Supplemental Materials for Temperature dependence of the Raman spectrum of orthorhombic Bi_2Se_3

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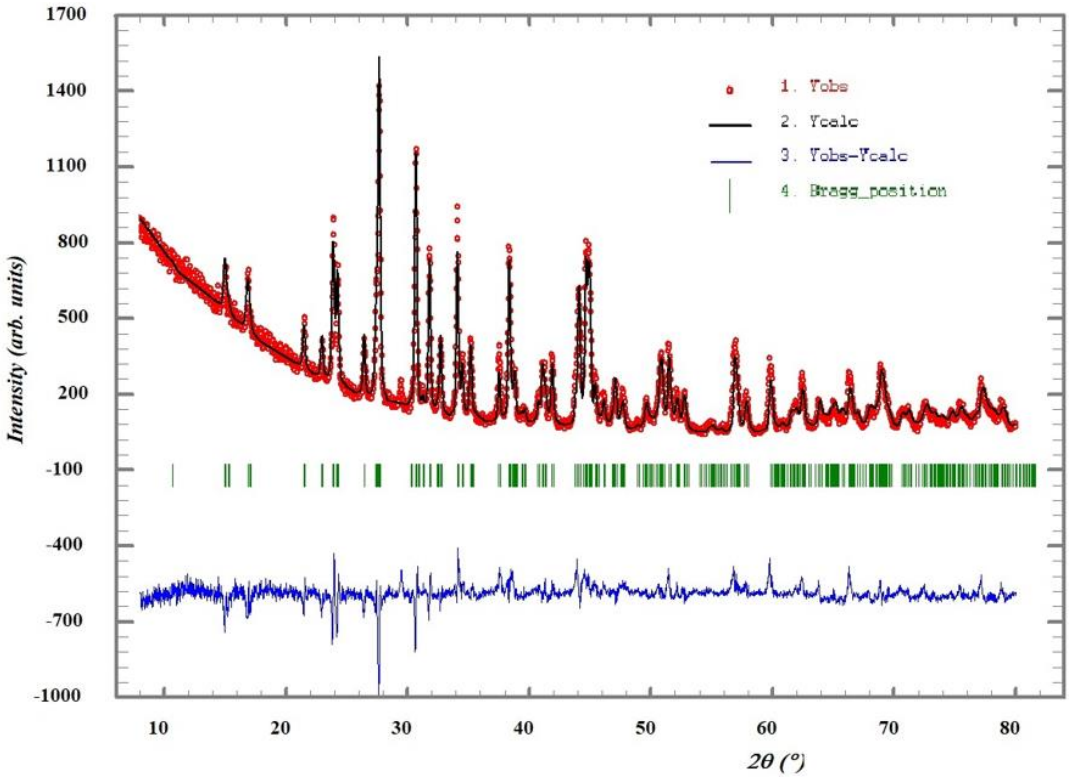
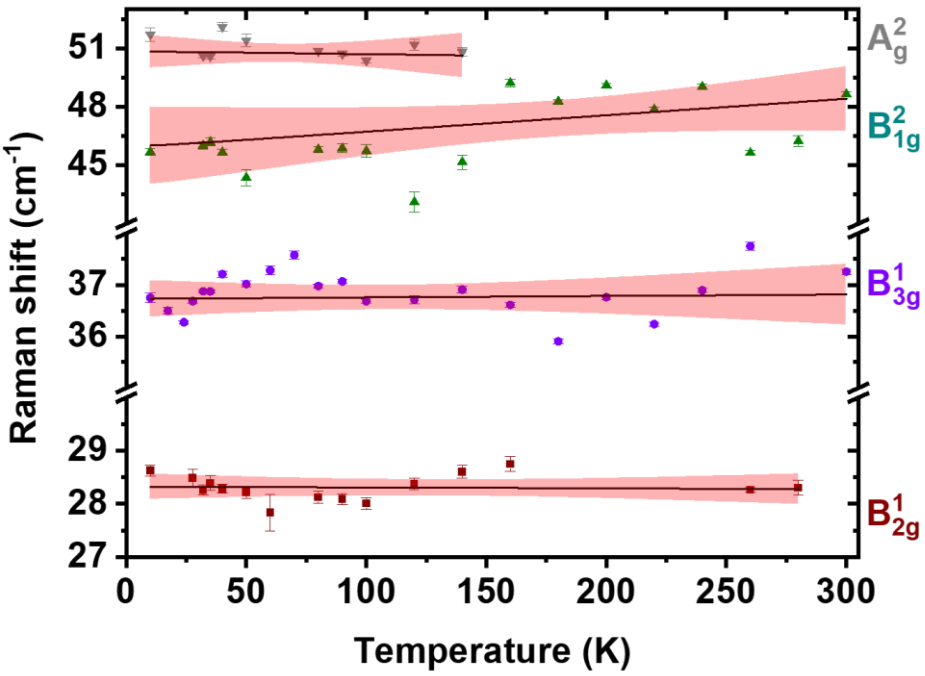
Figure SM.1 shows the x-ray diffraction pattern (symbols) of orthorhombic Pnma Bi2Se3 with the corresponding fit (red line) from the Rietveld analysis, displaying the 2θ value of the Bragg peaks (green).

Figures SM.2, SM.3, and SM.4 display additional information on the temperature dependence of Raman phonon frequencies for the lower frequency modes. The lines display fits with Eq. 1 (Klemens' Ansatz) of the main text. The red bands show the 99% confidence intervals [1]. Unfortunately the scattering in the linewidths prevented to do an analysis of the anharmonic effects similar to that reported in the main text for other Raman modes.

