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Two new Rb–Ga arsenates: $RbGa(HAsO_4)_2$ and $RbGa_2As(HAsO_4)_6$

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The crystal structures of hydrothermally synthesized (T = 493 K, 7–9 d) rubidium gallium bis[hydrogenarsenate(V)], $RbGa(HAsO_4)_2$, and rubidium digallium arsenic(V) hexa[hydrogenarsenate(V)], $RbGa_2As(HAsO_4)_6$, were solved by single-crystal X-ray diffraction. Both compounds have tetrahedral–octahedral framework topologies. The M^+ cations are located in channels of the respective framework. $RbGa(HAsO_4)_2$ crystallizes in the $RbFe(HPO_4)_2$ structure type ($R\bar{3}c$), while $RbGa_2As(HAsO_4)_6$ adopts the structure type of $RbAl_2As(HAsO_4)_6$ ($R\bar{3}c$), which represents a modification of the $RbFe(HPO_4)_2$ structure type. In this modification, one third of the $M^{3+}O_6$ octahedra are replaced by AsO_6 octahedra, and two thirds of the voids in the structure, which are usually filled by M^+ cations, remain empty to achieve charge balance.

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 nonlinear optical features (frequency doubling) (Sun *et al.*, 2017). In order to further increase the insufficient knowledge about the crystal chemistry and structure types of arsenates, a comprehensive 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) was undertaken, which led to a large number of new compounds, most of which have been published (Schwendtner & Kolitsch, 2007, 2017, 2018*a*,*b*, and references therein).

Among the many different structure types found during our study, one atomic arrangement, *i.e.* the $RbFe(HPO_4)_2$ type (Lii & Wu, 1994; rhombohedral, $R\bar{3}c$), was found to show a large crystal–chemical flexibility which allows the incorporation of a wide variety of cations. A total of nine representatives of this structure type are presently known among $M^+M^{3+}(HTO_4)_2$ (T = P, As) compounds containing Rb or Cs as the M^+ cation and Al, Ga, Fe or In as the M^{3+} cation (Lesage *et al.*, 2007; Lii & Wu, 1994; Schwendtner & Kolitsch, 2017, 2018*a*,*b*), including $RbGa(HPO_4)_2$ (Lesage *et al.*, 2007). One of the title compounds, $RbGa(HAsO_4)_2$, is another new representative of the $RbFe(HPO_4)_2$ structure type. The second title compound, $RbGa_2As(HAsO_4)_6$, is the third representative of a recently described variation of the $RbFe(HPO_4)_2$ type, the $RbAl_2As(HAsO_4)_6$ type. It also crystallizes in $R\bar{3}c$ and up to now members with RbAl and CsFe as M^+M^{3+} cation combinations

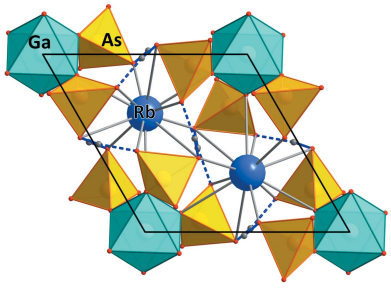

Table 1
Hydrogen-bond geometry (Å, °) for $RbGa(HAsO_4)_2$.

D—H···A	D—H	H···A	D···A	D—H···A
O3—H···O4^{xxi}	0.85 (3)	1.76 (3)	2.598 (2)	168 (4)

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

Table 2
Hydrogen-bond geometry (Å, °) for $RbGa_2As(HAsO_4)_6$.

D—H···A	D—H	H···A	D···A	D—H···A
O3—H···O4^{xiv}	0.80 (3)	1.98 (3)	2.7314 (17)	158 (3)

