{3-x}\text{H}_x$ , upper tick marks (green) elemental vanadium.

**Table S3.** Structural details from the 4-phase refinement of reduced ceramic  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  against synchrotron X-ray powder diffraction data.

### 4. Compositional characterization of reduced ‘ceramic’ $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$

**Figure S3.** Thermogravimetric data collected during the reoxidation of reduced  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via ceramic route.

### 5. Compositional characterization of $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_{1.5}\text{H}_{1.5}$

**Figure S4.** Thermogravimetric data collected during the reoxidation of reduced  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via arc-melt route.

**Table S4.** Parameters from the manganometric titration of reduced  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via arc-melt route.

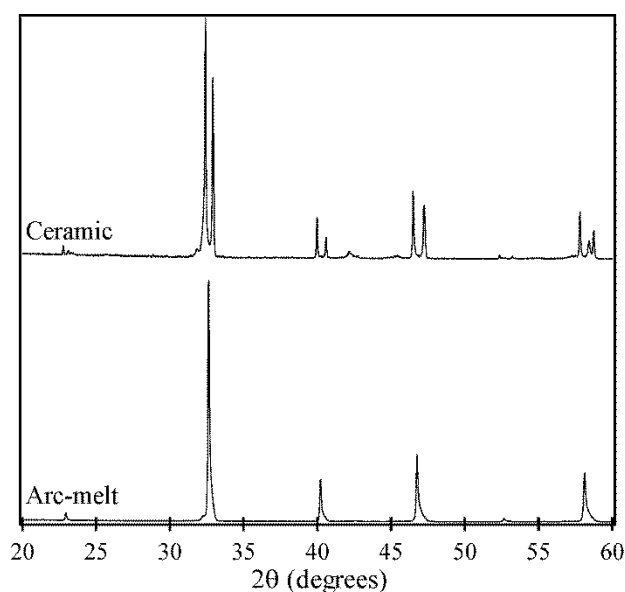
### 6. $\mu^+\text{SR}$ data collected from reduced ‘ceramic’ $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$ and $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_{1.5}\text{H}_{1.5}$

**Figure S5.** Plots of the asymmetry of  $\mu^+\text{SR}$  data collected from reduced ‘ceramic’  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  (top) and  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_{1.5}\text{H}_{1.5}$  (bottom) at low temperature. Oscillations in the data collected from reduced ‘ceramic’  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  are consistent with observation of antiferromagnetic order in  $\text{SrVO}_2\text{H}$ .

### 7. Details of calculations

**Table S5.** Optimized lattice parameters and fractional coordinates and total energies for  $\text{SrVO}_2\text{H}$ ,  $\text{SrTiO}_2\text{H}$  and  $\text{SrV}_{0.75}\text{Ti}_{0.25}\text{H}$ .

## 1. X-ray powder diffraction data from samples of composition $\text{SrV}_{0.5}\text{Ti}_{0.5}\text{O}_3$ prepared by ceramic and arc-melt routes



**Figure S1.** X-ray powder diffraction data collected from samples of nominal composition  $\text{SrV}_{0.5}\text{Ti}_{0.5}\text{O}_3$  prepared by ceramic and arc-melt routes.

## 2. Manganometric titrations of ceramic and arc-melted samples of $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$

Manganometric titrations were performed by dissolving samples in 5M  $\text{H}_2\text{SO}_4$  and then titrating the resulting solution against a standard solution of  $\text{KMnO}_4$ .

Measurement number	1	2	3
Mass of sample (g)	0.0400(2)	0.0402(3)	0.0401(3)
No. moles of V	$2.03(1) \times 10^{-4}$	$2.04(1) \times 10^{-4}$	$2.04(1) \times 10^{-4}$
Titre Volume ( $\text{cm}^3$ )	33.0(1)	33.1(1)	33.0(1)
No. moles $\text{MnO}_4^-$	$4.10(1) \times 10^{-5}$	$4.11(1) \times 10^{-5}$	$4.10(1) \times 10^{-5}$
average V oxidation state	+3.99(2)	+3.98(2)	+3.99(2)

