Supplementary Materials: Structure and Anharmonicity of α- and β-Sb_2O_3 at Low Temperature

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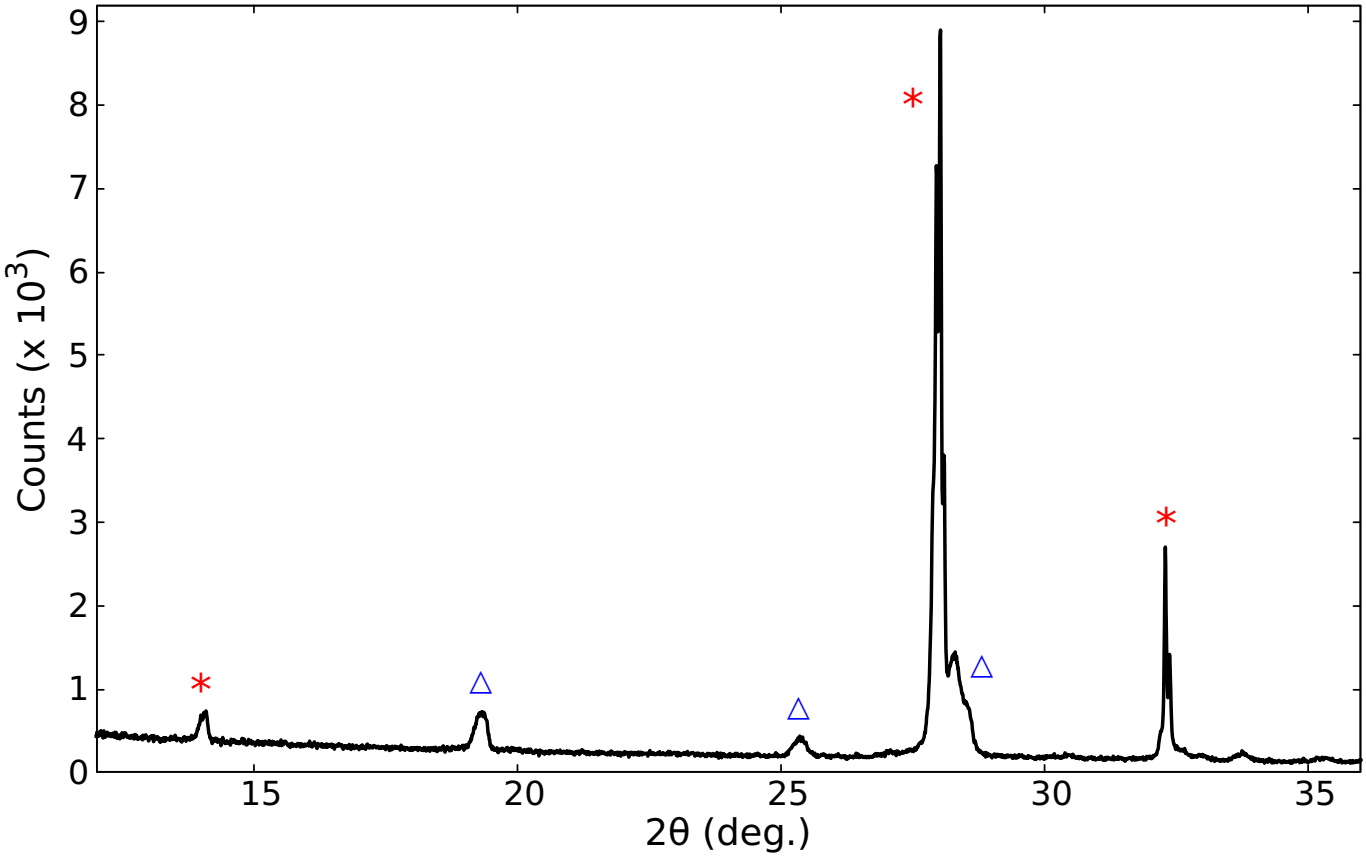

Figure S1. Powder x-ray diffraction pattern of commercial Sb_2O_3 powder. The powder contains a mixture of α and β, indicated by red asterisks and blue triangles, respectively. Phase mixture can differ between batches.

