Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for "Is $RuAs_2$ a candidate for high temperature thermoelectric applications?"

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S1. X-ray diffraction data and refinements

Powder X-ray diffraction (PXRD) has been used extensively throughout this study, to the extent that some of the finer details are out of the scope of the main article are covered here.

In order to measure PXRD data for the pressed pellet at SPring-8 some powder was filed off the edge of the pellet. PXRD data from the in-house Rigaku Smatlab and SPring-8 is compared in Figure S1 to ensure that the PXRD data from the powder filed off the pellet are representative of the pellet itself. As expected the PXRD patterns from the as prepared powder are practically identical, with the exception of the background from the silica capillary. The two patterns from the pellet from SPring-8 and the Rigaku are also nearly identical; therefore, all SPring-8 data is concluded to be representative of the bulk pellet. There are a few impurity peaks, which all have a very low intensity; thus it is assumed that any phases creating these peaks have a negligible contribution to all property measurements. As of writing no phase fitting any of these peaks have been identified.

During the laser flash analysis (LFA) some surface reaction was observed. This is only a surface reaction, as the new peaks in the diffraction pattern are removed upon polishing of the pellet (see Figure S2). Additionally, the measured thermal diffusivity is the same on heating and cooling, which also shows that this was only a surface reaction. This reaction is most likely a reaction with the graphite spray, as no phase changes were observed between any other property measurements and the same change was observed on both sides of the pellet. No phases fitting the new peaks have been identified and work on this is ongoing.

All PXRD patterns collected at SPring-8 are shown in Figure S3 for the as prepared powder and in Figure S4 for the densified pellet, while refinement evaluation parameters and refined arsenic occupancy is summarized in the tables next to the figures. Some peaks appear at 1000 K for the pellet sample; this is, however, believed to be related to sample preparation rather than any transformation related to $RuAs_2$ itself, as no such transformation has been observed at any point.