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

are known (Schwendtner & Kolitsch, 2018*b*). Interestingly, all presently known M^+M^{3+} combinations adopting this new structure type also have representatives adopting the $RbFe(HPO_4)_2$ type. It thus seems likely that more of the known $RbFe(HPO_4)_2$-type arsenates would also adopt the new $RbAl_2As(HAsO_4)_6$-type atomic arrangement under formally 'dry' synthesis conditions (see §3). $RbGa_2As(HAsO_4)_6$ is a rare example of a compound containing AsO_6 octahedra. Out of all reported arsenates(V), only about 3% contain AsO_6 polyhedra, according to our earlier review paper (Schwendtner & Kolitsch, 2007), which provides an overview of all known compounds containing AsO_6 groups and their bond-length statistics. At present, 37 compounds containing As in an octahedral coordination are known (Schwendtner & Kolitsch, 2018*b*); $RbGa_2As(HAsO_4)_6$ represents the 38th member of this class of compounds. While 12 Rb- and Ga-containing phosphates are contained in the ICSD (FIZ, 2018), only one Rb–Ga arsenate, *i.e.* $RbGaF_3(H_2AsO_4)$ (Marshall *et al.*, 2015), is known so far. Since submitting this paper, another paper dealing with isotypic $M^+M_2^{3+}As(HAsO_4)_6$ compounds (M^+M^{3+} = TlGa, CsGa, CsAl) has been published (Schwendtner & Kolitsch, 2018*c*).

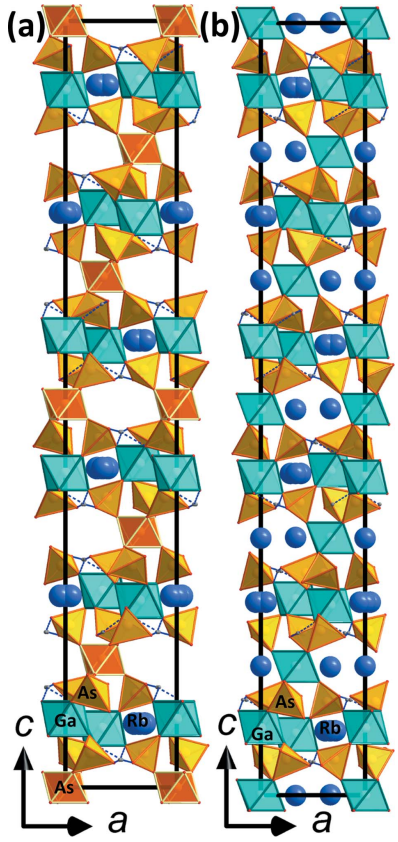

Figure 1
Crystal structure drawings of (*a*) $RbGa_2As(HAsO_4)_6$ and (*b*) $RbGa(HAsO_4)_2$ in views along the *b* axis. A part of the GaO_6 octahedra is replaced by AsO_6 octahedra in $RbGa_2As(HAsO_4)_6$; the corresponding layers (see Figs. 2 and 3) are compressed along *c* and the corresponding void remains vacant of Rb atoms.

2. Structural commentary

The two title compounds are very closely related to each other and are modifications of a basic tetrahedral–octahedral framework structure featuring interpenetrating channels, which host the M^+ cations (Fig. 1). The two structure types, first reported for $RbFe(HPO_4)_2$ ($R\overline{3}c$; Lii & Wu, 1994) and $RbAl_2As(HAsO_4)_6$ ($R\overline{3}c$; Schwendtner & Kolitsch, 2018*b*), are

