

Supporting Information

To

Site Specific and Localized Structural Displacements in Open Structured Multimetallic Oxides

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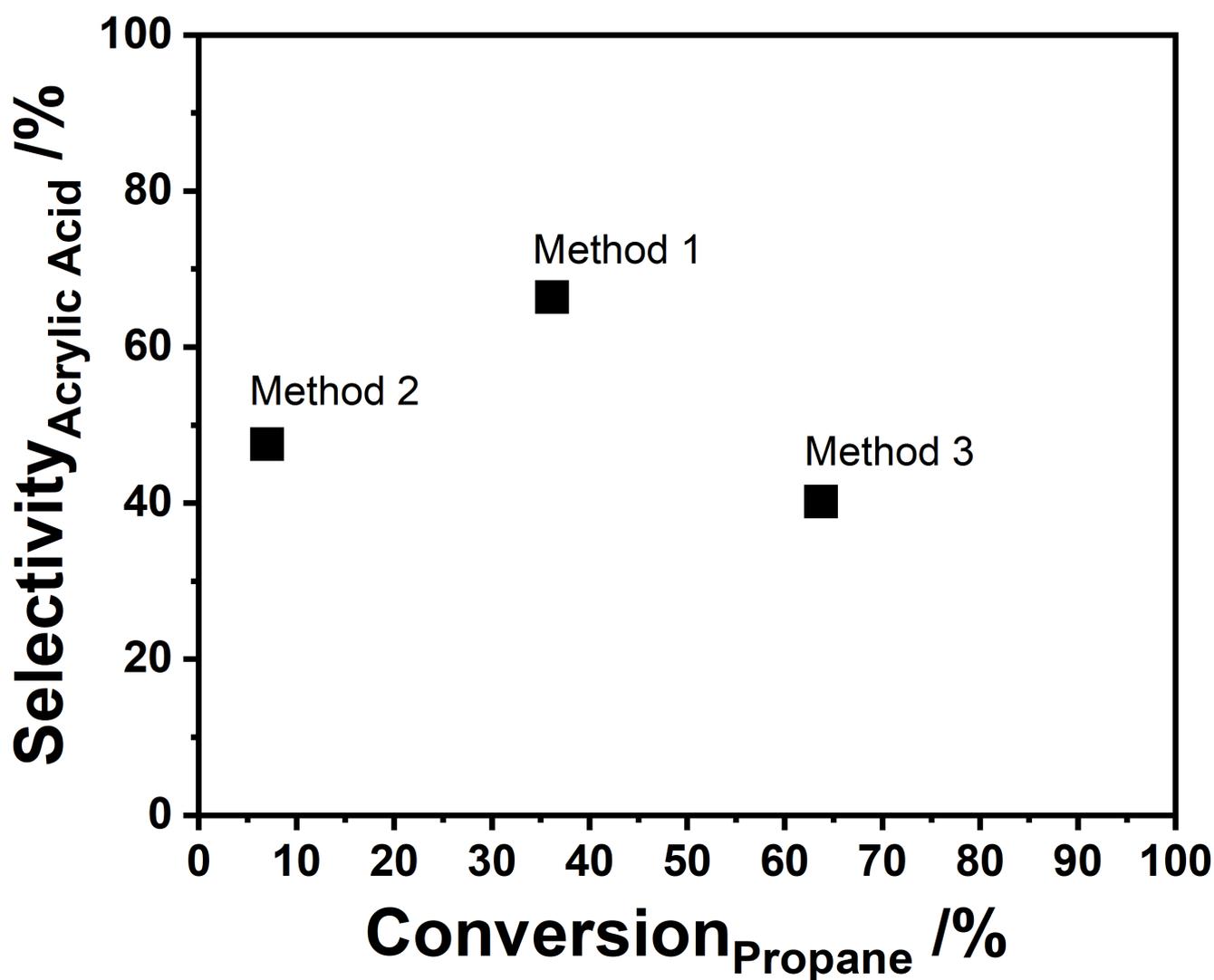


Figure S 1. Selectivity towards acrylic acid formation and conversion of propane at 400°C of the different (Mo,V,Te,Nb)O_x catalysts presented in the manuscript. Conditions: C₃H₈/O₂/N₂/H₂O= 3/6/51/40; gas flow: 14.7 ml/min (method 1), 10 ml/min (method 2), 16.7 ml/min (method 3); mass: 90 mg (method 1), mass: 300 mg (method 2), 100 mg (method 3).