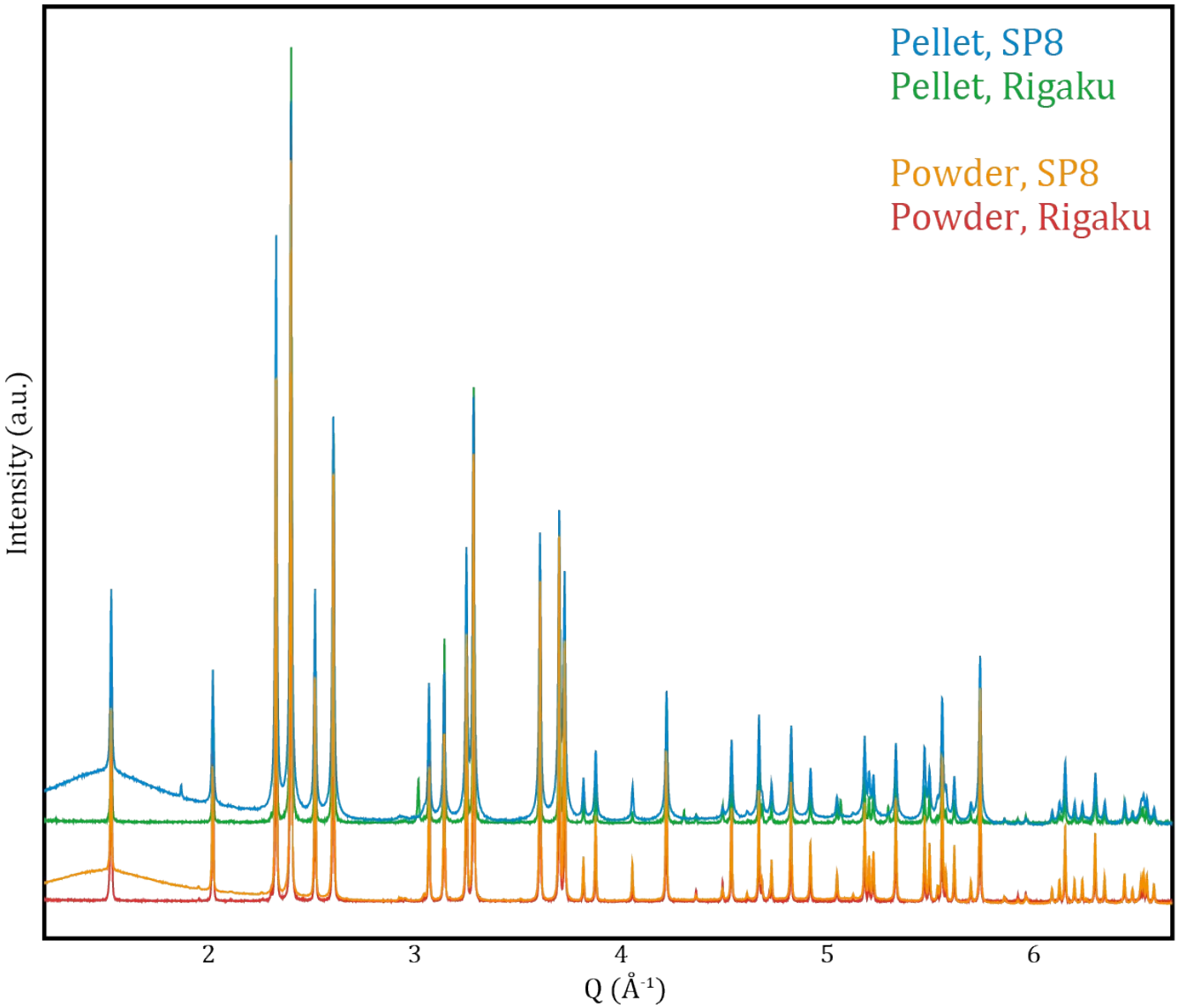

Figure S1. Comparison of PXRD patterns from SPring-8 and the in-house Riguka SmartLab in Q space

