Synthesis, crystal structure, and electronic structure of Ba2GeTe3(Te2)

Jai Prakash, Adel Mesbah, Sébastien Lebègue, James Ibers

Synthesis, crystal structure, and electronic structure of $Ba_2GeTe_3(Te_2)$

Jai Prakash[a,b], Adel Mesbah[b,c], Sébastien Lebègue[d], and James A. Ibers[b,*]

[a]*Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana 502285, India*

[b]*Department of Chemistry, Northwestern University, Evanston, IL 60208-3113, USA*

[c]*ICSM, UMR 5257, CEA CNRS, ENSCM, Univ. Montpellier, Site de Marcoule-Bât.426, BP 17171, 30207 Bagnols-sur-Cèze, France*

[d]*Laboratoire de Physique et Chimie Théoriques (LPCT, UMR CNRS 7019), Institut Jean Barriol, Université de Lorraine, BP 239, Boulevard des Aiguillettes, Vandoeuvre-lès-Nancy 54506, France*

Keywords: Barium germanium telluride, solid-state synthesis; crystal structure, Te–Te single bond, electronic structure

Abstract

Black crystals of $Ba_2GeTe_3(Te_2)$ were obtained by the "U-assisted" reaction of U, Ba, Ge, and Te at 1173 K using the sealed-tube method. The crystal structure of $Ba_2GeTe_3(Te_2)$ was determined by a single crystal X-ray study at 100(2) K. It crystallizes in space group *Pnma* of the orthorhombic crystal system with four formula units in a cell with constants a = 6.7900(14) Å, b = 23.720(5) Å, and c = 6.9300(14) Å. The crystal structure of $Ba_2GeTe_3(Te_2)$ can be described as pseudo one-dimensional with zig-zag chains $^1_\infty[GeTe_3^{2-}]$ where each Ge atom is bonded to four Te atoms in a distorted tetrahedron. These chains are separated by the Ba^{2+} cations and homoatomic dimers of Te_2^{2-}. Around each Ba atom there are nine Te atoms in a distorted tricapped trigonal prism. Charge balance in $Ba_2GeTe_3(Te_2)$ is achieved with 2 × Ba^{2+}, 1 × Ge^{4+}, 3 × Te^{2-}, and 1 × Te_2^{2-}. Density functional theory (DFT) calculations suggest $Ba_2GeTe_3(Te_2)$ is a metal with Ge- and Te-derived states contributing the most around the Fermi level.

Corresponding author. Fax: +1 847 491 2976

E-mail address: ibers@chem.northwestern.edu (J. A. Ibers)

1. Introduction

The compounds A/Q/T and Ak/Q/T, where A = alkali metal = Li-Cs ; Ak = alkaline-earth metal = Mg, Ca, Sr, Ba; Q = chalcogen = S, Se, and Te; and T = Si, Ge, and Sn, have been extensively studied because of their rich structural chemistry. These compounds show diverse physical properties, such as semiconducting, nonlinear optics (NLO) materials, thermoelectric properties, solar energy converters, and detector materials [1-4]. For example, $Li_2Ga_2GeS_6$ shows a strong second harmonic generation (SHG) effect [5] and the $Li_2In_2TQ_6$ (T = Si, Ge; Q = S, Se) compounds are the few examples of IR NLO materials [6].

The structures of most of these compounds contain tetrahedral TQ_4 units. The condensation of TQ_4 units results in the formation of infinite chains, layers, and networks of $[T_xQ_y^{n-}]$ units. Compounds such as Mg_2SnS_4 [2] and Ba_3GeS_5 [7] contain discrete units of $[TQ_4^{4-}]$ and are classified as zero-dimensional. Other examples of $[T_xQ_y^{n-}]$ units include the $[Ge_4S_{10}^{4-}]$ clusters in $Ba_2Ge_4S_{10}$ [8], the infinite chains of $[GeS_3^{2-}]$ in $Ba_2Ge_2S_6$ [1], and the $[SnS_5^{6-}]$ units in the $BaSn_2S_5$ structure [9]. Apart from TQ_4 units, a few compounds also contain ethane-like $[T_2Q_6^{6-}]$ units with homonuclear T–T bonds, an example being $K_6Ge_2S_6$ [10].