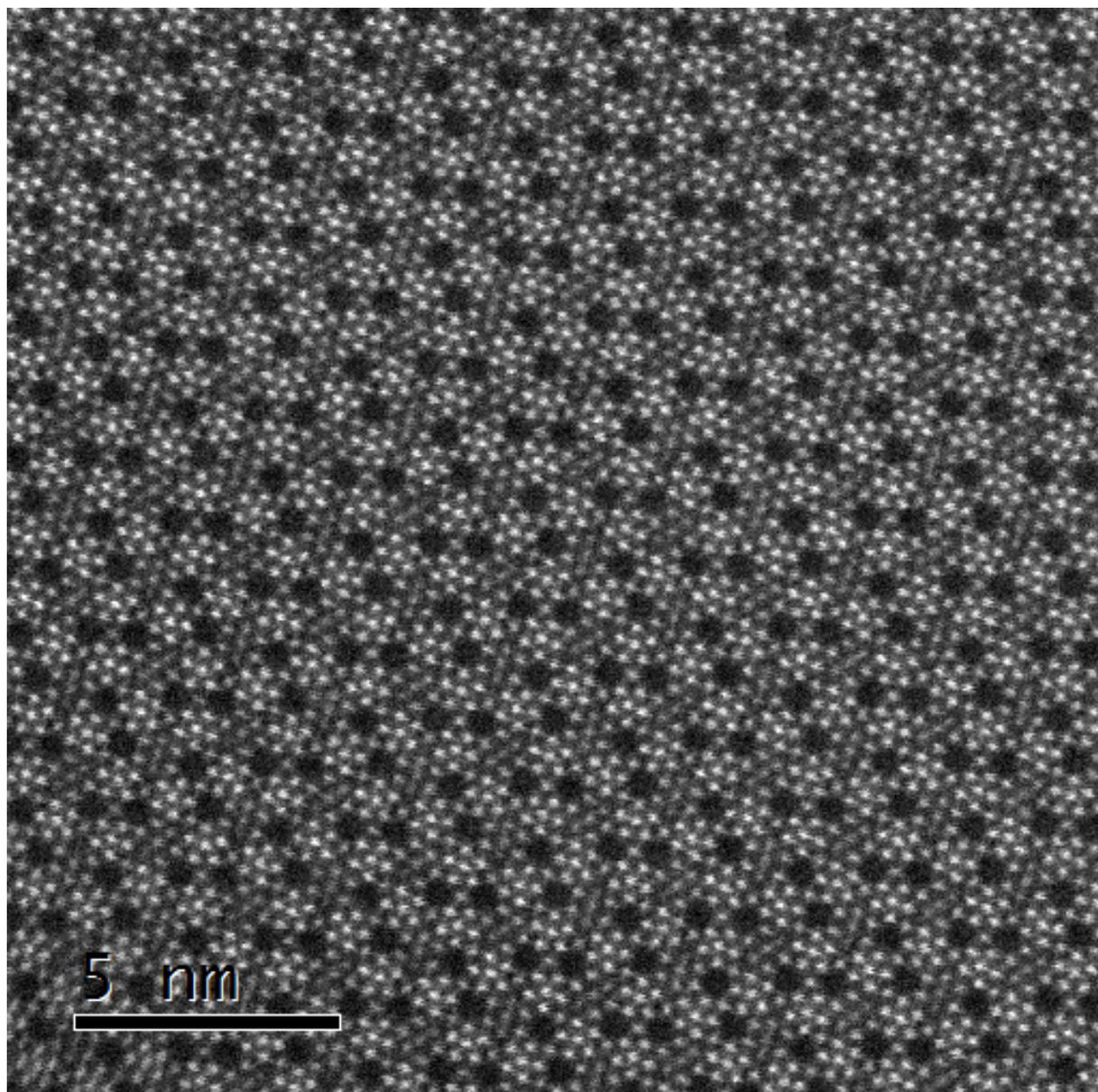


Figure S 2. Original ADF-STEM image of the M1 sample prepared by Method 1.

