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$M^+M^{3+}_2As(HAsO_4)_6$ (M^+M^{3+} = TlGa, CsGa, CsAl): three new metal arsenates containing AsO_6 octahedra

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The crystal structures of hydrothermally synthesized (T = 493 K, 7 d) thallium(I) digallium arsenic(V) hexakis[hydrogenarsenate(V)], $TlGa_2As(HAsO_4)_6$, caesium digallium arsenic(V) hexakis[hydrogenarsenate(V)], $CsGa_2As(HAsO_4)_6$, and caesium dialuminium arsenic(V) hexakis[hydrogenarsenate(V)], $CsAl_2As(HAsO_4)_6$, were solved by single-crystal X-ray diffraction. The three compounds are isotypic and adopt the structure type of $RbAl_2As(HAsO_4)_6$ ($R\bar{3}c$), which itself represents a modification of the $RbFe(HPO_4)_2$ structure type and consists of a tetrahedral–octahedral framework in which the slightly disordered M^+ cations are located in channels. The three new compounds contain AsO_6 octahedra assuming the topological role of $M^{3+}O_6$ octahedra. The As—O bond lengths are among the shortest As—O bond lengths known so far in AsO_6 octahedra.

1. Chemical context

Compounds with mixed tetrahedral–octahedral (T–O) framework structures feature a broad range of different atomic arrangements, resulting in topologies with various interesting properties such as ion exchange (Masquelier *et al.*, 1996) and ion conductivity (Chouchene *et al.*, 2017), as well as unusual piezoelectric (Ren *et al.*, 2015), magnetic (Ouerfelli *et al.*, 2007) or non-linear optical features (frequency doubling) (Sun *et al.*, 2017).

The three new compounds were obtained during an extensive experimental study of the system M^+–M^{3+}–O–(H)–As^{5+} (M^+ = Li, Na, K, Rb, Cs, Ag, Tl, NH_4; M^{3+} = Al, Ga, In, Sc, Fe, Cr, Tl). This system was found to contain representatives of a large variety of new structure types (Schwendtner & Kolitsch, 2004, 2005, 2007*a*,*b*,*c*, 2017*a*, 2018*a*; Schwendtner, 2006).

Among the many different structure types found during our study, one atomic arrangement, the $RbFe(HPO_4)_2$-type (Lii & Wu, 1994; $R\bar{3}c$), and relatives thereof (Schwendtner & Kolitsch, 2018*a*) was observed to show a large crystal–chemical flexibility that allows the incorporation of a wide variety of cations. The three title compounds, $TlGa_2As(HAsO_4)_6$, $CsGa_2As(HAsO_4)_6$ and $CsAl_2As(HAsO_4)_6$ are further representatives of one of these recently described variations of the $RbFe(HPO_4)_2$ type, *viz*. the $RbAl_2As(HAsO_4)_6$ type (Schwendtner & Kolitsch, 2018*a*). It also crystallizes in $R\bar{3}c$ and up to now members with RbAl and CsFe

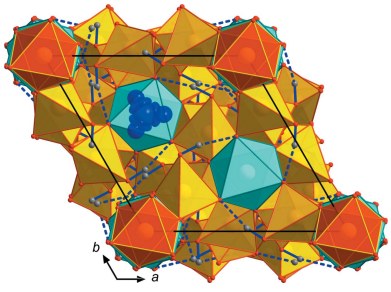

Table 1
Comparison of unit-cell parameters (Å, Å^3) for the six known isotypic compounds.

Compound	*a*	*c*	*V*
$TlGa_2As(HAsO_4)_6$	8.484 (1)	50.724 (11)	3161.9 (10)
$RbGa_2As(HAsO_4)_6$	8.491 (1)	50.697 (11)	3165.4 (10)
$CsGa_2As(HAsO_4)_6$	8.520 (1)	50.608 (11)	3181.4 (10)
$RbAl_2As(HAsO_4)_6$	8.410 (1)	50.287 (11)	3080.2 (10)
$CsAl_2As(HAsO_4)_6$	8.439 (1)	50.169 (11)	3094.2 (10)
$CsFe_2As(HAsO_4)_6$	8.582 (1)	50.942 (11)	3249.3 (10)

(Schwendtner & Kolitsch, 2018*a*) and RbGa (Schwendtner & Kolitsch, 2018*c*) as M^+M^{3+} cation combinations are known (Table 1). While all previously known M^+M^{3+} combinations adopting this structure type also have representatives adopting the $RbFe(HPO_4)_2$ type, this is not the case for the three new members.

The title compounds are rare examples of compounds containing AsO_6 octahedra. According to our review article, only about 3% of all reported arsenates(V) contain AsO_6 polyhedra (Schwendtner & Kolitsch, 2007*a*). Presently (Schwendtner & Kolitsch, 2018*a*), 41 inorganic compounds containing As in an octahedral coordination are known, including the recently published $RbGa_2As(HAsO_4)_6$ (Schwendtner & Kolitsch, 2018*c*) and the three new compounds of this study. While no arsenates(V) containing both Tl and Ga are known in the ICSD (FIZ, 2018) so far, there are two arsenates(V) containing both Cs and Ga, namely $Cs_2Ga_3(As_3O_{10})(AsO_4)_2$ (Lin & Lii, 1996) and $CsGa(H_{1.5}AsO_4)_2(H_2AsO_4)$ (Schwendtner & Kolitsch, 2005), and one arsenate(V) containing both Cs and Al, $CsAl(H_2AsO_4)(HAsO_4)$ (Schwendtner & Kolitsch, 2007*b*). In addition to the crystal structures contained in the ICSD, an indexed powder diffraction pattern of the diarsenate $CsAlAs_2O_7$ has been published (Boughzala & Jouini, 1992).

2. Structural commentary

The three title compounds are isotypic and new representatives of the $RbAl_2As(HAsO_4)_6$-structure type ($R\bar{3}c$; Schwendtner & Kolitsch, 2018*a*), which is a recently described variation of the $RbFe(HPO_4)_2$ structure type ($R\bar{3}c$; Lii & Wu, 1994) and closely related to the following two structure types: $(NH_4)Fe(HPO_4)_2$ ($P\bar{1}$; Yakubovich, 1993) and $RbAl(HAsO_4)_2$ ($R32$; Schwendtner & Kolitsch, 2018*a*). The reader is referred to our latest papers for a detailed discussion of the four related structure types (Schwendtner & Kolitsch, 2018*a*) and a review of compounds crystallizing in the $RbFe(HPO_4)_2$ and $(NH_4)Fe(HPO_4)_2$ structure types (Schwendtner & Kolitsch, 2018*b*). All of these modifications share a basic tetrahedral–octahedral framework structure featuring interpenetrating channels, which host the M^+ cations (Figs. 1, 2). The fundamental building unit in all these structure types contains $M^{3+}O_6$ octahedra, which are connected *via* their six corners to six protonated AsO_4 tetrahedra, thereby forming an $M^{3+}As_6O_{24}$ unit (Fig. 3). These units are in turn connected *via* three corners to other $M^{3+}O_6$ octahedra. The free, protonated corner of each AsO_4 tetrahedron forms a hydrogen bond to the neighbouring $M^{3+}As_6O_{24}$ group (Table 2). The $M^{3+}As_6O_{24}$ units are arranged in layers perpendicular to the c_{hex} axis (Fig. 2). When compared to the $RbFe(HPO_4)_2$ structure type, in $TlGa_2As(HAsO_4)_6$, $CsGa_2As(HAsO_4)_6$ and $CsAl_2As(HAsO_4)_6$ one third of all M^{3+} cations are replaced by As^{5+}.

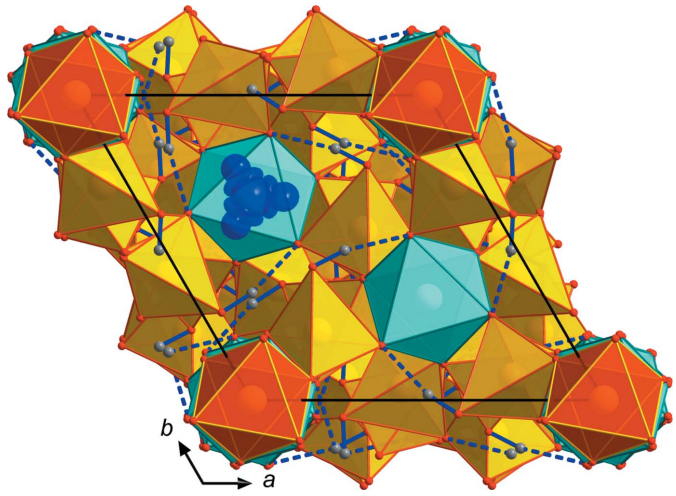

Figure 2
Structure drawing of $TlGa_2As(HAsO_4)_6$ viewed along *c*. Red octahedra = AsO_6, blue–green octahedra = GaO_6, yellow tetrahedra = AsO_4; hydrogen atoms are shown as small grey spheres. Hydrogen bonds are shown as blue lines (solid for D—H and dotted for H$\cdots A$). For the three disordered Tl positions, the displacement parameters are drawn at the 80% probability level. The unit cell is outlined.

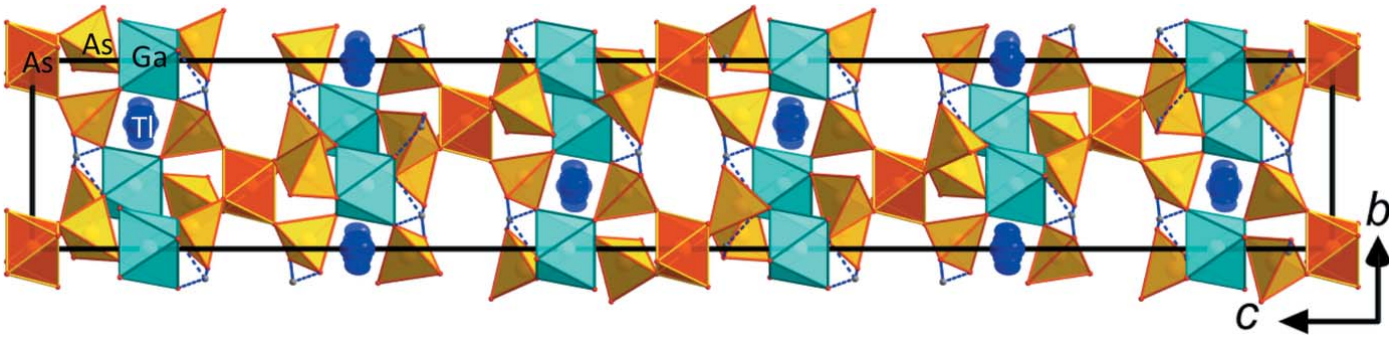

Figure 1
Structure drawing of the framework structure of $TlGa_2As(HAsO_4)_6$ viewed along *a*. The unit cell is outlined.

Table 2
Hydrogen-bond geometry (Å, °) for $CsAl_2As(HAsO_4)_6$, $CsGa_2As(HAsO_4)_6$ and $TlGa_2As(HAsO_4)_6$.

	D—H···A	D—H	H···A	D···A	D—H···A
$CsAl_2As(HAsO_4)_6$	O3—H···O4^{xiv}	0.875 (19)	1.94 (2)	2.7321 (18)	150 (3)
$CsGa_2As(HAsO_4)_6$	O3—H···O4^{xiv}	0.861 (18)	1.93 (2)	2.727 (2)	154 (3)
$TlGa_2As(HAsO_4)_6$	O3—H···O4^{xiv}	0.871 (19)	1.94 (3)	2.728 (2)	150 (4)

Symmetry code: (xiv) $y, x-1, -z+\frac{3}{2}$.

This requires that two thirds of all M^+ cations are omitted to achieve charge balance.

Like many other and all isotypic compounds containing AsO_6 octahedra, the three title compounds were grown by 'dry' hydrothermal techniques (using arsenic acid without the addition of water). The extreme abundance of As during the synthesis and the formation of a melt of arsenic acid promotes the octahedral coordination of As. As a result of the smaller ionic radius of As^{5+} this substitution also has an effect on the unit-cell parameters (Table 3) and the pore diameter. While the lengths of the c axis of all so far known $RbFe(HPO_4)_2$-type arsenates range from 52.87 (1) to 56.99 (1) Å (Schwendtner and Kolitsch, 2018*b*) and correlate well with the sizes of the involved M^+ and M^{3+} cations, the length of this axis in the $RbAl_2As(HAsO_4)_6$-type compounds is much smaller and the range of lengths much narrower [50.17 (1)–50.94 (1) Å, see Table 1]. The c unit-cell parameter correlates with the size of the involved M^{3+} cation, while the M^+ cations seem to show a negative correlation with the c parameter (Table 1). The unit-cell parameters a and V correlate well with the size of both cations, but the influence of the M^+ cations is stronger. It seems that in order to incorporate the small AsO_6 octahedron in the structure the cell widens along the a axis to incorporate the large M^+ cations and is strongly compressed along c. This effect is also visible in the hydrogen bonds that are very strong in the $RbFe(HPO_4)_2$-type arsenates with D—H···A bond lengths ranging from 2.598 (2) to 2.634 (2) Å, while for the $RbAl_2As(HAsO_4)_6$-type arsenates they range from 2.727 (2) to 2.7481 (19) Å (Schwendtner & Kolitsch, 2017*b*, 2018*a*,*b*,*c*; this paper).

Table 3
Comparison of selected bond lengths (Å) and BVSs[a] for $CsAl_2As(HAsO_4)_6$, $CsGa_2As(HAsO_4)_6$ and $TlGa_2As(HAsO_4)_6$.

	$CsAl_2As(HAsO_4)_6$	$CsGa_2As(HAsO_4)_6$	$TlGa_2As(HAsO_4)_6$
M^+1A—O2 (6×)	3.4707 (12)	3.4719 (15)	3.4419 (15)
M^+1A—O3 (6×)	3.4066 (16)	3.4829 (19)	3.4358 (19)
<M^+1A—O>/BVS	**3.439/0.75**	**3.477/0.68**	**3.439/0.46**
M^{3+}—O2 (3×)	1.8933 (13)	1.9612 (15)	1.9648 (14)
M^{3+}—O4 (3×)	1.8963 (12)	1.9679 (15)	1.9609 (14)
<M^{3+}—O>/BVS	**1.895/3.07**	**1.965/3.09**	**1.963/3.11**
$^{[6]}$As—O (6×)	1.8104 (11)	1.8109 (14)	1.8062 (14)
<$^{[6]}$As—O>/BVS	**1.810/5.27**	**1.811/5.27**	**1.806/5.34**
$^{[4]}$As—O1	1.7094 (12)	1.7089 (14)	1.7094 (14)
$^{[4]}$As—O2	1.6641 (11)	1.6646 (14)	1.6641 (14)
$^{[4]}$As—O4	1.6639 (12)	1.6670 (15)	1.6672 (14)
$^{[4]}$As—O3(H)	1.7108 (13)	1.7125 (17)	1.7115 (16)
<$^{[4]}$As—O>/BVS	**1.687/5.00**	**1.688/4.98**	**1.688/4.99**

Note: (*a*) Gagné & Hawthorne (2015).

In all three title compounds, the M^+ cations are 12-coordinated (Figs. 3, 4), and the average M^+—O bond lengths (Table 3) are longer than the average bond lengths of M^+O_{12} polyhedra of 3.377 Å for Cs (Gagné & Hawthorne, 2016) and 3.195 Å for Tl^+ (Gagné & Hawthorne, 2018), thus leading to rather low bond-valence sums (BVSs) (Gagné & Hawthorne, 2015) of only 0.46–0.75 valence units (v.u.). The lowest BVS sum was found for $^{[12]}$Tl, which shows an extremely long average Tl—O bond length (3.439 Å), considerably longer than the longest previously reported value in the literature, 3.304 Å (Gagné & Hawthorne, 2018). Considering the positions of the disordered Tl-atom positions, the BVSs would increase to 0.54 (Tl1*B*) and 0.68 v.u. (Tl1*C*).

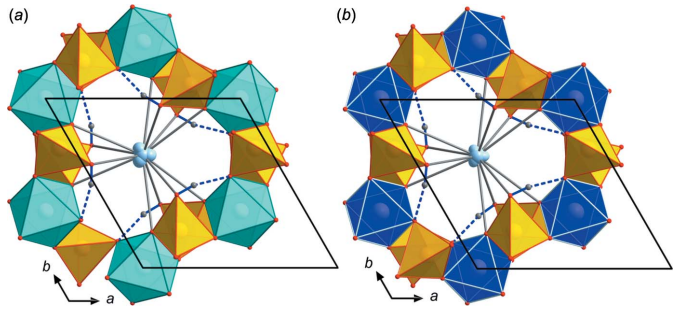

Figure 3
Comparison of the Cs atom disorder, Cs—O bonds and hydrogen-bonding scheme in (*a*) $CsGa_2As(HAsO_4)_6$ and (*b*) $CsAl_2As(HAsO_4)_6$, viewed along c. Displacement ellipsoids for Cs are drawn at the 80% probability level.

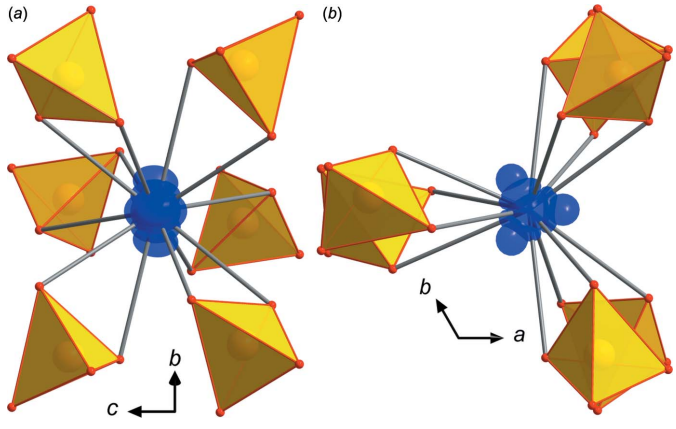

Figure 4
Tl positional disorder and Tl—O bonding scheme for $TlGa_2As(HAsO_4)_6$ viewed along a (*a*) and c (*b*). Displacement ellipsoids for Tl are drawn at the 80% probability level.

Table 4
Experimental details.

	$CsAl_2As(HAsO_4)_6$	$CsGa_2As(HAsO_4)_6$	$TlGa_2As(HAsO_4)_6$
Crystal data			
M_r	1101.36	1186.84	1258.30
Crystal system, space group	Trigonal, $R\bar{3}c$:*H*	Trigonal, $R\bar{3}c$:*H*	Trigonal, $R\bar{3}c$:*H*
Temperature (K)	293	293	293
a, *c* (Å)	8.439 (1), 50.169 (11)	8.5199 (10), 50.608 (11)	8.484 (1), 50.724 (11)
V (Å^3)	3094.2 (10)	3181.4 (10)	3161.9 (10)
Z	6	6	6
Radiation type	Mo *Kα*	Mo *Kα*	Mo *Kα*
μ (mm^{-1})	13.14	15.18	21.18
Crystal size (mm)	0.08 × 0.07 × 0.06	0.07 × 0.07 × 0.07	0.08 × 0.07 × 0.05
Data collection			
Diffractometer	Nonius KappaCCD single-crystal four-circle	Nonius KappaCCD single-crystal four-circle	Nonius KappaCCD single-crystal four-circle
Absorption correction	Multi-scan (*HKL SCALEPACK*; Otwinowski *et al.*, 2003)	Multi-scan (*HKL SCALEPACK*; Otwinowski *et al.*, 2003)	Multi-scan *HKL SCALEPACK* (Otwinowski *et al.*, 2003)
T_{min}, T_{max}	0.420, 0.506	0.416, 0.416	0.200, 0.347
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4584, 1259, 1153	4712, 1293, 1134	4682, 1285, 1129
R_{int}	0.014	0.018	0.024
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.757	0.757	0.757
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.015, 0.034, 1.11	0.018, 0.041, 1.16	0.018, 0.041, 1.10
No. of reflections	1259	1293	1285
No. of parameters	65	65	71
No. of restraints	2	2	2
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.61, −0.45	0.86, −0.73	0.74, −0.73

Computer programs: *COLLECT* (Nonius, 2003), *HKL DENZO*, *SCALEPACK* (Otwinowski *et al.*, 2003), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2005) and *publCIF* (Westrip, 2010).

These loose bondings lead to considerable positional disorder of the M^+ cations in their hosting voids, which were modelled by two overlapping Cs positions between 0.15 (2) and 0.25 (5) Å apart (Fig. 3). The main Cs-atom electron densities with 62 and 72% for the Al- and Ga-containing compounds, respectively, are located on the central position Cs1*A*. For the Tl compound, only 33% of the electron-density distribution is explained by the central Tl1*A* position, 36% by the next nearest position Tl1*B* 0.407 (7) Å away and 27% by the furthest Tl1*C* position 0.766 (9) Å apart from the central position – so three positions for Tl were needed to get a good fit explaining the electron-density distribution (Fig. 4). The effect of slightly disordered M^+ cations in this type of compound is well known and was found for most of the previously cited compounds crystallizing in these related structure types; in $TlGa_2As(HAsO_4)_6$ the positional disorder shows its most extreme form, probably as a result of the influence of the lone electron pair on the Tl^+ cation.

In contrast to the underbonded M^+ cations the AsO_6 octahedra are overbonded. The six As—O distances in each of these isotypic compounds are identical and among the shortest of all known AsO_6-containing compounds. $TlGa_2As(HAsO_4)_6$ shows the shortest average $^{[6]}$As—O distance known so far of 1.806 Å, leading to rather high BVSs of 5.34 v.u. (after Gagné & Hawthorne, 2015). The grand mean As—O bond distance in AsO_6 octahedra in inorganic compounds is 1.830 (2) Å according to Schwendtner & Kolitsch (2007*a*); this value was determined from 33 AsO_6 octahedra of 31 compounds. Gagné & Hawthorne (2018) determined an identical, but less precise, value of 1.83 (3) Å, based on only 13 AsO_6 octahedra in AsO_6-containing compounds.

A further, indirect effect of the substituting AsO_6 octahedra is a notable change in the As—O distances of the protonated AsO_4 tetrahedra. The average As—O distance in these AsO_4 tetrahedra, with values between 1.687 and 1.688 Å, is slightly larger in all three compounds than the statistical average of 1.686 (10) Å (Schwendtner, 2008). The BVSs (Gagné & Hawthorne, 2015) are close to ideal values (4.98–5.00 v.u.). The AsO_4 tetrahedra have two short bond lengths to connected $M^{3+}O_6$ octahedra, but the $^{[4]}$As—O bond length of the O atom shared with the AsO_6 octahedra is elongated (Table 3) because of $^{[4]}$As—O—$^{[6]}$As repulsion. The $^{[4]}$As—O···H bond is therefore shorter than the average distance of As—O···H bonds in $HAsO_4$ groups [1.72 (3) Å; Schwendtner, 2008].

The average M^{3+}—O bond lengths of the octahedrally coordinated Ga cations (1.963–1.965 Å) and Al cations (1.895 Å) are slightly shorter than the grand mean averages of 1.978 (17) and 1.903 (14) Å for $^{[6]}$Ga—O and $^{[6]}$Al—O, respectively (Gagné & Hawthorne, 2018), explaining the slightly higher corresponding BVSs of 3.07 to 3.11 v.u.

3. Synthesis and crystallization

The compounds were grown by hydrothermal synthesis at 493 K (7 d, autogeneous pressure, slow furnace cooling) using

Teflon-lined stainless steel autoclaves with an approximate filling volume of 2 cm^3. Reagent-grade Cs_2CO_3, Tl_2CO_3, Ga_2O_3, Al_2O_3 and $H_3AsO_4{\cdot}0.5H_2O$ were used as starting reagents in approximate volume ratios of M^+:M^{3+}:As of 1:1:3, 1:2:4 and 1:1:2 for the TlGa-, CsGa- and CsAl-synthesis batches, respectively. No additional water was added and arsenic acid was present in excess to promote the growth of crystals from a melt or even vapor of arsenic acid under extremely acidic conditions. All three compounds formed large, colourless, pseudo-octahedral crystals, $TlGa_2As(HAsO_4)_6$ was accompanied by colourless, acicular-to-prismatic crystals of $Ga(H_2AsO_4)(H_2As_2O_7)$ (Schwendtner & Kolitsch, 2017*a*). All crystals were extracted mechanically and not further washed; they are slightly hygroscopic and decompose slowly over a period of several years.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4.