The current ICSD database [11] shows very few compounds in the ternary Ak/Ge/Q system: $Ba_2Ge_4S_{10}$ [8], $Ba_2Ge_2S_6$ [1], Ba_3GeS_5 [12], Ak_2GeQ_4 (Ak = Mg, Ca, Sr, and Ba; Q = S and Se) [1,2,12], $Sr_2Ge_2Se_5$ [13], $Ba_2Ge_2Se_5$ [13], and only one telluride $Ba_2Ge_2Te_5$ [14]. Most of these compounds contain Ge^{4+}. However, there are few compounds with Ge^{3+} or mixed $Ge^{2+/4+}$. For example, $Sr_2Ge_2Se_5$ [13] and $Ba_2Ge_2Te_5$ [14] contain exclusively Ge^{3+} whereas Ge^{2+} and Ge^{4+} coexist in a mixed-valence compound $Ba_2Ge_2Se_5$ [13]. Surprisingly, there appear to be no known Ak/Ge/Q compounds with structures that have any homoatomic Q–Q bonds. Here we present the first such example: the synthesis, crystal structure, and electronic structure of the new ternary polytelluride $Ba_2GeTe_3(Te_2)$.

2. Experimental

2.1. Synthesis

Caution! *Depleted uranium is an α-emitting radioisotope and its manipulation is considered a health risk. Its use requires appropriate infrastructure and personnel trained in the handling of radioactive materials.*

The following reactants were used as received: Ba (Alfa 99.5%), Ge (Aesar 99.99%), and Te (Aldrich 99.8%). U powder was obtained through the hydridization of depleted-U turnings (Mfg Sci. Corp.) followed by decomposition of the hydride under vacuum [15].

Synthesis of single crystals of $Ba_2GeTe_3(Te_2)$. Black crystals of $Ba_2GeTe_3(Te_2)$ were serendipitously obtained by combining the elements Ba, Ge, U, and Te. The aim of the reaction was to synthesize a new quaternary compound of Ba, Ge, U, and Te. The reactants were loaded into carbon-coated fused-silica tubes in an Ar-filled glove box, evacuated to 10^{-4} Torr, and flame sealed. The reaction contained 0.0346 g (0.252 mmol) Ba, 0.01g (0.042 mmol) U, 0.0061g (0.084 mmol) Ge, and 0.0965g (0.756 mmol) Te. The sealed tube containing the reaction mixture was heated from 298 K to 1053 K in 36 h, held there for 15 h, further heated to 1173 K in 24 h, and held there for 192 h. The tube was then cooled to 993 K over 99 h and finally to 298 K in a further 122 h. Semi-quantitative elemental analysis of the products was carried out with the use of a Hitachi S-3400 SEM equipped for EDX analysis. The black irregular shaped crystals showed Ba:Ge:Te ≈ 2:1:5. The sizes of these crystals were in the range of ~ 30 μm to 150 μm. The reaction product also contained crystals of UOTe and BaTe. The crystals of $Ba_2GeTe_3(Te_2)$ were stable in air for at least one week as judged from unit-cell determinations.

2.2. Structure Determination

Single-crystal X-ray diffraction data were collected at 100(2) K on an APEX2 X-ray diffractometer equipped with graphite-monochromatized Mo$K\alpha$ radiation [16]. The crystal-to-detector distance was 60 mm; the exposure time was 15 sec/frame. Collection of

intensity data, cell refinement, and data reduction were performed using APEX2 as a series of 0.3° scans in φ and ω [16]. Face-indexed absorption, incident beam, and decay corrections were performed by the program SADABS [17]. The crystal structure was solved using the SHELX14 suite of programs [18]. Atom positions were standardized using the program STRUCTURE TIDY [19]. Structure drawings were made using the program CRYSTALMAKER [20]. Further details are given in Tables 1 and 2, and in the Supporting Information.

