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$Ba_{14}Si_4Sb_8Te_{32}(Te_3)$: hypervalent Te in a new structure type with low thermal conductivity

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Electronic Supplementary Information (ESI)

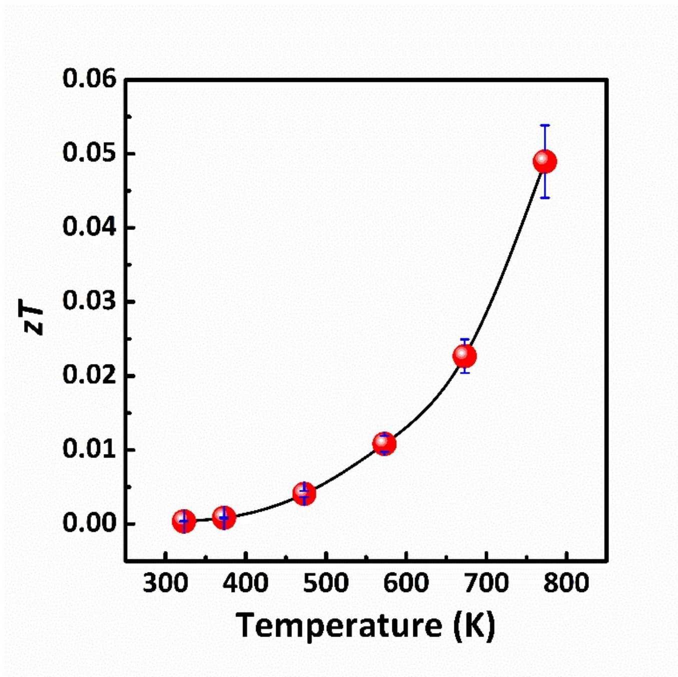

Fig. SI1: (a) The variation of temperature-dependent thermoelectric figure of merit (*zT*) for the polycrystalline $Ba_{14}Si_4Sb_8Te_{32}(Te_3)$ with temperature. The *zT* value of the sample is calculated by assuming the transport properties of the compact polycrystalline sample as direction independent.

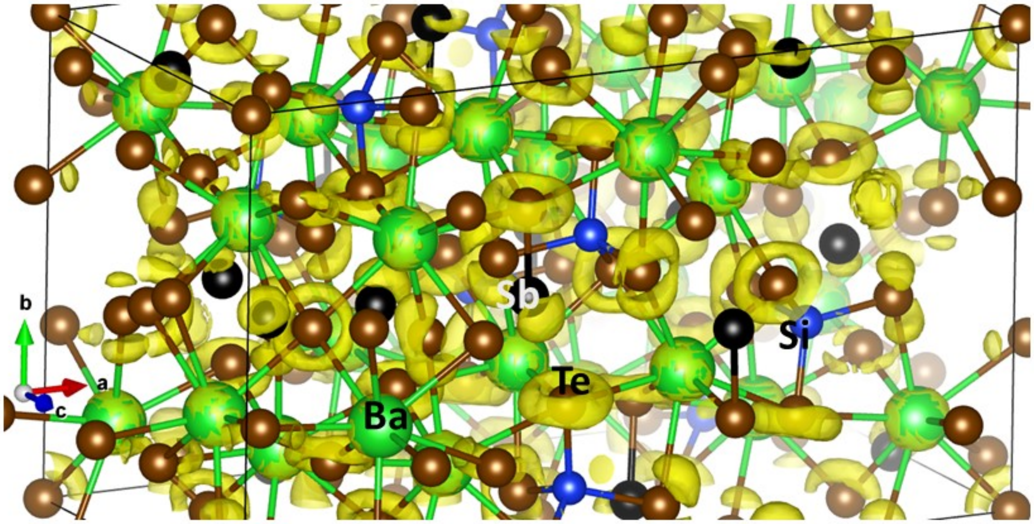

Fig. SI2: The 3D iso-surfaces of the electron localization function (ELF) for the $Ba_{14}Si_4Sb_8Te_{32}(Te_3)$ structure. The yellow cloud on the Te atoms indicates the density of transferred electrons. The yellow clouds on the Sb atoms show 5s^2 electron pair. The Ba, Si, Sb, and Te atoms are represented by green, blue, black, and brown spheres, respectively.

S1: Optical Properties

The optical absorption coefficient (α) is obtained from the complex dielectric function $\varepsilon(\omega) = \varepsilon^{'}(\omega) + \varepsilon^{''}(\omega)$. The imaginary part of the dielectric function $\varepsilon^{''}(\omega)$ can be expressed as:[1,2]

$$\varepsilon^{''}_{ij}(\omega) = \frac{4\pi^2 e^2}{V_c} \lim_{q \to 0} \sum_{c,v,\vec{k}} 2 w_{\vec{k}} \delta\left(\varepsilon_{c\vec{k}} - \varepsilon_{v\vec{k}} - \omega\right) \times \left\langle u_{c\vec{k} + \hat{e}_i q} \middle| u_{v\vec{k}} \right\rangle \left\langle u_{c\vec{k} + \hat{e}_j q} \middle| u_{v\vec{k}} \right\rangle^{*} \tag{S1-1}$$

where; indices *v* indicates the valence band (VB) and the *c* indicates the conduction band (CB) states; $u_{c\vec{k}}$ is the cell periodic part of the single-particle wavefunctions; $\varepsilon_{c\vec{k}}$ and $\varepsilon_{v\vec{k}}$ are CB and VB single-electron energy; $w_{\vec{k}}$ is the weight of the k-points; V_c is the volume of the unit cell.

The real part of the dielectric function $\varepsilon^{'}(\omega)$ can be expressed in terms of $\varepsilon^{''}(\omega)$ via Kramers-Kronig transformation as:

$$\varepsilon_{ij}^{'}(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\varepsilon_{ij}^{''}(\omega^{'})\omega^{'}}{\omega^{'2} - \omega^2 + i\eta} d\omega^{'} \tag{S1-2}$$

where η is a small complex shift and P is the principal value. The absorption coefficient $\alpha(\omega)$ can be computed using $\varepsilon^{'}(\omega)$ and $\varepsilon^{''}(\omega)$ as:

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c}\left[\sqrt{\varepsilon^{'}(\omega)^2 + \varepsilon^{''}(\omega)^2} - \varepsilon^{'}(\omega)\right]^{1/2} \tag{S1-3}$$

S2: Thermoelectric properties

The thermoelectric parameters are computed using semi-classical Boltzmann transport theory within the rigid band approach.[3] The carrier concentration (*p*- or *n*-type) in the system is modelled by creating shifts in the chemical potential. The electrical conductivity (σ_{ij}) as a function of temperature (T) and chemical potential (μ) is. given as:

$$\sigma_{ij}(T;\mu) = \frac{1}{V}\int \sigma_{ij}(\epsilon)\left[-\frac{\partial f_{\mu}(T;\mu)}{\partial \epsilon}\right] d\epsilon \tag{S2-1}$$

where $f_{\mu}(T;\mu)$ is the Fermi function, ϵ is the energy and V is the volume. σ_{ij} as function of energy (ϵ) can be expressed as:

$$\sigma_{ij}(\epsilon) = \frac{1}{N}\sum_{n,\vec{k}} \sigma_{ij}(n,\vec{k})\, \delta(\epsilon - \epsilon_{n,\vec{k}}) \tag{S2-2}$$

where $\epsilon_{n,\vec{k}}$ are the band energies and N is the number of $\vec{k}$ points in the Brillouin zone. $\sigma_{ij}(n,\vec{k})$ in terms of relaxation time $\tau_{n,\vec{k}}$ and group velocity $\vec{v}(n,\vec{k})$ is given as:

$$\sigma_{ij}(n,\vec{k}) = e^2 \tau_{n,\vec{k}} v_i(n,\vec{k}) v_j(n,\vec{k}) \tag{S2-3}$$