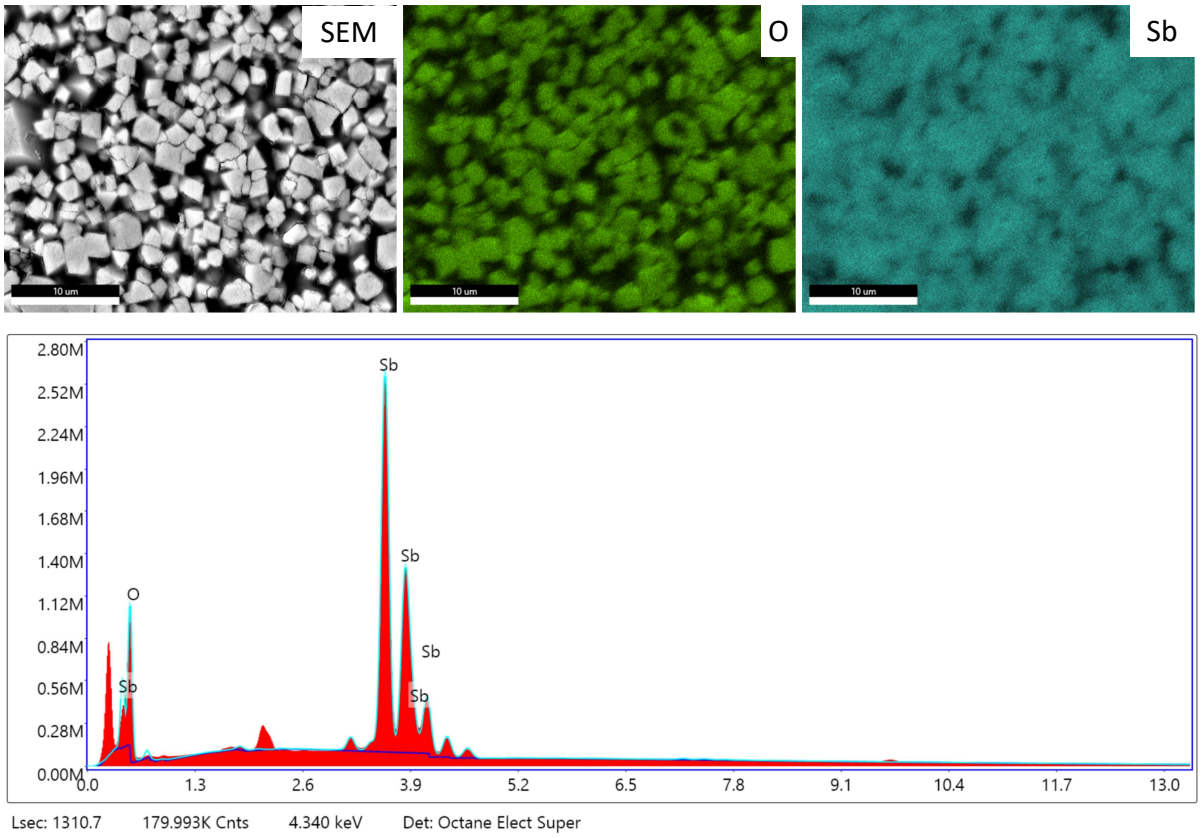

Figure S2. SEM images of α-Sb_2O_3 with EDS analysis for both O and Sb atoms.