2.3. Electronic structure calculation

To conduct our calculations we have used the VASP (Vienna ab Initio Simulation Package) [21] code which implements density functional theory [22,23] using the projector augmented wave basis set [24]. For the exchange-correlation functional, we have chosen the one of Heyd, Scuseria, and Ernzerhof [25-27]. The crystal structure was kept identical to the experimental one, while to ensure proper convergence of our calculations, a 12 × 4 × 12 mesh was used to integrate over the Brillouin zone. The default cut-off was used for the plane wave part of the wave functions.

3. Results and discussion

3.1. Synthesis and Structure

Black single crystals of $Ba_2GeTe_3(Te_2)$ were first obtained using the sealed tube method by heating the elements Ba, Ge, U, and Te at 1173 K. A yield of $Ba_2GeTe_3(Te_2)$ crystals was about 25% (based on Ge). The reaction of stoichiometric amount of Ba, Ge, and Te did not yield the target $Ba_2GeTe_3(Te_2)$ phase, but instead a mixture of the phases BaTe, GeTe, $Ba_2Ge_2Te_5$, and unreacted Te powder was obtained. The reaction of Ba, Ge, and Te in the same ratio as loaded in the initial reaction that involved uranium also tried using the same heating profile. However, the reaction product showed the presence of $Ba_2Ge_2Te_5$ as a major phase. Our further attempts to synthesize this compound by varying the heating conditions failed. It appears that this compound cannot be synthesized without the participation of U in the reaction. There are other known examples of compounds such as $CsTi_5Te_8$ [28] that can only be synthesized by U-assisted reactions.

The single-crystal X-ray diffraction study of $Ba_2GeTe_3(Te_2)$ shows that it crystallizes with four formula units in the space group *Pnma* of the orthorhombic system in a cell of dimensions a = 6.790(1), b = 23.720(5), and c = 6.930(1) Å. The site symmetries of the atoms in the asymmetric unit are: Ba1 (1), Ge1 (.*m*.), Te1 (1), Te2 (1), and Te3 (.*m*.). The crystal structure of $Ba_2GeTe_3(Te_2)$ is one-dimensional (Fig. 1).