The Seebeck coefficient tensor (S_{ij}) as a function of temperature (T) and chemical potential (μ) is given as:

$$S_{ij}(T;\mu) = \frac{1}{eTV\sigma_{ij}(T;\mu)} \int \sigma_{ij}(\epsilon)(\epsilon - \mu)\left[-\frac{\partial f_\mu(T;\mu)}{\partial \epsilon} \right] d\epsilon \qquad \text{(S2-4)}$$

The total thermal conductivity (κ) is given as $\kappa_{tot} = \kappa_{lat} + \kappa_{el}$, where κ_{lat} is the lattice (phonon) component and κ_{el} is the electronic component of κ_{tot}. The electronic part of thermal conductivity (κ_{el}) and the electrical conductivity (σ) are related as $\kappa_{el} = L_0 \sigma T$ (Wiedemann-Franz relation), where $L_0 = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$ is the Lorentz number. The quantities σ and κ_{el} are computed with respect to the relaxation time $\tau = \left(T_0 \times n_0^{1/3}\right)/\left(Tn^{1/3}\right) \times 10^{-14} s$ where n_0 is the carrier concentration at $T_0 = 300\ K$. The figure of merit (zT) is calculated using $zT = \frac{S^2 \sigma T}{(\kappa_{el} + \kappa_{lat})}$.

Table SI1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for the $Ba_{14}Si_4Sb_8Te_{32}(Te_3)$ structure.

Atoms	Wyckoff Positions	Site Symmetry	*x*	*y*	*z*	U_{iso}/U_{eq}[a]	SOF
Ba(1)	4*e*	1	0.04343(2)	0.18833(5)	0.18477(4)	0.02623(13)	1
Ba(2)	4*e*	1	0.09742(2)	0.81900(4)	0.10772(4)	0.02136(12)	1
Ba(3)	4*e*	1	0.18167(2)	0.17380(4)	0.48300(4)	0.02183(12)	1
Ba(4)	4*e*	1	0.32216(2)	0.32772(4)	0.26481(4)	0.01935(11)	1
Ba(5)	4*e*	1	0.46798(2)	0.18377(4)	0.05881(4)	0.01819(11)	1
Ba(6)	4*e*	1	0.61322(2)	0.17238(4)	0.32879(4)	0.01964(12)	1
Ba(7)	4*e*	1	0.76305(2)	0.32426(4)	0.11997(4)	0.02005(12)	1
Si(1)	4*e*	1	0.23117(10)	0.6025(2)	0.15287(18)	0.0205(5)	1
Si(2)	4*e*	1	0.48135(9)	0.40274(19)	0.27996(16)	0.0150(5)	1
Sb(1)	4*e*	1	0.05367(4)	0.94982(9)	0.39263(6)	0.0682(3)	1
Sb(2)	4*e*	1	0.14703(3)	0.48746(6)	0.31953(5)	0.02730(15)	1

Sb(3)	4*e*	1	0.27961(2)	0.03296(5)	0.07204(5)	0.02389(14)	1
Sb(4)	4*e*	1	0.59866(2)	0.48145(5)	0.14259(5)	0.02353(14)	1
Te(1)	4*e*	1	0.02298(2)	0.43675(6)	0.29172(5)	0.02245(15)	0.91
Te(2)	4*e*	1	0.0325(3)	0.3819(7)	0.3403(6)	0.0285(17)	0.09
Te(3)	4*e*	1	0.03416(2)	0.17787(7)	0.44546(5)	0.03643(19)	1
Te(4)	4*e*	1	0.10159(2)	0.72154(5)	0.35468(4)	0.02038(13)	1
Te(5)	4*e*	1	0.13133(2)	0.55879(5)	0.10113(4)	0.02545(14)	1
Te(6)	4*e*	1	0.13902(2)	0.00681(5)	0.28984(4)	0.02057(13)	1
Te(7)	4*e*	1	0.16376(2)	0.06408(5)	0.03331(4)	0.02077(13)	1
Te(8)	4*e*	1	0.17873(2)	0.29443(5)	0.24775(4)	0.01854(12)	1
Te(9)	4*e*	1	0.24942(2)	0.78443(5)	0.12369(4)	0.01919(12)	1
Te(10)	4*e*	1	0.26354(2)	0.56712(5)	0.33512(4)	0.01839(12)	1
Te(11)	4*e*	1	0.29002(2)	0.05889(5)	0.28283(4)	0.01949(13)	1
Te(12)	4*e*	1	0.29250(2)	0.49647(5)	0.05945(4)	0.02134(13)	1
Te(13)	4*e*	1	0.32041(2)	0.22014(5)	0.02389(4)	0.01839(12)	1
Te(14)	4*e*	1	0.45953(2)	0.44316(5)	0.10223(4)	0.02253(13)	1
Te(15)	4*e*	1	0.46604(2)	0.22048(4)	0.31459(4)	0.01694(12)	1
Te(16)	4*e*	1	0.57652(2)	0.00507(4)	0.11982(4)	0.01680(12)	1
Te(17)	4*e*	1	0.58393(2)	0.44434(5)	0.34105(4)	0.01814(12)	1
Te(18)	4*e*	1	0.61415(2)	0.28283(5)	0.09010(4)	0.01804(12)	1
Te(19)	2*a*	−1	0.000000	0.000000	0.000000	0.0349(2)	1

[a] U_{iso}/U_{eq} is one-third trace value of the orthogonalized U_{ij} tensor.