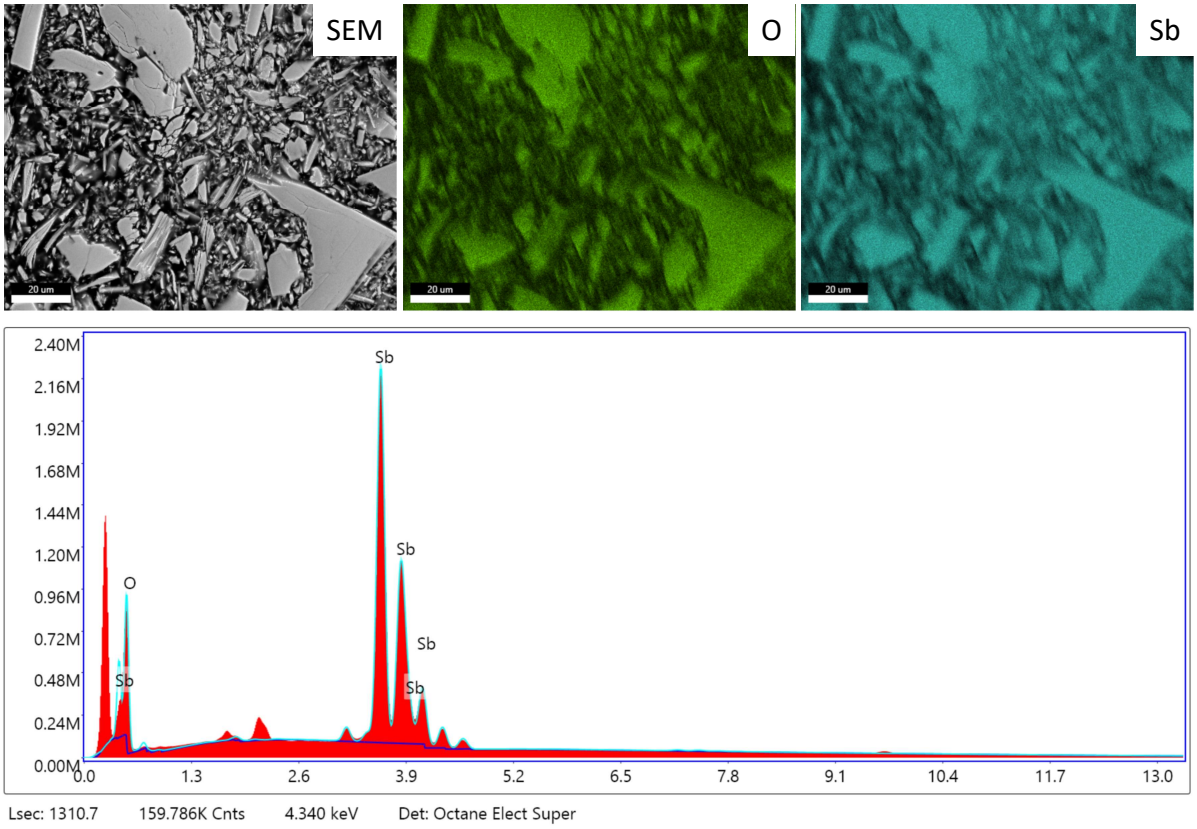

Figure S3. SEM images of β-Sb_2O_3 with EDS analysis for both O and Sb atoms.

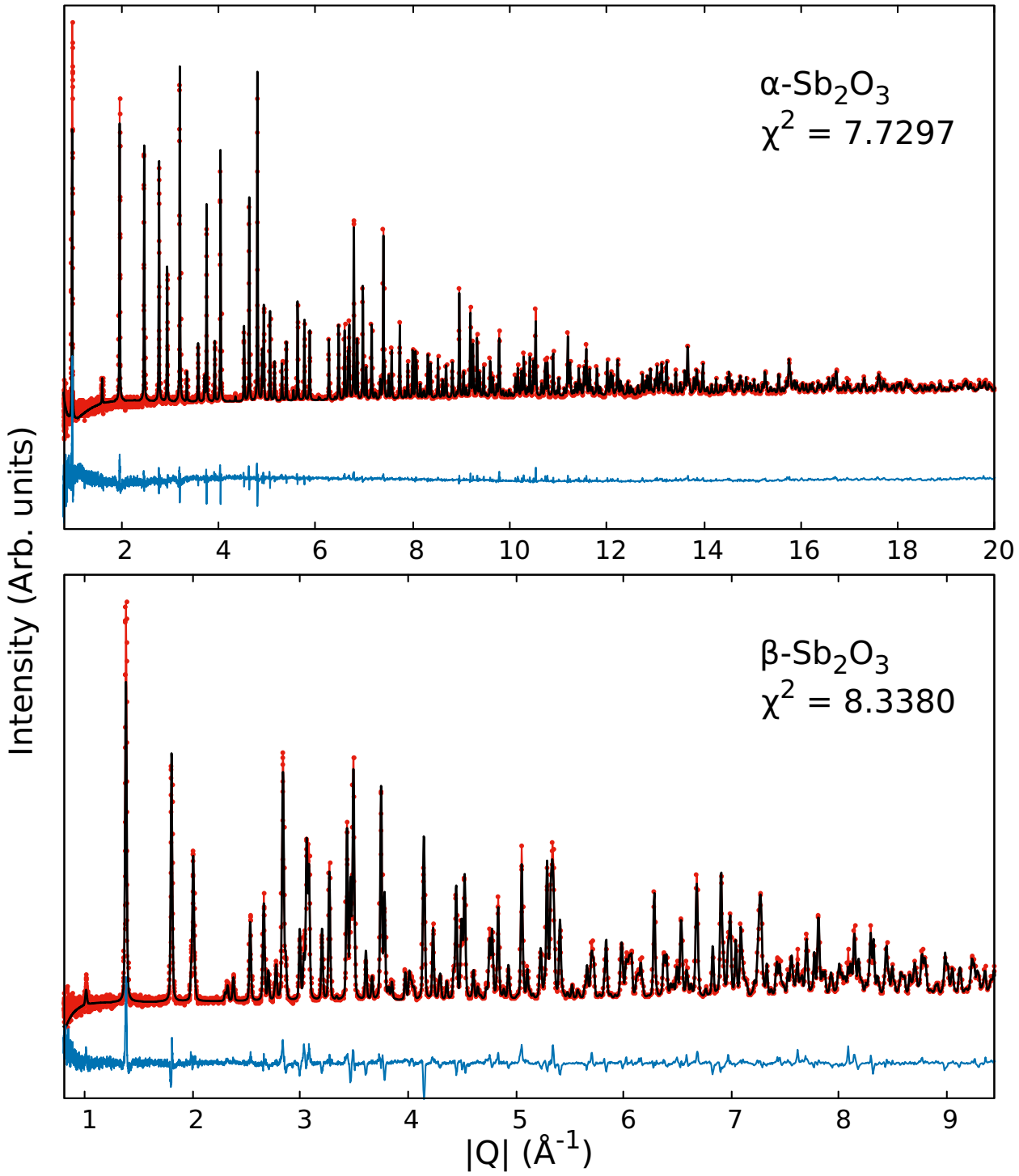

Figure S4. (Red points) Powder neutron diffractograms in q-space of (Top) α- and (Bottom) β-Sb_2O_3 and (black curves) Rietveld fit at 20 K. Blue curves are fitting residuals.

