

Electronic Supplementary Information for “Temperature-induced abrupt volume inflation in the mixed-valence ternary Zintl phase $\text{Yb}_8\text{Ge}_3\text{Sb}_5$ ”

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Table 1S. Refined structural parameters for $\text{Yb}_8\text{Ge}_3\text{Sb}_5$ obtained from the Rietveld refinement of the synchrotron X-ray diffraction data at 5 K.

Structural Parameters						
	Site	x/a	y/b	z/c	N	$B (\text{\AA}^2)$
Yb(1)	$8i$	0.1836(1)	0	0	0.99(3)	1.57(5)
Yb(2)	$8h$	0.1282(1)	0.1282(1)	$\frac{1}{2}$	0.99(3)	3.14(8)
Yb(3)	$16k$	0.3548(1)	0.1452(1)	$\frac{1}{4}$	1.01(2)	1.30(3)
Sb(1)	$8h$	0.1987(1)	0.1987(1)	0	1.07(5)	3.60(10)
Sb(2)	$8j$	0.2713(2)	0	$\frac{1}{2}$	1.07(5)	2.12(8)
Sb(3)	$4e$	0	0	-0.2442(1)	0.96(6)	3.21(9)
Ge(1)	$8i$	0.3841(3)	0	0	0.98(9)	1.36(9)
Ge(2)	$4d$	$\frac{1}{2}$	0	$\frac{1}{4}$	0.95(9)	1.46(9)