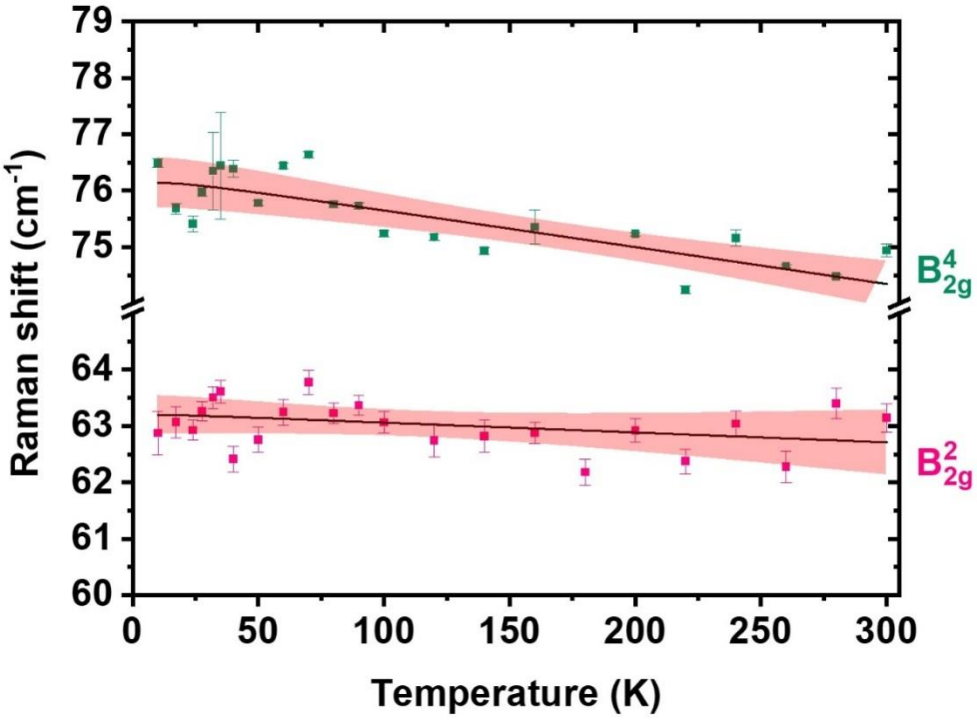


SM. 1 X-ray diffraction pattern of the sample investigated, together with the result of a Rietveld fit (black line), displaying the angular position of the Bragg peaks (green, vertical lines) and the fit error (blue).

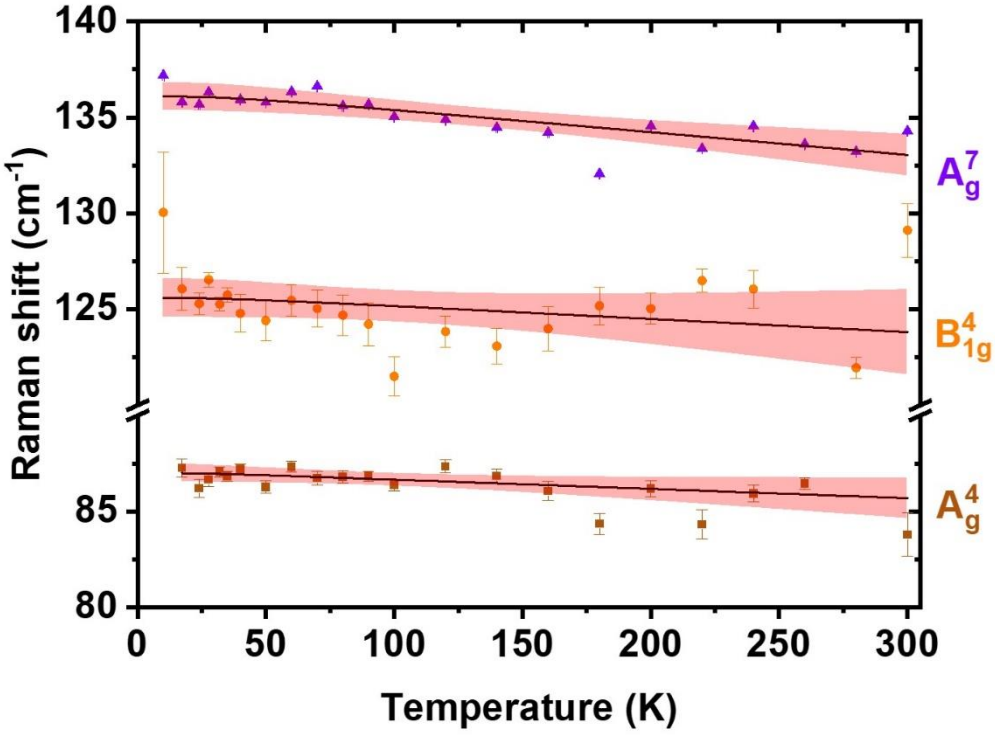


SM. 2 Temperature dependence of the phonon frequency for the Raman modes observed between 20 and 55 cm^{-1}, from 10 to 300 K. The solid lines display fits with a

two oscillator model according to Eq. 1 in the main text (Klemens' Ansatz),and the red bands show the 99% confidence interval.



SM. 3 Temperature dependence of the phonon frequency for the Raman modes observed between 55 and 80 cm^{-1}, from 10 to 300 K. The solid lines display fits with a two oscillator model according to Eq. 1 in the main text (Klemens' Ansatz),and the red bands show the 99% confidence interval.



SM. 4 Temperature dependence of the phonon frequency for the Raman modes observed between 80 and 140 cm^{-1}, from 10 to 300 K. The solid lines display fits with a two oscillator model according to Eq. 1 in the main text (Klemens' Ansatz), and the red bands show the 99% confidence interval.

References:

[1] A. Hazra, *Using the confidence interval confidently*, J. Thorac Dis **9** (10), 4125 (2017).