Table SI2: The atomic displacement parameters (Å^2) for the $Ba_{14}Si_4Sb_8Te_{32}(Te_3)$ structure.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0215(3)	0.0259(3)	0.0297(3)	-0.0004(2)	-0.0023(2)	0.0003(2)
Ba2	0.0229(2)	0.0219(3)	0.0185(3)	0.0050(2)	-0.00036(19)	-0.0005(2)
Ba3	0.0219(2)	0.0199(3)	0.0222(3)	-0.0011(2)	-0.0023(2)	-0.0007(2)
Ba4	0.0198(2)	0.0188(3)	0.0186(3)	0.0004(2)	-0.00071(18)	-0.0009(2)
Ba5	0.0206(2)	0.0174(3)	0.0159(2)	0.0012(2)	0.00010(18)	-0.0010(2)
Ba6	0.0208(2)	0.0191(3)	0.0180(3)	0.0007(2)	-0.00135(19)	0.0010(2)
Ba7	0.0215(2)	0.0179(3)	0.0197(3)	0.0002(2)	-0.00118(19)	0.0005(2)
Si1	0.0242(12)	0.0192(14)	0.0185(12)	-0.0009(10)	0.0038(9)	-0.0003(10)
Si2	0.0153(10)	0.0133(13)	0.0162(11)	0.0011(9)	0.0009(8)	-0.0019(9)
Sb1	0.0495(5)	0.1205(10)	0.0336(5)	-0.0442(6)	0.0015(4)	0.0158(5)
Sb2	0.0277(3)	0.0319(4)	0.0218(3)	-0.0058(3)	0.0013(2)	0.0002(3)
Sb3	0.0245(3)	0.0210(4)	0.0250(3)	0.0004(2)	-0.0007(2)	0.0015(3)
Sb4	0.0296(3)	0.0174(3)	0.0229(3)	0.0022(3)	0.0011(2)	0.0009(3)
Te1	0.0155(3)	0.0274(4)	0.0237(4)	-0.0011(3)	-0.0001(2)	-0.0019(3)
Te2	0.020(3)	0.039(5)	0.028(4)	-0.007(3)	0.009(3)	-0.018(4)
Te3	0.0218(3)	0.0580(6)	0.0289(4)	0.0049(3)	0.0016(2)	-0.0086(3)
Te4	0.0205(3)	0.0226(3)	0.0181(3)	-0.0036(2)	0.0027(2)	0.0021(2)
Te5	0.0272(3)	0.0236(4)	0.0227(3)	0.0021(3)	-0.0072(2)	-0.0016(3)
Te6	0.0252(3)	0.0157(3)	0.0209(3)	0.0010(2)	0.0034(2)	-0.0005(2)
Te7	0.0226(3)	0.0221(3)	0.0175(3)	-0.0011(2)	0.0023(2)	0.0009(2)
Te8	0.0185(2)	0.0168(3)	0.0199(3)	-0.0012(2)	0.0012(2)	-0.0005(2)
Te9	0.0240(3)	0.0149(3)	0.0190(3)	0.0011(2)	0.0042(2)	0.0007(2)
Te10	0.0203(3)	0.0170(3)	0.0173(3)	-0.0018(2)	0.0003(2)	0.0000(2)

Te11	0.0205(3)	0.0194(3)	0.0187(3)	0.0016(2)	0.0033(2)	0.0023(2)
Te12	0.0266(3)	0.0158(3)	0.0215(3)	-0.0009(2)	0.0029(2)	-0.0004(2)
Te13	0.0191(3)	0.0180(3)	0.0180(3)	0.0010(2)	0.0025(2)	-0.0001(2)
Te14	0.0312(3)	0.0182(3)	0.0170(3)	0.0052(2)	-0.0013(2)	0.0008(2)
Te15	0.0206(3)	0.0129(3)	0.0175(3)	-0.0005(2)	0.0032(2)	-0.0004(2)
Te16	0.0175(2)	0.0140(3)	0.0194(3)	-0.0005(2)	0.00401(19)	0.0001(2)
Te17	0.0161(2)	0.0197(3)	0.0185(3)	-0.0015(2)	0.00173(19)	-0.0027(2)
Te18	0.0210(3)	0.0158(3)	0.0176(3)	-0.0007(2)	0.0034(2)	0.0002(2)
Te19	0.0192(4)	0.0256(6)	0.0572(6)	0.0070(4)	-0.0042(4)	-0.0121(5)

Table SI3: The geometric parameters (Å) for the $Ba_{14}Si_4Sb_8Te_{32}(Te_3)$ structure.

Ba1—Te2	3.380 (7)	Ba5—Ba6	4.7372 (8)
Ba1—Te4^{i}	3.5098 (8)	Ba6—Te12^{ix}	3.4853 (8)
Ba1—Te6	3.5253 (9)	Ba6—Te18	3.5730 (8)
Ba1—Te8	3.5693 (8)	Ba6—Te15	3.6020 (8)
Ba1—Te3	3.5885 (10)	Ba6—Te18^{vii}	3.6044 (8)
Ba1—Te19	3.6173 (7)	Ba6—Te9^{ix}	3.6279 (8)
Ba1—Te1	3.6913 (10)	Ba6—Te16	3.6367 (8)
Ba1—Te3^{ii}	3.6984 (10)	Ba6—Te17	3.7186 (9)
Ba1—Te1^{i}	3.7656 (10)	Ba6—Te14^{ix}	3.7220 (9)
Ba2—Te2^{iii}	3.422 (6)	Ba7—Te6^{vi}	3.5113 (8)
Ba2—Te4^{iv}	3.5019 (8)	Ba7—Te4^{ix}	3.5293 (8)
Ba2—Te19^{v}	3.5589 (6)	Ba7—Te12^{x}	3.5579 (8)
Ba2—Te6^{v}	3.5803 (8)	Ba7—Te10^{ix}	3.5710 (9)

Ba2—Te5	3.5842 (10)	Ba7—Te9^{ix}	3.5826 (8)
Ba2—Te4	3.5951 (8)	Ba7—Te9^{x}	3.5977 (8)
Ba2—Te9	3.6879 (8)	Ba7—Te18	3.6176 (8)
Ba2—Te3^{iii}	3.6926 (9)	Ba7—Te11^{vi}	3.7057 (9)
Ba2—Te1^{iii}	3.7330 (9)	Si1—Te5	2.496 (2)
Ba2—Te7^{v}	3.8491 (9)	Si1—Te9	2.517 (3)
Ba2—Ba7^{vi}	4.6701 (8)	Si1—Te12	2.519 (3)
Ba3—Te6	3.5007 (8)	Si1—Te10	2.544 (2)
Ba3—Te3	3.5411 (8)	Si2—Te14	2.466 (2)
Ba3—Te12^{vii}	3.5693 (8)	Si2—Te16^{vi}	2.493 (2)
Ba3—Te8	3.5790 (9)	Si2—Te15	2.523 (3)
Ba3—Te7^{vii}	3.6137 (10)	Si2—Te17	2.573 (2)
Ba3—Te13^{vii}	3.6219 (8)	Sb1—Te6^{v}	2.7549 (10)
Ba3—Te8^{vii}	3.6393 (9)	Sb1—Te1^{iii}	2.9201 (11)
Ba3—Te5^{vii}	3.7814 (9)	Sb1—Te3^{v}	3.1873 (16)
Ba3—Ba4^{vii}	4.7747 (8)	Sb1—Te5^{xi}	3.1901 (10)
Ba4—Te8	3.4792 (8)	Sb2—Te8	2.9030 (10)
Ba4—Te13	3.5772 (8)	Sb2—Te7^{vii}	2.9652 (9)
Ba4—Te13^{vii}	3.5904 (8)	Sb2—Te10	2.9978 (8)
Ba4—Te12	3.5917 (8)	Sb2—Te1	3.0538 (9)
Ba4—Te16^{vi}	3.6191 (8)	Sb2—Te5	3.0973 (9)
Ba4—Te10	3.6843 (9)	Sb2—Te2	3.159 (7)
Ba4—Te11	3.6984 (9)	Sb3—Te13	2.8043 (9)
Ba4—Te15	3.7462 (8)	Sb3—Te7	2.8159 (8)