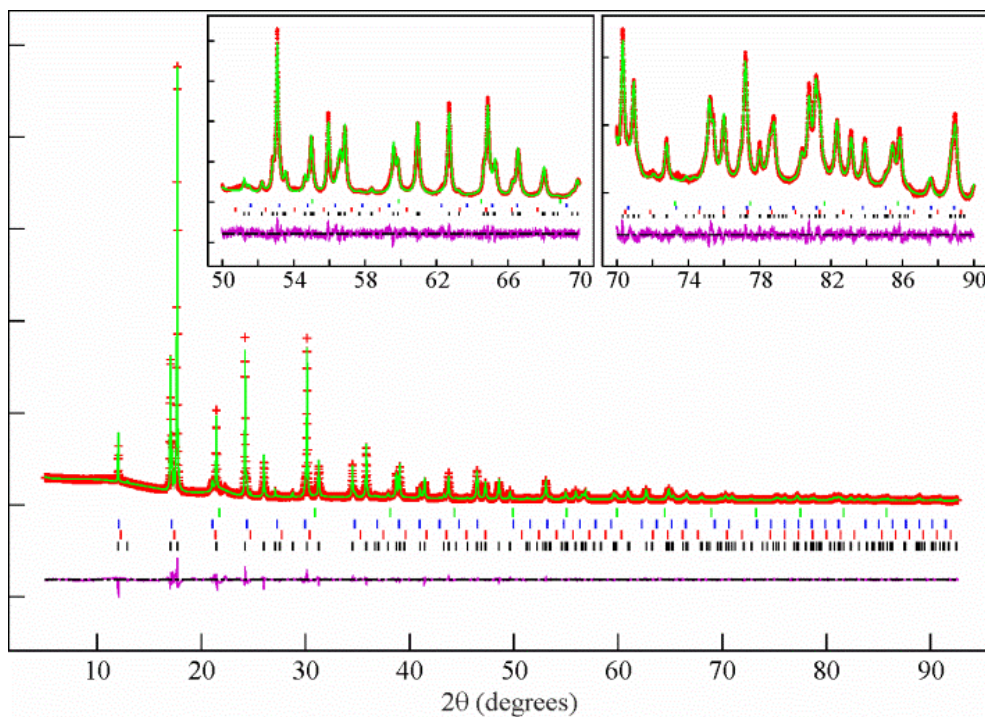
**Table S1.** Parameters from the manganometric titration of  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via ceramic route.

Measurement number	1	2	3
Mass of sample (g)	0.0401(3)	0.0402(3)	0.0400(3)
No. moles of V	$2.04(1) \times 10^{-4}$	$2.04(1) \times 10^{-4}$	$2.03(1) \times 10^{-4}$
Titre Volume ( $\text{cm}^3$ )	32.8(1)	32.9(1)	32.8(1)
No. moles $\text{MnO}_4^-$	$4.08(1) \times 10^{-5}$	$4.09(1) \times 10^{-5}$	$4.08(1) \times 10^{-5}$
average V oxidation state	+4.00(2)	+4.00(2)	+4.00(2)

**Table S2.** Parameters from the manganometric titration of  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via arc-melt route.

### 3. Structural characterization of reduced ‘ceramic’ $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$

A 4-phase structural model consisting of tetragonal  $\text{SrVO}_2\text{H}$ , cubic  $\text{SrVO}_{3-x}$ ,  $\text{SrTiO}_x\text{H}_y$  and elemental vanadium was refined against synchrotron X-ray powder diffraction data collected from the product of reaction between ‘ceramic’  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  and  $\text{CaH}_2$ . Observed and calculated data are shown in Figure S2, with full details of the refined structural model given in Table S1.