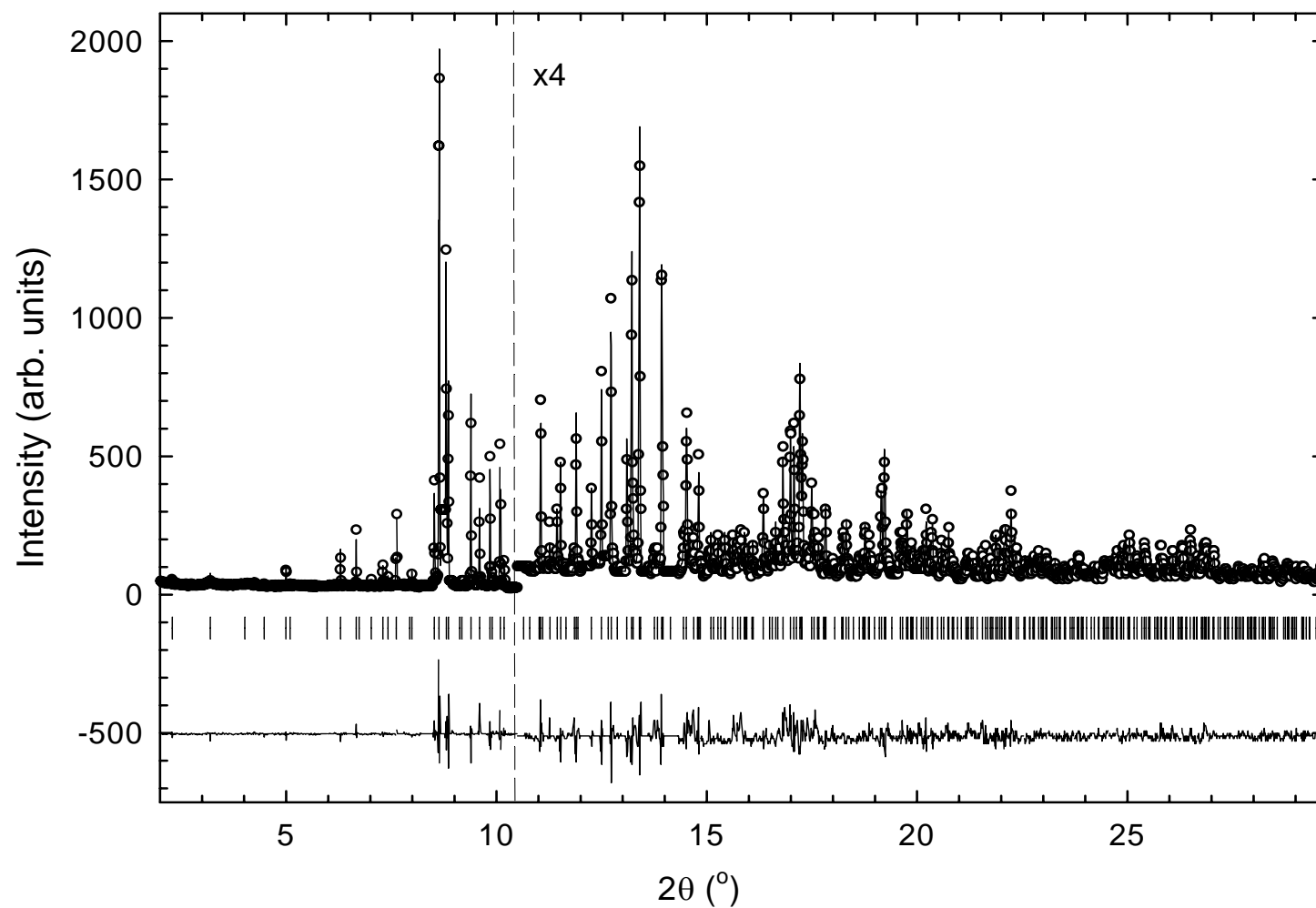


Figure 1S. Final observed (\circ) and calculated (solid line) synchrotron X-ray powder ($\lambda = 0.42976 \text{ \AA}$) diffraction profiles for $\text{Yb}_8\text{Ge}_3\text{Sb}_5$ at 5 K. The lower solid line shows the difference profile and the tick marks show the reflection positions. Some impurity peaks were excluded from the refinement.

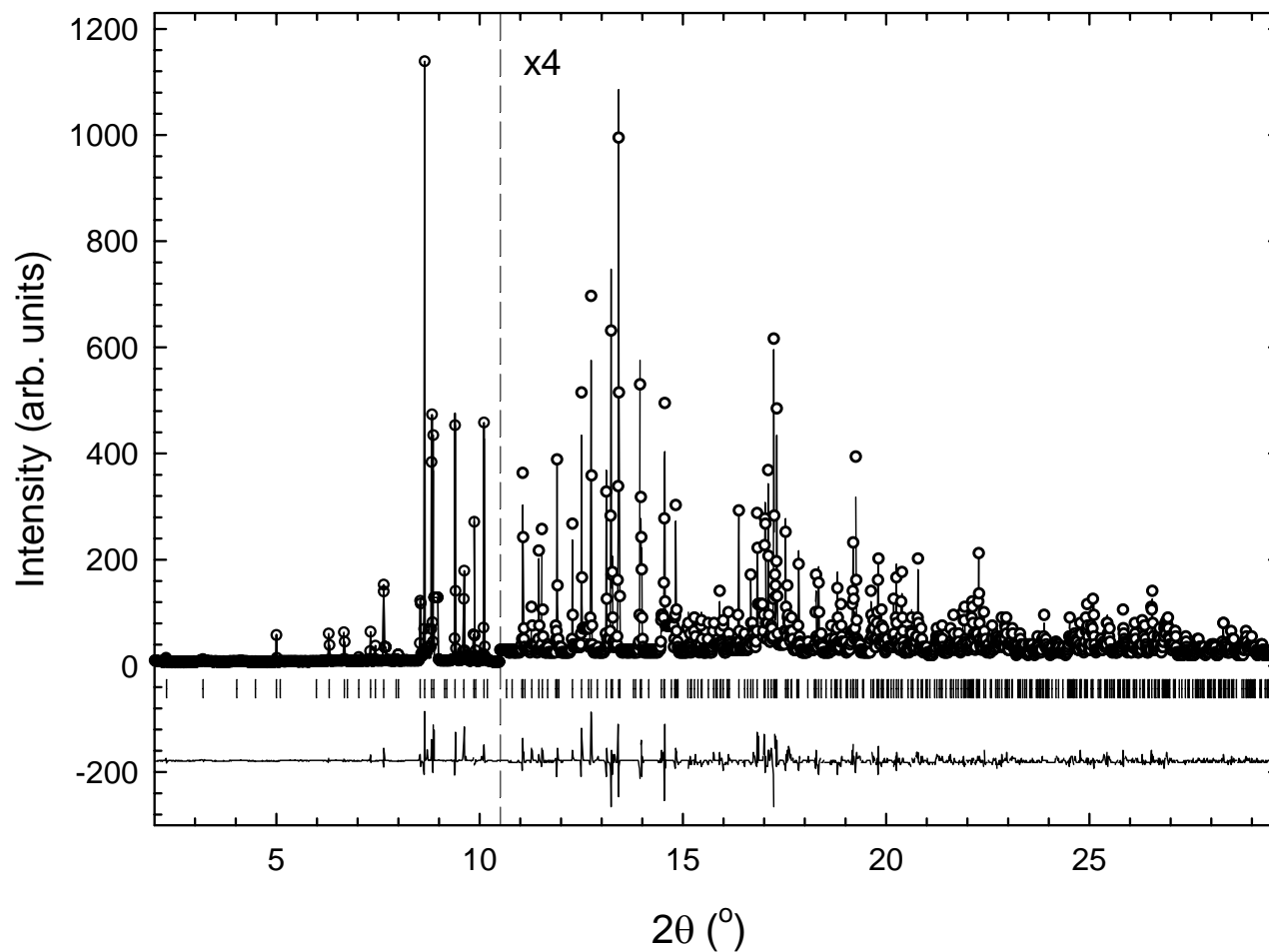


Figure 2S. Final observed (\circ) and calculated (solid line) synchrotron X-ray powder ($\lambda = 0.42976 \text{ \AA}$) diffraction profiles for $\text{Yb}_8\text{Ge}_3\text{Sb}_5$ at 300 K. The lower solid line shows the difference profile and the tick marks show the reflection positions. Some impurity peaks were excluded from the refinement