For reasons of comparison, the coordinates of $RbAl_2As(HAsO_4)_6$ (Schwendtner & Kolitsch, 2018*a*) were used for the refinement. These coordinates are also comparable to the related $RbFe(HPO_4)_2$ structure type ($R\bar{3}c$; Lii & Wu, 1994). In all compounds, O—H bonds were restrained to 0.9±0.02 Å. During the last refinement steps, residual electron-density peaks of up to 5.54 e $Å^{-3}$ were located close to the M^+ sites, suggesting irregular displacement parameters and split positions, similar to what was found for many other $RbFe(HPO_4)_2$-type compounds and relatives thereof (Lesage *et al.*, 2007; Schwendtner and Kolitsch, 2018*a*,*b*). Therefore, a further position M^+1B was included in the refinements, which refined to low occupancies and led to considerable decreases in the R factors and weight parameters for all compounds.

This, however, was not satisfactory for $TlGa_2As(HAsO_4)_6$, where it led to negative electron densities of −2.3 e $Å^{-3}$ at the centre of the Tl1A position, probably an effect of the lone electron pair. Therefore, the Tl atoms were again removed from the model and the three highest residual electron densities from the difference-Fourier map were then refined simultaneously as Tl1a, Tl1b and Tl1c. This led to a much better fit explaining the disordered electron density. The refined bulk occupancies on the disordered M^+ positions in all compounds were very close to 1, but a restraint was still set in all cases to give a total occupancy of 1.00. The final residual electron densities in all title compounds are < 1 e $Å^{-3}$.

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supporting information

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$M^+M^{3+}{}_2As(HAsO_4)_6$ (M^+M^{3+} = TlGa, CsGa, CsAl): three new metal arsenates containing AsO_6 octahedra

Karolina Schwendtner and Uwe Kolitsch

Computing details

For all structures, data collection: *COLLECT* (Nonius, 2003). Cell refinement: (*HKL SCALEPACK*; Otwinowski *et al.*, 2003) for CsAl2AsHAsO46; *HKL SCALEPACK* (Otwinowski *et al.*, 2003) for CsGa2AsHAsO46, TlGa2AsHAsO46. For all structures, data reduction: *HKL DENZO*, *SCALEPACK* (Otwinowski *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Caesium dialuminium arsenic(V) hexakis[hydrogen arsenate(V)] (CsAl2AsHAsO46)

Crystal data

$CsAl_2As(HAsO_4)_6$
M_r = 1101.36
Trigonal, $R\bar{3}c$:*H*
a = 8.439 (1) Å
c = 50.169 (11) Å
V = 3094.2 (10) Å^3
Z = 6
F(000) = 3060
D_x = 3.546 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2513 reflections
θ = 2.4–32.5°
μ = 13.14 mm^{-1}
T = 293 K
Large pseudo-octahedra, colourless
0.08 × 0.07 × 0.06 mm

Data collection

Nonius KappaCCD single-crystal four-circle diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (HKL SCALEPACK; Otwinowski *et al.*, 2003)
T_{min} = 0.420, T_{max} = 0.506
4584 measured reflections
1259 independent reflections
1153 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 32.5°, θ_{min} = 2.4°
h = −12→12
k = −10→10
l = −75→75

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.034
S = 1.11
1259 reflections
65 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0121P)^2 + 14.2108P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Extinction correction: SHELXL-2016/6 (Sheldrick 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000152 (15)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cs1A	0.000000	0.000000	0.750000	0.0317 (19)	0.624 (3)
Cs1B	0.000000	−0.018 (3)	0.750000	0.023 (2)	0.1254 (9)
Al1	0.333333	0.666667	0.75637 (2)	0.00616 (14)	
As2	0.333333	0.666667	0.666667	0.00670 (8)	
As1	−0.44835 (2)	−0.41203 (2)	0.71182 (2)	0.00739 (5)	
O1	0.39564 (16)	−0.47264 (16)	0.68660 (2)	0.0100 (2)	
O2	−0.46035 (16)	−0.27705 (16)	0.73495 (2)	0.0099 (2)	
O3	−0.23352 (18)	−0.28644 (19)	0.69863 (3)	0.0178 (3)	
O4	0.48577 (16)	−0.13040 (16)	0.77831 (2)	0.0102 (2)	
H	−0.184 (5)	−0.355 (5)	0.7004 (7)	0.066 (11)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1A	0.029 (2)	0.029 (2)	0.0366 (19)	0.0146 (12)	0.000	0.000
Cs1B	0.016 (3)	0.028 (4)	0.021 (2)	0.0082 (15)	0.0021 (18)	0.0011 (9)
Al1	0.0066 (2)	0.0066 (2)	0.0053 (3)	0.00329 (11)	0.000	0.000
As2	0.00756 (11)	0.00756 (11)	0.00499 (15)	0.00378 (5)	0.000	0.000
As1	0.00831 (8)	0.00780 (8)	0.00710 (8)	0.00481 (6)	−0.00008 (5)	0.00030 (5)
O1	0.0132 (5)	0.0097 (5)	0.0085 (5)	0.0067 (4)	−0.0030 (4)	0.0000 (4)
O2	0.0106 (5)	0.0099 (5)	0.0097 (5)	0.0055 (4)	0.0007 (4)	−0.0017 (4)
O3	0.0104 (5)	0.0177 (6)	0.0245 (6)	0.0065 (5)	0.0071 (5)	0.0057 (5)
O4	0.0115 (5)	0.0082 (5)	0.0123 (5)	0.0060 (4)	−0.0028 (4)	−0.0035 (4)

Geometric parameters (Å, º)

Cs1A—Cs1B^{i}	0.15 (2)	Cs1B—O2^{iii}	3.457 (2)
Cs1A—Cs1B^{ii}	0.15 (2)	Cs1B—O3^{ii}	3.507 (14)
Cs1A—O3^{iii}	3.4066 (15)	Cs1B—O3^{v}	3.507 (14)
Cs1A—O3^{ii}	3.4066 (16)	Cs1B—O2^{v}	3.609 (19)
Cs1A—O3^{iv}	3.4066 (16)	Cs1B—O2^{ii}	3.609 (19)
Cs1A—O3	3.4066 (16)	Cs1B—O4^{vi}	4.018 (19)
Cs1A—O3^{v}	3.4066 (15)	Cs1B—O4^{vii}	4.018 (19)
Cs1A—O3^{i}	3.4066 (16)	Cs1B—As1^{i}	4.039 (10)
Cs1A—O2	3.4707 (13)	Cs1B—As1^{iv}	4.039 (10)

Cs1A—O2^{v}	3.4707 (12)	Cs1B—As1	4.057 (7)
Cs1A—O2^{i}	3.4707 (12)	Cs1B—As1^{iii}	4.057 (7)
Cs1A—O2^{iv}	3.4708 (13)	Al1—O2^{viii}	1.8933 (12)
Cs1A—O2^{iii}	3.4708 (13)	Al1—O2^{ii}	1.8933 (13)
Cs1A—O2^{ii}	3.4708 (13)	Al1—O2^{ix}	1.8934 (12)
Cs1A—As1	4.1132 (5)	Al1—O4^{x}	1.8963 (13)
Cs1A—As1^{v}	4.1132 (4)	Al1—O4^{i}	1.8963 (12)
Cs1A—As1^{i}	4.1132 (5)	Al1—O4^{xi}	1.8963 (12)
Cs1A—As1^{iv}	4.1133 (4)	As2—O1^{xii}	1.8103 (12)
Cs1A—As1^{iii}	4.1133 (4)	As2—O1^{xiii}	1.8103 (12)
Cs1A—As1^{ii}	4.1133 (5)	As2—O1^{xi}	1.8104 (11)
Cs1B—Cs1B^{i}	0.27 (4)	As2—O1^{i}	1.8104 (12)
Cs1B—Cs1B^{ii}	0.27 (4)	As2—O1^{xiv}	1.8104 (11)
Cs1B—O3^{iii}	3.345 (8)	As2—O1^{x}	1.8104 (11)
Cs1B—O3	3.345 (8)	As1—O4^{iii}	1.6639 (12)
Cs1B—O2^{i}	3.352 (16)	As1—O2	1.6641 (11)
Cs1B—O2^{iv}	3.352 (16)	As1—O1^{xv}	1.7094 (12)
Cs1B—O3^{iv}	3.376 (4)	As1—O3	1.7108 (13)
Cs1B—O3^{i}	3.376 (4)	O3—H	0.875 (19)
Cs1B—O2	3.457 (2)		

Cs1B^{i}—Cs1A—Cs1B^{ii}	120.0 (2)	O3^{v}—Cs1B—O4^{vii}	153.1 (3)
Cs1B^{i}—Cs1A—O3^{iii}	77.07 (3)	O2^{v}—Cs1B—O4^{vii}	143.57 (3)
Cs1B^{ii}—Cs1A—O3^{iii}	130.09 (4)	O2^{ii}—Cs1B—O4^{vii}	146.38 (3)
Cs1B^{i}—Cs1A—O3^{ii}	77.07 (3)	O4^{vi}—Cs1B—O4^{vii}	50.4 (3)
Cs1B^{ii}—Cs1A—O3^{ii}	65.14 (12)	Cs1B^{i}—Cs1B—As1^{i}	91.9 (2)
O3^{iii}—Cs1A—O3^{ii}	154.15 (5)	Cs1B^{ii}—Cs1B—As1^{i}	141.11 (14)
Cs1B^{i}—Cs1A—O3^{iv}	130.09 (3)	O3^{iii}—Cs1B—As1^{i}	78.8 (2)
Cs1B^{ii}—Cs1A—O3^{iv}	65.14 (12)	O3—Cs1B—As1^{i}	80.6 (2)
O3^{iii}—Cs1A—O3^{iv}	68.99 (4)	O2^{i}—Cs1B—As1^{i}	23.77 (5)
O3^{ii}—Cs1A—O3^{iv}	130.29 (5)	O2^{iv}—Cs1B—As1^{i}	101.5 (5)
Cs1B^{i}—Cs1A—O3	130.09 (3)	O3^{iv}—Cs1B—As1^{i}	137.7 (6)
Cs1B^{ii}—Cs1A—O3	77.07 (14)	O3^{i}—Cs1B—As1^{i}	24.66 (9)
O3^{iii}—Cs1A—O3	130.29 (5)	O2—Cs1B—As1^{i}	126.1 (3)
O3^{ii}—Cs1A—O3	68.99 (4)	O2^{iii}—Cs1B—As1^{i}	49.09 (10)
O3^{iv}—Cs1A—O3	99.81 (5)	O3^{ii}—Cs1B—As1^{i}	92.71 (5)
Cs1B^{i}—Cs1A—O3^{v}	65.14 (4)	O3^{v}—Cs1B—As1^{i}	125.43 (12)
Cs1B^{ii}—Cs1A—O3^{v}	77.07 (14)	O2^{v}—Cs1B—As1^{i}	143.1 (4)
O3^{iii}—Cs1A—O3^{v}	68.99 (4)	O2^{ii}—Cs1B—As1^{i}	92.74 (12)
O3^{ii}—Cs1A—O3^{v}	99.81 (5)	O4^{vi}—Cs1B—As1^{i}	64.3 (3)
O3^{iv}—Cs1A—O3^{v}	68.99 (4)	O4^{vii}—Cs1B—As1^{i}	65.5 (3)
O3—Cs1A—O3^{v}	154.15 (5)	Cs1B^{i}—Cs1B—As1^{iv}	141.1 (3)
Cs1B^{i}—Cs1A—O3^{i}	65.14 (4)	Cs1B^{ii}—Cs1B—As1^{iv}	91.9 (4)
Cs1B^{ii}—Cs1A—O3^{i}	130.09 (4)	O3^{iii}—Cs1B—As1^{iv}	80.6 (2)
O3^{iii}—Cs1A—O3^{i}	99.81 (5)	O3—Cs1B—As1^{iv}	78.8 (2)
O3^{ii}—Cs1A—O3^{i}	68.99 (4)	O2^{i}—Cs1B—As1^{iv}	101.5 (5)
O3^{iv}—Cs1A—O3^{i}	154.15 (5)	O2^{iv}—Cs1B—As1^{iv}	23.77 (5)
O3—Cs1A—O3^{i}	68.99 (4)	O3^{iv}—Cs1B—As1^{iv}	24.66 (9)

O3^{v}—Cs1A—O3^{i}	130.29 (5)	O3^{i}—Cs1B—As1^{iv}	137.7 (6)
Cs1B^{i}—Cs1A—O2	153.70 (4)	O2—Cs1B—As1^{iv}	49.09 (10)
Cs1B^{ii}—Cs1A—O2	38.5 (2)	O2^{iii}—Cs1B—As1^{iv}	126.1 (3)
O3^{iii}—Cs1A—O2	127.04 (3)	O3^{ii}—Cs1B—As1^{iv}	125.43 (12)
O3^{ii}—Cs1A—O2	78.39 (3)	O3^{v}—Cs1B—As1^{iv}	92.71 (5)
O3^{iv}—Cs1A—O2	62.83 (3)	O2^{v}—Cs1B—As1^{iv}	92.74 (12)
O3—Cs1A—O2	45.72 (3)	O2^{ii}—Cs1B—As1^{iv}	143.1 (4)
O3^{v}—Cs1A—O2	110.37 (3)	O4^{vi}—Cs1B—As1^{iv}	65.5 (3)
O3^{i}—Cs1A—O2	113.93 (3)	O4^{vii}—Cs1B—As1^{iv}	64.3 (3)
Cs1B^{i}—Cs1A—O2^{v}	83.46 (2)	As1^{i}—Cs1B—As1^{iv}	124.1 (5)
Cs1B^{ii}—Cs1A—O2^{v}	38.5 (2)	Cs1B^{i}—Cs1B—As1	135.2 (3)
O3^{iii}—Cs1A—O2^{v}	113.93 (3)	Cs1B^{ii}—Cs1B—As1	84.4 (4)
O3^{ii}—Cs1A—O2^{v}	62.83 (3)	O3^{iii}—Cs1B—As1	129.9 (5)
O3^{iv}—Cs1A—O2^{v}	78.39 (3)	O3—Cs1B—As1	24.38 (5)
O3—Cs1A—O2^{v}	110.37 (3)	O2^{i}—Cs1B—As1	96.4 (4)
O3^{v}—Cs1A—O2^{v}	45.72 (3)	O2^{iv}—Cs1B—As1	49.35 (14)
O3^{i}—Cs1A—O2^{v}	127.04 (3)	O3^{iv}—Cs1B—As1	78.22 (15)
O2—Cs1A—O2^{v}	77.02 (4)	O3^{i}—Cs1B—As1	94.4 (2)
Cs1B^{i}—Cs1A—O2^{i}	83.46 (2)	O2—Cs1B—As1	23.92 (7)
Cs1B^{ii}—Cs1A—O2^{i}	153.70 (19)	O2^{iii}—Cs1B—As1	149.8 (5)
O3^{iii}—Cs1A—O2^{i}	62.83 (3)	O3^{ii}—Cs1B—As1	78.48 (6)
O3^{ii}—Cs1A—O2^{i}	113.93 (3)	O3^{v}—Cs1B—As1	132.2 (2)
O3^{iv}—Cs1A—O2^{i}	110.37 (3)	O2^{v}—Cs1B—As1	96.79 (18)
O3—Cs1A—O2^{i}	78.39 (3)	O2^{ii}—Cs1B—As1	121.4 (3)
O3^{v}—Cs1A—O2^{i}	127.04 (3)	O4^{vi}—Cs1B—As1	92.2 (4)
O3^{i}—Cs1A—O2^{i}	45.72 (3)	O4^{vii}—Cs1B—As1	47.32 (16)
O2—Cs1A—O2^{i}	115.404 (13)	As1^{i}—Cs1B—As1	102.3 (3)
O2^{v}—Cs1A—O2^{i}	166.91 (4)	As1^{iv}—Cs1B—As1	57.07 (13)
Cs1B^{i}—Cs1A—O2^{iv}	153.70 (4)	Cs1B^{i}—Cs1B—As1^{iii}	84.4 (2)
Cs1B^{ii}—Cs1A—O2^{iv}	83.5 (2)	Cs1B^{ii}—Cs1B—As1^{iii}	135.20 (15)
O3^{iii}—Cs1A—O2^{iv}	78.39 (3)	O3^{iii}—Cs1B—As1^{iii}	24.38 (5)
O3^{ii}—Cs1A—O2^{iv}	127.04 (3)	O3—Cs1B—As1^{iii}	129.9 (5)
O3^{iv}—Cs1A—O2^{iv}	45.72 (3)	O2^{i}—Cs1B—As1^{iii}	49.35 (14)
O3—Cs1A—O2^{iv}	62.83 (3)	O2^{iv}—Cs1B—As1^{iii}	96.4 (4)
O3^{v}—Cs1A—O2^{iv}	113.93 (3)	O3^{iv}—Cs1B—As1^{iii}	94.4 (2)
O3^{i}—Cs1A—O2^{iv}	110.37 (3)	O3^{i}—Cs1B—As1^{iii}	78.22 (15)
O2—Cs1A—O2^{iv}	52.60 (4)	O2—Cs1B—As1^{iii}	149.8 (5)
O2^{v}—Cs1A—O2^{iv}	115.404 (13)	O2^{iii}—Cs1B—As1^{iii}	23.92 (7)
O2^{i}—Cs1A—O2^{iv}	77.02 (4)	O3^{ii}—Cs1B—As1^{iii}	132.2 (2)
Cs1B^{i}—Cs1A—O2^{iii}	38.51 (2)	O3^{v}—Cs1B—As1^{iii}	78.48 (6)
Cs1B^{ii}—Cs1A—O2^{iii}	153.70 (19)	O2^{v}—Cs1B—As1^{iii}	121.4 (3)
O3^{iii}—Cs1A—O2^{iii}	45.72 (3)	O2^{ii}—Cs1B—As1^{iii}	96.80 (18)
O3^{ii}—Cs1A—O2^{iii}	110.37 (3)	O4^{vi}—Cs1B—As1^{iii}	47.32 (16)
O3^{iv}—Cs1A—O2^{iii}	113.93 (3)	O4^{vii}—Cs1B—As1^{iii}	92.2 (4)
O3—Cs1A—O2^{iii}	127.04 (3)	As1^{i}—Cs1B—As1^{iii}	57.07 (13)
O3^{v}—Cs1A—O2^{iii}	78.39 (3)	As1^{iv}—Cs1B—As1^{iii}	102.3 (3)
O3^{i}—Cs1A—O2^{iii}	62.83 (3)	As1—Cs1B—As1^{iii}	138.7 (6)
O2—Cs1A—O2^{iii}	166.91 (4)	O2^{viii}—Al1—O2^{ii}	90.96 (6)

O2^{v}—Cs1A—O2^{iii}	115.403 (13)	O2^{viii}—Al1—O2^{ix}	90.96 (6)
O2^{i}—Cs1A—O2^{iii}	52.60 (4)	O2^{ii}—Al1—O2^{ix}	90.96 (6)
O2^{iv}—Cs1A—O2^{iii}	115.402 (13)	O2^{viii}—Al1—O4^{x}	88.82 (5)
Cs1B^{i}—Cs1A—O2^{ii}	38.51 (2)	O2^{ii}—Al1—O4^{x}	178.50 (6)
Cs1B^{ii}—Cs1A—O2^{ii}	83.5 (2)	O2^{ix}—Al1—O4^{x}	90.53 (5)
O3^{iii}—Cs1A—O2^{ii}	110.37 (3)	O2^{viii}—Al1—O4^{i}	178.50 (6)
O3^{ii}—Cs1A—O2^{ii}	45.72 (3)	O2^{ii}—Al1—O4^{i}	90.53 (5)
O3^{iv}—Cs1A—O2^{ii}	127.04 (3)	O2^{ix}—Al1—O4^{i}	88.82 (5)
O3—Cs1A—O2^{ii}	113.93 (3)	O4^{x}—Al1—O4^{i}	89.70 (6)
O3^{v}—Cs1A—O2^{ii}	62.83 (3)	O2^{viii}—Al1—O4^{xi}	90.53 (5)
O3^{i}—Cs1A—O2^{ii}	78.39 (3)	O2^{ii}—Al1—O4^{xi}	88.82 (5)
O2—Cs1A—O2^{ii}	115.404 (13)	O2^{ix}—Al1—O4^{xi}	178.50 (6)
O2^{v}—Cs1A—O2^{ii}	52.60 (4)	O4^{x}—Al1—O4^{xi}	89.70 (6)
O2^{i}—Cs1A—O2^{ii}	115.404 (13)	O4^{i}—Al1—O4^{xi}	89.70 (6)
O2^{iv}—Cs1A—O2^{ii}	166.91 (4)	O2^{viii}—Al1—Cs1B^{x}	123.30 (10)
O2^{iii}—Cs1A—O2^{ii}	77.02 (4)	O2^{ii}—Al1—Cs1B^{x}	99.54 (13)
Cs1B^{i}—Cs1A—As1	151.960 (16)	O2^{ix}—Al1—Cs1B^{x}	33.98 (6)
Cs1B^{ii}—Cs1A—As1	60.19 (18)	O4^{x}—Al1—Cs1B^{x}	81.81 (12)
O3^{iii}—Cs1A—As1	126.11 (2)	O4^{i}—Al1—Cs1B^{x}	56.21 (9)
O3^{ii}—Cs1A—As1	78.79 (2)	O4^{xi}—Al1—Cs1B^{x}	144.65 (7)
O3^{iv}—Cs1A—As1	77.08 (3)	O2^{viii}—Al1—Cs1B^{i}	99.54 (12)
O3—Cs1A—As1	24.02 (2)	O2^{ii}—Al1—Cs1B^{i}	33.98 (5)
O3^{v}—Cs1A—As1	133.70 (2)	O2^{ix}—Al1—Cs1B^{i}	123.30 (9)
O3^{i}—Cs1A—As1	92.93 (3)	O4^{x}—Al1—Cs1B^{i}	144.65 (6)
O2—Cs1A—As1	23.442 (18)	O4^{i}—Al1—Cs1B^{i}	81.81 (12)
O2^{v}—Cs1A—As1	98.010 (19)	O4^{xi}—Al1—Cs1B^{i}	56.21 (9)
O2^{i}—Cs1A—As1	93.54 (2)	Cs1B^{x}—Al1—Cs1B^{i}	119.552 (13)
O2^{iv}—Cs1A—As1	48.32 (2)	O2^{viii}—Al1—Cs1B^{xi}	33.98 (6)
O2^{iii}—Cs1A—As1	146.060 (19)	O2^{ii}—Al1—Cs1B^{xi}	123.30 (10)
O2^{ii}—Cs1A—As1	123.48 (2)	O2^{ix}—Al1—Cs1B^{xi}	99.54 (14)
Cs1B^{i}—Cs1A—As1^{v}	67.330 (11)	O4^{x}—Al1—Cs1B^{xi}	56.21 (10)
Cs1B^{ii}—Cs1A—As1^{v}	60.19 (18)	O4^{i}—Al1—Cs1B^{xi}	144.65 (7)
O3^{iii}—Cs1A—As1^{v}	92.93 (3)	O4^{xi}—Al1—Cs1B^{xi}	81.81 (14)
O3^{ii}—Cs1A—As1^{v}	77.09 (3)	Cs1B^{x}—Al1—Cs1B^{xi}	119.552 (7)
O3^{iv}—Cs1A—As1^{v}	78.78 (2)	Cs1B^{i}—Al1—Cs1B^{xi}	119.552 (4)
O3—Cs1A—As1^{v}	133.71 (2)	O2^{viii}—Al1—Cs1A^{x}	122.73 (4)
O3^{v}—Cs1A—As1^{v}	24.02 (2)	O2^{ii}—Al1—Cs1A^{x}	100.35 (4)
O3^{i}—Cs1A—As1^{v}	126.11 (2)	O2^{ix}—Al1—Cs1A^{x}	33.72 (4)
O2—Cs1A—As1^{v}	98.010 (19)	O4^{x}—Al1—Cs1A^{x}	81.01 (3)
O2^{v}—Cs1A—As1^{v}	23.441 (19)	O4^{i}—Al1—Cs1A^{x}	56.75 (4)
O2^{i}—Cs1A—As1^{v}	146.06 (2)	O4^{xi}—Al1—Cs1A^{x}	144.92 (4)
O2^{iv}—Cs1A—As1^{v}	123.484 (19)	Cs1B^{x}—Al1—Cs1A^{x}	0.93 (14)
O2^{iii}—Cs1A—As1^{v}	93.54 (2)	Cs1B^{i}—Al1—Cs1A^{x}	120.48 (13)
O2^{ii}—Cs1A—As1^{v}	48.32 (2)	Cs1B^{xi}—Al1—Cs1A^{x}	118.65 (14)
As1—Cs1A—As1^{v}	120.371 (6)	O2^{viii}—Al1—Cs1A	100.35 (4)
Cs1B^{i}—Cs1A—As1^{i}	67.330 (8)	O2^{ii}—Al1—Cs1A	33.72 (4)
Cs1B^{ii}—Cs1A—As1^{i}	151.96 (3)	O2^{ix}—Al1—Cs1A	122.73 (4)
O3^{iii}—Cs1A—As1^{i}	77.09 (3)	O4^{x}—Al1—Cs1A	144.92 (4)