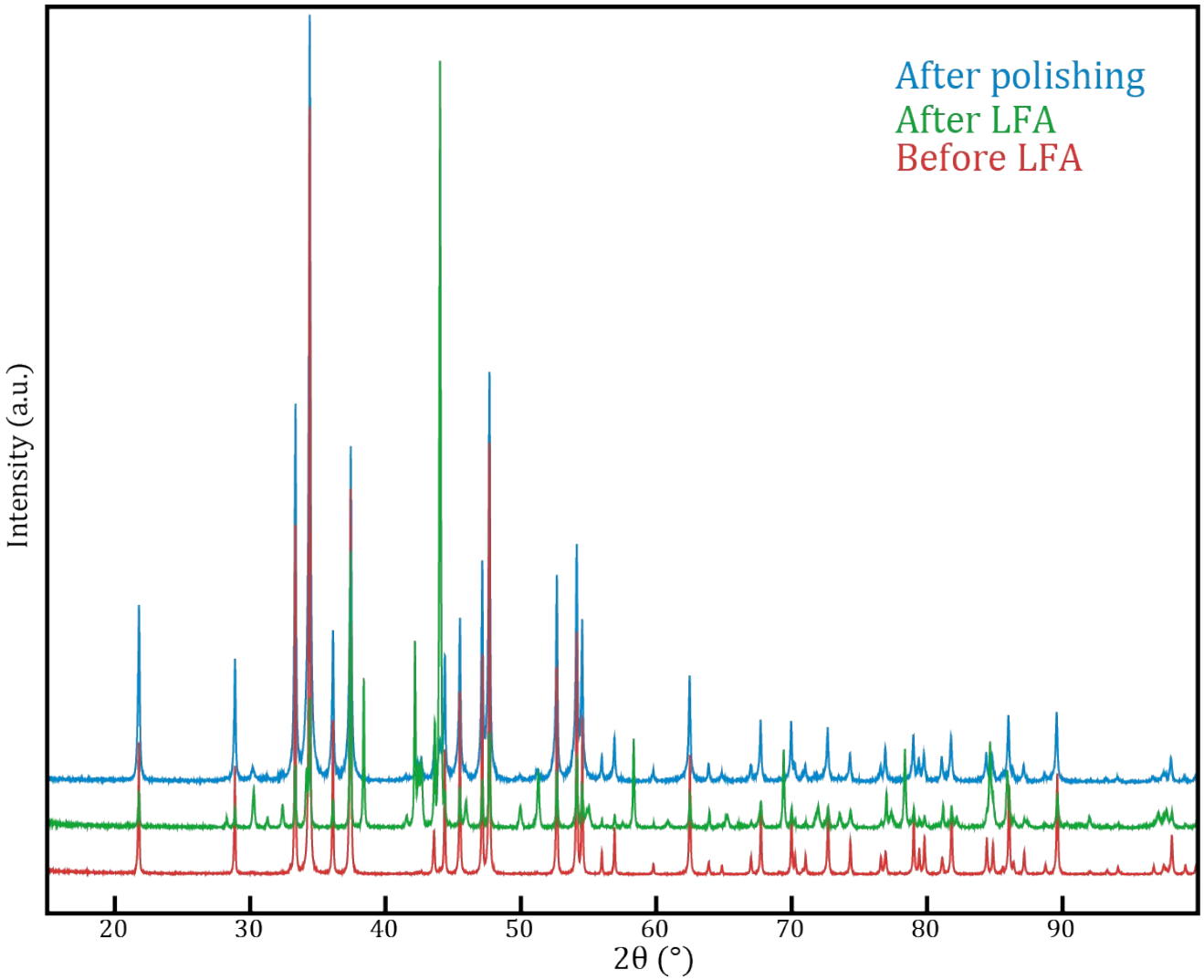

Figure S2. Comparison of PXRD patterns before and after LFA measurement

As prepared powder

Temperatur [K]	Occupancy (As)	R_F	R_{wp}	X^2
300	0.5024(9)	2.29	8.12	2.29
400	0.5023(8)	3.41	8.12	2.24
500	0.5028(9)	2.91	8.23	2.29
600	0.5030(9)	3.05	8.15	2.21
700	0.5036(8)	3.06	8.13	2.16
800	0.5035(9)	2.89	8.39	2.29
900	0.5017(9)	3.19	8.54	2.33
1000	0.5019(9)	3.66	8.93	2.52

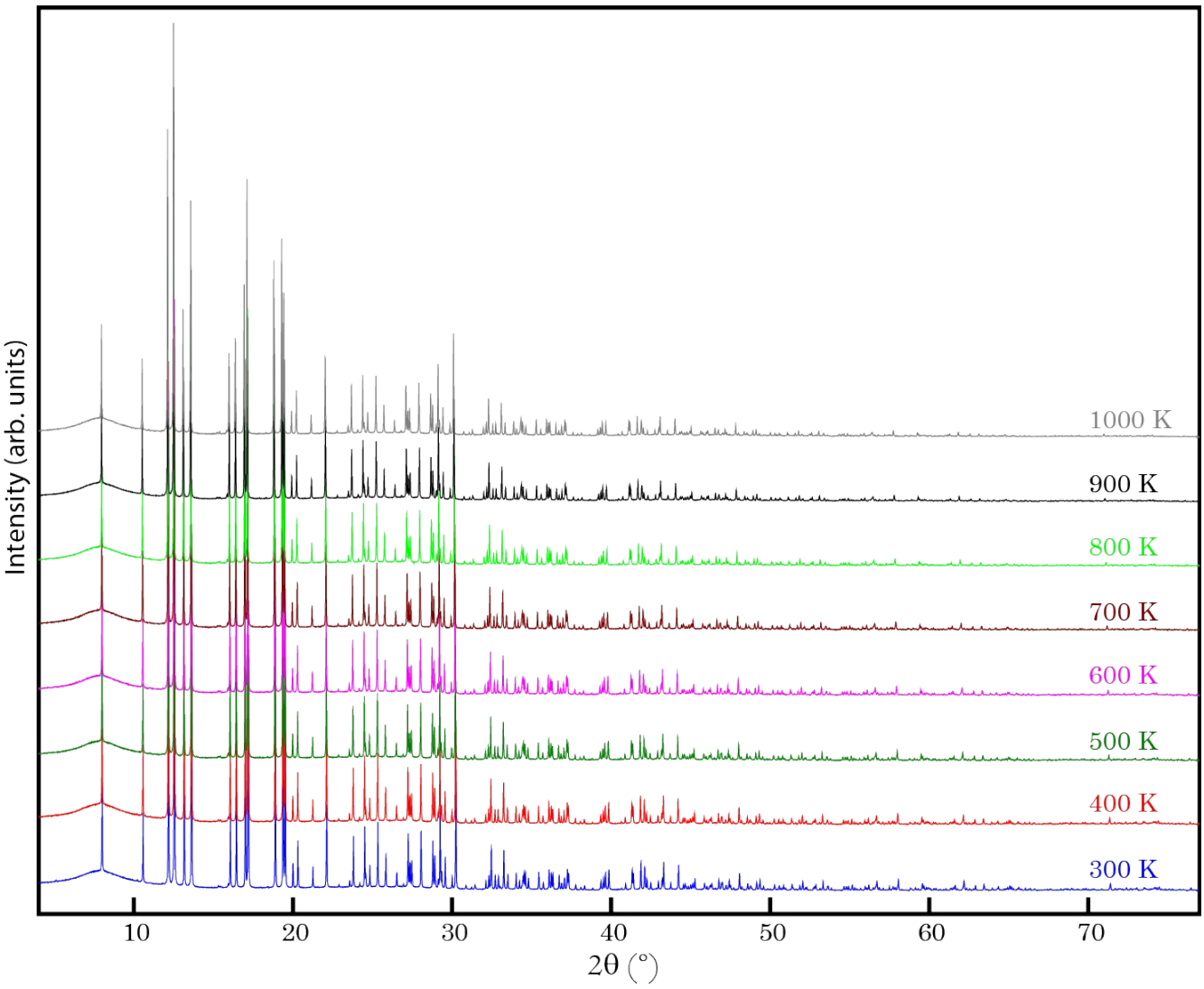

Figure S3. Comparison of the collected PXRD patterns from the as prepared $RuAs_2$ powder

