**Synthesis of silicon monotelluride (CH5985)**

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Against all expectations based on theoretical studies in the literature, in our recent exploration of the high-pressure high-temperature Si-Te phase diagram using the multi-anvil at ID06-LVP, we have found out that no silicon monotelluride SiTe is formed from various mixtures of elemental Si and Te up to about 10 GPa [**1**]. Only the $Te_8$@($Si_{38}Te_8$)-type clathrates (*P*4-3*n*), recoverable to ambient, and a hexagonal phase (*hex*) of the $Mn_5Si_3$-structure type (*P*$6_3$/*mcm*) with the composition $Si_{0.14}Te$ were obtained (**Figure 1**). *hex* survives decompression until the press is opened, whereupon it amorphizes. We also demonstrated that it is an unstable product of the decomposition of silicon sesquitelluride $Si_2Te_3$. Temperature cycling at high pressures shows that the melting and crystallization of *hex* are reversible. The most noteworthy result of our study is the high degree of interchangeability of Si and Te in the *hex* phase. Three different Wyckoff positions are occupied: the *4d* site (1/3,2/3,0) and two *6g* sites (*x*,0,1/4 with $x \approx 0.24$ and 0.62). The *4d* site is exclusively occupied by Te. This Te1 site is octahedrally coordinated by Te3/Si2 (0.94:0.06). The Te-centered octahedra share common faces and form columns along the *c* axis. Neighboring columns are interconnected via common edges. The Te2/Si1 (0.75:0.25) atoms on the other *6g* site are interconnected to form chains of face-sharing distorted empty octahedra along the *c* direction.

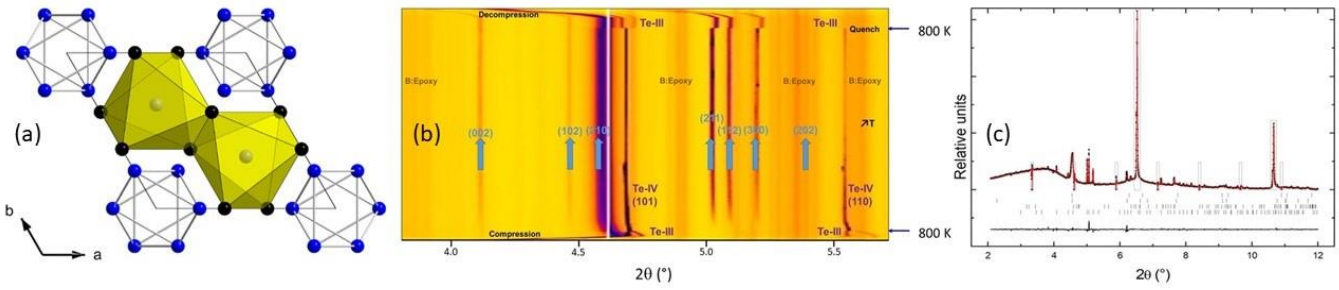


***Figure 1** [1] – **(a)** Crystal structure of the $Mn_5Si_3$-like phase. Te1, Te2/Si1, and Te3/Si2 atoms are drawn as grey, blue, and black symbols, respectively. **(b)** Measured powder patterns at 10 GPa (λ = 0.23437 Å). Reflections due to the $Mn_5Si_3$-like phase are indicated. **(c)** Observed diagram compared with the calculated and difference diagrams at 10 GPa and room temperature (λ = 0.23393 Å). Vertical markers indicate the positions of the calculated Bragg reflections for (from bottom to top) the $Mn_5Si_3$ –like phase, Te-III, hBN, and graphite.*

[**1**] A. Grzechnik *et al.*, Inorg. Chem. 2022, 61, 7349.