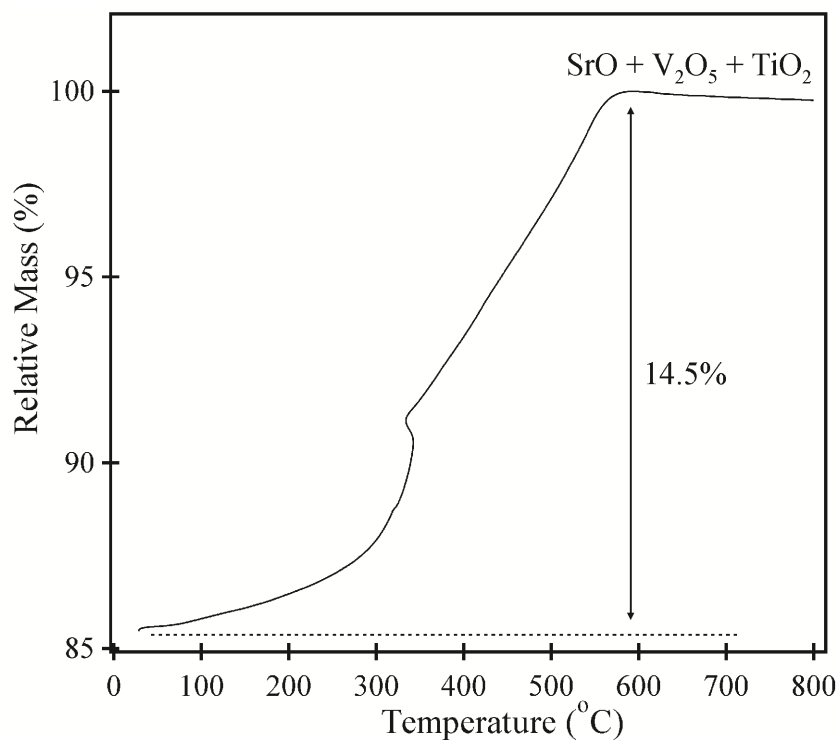
**Figure S2.** Observed, calculated and difference plot from the refinement of reduced ceramic  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  against synchrotron X-ray powder diffraction data. Lower tick marks (black) indicate peak positions of the majority  $\text{SrVO}_2\text{H}$  phase, middle tick marks (red)  $\text{SrVO}_3$ , middle tick marks (blue)  $\text{SrTiO}_{3-x}\text{H}_x$ , upper tick marks (green) elemental vanadium.

SrVO <sub>2</sub> H					
Atom	x	y	z	Fraction	U <sub>iso</sub> (Å <sup>2</sup> )
Sr	½	½	½	1	0.0040(2)
V	0	0	0	1	0.0033(1)
O	½	0	0	1	0.0028(5)
H	0	0	½	1	0.002†
SrVO <sub>2</sub> H space group <i>P4/mmm</i> (#123) Formula weight : 171.55 g mol <sup>-1</sup> , Z = 1 Mass Fraction: 81.3(1) % <i>a</i> = 3.935(1) Å, <i>c</i> = 3.665(1) Å					
SrVO <sub>3-x</sub>					
Atom	x	y	z	Fraction	U <sub>iso</sub> (Å <sup>2</sup> )
Sr	½	½	½	1	0.0040(2)
V	0	0	0	1	0.0029(1)
O	0.5	0	0	0.92‡	0.0026(2)
SrVO <sub>3-x</sub> space group <i>Pm-3m</i> (#221) Formula weight : 182.71 g mol <sup>-1</sup> , Z = 1 Mass Fraction: 6.8(1) % <i>a</i> = 3.852(1) Å					
SrTiO <sub>3-x</sub> H <sub>x</sub>					
Atom	x	y	z	Fraction	U <sub>iso</sub> (Å <sup>2</sup> )
Sr	½	½	½	1	0.0041(3)
Ti	0	0	0	1	0.0028(2)
O	½	0	0	0.96	0.0017(3)
SrTiO <sub>3-x</sub> H <sub>x</sub> space group <i>Pm-3m</i> (#221) Formula weight : 181.57 g mol <sup>-1</sup> , Z = 1 Mass Fraction: 4.8(2) % <i>a</i> = 3.911(1) Å					
Vanadium					
Atom	x	y	z	Fraction	U <sub>iso</sub> (Å <sup>2</sup> )
V	0	0	0	1	0.0020(3)
V space group <i>Im-3m</i> (#229) Formula weight : 50.94 g mol <sup>-1</sup> , Z = 2 Mass Fraction: 7.1(4) % <i>a</i> = 3.026(1) Å					
Radiation source: Synchrotron X-ray, λ = 0.82626(1) Temperature: 298 K χ <sup>2</sup> = 7.534; <i>wRp</i> = 3.31 %; <i>Rp</i> = 2.06 %.					