Pressed pellet

Temperatur [K]	Occupancy (As)	R_F	R_{wp}	X^2
300	0.500(1)	1.94	10.7	2.70
400	0.500(1)	2.09	10.9	2.78
500	0.501(1)	1.96	10.8	2.70
600	0.500(1)	2.83	10.8	2.72
700	0.500(1)	2.80	10.9	2.80
800	0.502(1)	2.58	10.6	2.77
900	0.503(1)	2.88	9.76	2.57
1000	0.504(2)	3.01	10.1	2.97

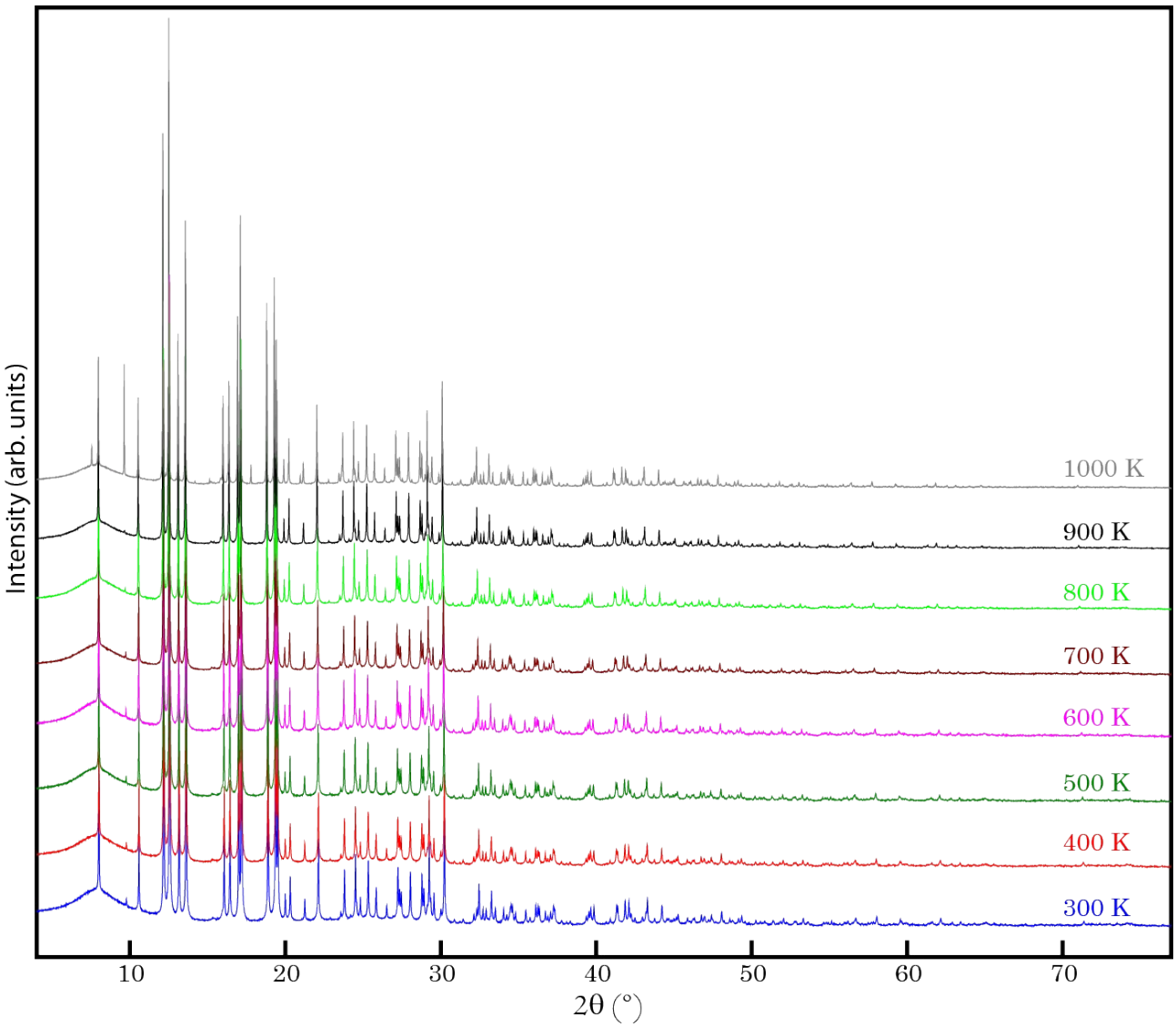

Figure S4. Comparison of the collected PXRD patterns from the pressed $RuAs_2$ pellet

S2. Debye fit

The fit was done using MATLAB and the fitted points and line is shown below. The main manuscript uses B_{iso}, which here has been converted using $U_{iso} = \frac{B_{iso}}{8\pi^2}$.