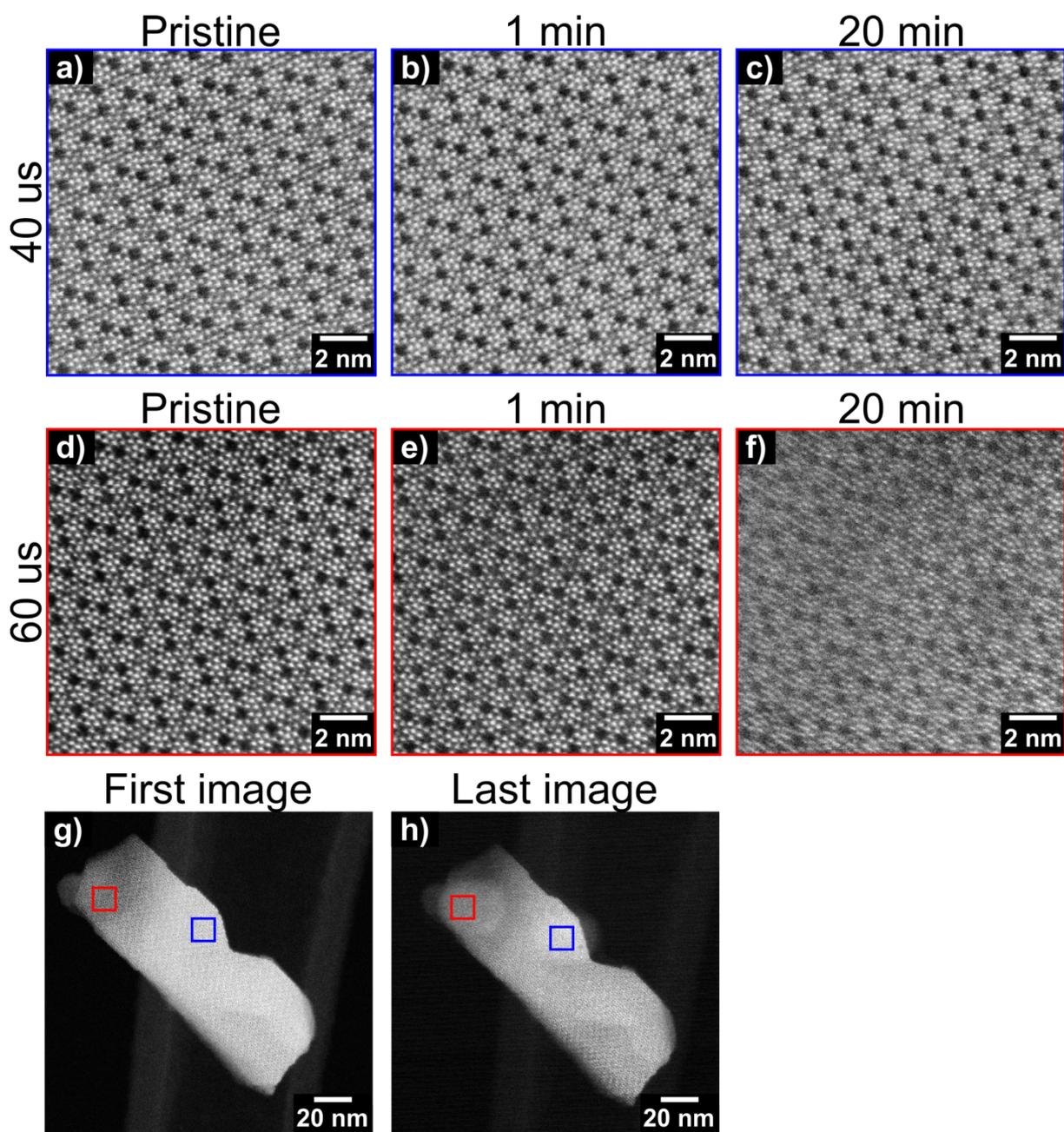


Figure S 3. ADF-STEM study of the influence of the electron beam on the microstructure of $(\text{Mo,V,Te,Nb})\text{O}_x$ synthesized by Method 1. The sample was continuously exposed to the electron beam for 1 min and 20 min: (a)–(c) acquisition time: 40 μs and for comparison (d)–(f) acquisition time: 60 μs . (g) and (h) denote overview ADF-STEM images before and after the beam damage study. Changes are observed only for the sample acquired with 60 $\mu\text{s}/\text{pixel}$ after 20 min. Carbon contamination can be observed at the exposed area. Beam dose rate: 6200 $\text{e}/\text{\AA}^2\text{s}$.