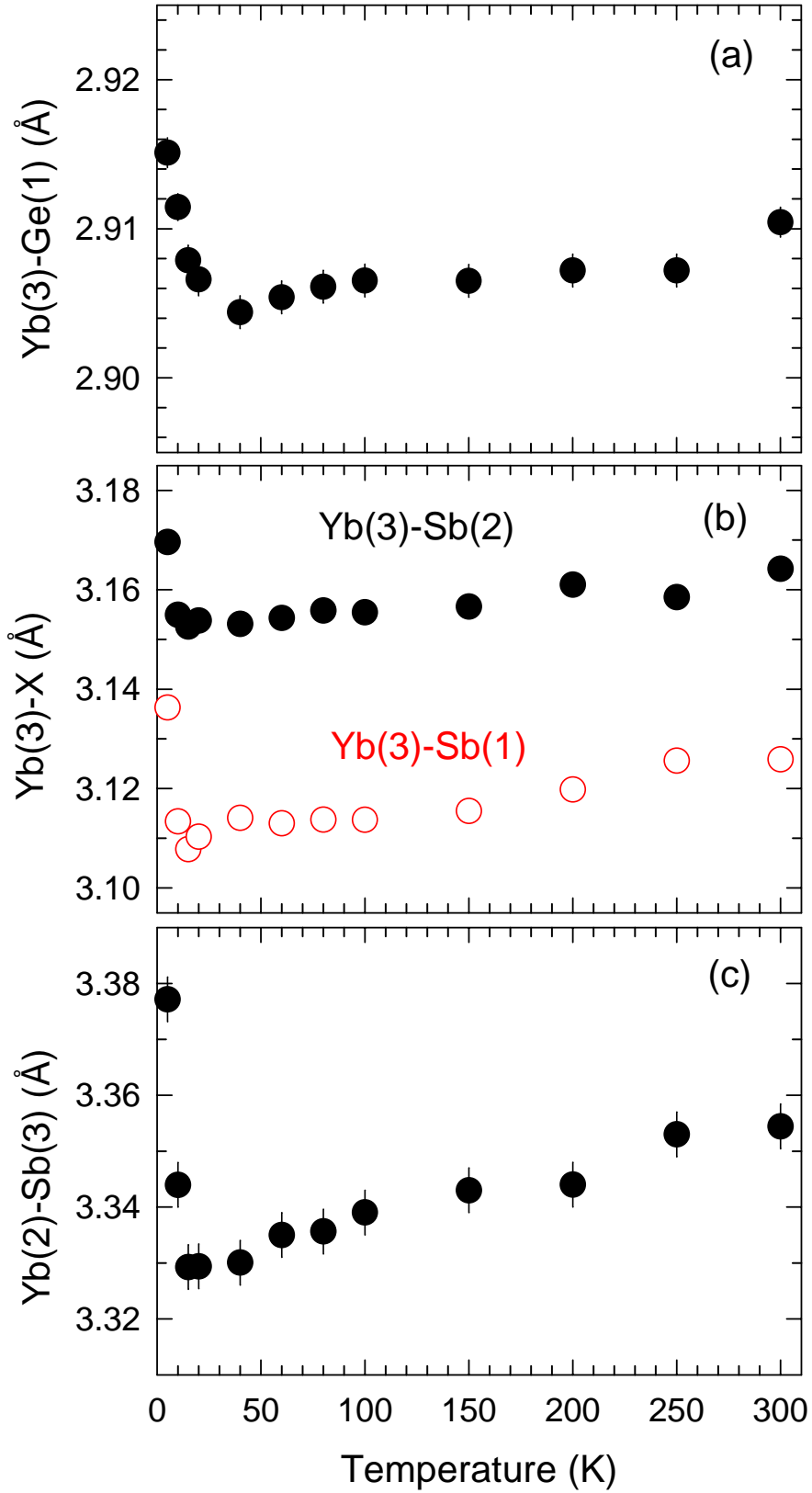


Figure 3S. Temperature dependence of selected interatomic distances in $\text{Yb}_8\text{Ge}_3\text{Sb}_5$ as obtained from Rietveld refinements of the synchrotron X-ray powder diffraction profiles. (a) Yb(3)-Ge(1). (b) Yb(3)-Sb(1) and Yb(3)-Sb(2). (c) Yb(2)-Sb(3).