O3^{ii}—Cs1A—As1^{i}	92.93 (3)	O4^{i}—Al1—Cs1A	81.01 (4)
O3^{iv}—Cs1A—As1^{i}	133.71 (2)	O4^{xi}—Al1—Cs1A	56.75 (4)
O3—Cs1A—As1^{i}	78.79 (2)	Cs1B^{x}—Al1—Cs1A	118.65 (14)
O3^{v}—Cs1A—As1^{i}	126.11 (2)	Cs1B^{i}—Al1—Cs1A	0.93 (13)
O3^{i}—Cs1A—As1^{i}	24.02 (2)	Cs1B^{xi}—Al1—Cs1A	120.48 (13)
O2—Cs1A—As1^{i}	123.48 (2)	Cs1A^{x}—Al1—Cs1A	119.576 (2)
O2^{v}—Cs1A—As1^{i}	146.06 (2)	O2^{viii}—Al1—Cs1A^{viii}	33.72 (4)
O2^{i}—Cs1A—As1^{i}	23.441 (19)	O2^{ii}—Al1—Cs1A^{viii}	122.74 (4)
O2^{iv}—Cs1A—As1^{i}	98.010 (19)	O2^{ix}—Al1—Cs1A^{viii}	100.35 (4)
O2^{iii}—Cs1A—As1^{i}	48.32 (2)	O4^{x}—Al1—Cs1A^{viii}	56.75 (4)
O2^{ii}—Cs1A—As1^{i}	93.54 (2)	O4^{i}—Al1—Cs1A^{viii}	144.92 (4)
As1—Cs1A—As1^{i}	100.065 (9)	O4^{xi}—Al1—Cs1A^{viii}	81.01 (4)
As1^{v}—Cs1A—As1^{i}	134.660 (5)	Cs1B^{x}—Al1—Cs1A^{viii}	120.48 (14)
Cs1B^{i}—Cs1A—As1^{iv}	151.959 (16)	Cs1B^{i}—Al1—Cs1A^{viii}	118.65 (13)
Cs1B^{ii}—Cs1A—As1^{iv}	67.33 (18)	Cs1B^{xi}—Al1—Cs1A^{viii}	0.93 (14)
O3^{iii}—Cs1A—As1^{iv}	78.79 (2)	Cs1A^{x}—Al1—Cs1A^{viii}	119.576 (2)
O3^{ii}—Cs1A—As1^{iv}	126.11 (2)	Cs1A—Al1—Cs1A^{viii}	119.576 (2)
O3^{iv}—Cs1A—As1^{iv}	24.02 (2)	O1^{xii}—As2—O1^{xiii}	92.41 (5)
O3—Cs1A—As1^{iv}	77.08 (3)	O1^{xii}—As2—O1^{xi}	180.0
O3^{v}—Cs1A—As1^{iv}	92.93 (3)	O1^{xiii}—As2—O1^{xi}	87.59 (5)
O3^{i}—Cs1A—As1^{iv}	133.70 (2)	O1^{xii}—As2—O1^{i}	87.59 (5)
O2—Cs1A—As1^{iv}	48.31 (2)	O1^{xiii}—As2—O1^{i}	180.00 (10)
O2^{v}—Cs1A—As1^{iv}	93.54 (2)	O1^{xi}—As2—O1^{i}	92.41 (5)
O2^{i}—Cs1A—As1^{iv}	98.010 (19)	O1^{xii}—As2—O1^{xiv}	92.41 (5)
O2^{iv}—Cs1A—As1^{iv}	23.441 (18)	O1^{xiii}—As2—O1^{xiv}	92.41 (5)
O2^{iii}—Cs1A—As1^{iv}	123.482 (19)	O1^{xi}—As2—O1^{xiv}	87.59 (5)
O2^{ii}—Cs1A—As1^{iv}	146.060 (19)	O1^{i}—As2—O1^{xiv}	87.59 (5)
As1—Cs1A—As1^{iv}	56.080 (13)	O1^{xii}—As2—O1^{x}	87.59 (5)
As1^{v}—Cs1A—As1^{iv}	100.065 (7)	O1^{xiii}—As2—O1^{x}	87.59 (5)
As1^{i}—Cs1A—As1^{iv}	120.371 (6)	O1^{xi}—As2—O1^{x}	92.40 (5)
Cs1B^{i}—Cs1A—As1^{iii}	60.186 (15)	O1^{i}—As2—O1^{x}	92.40 (5)
Cs1B^{ii}—Cs1A—As1^{iii}	151.96 (3)	O1^{xiv}—As2—O1^{x}	180.00 (7)
O3^{iii}—Cs1A—As1^{iii}	24.02 (2)	O4^{iii}—As1—O2	117.14 (6)
O3^{ii}—Cs1A—As1^{iii}	133.70 (2)	O4^{iii}—As1—O1^{xv}	101.04 (6)
O3^{iv}—Cs1A—As1^{iii}	92.93 (3)	O2—As1—O1^{xv}	114.80 (6)
O3—Cs1A—As1^{iii}	126.11 (2)	O4^{iii}—As1—O3	110.50 (6)
O3^{v}—Cs1A—As1^{iii}	78.79 (2)	O2—As1—O3	104.71 (7)
O3^{i}—Cs1A—As1^{iii}	77.08 (3)	O1^{xv}—As1—O3	108.55 (7)
O2—Cs1A—As1^{iii}	146.058 (19)	O4^{iii}—As1—Cs1B^{ii}	111.95 (18)
O2^{v}—Cs1A—As1^{iii}	123.483 (19)	O2—As1—Cs1B^{ii}	54.3 (3)
O2^{i}—Cs1A—As1^{iii}	48.32 (2)	O1^{xv}—As1—Cs1B^{ii}	146.59 (15)
O2^{iv}—Cs1A—As1^{iii}	93.54 (2)	O3—As1—Cs1B^{ii}	55.4 (2)
O2^{iii}—Cs1A—As1^{iii}	23.441 (19)	O4^{iii}—As1—Cs1B	108.9 (3)
O2^{ii}—Cs1A—As1^{iii}	98.011 (19)	O2—As1—Cs1B	57.4 (2)
As1—Cs1A—As1^{iii}	134.660 (5)	O1^{xv}—As1—Cs1B	149.1 (2)
As1^{v}—Cs1A—As1^{iii}	100.065 (7)	O3—As1—Cs1B	53.82 (8)
As1^{i}—Cs1A—As1^{iii}	56.081 (12)	Cs1B^{ii}—As1—Cs1B	3.7 (5)
As1^{iv}—Cs1A—As1^{iii}	100.064 (7)	O4^{iii}—As1—Cs1A	110.78 (4)

Cs1B^{i}—Cs1A—As1^{ii}	60.186 (14)	O2—As1—Cs1A	56.07 (4)
Cs1B^{ii}—Cs1A—As1^{ii}	67.33 (18)	O1^{xv}—As1—Cs1A	147.44 (4)
O3^{iii}—Cs1A—As1^{ii}	133.70 (2)	O3—As1—Cs1A	54.16 (5)
O3^{ii}—Cs1A—As1^{ii}	24.02 (2)	Cs1B^{ii}—As1—Cs1A	1.9 (3)
O3^{iv}—Cs1A—As1^{ii}	126.11 (2)	Cs1B—As1—Cs1A	2.0 (3)
O3—Cs1A—As1^{ii}	92.93 (3)	O4^{iii}—As1—Cs1B^{i}	111.44 (10)
O3^{v}—Cs1A—As1^{ii}	77.08 (3)	O2—As1—Cs1B^{i}	56.52 (7)
O3^{i}—Cs1A—As1^{ii}	78.79 (2)	O1^{xv}—As1—Cs1B^{i}	146.64 (11)
O2—Cs1A—As1^{ii}	93.55 (2)	O3—As1—Cs1B^{i}	53.34 (12)
O2^{v}—Cs1A—As1^{ii}	48.32 (2)	Cs1B^{ii}—As1—Cs1B^{i}	2.2 (3)
O2^{i}—Cs1A—As1^{ii}	123.48 (2)	Cs1B—As1—Cs1B^{i}	2.5 (4)
O2^{iv}—Cs1A—As1^{ii}	146.060 (19)	Cs1A—As1—Cs1B^{i}	0.97 (13)
O2^{iii}—Cs1A—As1^{ii}	98.011 (19)	O4^{iii}—As1—Cs1B^{xvi}	44.17 (5)
O2^{ii}—Cs1A—As1^{ii}	23.441 (19)	O2—As1—Cs1B^{xvi}	93.27 (8)
As1—Cs1A—As1^{ii}	100.065 (9)	O1^{xv}—As1—Cs1B^{xvi}	78.98 (10)
As1^{v}—Cs1A—As1^{ii}	56.081 (13)	O3—As1—Cs1B^{xvi}	154.47 (5)
As1^{i}—Cs1A—As1^{ii}	100.065 (9)	Cs1B^{ii}—As1—Cs1B^{xvi}	129.10 (15)
As1^{iv}—Cs1A—As1^{ii}	134.660 (5)	Cs1B—As1—Cs1B^{xvi}	128.6 (2)
As1^{iii}—Cs1A—As1^{ii}	120.371 (6)	Cs1A—As1—Cs1B^{xvi}	129.41 (10)
Cs1B^{i}—Cs1B—Cs1B^{ii}	60.00 (4)	Cs1B^{i}—As1—Cs1B^{xvi}	130.38 (4)
Cs1B^{i}—Cs1B—O3^{iii}	94.4 (3)	O4^{iii}—As1—Cs1A^{xvii}	44.29 (4)
Cs1B^{ii}—Cs1B—O3^{iii}	125.9 (2)	O2—As1—Cs1A^{xvii}	93.71 (4)
Cs1B^{i}—Cs1B—O3	125.9 (3)	O1^{xv}—As1—Cs1A^{xvii}	78.36 (4)
Cs1B^{ii}—Cs1B—O3	94.4 (4)	O3—As1—Cs1A^{xvii}	154.48 (5)
O3^{iii}—Cs1B—O3	135.1 (7)	Cs1B^{ii}—As1—Cs1A^{xvii}	129.75 (5)
Cs1B^{i}—Cs1B—O2^{i}	111.1 (2)	Cs1B—As1—Cs1A^{xvii}	129.29 (11)
Cs1B^{ii}—Cs1B—O2^{i}	164.59 (9)	Cs1A—As1—Cs1A^{xvii}	130.055 (13)
O3^{iii}—Cs1B—O2^{i}	64.7 (3)	Cs1B^{i}—As1—Cs1A^{xvii}	131.03 (14)
O3—Cs1B—O2^{i}	80.9 (4)	Cs1B^{xvi}—As1—Cs1A^{xvii}	0.65 (10)
Cs1B^{i}—Cs1B—O2^{iv}	164.6 (2)	O4^{iii}—As1—Cs1B^{xviii}	45.8 (2)
Cs1B^{ii}—Cs1B—O2^{iv}	111.1 (4)	O2—As1—Cs1B^{xviii}	92.99 (12)
O3^{iii}—Cs1B—O2^{iv}	80.9 (4)	O1^{xv}—As1—Cs1B^{xviii}	77.45 (15)
O3—Cs1B—O2^{iv}	64.7 (3)	O3—As1—Cs1B^{xviii}	155.9 (2)
O2^{i}—Cs1B—O2^{iv}	80.3 (5)	Cs1B^{ii}—As1—Cs1B^{xviii}	130.167 (13)
Cs1B^{i}—Cs1B—O3^{iv}	117.8 (3)	Cs1B—As1—Cs1B^{xviii}	129.84 (3)
Cs1B^{ii}—Cs1B—O3^{iv}	81.1 (4)	Cs1A—As1—Cs1B^{xviii}	130.54 (7)
O3^{iii}—Cs1B—O3^{iv}	70.08 (15)	Cs1B^{i}—As1—Cs1B^{xviii}	131.5 (2)
O3—Cs1B—O3^{iv}	101.7 (3)	Cs1B^{xvi}—As1—Cs1B^{xviii}	1.8 (3)
O2^{i}—Cs1B—O3^{iv}	114.1 (5)	Cs1A^{xvii}—As1—Cs1B^{xviii}	1.5 (2)
O2^{iv}—Cs1B—O3^{iv}	46.81 (15)	O4^{iii}—As1—Cs1B^{xvii}	42.9 (2)
Cs1B^{i}—Cs1B—O3^{i}	81.1 (3)	O2—As1—Cs1B^{xvii}	94.85 (18)
Cs1B^{ii}—Cs1B—O3^{i}	117.8 (2)	O1^{xv}—As1—Cs1B^{xvii}	78.69 (8)
O3^{iii}—Cs1B—O3^{i}	101.7 (3)	O3—As1—Cs1B^{xvii}	153.1 (2)
O3—Cs1B—O3^{i}	70.08 (15)	Cs1B^{ii}—As1—Cs1B^{xvii}	129.92 (2)
O2^{i}—Cs1B—O3^{i}	46.81 (15)	Cs1B—As1—Cs1B^{xvii}	129.35 (12)
O2^{iv}—Cs1B—O3^{i}	114.1 (5)	Cs1A—As1—Cs1B^{xvii}	130.167 (19)
O3^{iv}—Cs1B—O3^{i}	159.2 (7)	Cs1B^{i}—As1—Cs1B^{xvii}	131.14 (15)
Cs1B^{i}—Cs1B—O2	123.2 (4)	Cs1B^{xvi}—As1—Cs1B^{xvii}	1.6 (2)

Cs1B^{ii}—Cs1B—O2	64.8 (5)	Cs1A^{xvii}—As1—Cs1B^{xvii}	1.4 (2)
O3^{iii}—Cs1B—O2	129.6 (3)	Cs1B^{xviii}—As1—Cs1B^{xvii}	2.9 (4)
O3—Cs1B—O2	46.24 (7)	As1^{xix}—O1—As2^{xx}	130.17 (7)
O2^{i}—Cs1B—O2	119.0 (5)	As1^{xix}—O1—Cs1B^{vi}	81.42 (16)
O2^{iv}—Cs1B—O2	53.68 (15)	As2^{xx}—O1—Cs1B^{vi}	129.94 (11)
O3^{iv}—Cs1B—O2	63.29 (6)	As1^{xix}—O1—Cs1A^{xx}	82.55 (4)
O3^{i}—Cs1B—O2	115.10 (14)	As2^{xx}—O1—Cs1A^{xx}	129.26 (5)
Cs1B^{i}—Cs1B—O2^{iii}	64.8 (3)	Cs1B^{vi}—O1—Cs1A^{xx}	1.14 (17)
Cs1B^{ii}—Cs1B—O2^{iii}	123.2 (2)	As1^{xix}—O1—Cs1B^{xxi}	83.66 (17)
O3^{iii}—Cs1B—O2^{iii}	46.23 (7)	As2^{xx}—O1—Cs1B^{xxi}	127.6 (2)
O3—Cs1B—O2^{iii}	129.7 (3)	Cs1B^{vi}—O1—Cs1B^{xxi}	2.5 (3)
O2^{i}—Cs1B—O2^{iii}	53.68 (15)	Cs1A^{xx}—O1—Cs1B^{xxi}	1.7 (2)
O2^{iv}—Cs1B—O2^{iii}	119.0 (5)	As1—O2—Al1^{xvii}	125.94 (7)
O3^{iv}—Cs1B—O2^{iii}	115.10 (14)	As1—O2—Cs1B^{ii}	101.9 (2)
O3^{i}—Cs1B—O2^{iii}	63.29 (6)	Al1^{xvii}—O2—Cs1B^{ii}	127.63 (17)
O2—Cs1B—O2^{iii}	172.0 (7)	As1—O2—Cs1B	98.7 (3)
Cs1B^{i}—Cs1B—O3^{ii}	58.4 (2)	Al1^{xvii}—O2—Cs1B	129.54 (14)
Cs1B^{ii}—Cs1B—O3^{ii}	50.60 (16)	Cs1B^{ii}—O2—Cs1B	4.1 (6)
O3^{iii}—Cs1B—O3^{ii}	151.4 (4)	As1—O2—Cs1A	100.49 (5)
O3—Cs1B—O3^{ii}	68.50 (9)	Al1^{xvii}—O2—Cs1A	128.67 (5)
O2^{i}—Cs1B—O3^{ii}	114.37 (6)	Cs1B^{ii}—O2—Cs1A	1.6 (2)
O2^{iv}—Cs1B—O3^{ii}	127.63 (7)	Cs1B—O2—Cs1A	2.5 (4)
O3^{iv}—Cs1B—O3^{ii}	127.8 (4)	As1—O2—Cs1B^{i}	100.86 (7)
O3^{i}—Cs1B—O3^{ii}	68.17 (13)	Al1^{xvii}—O2—Cs1B^{i}	128.74 (5)
O2—Cs1B—O3^{ii}	77.24 (17)	Cs1B^{ii}—O2—Cs1B^{i}	1.12 (16)
O2^{iii}—Cs1B—O3^{ii}	108.3 (3)	Cs1B—O2—Cs1B^{i}	3.5 (5)
Cs1B^{i}—Cs1B—O3^{v}	50.6 (2)	Cs1A—O2—Cs1B^{i}	1.08 (14)
Cs1B^{ii}—Cs1B—O3^{v}	58.37 (14)	As1—O3—Cs1B	101.80 (6)
O3^{iii}—Cs1B—O3^{v}	68.50 (9)	As1—O3—Cs1B^{ii}	99.9 (3)
O3—Cs1B—O3^{v}	151.4 (4)	Cs1B—O3—Cs1B^{ii}	4.5 (6)
O2^{i}—Cs1B—O3^{v}	127.63 (7)	As1—O3—Cs1A	101.82 (6)
O2^{iv}—Cs1B—O3^{v}	114.37 (6)	Cs1B—O3—Cs1A	2.4 (3)
O3^{iv}—Cs1B—O3^{v}	68.17 (13)	Cs1B^{ii}—O3—Cs1A	2.5 (4)
O3^{i}—Cs1B—O3^{v}	127.8 (4)	As1—O3—Cs1B^{i}	103.6 (2)
O2—Cs1B—O3^{v}	108.3 (3)	Cs1B—O3—Cs1B^{i}	3.5 (5)
O2^{iii}—Cs1B—O3^{v}	77.24 (17)	Cs1B^{ii}—O3—Cs1B^{i}	3.8 (5)
O3^{ii}—Cs1B—O3^{v}	96.0 (5)	Cs1A—O3—Cs1B^{i}	1.9 (3)
Cs1B^{i}—Cs1B—O2^{v}	53.28 (17)	As1—O3—H	105 (3)
Cs1B^{ii}—Cs1B—O2^{v}	14.29 (7)	Cs1B—O3—H	93 (3)
O3^{iii}—Cs1B—O2^{v}	112.0 (3)	Cs1B^{ii}—O3—H	98 (2)
O3—Cs1B—O2^{v}	108.5 (3)	Cs1A—O3—H	96 (2)
O2^{i}—Cs1B—O2^{v}	164.4 (4)	Cs1B^{i}—O3—H	96 (3)
O2^{iv}—Cs1B—O2^{v}	114.85 (9)	As1^{iii}—O4—Al1^{xx}	127.34 (7)
O3^{iv}—Cs1B—O2^{v}	76.9 (2)	As1^{iii}—O4—Cs1B^{xxii}	119.06 (10)
O3^{i}—Cs1B—O2^{v}	123.6 (5)	Al1^{xx}—O4—Cs1B^{xxii}	100.69 (5)
O2—Cs1B—O2^{v}	75.4 (2)	As1^{iii}—O4—Cs1A^{xix}	119.48 (5)
O2^{iii}—Cs1B—O2^{v}	112.3 (4)	Al1^{xx}—O4—Cs1A^{xix}	100.82 (4)
O3^{ii}—Cs1B—O2^{v}	60.5 (3)	Cs1B^{xxii}—O4—Cs1A^{xix}	0.90 (13)

O3^{v}—Cs1B—O2^{v}	44.1 (2)	As1^{iii}—O4—Cs1B^{xix}	121.4 (3)
Cs1B^{i}—Cs1B—O2^{ii}	14.29 (3)	Al1^{xx}—O4—Cs1B^{xix}	99.51 (19)
Cs1B^{ii}—Cs1B—O2^{ii}	53.28 (3)	Cs1B^{xxii}—O4—Cs1B^{xix}	2.7 (4)
O3^{iii}—Cs1B—O2^{ii}	108.5 (3)	Cs1A^{xix}—O4—Cs1B^{xix}	2.0 (3)
O3—Cs1B—O2^{ii}	112.0 (3)	As1^{iii}—O4—Cs1B^{xxiii}	117.9 (2)
O2^{i}—Cs1B—O2^{ii}	114.85 (9)	Al1^{xx}—O4—Cs1B^{xxiii}	102.2 (2)
O2^{iv}—Cs1B—O2^{ii}	164.4 (4)	Cs1B^{xxii}—O4—Cs1B^{xxiii}	1.5 (2)
O3^{iv}—Cs1B—O2^{ii}	123.6 (5)	Cs1A^{xix}—O4—Cs1B^{xxiii}	1.6 (2)
O3^{i}—Cs1B—O2^{ii}	76.9 (2)	Cs1B^{xix}—O4—Cs1B^{xxiii}	3.5 (5)
O2—Cs1B—O2^{ii}	112.3 (4)	As1^{iii}—O4—Cs1B	52.18 (19)
O2^{iii}—Cs1B—O2^{ii}	75.4 (2)	Al1^{xx}—O4—Cs1B	75.5 (2)
O3^{ii}—Cs1B—O2^{ii}	44.1 (2)	Cs1B^{xxii}—O4—Cs1B	135.11 (6)
O3^{v}—Cs1B—O2^{ii}	60.5 (3)	Cs1A^{xix}—O4—Cs1B	136.01 (8)
O2^{v}—Cs1B—O2^{ii}	50.4 (3)	Cs1B^{xix}—O4—Cs1B	137.3 (2)
Cs1B^{i}—Cs1B—O4^{vi}	131.69 (8)	Cs1B^{xxiii}—O4—Cs1B	135.55 (3)
Cs1B^{ii}—Cs1B—O4^{vi}	154.46 (10)	As1^{iii}—O4—Cs1B^{i}	49.73 (17)
O3^{iii}—Cs1B—O4^{vi}	42.3 (2)	Al1^{xx}—O4—Cs1B^{i}	78.1 (2)
O3—Cs1B—O4^{vi}	92.7 (5)	Cs1B^{xxii}—O4—Cs1B^{i}	133.5 (3)
O2^{i}—Cs1B—O4^{vi}	40.9 (2)	Cs1A^{xix}—O4—Cs1B^{i}	134.38 (18)
O2^{iv}—Cs1B—O4^{vi}	51.1 (3)	Cs1B^{xix}—O4—Cs1B^{i}	135.76 (3)
O3^{iv}—Cs1B—O4^{vi}	73.4 (3)	Cs1B^{xxiii}—O4—Cs1B^{i}	133.8 (3)
O3^{i}—Cs1B—O4^{vi}	87.7 (4)	Cs1B—O4—Cs1B^{i}	3.1 (4)
O2—Cs1B—O4^{vi}	104.2 (4)	As1^{iii}—O4—Cs1A	50.92 (3)
O2^{iii}—Cs1B—O4^{vi}	68.2 (2)	Al1^{xx}—O4—Cs1A	76.77 (3)
O3^{ii}—Cs1B—O4^{vi}	153.1 (3)	Cs1B^{xxii}—O4—Cs1A	134.61 (13)
O3^{v}—Cs1B—O4^{vi}	108.65 (13)	Cs1A^{xix}—O4—Cs1A	135.51 (3)
O2^{v}—Cs1B—O4^{vi}	146.38 (3)	Cs1B^{xix}—O4—Cs1A	136.84 (18)
O2^{ii}—Cs1B—O4^{vi}	143.57 (3)	Cs1B^{xxiii}—O4—Cs1A	135.01 (8)
Cs1B^{i}—Cs1B—O4^{vii}	154.46 (3)	Cs1B—O4—Cs1A	1.4 (2)
Cs1B^{ii}—Cs1B—O4^{vii}	131.7 (2)	Cs1B^{i}—O4—Cs1A	1.7 (3)
O3^{iii}—Cs1B—O4^{vii}	92.7 (5)	As1^{iii}—O4—Cs1B^{ii}	50.88 (4)
O3—Cs1B—O4^{vii}	42.3 (2)	Al1^{xx}—O4—Cs1B^{ii}	76.75 (4)
O2^{i}—Cs1B—O4^{vii}	51.1 (3)	Cs1B^{xxii}—O4—Cs1B^{ii}	135.21 (5)
O2^{iv}—Cs1B—O4^{vii}	40.9 (2)	Cs1A^{xix}—O4—Cs1B^{ii}	136.11 (9)
O3^{iv}—Cs1B—O4^{vii}	87.7 (4)	Cs1B^{xix}—O4—Cs1B^{ii}	137.4 (3)
O3^{i}—Cs1B—O4^{vii}	73.4 (3)	Cs1B^{xxiii}—O4—Cs1B^{ii}	135.61 (3)
O2—Cs1B—O4^{vii}	68.2 (2)	Cs1B—O4—Cs1B^{ii}	1.30 (19)
O2^{iii}—Cs1B—O4^{vii}	104.2 (4)	Cs1B^{i}—O4—Cs1B^{ii}	2.1 (3)
O3^{ii}—Cs1B—O4^{vii}	108.65 (13)	Cs1A—O4—Cs1B^{ii}	0.59 (8)

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) −*x*+*y*, −*x*, *z*; (iii) −*x*, −*x*+*y*, −*z*+3/2; (iv) *y*, *x*, −*z*+3/2; (v) *x*−*y*, −*y*, −*z*+3/2; (vi) −*y*, *x*−*y*−1, *z*; (vii) *y*, *x*−1, −*z*+3/2; (viii) *x*+1, *y*+1, *z*; (ix) −*y*, *x*−*y*+1, *z*; (x) *x*, *y*+1, *z*; (xi) −*x*+*y*+1, −*x*+1, *z*; (xii) *x*−*y*−1/3, *x*+1/3, −*z*+4/3; (xiii) *y*+2/3, −*x*+*y*+4/3, −*z*+4/3; (xiv) −*x*+2/3, −*y*+1/3, −*z*+4/3; (xv) *x*−1, *y*, *z*; (xvi) −*y*−1, *x*−*y*−1, *z*; (xvii) *x*−1, *y*−1, *z*; (xviii) −*x*+*y*−1, −*x*−1, *z*; (xix) *x*+1, *y*, *z*; (xx) *x*, *y*−1, *z*; (xxi) −*x*+*y*, −*x*−1, *z*; (xxii) −*x*+*y*+1, −*x*, *z*; (xxiii) −*y*+1, *x*−*y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O3—H···O4^{vii}	0.88 (2)	1.94 (2)	2.7321 (18)	150 (3)

Symmetry code: (vii) $y, x-1, -z+3/2$.