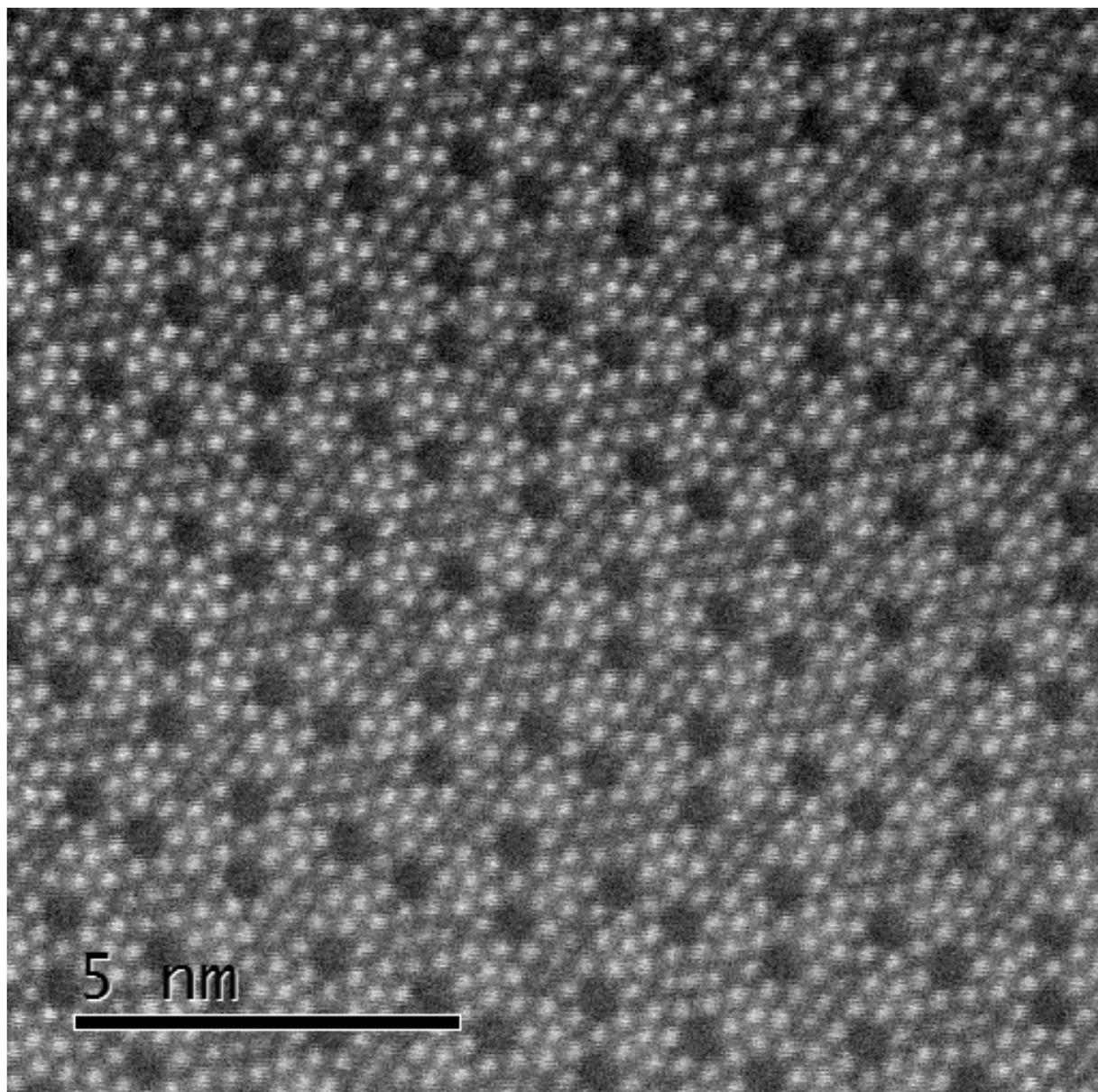


Figure S 4. Original ADF-STEM image of the M1 sample prepared by Method 2.