Ba5—Te15	3.5229 (8)	Sb3—Te11	2.8678 (9)
Ba5—Te14	3.5342 (9)	Sb4—Te18	2.7925 (9)
Ba5—Te15^{ii}	3.5578 (8)	Sb4—Te17	2.8163 (9)
Ba5—Te16	3.5697 (8)	Sb4—Te11^{vi}	2.9397 (8)
Ba5—Te16^{viii}	3.5732 (8)	Te1—Te2	0.995 (9)
Ba5—Te13	3.5752 (8)	Te1—Te19^{iii}	3.0804 (7)
Ba5—Te18	3.7511 (8)	Te2—Te19^{iii}	2.882 (7)
Ba5—Te17^{ix}	3.7654 (9)	Te2—Te3	3.082 (10)
Te2—Ba1—Te4^{i}	80.68 (11)	Te6^{vi}—Ba7—Te11^{vi}	62.300 (17)
Te2—Ba1—Te6	112.14 (15)	Te4^{ix}—Ba7—Te11^{vi}	131.13 (2)
Te4^{i}—Ba1—Te6	137.63 (2)	Te12^{x}—Ba7—Te11^{vi}	63.614 (17)
Te2—Ba1—Te8	71.97 (11)	Te10^{ix}—Ba7—Te11^{vi}	132.64 (2)
Te4^{i}—Ba1—Te8	148.66 (2)	Te9^{ix}—Ba7—Te11^{vi}	72.536 (17)
Te6—Ba1—Te8	69.216 (18)	Te9^{x}—Ba7—Te11^{vi}	132.997 (19)
Te2—Ba1—Te3	52.40 (16)	Te18—Ba7—Te11^{vi}	77.402 (17)
Te4^{i}—Ba1—Te3	87.840 (19)	Te6^{vi}—Ba7—Ba2^{ix}	49.451 (14)
Te6—Ba1—Te3	72.337 (19)	Te4^{ix}—Ba7—Ba2^{ix}	49.653 (14)
Te8—Ba1—Te3	87.423 (19)	Te12^{x}—Ba7—Ba2^{ix}	136.216 (19)
Te2—Ba1—Te19	158.52 (12)	Te10^{ix}—Ba7—Ba2^{ix}	88.711 (15)
Te4^{i}—Ba1—Te19	77.885 (15)	Te9^{ix}—Ba7—Ba2^{ix}	51.031 (14)
Te6—Ba1—Te19	85.143 (18)	Te9^{x}—Ba7—Ba2^{ix}	133.484 (18)
Te8—Ba1—Te19	128.076 (19)	Te18—Ba7—Ba2^{ix}	133.742 (18)
Te3—Ba1—Te19	127.56 (2)	Te11^{vi}—Ba7—Ba2^{ix}	88.746 (15)

Te2—Ba1—Te1	15.37 (15)	Te5—Si1—Te9	111.51 (10)
Te4^{i}—Ba1—Te1	76.216 (18)	Te5—Si1—Te12	109.86 (10)
Te6—Ba1—Te1	125.24 (2)	Te9—Si1—Te12	109.76 (9)
Te8—Ba1—Te1	73.371 (18)	Te5—Si1—Te10	113.07 (9)
Te3—Ba1—Te1	67.40 (2)	Te9—Si1—Te10	107.25 (9)
Te19—Ba1—Te1	149.400 (19)	Te12—Si1—Te10	105.17 (9)
Te2—Ba1—Te3^{ii}	100.35 (16)	Te14—Si2—Te16^{vi}	110.72 (9)
Te4^{i}—Ba1—Te3^{ii}	82.094 (18)	Te14—Si2—Te15	112.21 (9)
Te6—Ba1—Te3^{ii}	130.58 (2)	Te16^{vi}—Si2—Te15	108.79 (9)
Te8—Ba1—Te3^{ii}	87.944 (19)	Te14—Si2—Te17	109.89 (9)
Te3—Ba1—Te3^{ii}	152.32 (2)	Te16^{vi}—Si2—Te17	107.06 (9)
Te19—Ba1—Te3^{ii}	75.382 (19)	Te15—Si2—Te17	107.99 (8)
Te1—Ba1—Te3^{ii}	85.14 (2)	Te6^{v}—Sb1—Te1^{iii}	90.81 (3)
Te2—Ba1—Te1^{i}	124.25 (13)	Te6^{v}—Sb1—Te3^{v}	89.60 (3)
Te4^{i}—Ba1—Te1^{i}	72.314 (18)	Te1^{iii}—Sb1—Te3^{v}	98.91 (4)
Te6—Ba1—Te1^{i}	67.255 (19)	Te6^{v}—Sb1—Te5^{xi}	93.94 (3)
Te8—Ba1—Te1^{i}	136.45 (2)	Te1^{iii}—Sb1—Te5^{xi}	173.55 (4)
Te3—Ba1—Te1^{i}	78.29 (2)	Te3^{v}—Sb1—Te5^{xi}	85.49 (3)
Te19—Ba1—Te1^{i}	49.272 (14)	Te8—Sb2—Te7^{vii}	96.64 (3)
Te1—Ba1—Te1^{i}	133.744 (17)	Te8—Sb2—Te10	92.97 (2)
Te3^{ii}—Ba1—Te1^{i}	122.15 (2)	Te7^{vii}—Sb2—Te10	90.56 (2)
Te2^{iii}—Ba2—Te4^{iv}	112.95 (13)	Te8—Sb2—Te1	93.46 (3)
Te2^{iii}—Ba2—Te19^{v}	48.71 (12)	Te7^{vii}—Sb2—Te1	94.17 (3)
Te4^{iv}—Ba2—Te19^{v}	78.768 (15)	Te10—Sb2—Te1	171.52 (3)

$Te2^{iii}$—Ba2—$Te6^{v}$	82.26 (16)	Te8—Sb2—Te5	87.45 (2)
$Te4^{iv}$—Ba2—$Te6^{v}$	138.38 (2)	$Te7^{vii}$—Sb2—Te5	175.45 (3)
$Te19^{v}$—Ba2—$Te6^{v}$	85.204 (17)	Te10—Sb2—Te5	87.22 (2)
$Te2^{iii}$—Ba2—Te5	117.69 (15)	Te1—Sb2—Te5	87.56 (2)
$Te4^{iv}$—Ba2—Te5	77.747 (18)	Te8—Sb2—Te2	84.65 (15)
$Te19^{v}$—Ba2—Te5	142.504 (18)	$Te7^{vii}$—Sb2—Te2	79.28 (15)
$Te6^{v}$—Ba2—Te5	131.01 (2)	Te10—Sb2—Te2	169.20 (17)
$Te2^{iii}$—Ba2—Te4	78.91 (12)	Te1—Sb2—Te2	18.33 (16)
$Te4^{iv}$—Ba2—Te4	149.613 (19)	Te5—Sb2—Te2	103.16 (15)
$Te19^{v}$—Ba2—Te4	124.512 (18)	Te13—Sb3—Te7	101.39 (3)
$Te6^{v}$—Ba2—Te4	68.744 (18)	Te13—Sb3—Te11	98.00 (3)
Te5—Ba2—Te4	72.095 (18)	Te7—Sb3—Te11	96.97 (3)
$Te2^{iii}$—Ba2—Te9	163.17 (15)	Te18—Sb4—Te17	96.66 (3)
$Te4^{iv}$—Ba2—Te9	83.016 (17)	Te18—Sb4—$Te11^{vi}$	106.02 (3)
$Te19^{v}$—Ba2—Te9	135.34 (2)	Te17—Sb4—$Te11^{vi}$	87.66 (2)
$Te6^{v}$—Ba2—Te9	82.025 (17)	Te2—Te1—$Sb1^{i}$	132.9 (4)
Te5—Ba2—Te9	69.459 (16)	Te2—Te1—Sb2	86.8 (4)
Te4—Ba2—Te9	89.801 (17)	$Sb1^{i}$—Te1—Sb2	126.50 (3)
$Te2^{iii}$—Ba2—$Te3^{iii}$	51.17 (16)	Te2—Te1—$Te19^{iii}$	69.2 (4)
$Te4^{iv}$—Ba2—$Te3^{iii}$	82.283 (18)	$Sb1^{i}$—Te1—$Te19^{iii}$	127.02 (3)
$Te19^{v}$—Ba2—$Te3^{iii}$	76.152 (18)	Sb2—Te1—$Te19^{iii}$	96.94 (2)
$Te6^{v}$—Ba2—$Te3^{iii}$	130.60 (2)	Te2—Te1—Ba1	64.3 (4)
Te5—Ba2—$Te3^{iii}$	72.07 (2)	$Sb1^{i}$—Te1—Ba1	79.54 (3)
Te4—Ba2—$Te3^{iii}$	85.001 (19)	Sb2—Te1—Ba1	93.87 (2)