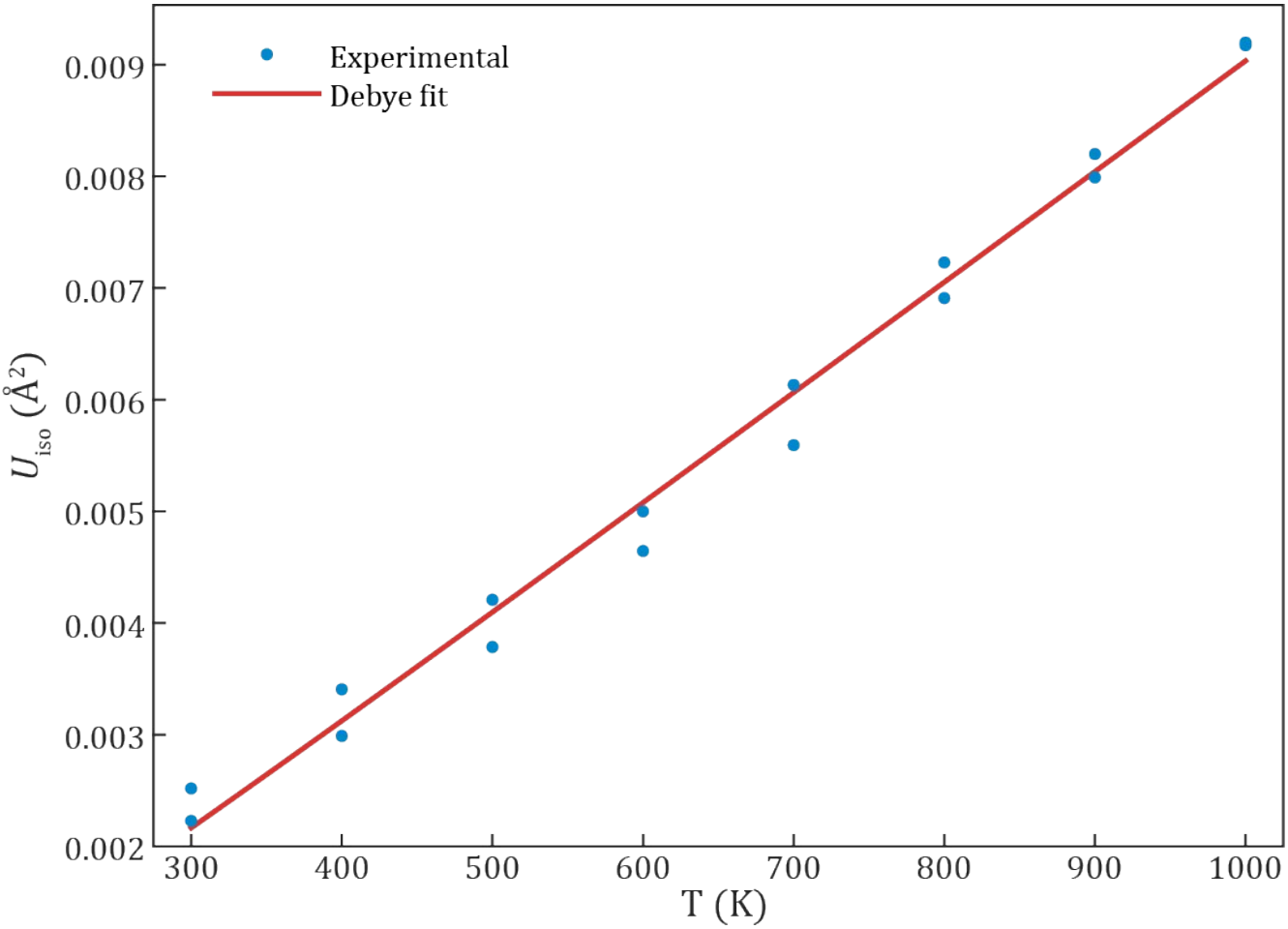

Figure S5. Debye fit of the isotropic thermal displacement parameters