Caesium digallium arsenic(V) hexakis[hydrogen arsenate(V)] (CsGa2AsHAsO46)

Crystal data

$CsGa_2As(HAsO_4)_6$
M_r = 1186.84
Trigonal, $R\bar{3}c$:*H*
a = 8.5199 (10) Å
c = 50.608 (11) Å
V = 3181.4 (10) Å^3
Z = 6
$F(000)$ = 3276
D_x = 3.717 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2582 reflections
θ = 2.9–32.6°
μ = 15.18 mm^{-1}
T = 293 K
Pseudo-octahedra, colourless
0.07 × 0.07 × 0.07 mm

Data collection

Nonius KappaCCD single-crystal four-circle diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (HKL SCALEPACK; Otwinowski *et al.*, 2003)
T_{min} = 0.416, T_{max} = 0.416
4712 measured reflections
1293 independent reflections
1134 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 32.6°, θ_{min} = 2.9°
h = −12→12
k = −10→10
l = −76→76

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.041
S = 1.16
1293 reflections
65 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0155P)^2 + 13.7864P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000080 (16)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cs1A	0.000000	0.000000	0.750000	0.033 (3)	0.720 (3)
Cs1B	0.000000	−0.030 (5)	0.750000	0.0264 (19)	0.0932 (9)
Ga1	0.333333	0.666667	0.75610 (2)	0.00886 (8)	
As2	0.333333	0.666667	0.666667	0.00779 (10)	
As1	−0.44795 (3)	−0.41187 (3)	0.71128 (2)	0.00894 (6)	

O1	0.3969 (2)	−0.47002 (19)	0.68643 (3)	0.0119 (3)
O2	−0.4545 (2)	−0.27504 (19)	0.73418 (3)	0.0113 (3)
O3	−0.2351 (2)	−0.2915 (2)	0.69800 (4)	0.0203 (3)
O4	0.4903 (2)	−0.1257 (2)	0.77880 (3)	0.0121 (3)
H	−0.179 (5)	−0.350 (5)	0.7009 (7)	0.045 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1A	0.030 (4)	0.030 (4)	0.041 (2)	0.015 (2)	0.000	0.000
Cs1B	0.021 (6)	0.024 (4)	0.034 (5)	0.010 (3)	0.002 (2)	0.0011 (11)
Ga1	0.00933 (11)	0.00933 (11)	0.00791 (16)	0.00466 (6)	0.000	0.000
As2	0.00862 (13)	0.00862 (13)	0.00615 (19)	0.00431 (7)	0.000	0.000
As1	0.00989 (10)	0.00944 (10)	0.00872 (9)	0.00576 (8)	0.00007 (7)	0.00054 (7)
O1	0.0154 (7)	0.0121 (6)	0.0097 (6)	0.0081 (6)	−0.0034 (5)	0.0000 (5)
O2	0.0114 (6)	0.0108 (6)	0.0114 (6)	0.0054 (5)	0.0004 (5)	−0.0020 (5)
O3	0.0122 (7)	0.0210 (8)	0.0281 (9)	0.0086 (7)	0.0080 (6)	0.0067 (7)
O4	0.0143 (7)	0.0101 (6)	0.0143 (6)	0.0079 (6)	−0.0036 (5)	−0.0039 (5)

Geometric parameters (Å, º)

Cs1A—Cs1B^{i}	0.25 (5)	Cs1B—O2	3.451 (2)
Cs1A—Cs1B^{ii}	0.25 (4)	Cs1B—O2^{iii}	3.451 (2)
Cs1A—O2	3.4719 (16)	Cs1B—O3^{ii}	3.65 (3)
Cs1A—O2^{iii}	3.4719 (15)	Cs1B—O3^{v}	3.65 (3)
Cs1A—O2^{iv}	3.4719 (16)	Cs1B—O2^{ii}	3.70 (4)
Cs1A—O2^{ii}	3.4719 (15)	Cs1B—O2^{v}	3.70 (4)
Cs1A—O2^{v}	3.4719 (15)	Cs1B—O4^{vi}	3.95 (4)
Cs1A—O2^{i}	3.4719 (15)	Cs1B—O4^{vii}	3.95 (4)
Cs1A—O3^{iii}	3.4828 (19)	Cs1B—As1^{iv}	4.043 (19)
Cs1A—O3^{ii}	3.4828 (19)	Cs1B—As1^{i}	4.043 (19)
Cs1A—O3^{iv}	3.4829 (19)	Cs1B—As1^{iii}	4.072 (14)
Cs1A—O3^{v}	3.4829 (19)	Cs1B—As1	4.072 (14)
Cs1A—O3^{i}	3.4829 (19)	Ga1—O2^{viii}	1.9612 (14)
Cs1A—O3	3.483 (2)	Ga1—O2^{ii}	1.9612 (15)
Cs1A—As1^{iii}	4.1625 (5)	Ga1—O2^{ix}	1.9612 (15)
Cs1A—As1^{v}	4.1625 (5)	Ga1—O4^{x}	1.9679 (15)
Cs1A—As1^{iv}	4.1625 (5)	Ga1—O4^{i}	1.9679 (15)
Cs1A—As1^{ii}	4.1625 (5)	Ga1—O4^{xi}	1.9679 (15)
Cs1A—As1^{i}	4.1625 (5)	As2—O1^{xii}	1.8109 (14)
Cs1A—As1	4.1626 (5)	As2—O1^{xiii}	1.8109 (15)
Cs1B—Cs1B^{i}	0.44 (8)	As2—O1^{xiv}	1.8109 (14)
Cs1B—Cs1B^{ii}	0.44 (7)	As2—O1^{i}	1.8109 (15)
Cs1B—O2^{iv}	3.28 (3)	As2—O1^{xi}	1.8109 (14)
Cs1B—O2^{i}	3.28 (3)	As2—O1^{x}	1.8109 (14)
Cs1B—O3^{iii}	3.383 (16)	As1—O2	1.6646 (14)
Cs1B—O3	3.383 (16)	As1—O4^{iii}	1.6670 (15)
Cs1B—O3^{iv}	3.436 (7)	As1—O1^{xv}	1.7089 (14)

Cs1B—O3^{i}	3.436 (7)	As1—O3	1.7125 (17)
Cs1B^{i}—Cs1A—Cs1B^{ii}	120.0 (3)	Cs1B^{ii}—Cs1B—O4^{vii}	153.66 (17)
Cs1B^{i}—Cs1A—O2	153.53 (4)	O2^{iv}—Cs1B—O4^{vii}	52.0 (6)
Cs1B^{ii}—Cs1A—O2	38.9 (2)	O2^{i}—Cs1B—O4^{vii}	43.4 (5)
Cs1B^{i}—Cs1A—O2^{iii}	38.93 (3)	O3^{iii}—Cs1B—O4^{vii}	42.8 (4)
Cs1B^{ii}—Cs1A—O2^{iii}	153.5 (2)	O3—Cs1B—O4^{vii}	94.6 (9)
O2—Cs1A—O2^{iii}	166.53 (5)	O3^{iv}—Cs1B—O4^{vii}	74.4 (6)
Cs1B^{i}—Cs1A—O2^{iv}	153.53 (4)	O3^{i}—Cs1B—O4^{vii}	90.2 (7)
Cs1B^{ii}—Cs1A—O2^{iv}	83.3 (3)	O2—Cs1B—O4^{vii}	105.9 (9)
O2—Cs1A—O2^{iv}	52.94 (5)	O2^{iii}—Cs1B—O4^{vii}	69.3 (5)
O2^{iii}—Cs1A—O2^{iv}	114.848 (17)	O3^{ii}—Cs1B—O4^{vii}	155.2 (6)
Cs1B^{i}—Cs1A—O2^{ii}	38.93 (3)	O3^{v}—Cs1B—O4^{vii}	108.8 (2)
Cs1B^{ii}—Cs1A—O2^{ii}	83.3 (3)	O2^{ii}—Cs1B—O4^{vii}	144.37 (3)
O2—Cs1A—O2^{ii}	114.849 (17)	O2^{v}—Cs1B—O4^{vii}	145.20 (3)
O2^{iii}—Cs1A—O2^{ii}	77.86 (5)	O4^{vi}—Cs1B—O4^{vii}	51.9 (5)
O2^{iv}—Cs1A—O2^{ii}	166.53 (5)	Cs1B^{i}—Cs1B—As1^{iv}	139.7 (5)
Cs1B^{i}—Cs1A—O2^{v}	83.27 (2)	Cs1B^{ii}—Cs1B—As1^{iv}	90.7 (7)
Cs1B^{ii}—Cs1A—O2^{v}	38.9 (2)	O2^{iv}—Cs1B—As1^{iv}	23.43 (7)
O2—Cs1A—O2^{v}	77.86 (5)	O2^{i}—Cs1B—As1^{iv}	104.5 (10)
O2^{iii}—Cs1A—O2^{v}	114.847 (17)	O3^{iii}—Cs1B—As1^{iv}	81.1 (5)
O2^{iv}—Cs1A—O2^{v}	114.848 (17)	O3—Cs1B—As1^{iv}	80.2 (5)
O2^{ii}—Cs1A—O2^{v}	52.94 (5)	O3^{iv}—Cs1B—As1^{iv}	24.81 (16)
Cs1B^{i}—Cs1A—O2^{i}	83.27 (2)	O3^{i}—Cs1B—As1^{iv}	140.9 (11)
Cs1B^{ii}—Cs1A—O2^{i}	153.5 (2)	O2—Cs1B—As1^{iv}	50.4 (2)
O2—Cs1A—O2^{i}	114.848 (17)	O2^{iii}—Cs1B—As1^{iv}	126.7 (7)
O2^{iii}—Cs1A—O2^{i}	52.94 (5)	O3^{ii}—Cs1B—As1^{iv}	124.7 (3)
O2^{iv}—Cs1A—O2^{i}	77.86 (5)	O3^{v}—Cs1B—As1^{iv}	92.41 (13)
O2^{ii}—Cs1A—O2^{i}	114.848 (17)	O2^{ii}—Cs1B—As1^{iv}	141.3 (8)
O2^{v}—Cs1A—O2^{i}	166.53 (5)	O2^{v}—Cs1B—As1^{iv}	91.9 (3)
Cs1B^{i}—Cs1A—O3^{iii}	77.37 (3)	O4^{vi}—Cs1B—As1^{iv}	66.4 (5)
Cs1B^{ii}—Cs1A—O3^{iii}	130.09 (5)	O4^{vii}—Cs1B—As1^{iv}	66.1 (5)
O2—Cs1A—O3^{iii}	127.26 (4)	Cs1B^{i}—Cs1B—As1^{i}	90.7 (5)
O2^{iii}—Cs1A—O3^{iii}	45.15 (4)	Cs1B^{ii}—Cs1B—As1^{i}	139.7 (4)
O2^{iv}—Cs1A—O3^{iii}	77.63 (4)	O2^{iv}—Cs1B—As1^{i}	104.5 (10)
O2^{ii}—Cs1A—O3^{iii}	111.42 (4)	O2^{i}—Cs1B—As1^{i}	23.43 (7)
O2^{v}—Cs1A—O3^{iii}	113.36 (4)	O3^{iii}—Cs1B—As1^{i}	80.2 (5)
O2^{i}—Cs1A—O3^{iii}	63.40 (4)	O3—Cs1B—As1^{i}	81.1 (5)
Cs1B^{i}—Cs1A—O3^{ii}	77.37 (3)	O3^{iv}—Cs1B—As1^{i}	140.9 (11)
Cs1B^{ii}—Cs1A—O3^{ii}	64.82 (14)	O3^{i}—Cs1B—As1^{i}	24.81 (16)
O2—Cs1A—O3^{ii}	77.64 (4)	O2—Cs1B—As1^{i}	126.7 (7)
O2^{iii}—Cs1A—O3^{ii}	111.42 (4)	O2^{iii}—Cs1B—As1^{i}	50.4 (2)
O2^{iv}—Cs1A—O3^{ii}	127.26 (4)	O3^{ii}—Cs1B—As1^{i}	92.41 (13)
O2^{ii}—Cs1A—O3^{ii}	45.15 (4)	O3^{v}—Cs1B—As1^{i}	124.7 (3)
O2^{v}—Cs1A—O3^{ii}	63.40 (4)	O2^{ii}—Cs1B—As1^{i}	91.9 (3)
O2^{i}—Cs1A—O3^{ii}	113.36 (4)	O2^{v}—Cs1B—As1^{i}	141.3 (8)
O3^{iii}—Cs1A—O3^{ii}	154.75 (6)	O4^{vi}—Cs1B—As1^{i}	66.1 (5)
Cs1B^{i}—Cs1A—O3^{iv}	130.09 (3)	O4^{vii}—Cs1B—As1^{i}	66.4 (5)

Cs1B^{ii}—Cs1A—O3^{iv}	64.82 (15)	As1^{iv}—Cs1B—As1^{i}	126.9 (11)
O2—Cs1A—O3^{iv}	63.40 (4)	Cs1B^{i}—Cs1B—As1^{iii}	83.1 (5)
O2^{iii}—Cs1A—O3^{iv}	113.36 (4)	Cs1B^{ii}—Cs1B—As1^{iii}	133.8 (4)
O2^{iv}—Cs1A—O3^{iv}	45.15 (4)	O2^{iv}—Cs1B—As1^{iii}	97.9 (8)
O2^{ii}—Cs1A—O3^{iv}	127.26 (4)	O2^{i}—Cs1B—As1^{iii}	50.8 (3)
O2^{v}—Cs1A—O3^{iv}	77.63 (4)	O3^{iii}—Cs1B—As1^{iii}	24.39 (9)
O2^{i}—Cs1A—O3^{iv}	111.42 (4)	O3—Cs1B—As1^{iii}	132.1 (10)
O3^{iii}—Cs1A—O3^{iv}	69.12 (4)	O3^{iv}—Cs1B—As1^{iii}	95.2 (4)
O3^{ii}—Cs1A—O3^{iv}	129.64 (6)	O3^{i}—Cs1B—As1^{iii}	79.1 (3)
Cs1B^{i}—Cs1A—O3^{v}	64.82 (4)	O2—Cs1B—As1^{iii}	152.4 (10)
Cs1B^{ii}—Cs1A—O3^{v}	77.37 (17)	O2^{iii}—Cs1B—As1^{iii}	23.78 (13)
O2—Cs1A—O3^{v}	111.41 (4)	O3^{ii}—Cs1B—As1^{iii}	131.7 (5)
O2^{iii}—Cs1A—O3^{v}	77.64 (4)	O3^{v}—Cs1B—As1^{iii}	77.69 (14)
O2^{iv}—Cs1A—O3^{v}	113.36 (4)	O2^{ii}—Cs1B—As1^{iii}	96.6 (4)
O2^{ii}—Cs1A—O3^{v}	63.40 (4)	O2^{v}—Cs1B—As1^{iii}	119.1 (6)
O2^{v}—Cs1A—O3^{v}	45.15 (4)	O4^{vi}—Cs1B—As1^{iii}	94.1 (8)
O2^{i}—Cs1A—O3^{v}	127.26 (4)	O4^{vii}—Cs1B—As1^{iii}	48.3 (3)
O3^{iii}—Cs1A—O3^{v}	69.12 (4)	As1^{iv}—Cs1B—As1^{iii}	103.2 (6)
O3^{ii}—Cs1A—O3^{v}	99.81 (6)	As1^{i}—Cs1B—As1^{iii}	58.3 (3)
O3^{iv}—Cs1A—O3^{v}	69.12 (4)	Cs1B^{i}—Cs1B—As1	133.8 (6)
Cs1B^{i}—Cs1A—O3^{i}	64.82 (3)	Cs1B^{ii}—Cs1B—As1	83.1 (7)
Cs1B^{ii}—Cs1A—O3^{i}	130.09 (5)	O2^{iv}—Cs1B—As1	50.8 (3)
O2—Cs1A—O3^{i}	113.36 (4)	O2^{i}—Cs1B—As1	97.9 (8)
O2^{iii}—Cs1A—O3^{i}	63.40 (4)	O3^{iii}—Cs1B—As1	132.1 (10)
O2^{iv}—Cs1A—O3^{i}	111.42 (4)	O3—Cs1B—As1	24.39 (9)
O2^{ii}—Cs1A—O3^{i}	77.64 (4)	O3^{iv}—Cs1B—As1	79.2 (3)
O2^{v}—Cs1A—O3^{i}	127.26 (4)	O3^{i}—Cs1B—As1	95.2 (4)
O2^{i}—Cs1A—O3^{i}	45.15 (4)	O2—Cs1B—As1	23.78 (13)
O3^{iii}—Cs1A—O3^{i}	99.81 (6)	O2^{iii}—Cs1B—As1	152.4 (10)
O3^{ii}—Cs1A—O3^{i}	69.12 (5)	O3^{ii}—Cs1B—As1	77.69 (14)
O3^{iv}—Cs1A—O3^{i}	154.75 (5)	O3^{v}—Cs1B—As1	131.7 (5)
O3^{v}—Cs1A—O3^{i}	129.64 (6)	O2^{ii}—Cs1B—As1	119.1 (6)
Cs1B^{i}—Cs1A—O3	130.09 (3)	O2^{v}—Cs1B—As1	96.6 (4)
Cs1B^{ii}—Cs1A—O3	77.37 (17)	O4^{vi}—Cs1B—As1	48.3 (3)
O2—Cs1A—O3	45.15 (4)	O4^{vii}—Cs1B—As1	94.1 (8)
O2^{iii}—Cs1A—O3	127.26 (4)	As1^{iv}—Cs1B—As1	58.3 (3)
O2^{iv}—Cs1A—O3	63.40 (4)	As1^{i}—Cs1B—As1	103.2 (6)
O2^{ii}—Cs1A—O3	113.36 (4)	As1^{iii}—Cs1B—As1	141.4 (11)
O2^{v}—Cs1A—O3	111.42 (4)	O2^{viii}—Ga1—O2^{ii}	91.15 (6)
O2^{i}—Cs1A—O3	77.63 (4)	O2^{viii}—Ga1—O2^{ix}	91.15 (6)
O3^{iii}—Cs1A—O3	129.64 (6)	O2^{ii}—Ga1—O2^{ix}	91.15 (6)
O3^{ii}—Cs1A—O3	69.12 (5)	O2^{viii}—Ga1—O4^{x}	90.84 (6)
O3^{iv}—Cs1A—O3	99.81 (6)	O2^{ii}—Ga1—O4^{x}	178.00 (6)
O3^{v}—Cs1A—O3	154.75 (6)	O2^{ix}—Ga1—O4^{x}	88.66 (6)
O3^{i}—Cs1A—O3	69.12 (5)	O2^{viii}—Ga1—O4^{i}	88.66 (6)
Cs1B^{i}—Cs1A—As1^{iii}	60.306 (12)	O2^{ii}—Ga1—O4^{i}	90.84 (6)
Cs1B^{ii}—Cs1A—As1^{iii}	151.64 (4)	O2^{ix}—Ga1—O4^{i}	178.00 (6)
O2—Cs1A—As1^{iii}	146.15 (2)	O4^{x}—Ga1—O4^{i}	89.35 (6)