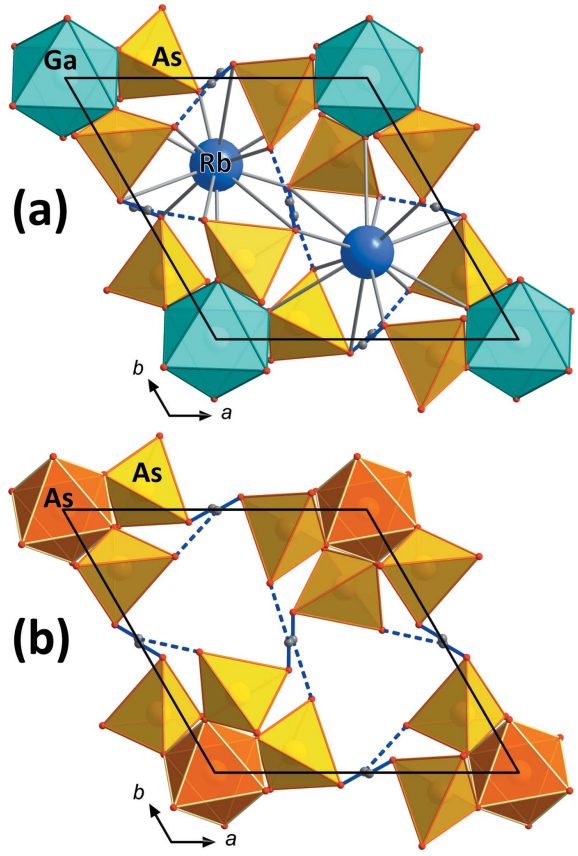

Figure 2
Crystal structure drawings of (*a*) $RbGa(HAsO_4)_2$ and (*b*) $RbGa_2As(HAsO_4)_6$ inequal layers, viewed along the *c* axis. In this layer, the GaO_6 octahedra are replaced by AsO_6 octahedra in $RbGa_2As(HAsO_4)_6$ (*b*). Since the unit-cell dimensions in directions *a* and *b* are slightly longer in $RbGa_2As(HAsO_4)_6$ and the AsO_6 octahedra are smaller than the corresponding GaO_6 octahedra, the $(Ga/As)As_6O_{24}$ units within this layer move further apart – leading to longer D—H···A distances and a compressed (along *c*) void that is too small for Rb atoms (compare Fig. 1).

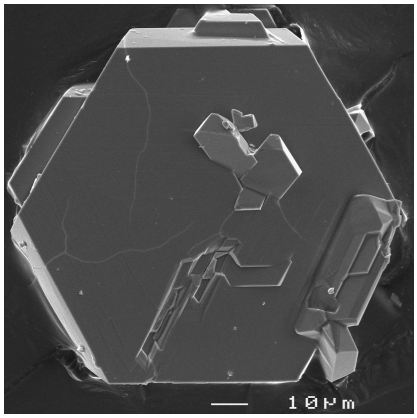

Figure 3
SEM micrograph of the pseudohexagonal tabular crystals of $RbGa(HAsO_4)_2$.

also related to the triclinic $(NH_4)Fe(HPO_4)_2$ type ($P\overline{1}$; Yakubovich, 1993) and the $RbAl(HAsO_4)_2$ type ($R32$; Schwendtner & Kolitsch, 2018*b*). 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. 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 (Fig. 2). The $M^{3+}As_6O_{24}$ units are arranged in layers perpendicular to the c_{hex} axis (Fig. 1). The units within these layers are held together by medium–strong hydrogen bonds (Tables 1 and 2). Both title compounds invariably show a very similar crystal habit: strongly pseudohexagonal to pseudo-octahedral (*cf.* Fig. 3).

The new compound $RbGa_2As(HAsO_4)_6$ could only be grown by 'dry' hydrothermal techniques (without the addition of water). The extreme abundance of As during the synthesis and the formation of a melt of arsenic acid promotes the formation of this novel structure type and endorses the octahedral coordination of As. The substitution of one third of all Ga^{3+} cations by As^{5+} requires that two thirds of all Rb^+ cations are omitted to achieve charge balance (compare Figs. 1*a*, 1*b*, 2*a* and 2*b*). This substitution also has an effect on the unit-cell parameters (Table 3) and the pore diameter. Since GaO_6 is only replaced by AsO_6 in every second layer (perpendicular to the *c* axis), the *a* axis must remain long enough to still be able to house the GaO_6 in the layers between. The effect of the smaller AsO_6 octahedra is therefore mainly reflected by a strong compression of about 5% along the *c* axis, while the *a* axis becomes even slightly longer compared to $RbGa(HAsO_4)_2$. Due to the comparatively smaller AsO_6 octahedra, the $(Ga/As)As_6O_{24}$ units are further apart in $RbGa_2As(HAsO_4)_6$ and the encased void is compressed along *c*, making it too small to house Rb^+ cations (Figs. 1 and 2). This effect is also reflected by the considerably elongated hydrogen bond in $RbGa_2As(HAsO_4)_6$. While these bonds, which connect neighbouring $(Ga/As)As_6O_{24}$ groups, are very strong in $RbGa(HAsO_4)_2$ [D—H$\cdots A$ = 2.598 (2) Å], they are much longer in $RbGa_2As(HAsO_4)_6$ [2.7314 (17) Å; compare Tables 1 and 2]. The second layer, in contrast, remains practically identical in both compounds and contains Rb atoms with a slight positional disorder (Fig. 4). In both compounds, the Rb atoms are 12-coordinated (Figs. 2 and 3), and the average Rb—O bond lengths in $RbGa_2As(HAsO_4)_6$ (3.433 Å) are longer than the longest average bond length in RbO_{12} polyhedra of 3.410 Å reported so far (Gagné & Hawthorne, 2016), thus leading to rather low bond-valence sums (BVSs; Gagné & Hawthorne, 2015) of only 0.59 valence units (v.u.), whereas the corresponding BVSs are 0.82 and 0.84 v.u. for $RbGa(HAsO_4)_2$. These loose bondings lead to considerable positional disorder of the Rb^+ cations in these voids, which were modelled with two Rb positions, between 0.41 (2) and 0.42 (4) Å apart. While position Rb1*A* in the centre of the large framework void in $RbGa_2As(HAsO_4)_6$ has only 77% occupancy compared to the off-centre position Rb1*B* (with occupancy 23%), in $RbGa(HAsO_4)_2$, the central position Rb1*A* has 91% occupancy. Similar behaviour was observed for the isotypic CsFe and RbAl compounds (Schwendtner & Kolitsch, 2018*b*), as well as isotypic phosphates (Lesage *et al.*, 2007).