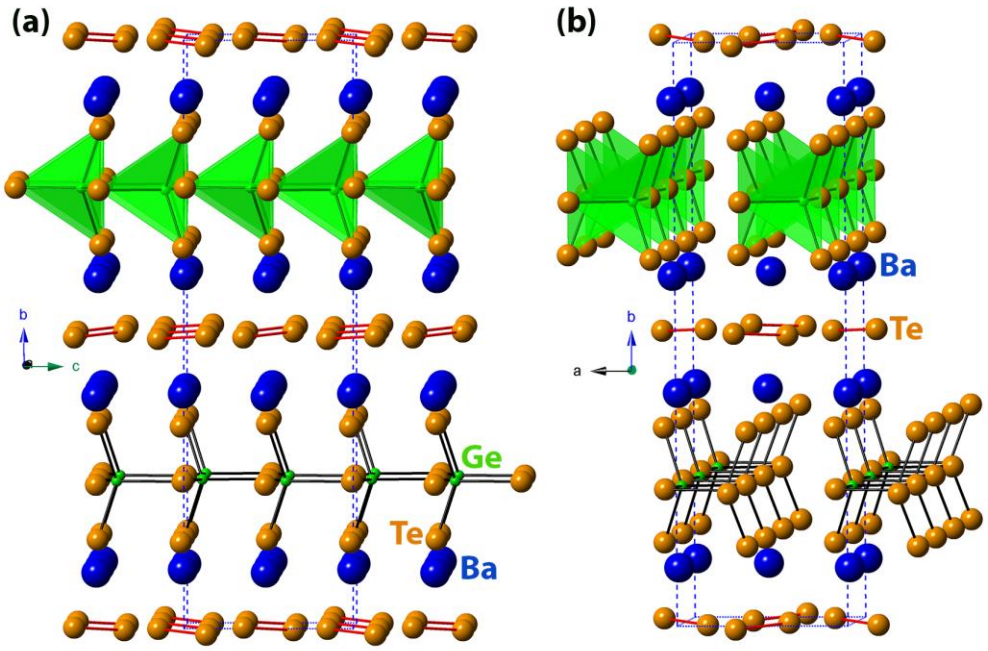

Fig. 1: The unit cell view of $Ba_2GeTe_3(Te_2)$ structure along (a) [100] and (b) [001] directions. The Ba, Ge, and Te atoms are shown in blue, green, and orange, respectively.

It consists of the zigzag chains that are made up of Ge1, Te1, and Te3 atoms. Each Ge atom is bonded to two Te1 and two Te3 atoms in a distorted tetrahedral fashion. Each $GeTe_4$ tetrahedron shares its two corners with the two neighboring $GeTe_4$ tetrahedra forming the infinite zigzag chain of $^1_\infty[GeTe_3^{2-}]$ composition (Fig. 2). The Ge1–Te distances are in the range of 2.571(1)–2.683(1) Å. These distances are in good agreement with the corresponding distances in some known related compounds (Table 3).

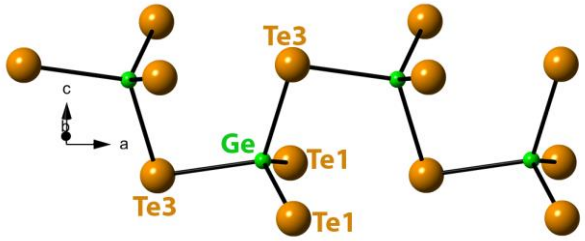

Fig. 2: A view of infinite zig-zag chain of $[GeTe_3^{2-}]$ in $Ba_2GeTe_3(Te_2)$ structure.

The Ba atoms in $Ba_2GeTe_3(Te_2)$ structure are surrounded by nine Te atoms (4 × Te1, 4 ×

Te2, and 1 × Te3) in a distorted tricapped trigonal prism geometry (Fig. 3).

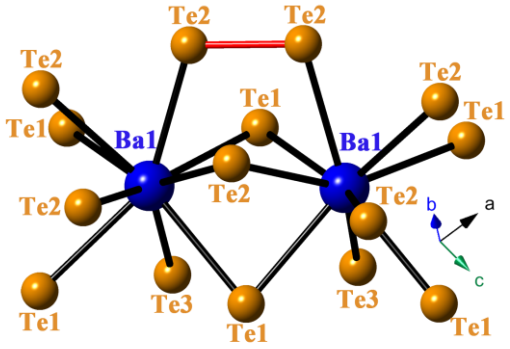

Fig. 3: Local coordination environment of Ba atoms in $Ba_2GeTe_3(Te_2)$ structure. The Ba–Te interactions are shown as black lines and Te–Te bond is shown as a red solid line.

The Ba–Te distances range between 3.5323(5) to 3.7110(7) Å. Compare these distances with $BaSbTe_3$, (3.406(1)–3.888(1) Å) [29], Ba_2SnTe_5 (3.583(1)–3.662(1) Å) [9], and $BaBiTe_3$ (3.404(2)–3.887(2) Å) [30] where the local coordination environments of Ba atoms are similar. This structure also features homoatomic Te–Te bonding between two Te2 atoms forming a Te_2^{2-} dimer with a distance of 2.7924(5) Å. This distance is comparable to the single bond Te–Te distances found in Cs_4GeTe_6 (2.735(1) and 2.746(1) Å) [31], Cs_2GeTe_4 (2.780(1) Å) [32], Tl_2GeTe_5 (2.905(1) Å) [33], K_2GeTe_4 (2.736(1) Å) [34], α-$ThTe_3$ (2.7631(8) Å) [35], and $BaThTe_4$ (2.766(1) Å) [36].