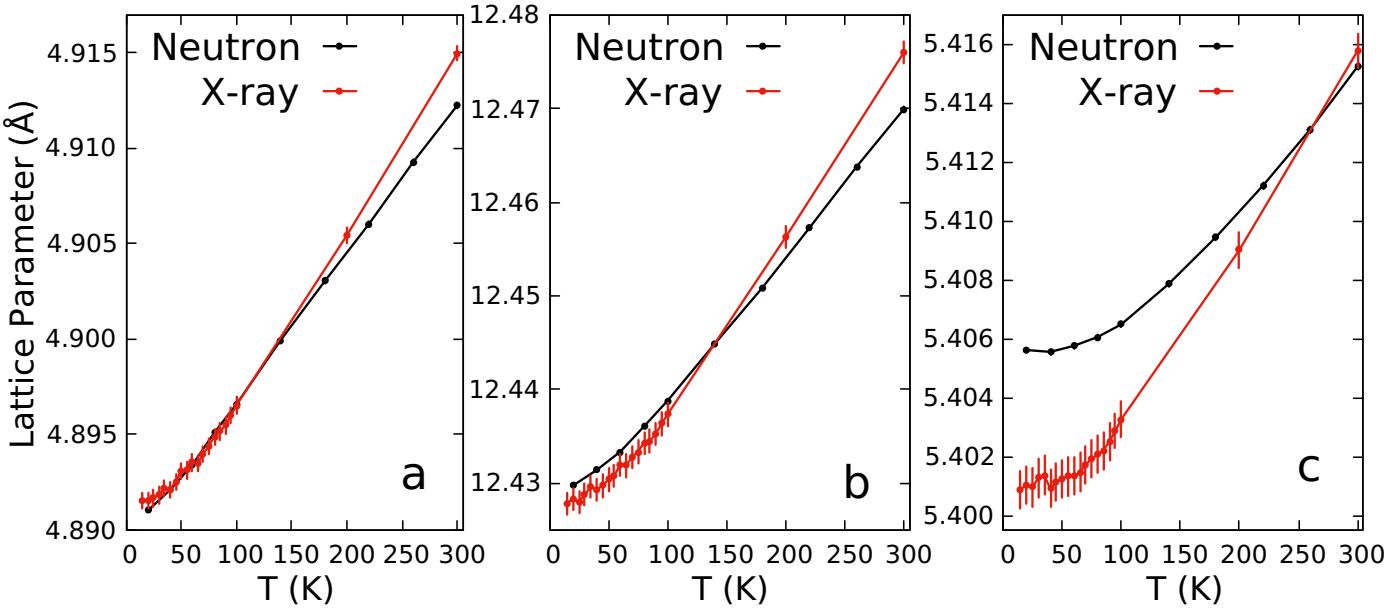

Figure S5. Temperature-dependent lattice constants of β-Sb_2O_3 from both powder neutron diffraction and powder x-ray diffraction. Lattice parameters *a*, *b*, and *c* are labeled accordingly. When not visible, error bars are equivalent to point size.

