

Hafnium germanium telluride

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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{Hf-Ge}) = 0.002$ Å; R factor = 0.024; wR factor = 0.055; data-to-parameter ratio = 23.9.

The title hafnium germanium telluride, HfGeTe_4 , has been synthesized by the use of a halide flux and structurally characterized by X-ray diffraction. HfGeTe_4 is isostructural with stoichiometric ZrGeTe_4 and the Hf site in this compound is also fully occupied. The crystal structure of HfGeTe_4 adopts a two-dimensional layered structure, each layer being composed of two unique one-dimensional chains of face-sharing Hf-centered bicapped trigonal prisms and corner-sharing Ge-centered tetrahedra. These layers stack on top of each other to complete the three-dimensional structure with undulating van der Waals gaps.

Related literature

For the synthesis, crystal structure, and electronic structure of $\text{Hf}_{0.85}\text{GeTe}_4$, see: Mar & Ibers (1993). For the synthesis and structure of ZrGeTe_4 , see: Lee *et al.* (2007). The title compound, HfGeTe_4 , is isostructural with $\text{Hf}_{0.85}\text{GeTe}_4$ and ZrGeTe_4 . However the Hf site in HfGeTe_4 is fully occupied. For related literature, see: Furuseth *et al.* (1973); Gelato & Parthé (1987); Smith & Bailey (1957); Zhao & Parthé (1990).

Experimental

Crystal data

HfGeTe_4	$V = 696.63$ (6) Å ³
$M_r = 761.48$	$Z = 4$
Orthorhombic, $Cmc2_1$	Mo $K\alpha$ radiation
$a = 3.97951$ (17) Å	$\mu = 35.50$ mm ⁻¹
$b = 15.9530$ (7) Å	$T = 290$ (1) K
$c = 10.9731$ (7) Å	$0.30 \times 0.02 \times 0.02$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	3348 measured reflections
Absorption correction: numerical (NUMABS; Higashi, 2000)	910 independent reflections
$T_{\min} = 0.425$, $T_{\max} = 0.510$	878 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$	$\Delta\rho_{\text{max}} = 1.55$ e Å ⁻³
$wR(F^2) = 0.054$	$\Delta\rho_{\text{min}} = -2.00$ e Å ⁻³
$S = 0.97$	Absolute structure: Flack (1983),
910 reflections	431 Friedel pairs
38 parameters	Flack parameter: 0.008 (14)
1 restraint	

Table 1

Selected geometric parameters (Å, °).

Hf—Ge ⁱ	2.8286 (15)	Hf—Te ⁱⁱ	2.9825 (8)
Hf—Te ³ⁱⁱ	2.9454 (8)	Hf—Te ^{4iv}	3.0312 (11)
Hf—Te ³ⁱⁱⁱ	2.9454 (8)	Ge—Te ^{4v}	2.6761 (10)
Hf—Te ¹ⁱⁱⁱ	2.9524 (7)	Ge—Te ^{4vi}	2.6761 (10)
Hf—Te ¹ⁱⁱ	2.9524 (7)	Ge—Te ³	2.6955 (17)
Hf—Te ²ⁱⁱⁱ	2.9825 (8)	Te ¹ —Te ²	2.7387 (13)
Te ^{4v} —Ge—Te ^{4vi}	96.07 (5)	Te ^{4v} —Ge—Hf ^{iv}	123.85 (4)
Te ^{4v} —Ge—Te ³	92.35 (4)	Te ³ —Ge—Hf ^{iv}	120.07 (5)

Symmetry codes: (i) $-x, -y + 1, z - \frac{1}{2}$; (ii) $x + \frac{1}{2}, y + \frac{1}{2}, z$; (iii) $x - \frac{1}{2}, y + \frac{1}{2}, z$; (iv) $-x, -y + 1, z + \frac{1}{2}$; (v) $-x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (vi) $-x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 2006); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: locally modified version of *ORTEP* (Johnson, 1965); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

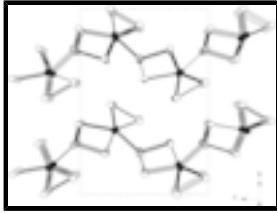
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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2040).

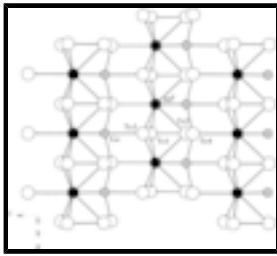
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