Te9—Ba2—Te3^{iii}	140.88 (2)	Te19^{iii}—Te1—Ba1	131.39 (3)
Te2^{iii}—Ba2—Te1^{iii}	15.19 (16)	Te2—Te1—Ba2^{i}	64.4 (4)
Te4^{iv}—Ba2—Te1^{iii}	123.58 (2)	Sb1^{i}—Te1—Ba2^{i}	84.41 (3)
Te19^{v}—Ba2—Te1^{iii}	49.909 (14)	Sb2—Te1—Ba2^{i}	148.47 (3)
Te6^{v}—Ba2—Te1^{iii}	67.079 (18)	Te19^{iii}—Te1—Ba2^{i}	62.111 (15)
Te5—Ba2—Te1^{iii}	127.79 (2)	Ba1—Te1—Ba2^{i}	85.22 (2)
Te4—Ba2—Te1^{iii}	74.686 (18)	Te2—Te1—Ba1^{iii}	131.9 (4)
Te9—Ba2—Te1^{iii}	148.67 (2)	Sb1^{i}—Te1—Ba1^{iii}	77.86 (3)
Te3^{iii}—Ba2—Te1^{iii}	65.92 (2)	Sb2—Te1—Ba1^{iii}	102.41 (3)
Te2^{iii}—Ba2—Te7^{v}	105.80 (14)	Te19^{iii}—Te1—Ba1^{iii}	62.857 (16)
Te4^{iv}—Ba2—Te7^{v}	78.770 (18)	Ba1—Te1—Ba1^{iii}	157.120 (19)
Te19^{v}—Ba2—Te7^{v}	65.664 (15)	Ba2^{i}—Te1—Ba1^{iii}	89.04 (2)
Te6^{v}—Ba2—Te7^{v}	59.640 (17)	Te1—Te2—Te19^{iii}	92.0 (5)
Te5—Ba2—Te7^{v}	135.83 (2)	Te1—Te2—Te3	161.9 (5)
Te4—Ba2—Te7^{v}	126.53 (2)	Te19^{iii}—Te2—Te3	97.1 (2)
Te9—Ba2—Te7^{v}	70.972 (17)	Te1—Te2—Sb2	74.8 (4)
Te3^{iii}—Ba2—Te7^{v}	139.87 (2)	Te19^{iii}—Te2—Sb2	98.9 (2)
Te1^{iii}—Ba2—Te7^{v}	96.34 (2)	Te3—Te2—Sb2	118.8 (2)
Te2^{iii}—Ba2—Ba7^{vi}	114.84 (14)	Te1—Te2—Ba1	100.4 (4)
Te4^{iv}—Ba2—Ba7^{vi}	132.063 (18)	Te19^{iii}—Te2—Ba1	161.0 (3)
Te19^{v}—Ba2—Ba7^{vi}	133.321 (17)	Te3—Te2—Ba1	67.28 (17)
Te6^{v}—Ba2—Ba7^{vi}	48.177 (14)	Sb2—Te2—Ba1	98.26 (17)
Te5—Ba2—Ba7^{vi}	83.721 (15)	Te1—Te2—Ba2^{i}	100.4 (4)
Te4—Ba2—Ba7^{vi}	48.434 (13)	Te19^{iii}—Te2—Ba2^{i}	68.12 (13)

Te9—Ba2—Ba7^{vi}	49.051 (13)	Te3—Te2—Ba2^{i}	68.95 (16)
Te3^{iii}—Ba2—Ba7^{vi}	132.615 (19)	Sb2—Te2—Ba2^{i}	166.3 (3)
Te1^{iii}—Ba2—Ba7^{vi}	102.728 (18)	Ba1—Te2—Ba2^{i}	95.27 (18)
Te7^{v}—Ba2—Ba7^{vi}	85.002 (15)	Te2—Te3—Sb1^{xii}	137.55 (13)
Te6—Ba3—Te3	73.198 (18)	Te2—Te3—Ba3	91.76 (12)
Te6—Ba3—Te12^{vii}	86.88 (2)	Sb1^{xii}—Te3—Ba3	80.83 (2)
Te3—Ba3—Te12^{vii}	139.18 (2)	Te2—Te3—Ba1	60.33 (13)
Te6—Ba3—Te8	69.375 (19)	Sb1^{xii}—Te3—Ba1	77.49 (2)
Te3—Ba3—Te8	88.002 (19)	Ba3—Te3—Ba1	87.004 (19)
Te12^{vii}—Ba3—Te8	118.25 (2)	Te2—Te3—Ba2^{i}	59.88 (12)
Te6—Ba3—Te7^{vii}	137.06 (2)	Sb1^{xii}—Te3—Ba2^{i}	126.61 (3)
Te3—Ba3—Te7^{vii}	82.41 (2)	Ba3—Te3—Ba2^{i}	149.75 (3)
Te12^{vii}—Ba3—Te7^{vii}	132.07 (2)	Ba1—Te3—Ba2^{i}	87.30 (2)
Te8—Ba3—Te7^{vii}	75.082 (18)	Te2—Te3—Ba1^{vii}	88.56 (13)
Te6—Ba3—Te13^{vii}	122.70 (2)	Sb1^{xii}—Te3—Ba1^{vii}	132.04 (3)
Te3—Ba3—Te13^{vii}	155.99 (3)	Ba3—Te3—Ba1^{vii}	86.520 (19)
Te12^{vii}—Ba3—Te13^{vii}	63.877 (18)	Ba1—Te3—Ba1^{vii}	147.97 (3)
Te8—Ba3—Te13^{vii}	82.376 (17)	Ba2^{i}—Te3—Ba1^{vii}	82.743 (19)
Te7^{vii}—Ba3—Te13^{vii}	73.884 (17)	Ba2^{xi}—Te4—Ba1^{iii}	88.319 (18)
Te6—Ba3—Te8^{vii}	140.86 (2)	Ba2^{xi}—Te4—Ba7^{vi}	96.493 (18)
Te3—Ba3—Te8^{vii}	89.305 (19)	Ba1^{iii}—Te4—Ba7^{vi}	164.12 (2)
Te12^{vii}—Ba3—Te8^{vii}	84.244 (17)	Ba2^{xi}—Te4—Ba2	167.21 (2)
Te8—Ba3—Te8^{vii}	146.374 (19)	Ba1^{iii}—Te4—Ba2	90.045 (18)
Te7^{vii}—Ba3—Te8^{vii}	71.338 (17)	Ba7^{vi}—Te4—Ba2	81.911 (17)