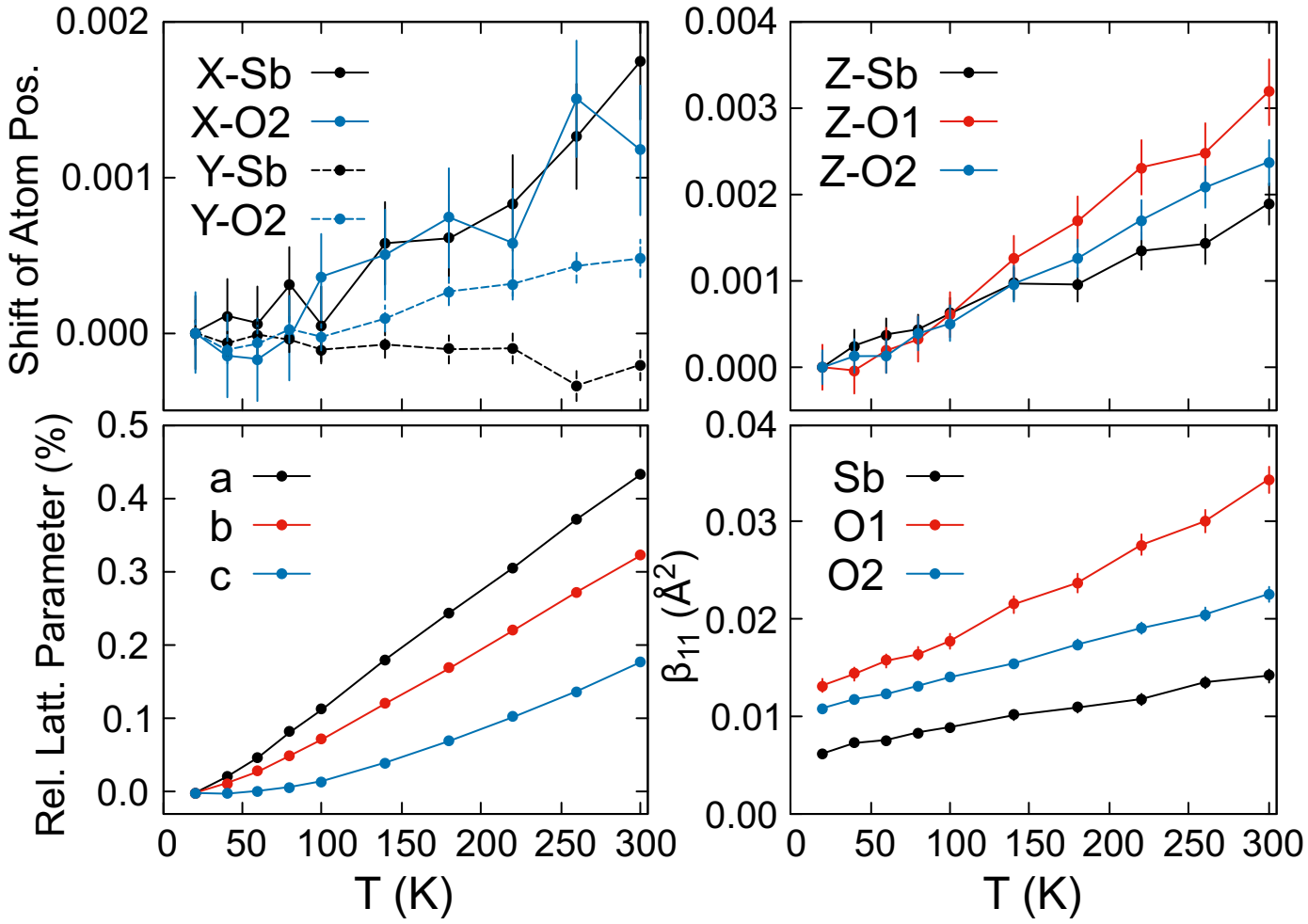

Figure S6. Temperature-dependent β-Sb_2O_3 Rietveld refinement parameters using anisotropic ADPs. (Top) Relative shift of atomic X, Y (Top-Left), and Z (Top-Right) coordinates for Sb and O atoms in fractional coordinates of the corresponding axis from 20 K. Values of X, Y, and Z for each atom at 20 K are given in Supplementary Table 1 below. (Bottom-Left) Relative lattice parameters given as a % difference from 20 K [a - 4.89103(7), b - 12.4297(2), c - 5.40561(7)]. (Bottom-Right) Anisotropic β_{11} ADP values for all atoms. Unless noted, error bars are approximately the size of the data points.