The charge balance in this ternary $Ba_2GeTe_3(Te_2)$ compound can be achieved with 2 × Ba^{2+}, 1 × Ge^{4+}, 3 × Te^{2-}, and 1 × Te_2^{2-}. Hence, the chemical formula of this closed shell Zintl compound is best described as $Ba_2GeTe_3(Te_2)$.

3.2. Electronic structure

In Fig. 4 we present our computed total (upper plot) and partial (lower plots) density of states (DOS) for $Ba_2GeTe_3(Te_2)$, as obtained with the HSE functional. Although relatively small, the total density has a finite value at the Fermi level; thus Ba_2GeTe_5 is a metal.

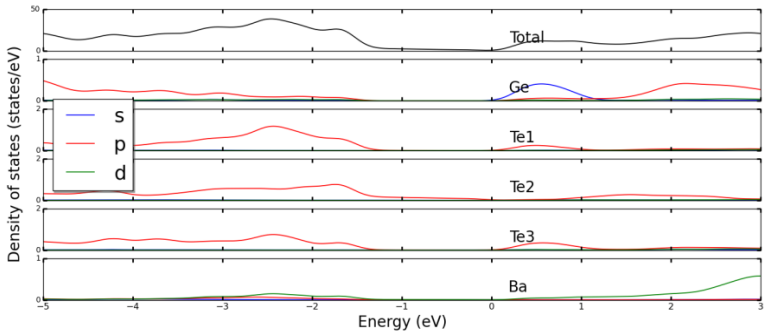

Fig. 4: Density of states (DOS) for $Ba_2GeTe_3(Te_2)$.

From our partial density of states, it can be seen that Ge- and Te-derived states contribute the most around the Fermi level, while the contribution from Ba is almost negligible.

4. Conclusions

Crystals of the new ternary polytelluride, $Ba_2GeTe_3(Te_2)$, have been obtained by the solid-state "U-assisted" reaction of U, Ba, Ge, and Te at 1173 K. The single crystal X-ray study at 100(2) K indicates that $Ba_2GeTe_3(Te_2)$ crystallizes in space group *Pnma* of the orthorhombic crystal system with four units in a cell with constants of a = 6.7900(14) Å, b = 23.720(5) Å, and c = 6.9300(14) Å. Charge balance in $Ba_2GeTe_3(Te_2)$ is achieved with 2 × Ba^{2+}, 1 × Ge^{4+}, 3 × Te^{2-}, and 1 × Te_2^{2-}: (Te–Te = 2.7924(5) Å). The crystal structure of $Ba_2GeTe_3(Te_2)$ can be described as pseudo one-dimensional with zig-zag chains of $^1_\infty[GeTe_3^{2-}]$, where each Ge atom, which has *m* symmetry, is coordinated to four Te atoms that form a distorted tetrahedron. Each Ba atom is surrounded by nine Te atoms in a distorted tricapped trigonal prism. The Te_2^{2-} units and Ba^{2+} cations separate the $^1_\infty[GeTe_3^{2-}]$ chains. $Ba_2GeTe_3(Te_2)$ is predicted to be a metal from the DFT calculations with Ge and Te-derived states contributing the most around the Fermi level.

5. Supporting information

The crystallographic CIF file for $Ba_2GeTe_3(Te_2)$ [i.e., Ba_2GeTe_5] has been deposited as entry CCDC-1935898 (https://www.ccdc.cam.ac.uk).

Acknowledgments

Use was made of the IMSERC X-ray Facility at Northwestern University, supported by the International Institute of Nanotechnology (IIN).

References

[1] K. Wu, X. Su, Z. Yang, S. Pan, An investigation of new infrared nonlinear optical material: $BaCdSnSe_4$, and three new related cetrosymmetric compounds: Ba_2SnSe_4, Mg_2GeSe_4, and $Ba_2Ge_2S_6$, Dalton Trans. 44 (2015) 19856-19864.