O2^{iii}—Cs1A—As1^{iii}	22.98 (2)	O2^{viii}—Ga1—O4^{xi}	178.00 (6)
O2^{iv}—Cs1A—As1^{iii}	93.23 (2)	O2^{ii}—Ga1—O4^{xi}	88.66 (6)
O2^{ii}—Cs1A—As1^{iii}	98.62 (2)	O2^{ix}—Ga1—O4^{xi}	90.84 (6)
O2^{v}—Cs1A—As1^{iii}	122.59 (2)	O4^{x}—Ga1—O4^{xi}	89.35 (6)
O2^{i}—Cs1A—As1^{iii}	49.10 (2)	O4^{i}—Ga1—O4^{xi}	89.35 (7)
O3^{iii}—Cs1A—As1^{iii}	23.83 (3)	O2^{viii}—Ga1—Cs1B^{x}	34.15 (10)
O3^{ii}—Cs1A—As1^{iii}	134.28 (3)	O2^{ii}—Ga1—Cs1B^{x}	99.2 (3)
O3^{iv}—Cs1A—As1^{iii}	92.90 (3)	O2^{ix}—Ga1—Cs1B^{x}	123.8 (2)
O3^{v}—Cs1A—As1^{iii}	78.30 (3)	O4^{x}—Ga1—Cs1B^{x}	82.5 (2)
O3^{i}—Cs1A—As1^{iii}	77.37 (3)	O4^{i}—Ga1—Cs1B^{x}	55.68 (16)
O3—Cs1A—As1^{iii}	125.98 (3)	O4^{xi}—Ga1—Cs1B^{x}	143.97 (12)
Cs1B^{i}—Cs1A—As1^{v}	67.383 (11)	O2^{viii}—Ga1—Cs1B^{i}	123.79 (17)
Cs1B^{ii}—Cs1A—As1^{v}	60.3 (2)	O2^{ii}—Ga1—Cs1B^{i}	34.15 (9)
O2—Cs1A—As1^{v}	98.62 (2)	O2^{ix}—Ga1—Cs1B^{i}	99.2 (2)
O2^{iii}—Cs1A—As1^{v}	93.23 (2)	O4^{x}—Ga1—Cs1B^{i}	143.97 (10)
O2^{iv}—Cs1A—As1^{v}	122.59 (2)	O4^{i}—Ga1—Cs1B^{i}	82.5 (2)
O2^{ii}—Cs1A—As1^{v}	49.10 (2)	O4^{xi}—Ga1—Cs1B^{i}	55.68 (16)
O2^{v}—Cs1A—As1^{v}	22.98 (2)	Cs1B^{x}—Ga1—Cs1B^{i}	119.57 (2)
O2^{i}—Cs1A—As1^{v}	146.15 (2)	O2^{viii}—Ga1—Cs1B^{xi}	99.2 (3)
O3^{iii}—Cs1A—As1^{v}	92.90 (3)	O2^{ii}—Ga1—Cs1B^{xi}	123.79 (19)
O3^{ii}—Cs1A—As1^{v}	77.37 (3)	O2^{ix}—Ga1—Cs1B^{xi}	34.15 (12)
O3^{iv}—Cs1A—As1^{v}	78.29 (3)	O4^{x}—Ga1—Cs1B^{xi}	55.68 (19)
O3^{v}—Cs1A—As1^{v}	23.82 (3)	O4^{i}—Ga1—Cs1B^{xi}	143.97 (13)
O3^{i}—Cs1A—As1^{v}	125.98 (3)	O4^{xi}—Ga1—Cs1B^{xi}	82.5 (3)
O3—Cs1A—As1^{v}	134.28 (3)	Cs1B^{x}—Ga1—Cs1B^{xi}	119.575 (14)
As1^{iii}—Cs1A—As1^{v}	99.647 (7)	Cs1B^{i}—Ga1—Cs1B^{xi}	119.575 (5)
Cs1B^{i}—Cs1A—As1^{iv}	151.635 (12)	O2^{viii}—Ga1—Cs1A^{x}	33.70 (4)
Cs1B^{ii}—Cs1A—As1^{iv}	67.4 (2)	O2^{ii}—Ga1—Cs1A^{x}	100.57 (4)
O2—Cs1A—As1^{iv}	49.10 (2)	O2^{ix}—Ga1—Cs1A^{x}	122.84 (4)
O2^{iii}—Cs1A—As1^{iv}	122.59 (2)	O4^{x}—Ga1—Cs1A^{x}	81.19 (4)
O2^{iv}—Cs1A—As1^{iv}	22.98 (2)	O4^{i}—Ga1—Cs1A^{x}	56.58 (4)
O2^{ii}—Cs1A—As1^{iv}	146.15 (2)	O4^{xi}—Ga1—Cs1A^{x}	144.45 (5)
O2^{v}—Cs1A—As1^{iv}	93.23 (2)	Cs1B^{x}—Ga1—Cs1A^{x}	1.6 (3)
O2^{i}—Cs1A—As1^{iv}	98.62 (2)	Cs1B^{i}—Ga1—Cs1A^{x}	121.1 (3)
O3^{iii}—Cs1A—As1^{iv}	78.30 (3)	Cs1B^{xi}—Ga1—Cs1A^{x}	118.1 (3)
O3^{ii}—Cs1A—As1^{iv}	125.98 (3)	O2^{viii}—Ga1—Cs1A	122.84 (4)
O3^{iv}—Cs1A—As1^{iv}	23.83 (3)	O2^{ii}—Ga1—Cs1A	33.70 (4)
O3^{v}—Cs1A—As1^{iv}	92.90 (3)	O2^{ix}—Ga1—Cs1A	100.57 (4)
O3^{i}—Cs1A—As1^{iv}	134.28 (3)	O4^{x}—Ga1—Cs1A	144.45 (5)
O3—Cs1A—As1^{iv}	77.37 (3)	O4^{i}—Ga1—Cs1A	81.19 (4)
As1^{iii}—Cs1A—As1^{iv}	99.647 (7)	O4^{xi}—Ga1—Cs1A	56.58 (4)
As1^{v}—Cs1A—As1^{iv}	99.647 (8)	Cs1B^{x}—Ga1—Cs1A	118.1 (3)
Cs1B^{i}—Cs1A—As1^{ii}	60.306 (11)	Cs1B^{i}—Ga1—Cs1A	1.6 (3)
Cs1B^{ii}—Cs1A—As1^{ii}	67.4 (2)	Cs1B^{xi}—Ga1—Cs1A	121.1 (3)
O2—Cs1A—As1^{ii}	93.23 (2)	Cs1A^{x}—Ga1—Cs1A	119.612 (1)
O2^{iii}—Cs1A—As1^{ii}	98.62 (2)	O2^{viii}—Ga1—Cs1A^{ix}	100.57 (4)
O2^{iv}—Cs1A—As1^{ii}	146.15 (2)	O2^{ii}—Ga1—Cs1A^{ix}	122.84 (4)
O2^{ii}—Cs1A—As1^{ii}	22.98 (2)	O2^{ix}—Ga1—Cs1A^{ix}	33.70 (4)

O2^{v}—Cs1A—As1^{ii}	49.10 (2)	O4^{x}—Ga1—Cs1A^{ix}	56.58 (4)
O2^{i}—Cs1A—As1^{ii}	122.59 (2)	O4^{i}—Ga1—Cs1A^{ix}	144.45 (5)
O3^{iii}—Cs1A—As1^{ii}	134.28 (3)	O4^{xi}—Ga1—Cs1A^{ix}	81.19 (4)
O3^{ii}—Cs1A—As1^{ii}	23.83 (3)	Cs1B^{x}—Ga1—Cs1A^{ix}	121.1 (3)
O3^{iv}—Cs1A—As1^{ii}	125.98 (3)	Cs1B^{i}—Ga1—Cs1A^{ix}	118.1 (3)
O3^{v}—Cs1A—As1^{ii}	77.37 (3)	Cs1B^{xi}—Ga1—Cs1A^{ix}	1.6 (3)
O3^{i}—Cs1A—As1^{ii}	78.30 (3)	Cs1A^{x}—Ga1—Cs1A^{ix}	119.612 (1)
O3—Cs1A—As1^{ii}	92.90 (3)	Cs1A—Ga1—Cs1A^{ix}	119.612 (1)
As1^{iii}—Cs1A—As1^{ii}	120.612 (7)	O1^{xii}—As2—O1^{xiii}	92.46 (6)
As1^{v}—Cs1A—As1^{ii}	56.729 (13)	O1^{xii}—As2—O1^{xiv}	92.45 (6)
As1^{iv}—Cs1A—As1^{ii}	134.766 (6)	O1^{xiii}—As2—O1^{xiv}	92.45 (6)
Cs1B^{i}—Cs1A—As1^{i}	67.383 (6)	O1^{xii}—As2—O1^{i}	87.55 (6)
Cs1B^{ii}—Cs1A—As1^{i}	151.64 (4)	O1^{xiii}—As2—O1^{i}	180.00 (12)
O2—Cs1A—As1^{i}	122.59 (2)	O1^{xiv}—As2—O1^{i}	87.55 (6)
O2^{iii}—Cs1A—As1^{i}	49.10 (2)	O1^{xii}—As2—O1^{xi}	180.0
O2^{iv}—Cs1A—As1^{i}	98.62 (2)	O1^{xiii}—As2—O1^{xi}	87.55 (6)
O2^{ii}—Cs1A—As1^{i}	93.23 (2)	O1^{xiv}—As2—O1^{xi}	87.55 (6)
O2^{v}—Cs1A—As1^{i}	146.15 (2)	O1^{i}—As2—O1^{xi}	92.45 (6)
O2^{i}—Cs1A—As1^{i}	22.98 (2)	O1^{xii}—As2—O1^{x}	87.55 (6)
O3^{iii}—Cs1A—As1^{i}	77.37 (3)	O1^{xiii}—As2—O1^{x}	87.55 (6)
O3^{ii}—Cs1A—As1^{i}	92.90 (3)	O1^{xiv}—As2—O1^{x}	180.00 (8)
O3^{iv}—Cs1A—As1^{i}	134.29 (3)	O1^{i}—As2—O1^{x}	92.45 (6)
O3^{v}—Cs1A—As1^{i}	125.98 (3)	O1^{xi}—As2—O1^{x}	92.45 (6)
O3^{i}—Cs1A—As1^{i}	23.82 (3)	O2—As1—O4^{iii}	117.09 (7)
O3—Cs1A—As1^{i}	78.30 (3)	O2—As1—O1^{xv}	115.06 (7)
As1^{iii}—Cs1A—As1^{i}	56.729 (13)	O4^{iii}—As1—O1^{xv}	100.76 (7)
As1^{v}—Cs1A—As1^{i}	134.766 (7)	O2—As1—O3	104.49 (8)
As1^{iv}—Cs1A—As1^{i}	120.612 (7)	O4^{iii}—As1—O3	110.80 (8)
As1^{ii}—Cs1A—As1^{i}	99.647 (9)	O1^{xv}—As1—O3	108.60 (8)
Cs1B^{i}—Cs1A—As1	151.634 (13)	O2—As1—Cs1B^{ii}	51.6 (5)
Cs1B^{ii}—Cs1A—As1	60.3 (2)	O4^{iii}—As1—Cs1B^{ii}	113.4 (3)
O2—Cs1A—As1	22.98 (2)	O1^{xv}—As1—Cs1B^{ii}	145.8 (3)
O2^{iii}—Cs1A—As1	146.15 (2)	O3—As1—Cs1B^{ii}	57.4 (4)
O2^{iv}—Cs1A—As1	49.10 (2)	O2—As1—Cs1B	56.7 (4)
O2^{ii}—Cs1A—As1	122.58 (2)	O4^{iii}—As1—Cs1B	108.4 (6)
O2^{v}—Cs1A—As1	98.62 (2)	O1^{xv}—As1—Cs1B	150.0 (5)
O2^{i}—Cs1A—As1	93.23 (2)	O3—As1—Cs1B	54.65 (13)
O3^{iii}—Cs1A—As1	125.98 (3)	Cs1B^{ii}—As1—Cs1B	6.2 (11)
O3^{ii}—Cs1A—As1	78.29 (3)	O2—As1—Cs1A	54.52 (5)
O3^{iv}—Cs1A—As1	77.37 (3)	O4^{iii}—As1—Cs1A	111.50 (5)
O3^{v}—Cs1A—As1	134.29 (3)	O1^{xv}—As1—Cs1A	147.27 (5)
O3^{i}—Cs1A—As1	92.89 (3)	O3—As1—Cs1A	55.24 (6)
O3—Cs1A—As1	23.82 (3)	Cs1B^{ii}—As1—Cs1A	3.1 (5)
As1^{iii}—Cs1A—As1	134.766 (6)	Cs1B—As1—Cs1A	3.3 (6)
As1^{v}—Cs1A—As1	120.613 (7)	O2—As1—Cs1B^{i}	55.25 (13)
As1^{iv}—Cs1A—As1	56.731 (13)	O4^{iii}—As1—Cs1B^{i}	112.60 (18)
As1^{ii}—Cs1A—As1	99.647 (9)	O1^{xv}—As1—Cs1B^{i}	146.0 (2)
As1^{i}—Cs1A—As1	99.646 (9)	O3—As1—Cs1B^{i}	53.9 (2)

Cs1B^{i}—Cs1B—Cs1B^{ii}	60.00 (6)	Cs1B^{ii}—As1—Cs1B^{i}	3.7 (6)
Cs1B^{i}—Cs1B—O2^{iv}	162.9 (4)	Cs1B—As1—Cs1B^{i}	4.2 (7)
Cs1B^{ii}—Cs1B—O2^{iv}	109.7 (7)	Cs1A—As1—Cs1B^{i}	1.6 (3)
Cs1B^{i}—Cs1B—O2^{i}	109.7 (5)	O2—As1—Cs1B^{xvi}	93.88 (14)
Cs1B^{ii}—Cs1B—O2^{i}	162.9 (3)	O4^{iii}—As1—Cs1B^{xvi}	42.74 (6)
O2^{iv}—Cs1B—O2^{i}	83.4 (10)	O1^{xv}—As1—Cs1B^{xvi}	79.72 (19)
Cs1B^{i}—Cs1B—O3^{iii}	93.3 (6)	O3—As1—Cs1B^{xvi}	153.38 (6)
Cs1B^{ii}—Cs1B—O3^{iii}	124.8 (5)	Cs1B^{ii}—As1—Cs1B^{xvi}	127.8 (3)
O2^{iv}—Cs1B—O3^{iii}	81.8 (7)	Cs1B—As1—Cs1B^{xvi}	127.1 (4)
O2^{i}—Cs1B—O3^{iii}	66.5 (5)	Cs1A—As1—Cs1B^{xvi}	128.4 (2)
Cs1B^{i}—Cs1B—O3	124.8 (6)	Cs1B^{i}—As1—Cs1B^{xvi}	129.96 (7)
Cs1B^{ii}—Cs1B—O3	93.3 (7)	O2—As1—Cs1A^{xvii}	94.63 (5)
O2^{iv}—Cs1B—O3	66.5 (5)	O4^{iii}—As1—Cs1A^{xvii}	42.93 (5)
O2^{i}—Cs1B—O3	81.8 (7)	O1^{xv}—As1—Cs1A^{xvii}	78.68 (5)
O3^{iii}—Cs1B—O3	137.4 (14)	O3—As1—Cs1A^{xvii}	153.41 (6)
Cs1B^{i}—Cs1B—O3^{iv}	116.2 (7)	Cs1B^{ii}—As1—Cs1A^{xvii}	128.92 (12)
Cs1B^{ii}—Cs1B—O3^{iv}	79.3 (8)	Cs1B—As1—Cs1A^{xvii}	128.2 (2)
O2^{iv}—Cs1B—O3^{iv}	46.8 (3)	Cs1A—As1—Cs1A^{xvii}	129.479 (13)
O2^{i}—Cs1B—O3^{iv}	117.7 (11)	Cs1B^{i}—As1—Cs1A^{xvii}	131.1 (3)
O3^{iii}—Cs1B—O3^{iv}	70.8 (3)	Cs1B^{xvi}—As1—Cs1A^{xvii}	1.1 (2)
O3—Cs1B—O3^{iv}	102.8 (5)	O2—As1—Cs1B^{xviii}	93.5 (2)
Cs1B^{i}—Cs1B—O3^{i}	79.3 (6)	O4^{iii}—As1—Cs1B^{xviii}	45.4 (4)
Cs1B^{ii}—Cs1B—O3^{i}	116.2 (5)	O1^{xv}—As1—Cs1B^{xviii}	77.2 (3)
O2^{iv}—Cs1B—O3^{i}	117.7 (11)	O3—As1—Cs1B^{xviii}	155.7 (4)
O2^{i}—Cs1B—O3^{i}	46.8 (3)	Cs1B^{ii}—As1—Cs1B^{xviii}	129.53 (5)
O3^{iii}—Cs1B—O3^{i}	102.8 (5)	Cs1B—As1—Cs1B^{xviii}	129.12 (6)
O3—Cs1B—O3^{i}	70.8 (3)	Cs1A—As1—Cs1B^{xviii}	130.25 (12)
O3^{iv}—Cs1B—O3^{i}	163.0 (14)	Cs1B^{i}—As1—Cs1B^{xviii}	131.8 (4)
Cs1B^{i}—Cs1B—O2	121.6 (7)	Cs1B^{xvi}—As1—Cs1B^{xviii}	3.0 (5)
Cs1B^{ii}—Cs1B—O2	63.4 (9)	Cs1A^{xvii}—As1—Cs1B^{xviii}	2.5 (4)
O2^{iv}—Cs1B—O2	54.7 (3)	O2—As1—Cs1B^{xvii}	96.5 (3)
O2^{i}—Cs1B—O2	120.8 (10)	O4^{iii}—As1—Cs1B^{xvii}	40.7 (4)
O3^{iii}—Cs1B—O2	131.5 (6)	O1^{xv}—As1—Cs1B^{xvii}	79.23 (14)
O3—Cs1B—O2	45.98 (12)	O3—As1—Cs1B^{xvii}	151.1 (4)
O3^{iv}—Cs1B—O2	64.09 (9)	Cs1B^{ii}—As1—Cs1B^{xvii}	129.27 (4)
O3^{i}—Cs1B—O2	115.1 (2)	Cs1B—As1—Cs1B^{xvii}	128.2 (3)
Cs1B^{i}—Cs1B—O2^{iii}	63.4 (7)	Cs1A—As1—Cs1B^{xvii}	129.66 (3)
Cs1B^{ii}—Cs1B—O2^{iii}	121.6 (5)	Cs1B^{i}—As1—Cs1B^{xvii}	131.2 (3)
O2^{iv}—Cs1B—O2^{iii}	120.8 (10)	Cs1B^{xvi}—As1—Cs1B^{xvii}	2.7 (4)
O2^{i}—Cs1B—O2^{iii}	54.7 (3)	Cs1A^{xvii}—As1—Cs1B^{xvii}	2.3 (4)
O3^{iii}—Cs1B—O2^{iii}	45.98 (12)	Cs1B^{xviii}—As1—Cs1B^{xvii}	4.7 (8)
O3—Cs1B—O2^{iii}	131.5 (6)	As1^{xix}—O1—As2^{xx}	131.05 (8)
O3^{iv}—Cs1B—O2^{iii}	115.1 (2)	As1^{xix}—O1—Cs1B^{vii}	80.6 (3)
O3^{i}—Cs1B—O2^{iii}	64.09 (9)	As2^{xx}—O1—Cs1B^{vii}	130.0 (2)
O2—Cs1B—O2^{iii}	174.9 (14)	As1—O2—Ga1^{xvii}	124.47 (8)
Cs1B^{i}—Cs1B—O3^{ii}	57.6 (4)	As1—O2—Cs1B^{ii}	105.0 (5)
Cs1B^{ii}—Cs1B—O3^{ii}	49.5 (3)	Ga1^{xvii}—O2—Cs1B^{ii}	126.2 (4)
O2^{iv}—Cs1B—O3^{ii}	128.02 (8)	As1—O2—Cs1B	99.5 (5)

O2^{i}—Cs1B—O3^{ii}	113.88 (5)	Ga1^{xvii}—O2—Cs1B	129.4 (2)
O3^{iii}—Cs1B—O3^{ii}	150.1 (9)	Cs1B^{ii}—O2—Cs1B	6.9 (12)
O3—Cs1B—O3^{ii}	68.2 (2)	As1—O2—Cs1A	102.50 (6)
O3^{iv}—Cs1B—O3^{ii}	125.6 (7)	Ga1^{xvii}—O2—Cs1A	128.04 (6)
O3^{i}—Cs1B—O3^{ii}	67.7 (3)	Cs1B^{ii}—O2—Cs1A	2.8 (5)
O2—Cs1B—O3^{ii}	75.7 (4)	Cs1B—O2—Cs1A	4.2 (7)
O2^{iii}—Cs1B—O3^{ii}	108.0 (6)	As1—O2—Cs1B^{i}	103.06 (11)
Cs1B^{i}—Cs1B—O3^{v}	49.5 (4)	Ga1^{xvii}—O2—Cs1B^{i}	128.20 (6)
Cs1B^{ii}—Cs1B—O3^{v}	57.6 (3)	Cs1B^{ii}—O2—Cs1B^{i}	2.0 (4)
O2^{iv}—Cs1B—O3^{v}	113.88 (5)	Cs1B—O2—Cs1B^{i}	5.8 (10)
O2^{i}—Cs1B—O3^{v}	128.02 (8)	Cs1A—O2—Cs1B^{i}	1.8 (3)
O3^{iii}—Cs1B—O3^{v}	68.2 (2)	As1—O3—Cs1B	100.96 (8)
O3—Cs1B—O3^{v}	150.1 (8)	As1—O3—Cs1B^{ii}	97.8 (5)
O3^{iv}—Cs1B—O3^{v}	67.7 (3)	Cs1B—O3—Cs1B^{ii}	7.3 (13)
O3^{i}—Cs1B—O3^{v}	125.6 (7)	As1—O3—Cs1A	100.94 (7)
O2—Cs1B—O3^{v}	107.9 (6)	Cs1B—O3—Cs1A	3.9 (7)
O2^{iii}—Cs1B—O3^{v}	75.7 (4)	Cs1B^{ii}—O3—Cs1A	4.1 (7)
O3^{ii}—Cs1B—O3^{v}	93.7 (10)	As1—O3—Cs1B^{i}	103.8 (5)
Cs1B^{i}—Cs1B—O2^{ii}	15.07 (4)	Cs1B—O3—Cs1B^{i}	5.7 (10)
Cs1B^{ii}—Cs1B—O2^{ii}	52.57 (10)	Cs1B^{ii}—O3—Cs1B^{i}	6.2 (10)
O2^{iv}—Cs1B—O2^{ii}	162.2 (7)	Cs1A—O3—Cs1B^{i}	3.1 (5)
O2^{i}—Cs1B—O2^{ii}	113.8 (2)	As1^{iii}—O4—Ga1^{xx}	126.05 (8)
O3^{iii}—Cs1B—O2^{ii}	108.3 (6)	As1^{iii}—O4—Cs1B^{xxi}	120.63 (19)
O3—Cs1B—O2^{ii}	110.2 (6)	Ga1^{xx}—O4—Cs1B^{xxi}	100.03 (7)
O3^{iv}—Cs1B—O2^{ii}	121.6 (10)	As1^{iii}—O4—Cs1A^{xix}	121.31 (6)
O3^{i}—Cs1B—O2^{ii}	75.2 (4)	Ga1^{xx}—O4—Cs1A^{xix}	100.29 (5)
O2—Cs1B—O2^{ii}	109.7 (9)	Cs1B^{xxi}—O4—Cs1A^{xix}	1.5 (3)
O2^{iii}—Cs1B—O2^{ii}	75.1 (5)	As1^{iii}—O4—Cs1B^{xix}	124.5 (6)
O3^{ii}—Cs1B—O2^{ii}	42.6 (4)	Ga1^{xx}—O4—Cs1B^{xix}	98.2 (4)
O3^{v}—Cs1B—O2^{ii}	59.6 (6)	Cs1B^{xxi}—O4—Cs1B^{xix}	4.5 (8)
Cs1B^{i}—Cs1B—O2^{v}	52.6 (3)	Cs1A^{xix}—O4—Cs1B^{xix}	3.3 (5)
Cs1B^{ii}—Cs1B—O2^{v}	15.07 (11)	As1^{iii}—O4—Cs1B^{xxii}	118.8 (4)
O2^{iv}—Cs1B—O2^{v}	113.8 (2)	Ga1^{xx}—O4—Cs1B^{xxii}	102.6 (4)
O2^{i}—Cs1B—O2^{v}	162.2 (7)	Cs1B^{xxi}—O4—Cs1B^{xxii}	2.6 (4)
O3^{iii}—Cs1B—O2^{v}	110.2 (6)	Cs1A^{xix}—O4—Cs1B^{xxii}	2.6 (4)
O3—Cs1B—O2^{v}	108.3 (6)	Cs1B^{xix}—O4—Cs1B^{xxii}	5.7 (10)
O3^{iv}—Cs1B—O2^{v}	75.2 (4)	As1^{iii}—O4—Cs1B	52.6 (4)
O3^{i}—Cs1B—O2^{v}	121.6 (10)	Ga1^{xx}—O4—Cs1B	73.8 (4)
O2—Cs1B—O2^{v}	75.1 (5)	Cs1B^{xxi}—O4—Cs1B	134.69 (14)
O2^{iii}—Cs1B—O2^{v}	109.7 (9)	Cs1A^{xix}—O4—Cs1B	136.21 (14)
O3^{ii}—Cs1B—O2^{v}	59.6 (6)	Cs1B^{xix}—O4—Cs1B	138.2 (4)
O3^{v}—Cs1B—O2^{v}	42.6 (4)	Cs1B^{xxii}—O4—Cs1B	135.56 (6)
O2^{ii}—Cs1B—O2^{v}	49.4 (6)	As1^{iii}—O4—Cs1B^{i}	48.6 (3)
Cs1B^{i}—Cs1B—O4^{vi}	153.66 (8)	Ga1^{xx}—O4—Cs1B^{i}	78.2 (4)
Cs1B^{ii}—Cs1B—O4^{vi}	131.4 (4)	Cs1B^{xxi}—O4—Cs1B^{i}	132.1 (6)
O2^{iv}—Cs1B—O4^{vi}	43.4 (5)	Cs1A^{xix}—O4—Cs1B^{i}	133.6 (4)
O2^{i}—Cs1B—O4^{vi}	52.0 (6)	Cs1B^{xix}—O4—Cs1B^{i}	135.86 (5)
O3^{iii}—Cs1B—O4^{vi}	94.6 (9)	Cs1B^{xxii}—O4—Cs1B^{i}	132.7 (5)

O3—Cs1B—O4^{vi}	42.8 (4)	Cs1B—O4—Cs1B^{i}	5.1 (9)
O3^{iv}—Cs1B—O4^{vi}	90.2 (7)	As1^{iii}—O4—Cs1A	50.49 (4)
O3^{i}—Cs1B—O4^{vi}	74.4 (6)	Ga1^{xx}—O4—Cs1A	76.01 (4)
O2—Cs1B—O4^{vi}	69.3 (5)	Cs1B^{xxi}—O4—Cs1A	133.9 (3)
O2^{iii}—Cs1B—O4^{vi}	105.9 (9)	Cs1A^{xix}—O4—Cs1A	135.46 (4)
O3^{ii}—Cs1B—O4^{vi}	108.8 (2)	Cs1B^{xix}—O4—Cs1A	137.6 (3)
O3^{v}—Cs1B—O4^{vi}	155.2 (6)	Cs1B^{xxii}—O4—Cs1A	134.68 (14)
O2^{ii}—Cs1B—O4^{vi}	145.19 (3)	Cs1B—O4—Cs1A	2.3 (4)
O2^{v}—Cs1B—O4^{vi}	144.37 (3)	Cs1B^{i}—O4—Cs1A	2.8 (5)
Cs1B^{i}—Cs1B—O4^{vii}	131.4 (2)		

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) −*x*+*y*, −*x*, *z*; (iii) −*x*, −*x*+*y*, −*z*+3/2; (iv) *y*, *x*, −*z*+3/2; (v) *x*−*y*, −*y*, −*z*+3/2; (vi) *y*, *x*−1, −*z*+3/2; (vii) −*y*, *x*−*y*−1, *z*; (viii) −*y*, *x*−*y*+1, *z*; (ix) *x*+1, *y*+1, *z*; (x) *x*, *y*+1, *z*; (xi) −*x*+*y*+1, −*x*+1, *z*; (xii) *x*−*y*−1/3, *x*+1/3, −*z*+4/3; (xiii) *y*+2/3, −*x*+*y*+4/3, −*z*+4/3; (xiv) −*x*+2/3, −*y*+1/3, −*z*+4/3; (xv) *x*−1, *y*, *z*; (xvi) −*y*−1, *x*−*y*−1, *z*; (xvii) *x*−1, *y*−1, *z*; (xviii) −*x*+*y*−1, −*x*−1, *z*; (xix) *x*+1, *y*, *z*; (xx) *x*, *y*−1, *z*; (xxi) −*x*+*y*+1, −*x*, *z*; (xxii) −*y*+1, *x*−*y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H···O4^{vi}	0.86 (2)	1.93 (2)	2.727 (2)	154 (3)

Symmetry code: (vi) *y*, *x*−1, −*z*+3/2.