Te13^{vii}—Ba3—Te8^{vii}	86.724 (17)	Si1—Te5—Sb2	79.15 (6)
Te6—Ba3—Te5^{vii}	73.364 (19)	Si1—Te5—Sb1^{iv}	133.87 (6)
Te3—Ba3—Te5^{vii}	72.393 (19)	Sb2—Te5—Sb1^{iv}	145.57 (3)
Te12^{vii}—Ba3—Te5^{vii}	67.823 (18)	Si1—Te5—Ba2	88.93 (7)
Te8—Ba3—Te5^{vii}	141.57 (2)	Sb2—Te5—Ba2	105.96 (2)
Te7^{vii}—Ba3—Te5^{vii}	131.75 (2)	Sb1^{iv}—Te5—Ba2	87.00 (3)
Te13^{vii}—Ba3—Te5^{vii}	127.088 (19)	Si1—Te5—Ba3^{ii}	87.59 (6)
Te8^{vii}—Ba3—Te5^{vii}	67.973 (17)	Sb2—Te5—Ba3^{ii}	98.57 (2)
Te6—Ba3—Ba4^{vii}	135.041 (19)	Sb1^{iv}—Te5—Ba3^{ii}	77.12 (2)
Te3—Ba3—Ba4^{vii}	135.452 (19)	Ba2—Te5—Ba3^{ii}	154.09 (2)
Te12^{vii}—Ba3—Ba4^{vii}	48.383 (14)	Sb1^{xii}—Te6—Ba3	87.79 (3)
Te8—Ba3—Ba4^{vii}	130.350 (17)	Sb1^{xii}—Te6—Ba7^{ix}	98.47 (3)
Te7^{vii}—Ba3—Ba4^{vii}	86.711 (15)	Ba3—Te6—Ba7^{ix}	93.704 (19)
Te13^{vii}—Ba3—Ba4^{vii}	48.053 (13)	Sb1^{xii}—Te6—Ba1	84.28 (3)
Te8^{vii}—Ba3—Ba4^{vii}	46.467 (13)	Ba3—Te6—Ba1	88.62 (2)
Te5^{vii}—Ba3—Ba4^{vii}	83.714 (15)	Ba7^{ix}—Te6—Ba1	176.46 (2)
Te8—Ba4—Te13	89.895 (17)	Sb1^{xii}—Te6—Ba2^{xii}	89.79 (3)
Te8—Ba4—Te13^{vii}	84.238 (17)	Ba3—Te6—Ba2^{xii}	175.05 (2)
Te13—Ba4—Te13^{vii}	145.938 (18)	Ba7^{ix}—Te6—Ba2^{xii}	82.371 (19)
Te8—Ba4—Te12	86.267 (17)	Ba1—Te6—Ba2^{xii}	95.44 (2)
Te13—Ba4—Te12	64.103 (18)	Sb3—Te7—Sb2^{ii}	98.69 (3)
Te13^{vii}—Ba4—Te12	148.15 (2)	Sb3—Te7—Ba3^{ii}	92.14 (2)
Te8—Ba4—Te16^{vi}	136.55 (2)	Sb2^{ii}—Te7—Ba3^{ii}	92.54 (2)
Te13—Ba4—Te16^{vi}	125.89 (2)	Sb3—Te7—Ba2^{xii}	105.37 (2)

Te13^{vii}—Ba4—Te16^{vi}	77.726 (16)	Sb2^{ii}—Te7—Ba2^{xii}	93.03 (2)
Te12—Ba4—Te16^{vi}	88.747 (19)	Ba3^{ii}—Te7—Ba2^{xii}	160.58 (2)
Te8—Ba4—Te10	73.308 (17)	Sb2—Te8—Ba4	99.80 (2)
Te13—Ba4—Te10	129.124 (19)	Sb2—Te8—Ba1	99.19 (2)
Te13^{vii}—Ba4—Te10	81.054 (18)	Ba4—Te8—Ba1	160.63 (2)
Te12—Ba4—Te10	67.097 (18)	Sb2—Te8—Ba3	94.31 (2)
Te16^{vi}—Ba4—Te10	65.082 (16)	Ba4—Te8—Ba3	95.631 (18)
Te8—Ba4—Te11	70.279 (16)	Ba1—Te8—Ba3	86.722 (18)
Te13—Ba4—Te11	72.063 (17)	Sb2—Te8—Ba3^{ii}	105.69 (2)
Te13^{vii}—Ba4—Te11	74.382 (17)	Ba4—Te8—Ba3^{ii}	84.217 (17)
Te12—Ba4—Te11	129.956 (19)	Ba1—Te8—Ba3^{ii}	87.008 (18)
Te16^{vi}—Ba4—Te11	138.292 (19)	Ba3—Te8—Ba3^{ii}	159.75 (2)
Te10—Ba4—Te11	137.56 (2)	Si1—Te9—Ba7^{vi}	87.18 (6)
Te8—Ba4—Te15	149.24 (2)	Si1—Te9—Ba7^{x}	76.06 (6)
Te13—Ba4—Te15	84.715 (17)	Ba7^{vi}—Te9—Ba7^{x}	161.92 (2)
Te13^{vii}—Ba4—Te15	83.511 (16)	Si1—Te9—Ba6^{vi}	75.39 (6)
Te12—Ba4—Te15	117.789 (19)	Ba7^{vi}—Te9—Ba6^{vi}	94.755 (18)
Te16^{vi}—Ba4—Te15	67.219 (16)	Ba7^{x}—Te9—Ba6^{vi}	87.637 (17)
Te10—Ba4—Te15	131.922 (19)	Si1—Te9—Ba2	86.32 (6)
Te11—Ba4—Te15	79.267 (17)	Ba7^{vi}—Te9—Ba2	79.918 (16)
Te8—Ba4—Ba3^{ii}	49.316 (14)	Ba7^{x}—Te9—Ba2	92.096 (17)
Te13—Ba4—Ba3^{ii}	48.856 (13)	Ba6^{vi}—Te9—Ba2	161.22 (2)
Te13^{vii}—Ba4—Ba3^{ii}	133.436 (17)	Si1—Te10—Sb2	80.39 (6)
Te12—Ba4—Ba3^{ii}	47.982 (14)	Si1—Te10—Ba7^{vi}	87.03 (6)