[2] K. Wu, S. Pan, Z. Yang, Ba_2GeS_4 and Mg_2SnS_4: synthesis, structures, optical properties and electronic structures, RSC Adv. 5 (2015) 33646-33652.

[3] A. Assoud, N. Soheilnia, H. Kleinke, New Quaternary Barium Copper/Silver Selenostannates: Different Coordination Spheres, Metal-Metal Interactions, and Physical Properties, Chem. Mater. 17 (2005) 2255-2261.

[4] G.A. Marking, J.A. Hanko, M.G. Kanatzidis, New Quaternary Thiostannates and Thiogermanates. $A_2Hg_3M_2S_8$ (A = Cs, Rb; M = Sn, Ge) through Molten A_2S_x. Reversible Glass Formation in $Cs_2Hg_3M_2S_8$, Chem. Mater. 10 (1998) 1191-1199.

[5] Y. Kim, I.-seok Seo, S.W. Martin, J. Baek, P.S. Halasyamani, N. Arumugam, H. Steinfink, Characterization of New Infrared Nonlinear Optical Material with High Laser Damage Threshold, $Li_2Ga_2GeS_6$, Chem. Mater. 20 (2008) 6048-6052.

[6] W. Yin, K. Feng, W. Hao, J. Yao, Y. Wu, Synthesis, Structure, and Properties of $Li_2In_2MQ_6$ (M = Si, Ge; Q = S, Se): A New Series of IR Nonlinear Optical Materials, Inorg. Chem. 51 (2012) 5839-5843.

[7] M.-Y. Pan, S.-Q. Xia, X.-C. Liu, X.-T. Tao, Ba_3GeS_5 and Ba_3InS_4Cl: Interesting size effects originated from the tetrahedral anions, J. Solid State Chem. 219 (2014) 74-79.

[8] M. Ribes, J. Olivier-Fourcade, E. Philippot, M. Maurin, Etude Structurale de Thiocomposés à Groupement Anionique de Type Tetrane $Na_4X_4S_{10}$ (X = Ge, Si) et $Ba_2Ge_4S_{10}$, J. Solid State Chem. 8 (1973) 195-205.

[9] J. Li, Y.Y. Liszewski, L.A. MacAdams, Synthesis and Characterization of Ba_2SnTe_5: A New Zintl Phase Containing Unique One-Dimensional Chains of $(SnTe_3)^{2-}$ and Dimeric Units of $(Te_2)^{2-}$, Chem. Mater. 8 (1996) 598-600.

[10] B. Eisenmann, E. Kieselbach, H. Schäfer, H. Schrod, Über Thio-, Selenido- und Telluridogermanate(III): Zur Kenntnis von $K_6Ge_2S_6$, $K_6Ge_2Se_6$ und $Na_6Ge_2Te_6$, Z. Anorg. Allg. Chem. 516 (1984) 49-54.

[11] The Inorganic Crystal Structure Database (ICSD) Web. http://www2.fiz-karlsruhe.de/icsd_web.html (accessed 27 June 2019).

[12] A. Assoud, N. Soheilnia, H. Kleinke, From Yellow to Black: New Semiconducting Ba Chalcogeno-Germanates, Z. Naturforsch. B: Anorg. Chem. Org. Chem. 59b (2004) 975-979.

[13] D. Johrendt, M. Tampier, Strontium Selenogermanate(III) and Barium Selenogermanate(II,IV): Synthesis, Crystal Structures, and Chemical Bonding, Chem. Eur. J. 6 (2000) 994-998.

[14] C. Brinkmann, B. Eisenmann, H. Schäfer, $Ba_2Ge_2Te_5$, ein neues Kettentelluridogermanat(III), Z. Anorg. Allg. Chem. 517 (1984) 143-148.