Thallium digallium arsenic(V) hexakis[hydrogen arsenate(V)] (TlGa2AsHAsO46)

Crystal data

$TlGa_2As(HAsO_4)_6$
M_r = 1258.30
Trigonal, $R\bar{3}c$:*H*
a = 8.484 (1) Å
c = 50.724 (11) Å
V = 3161.9 (10) Å^3
Z = 6
F(000) = 3432
D_x = 3.965 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 2570 reflections
θ = 2.4–32.6°
μ = 21.18 mm^{-1}
T = 293 K
Large pseudo-octahedra, colourless
0.08 × 0.07 × 0.05 mm

Data collection

Nonius KappaCCD single-crystal four-circle diffractometer
Radiation source: fine-focus sealed tube
φ and *ω* scans
Absorption correction: multi-scan HKL SCALEPACK (Otwinowski *et al.*, 2003)
T_{min} = 0.200, T_{max} = 0.347
4682 measured reflections
1285 independent reflections
1129 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 32.6°, θ_{min} = 2.4°
h = −12→12
k = −10→10
l = −76→76

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.041
S = 1.10
1285 reflections
71 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0174P)^2 + 10.0458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005

$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Extinction correction: SHELXL-2016/6 (Sheldrick 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000237 (18)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Tl1A	0.000000	0.000000	0.750000	0.074 (4)	0.329 (3)
Tl1B	0.000000	−0.0480 (7)	0.750000	0.0496 (15)	0.1294 (11)
Tl1C	0.000000	−0.0903 (10)	0.750000	0.0387 (10)	0.0941 (11)
Ga1	0.333333	0.666667	0.75604 (2)	0.00849 (8)	
As2	0.333333	0.666667	0.666667	0.00754 (9)	
As1	−0.44448 (3)	−0.40820 (3)	0.71139 (2)	0.00861 (6)	
O1	0.40173 (19)	−0.46663 (18)	0.68629 (3)	0.0112 (3)	
O2	−0.45247 (19)	−0.27070 (18)	0.73408 (3)	0.0116 (3)	
O3	−0.2297 (2)	−0.2872 (2)	0.69852 (4)	0.0209 (3)	
O4	0.48864 (18)	−0.12491 (19)	0.77863 (3)	0.0117 (3)	
H	−0.176 (5)	−0.351 (5)	0.7005 (8)	0.069 (14)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tl1A	0.056 (4)	0.056 (4)	0.109 (4)	0.028 (2)	0.000	0.000
Tl1B	0.061 (2)	0.029 (3)	0.069 (2)	0.0305 (10)	0.0008 (16)	0.0004 (8)
Tl1C	0.0285 (14)	0.030 (3)	0.0566 (17)	0.0142 (7)	0.0073 (11)	0.0037 (5)
Ga1	0.00891 (11)	0.00891 (11)	0.00765 (16)	0.00446 (5)	0.000	0.000
As2	0.00849 (13)	0.00849 (13)	0.00563 (19)	0.00425 (6)	0.000	0.000
As1	0.00960 (10)	0.00911 (10)	0.00843 (9)	0.00564 (7)	0.00016 (6)	0.00061 (6)
O1	0.0147 (6)	0.0116 (6)	0.0096 (6)	0.0082 (5)	−0.0029 (5)	−0.0001 (5)
O2	0.0112 (6)	0.0109 (6)	0.0125 (6)	0.0055 (5)	0.0005 (5)	−0.0023 (5)
O3	0.0137 (7)	0.0206 (8)	0.0291 (9)	0.0092 (6)	0.0089 (6)	0.0085 (7)
O4	0.0133 (6)	0.0105 (6)	0.0136 (6)	0.0077 (5)	−0.0024 (5)	−0.0032 (5)

Geometric parameters (Å, º)

Tl1A—Tl1B^{i}	0.408 (7)	Tl1B—O4^{vii}	3.810 (6)
Tl1A—Tl1B^{ii}	0.408 (6)	Tl1B—As1^{iv}	3.936 (3)
Tl1A—Tl1C	0.766 (9)	Tl1B—As1^{i}	3.936 (3)
Tl1A—Tl1C^{i}	0.766 (9)	Tl1C—Tl1C^{i}	1.327 (15)
Tl1A—Tl1C^{ii}	0.766 (9)	Tl1C—Tl1C^{ii}	1.327 (15)
Tl1A—O3	3.4357 (19)	Tl1C—O2^{iv}	2.883 (6)
Tl1A—O3^{iii}	3.4358 (19)	Tl1C—O2^{i}	2.883 (6)

Tl1A—O3^{i}	3.4358 (19)	Tl1C—O3	3.186 (3)
Tl1A—O3^{iv}	3.4358 (19)	Tl1C—O3^{v}	3.186 (3)
Tl1A—O3^{v}	3.4358 (19)	Tl1C—O3^{iv}	3.3574 (19)
Tl1A—O3^{ii}	3.4358 (19)	Tl1C—O3^{i}	3.3574 (19)
Tl1A—O2^{v}	3.4419 (15)	Tl1C—O2^{v}	3.4432 (18)
Tl1A—O2^{iv}	3.4419 (15)	Tl1C—O2	3.4432 (18)
Tl1A—O2^{ii}	3.4419 (15)	Tl1C—O4^{vi}	3.494 (8)
Tl1A—O2^{iii}	3.4419 (14)	Tl1C—O4^{vii}	3.494 (8)
Tl1A—O2^{i}	3.4419 (14)	Tl1C—As1^{iv}	3.802 (3)
Tl1A—O2	3.4419 (15)	Tl1C—As1^{i}	3.802 (3)
Tl1A—As1^{v}	4.1219 (5)	Tl1C—As1^{v}	3.8935 (19)
Tl1A—As1^{iii}	4.1219 (5)	Tl1C—As1	3.8936 (19)
Tl1A—As1^{iv}	4.1219 (5)	Tl1C—O3^{iii}	3.969 (7)
Tl1B—Tl1B^{i}	0.706 (11)	Ga1—O4^{viii}	1.9609 (14)
Tl1B—Tl1B^{ii}	0.706 (11)	Ga1—O4^{ix}	1.9609 (15)
Tl1B—Tl1C^{i}	1.032 (12)	Ga1—O4^{i}	1.9609 (14)
Tl1B—Tl1C^{ii}	1.032 (11)	Ga1—O2^{x}	1.9648 (14)
Tl1B—O2^{iv}	3.134 (5)	Ga1—O2^{ii}	1.9648 (15)
Tl1B—O2^{i}	3.134 (5)	Ga1—O2^{xi}	1.9648 (14)
Tl1B—O3	3.283 (3)	As2—O1^{xii}	1.8062 (14)
Tl1B—O3^{v}	3.283 (3)	As2—O1^{xiii}	1.8062 (14)
Tl1B—O3^{i}	3.373 (2)	As2—O1^{ix}	1.8062 (14)
Tl1B—O3^{iv}	3.373 (2)	As2—O1^{xiv}	1.8062 (14)
Tl1B—O2^{v}	3.4213 (15)	As2—O1^{i}	1.8063 (14)
Tl1B—O2	3.4213 (15)	As2—O1^{viii}	1.8063 (14)
Tl1B—O3^{iii}	3.709 (5)	As1—O2	1.6641 (14)
Tl1B—O3^{ii}	3.709 (5)	As1—O4^{v}	1.6672 (14)
Tl1B—O2^{ii}	3.810 (6)	As1—O1^{xv}	1.7094 (14)
Tl1B—O2^{iii}	3.810 (6)	As1—O3	1.7115 (16)
Tl1B—O4^{vi}	3.810 (6)		

Tl1B^{i}—Tl1A—Tl1B^{ii}	120.00 (2)	O2^{i}—Tl1C—O3^{i}	49.88 (5)
Tl1B^{i}—Tl1A—Tl1C	120.000 (17)	O3—Tl1C—O3^{i}	72.40 (6)
Tl1B^{ii}—Tl1A—Tl1C	120.00 (7)	O3^{v}—Tl1C—O3^{i}	107.87 (7)
Tl1B^{i}—Tl1A—Tl1C^{i}	0 (2)	O3^{iv}—Tl1C—O3^{i}	178.8 (3)
Tl1B^{ii}—Tl1A—Tl1C^{i}	120.00 (2)	Tl1A—Tl1C—O2^{v}	83.51 (14)
Tl1C—Tl1A—Tl1C^{i}	120.000 (19)	Tl1B^{i}—Tl1C—O2^{v}	64.1 (2)
Tl1B^{i}—Tl1A—Tl1C^{ii}	120.000 (17)	Tl1B^{ii}—Tl1C—O2^{v}	102.9 (3)
Tl1B^{ii}—Tl1A—Tl1C^{ii}	0.000 (19)	Tl1C^{i}—Tl1C—O2^{v}	54.51 (14)
Tl1C—Tl1A—Tl1C^{ii}	120.00 (5)	Tl1C^{ii}—Tl1C—O2^{v}	112.64 (13)
Tl1C^{i}—Tl1A—Tl1C^{ii}	120.000 (17)	O2^{iv}—Tl1C—O2^{v}	132.5 (2)
Tl1B^{i}—Tl1A—O3	129.66 (3)	O2^{i}—Tl1C—O2^{v}	58.33 (6)
Tl1B^{ii}—Tl1A—O3	77.72 (3)	O3—Tl1C—O2^{v}	136.75 (5)
Tl1C—Tl1A—O3	64.82 (3)	O3^{v}—Tl1C—O2^{v}	47.23 (4)
Tl1C^{i}—Tl1A—O3	129.66 (3)	O3^{iv}—Tl1C—O2^{v}	115.03 (5)
Tl1C^{ii}—Tl1A—O3	77.72 (3)	O3^{i}—Tl1C—O2^{v}	64.82 (4)
Tl1B^{i}—Tl1A—O3^{iii}	64.82 (3)	Tl1A—Tl1C—O2	83.51 (14)
Tl1B^{ii}—Tl1A—O3^{iii}	77.72 (3)	Tl1B^{i}—Tl1C—O2	102.9 (3)

Tl1C—Tl1A—O3^{iii}	129.65 (3)	Tl1B^{ii}—Tl1C—O2	64.1 (2)
Tl1C^{i}—Tl1A—O3^{iii}	64.82 (3)	Tl1C^{i}—Tl1C—O2	112.64 (14)
Tl1C^{ii}—Tl1A—O3^{iii}	77.72 (3)	Tl1C^{ii}—Tl1C—O2	54.51 (15)
O3—Tl1A—O3^{iii}	155.44 (5)	O2^{iv}—Tl1C—O2	58.33 (6)
Tl1B^{i}—Tl1A—O3^{i}	64.82 (3)	O2^{i}—Tl1C—O2	132.5 (2)
Tl1B^{ii}—Tl1A—O3^{i}	129.65 (3)	O3—Tl1C—O2	47.23 (4)
Tl1C—Tl1A—O3^{i}	77.72 (3)	O3^{v}—Tl1C—O2	136.75 (5)
Tl1C^{i}—Tl1A—O3^{i}	64.82 (3)	O3^{iv}—Tl1C—O2	64.82 (4)
Tl1C^{ii}—Tl1A—O3^{i}	129.65 (3)	O3^{i}—Tl1C—O2	115.03 (5)
O3—Tl1A—O3^{i}	68.50 (4)	O2^{v}—Tl1C—O2	167.0 (3)
O3^{iii}—Tl1A—O3^{i}	129.64 (6)	Tl1A—Tl1C—O4^{vi}	150.55 (7)
Tl1B^{i}—Tl1A—O3^{iv}	129.65 (3)	Tl1B^{i}—Tl1C—O4^{vi}	136.76 (15)
Tl1B^{ii}—Tl1A—O3^{iv}	64.82 (3)	Tl1B^{ii}—Tl1C—O4^{vi}	155.25 (6)
Tl1C—Tl1A—O3^{iv}	77.72 (3)	Tl1C^{i}—Tl1C—O4^{vi}	128.52 (6)
Tl1C^{i}—Tl1A—O3^{iv}	129.65 (3)	Tl1C^{ii}—Tl1C—O4^{vi}	152.31 (4)
Tl1C^{ii}—Tl1A—O3^{iv}	64.82 (3)	O2^{iv}—Tl1C—O4^{vi}	58.91 (14)
O3—Tl1A—O3^{iv}	100.69 (6)	O2^{i}—Tl1C—O4^{vi}	49.76 (12)
O3^{iii}—Tl1A—O3^{iv}	68.50 (4)	O3—Tl1C—O4^{vi}	106.8 (2)
O3^{i}—Tl1A—O3^{iv}	155.44 (5)	O3^{v}—Tl1C—O4^{vi}	47.94 (9)
Tl1B^{i}—Tl1A—O3^{v}	77.72 (3)	O3^{iv}—Tl1C—O4^{vi}	81.43 (12)
Tl1B^{ii}—Tl1A—O3^{v}	129.65 (3)	O3^{i}—Tl1C—O4^{vi}	99.64 (15)
Tl1C—Tl1A—O3^{v}	64.82 (3)	O2^{v}—Tl1C—O4^{vi}	75.36 (9)
Tl1C^{i}—Tl1A—O3^{v}	77.72 (3)	O2—Tl1C—O4^{vi}	116.71 (18)
Tl1C^{ii}—Tl1A—O3^{v}	129.65 (3)	Tl1A—Tl1C—O4^{vii}	150.55 (7)
O3—Tl1A—O3^{v}	129.64 (6)	Tl1B^{i}—Tl1C—O4^{vii}	155.24 (6)
O3^{iii}—Tl1A—O3^{v}	68.50 (4)	Tl1B^{ii}—Tl1C—O4^{vii}	136.76 (16)
O3^{i}—Tl1A—O3^{v}	100.69 (5)	Tl1C^{i}—Tl1C—O4^{vii}	152.31 (4)
O3^{iv}—Tl1A—O3^{v}	68.50 (4)	Tl1C^{ii}—Tl1C—O4^{vii}	128.52 (7)
Tl1B^{i}—Tl1A—O3^{ii}	77.72 (3)	O2^{iv}—Tl1C—O4^{vii}	49.76 (12)
Tl1B^{ii}—Tl1A—O3^{ii}	64.82 (3)	O2^{i}—Tl1C—O4^{vii}	58.91 (15)
Tl1C—Tl1A—O3^{ii}	129.65 (3)	O3—Tl1C—O4^{vii}	47.94 (9)
Tl1C^{i}—Tl1A—O3^{ii}	77.72 (3)	O3^{v}—Tl1C—O4^{vii}	106.8 (2)
Tl1C^{ii}—Tl1A—O3^{ii}	64.82 (3)	O3^{iv}—Tl1C—O4^{vii}	99.64 (15)
O3—Tl1A—O3^{ii}	68.50 (4)	O3^{i}—Tl1C—O4^{vii}	81.43 (12)
O3^{iii}—Tl1A—O3^{ii}	100.69 (5)	O2^{v}—Tl1C—O4^{vii}	116.71 (18)
O3^{i}—Tl1A—O3^{ii}	68.50 (4)	O2—Tl1C—O4^{vii}	75.36 (9)
O3^{iv}—Tl1A—O3^{ii}	129.64 (6)	O4^{vi}—Tl1C—O4^{vii}	58.90 (15)
O3^{v}—Tl1A—O3^{ii}	155.44 (6)	Tl1A—Tl1C—As1^{iv}	109.57 (12)
Tl1B^{i}—Tl1A—O2^{v}	38.59 (2)	Tl1B^{i}—Tl1C—As1^{iv}	125.8 (2)
Tl1B^{ii}—Tl1A—O2^{v}	153.03 (3)	Tl1B^{ii}—Tl1C—As1^{iv}	92.58 (19)
Tl1C—Tl1A—O2^{v}	83.71 (3)	Tl1C^{i}—Tl1C—As1^{iv}	133.20 (11)
Tl1C^{i}—Tl1A—O2^{v}	38.59 (2)	Tl1C^{ii}—Tl1C—As1^{iv}	84.00 (13)
Tl1C^{ii}—Tl1A—O2^{v}	153.03 (3)	O2^{iv}—Tl1C—As1^{iv}	24.19 (3)
O3—Tl1A—O2^{v}	127.32 (4)	O2^{i}—Tl1C—As1^{iv}	117.7 (2)
O3^{iii}—Tl1A—O2^{v}	76.88 (4)	O3—Tl1C—As1^{iv}	86.06 (8)
O3^{i}—Tl1A—O2^{v}	64.02 (4)	O3^{v}—Tl1C—As1^{iv}	85.56 (8)
O3^{iv}—Tl1A—O2^{v}	113.04 (4)	O3^{iv}—Tl1C—As1^{iv}	26.75 (4)
O3^{v}—Tl1A—O2^{v}	45.62 (4)	O3^{i}—Tl1C—As1^{iv}	154.2 (2)

O3^{ii}—Tl1A—O2^{v}	111.53 (4)	O2^{v}—Tl1C—As1^{iv}	132.74 (7)
Tl1B^{i}—Tl1A—O2^{iv}	153.03 (2)	O2—Tl1C—As1^{iv}	52.91 (3)
Tl1B^{ii}—Tl1A—O2^{iv}	83.71 (4)	O4^{vi}—Tl1C—As1^{iv}	72.63 (12)
Tl1C—Tl1A—O2^{iv}	38.59 (3)	O4^{vii}—Tl1C—As1^{iv}	73.46 (12)
Tl1C^{i}—Tl1A—O2^{iv}	153.03 (2)	Tl1A—Tl1C—As1^{i}	109.57 (12)
Tl1C^{ii}—Tl1A—O2^{iv}	83.71 (3)	Tl1B^{i}—Tl1C—As1^{i}	92.58 (18)
O3—Tl1A—O2^{iv}	64.02 (4)	Tl1B^{ii}—Tl1C—As1^{i}	125.8 (2)
O3^{iii}—Tl1A—O2^{iv}	113.04 (4)	Tl1C^{i}—Tl1C—As1^{i}	84.00 (12)
O3^{i}—Tl1A—O2^{iv}	111.53 (4)	Tl1C^{ii}—Tl1C—As1^{i}	133.20 (11)
O3^{iv}—Tl1A—O2^{iv}	45.62 (3)	O2^{iv}—Tl1C—As1^{i}	117.7 (2)
O3^{v}—Tl1A—O2^{iv}	76.88 (4)	O2^{i}—Tl1C—As1^{i}	24.19 (3)
O3^{ii}—Tl1A—O2^{iv}	127.32 (4)	O3—Tl1C—As1^{i}	85.56 (8)
O2^{v}—Tl1A—O2^{iv}	114.671 (18)	O3^{v}—Tl1C—As1^{i}	86.06 (8)
Tl1B^{i}—Tl1A—O2^{ii}	38.59 (2)	O3^{iv}—Tl1C—As1^{i}	154.2 (2)
Tl1B^{ii}—Tl1A—O2^{ii}	83.71 (3)	O3^{i}—Tl1C—As1^{i}	26.75 (4)
Tl1C—Tl1A—O2^{ii}	153.03 (3)	O2^{v}—Tl1C—As1^{i}	52.91 (3)
Tl1C^{i}—Tl1A—O2^{ii}	38.59 (2)	O2—Tl1C—As1^{i}	132.74 (7)
Tl1C^{ii}—Tl1A—O2^{ii}	83.71 (3)	O4^{vi}—Tl1C—As1^{i}	73.46 (12)
O3—Tl1A—O2^{ii}	113.05 (4)	O4^{vii}—Tl1C—As1^{i}	72.63 (12)
O3^{iii}—Tl1A—O2^{ii}	64.02 (4)	As1^{iv}—Tl1C—As1^{i}	140.9 (2)
O3^{i}—Tl1A—O2^{ii}	76.88 (4)	Tl1A—Tl1C—As1^{v}	102.03 (12)
O3^{iv}—Tl1A—O2^{ii}	127.32 (4)	Tl1B^{i}—Tl1C—As1^{v}	84.78 (18)
O3^{v}—Tl1A—O2^{ii}	111.53 (4)	Tl1B^{ii}—Tl1C—As1^{v}	118.9 (2)
O3^{ii}—Tl1A—O2^{ii}	45.62 (4)	Tl1C^{i}—Tl1C—As1^{v}	76.18 (12)
O2^{v}—Tl1A—O2^{ii}	77.17 (4)	Tl1C^{ii}—Tl1C—As1^{v}	126.86 (11)
O2^{iv}—Tl1A—O2^{ii}	167.42 (5)	O2^{iv}—Tl1C—As1^{v}	107.38 (17)
Tl1B^{i}—Tl1A—O2^{iii}	83.71 (2)	O2^{i}—Tl1C—As1^{v}	54.77 (6)
Tl1B^{ii}—Tl1A—O2^{iii}	38.59 (4)	O3—Tl1C—As1^{v}	144.21 (19)
Tl1C—Tl1A—O2^{iii}	153.03 (3)	O3^{v}—Tl1C—As1^{v}	25.57 (3)
Tl1C^{i}—Tl1A—O2^{iii}	83.71 (2)	O3^{iv}—Tl1C—As1^{v}	97.93 (5)
Tl1C^{ii}—Tl1A—O2^{iii}	38.59 (3)	O3^{i}—Tl1C—As1^{v}	82.32 (4)
O3—Tl1A—O2^{iii}	111.53 (4)	O2^{v}—Tl1C—As1^{v}	25.27 (3)
O3^{iii}—Tl1A—O2^{iii}	45.62 (3)	O2—Tl1C—As1^{v}	162.06 (9)
O3^{i}—Tl1A—O2^{iii}	127.31 (4)	O4^{vi}—Tl1C—As1^{v}	52.35 (7)
O3^{iv}—Tl1A—O2^{iii}	76.88 (4)	O4^{vii}—Tl1C—As1^{v}	104.36 (18)
O3^{v}—Tl1A—O2^{iii}	113.04 (4)	As1^{iv}—Tl1C—As1^{v}	109.44 (10)
O3^{ii}—Tl1A—O2^{iii}	64.02 (4)	As1^{i}—Tl1C—As1^{v}	61.81 (4)
O2^{v}—Tl1A—O2^{iii}	114.671 (18)	Tl1A—Tl1C—As1	102.03 (12)
O2^{iv}—Tl1A—O2^{iii}	114.671 (18)	Tl1B^{i}—Tl1C—As1	118.9 (2)
O2^{ii}—Tl1A—O2^{iii}	53.93 (5)	Tl1B^{ii}—Tl1C—As1	84.78 (19)
Tl1B^{i}—Tl1A—O2^{i}	83.71 (2)	Tl1C^{i}—Tl1C—As1	126.86 (12)
Tl1B^{ii}—Tl1A—O2^{i}	153.03 (4)	Tl1C^{ii}—Tl1C—As1	76.18 (13)
Tl1C—Tl1A—O2^{i}	38.59 (3)	O2^{iv}—Tl1C—As1	54.77 (6)
Tl1C^{i}—Tl1A—O2^{i}	83.71 (2)	O2^{i}—Tl1C—As1	107.38 (17)
Tl1C^{ii}—Tl1A—O2^{i}	153.03 (3)	O3—Tl1C—As1	25.56 (3)
O3—Tl1A—O2^{i}	76.88 (4)	O3^{v}—Tl1C—As1	144.21 (19)
O3^{iii}—Tl1A—O2^{i}	127.31 (4)	O3^{iv}—Tl1C—As1	82.32 (4)
O3^{i}—Tl1A—O2^{i}	45.62 (3)	O3^{i}—Tl1C—As1	97.93 (5)