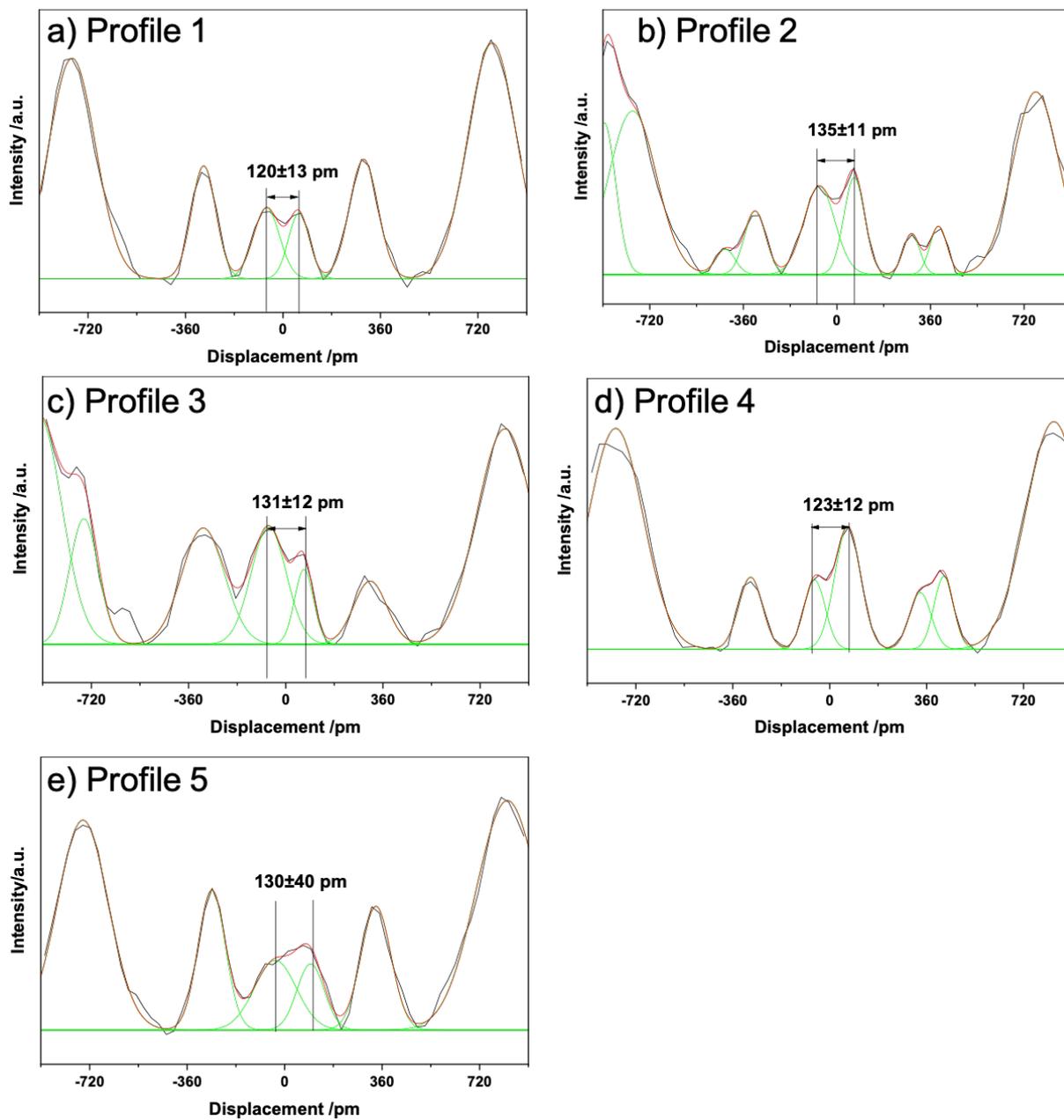


Figure S 5. Gaussian fitted line profiles (a)-(e) that are presented in Figure 2. The distances denote the displacement of the S2 sites including the error.