A further indirect effect of the substituting AsO_6 octahedra is a distinct change in the As—O distances of the AsO_4 tetrahedra. The average As—O distance in the protonated AsO_4 tetrahedra, with values between 1.688 and 1.689 Å, is in

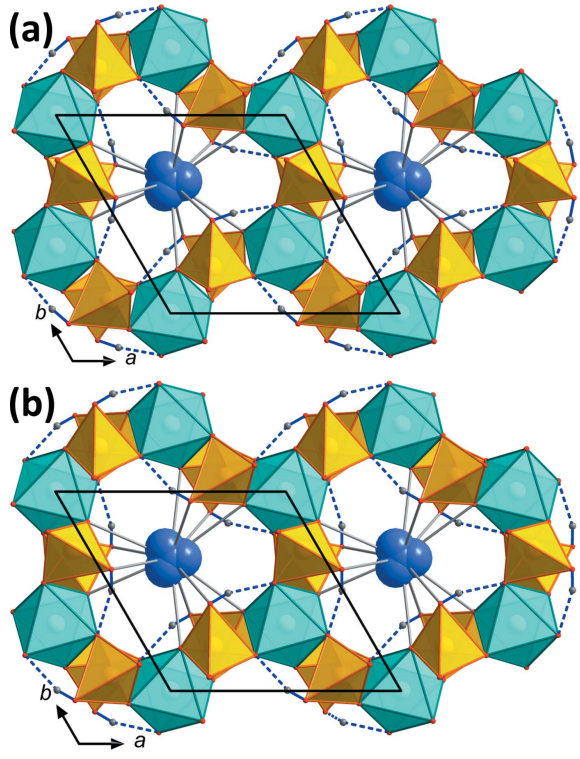

Figure 4
Crystal structure drawing of (*a*) $RbGa(HAsO_4)_2$ and (*b*) $RbGa_2As(HAsO_4)_6$ equal layers, viewed along the *a* axis. In these topologically equivalent layers, there are no visible differences between the two structure types apart from very minor changes in the hydrogen-bond geometries. The Rb atoms in both compounds show a slight positional disorder and are 12-coordinated.

Table 3
Experimental details.

	$RbGa(HAsO_4)_2$	$RbGa_2As(HAsO_4)_6$
Crystal data		
Chemical formula	$RbGa(HAsO_4)_2$	$RbGa_2As(HAsO_4)_6$
M_r	435.05	1139.40
Crystal system, space group	Trigonal, $R\bar{3}c$:*H*	Trigonal, $R\bar{3}c$:*H*
Temperature (K)	293	293
a, *c* (Å)	8.385 (1), 53.880 (11)	8.491 (1), 50.697 (11)
V (Å^3)	3280.7 (10)	3165.4 (10)
Z	18	6
Radiation type	Mo *Kα*	Mo *Kα*
μ (mm^{-1})	19.42	15.85
Crystal size (mm)	0.07 × 0.07 × 0.02	0.13 × 0.12 × 0.12
Data collection		
Diffractometer	Nonius KappaCCD single-crystal four-circle	Nonius KappaCCD single-crystal four-circle
Absorption correction	Multi-scan (*SCALEPACK*; Otwinowski *et al.*, 2003)	Multi-scan (*SCALEPACK*; Otwinowski *et al.*, 2003)
T_{min}, T_{max}	0.343, 0.697	0.232, 0.252
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3896, 1079, 1027	4684, 1287, 1196
R_{int}	0.016	0.016
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.704	0.757
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.016, 0.040, 1.11	0.014, 0.034, 1.13
No. of reflections	1079	1287
No. of parameters	68	65
No. of restraints	2	2
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.53	0.75, −0.84