O3^{iv}—Tl1A—O2^{i}	111.52 (4)	O2^{v}—Tl1C—As1	162.06 (9)
O3^{v}—Tl1A—O2^{i}	64.02 (4)	O2—Tl1C—As1	25.27 (3)
O3^{ii}—Tl1A—O2^{i}	113.04 (4)	O4^{vi}—Tl1C—As1	104.36 (18)
O2^{v}—Tl1A—O2^{i}	53.93 (5)	O4^{vii}—Tl1C—As1	52.35 (7)
O2^{iv}—Tl1A—O2^{i}	77.17 (4)	As1^{iv}—Tl1C—As1	61.81 (4)
O2^{ii}—Tl1A—O2^{i}	114.671 (18)	As1^{i}—Tl1C—As1	109.44 (10)
O2^{iii}—Tl1A—O2^{i}	167.42 (5)	As1^{v}—Tl1C—As1	155.9 (2)
Tl1B^{i}—Tl1A—O2	153.03 (2)	Tl1A—Tl1C—O3^{iii}	41.80 (9)
Tl1B^{ii}—Tl1A—O2	38.59 (3)	Tl1B^{i}—Tl1C—O3^{iii}	42.53 (9)
Tl1C—Tl1A—O2	83.71 (3)	Tl1B^{ii}—Tl1C—O3^{iii}	48.38 (13)
Tl1C^{i}—Tl1A—O2	153.03 (2)	Tl1C^{i}—Tl1C—O3^{iii}	45.67 (7)
Tl1C^{ii}—Tl1A—O2	38.59 (3)	Tl1C^{ii}—Tl1C—O3^{iii}	53.67 (6)
O3—Tl1A—O2	45.61 (3)	O2^{iv}—Tl1C—O3^{iii}	112.74 (5)
O3^{iii}—Tl1A—O2	111.53 (4)	O2^{i}—Tl1C—O3^{iii}	127.49 (5)
O3^{i}—Tl1A—O2	113.04 (4)	O3—Tl1C—O3^{iii}	139.3 (2)
O3^{iv}—Tl1A—O2	64.02 (4)	O3^{v}—Tl1C—O3^{iii}	64.35 (8)
O3^{v}—Tl1A—O2	127.32 (4)	O3^{iv}—Tl1C—O3^{iii}	63.07 (9)
O3^{ii}—Tl1A—O2	76.88 (4)	O3^{i}—Tl1C—O3^{iii}	115.92 (18)
O2^{v}—Tl1A—O2	167.42 (5)	O2^{v}—Tl1C—O3^{iii}	70.05 (10)
O2^{iv}—Tl1A—O2	53.93 (5)	O2—Tl1C—O3^{iii}	99.95 (14)
O2^{ii}—Tl1A—O2	114.671 (18)	O4^{vi}—Tl1C—O3^{iii}	110.35 (4)
O2^{iii}—Tl1A—O2	77.17 (5)	O4^{vii}—Tl1C—O3^{iii}	161.91 (11)
O2^{i}—Tl1A—O2	114.671 (18)	As1^{iv}—Tl1C—O3^{iii}	89.69 (6)
Tl1B^{i}—Tl1A—As1^{v}	60.345 (3)	As1^{i}—Tl1C—O3^{iii}	120.32 (10)
Tl1B^{ii}—Tl1A—As1^{v}	151.344 (7)	As1^{v}—Tl1C—O3^{iii}	74.64 (6)
Tl1C—Tl1A—As1^{v}	67.496 (15)	As1—Tl1C—O3^{iii}	125.14 (13)
Tl1C^{i}—Tl1A—As1^{v}	60.345 (3)	O4^{viii}—Ga1—O4^{ix}	89.32 (6)
Tl1C^{ii}—Tl1A—As1^{v}	151.344 (7)	O4^{viii}—Ga1—O4^{i}	89.32 (6)
O3—Tl1A—As1^{v}	125.98 (3)	O4^{ix}—Ga1—O4^{i}	89.32 (6)
O3^{iii}—Tl1A—As1^{v}	77.63 (3)	O4^{viii}—Ga1—O2^{x}	177.75 (6)
O3^{i}—Tl1A—As1^{v}	78.07 (3)	O4^{ix}—Ga1—O2^{x}	91.19 (6)
O3^{iv}—Tl1A—As1^{v}	92.52 (3)	O4^{i}—Ga1—O2^{x}	88.50 (6)
O3^{v}—Tl1A—As1^{v}	24.05 (3)	O4^{viii}—Ga1—O2^{ii}	88.50 (6)
O3^{ii}—Tl1A—As1^{v}	134.64 (3)	O4^{ix}—Ga1—O2^{ii}	177.75 (6)
O2^{v}—Tl1A—As1^{v}	23.26 (2)	O4^{i}—Ga1—O2^{ii}	91.19 (6)
O2^{iv}—Tl1A—As1^{v}	92.70 (2)	O2^{x}—Ga1—O2^{ii}	91.01 (6)
O2^{ii}—Tl1A—As1^{v}	98.35 (2)	O4^{viii}—Ga1—O2^{xi}	91.19 (6)
O2^{iii}—Tl1A—As1^{v}	122.48 (2)	O4^{ix}—Ga1—O2^{xi}	88.50 (6)
O2^{i}—Tl1A—As1^{v}	49.80 (3)	O4^{i}—Ga1—O2^{xi}	177.75 (6)
O2—Tl1A—As1^{v}	146.60 (2)	O2^{x}—Ga1—O2^{xi}	91.01 (6)
Tl1B^{i}—Tl1A—As1^{iii}	67.496 (3)	O2^{ii}—Ga1—O2^{xi}	91.01 (6)
Tl1B^{ii}—Tl1A—As1^{iii}	60.35 (2)	O4^{viii}—Ga1—Tl1C^{ix}	142.93 (5)
Tl1C—Tl1A—As1^{iii}	151.344 (7)	O4^{ix}—Ga1—Tl1C^{ix}	85.12 (7)
Tl1C^{i}—Tl1A—As1^{iii}	67.496 (3)	O4^{i}—Ga1—Tl1C^{ix}	54.06 (6)
Tl1C^{ii}—Tl1A—As1^{iii}	60.345 (15)	O2^{x}—Ga1—Tl1C^{ix}	35.00 (5)
O3—Tl1A—As1^{iii}	134.64 (3)	O2^{ii}—Ga1—Tl1C^{ix}	96.95 (7)
O3^{iii}—Tl1A—As1^{iii}	24.05 (3)	O2^{xi}—Ga1—Tl1C^{ix}	125.17 (6)
O3^{i}—Tl1A—As1^{iii}	125.98 (3)	O4^{viii}—Ga1—Tl1C^{viii}	85.12 (8)

O3^{iv}—Tl1A—As1^{iii}	77.63 (3)	O4^{ix}—Ga1—Tl1C^{viii}	54.06 (6)
O3^{v}—Tl1A—As1^{iii}	92.52 (3)	O4^{i}—Ga1—Tl1C^{viii}	142.93 (6)
O3^{ii}—Tl1A—As1^{iii}	78.07 (3)	O2^{x}—Ga1—Tl1C^{viii}	96.95 (8)
O2^{v}—Tl1A—As1^{iii}	92.70 (2)	O2^{ii}—Ga1—Tl1C^{viii}	125.17 (6)
O2^{iv}—Tl1A—As1^{iii}	122.48 (2)	O2^{xi}—Ga1—Tl1C^{viii}	35.00 (5)
O2^{ii}—Tl1A—As1^{iii}	49.80 (2)	Tl1C^{ix}—Ga1—Tl1C^{viii}	119.488 (4)
O2^{iii}—Tl1A—As1^{iii}	23.26 (2)	O4^{viii}—Ga1—Tl1C^{i}	54.06 (6)
O2^{i}—Tl1A—As1^{iii}	146.60 (2)	O4^{ix}—Ga1—Tl1C^{i}	142.93 (5)
O2—Tl1A—As1^{iii}	98.35 (2)	O4^{i}—Ga1—Tl1C^{i}	85.13 (7)
As1^{v}—Tl1A—As1^{iii}	99.284 (8)	O2^{x}—Ga1—Tl1C^{i}	125.17 (6)
Tl1B^{i}—Tl1A—As1^{iv}	151.344 (7)	O2^{ii}—Ga1—Tl1C^{i}	35.00 (5)
Tl1B^{ii}—Tl1A—As1^{iv}	67.50 (2)	O2^{xi}—Ga1—Tl1C^{i}	96.95 (7)
Tl1C—Tl1A—As1^{iv}	60.345 (15)	Tl1C^{ix}—Ga1—Tl1C^{i}	119.488 (6)
Tl1C^{i}—Tl1A—As1^{iv}	151.344 (7)	Tl1C^{viii}—Ga1—Tl1C^{i}	119.488 (1)
Tl1C^{ii}—Tl1A—As1^{iv}	67.496 (15)	O4^{viii}—Ga1—Tl1B^{ix}	143.88 (5)
O3—Tl1A—As1^{iv}	78.07 (3)	O4^{ix}—Ga1—Tl1B^{ix}	82.88 (5)
O3^{iii}—Tl1A—As1^{iv}	92.52 (3)	O4^{i}—Ga1—Tl1B^{ix}	55.53 (5)
O3^{i}—Tl1A—As1^{iv}	134.64 (3)	O2^{x}—Ga1—Tl1B^{ix}	34.12 (4)
O3^{iv}—Tl1A—As1^{iv}	24.05 (3)	O2^{ii}—Ga1—Tl1B^{ix}	99.21 (6)
O3^{v}—Tl1A—As1^{iv}	77.63 (3)	O2^{xi}—Ga1—Tl1B^{ix}	123.61 (5)
O3^{ii}—Tl1A—As1^{iv}	125.98 (3)	Tl1C^{ix}—Ga1—Tl1B^{ix}	2.61 (6)
O2^{v}—Tl1A—As1^{iv}	122.48 (2)	Tl1C^{viii}—Ga1—Tl1B^{ix}	116.94 (6)
O2^{iv}—Tl1A—As1^{iv}	23.26 (2)	Tl1C^{i}—Ga1—Tl1B^{ix}	122.10 (5)
O2^{ii}—Tl1A—As1^{iv}	146.60 (2)	O4^{viii}—Ga1—Tl1B^{i}	55.53 (5)
O2^{iii}—Tl1A—As1^{iv}	92.70 (2)	O4^{ix}—Ga1—Tl1B^{i}	143.88 (5)
O2^{i}—Tl1A—As1^{iv}	98.35 (2)	O4^{i}—Ga1—Tl1B^{i}	82.88 (5)
O2—Tl1A—As1^{iv}	49.80 (2)	O2^{x}—Ga1—Tl1B^{i}	123.61 (5)
As1^{v}—Tl1A—As1^{iv}	99.284 (8)	O2^{ii}—Ga1—Tl1B^{i}	34.12 (4)
As1^{iii}—Tl1A—As1^{iv}	99.284 (8)	O2^{xi}—Ga1—Tl1B^{i}	99.21 (5)
Tl1B^{i}—Tl1B—Tl1B^{ii}	60.001 (6)	Tl1C^{ix}—Ga1—Tl1B^{i}	116.94 (6)
Tl1B^{i}—Tl1B—Tl1C^{i}	10.01 (19)	Tl1C^{viii}—Ga1—Tl1B^{i}	122.10 (6)
Tl1B^{ii}—Tl1B—Tl1C^{i}	70.01 (18)	Tl1C^{i}—Ga1—Tl1B^{i}	2.61 (6)
Tl1B^{i}—Tl1B—Tl1C^{ii}	70.01 (19)	Tl1B^{ix}—Ga1—Tl1B^{i}	119.553 (4)
Tl1B^{ii}—Tl1B—Tl1C^{ii}	10.0 (2)	O4^{viii}—Ga1—Tl1B^{viii}	82.88 (6)
Tl1C^{i}—Tl1B—Tl1C^{ii}	80.0 (4)	O4^{ix}—Ga1—Tl1B^{viii}	55.53 (5)
Tl1B^{i}—Tl1B—O2^{iv}	161.49 (7)	O4^{i}—Ga1—Tl1B^{viii}	143.88 (5)
Tl1B^{ii}—Tl1B—O2^{iv}	108.27 (9)	O2^{x}—Ga1—Tl1B^{viii}	99.21 (6)
Tl1C^{i}—Tl1B—O2^{iv}	165.03 (5)	O2^{ii}—Ga1—Tl1B^{viii}	123.61 (5)
Tl1C^{ii}—Tl1B—O2^{iv}	98.63 (15)	O2^{xi}—Ga1—Tl1B^{viii}	34.12 (5)
Tl1B^{i}—Tl1B—O2^{i}	108.27 (8)	Tl1C^{ix}—Ga1—Tl1B^{viii}	122.10 (6)
Tl1B^{ii}—Tl1B—O2^{i}	161.49 (6)	Tl1C^{viii}—Ga1—Tl1B^{viii}	2.61 (6)
Tl1C^{i}—Tl1B—O2^{i}	98.63 (14)	Tl1C^{i}—Ga1—Tl1B^{viii}	116.94 (6)
Tl1C^{ii}—Tl1B—O2^{i}	165.03 (5)	Tl1B^{ix}—Ga1—Tl1B^{viii}	119.553 (2)
O2^{iv}—Tl1B—O2^{i}	86.48 (16)	Tl1B^{i}—Ga1—Tl1B^{viii}	119.553 (1)
Tl1B^{i}—Tl1B—O3	122.35 (9)	O1^{xii}—As2—O1^{xiii}	92.56 (6)
Tl1B^{ii}—Tl1B—O3	91.20 (11)	O1^{xii}—As2—O1^{ix}	87.44 (6)
Tl1C^{i}—Tl1B—O3	125.20 (11)	O1^{xiii}—As2—O1^{ix}	87.44 (6)
Tl1C^{ii}—Tl1B—O3	85.15 (9)	O1^{xii}—As2—O1^{xiv}	92.56 (6)

O2^{iv}—Tl1B—O3	69.19 (9)	O1^{xiii}—As2—O1^{xiv}	92.56 (6)
O2^{i}—Tl1B—O3	83.53 (11)	O1^{ix}—As2—O1^{xiv}	179.99 (7)
Tl1B^{i}—Tl1B—O3^{v}	91.20 (10)	O1^{xii}—As2—O1^{i}	87.44 (6)
Tl1B^{ii}—Tl1B—O3^{v}	122.35 (9)	O1^{xiii}—As2—O1^{i}	180.0
Tl1C^{i}—Tl1B—O3^{v}	85.15 (9)	O1^{ix}—As2—O1^{i}	92.56 (6)
Tl1C^{ii}—Tl1B—O3^{v}	125.20 (11)	O1^{xiv}—As2—O1^{i}	87.44 (6)
O2^{iv}—Tl1B—O3^{v}	83.53 (11)	O1^{xii}—As2—O1^{viii}	180.0
O2^{i}—Tl1B—O3^{v}	69.19 (9)	O1^{xiii}—As2—O1^{viii}	87.44 (6)
O3—Tl1B—O3^{v}	142.5 (2)	O1^{ix}—As2—O1^{viii}	92.56 (6)
Tl1B^{i}—Tl1B—O3^{i}	76.72 (10)	O1^{xiv}—As2—O1^{viii}	87.44 (6)
Tl1B^{ii}—Tl1B—O3^{i}	113.31 (9)	O1^{i}—As2—O1^{viii}	92.56 (6)
Tl1C^{i}—Tl1B—O3^{i}	70.81 (8)	O2—As1—O4^{v}	117.11 (7)
Tl1C^{ii}—Tl1B—O3^{i}	118.40 (16)	O2—As1—O1^{xv}	115.20 (7)
O2^{iv}—Tl1B—O3^{i}	121.79 (16)	O4^{v}—As1—O1^{xv}	100.55 (7)
O2^{i}—Tl1B—O3^{i}	48.21 (5)	O2—As1—O3	104.32 (8)
O3—Tl1B—O3^{i}	71.03 (6)	O4^{v}—As1—O3	111.00 (7)
O3^{v}—Tl1B—O3^{i}	105.28 (8)	O1^{xv}—As1—O3	108.62 (8)
Tl1B^{i}—Tl1B—O3^{iv}	113.32 (10)	O2—As1—Tl1C^{ii}	45.23 (13)
Tl1B^{ii}—Tl1B—O3^{iv}	76.72 (11)	O4^{v}—As1—Tl1C^{ii}	117.24 (9)
Tl1C^{i}—Tl1B—O3^{iv}	118.40 (16)	O1^{xv}—As1—Tl1C^{ii}	142.08 (9)
Tl1C^{ii}—Tl1B—O3^{iv}	70.81 (9)	O3—As1—Tl1C^{ii}	62.00 (11)
O2^{iv}—Tl1B—O3^{iv}	48.21 (5)	O2—As1—Tl1C	62.05 (11)
O2^{i}—Tl1B—O3^{iv}	121.79 (16)	O4^{v}—As1—Tl1C	101.81 (13)
O3—Tl1B—O3^{iv}	105.28 (8)	O1^{xv}—As1—Tl1C	155.50 (11)
O3^{v}—Tl1B—O3^{iv}	71.03 (6)	O3—As1—Tl1C	53.44 (7)
O3^{i}—Tl1B—O3^{iv}	169.0 (2)	Tl1C^{ii}—As1—Tl1C	19.8 (2)
Tl1B^{i}—Tl1B—O2^{v}	60.43 (10)	O2—As1—Tl1B^{ii}	49.87 (9)
Tl1B^{ii}—Tl1B—O2^{v}	118.57 (9)	O4^{v}—As1—Tl1B^{ii}	114.51 (7)
Tl1C^{i}—Tl1B—O2^{v}	50.84 (13)	O1^{xv}—As1—Tl1B^{ii}	144.91 (7)
Tl1C^{ii}—Tl1B—O2^{v}	128.2 (3)	O3—As1—Tl1B^{ii}	58.46 (9)
O2^{iv}—Tl1B—O2^{v}	124.22 (15)	Tl1C^{ii}—As1—Tl1B^{ii}	4.93 (10)
O2^{i}—Tl1B—O2^{v}	56.67 (6)	Tl1C—As1—Tl1B^{ii}	15.14 (18)
O3—Tl1B—O2^{v}	133.64 (8)	O2—As1—Tl1B	58.46 (8)
O3^{v}—Tl1B—O2^{v}	46.81 (4)	O4^{v}—As1—Tl1B	106.50 (9)
O3^{i}—Tl1B—O2^{v}	64.90 (4)	O1^{xv}—As1—Tl1B	151.78 (9)
O3^{iv}—Tl1B—O2^{v}	115.21 (4)	O3—As1—Tl1B	53.97 (7)
Tl1B^{i}—Tl1B—O2	118.57 (11)	Tl1C^{ii}—As1—Tl1B	15.00 (18)
Tl1B^{ii}—Tl1B—O2	60.43 (12)	Tl1C—As1—Tl1B	5.05 (10)
Tl1C^{i}—Tl1B—O2	128.2 (3)	Tl1B^{ii}—As1—Tl1B	10.20 (16)
Tl1C^{ii}—Tl1B—O2	50.84 (14)	O2—As1—Tl1A	54.77 (5)
O2^{iv}—Tl1B—O2	56.67 (6)	O4^{v}—As1—Tl1A	111.51 (5)
O2^{i}—Tl1B—O2	124.22 (15)	O1^{xv}—As1—Tl1A	147.41 (5)
O3—Tl1B—O2	46.81 (4)	O3—As1—Tl1A	54.89 (6)
O3^{v}—Tl1B—O2	133.64 (9)	Tl1C^{ii}—As1—Tl1A	10.09 (12)
O3^{i}—Tl1B—O2	115.21 (4)	Tl1C—As1—Tl1A	10.48 (13)
O3^{iv}—Tl1B—O2	64.90 (4)	Tl1B^{ii}—As1—Tl1A	5.16 (8)
O2^{v}—Tl1B—O2	179.0 (2)	Tl1B—As1—Tl1A	5.42 (9)
Tl1B^{i}—Tl1B—O3^{iii}	48.40 (6)	O2—As1—Tl1B^{i}	55.93 (5)