**Table S3.** Structural details from the 4-phase refinement of reduced ceramic SrV<sub>0.95</sub>Ti<sub>0.05</sub>O<sub>3</sub> against synchrotron X-ray powder diffraction data. ‡ The fractional occupancy of the oxide ions in SrVO<sub>3-x</sub> was taken from the previous refinement of SrVO<sub>2</sub>H.<sup>12</sup>

#### 4. Compositional characterization of reduced ‘ceramic’ $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$

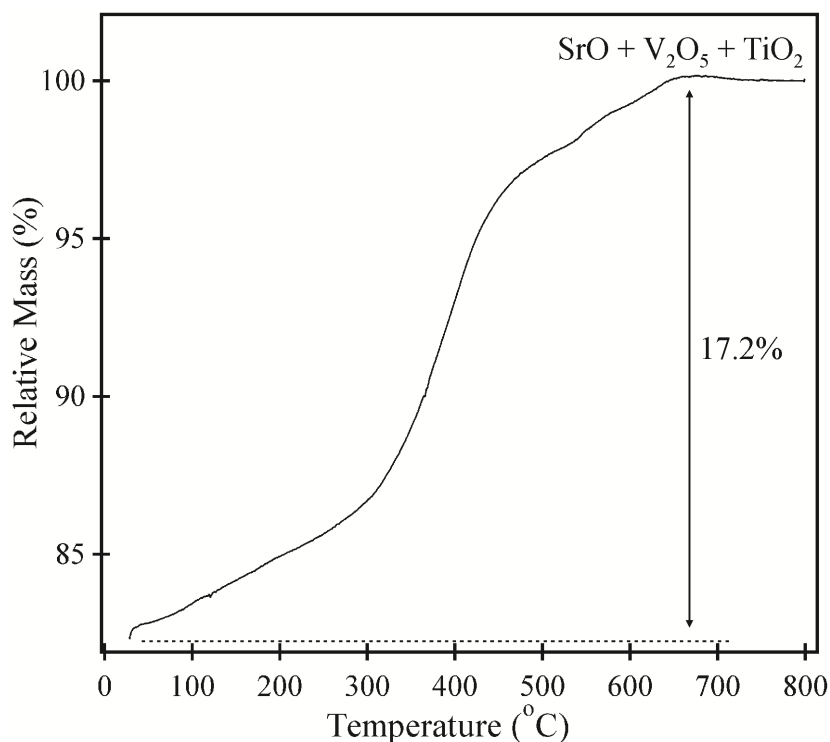
Thermogravimetric measurements were performed by heating powder samples at a rate of  $5\text{ }^\circ\text{C min}^{-1}$  under an oxygen atmosphere, using a Mettler-Toledo MX1 thermogravimetric microbalance. Figure S3 shows a plot of sample mass against temperature as the sample is oxidized to  $\text{SrO}$ ,  $\text{V}_2\text{O}_5$  and  $\text{TiO}_2$  (confirmed by X-ray powder diffraction). The observed mass gain (14.5%) is consistent with the formulation shown in Table S1.



**Figure S3.** Thermogravimetric data collected during the reoxidation of reduced  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  prepared via ceramic route.

## 5. Compositional characterization of SrV<sub>0.95</sub>Ti<sub>0.05</sub>O<sub>1.5</sub>H<sub>1.5</sub>

Thermogravimetric measurements were performed by heating powder samples at a rate of 5 °C min<sup>-1</sup> under an oxygen atmosphere, using a Mettler-Toledo MX1 thermogravimetric microbalance. Figure S4 shows a plot of sample mass against temperature as the sample is oxidized to SrO, V<sub>2</sub>O<sub>5</sub> and TiO<sub>2</sub> (confirmed by X-ray powder diffraction). The observed mass gain (17.2%) is consistent with the formulation shown in Table 2 in the main manuscript.