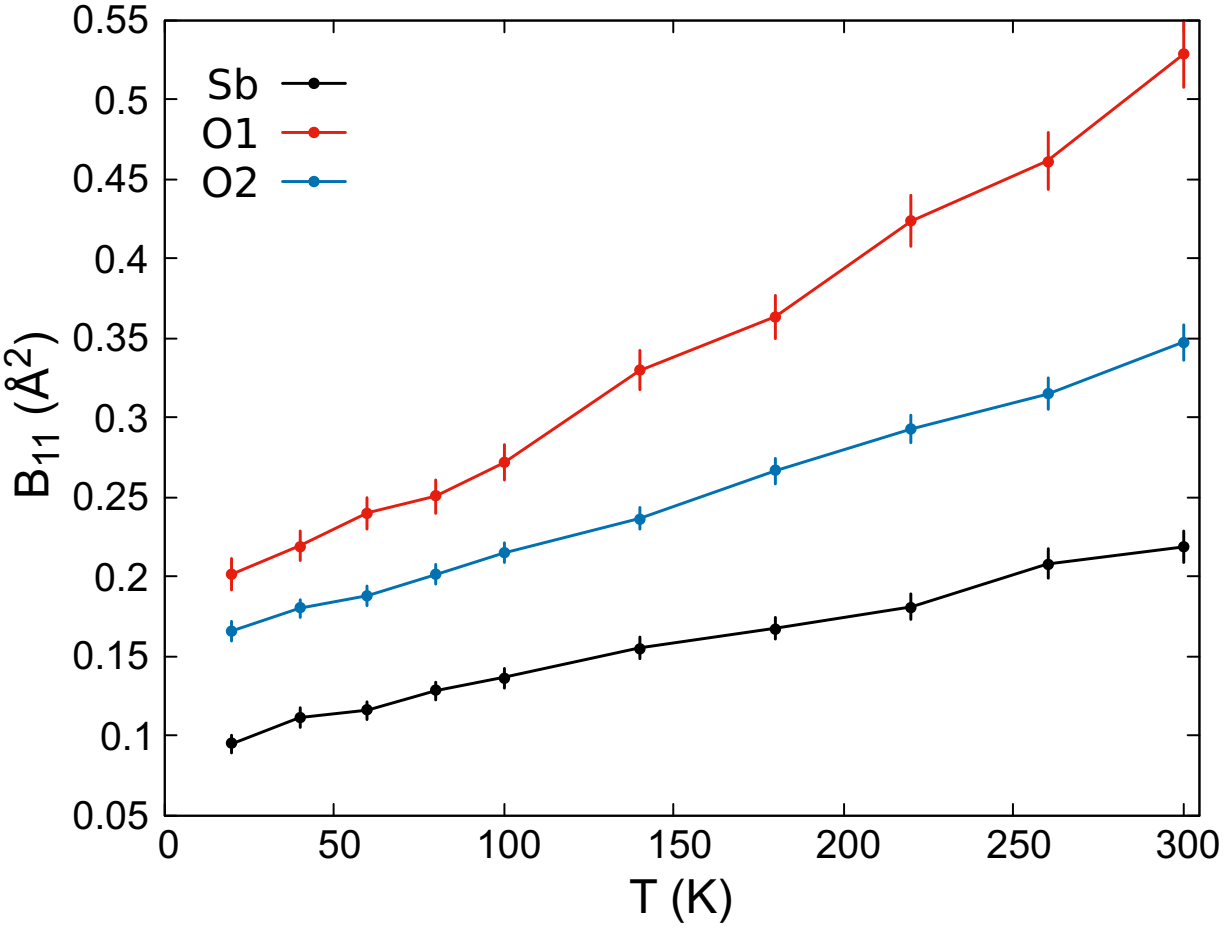

Figure S7. Temperature-dependent B_{11} parameters of β-Sb_2O_3 converted from the β_{11} values in Supplementary Fig. 2 as $B_{11} = \beta_{11} \times 4/a^{*2}$, where a^* is the reciprocal lattice vector. B_{11} is presented here for better comparison with the B_{iso} values presented in the main text.