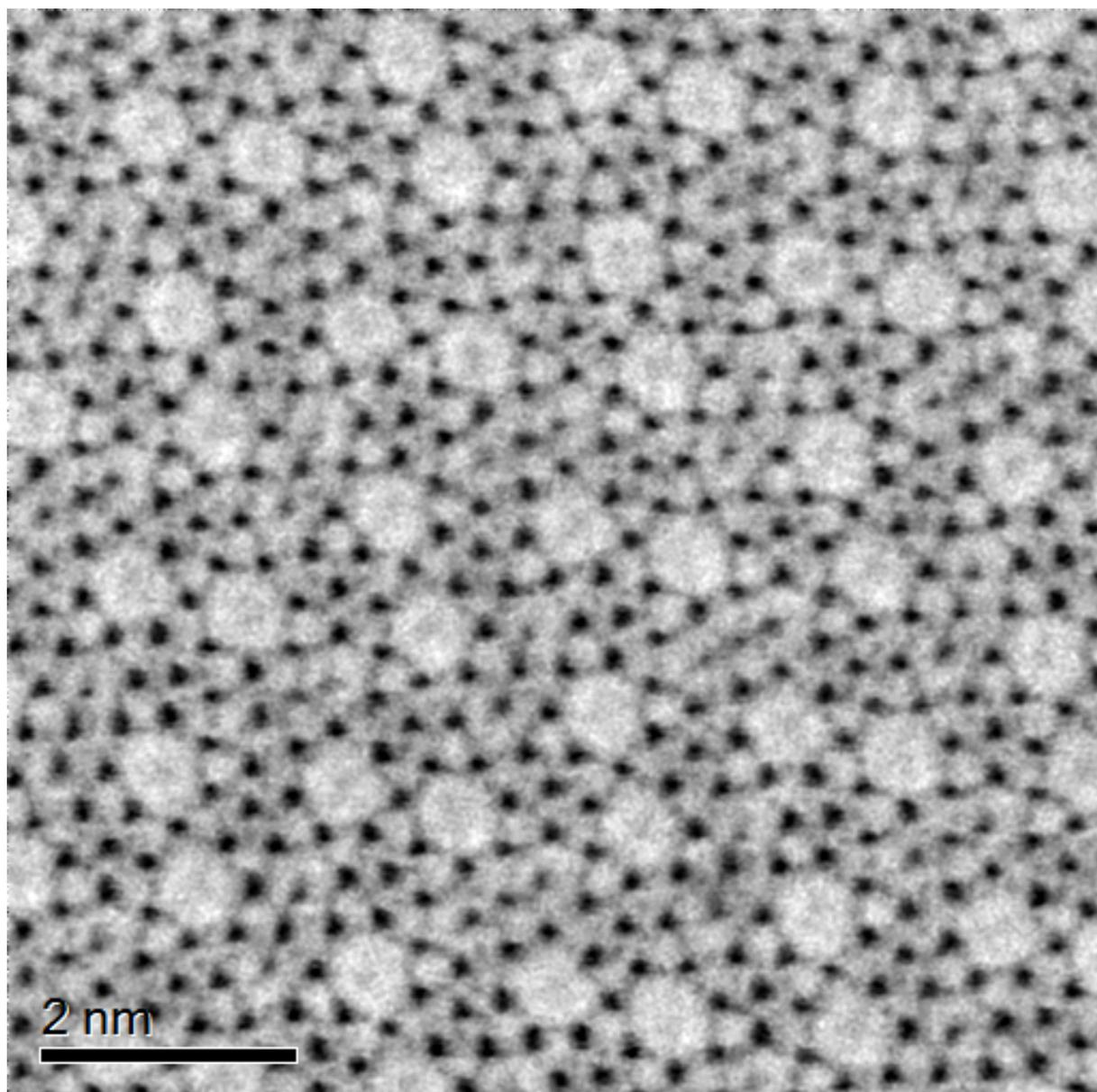


Figure S 6. Original ABF-STEM image of the M1 sample prepared by Method 3.

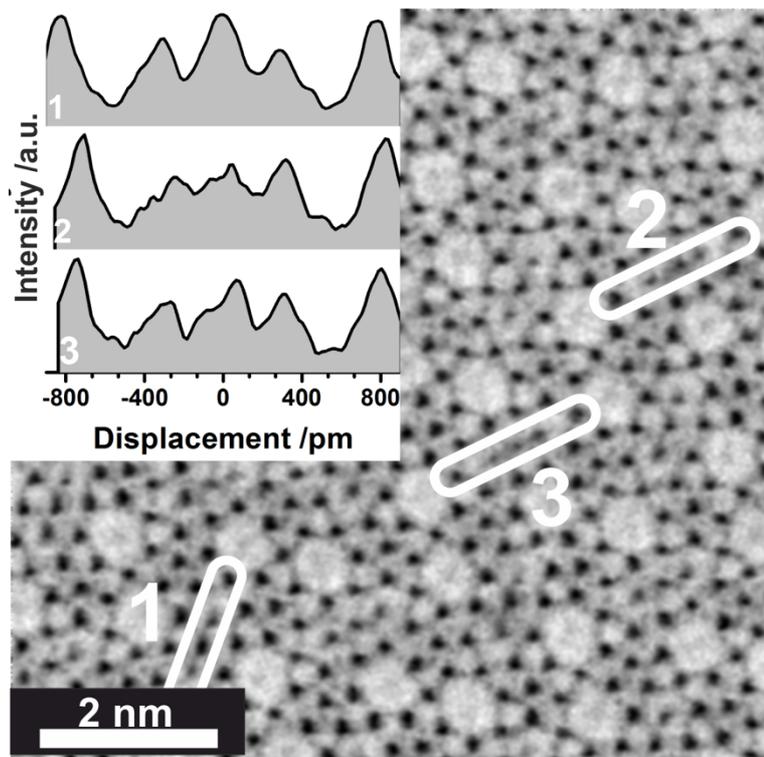


Figure S 7. Smoothed ABF-STEM image of orthorhombic (Mo,V,Te,Nb)Ox viewed along [001]. The M1 oxide was prepared by method 3. The inset denotes the corresponding line profiles taken from different ROIs. The original image is also shown in the supporting information (Figure S6).