$Te16^{vi}$—Ba4—$Ba3^{ii}$	136.079 (18)	Sb2—Te10—$Ba7^{vi}$	99.53 (2)
Te10—Ba4—$Ba3^{ii}$	87.392 (15)	Si1—Te10—Ba4	89.31 (6)
Te11—Ba4—$Ba3^{ii}$	85.152 (14)	Sb2—Te10—Ba4	93.66 (2)
Te15—Ba4—$Ba3^{ii}$	133.571 (17)	$Ba7^{vi}$—Te10—Ba4	165.52 (2)
Te15—Ba5—Te14	71.868 (17)	Sb3—Te11—$Sb4^{ix}$	104.86 (2)
Te15—Ba5—$Te15^{ii}$	150.812 (18)	Sb3—Te11—Ba4	92.44 (2)
Te14—Ba5—$Te15^{ii}$	78.944 (18)	$Sb4^{ix}$—Te11—Ba4	100.07 (2)
Te15—Ba5—Te16	88.309 (17)	Sb3—Te11—$Ba7^{ix}$	105.45 (2)
Te14—Ba5—Te16	132.64 (2)	$Sb4^{ix}$—Te11—$Ba7^{ix}$	85.61 (2)
$Te15^{ii}$—Ba5—Te16	112.094 (19)	Ba4—Te11—$Ba7^{ix}$	159.27 (2)
Te15—Ba5—$Te16^{viii}$	136.77 (2)	Si1—Te12—$Ba6^{vi}$	78.16 (6)
Te14—Ba5—$Te16^{viii}$	142.24 (2)	Si1—Te12—$Ba7^{x}$	76.81 (6)
$Te15^{ii}$—Ba5—$Te16^{viii}$	69.765 (17)	$Ba6^{vi}$—Te12—$Ba7^{x}$	90.51 (2)
Te16—Ba5—$Te16^{viii}$	80.178 (18)	Si1—Te12—$Ba3^{ii}$	92.06 (6)
Te15—Ba5—Te13	88.110 (17)	$Ba6^{vi}$—Te12—$Ba3^{ii}$	169.18 (2)
Te14—Ba5—Te13	78.995 (17)	$Ba7^{x}$—Te12—$Ba3^{ii}$	91.745 (19)
$Te15^{ii}$—Ba5—Te13	86.493 (17)	Si1—Te12—Ba4	91.82 (6)
Te16—Ba5—Te13	144.51 (2)	$Ba6^{vi}$—Te12—Ba4	91.979 (19)
$Te16^{viii}$—Ba5—Te13	78.519 (16)	$Ba7^{x}$—Te12—Ba4	167.60 (2)
Te15—Ba5—Te18	88.610 (16)	$Ba3^{ii}$—Te12—Ba4	83.635 (19)
Te14—Ba5—Te18	73.039 (17)	Sb3—Te13—Ba5	102.97 (2)
$Te15^{ii}$—Ba5—Te18	82.687 (17)	Sb3—Te13—Ba4	96.14 (2)
Te16—Ba5—Te18	63.657 (17)	Ba5—Te13—Ba4	92.529 (17)
$Te16^{viii}$—Ba5—Te18	121.437 (18)	Sb3—Te13—$Ba4^{ii}$	96.95 (2)

Te13—Ba5—Te18	151.45 (2)	Ba5—Te13—Ba4^{ii}	87.891 (17)
Te15—Ba5—Te17^{ix}	73.248 (17)	Ba4—Te13—Ba4^{ii}	166.47 (2)
Te14—Ba5—Te17^{ix}	138.31 (2)	Sb3—Te13—Ba3^{ii}	92.16 (2)
Te15^{ii}—Ba5—Te17^{ix}	132.994 (19)	Ba5—Te13—Ba3^{ii}	164.64 (2)
Te16—Ba5—Te17^{ix}	67.425 (17)	Ba4—Te13—Ba3^{ii}	83.091 (17)
Te16^{viii}—Ba5—Te17^{ix}	63.819 (17)	Ba4^{ii}—Te13—Ba3^{ii}	92.972 (17)
Te13—Ba5—Te17^{ix}	77.751 (17)	Si2—Te14—Ba5	86.49 (6)
Te18—Ba5—Te17^{ix}	128.015 (18)	Si2—Te14—Ba6^{vi}	88.86 (6)
Te15—Ba5—Ba6	49.045 (13)	Ba5—Te14—Ba6^{vi}	153.23 (2)
Te14—Ba5—Ba6	87.449 (15)	Si2—Te15—Ba5	85.91 (5)
Te15^{ii}—Ba5—Ba6	130.695 (17)	Si2—Te15—Ba5^{vii}	80.91 (5)
Te16—Ba5—Ba6	49.514 (13)	Ba5—Te15—Ba5^{vii}	166.81 (2)
Te16^{viii}—Ba5—Ba6	129.057 (18)	Si2—Te15—Ba6	90.80 (5)
Te13—Ba5—Ba6	137.120 (18)	Ba5—Te15—Ba6	83.340 (16)
Te18—Ba5—Ba6	48.076 (13)	Ba5^{vii}—Te15—Ba6	97.194 (17)
Te17^{ix}—Ba5—Ba6	86.617 (15)	Si2—Te15—Ba4	75.62 (5)
Te12^{ix}—Ba6—Te18	126.39 (2)	Ba5—Te15—Ba4	90.569 (17)
Te12^{ix}—Ba6—Te15	136.89 (2)	Ba5^{vii}—Te15—Ba4	85.775 (17)
Te18—Ba6—Te15	90.222 (17)	Ba6—Te15—Ba4	165.52 (2)
Te12^{ix}—Ba6—Te18^{vii}	76.384 (17)	Si2^{ix}—Te16—Ba5	92.60 (6)
Te18—Ba6—Te18^{vii}	145.957 (18)	Si2^{ix}—Te16—Ba5^{viii}	80.96 (6)
Te15—Ba6—Te18^{vii}	84.176 (17)	Ba5—Te16—Ba5^{viii}	99.821 (18)
Te12^{ix}—Ba6—Te9^{ix}	70.744 (18)	Si2^{ix}—Te16—Ba4^{ix}	78.47 (5)
Te18—Ba6—Te9^{ix}	82.737 (17)	Ba5—Te16—Ba4^{ix}	167.52 (2)

Te15—Ba6—Te9^{ix}	144.38 (2)	Ba5^{viii}—Te16—Ba4^{ix}	87.479 (19)
Te18^{vii}—Ba6—Te9^{ix}	82.580 (17)	Si2^{ix}—Te16—Ba6	90.41 (6)
Te12^{ix}—Ba6—Te16	90.13 (2)	Ba5—Te16—Ba6	82.194 (18)
Te18—Ba6—Te16	64.807 (17)	Ba5^{viii}—Te16—Ba6	171.20 (2)
Te15—Ba6—Te16	86.086 (17)	Ba4^{ix}—Te16—Ba6	89.106 (18)
Te18^{vii}—Ba6—Te16	147.46 (2)	Si2—Te17—Sb4	88.23 (5)
Te9^{ix}—Ba6—Te16	121.100 (19)	Si2—Te17—Ba6	87.43 (6)
Te12^{ix}—Ba6—Te17	139.48 (2)	Sb4—Te17—Ba6	94.61 (2)
Te18—Ba6—Te17	70.113 (17)	Si2—Te17—Ba5^{vi}	86.94 (6)
Te15—Ba6—Te17	68.523 (16)	Sb4—Te17—Ba5^{vi}	106.76 (2)
Te18^{vii}—Ba6—Te17	76.627 (17)	Ba6—Te17—Ba5^{vi}	157.70 (2)
Te9^{ix}—Ba6—Te17	76.278 (17)	Sb4—Te18—Ba6	98.29 (2)
Te16—Ba6—Te17	127.621 (19)	Sb4—Te18—Ba6^{ii}	96.36 (2)
Te12^{ix}—Ba6—Te14^{ix}	68.719 (18)	Ba6—Te18—Ba6^{ii}	165.11 (2)
Te18—Ba6—Te14^{ix}	129.176 (19)	Sb4—Te18—Ba7	89.50 (2)
Te15—Ba6—Te14^{ix}	70.274 (17)	Ba6—Te18—Ba7	95.099 (17)
Te18^{vii}—Ba6—Te14^{ix}	80.148 (17)	Ba6^{ii}—Te18—Ba7	87.692 (17)
Te9^{ix}—Ba6—Te14^{ix}	138.59 (2)	Sb4—Te18—Ba5	102.05 (2)
Te16—Ba6—Te14^{ix}	67.344 (17)	Ba6—Te18—Ba5	80.562 (16)
Te17—Ba6—Te14^{ix}	134.18 (2)	Ba6^{ii}—Te18—Ba5	93.774 (17)
Te12^{ix}—Ba6—Ba5	137.342 (19)	Ba7—Te18—Ba5	168.10 (2)
Te18—Ba6—Ba5	51.363 (13)	Te2^{ii}—Te19—Te2^{i}	180.0 (4)
Te15—Ba6—Ba5	47.615 (13)	Te2^{ii}—Te19—Te1^{ii}	18.83 (19)
Te18^{vii}—Ba6—Ba5	131.766 (17)	Te2^{i}—Te19—Te1^{ii}	161.17 (19)