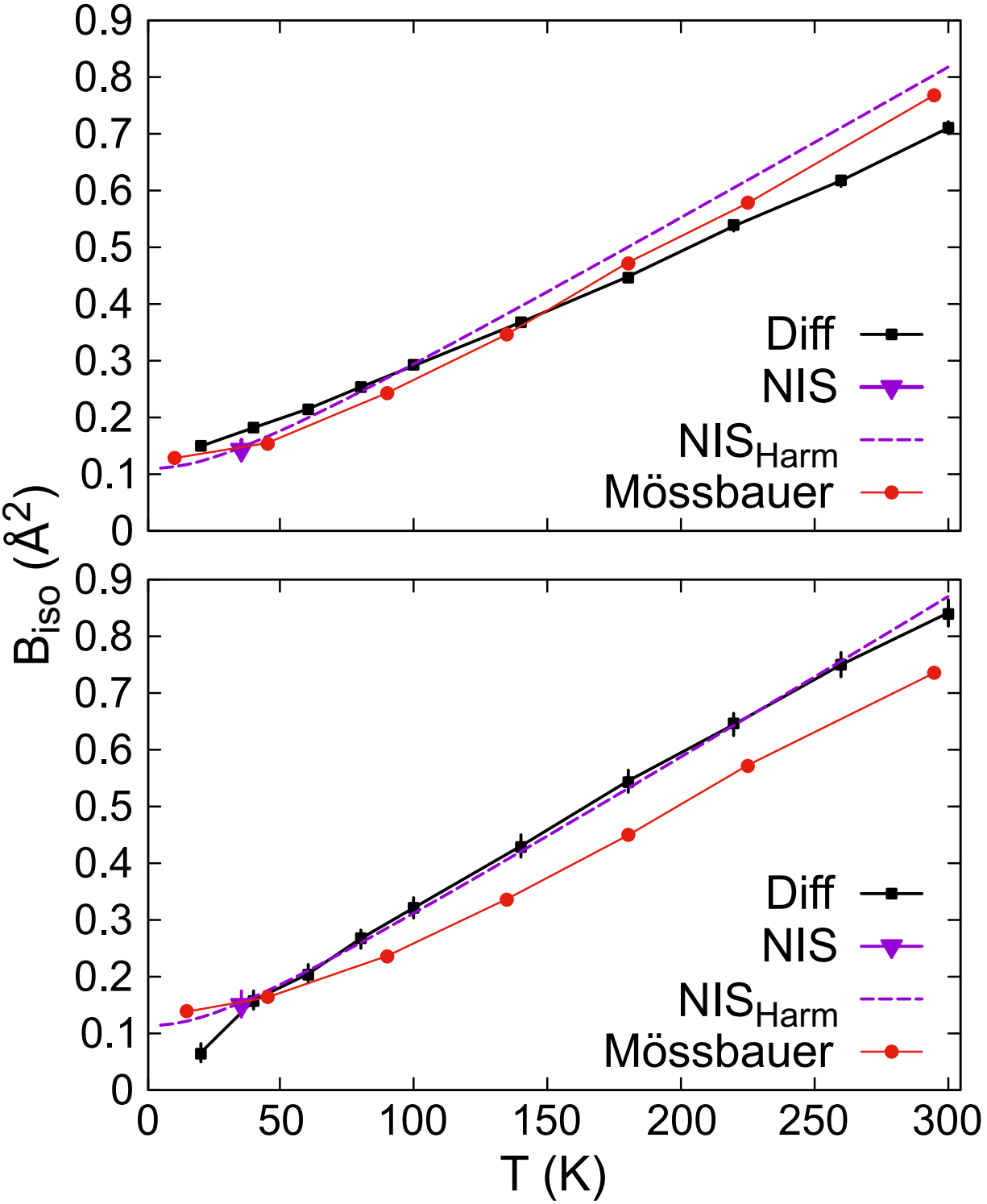

Figure S8. Temperature-dependent isotropic ADP values in α- (Top) and β-Sb_2O_3 (Bottom) compared with displacement parameters extracted from NIS and Mössbauer spectroscopy (Ref. 29 in the main text).

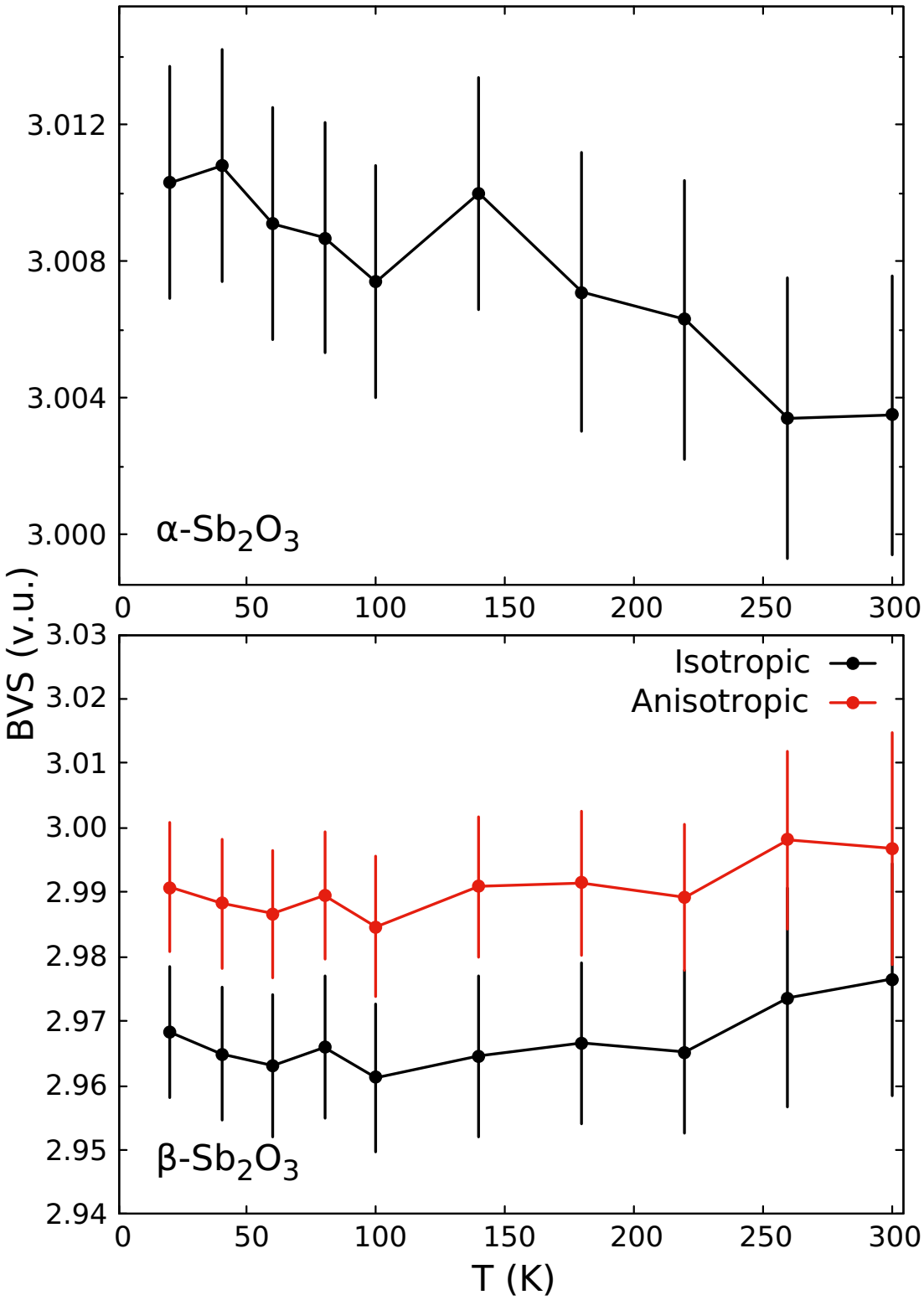

Figure S9. Comparison of temperature-dependent bond valence sum in α- (Top) and β-Sb_2O_3 (Bottom). The β phase values are from fits with isotropic (black) and anisotropic (red) ADPs.