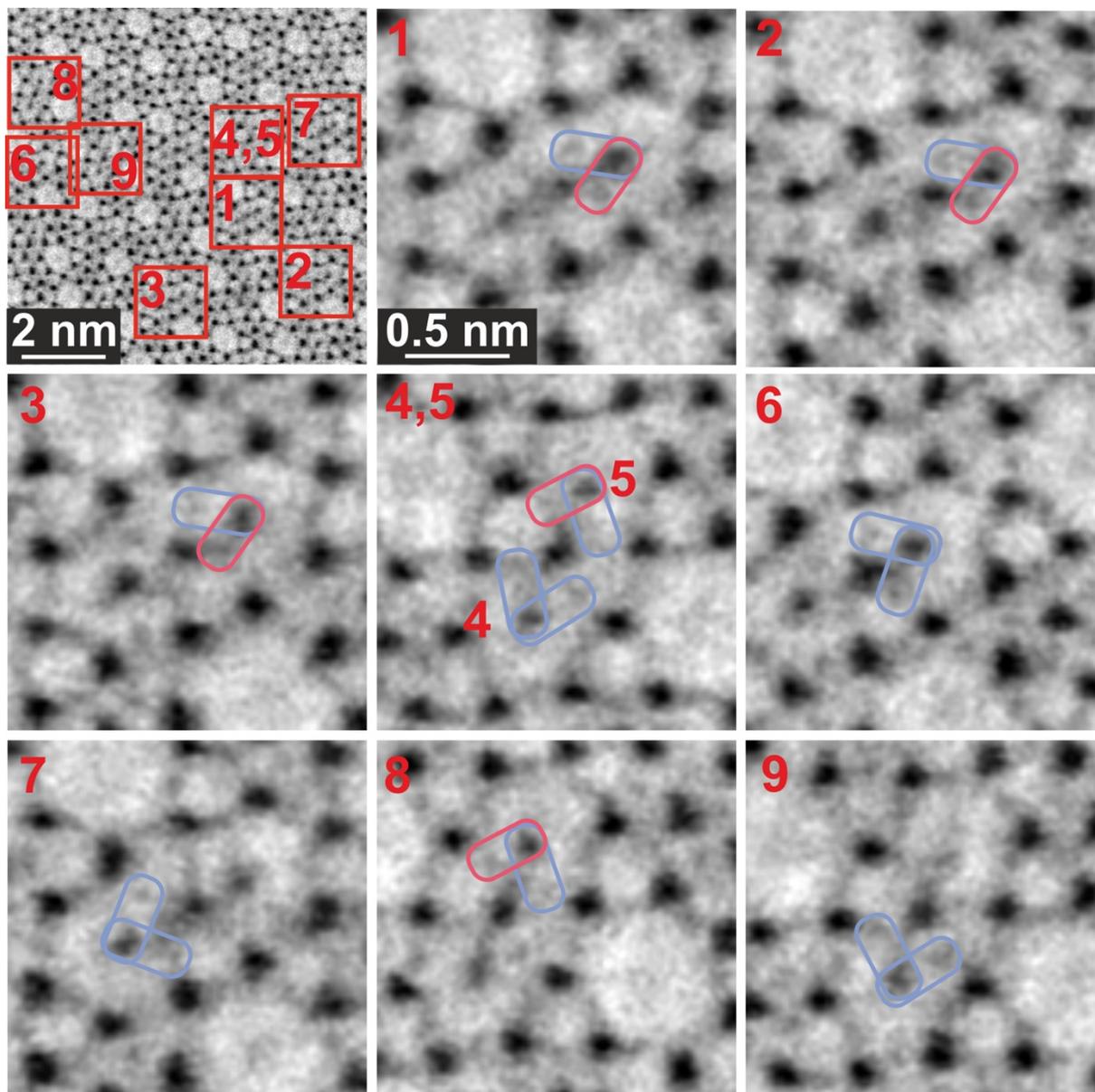


Figure S 8. Magnified ABF-STEM images highlighting the S2-O-Te relationship and indicate the presence of different Te-O distances. From these images the Te-O distances were measured as presented in Figure 3D. The different numbers correspond to the different Te-O positions and are identical with the numbers in Figure 3D. Pink and violet ellipses correspond to short and long Te-O distances, respectively. The red boxes in the top left image denote the regions of interests from which the magnified images were taken.