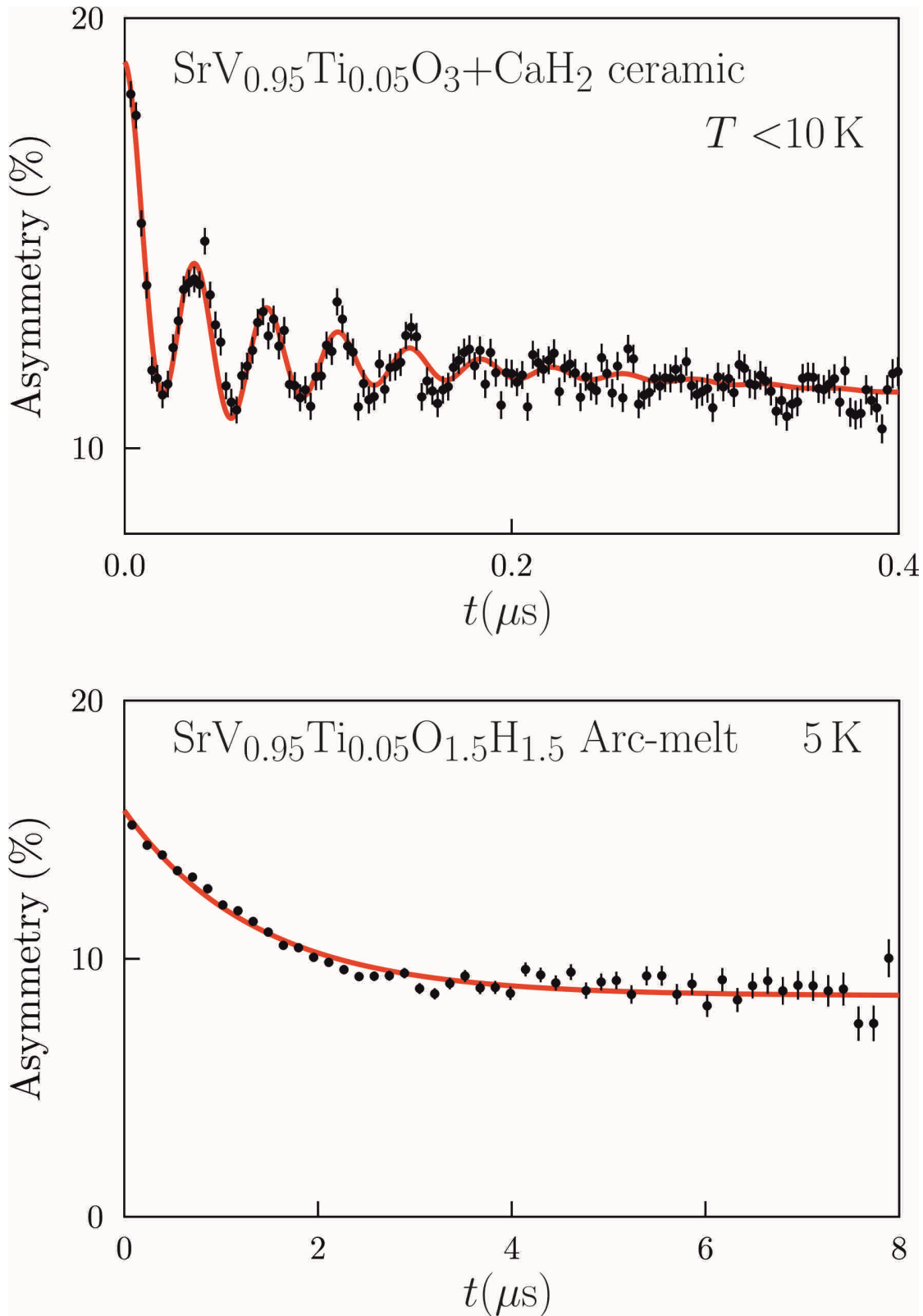
**Figure S4.** Thermogravimetric data collected during the reoxidation of reduced SrV<sub>0.95</sub>Ti<sub>0.05</sub>O<sub>3</sub> prepared via arc-melt route.

Manganometric titrations were performed by dissolving samples in 5M H<sub>2</sub>SO<sub>4</sub> and then titrating the resulting solution against a standard solution of KMnO<sub>4</sub>.

Measurement number	1	2	3
Mass of sample (g)	0.0251(3)	0.0252(3)	0.0252(3)
No. moles of V	$1.70(2) \times 10^{-4}$	$1.70(2) \times 10^{-4}$	$1.70(2) \times 10^{-4}$
Titre Volume (cm <sup>3</sup> )	28.2(1)	28.5(1)	28.4(1)
No. moles MnO <sub>4</sub> <sup>-</sup>	$9.75(3) \times 10^{-5}$	$9.86(3) \times 10^{-5}$	$9.82(3) \times 10^{-5}$
average V oxidation state	+2.14(4)	+2.10(5)	2.11(4)

**Table S4.** Parameters from the manganometric titration of reduced SrV<sub>0.95</sub>Ti<sub>0.05</sub>O<sub>3</sub> prepared via arc-melt route.

