

Supporting information S1: Results of the Rietveld refinement of the sample prepared by heating the sol-gel precursor to 300 °C.

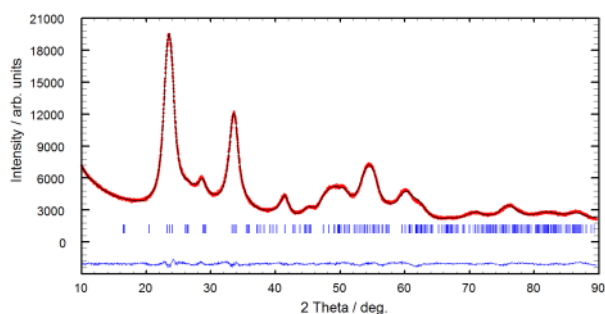


Figure S1.1 – Graphical results of the Rietveld refinement of the sample heated to 300 °C. Red line: observed profile; black line: calculated profile; blue line: differential plot for observed and calculated data; blue vertical bars indicate the theoretical positions of Bragg-reflections.

Table S1.1 – Numerical results of the Rietveld refinement of the sample heated to 300 °C.

composition	WO ₃
space group	<i>Pnma</i>
lattice parameters	$a = 754.99(21)$ pm $b = 742.1(2)$ pm $c = 767.1(2)$ pm
formula units	8
unit cell volume	53.73×10^6 pm ³
(normalized to one formula unit)	
calculated density	7.17 g/cm ³
diffractometer	PANalytical Empyrean MPD
wavelength	Cu K α ($\lambda_1 = 154.056$ pm; $\lambda_2 = 154.539$ pm; $I(\lambda_1/\lambda_2 = 0.5)$)
profile points	3070
2 θ range	10–90°
R_{Bragg}	0.007
R_{wp}	0.019
R_{exp}	0.015
S	1.3

Table S1.2 – Structural parameters for the sample heated to 300 °C. Owing to the nanocrystalline nature of the sample, atomic positions of oxygen atoms were not refined. Isotropic Debye-Waller factors were refined to a combined value for all atoms of $B_{overall} = 1.312$ Å².

Atom	site	x	y	z

W1	4c	0.0073(4)	¼	0.9760(8)
W2	4c	0.0264(6)	¼	0.472(7)
O1	4a	0	0	0
O2	4b	0	0	½
O3	4c	0.269	¼	0.973
O4	4c	0.278	¼	0.529
O5	4c	0.004	¼	0.738
O6	4c	0.015	¼	0.224

Supporting information S2: Results of the Rietveld refinement of the sample prepared by heating the sol-gel precursor to 450 °C.

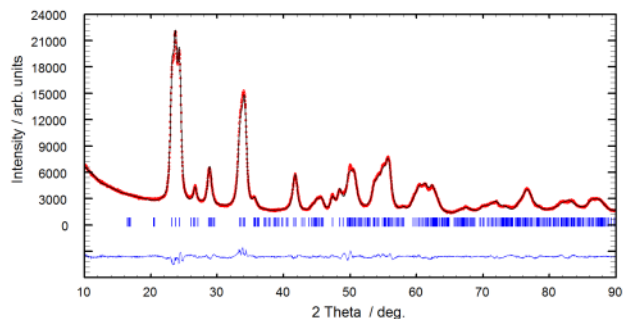


Figure S2.1 – Graphical results of the Rietveld refinement of the sample heated to 450 °C. Red line: observed profile; black line: calculated profile; blue line: differential plot for observed and calculated data; blue vertical bars indicate the theoretical positions of Bragg-reflections.

Table S2.1 – Numerical results of the Rietveld refinement of the sample heated to 450 °C.

composition	WO ₃
space group	<i>P2₁/n</i>
lattice parameters	<i>a</i> = 733.83(6) pm <i>b</i> = 751.94(7) pm <i>c</i> = 768.41(7) pm <i>β</i> = 90.53(1)°
formula units	8
unit cell volume	54.12 × 10 ⁶ pm ³
(normalized to one formula unit)	
calculated density	7.259 g/cm ³
diffractometer	PANalytical Empyrean MPD
wavelength	Cu K _α (<i>λ</i> ₁ = 154.056 pm; <i>λ</i> ₂ = 154.539 pm; 1(<i>λ</i> ₁ / <i>λ</i> ₂) = 0.5)
profile points	3070
2θ range	10–90°
<i>R</i> _{Bragg}	0.014
<i>R</i> _{wp}	0.034
<i>R</i> _{exp}	0.017
<i>S</i>	2.02

Table S2.2 – Structural parameters for the sample heated to 450 °C. Owing to the nanocrystalline nature of the sample, atomic positions were not refined. Isotropic Debye-Waller factors were refined to a combined value for all atoms of *B*_{overall} = 1.253 Å².

Atom	site	<i>x</i>	<i>y</i>	<i>z</i>
W1	4e	0.25346	0.02452	0.28322
W2	4e	0.25076	0.02197	0.78284
O1	4e	0.0025	0.035	0.2106
O2	4e	0.9974	0.46360	0.2161
O3	4e	0.284	0.26050	0.2848
O4	4e	0.2099	0.2568	0.7318
O5	4e	0.2827	0.0383	0.0046
O6	4e	0.2856	0.484	0.9944