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

both compounds very close to the statistical average of 1.686 (10) Å (Schwendtner, 2008). Also the BVSs (Gagné & Hawthorne, 2015) are close to ideal values (4.98–5.00 v.u.). In $RbGa(HAsO_4)_2$, the $HAsO_4$ tetrahedra show a typical distortion, with three short As—O distances to attached GaO_6 octahedra and one elongated As—O bond length for the protonated O atom involved in the O—H bond. That bond length (Table 4) in $RbGa(HAsO_4)_2$ is slightly longer [1.7417 (17) Å] than the average distance of As—O···H bonds in $HAsO_4$ groups [1.72 (3) Å; Schwendtner, 2008]. In contrast, $RbGa_2As(HAsO_4)_6$ has two short $^{[4]}$As—O bond lengths to neighbouring GaO_6 octahedra, but the $^{[4]}$As—O bond length of the O atom shared with the AsO_6 octahedra is also elongated [1.7100 (11) Å] due to $^{[4]}$As—O—$^{[6]}$As repulsion. The $^{[4]}$As—OH bond is therefore shortened to 1.7122 (13) Å (Table 5). The average As—O distances in the AsO_6 octahedra are the shortest average distances of AsO_6 octahedra found so far, *i.e.* 1.807 Å, leading to rather high BVSs of 5.33 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 on 33 AsO_6 octahedra of 31 compounds. Gagné & Hawthorne (2018) determined an identical, but less precise, value of 1.830 (28) Å, based on only 13 AsO_6 octahedra in AsO_6-containing compounds meeting all selection criteria as defined in Gagné & Hawthorne (2016). However, a larger number of compounds meeting these criteria were not used by Gagné & Hawthorne (2018) for unknown reasons. The average Ga—O bond lengths of the octahedrally coordinated Ga cations (1.962–1.964 Å) are slightly shorter than the grand mean average of 1.978 (17) Å (Gagné & Hawthorne, 2018), explaining the corresponding BVSs of 3.10 to 3.11 v.u.

Table 4
Selected bond lengths (Å) for $RbGa(HAsO_4)_2$.

Rb1*A*—O3^{i}	3.197 (2)	Rb2—O4^{xi}	3.4960 (16)
Rb1*A*—O3^{ii}	3.197 (2)	Rb2—O3^{xii}	3.5327 (19)
Rb1*A*—O3^{iii}	3.197 (2)	Rb2—O3^{xiii}	3.533 (2)
Rb1*A*—O3^{iv}	3.197 (2)	Rb2—O3^{xiv}	3.5328 (19)
Rb1*A*—O3^{v}	3.197 (2)	Ga1—O2^{xv}	1.9596 (14)
Rb1*A*—O3	3.197 (2)	Ga1—O2^{iii}	1.9597 (15)
Rb1*A*—O2^{ii}	3.3698 (16)	Ga1—O2^{xvi}	1.9597 (15)
Rb1*A*—O2^{iii}	3.3698 (16)	Ga1—O4^{xvii}	1.9690 (15)
Rb1*A*—O2^{v}	3.3699 (16)	Ga1—O4^{iv}	1.9690 (15)
Rb1*A*—O2	3.3699 (16)	Ga1—O4^{xviii}	1.9690 (15)
Rb1*A*—O2^{i}	3.3699 (15)	Ga2—O1^{viii}	1.9625 (15)
Rb1*A*—O2^{iv}	3.3699 (15)	Ga2—O1^{xiv}	1.9625 (16)
Rb2—O3	2.9346 (17)	Ga2—O1^{xix}	1.9625 (15)
Rb2—O3^{iv}	2.9347 (17)	Ga2—O1^{iv}	1.9626 (15)
Rb2—O3^{iii}	2.9347 (17)	Ga2—O1^{xviii}	1.9626 (16)
Rb2—O1^{vi}	3.3714 (16)	Ga2—O1^{xvii}	1.9626 (15)
Rb2—O1^{vii}	3.3715 (16)	As—O1^{xx}	1.6576 (15)
Rb2—O1^{viii}	3.3715 (17)	As—O2	1.6724 (15)
Rb2—O4^{ix}	3.4960 (16)	As—O4^{ii}	1.6805 (15)
Rb2—O4^{x}	3.4960 (17)	As—O3	1.7417 (17)