6.  $\mu^+$ SR data collected from reduced ‘ceramic’  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  and  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_{1.5}\text{H}_{1.5}$



**Figure S5.** Plots of the asymmetry of  $\mu^+$ SR data collected from reduced ‘ceramic’  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  (top) and  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_{1.5}\text{H}_{1.5}$  (bottom) at low temperature. Oscillations in the data collected from reduced ‘ceramic’  $\text{SrV}_{0.95}\text{Ti}_{0.05}\text{O}_3$  are consistent with observation of antiferromagnetic order in  $\text{SrVO}_2\text{H}$ .

## 6. Details of calculations

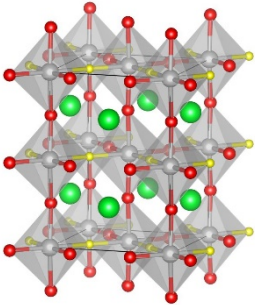
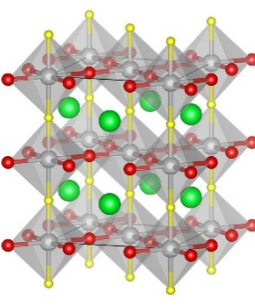
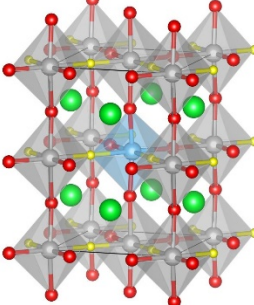
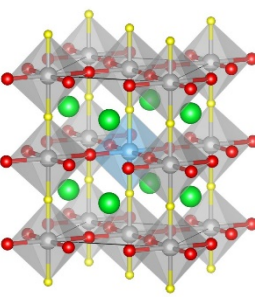
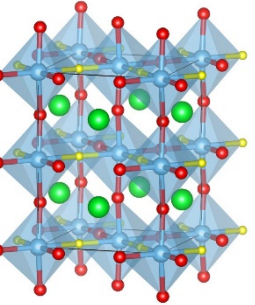
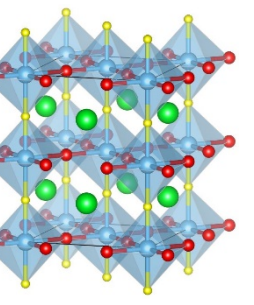
Structure	SrVO <sub>2</sub> H - <i>cis</i>	SrVO <sub>2</sub> H - <i>trans</i>	SrV <sub>0.75</sub> Ti <sub>0.25</sub> O <sub>2</sub> H - <i>cis</i>	SrV <sub>0.75</sub> Ti <sub>0.25</sub> O <sub>2</sub> H - <i>trans</i>	SrTiO <sub>2</sub> H - <i>cis</i>	SrTiO <sub>2</sub> H - <i>trans</i>																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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Energy	-128.865 eV	-129.923 eV	-129.560 eV	-129.924 eV	-130.022 eV	-129.166 eV																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Lattice Parameters	a = 5.448 Å b = 5.608 Å c = 7.864 Å γ = 90.000°	a = 5.634 Å b = 5.634 Å c = 7.385 Å γ = 90.000°	a = 5.540 Å b = 5.527 Å c = 7.914 Å γ = 90.000°	a = 5.672 Å b = 5.672 Å c = 7.412 Å γ = 90.000°	a = 5.679 Å b = 5.683 Å c = 7.819 Å γ = 90.000°	a = 5.694 Å b = 5.694 Å c = 7.517 Å γ = 90.000°																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Fractional Coordinates	<table border="1"> <tr><td>0.474</td><td>0.000</td><td>0.250</td><td>Sr</td></tr> <tr><td>0.026</td><td>0.500</td><td>0.250</td><td>Sr</td></tr> <tr><td>0.474</td><td>0.000</td><td>0.750</td><td>Sr</td></tr> <tr><td>0.026</td><td>0.500</td><td>0.750</td><td>Sr</td></tr> <tr><td>-0.006</td><td>0.000</td><td>0.000</td><td>V</td></tr> <tr><td>0.506</td><td>0.500</td><td>0.000</td><td>V</td></tr> <tr><td>-0.006</td><td>0.000</td><td>0.500</td><td>V</td></tr> <tr><td>0.506</td><td>0.500</td><td>0.500</td><td>V</td></tr> <tr><td>0.250</td><td>0.250</td><td>0.000</td><td>O</td></tr> <tr><td>0.250</td><td>0.750</td><td>0.000</td><td>O</td></tr> <tr><td>-0.034</td><td>0.000</td><td>0.250</td><td>O</td></tr> <tr><td>0.534</td><td>0.500