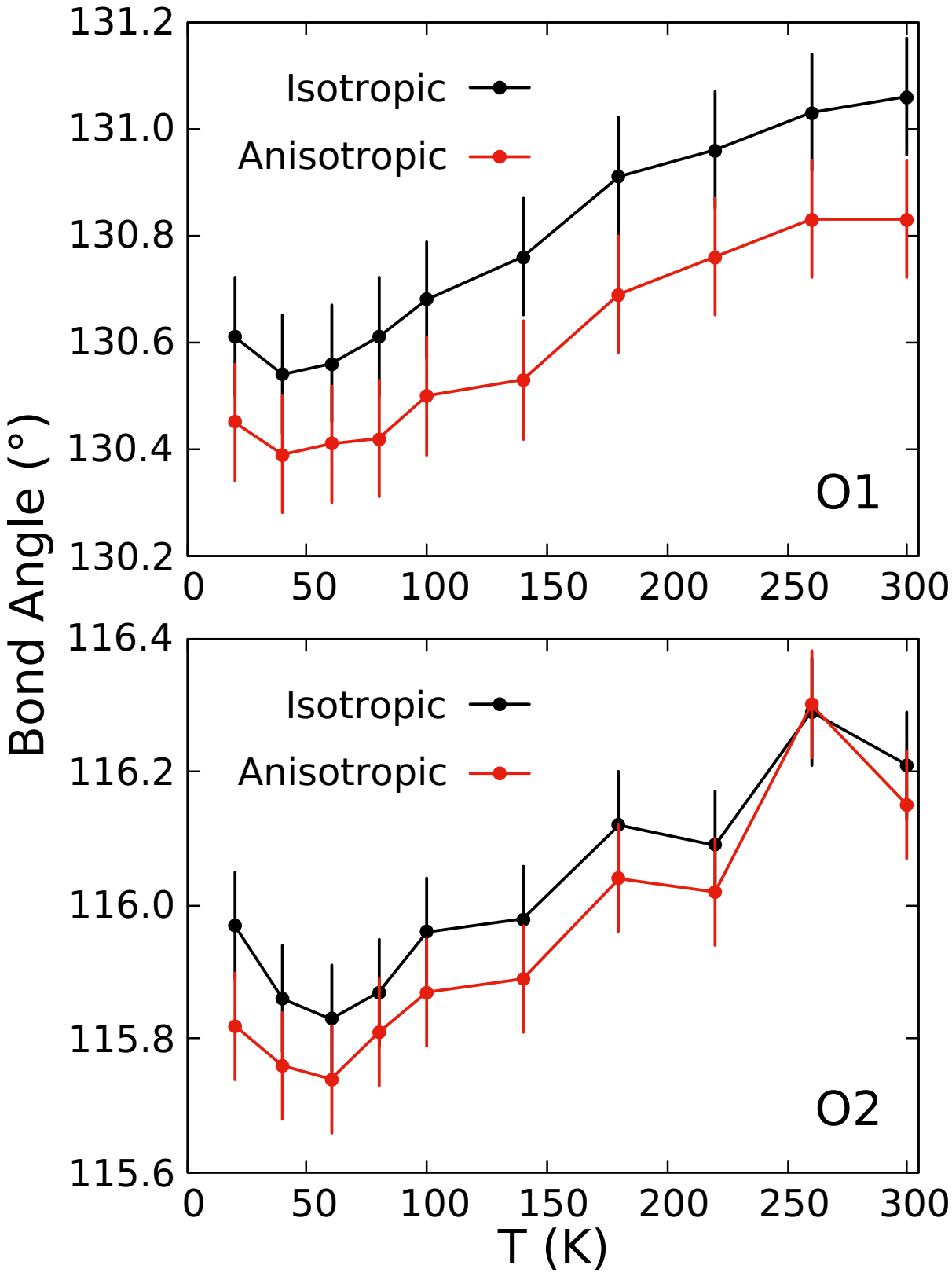

Figure S10. Comparison of temperature-dependent bond angles in β-Sb_2O_3 for both oxygen atoms O1 (Top) and O2 (Bottom) refined with either isotropic (black) or anisotropic (red) ADPs.