Symmetry codes: (i) $x-y, -y, -z+\frac{3}{2}$; (ii) $-x, -x+y, -z+\frac{3}{2}$; (iii) $-x+y, -x, z$; (iv) $-y, x-y, z$; (v) $y, x, -z+\frac{3}{2}$; (vi) $-x+\frac{2}{3}, -y-\frac{2}{3}, -z+\frac{4}{3}$; (vii) $x-y-\frac{4}{3}, x-\frac{2}{3}, -z+\frac{4}{3}$;

Table 5
Selected bond lengths (Å) for $RbGa_2As(HAsO_4)_6$.

Rb1*A*—O3^{i}	3.4212 (16)	Ga1—O4^{vii}	1.9623 (11)
Rb1*A*—O3^{ii}	3.4212 (16)	Ga1—O2^{viii}	1.9625 (11)
Rb1*A*—O3^{iii}	3.4212 (15)	Ga1—O2^{iii}	1.9625 (11)
Rb1*A*—O3^{iv}	3.4212 (16)	Ga1—O2^{ix}	1.9625 (11)
Rb1*A*—O3^{v}	3.4212 (15)	As1—O1^{x}	1.8067 (11)
Rb1*A*—O3	3.4213 (16)	As1—O1^{xi}	1.8068 (11)
Rb1*A*—O2^{ii}	3.4438 (12)	As1—O1^{xii}	1.8068 (11)
Rb1*A*—O2^{iii}	3.4438 (12)	As1—O1^{v}	1.8068 (11)
Rb1*A*—O2	3.4438 (12)	As1—O1^{vii}	1.8068 (11)
Rb1*A*—O2^{iv}	3.4438 (12)	As1—O1^{vi}	1.8068 (11)
Rb1*A*—O2^{i}	3.4438 (12)	As2—O2	1.6658 (11)
Rb1*A*—O2^{v}	3.4438 (12)	As2—O4^{ii}	1.6670 (11)
Ga1—O4^{vi}	1.9623 (12)	As2—O1^{xiii}	1.7100 (11)
Ga1—O4^{v}	1.9623 (11)	As2—O3	1.7122 (13)

Symmetry codes: (i) $x-y,-y,-z+\frac{3}{2}$; (ii) $-x,-x+y,-z+\frac{3}{2}$; (iii) $-x+y,-x,z$; (iv) $y,x,-z+\frac{3}{2}$; (v) $-y,x-y,z$; (vi) $x,y+1,z$; (vii) $-x+y+1,-x+1,z$; (viii) $-y,x-y+1,z$; (ix) $x+1,y+1,z$; (x) $x-y-\frac{1}{3},x+\frac{1}{3},-z+\frac{4}{3}$; (xi) $y+\frac{2}{3},-x+y+\frac{4}{3},-z+\frac{4}{3}$; (xii) $-x+\frac{2}{3},-y+\frac{1}{3},-z+\frac{4}{3}$; (xiii) $x-1,y,z$.

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 ml. Reagent-grade Rb_2CO_3, Ga_2O_3 and $H_3AsO_4{\cdot}0.5H_2O$ were used as starting reagents in approximate volume ratios of Rb:Ga:As of 1:1:3 for both synthesis batches. For $RbGa(HAsO_4)_2$ the vessels were filled with distilled water to about 70% of their inner volumes, which led to initial and final pH values of 1.5. The reaction product was washed thoroughly with distilled water, filtered and dried at room temperature. $RbGa(HAsO_4)_2$ formed colourless pseudohexagonal platelets (Fig. 3) and is stable in air.

