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# Disorder in layered tellurides Tt1Pn2Te4 (Tt = Ge, Sn, Pb; Pn = As, Sb, Bi)

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The crystal structure of the mineral tetradymite Bi2S2Te has inspired discussions about its details for a long time.[1,2] Variations of this structure led to a large family of chalcogenides composed of slabs with alternating cation and anion layers stacked in rocksalt-type fashion, which show characteristic van der Waals gaps between anion layers.[3] These compounds are of interest not only for their exact crystal structures but also for their thermoelectric properties and their high likelihood of being topologically non-trivial systems insulators.[4,5]
The rhombohedral compounds Tt1Pn2Te4 (*Tt* = Ge, Sn, Pb; *Pn* = As, Sb, Bi) feature septuple layers, in which the multiplicity of Wyckoff positions would allow complete cation ordering, which has been postulated in some cases.[6] However, more detailed studies based on single-crystal diffraction data almost always revealed cation disorder.[7] In the case of small scattering contrast, resonant X-ray diffraction corroborated the disorder.[8] Here we present a systematic investigation of these compounds with high-quality single crystal diffraction data collected with synchrotron radiation in order to establish exact site occupancy factors. As diffraction data cannot exclude short-range ordering, Z-contrast imaging by STEM-HAADF was used as a local probe, complemented by EDX spectroscopy with atomic resolution. All of these data confirm the cation disorder and could not even demonstrate short-range ordering.
The disorder observed might be explained as an interplay between charge balance at the vdW-gap and octahedron size mismatch in the layer.

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