</td><td>0.250</td><td>O</td></tr> <tr><td>0.250</td><td>0.250</td><td>0.500</td><td>O</td></tr> <tr><td>0.250</td><td>0.750</td><td>0.500</td><td>O</td></tr> <tr><td>-0.034</td><td>0.000</td><td>0.750</td><td>O</td></tr> <tr><td>0.534</td><td>0.500</td><td>0.750</td><td>O</td></tr> <tr><td>0.750</td><td>0.250</td><td>0.000</td><td>H</td></tr> <tr><td>0.750</td><td>0.250</td><td>0.500</td><td>H</td></tr> <tr><td>0.750</td><td>0.750</td><td>0.000</td><td>H</td></tr> <tr><td>0.750</td><td>0.750</td><td>0.500</td><td>H</td></tr> </table>	0.474	0.000	0.250	Sr	0.026	0.500	0.250	Sr	0.474	0.000	0.750	Sr	0.026	0.500	0.750	Sr	-0.006	0.000	0.000	V	0.506	0.500	0.000	V	-0.006	0.000	0.500	V	0.506	0.500	0.500	V	0.250	0.250	0.000	O	0.250	0.750	0.000	O	-0.034	0.000	0.250	O	0.534	0.500	0.250	O	0.250	0.250	0.500	O	0.250	0.750	0.500	O	-0.034	0.000	0.750	O	0.534	0.500	0.750	O	0.750	0.250	0.000	H	0.750	0.250	0.500	H	0.750	0.750	0.000	H	0.750	0.750	0.500	H	<table border="1"> <tr><td>0.500</td><td>0.000</td><td>0.250</td><td>Sr</td></tr> <tr><td>0.000</td><td>0.500</td><td>0.250</td><td>Sr</td></tr> <tr><td>0.500</td><td>0.000</td><td>0.750</td><td>Sr</td></tr> <tr><td>0.000</td><td>0.500</td><td>0.750</td><td>Sr</td></tr> 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</table>	0.500	0.000	0.250	Sr	0.000	0.500	0.250	Sr	0.500	0.000	0.750	Sr	0.000	0.500	0.750	Sr	0.000	0.000	0.000	V	0.500	0.500	0.000	V	0.000	0.000	0.500	V	0.500	0.500	0.500	V	0.250	0.250	0.000	O	0.250	0.750	0.000	O	0.750	0.250	0.000	O	0.750	0.750	0.000	O	0.250	0.250	0.500	O	0.250	0.750	0.500	O	0.750	0.250	0.500	O	0.750	0.750	0.500	O	0.000	0.000	0.250	H	0.500	0.500	0.250	H	0.000	0.000	0.750	H	0.500	0.500	0.750	H	<table border="1"> <tr><td>0.480</td><td>0.000</td><td>0.241</td><td>Sr</td></tr> <tr><td>0.014</td><td>0.500</td><td>0.238</td><td>Sr</td></tr> <tr><td>0.480</td><td>0.000</td><td>0.759</td><td>Sr</td></tr> <tr><td>0.014</td><td>0.500</td><td>0.762</td><td>Sr</td></tr> <tr><td>-0.005</td><td>0.000</td><td>0.000</td><td>V</td></tr> <tr><td>0.518</td><td>0.500</td><td>0.000</td><td>V</td></tr> <tr><td>-0.012</td><td>0.000</td><td>0.500</td><td>V</td></tr> <tr><td>0.484</td><td>0.500</td><td>0.500</td><td>Ti</td></tr> <tr><td>0.249</td><td>0.246</td><td>0.000</td><td>O</td></tr> <tr><td>0.249</td><td>0.754</td><td>0.000</td><td>O</td></tr> <tr><td>-0.046</td><td>0.000</td><td>0.251</td><td>O</td></tr> <tr><td>0.538</td><td>0.500</td><td>0.261</td><td>O</td></tr> <tr><td>0.257</td><td>0.246</td><td>0.500</td><td>O</td></tr> <tr><td>0.257</td><td>0.754</td><td>0.500</td><td>O</td></tr> <tr><td>-0.046</td><td>0.000</td><td>0.749</td><td>O</td></tr> <tr><td>0.538</td><td>0.500</td><td>0.739</td><td>O</td></tr> <tr><td>0.756</td><td>0.251</td><td>0.000</td><td>H</td></tr> <tr><td>0.759</td><td>0.252</td><td>0.500</td><td>H</td></tr> <tr><td>0.756</td><td>0.749</td><td>0.000</td><td>H</td></tr> <tr><td>0.759</td><td>0.748</td><td>0.500</td><td>H</td></tr> </table>	