[15] A.J.K. Haneveld, F. Jellinek, Some Ternary Uranium Chalcogenides, J. Less-Common Met. 18 (1969) 123-129.

[16] Bruker APEX2 Version 2009.5-1 Data Collection and Processing Software, Bruker Analytical X-Ray Instruments, Inc., Madison, WI, USA, 2009.

[17] G.M. Sheldrick, SADABS, 2008. Department of Structural Chemistry, University of

Göttingen, Göttingen, Germany.

[18] G.M. Sheldrick, A short history of SHELX, Acta Crystallogr. Sect. A: Found. Crystallogr. 64 (2008) 112-122.

[19] L.M. Gelato, E. Parthé, STRUCTURE TIDY - a computer program to standardize crystal structure data, J. Appl. Crystallogr. 20 (1987) 139-143.

[20] D. Palmer, CrystalMaker Software Version 2.7.7, 2013. CrystalMaker Software Ltd., Oxford, England

[21] G. Kresse, D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, Phys. Rev. B 59 (1999) 1758-1775.

[22] W. Kohn, L.J. Sham, Self-Consistent Equations Including Exchange and Correlation Effects, Phys. Rev. 140 (1965) 1133-1138.

[23] P. Hohenberg, W. Kohn, Inhomogeneous Electron Gas, Phys. Rev. 136 (1964) 864-871.

[24] P.E. Blöchl, Projector augmented-wave method, Phys. Rev. B 50 (1994) 17953-17979.

[25] J. Heyd, G.E. Scuseria, M. Ernzerhof, Hybrid functionals based on a screened Coulomb potential, J. Chem. Phys. 118 (2003) 8207-8215.

[26] J. Heyd, G.E. Scuseria, M. Ernzerhot, Erratum: "Hybrid functionals based on a screened Coulumb potential" [J. Chem. Phys. 118, 8207 (2003)], J. Chem. Phys. 124 (2006) 219906.

[27] J. Paier, M. Marsman, K. Hummer, G. Kresse, I.C. Gerber, J.G. Angyan, Screened hybrid density functionals applied to solids, J. Chem. Phys. 124 (2006) 154709.

[28] D.L. Gray, J.A. Ibers, Synthesis and structure of $CsTi_5Te_8$: Relation to the TlV_5S_8, $TlCr_3S_5$, and similar channel structures, J. Alloys Compd. 440 (2007) 74-77.

[29] K. Volk, G. Cordier, R. Cook, H. Schäfer, $BaSbTe_3$ und $BaBiSe_3$ Verbindungen mit BiSe- bzw. SbTe-Schichtverbänden, Z. Naturforsch. B: Chem. Sci. 35b (1980) 136-140.

[30] D.-Y. Chung, S. Jobic, T. Hogan, C.R. Kannewurf, R. Brec, J. Rouxel, M.G. Kanatzidi, Oligomerization Versus Polymerization of Texn- in the Polytelluride Compound $BaBiTe_3$. Structural Characterization, Electronic Structure, and Thermoelectric Properties, J. Am. Chem. Soc. 119 (1997) 2505-2515.

[31] C. Brinkmann, B. Eisenmann, H. Schäfer, Cs_4GeTe_6, ein o-Pertelluridogermanat(IV), Mater. Res. Bull. 20 (1985) 1207-1211.

[32] W.S. Sheldrick, B. Schaaf, Methanolothermale Synthese und Kristallstruktur von Diselenido- und Ditelluridogermanaten(IV) der Alkalimetalle K-Cs, Z. Naturforsch. B: Chem. Sci. 50b (1995) 1469-1475.

[33] A.A. Toure, G. Kra, R. Eholie, J. Olivier-Fourcade, J.-C. Jumas, M. Maurin, Sur le ternaire Tl-Ge-Te: Etude structurale de la phase Tl_2GeTe_5, J. Solid State Chem. 84 (1990) 245-252.

[34] B. Eisenmann, H. Schrod, H. Schäfer, K_2GeTe_4, ein pertelluridogermanat mit kettenstruktur, Mater. Res. Bull. 19 (1984) 293-298.