Tl1B^{ii}—Tl1B—O3^{iii}	56.62 (5)	O4^{v}—As1—Tl1B^{i}	113.25 (6)
Tl1C^{i}—Tl1B—O3^{iii}	52.40 (12)	O1^{xv}—As1—Tl1B^{i}	145.33 (6)
Tl1C^{ii}—Tl1B—O3^{iii}	62.37 (15)	O3—As1—Tl1B^{i}	52.81 (7)
O2^{iv}—Tl1B—O3^{iii}	113.67 (4)	Tl1C^{ii}—As1—Tl1B^{i}	10.77 (13)
O2^{i}—Tl1B—O3^{iii}	128.31 (4)	Tl1C—As1—Tl1B^{i}	11.63 (13)
O3—Tl1B—O3^{iii}	147.52 (14)	Tl1B^{ii}—As1—Tl1B^{i}	6.08 (9)
O3^{v}—Tl1B—O3^{iii}	66.83 (6)	Tl1B—As1—Tl1B^{i}	6.76 (10)
O3^{i}—Tl1B—O3^{iii}	122.76 (13)	Tl1A—As1—Tl1B^{i}	2.50 (3)
O3^{iv}—Tl1B—O3^{iii}	66.00 (6)	O2—As1—Tl1C^{xvi}	92.14 (6)
O2^{v}—Tl1B—O3^{iii}	73.56 (7)	O4^{v}—As1—Tl1C^{xvi}	41.91 (5)
O2—Tl1B—O3^{iii}	105.70 (10)	O1^{xv}—As1—Tl1C^{xvi}	82.53 (7)
Tl1B^{i}—Tl1B—O3^{ii}	56.62 (6)	O3—As1—Tl1C^{xvi}	152.91 (6)
Tl1B^{ii}—Tl1B—O3^{ii}	48.40 (5)	Tl1C^{ii}—As1—Tl1C^{xvi}	123.42 (8)
Tl1C^{i}—Tl1B—O3^{ii}	62.37 (15)	Tl1C—As1—Tl1C^{xvi}	121.18 (11)
Tl1C^{ii}—Tl1B—O3^{ii}	52.40 (12)	Tl1B^{ii}—As1—Tl1C^{xvi}	124.63 (6)
O2^{iv}—Tl1B—O3^{ii}	128.31 (4)	Tl1B—As1—Tl1C^{xvi}	123.45 (8)
O2^{i}—Tl1B—O3^{ii}	113.67 (4)	Tl1A—As1—Tl1C^{xvi}	125.61 (5)
O3—Tl1B—O3^{ii}	66.84 (6)	Tl1B^{i}—As1—Tl1C^{xvi}	128.10 (4)
O3^{v}—Tl1B—O3^{ii}	147.52 (14)	O2—As1—Tl1C^{i}	56.83 (5)
O3^{i}—Tl1B—O3^{ii}	66.00 (6)	O4^{v}—As1—Tl1C^{i}	114.55 (6)
O3^{iv}—Tl1B—O3^{ii}	122.76 (13)	O1^{xv}—As1—Tl1C^{i}	143.72 (6)
O2^{v}—Tl1B—O3^{ii}	105.70 (10)	O3—As1—Tl1C^{i}	51.27 (7)
O2—Tl1B—O3^{ii}	73.56 (7)	Tl1C^{ii}—As1—Tl1C^{i}	11.61 (14)
O3^{iii}—Tl1B—O3^{ii}	90.99 (15)	Tl1C—As1—Tl1C^{i}	12.76 (15)
Tl1B^{i}—Tl1B—O2^{ii}	15.14 (2)	Tl1B^{ii}—As1—Tl1C^{i}	7.28 (9)
Tl1B^{ii}—Tl1B—O2^{ii}	52.07 (3)	Tl1B—As1—Tl1C^{i}	8.14 (10)
Tl1C^{i}—Tl1B—O2^{ii}	22.47 (14)	Tl1A—As1—Tl1C^{i}	4.38 (4)
Tl1C^{ii}—Tl1B—O2^{ii}	61.7 (2)	Tl1B^{i}—As1—Tl1C^{i}	1.88 (4)
O2^{iv}—Tl1B—O2^{ii}	160.34 (12)	Tl1C^{xvi}—As1—Tl1C^{i}	129.990 (14)
O2^{i}—Tl1B—O2^{ii}	112.79 (4)	As1^{xvii}—O1—As2^{xviii}	131.79 (8)
O3—Tl1B—O2^{ii}	107.73 (10)	As1^{xvii}—O1—Tl1C^{vi}	76.09 (10)
O3^{v}—Tl1B—O2^{ii}	106.34 (9)	As2^{xviii}—O1—Tl1C^{vi}	131.19 (7)
O3^{i}—Tl1B—O2^{ii}	72.78 (8)	As1^{xvii}—O1—Tl1B^{vi}	79.08 (7)
O3^{iv}—Tl1B—O2^{ii}	118.09 (14)	As2^{xviii}—O1—Tl1B^{vi}	129.47 (6)
O2^{v}—Tl1B—O2^{ii}	72.62 (8)	Tl1C^{vi}—O1—Tl1B^{vi}	3.04 (7)
O2—Tl1B—O2^{ii}	106.41 (13)	As1—O2—Ga1^{xix}	123.98 (8)
O3^{iii}—Tl1B—O2^{ii}	57.99 (9)	As1—O2—Tl1C^{ii}	110.58 (14)
O3^{ii}—Tl1B—O2^{ii}	41.51 (7)	Ga1^{xix}—O2—Tl1C^{ii}	121.99 (11)
Tl1B^{i}—Tl1B—O2^{iii}	52.07 (4)	As1—O2—Tl1B^{ii}	106.18 (10)
Tl1B^{ii}—Tl1B—O2^{iii}	15.14 (3)	Ga1^{xix}—O2—Tl1B^{ii}	125.29 (8)
Tl1C^{i}—Tl1B—O2^{iii}	61.7 (2)	Tl1C^{ii}—O2—Tl1B^{ii}	4.89 (11)
Tl1C^{ii}—Tl1B—O2^{iii}	22.47 (15)	As1—O2—Tl1B	97.04 (10)
O2^{iv}—Tl1B—O2^{iii}	112.79 (4)	Ga1^{xix}—O2—Tl1B	130.25 (7)
O2^{i}—Tl1B—O2^{iii}	160.34 (12)	Tl1C^{ii}—O2—Tl1B	16.1 (2)
O3—Tl1B—O2^{iii}	106.34 (9)	Tl1B^{ii}—O2—Tl1B	11.30 (18)
O3^{v}—Tl1B—O2^{iii}	107.73 (10)	As1—O2—Tl1A	101.96 (6)
O3^{i}—Tl1B—O2^{iii}	118.09 (14)	Ga1^{xix}—O2—Tl1A	128.28 (6)
O3^{iv}—Tl1B—O2^{iii}	72.78 (8)	Tl1C^{ii}—O2—Tl1A	9.54 (13)

O2^{v}—Tl1B—O2^{iii}	106.41 (13)	Tl1B^{ii}—O2—Tl1A	4.65 (8)
O2—Tl1B—O2^{iii}	72.62 (8)	Tl1B—O2—Tl1A	6.80 (10)
O3^{iii}—Tl1B—O2^{iii}	41.51 (7)	As1—O2—Tl1C	92.68 (12)
O3^{ii}—Tl1B—O2^{iii}	57.99 (9)	Ga1^{xix}—O2—Tl1C	131.46 (7)
O2^{ii}—Tl1B—O2^{iii}	48.37 (9)	Tl1C^{ii}—O2—Tl1C	22.0 (3)
Tl1B^{i}—Tl1B—O4^{vi}	130.74 (4)	Tl1B^{ii}—O2—Tl1C	17.2 (2)
Tl1B^{ii}—Tl1B—O4^{vi}	153.31 (3)	Tl1B—O2—Tl1C	5.98 (12)
Tl1C^{i}—Tl1B—O4^{vi}	121.93 (15)	Tl1A—O2—Tl1C	12.78 (14)
Tl1C^{ii}—Tl1B—O4^{vi}	146.99 (14)	As1—O2—Tl1B^{i}	102.86 (6)
O2^{iv}—Tl1B—O4^{vi}	53.44 (9)	Ga1^{xix}—O2—Tl1B^{i}	128.59 (6)
O2^{i}—Tl1B—O4^{vi}	45.18 (8)	Tl1C^{ii}—O2—Tl1B^{i}	7.87 (11)
O3—Tl1B—O4^{vi}	98.07 (15)	Tl1B^{ii}—O2—Tl1B^{i}	3.37 (6)
O3^{v}—Tl1B—O4^{vi}	44.48 (7)	Tl1B—O2—Tl1B^{i}	9.37 (14)
O3^{i}—Tl1B—O4^{vi}	93.37 (11)	Tl1A—O2—Tl1B^{i}	2.78 (4)
O3^{iv}—Tl1B—O4^{vi}	76.71 (9)	Tl1C—O2—Tl1B^{i}	15.31 (17)
O2^{v}—Tl1B—O4^{vi}	71.57 (8)	As1—O2—Tl1C^{i}	103.50 (6)
O2—Tl1B—O4^{vi}	109.39 (13)	Ga1^{xix}—O2—Tl1C^{i}	128.74 (6)
O3^{iii}—Tl1B—O4^{vi}	109.27 (4)	Tl1C^{ii}—O2—Tl1C^{i}	7.09 (10)
O3^{ii}—Tl1B—O4^{vi}	157.13 (10)	Tl1B^{ii}—O2—Tl1C^{i}	3.69 (4)
O2^{ii}—Tl1B—O4^{vi}	144.16 (3)	Tl1B—O2—Tl1C^{i}	11.31 (13)
O2^{iii}—Tl1B—O4^{vi}	144.88 (3)	Tl1A—O2—Tl1C^{i}	4.82 (5)
Tl1B^{i}—Tl1B—O4^{vii}	153.31 (3)	Tl1C—O2—Tl1C^{i}	17.21 (19)
Tl1B^{ii}—Tl1B—O4^{vii}	130.74 (5)	Tl1B^{i}—O2—Tl1C^{i}	2.03 (4)
Tl1C^{i}—Tl1B—O4^{vii}	146.99 (13)	As1—O2—Tl1C^{xvi}	68.04 (4)
Tl1C^{ii}—Tl1B—O4^{vii}	121.93 (15)	Ga1^{xix}—O2—Tl1C^{xvi}	59.62 (4)
O2^{iv}—Tl1B—O4^{vii}	45.18 (8)	Tl1C^{ii}—O2—Tl1C^{xvi}	140.65 (6)
O2^{i}—Tl1B—O4^{vii}	53.44 (9)	Tl1B^{ii}—O2—Tl1C^{xvi}	137.61 (6)
O3—Tl1B—O4^{vii}	44.48 (7)	Tl1B—O2—Tl1C^{xvi}	128.34 (12)
O3^{v}—Tl1B—O4^{vii}	98.07 (15)	Tl1A—O2—Tl1C^{xvi}	134.48 (5)
O3^{i}—Tl1B—O4^{vii}	76.70 (9)	Tl1C—O2—Tl1C^{xvi}	122.85 (17)
O3^{iv}—Tl1B—O4^{vii}	93.37 (11)	Tl1B^{i}—O2—Tl1C^{xvi}	137.26 (5)
O2^{v}—Tl1B—O4^{vii}	109.39 (13)	Tl1C^{i}—O2—Tl1C^{xvi}	139.30 (4)
O2—Tl1B—O4^{vii}	71.57 (8)	As1—O3—Tl1C	100.99 (8)
O3^{iii}—Tl1B—O4^{vii}	157.14 (10)	As1—O3—Tl1B	101.09 (7)
O3^{ii}—Tl1B—O4^{vii}	109.27 (4)	Tl1C—O3—Tl1B	6.12 (13)
O2^{ii}—Tl1B—O4^{vii}	144.87 (3)	As1—O3—Tl1C^{ii}	91.25 (13)
O2^{iii}—Tl1B—O4^{vii}	144.16 (3)	Tl1C—O3—Tl1C^{ii}	23.2 (3)
O4^{vi}—Tl1B—O4^{vii}	53.60 (10)	Tl1B—O3—Tl1C^{ii}	17.8 (2)
Tl1B^{i}—Tl1B—As1^{iv}	137.73 (8)	As1—O3—Tl1B^{ii}	95.92 (11)
Tl1B^{ii}—Tl1B—As1^{iv}	88.74 (9)	Tl1C—O3—Tl1B^{ii}	17.8 (2)
Tl1C^{i}—Tl1B—As1^{iv}	143.84 (15)	Tl1B—O3—Tl1B^{ii}	12.08 (19)
Tl1C^{ii}—Tl1B—As1^{iv}	80.08 (13)	Tl1C^{ii}—O3—Tl1B^{ii}	6.11 (13)
O2^{iv}—Tl1B—As1^{iv}	23.96 (3)	As1—O3—Tl1A	101.07 (7)
O2^{i}—Tl1B—As1^{iv}	108.05 (16)	Tl1C—O3—Tl1A	12.57 (15)
O3—Tl1B—As1^{iv}	82.58 (7)	Tl1B—O3—Tl1A	6.45 (10)
O3^{v}—Tl1B—As1^{iv}	82.12 (7)	Tl1C^{ii}—O3—Tl1A	12.89 (15)
O3^{i}—Tl1B—As1^{iv}	145.30 (16)	Tl1B^{ii}—O3—Tl1A	6.78 (11)
O3^{iv}—Tl1B—As1^{iv}	25.63 (4)	As1—O3—Tl1B^{i}	105.62 (10)

O2^{v}—Tl1B—As1^{iv}	128.80 (9)	Tl1C—O3—Tl1B^{i}	14.88 (17)
O2—Tl1B—As1^{iv}	51.74 (4)	Tl1B—O3—Tl1B^{i}	9.25 (14)
O3^{iii}—Tl1B—As1^{iv}	91.55 (4)	Tl1C^{ii}—O3—Tl1B^{i}	15.81 (18)
O3^{ii}—Tl1B—As1^{iv}	123.66 (5)	Tl1B^{ii}—O3—Tl1B^{i}	10.07 (15)
O2^{ii}—Tl1B—As1^{iv}	138.66 (12)	Tl1A—O3—Tl1B^{i}	4.85 (7)
O2^{iii}—Tl1B—As1^{iv}	90.32 (5)	As1—O3—Tl1C^{i}	109.08 (11)
O4^{vi}—Tl1B—As1^{iv}	67.91 (8)	Tl1C—O3—Tl1C^{i}	17.3 (2)
O4^{vii}—Tl1B—As1^{iv}	68.66 (8)	Tl1B—O3—Tl1C^{i}	12.27 (13)
Tl1B^{i}—Tl1B—As1^{i}	88.74 (8)	Tl1C^{ii}—O3—Tl1C^{i}	18.6 (2)
Tl1B^{ii}—Tl1B—As1^{i}	137.73 (6)	Tl1B^{ii}—O3—Tl1C^{i}	13.23 (14)
Tl1C^{i}—Tl1B—As1^{i}	80.08 (12)	Tl1A—O3—Tl1C^{i}	8.55 (8)
Tl1C^{ii}—Tl1B—As1^{i}	143.84 (15)	Tl1B^{i}—O3—Tl1C^{i}	3.70 (7)
O2^{iv}—Tl1B—As1^{i}	108.05 (16)	As1^{v}—O4—Ga1^{xviii}	126.29 (8)
O2^{i}—Tl1B—As1^{i}	23.96 (3)	As1^{v}—O4—Tl1C^{xx}	119.50 (8)
O3—Tl1B—As1^{i}	82.12 (7)	Ga1^{xviii}—O4—Tl1C^{xx}	98.90 (5)
O3^{v}—Tl1B—As1^{i}	82.59 (7)	As1^{v}—O4—Tl1B^{xx}	120.75 (7)
O3^{i}—Tl1B—As1^{i}	25.63 (3)	Ga1^{xviii}—O4—Tl1B^{xx}	99.36 (5)
O3^{iv}—Tl1B—As1^{i}	145.30 (16)	Tl1C^{xx}—O4—Tl1B^{xx}	2.65 (6)
O2^{v}—Tl1B—As1^{i}	51.74 (4)	As1^{v}—O4—Tl1A^{xvii}	121.89 (6)
O2—Tl1B—As1^{i}	128.80 (9)	Ga1^{xviii}—O4—Tl1A^{xvii}	99.79 (5)
O3^{iii}—Tl1B—As1^{i}	123.66 (5)	Tl1C^{xx}—O4—Tl1A^{xvii}	5.17 (7)
O3^{ii}—Tl1B—As1^{i}	91.55 (4)	Tl1B^{xx}—O4—Tl1A^{xvii}	2.52 (4)
O2^{ii}—Tl1B—As1^{i}	90.32 (5)	As1^{v}—O4—Tl1B^{xvii}	126.95 (10)
O2^{iii}—Tl1B—As1^{i}	138.66 (12)	Ga1^{xviii}—O4—Tl1B^{xvii}	96.40 (7)
O4^{vi}—Tl1B—As1^{i}	68.66 (8)	Tl1C^{xx}—O4—Tl1B^{xvii}	9.46 (12)
O4^{vii}—Tl1B—As1^{i}	67.90 (8)	Tl1B^{xx}—O4—Tl1B^{xvii}	7.14 (11)
As1^{iv}—Tl1B—As1^{i}	131.02 (16)	Tl1A^{xvii}—O4—Tl1B^{xvii}	5.24 (8)
Tl1A—Tl1C—Tl1B^{i}	19.99 (19)	As1^{v}—O4—Tl1C^{xvii}	131.11 (13)
Tl1A—Tl1C—Tl1B^{ii}	19.99 (19)	Ga1^{xviii}—O4—Tl1C^{xvii}	93.57 (8)
Tl1B^{i}—Tl1C—Tl1B^{ii}	40.0 (4)	Tl1C^{xx}—O4—Tl1C^{xvii}	13.52 (16)
Tl1A—Tl1C—Tl1C^{i}	30.0	Tl1B^{xx}—O4—Tl1C^{xvii}	11.37 (12)
Tl1B^{i}—Tl1C—Tl1C^{i}	10.01 (19)	Tl1A^{xvii}—O4—Tl1C^{xvii}	9.57 (10)
Tl1B^{ii}—Tl1C—Tl1C^{i}	50.00 (19)	Tl1B^{xvii}—O4—Tl1C^{xvii}	4.33 (9)
Tl1A—Tl1C—Tl1C^{ii}	30.001 (5)	As1^{v}—O4—Tl1B^{xxi}	117.93 (8)
Tl1B^{i}—Tl1C—Tl1C^{ii}	50.00 (19)	Ga1^{xviii}—O4—Tl1B^{xxi}	103.39 (7)
Tl1B^{ii}—Tl1C—Tl1C^{ii}	10.01 (19)	Tl1C^{xx}—O4—Tl1B^{xxi}	5.57 (7)
Tl1C^{i}—Tl1C—Tl1C^{ii}	60.001 (5)	Tl1B^{xx}—O4—Tl1B^{xxi}	4.08 (6)
Tl1A—Tl1C—O2^{iv}	131.87 (13)	Tl1A^{xvii}—O4—Tl1B^{xxi}	4.01 (6)
Tl1B^{i}—Tl1C—O2^{iv}	149.7 (2)	Tl1B^{xvii}—O4—Tl1B^{xxi}	9.04 (13)
Tl1B^{ii}—Tl1C—O2^{iv}	113.0 (2)	Tl1C^{xvii}—O4—Tl1B^{xxi}	13.33 (14)
Tl1C^{i}—Tl1C—O2^{iv}	157.37 (11)	As1^{v}—O4—Tl1C	57.11 (10)
Tl1C^{ii}—Tl1C—O2^{iv}	103.48 (14)	Ga1^{xviii}—O4—Tl1C	69.38 (10)
Tl1A—Tl1C—O2^{i}	131.87 (13)	Tl1C^{xx}—O4—Tl1C	132.52 (6)
Tl1B^{i}—Tl1C—O2^{i}	113.0 (2)	Tl1B^{xx}—O4—Tl1C	135.13 (5)
Tl1B^{ii}—Tl1C—O2^{i}	149.7 (2)	Tl1A^{xvii}—O4—Tl1C	137.61 (4)
Tl1C^{i}—Tl1C—O2^{i}	103.48 (13)	Tl1B^{xvii}—O4—Tl1C	140.03 (5)
Tl1C^{ii}—Tl1C—O2^{i}	157.37 (11)	Tl1C^{xvii}—O4—Tl1C	141.67 (5)
O2^{iv}—Tl1C—O2^{i}	96.3 (3)	Tl1B^{xxi}—O4—Tl1C	137.05 (4)

Tl1A—Tl1C—O3	102.61 (15)	As1^{v}—O4—Tl1C^{xxi}	114.85 (9)
Tl1B^{i}—Tl1C—O3	112.72 (18)	Ga1^{xviii}—O4—Tl1C^{xxi}	106.19 (8)
Tl1B^{ii}—Tl1C—O3	91.37 (17)	Tl1C^{xx}—O4—Tl1C^{xxi}	7.53 (9)
Tl1C^{i}—Tl1C—O3	116.99 (14)	Tl1B^{xx}—O4—Tl1C^{xxi}	6.86 (7)
Tl1C^{ii}—Tl1C—O3	85.65 (15)	Tl1A^{xvii}—O4—Tl1C^{xxi}	7.13 (7)
O2^{iv}—Tl1C—O3	73.65 (11)	Tl1B^{xvii}—O4—Tl1C^{xxi}	12.10 (13)
O2^{i}—Tl1C—O3	89.44 (14)	Tl1C^{xvii}—O4—Tl1C^{xxi}	16.34 (17)
Tl1A—Tl1C—O3^{v}	102.61 (15)	Tl1B^{xxi}—O4—Tl1C^{xxi}	3.13 (6)
Tl1B^{i}—Tl1C—O3^{v}	91.37 (16)	Tl1C—O4—Tl1C^{xxi}	136.41 (4)
Tl1B^{ii}—Tl1C—O3^{v}	112.72 (18)	As1^{v}—O4—Tl1B	53.77 (7)
Tl1C^{i}—Tl1C—O3^{v}	85.65 (14)	Ga1^{xviii}—O4—Tl1B	72.86 (7)
Tl1C^{ii}—Tl1C—O3^{v}	116.99 (13)	Tl1C^{xx}—O4—Tl1B	131.57 (7)
O2^{iv}—Tl1C—O3^{v}	89.44 (14)	Tl1B^{xx}—O4—Tl1B	134.21 (4)
O2^{i}—Tl1C—O3^{v}	73.65 (11)	Tl1A^{xvii}—O4—Tl1B	136.72 (4)
O3—Tl1C—O3^{v}	154.8 (3)	Tl1B^{xvii}—O4—Tl1B	139.57 (6)
Tl1A—Tl1C—O3^{iv}	89.40 (15)	Tl1C^{xvii}—O4—Tl1B	141.61 (6)
Tl1B^{i}—Tl1C—O3^{iv}	101.8 (2)	Tl1B^{xxi}—O4—Tl1B	135.80 (4)
Tl1B^{ii}—Tl1C—O3^{iv}	77.01 (17)	Tl1C—O4—Tl1B	3.71 (8)
Tl1C^{i}—Tl1C—O3^{iv}	107.76 (14)	Tl1C^{xxi}—O4—Tl1B	134.90 (4)
Tl1C^{ii}—Tl1C—O3^{iv}	71.13 (14)	As1^{v}—O4—Tl1C^{i}	44.77 (8)
O2^{iv}—Tl1C—O3^{iv}	49.88 (5)	Ga1^{xviii}—O4—Tl1C^{i}	83.27 (9)
O2^{i}—Tl1C—O3^{iv}	131.2 (2)	Tl1C^{xx}—O4—Tl1C^{i}	124.50 (15)
O3—Tl1C—O3^{iv}	107.87 (7)	Tl1B^{xx}—O4—Tl1C^{i}	127.13 (11)
O3^{v}—Tl1C—O3^{iv}	72.40 (6)	Tl1A^{xvii}—O4—Tl1C^{i}	129.62 (9)
Tl1A—Tl1C—O3^{i}	89.39 (15)	Tl1B^{xvii}—O4—Tl1C^{i}	133.50 (7)
Tl1B^{i}—Tl1C—O3^{i}	77.01 (16)	Tl1C^{xvii}—O4—Tl1C^{i}	136.55 (3)
Tl1B^{ii}—Tl1C—O3^{i}	101.8 (2)	Tl1B^{xxi}—O4—Tl1C^{i}	127.83 (11)
Tl1C^{i}—Tl1C—O3^{i}	71.13 (14)	Tl1C—O4—Tl1C^{i}	16.03 (19)
Tl1C^{ii}—Tl1C—O3^{i}	107.76 (13)	Tl1C^{xxi}—O4—Tl1C^{i}	126.30 (13)
O2^{iv}—Tl1C—O3^{i}	131.2 (2)	Tl1B—O4—Tl1C^{i}	12.41 (14)

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) −*x*+*y*, −*x*, *z*; (iii) *x*−*y*, −*y*, −*z*+3/2; (iv) *y*, *x*, −*z*+3/2; (v) −*x*, −*x*+*y*, −*z*+3/2; (vi) −*y*, *x*−*y*−1, *z*; (vii) *y*, *x*−1, −*z*+3/2; (viii) −*x*+*y*+1, −*x*+1, *z*; (ix) *x*, *y*+1, *z*; (x) −*y*, *x*−*y*+1, *z*; (xi) *x*+1, *y*+1, *z*; (xii) *x*−*y*−1/3, *x*+1/3, −*z*+4/3; (xiii) *y*+2/3, −*x*+*y*+4/3, −*z*+4/3; (xiv) −*x*+2/3, −*y*+1/3, −*z*+4/3; (xv) *x*−1, *y*, *z*; (xvi) −*y*−1, *x*−*y*−1, *z*; (xvii) *x*+1, *y*, *z*; (xviii) *x*, *y*−1, *z*; (xix) *x*−1, *y*−1, *z*; (xx) −*x*+*y*+1, −*x*, *z*; (xxi) −*y*+1, *x*−*y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H···O4^{vii}	0.87 (2)	1.94 (3)	2.728 (2)	150 (4)

Symmetry code: (vii) *y*, *x*−1, −*z*+3/2.