Te9^{ix}—Ba6—Ba5	133.863 (18)	Te2^{ii}—Te19—Te1^{i}	161.17 (19)
Te16—Ba6—Ba5	48.293 (13)	Te2^{i}—Te19—Te1^{i}	18.83 (19)
Te17—Ba6—Ba5	82.934 (14)	Te1^{ii}—Te19—Te1^{i}	180.00 (4)
Te14^{ix}—Ba6—Ba5	83.962 (15)	Te2^{ii}—Te19—Ba2^{xii}	116.83 (13)
Te6^{vi}—Ba7—Te4^{ix}	70.252 (18)	Te2^{i}—Te19—Ba2^{xii}	63.17 (13)
Te6^{vi}—Ba7—Te12^{x}	86.90 (2)	Te1^{ii}—Te19—Ba2^{xii}	112.020 (16)
Te4^{ix}—Ba7—Te12^{x}	126.23 (2)	Te1^{i}—Te19—Ba2^{xii}	67.980 (16)
Te6^{vi}—Ba7—Te10^{ix}	137.77 (2)	Te2^{ii}—Te19—Ba2^{xiii}	63.17 (13)
Te4^{ix}—Ba7—Te10^{ix}	78.105 (18)	Te2^{i}—Te19—Ba2^{xiii}	116.83 (13)
Te12^{x}—Ba7—Te10^{ix}	135.06 (2)	Te1^{ii}—Te19—Ba2^{xiii}	67.980 (16)
Te6^{vi}—Ba7—Te9^{ix}	84.505 (17)	Te1^{i}—Te19—Ba2^{xiii}	112.020 (16)
Te4^{ix}—Ba7—Te9^{ix}	92.587 (17)	Ba2^{xii}—Te19—Ba2^{xiii}	180.000 (18)
Te12^{x}—Ba7—Te9^{ix}	134.08 (2)	Te2^{ii}—Te19—Ba1^{xiv}	86.65 (19)
Te10^{ix}—Ba7—Te9^{ix}	69.451 (17)	Te2^{i}—Te19—Ba1^{xiv}	93.35 (19)
Te6^{vi}—Ba7—Te9^{x}	124.99 (2)	Te1^{ii}—Te19—Ba1^{xiv}	67.872 (19)
Te4^{ix}—Ba7—Te9^{x}	83.951 (18)	Te1^{i}—Te19—Ba1^{xiv}	112.128 (19)
Te12^{x}—Ba7—Te9^{x}	70.292 (18)	Ba2^{xii}—Te19—Ba1^{xiv}	85.792 (15)
Te10^{ix}—Ba7—Te9^{x}	76.875 (18)	Ba2^{xiii}—Te19—Ba1^{xiv}	94.208 (15)
Te9^{ix}—Ba7—Te9^{x}	146.115 (19)	Te2^{ii}—Te19—Ba1	93.35 (19)
Te6^{vi}—Ba7—Te18	139.69 (2)	Te2^{i}—Te19—Ba1	86.65 (19)
Te4^{ix}—Ba7—Te18	148.23 (2)	Te1^{ii}—Te19—Ba1	112.129 (19)
Te12^{x}—Ba7—Te18	75.325 (17)	Te1^{i}—Te19—Ba1	67.871 (19)
Te10^{ix}—Ba7—Te18	70.816 (16)	Ba2^{xii}—Te19—Ba1	94.208 (15)
Te9^{ix}—Ba7—Te18	82.749 (17)	Ba2^{xiii}—Te19—Ba1	85.792 (15)

Te9^{x}—Ba7—Te18	82.819 (16)	Ba1^{xiv}—Te19—Ba1	180.0
Sb1^{i}—Te1—Te2—Te19^{iii}	-121.8 (3)	Ba1—Te1—Te2—Sb2	95.84 (18)
Sb2—Te1—Te2—Te19^{iii}	98.65 (15)	Ba2^{i}—Te1—Te2—Sb2	-166.8 (2)
Ba1—Te1—Te2—Te19^{iii}	-165.5 (3)	Ba1^{iii}—Te1—Te2—Sb2	-103.9 (3)
Ba2^{i}—Te1—Te2—Te19^{iii}	-68.11 (19)	Sb1^{i}—Te1—Te2—Ba1	43.7 (5)
Ba1^{iii}—Te1—Te2—Te19^{iii}	-5.2 (5)	Sb2—Te1—Te2—Ba1	-95.84 (18)
Sb1^{i}—Te1—Te2—Te3	-1.4 (19)	Te19^{iii}—Te1—Te2—Ba1	165.5 (3)
Sb2—Te1—Te2—Te3	-141.0 (16)	Ba2^{i}—Te1—Te2—Ba1	97.4 (3)
Te19^{iii}—Te1—Te2—Te3	120.3 (16)	Ba1^{iii}—Te1—Te2—Ba1	160.30 (19)
Ba1—Te1—Te2—Te3	-45.2 (15)	Sb1^{i}—Te1—Te2—Ba2^{i}	-53.6 (5)
Ba2^{i}—Te1—Te2—Te3	52.2 (15)	Sb2—Te1—Te2—Ba2^{i}	166.8 (2)
Ba1^{iii}—Te1—Te2—Te3	115.1 (15)	Te19^{iii}—Te1—Te2—Ba2^{i}	68.11 (19)
Sb1^{i}—Te1—Te2—Sb2	139.6 (3)	Ba1—Te1—Te2—Ba2^{i}	-97.4 (3)
Te19^{iii}—Te1—Te2—Sb2	-98.65 (15)	Ba1^{iii}—Te1—Te2—Ba2^{i}	62.9 (5)

Symmetry codes: (i) -*x*, *y*-1/2, -*z*+1/2; (ii) *x*, -*y*+1/2, *z*-1/2; (iii) -*x*, *y*+1/2, -*z*+1/2; (iv) *x*, -*y*+3/2, *z*-1/2; (v) *x*, *y*+1, *z*; (vi) -*x*+1, *y*+1/2, -*z*+1/2; (vii) *x*, -*y*+1/2, *z*+1/2; (viii) -*x*+1, -*y*, -*z*; (ix) -*x*+1, *y*-1/2, -*z*+1/2; (x) -*x*+1, -*y*+1, -*z*; (xi) *x*, -*y*+3/2, *z*+1/2; (xii) *x*, *y*-1, *z*; (xiii) -*x*, -*y*+1, -*z*; (xiv) -*x*, -*y*, -*z*.

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