[35] J. Prakash, J.A. Ibers, Synthesis and Crystal Structure of α-$ThTe_3$, Z. Anorg. Allg. Chem. 640 (2014) 1943-1945.

[36] J. Prakash, S. Lebègue, C.D. Malliakas, J.A. Ibers, Syntheses, Crystal Structures,

Resistivity Stuides, and Electronic Properties of Three New Barium Actinide Tellurides: $BaThTe_4$, $BaUTe_4$, and $BaUTe_6$, Inorg. Chem. 53 (2014) 12610-12616.

[37] K.O. Klepp, P. Ecker, The Crystal Structure of Tl_2GeTe_3: A Tellurogermanate(IV) with Bitetrahedral Anions, J. Solid State Chem. 117 (1995) 351-355.

[38] R.E. Marsh, On the Structure of Tl_2GeTe_5, J. Solid State Chem. 87 (1990) 467-468.

Table 1. Crystallographic Data and Structure Refinement Details for $Ba_2GeTe_3(Te_2)$ structure[a].

	Ba_2GeTe_5
Space group	*Pnma*
a (Å)	6.7900(14)
b (Å)	23.720(5)
c (Å)	6.9300(14)
V (Å^3)	1116.1(4)
Z	4
ρ (g cm^{-3})	5.863
μ (mm^{-1})	22.39
$R(F)$[b]	0.016
$R_w(F_{o2})$[c]	0.027

[a] λ = 0.71073 Å, T = 100(2) K.

[b] $R(F) = \Sigma\ ||F_o|-|F_c|| / \Sigma|F_o|$ for $F_o^2 > 2\sigma(F_o^2)$.

[c] $R_w(F_o^2) = \{\Sigma\ [w(F_o^2 - F_c^2)^2] / \Sigma w F_o^4\}^{1/2}$. For $F_o^2 < 0$, $w^{-1} = \sigma^2(F_o^2)$; for $F_o^2 \geq 0$, $w^{-1} = \sigma^2(F_o^2) + 0.0074\ F_o^2$.

Table 2: Selected Metrical Data for $Ba_2GeTe_3(Te_2)$.[a]

Atom pair	Distances (Å)	Angle (deg)
Ge1–Te1	2.5713(5) × 2	Te1–Ge1–Te1 130.05(2)
Ge1–Te3	2.6316(7)	Te1–Ge1–Te3 102.44(1) × 2
	2.6827(7)	Te1–Ge1–Te3 103.85(1) × 2
		Te3–Ge1–Te3 114.78(2)
Te2–Te2	2.7924(5)	
Ba1–Te1	3.6048(7)	
	3.6202(7)	
	3.6332(7)	
	3.7110(7)	
Ba1–Te2	3.5323(5)	
	3.5381(5)	
	3.5678(5)	
	3.5859(5)	
Ba1–Te3	3.5514(7)	

[a]Some entries have been rounded to three significant figures to facilitate comparisons.

Table 3 :Ge!Te Distances in Some Related Compounds with 4-Coordinated Ge atoms[a].

Compound	Structure	Ge!Te (Å)	Ref.
Ba_2GeTe_5	one-dimensional	2.571(1)–2.683(1)	this work
Cs_4GeTe_6	zero-dimensional	2.537(3)–2.623(2)	[31]
Cs_2GeTe_4	one-dimensional	2.549(1)–2.650(3)	[32]
Tl_2GeTe_3	zero-dimensional	2.580(3)–2.643(3)	[37]
α -Tl_2GeTe_5	zero-dimensional	2.604(1)–2.664(5)	[33]
β-Tl_2GeTe_5	zero-dimensional	2.616(1)–2.639(1)	[38]
K_2GeTe_4	one-dimensional	2.508(2)–2.640(2)	[34]

[a]Some distances have been rounded for comparison. All the compounds contain germanium in +4 oxidation state.