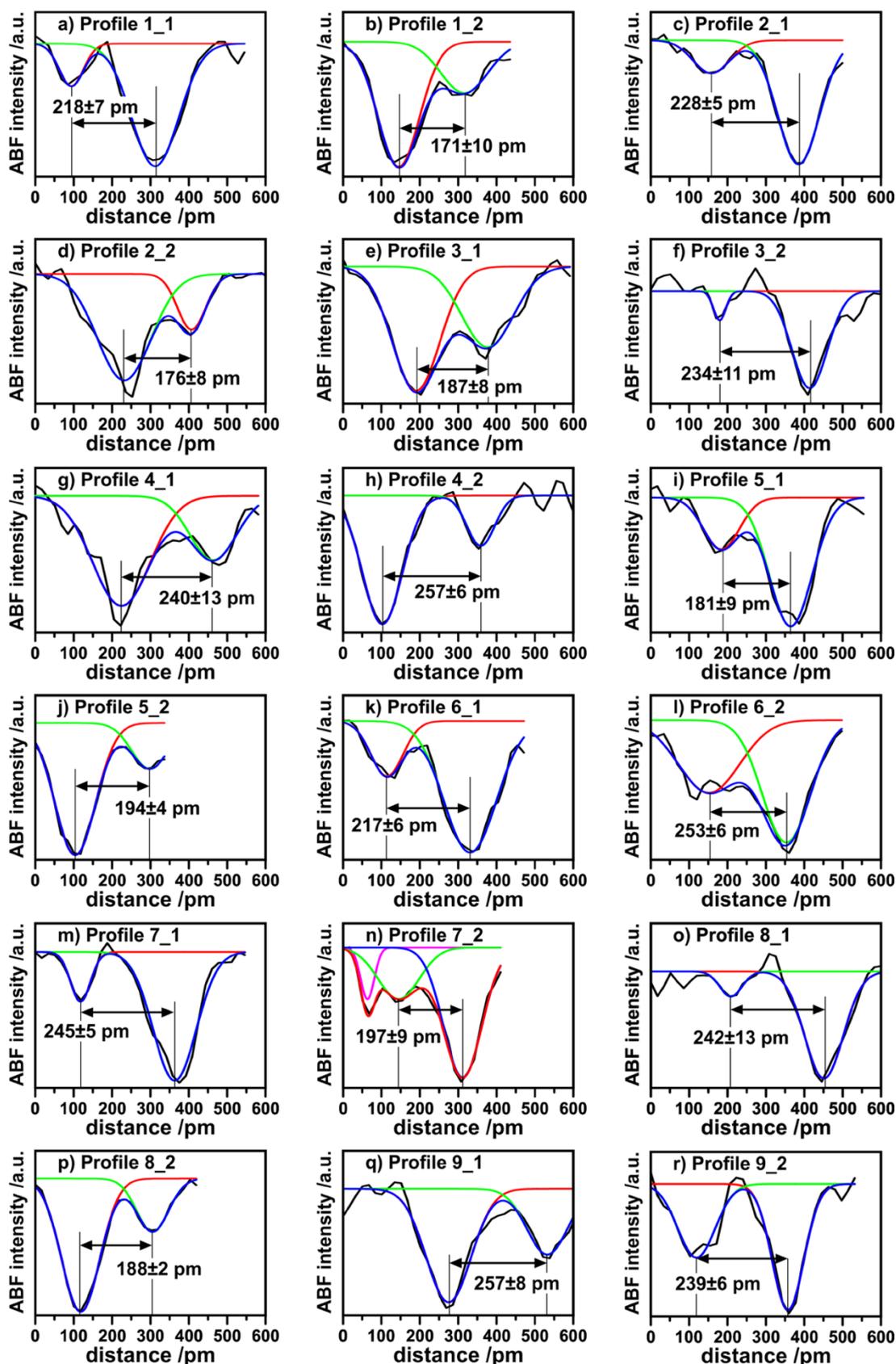


Figure S9. Line profiles and Gaussian fittings of Te-O distances around different S2 sites. The distances within the graphs denote the Te-O distance and the error. The labelling corresponds to the labelling and positions presented in Figure 3D.