0.480	0.000	0.241	Sr	0.014	0.500	0.238	Sr	0.480	0.000	0.759	Sr	0.014	0.500	0.762	Sr	-0.005	0.000	0.000	V	0.518	0.500	0.000	V	-0.012	0.000	0.500	V	0.484	0.500	0.500	Ti	0.249	0.246	0.000	O	0.249	0.754	0.000	O	-0.046	0.000	0.251	O	0.538	0.500	0.261	O	0.257	0.246	0.500	O	0.257	0.754	0.500	O	-0.046	0.000	0.749	O	0.538	0.500	0.739	O	0.756	0.251	0.000	H	0.759	0.252	0.500	H	0.756	0.749	0.000	H	0.759	0.748	0.500	H	<table border="1"> <tr><td>0.500</td><td>0.000</td><td>0.248</td><td>Sr</td></tr> <tr><td>0.000</td><td>0.500</td><td>0.248</td><td>Sr</td></tr> <tr><td>0.500</td><td>0.000</td><td>0.752</td><td>Sr</td></tr> <tr><td>0.000</td><td>0.500</td><td>0.752</td><td>Sr</td></tr> <tr><td>0.000</td><td>0.000</td><td>0.000</td><td>V</td></tr> <tr><td>0.500</td><td>0.500</td><td>0.000</td><td>V</td></tr> <tr><td>0.000</td><td>0.000</td><td>0.500</td><td>V</td></tr> <tr><td>0.500</td><td>0.500</td><td>0.500</td><td>Ti</td></tr> <tr><td>0.250</td><td>0.250</td><td>0.000</td><td>O</td></tr> 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</table>	0.500	0.000	0.248	Sr	0.000	0.500	0.248	Sr	0.500	0.000	0.752	Sr	0.000	0.500	0.752	Sr	0.000	0.000	0.000	V	0.500	0.500	0.000	V	0.000	0.000	0.500	V	0.500	0.500	0.500	Ti	0.250	0.250	0.000	O	0.250	0.750	0.000	O	0.750	0.250	0.000	O	0.750	0.750	0.000	O	0.258	0.258	0.500	O	0.258	0.742	0.500	O	0.742	0.258	0.500	O	0.742	0.742	0.500	O	0.000	0.000	0.249	H	0.500	0.500	0.247	H	0.000	0.000	0.751	H	0.500	0.500	0.753	H	<table border="1"> <tr><td>0.479</td><td>0.000</td><td>0.250</td><td>Sr</td></tr> <tr><td>0.021</td><td>0.500</td><td>0.250</td><td>Sr</td></tr> <tr><td>0.479</td><td>0.000</td><td>0.750</td><td>Sr</td></tr> <tr><td>0.021</td><td>0.500</td><td>0.750</td><td>Sr</td></tr> <tr><td>-0.007</td><td>0.000</td><td>0.000</td><td>Ti</td></tr> <tr><td>0.507</td><td>0.500</td><td>0.000</td><td>Ti</td></tr> <tr><td>-0.007</td><td>0.000</td><td>0.500</td><td>Ti</td></tr> <tr><td>0.507</td><td>0.500</td><td>0.500</td><td>Ti</td></tr> <tr><td>0.250</td><td>0.250</td><td>0.000</td><td>O</td></tr> 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Table S5. Optimized lattice parameters and fractional coordinates and total energies for SrVO<sub>2</sub>H, SrTiO<sub>2</sub>H and SrV<sub>0.75</sub>Ti<sub>0.25</sub>H.