For $RbGa_2As(HAsO_4)_6$, which contains As in both tetrahedral and octahedral coordination, no additional water was added and arsenic acid was present in excess to promote the growth of crystals from a melt or even vapour of arsenic acid under extremely acidic conditions. $RbGa_2As(HAsO_4)_6$ formed large colourless pseudo-octahedral crystals accompanied by small colourless twinned crystals of $RbH_3As_4O_{12}$ (Schwendtner & Kolitsch, 2007). The crystals of $RbGa_2As(HAsO_4)_6$ were extracted mechanically and not further washed; they are hygroscopic and decompose slowly over a period of several years to an amorphous gel and a new, strongly protonated diarsenate containing Rb and Ga (*P*321, publication in preparation). This slow partial alteration is illustrated in an X-ray powder diffraction pattern (Fig. 5).

A measured X-ray powder diffraction diagram of $RbGa(HAsO_4)_2$ was deposited at the International Centre for Diffraction Data under PDF number 00-057-0239 (Wohlschlaeger *et al.*, 2006).

4. Experimental and refinement

Crystal data, data collection and structure refinement are given in Table 3. For the refinement of $RbGa(HAsO_4)_2$, the coordinates of $RbFe(HPO_4)_2$ (Lii & Wu, 1994) were used for the final refinement steps. H atoms were then located from difference Fourier maps and added to the model. For the refinement of $RbGa_2As(HAsO_4)_6$, the model for $RbAl_2As(HAsO_4)_6$ (Schwendtner & Kolitsch, 2018*b*) was used as a starting point. In both compounds, O—H bonds were restrained to 0.9±0.04 Å. During the last refinement steps, residual electron-density peaks of up to 3.83 and 1.16 e Å^{-3} were located 0.63 and 0.68 Å from the Rb sites in $RbGa_2As(HAsO_4)_6$ and $RbGa(HAsO_4)_2$, respectively, suggesting irregular displacement parameters and split positions, similar to what was found for $RbFe(HPO_4)_2$-type $RbAl(HPO_4)_2$ (Lesage *et al.*, 2007). Therefore, a further position, Rb1*B*, was included in both refinements, which refined to low occupancies and led to considerable decreases in the *R* factors and weight parameters for both compounds. The bulk occupancies of Rb1*A* + Rb1*B* were constrained to give a total occupancy of 1.00. The final residual electron densities in both compounds are < 1 e Å^{-3}.

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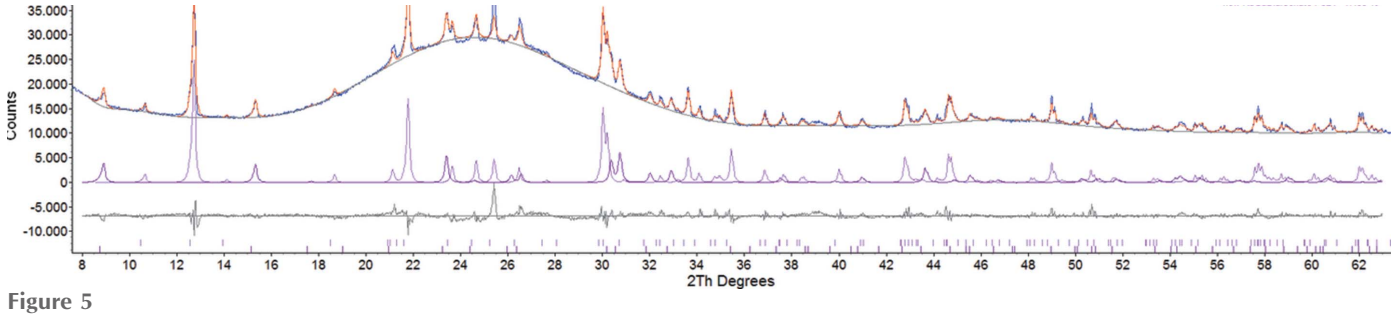

Figure 5
Graph of the Rietveld refinement (*TOPAS*; Bruker, 2009) of $RbGa_2As(HAsO_4)_6$, showing the partial alteration of the pseudo-octahedral crystals after an 11-year storage in air. The crystals were hygroscopic and had partly transformed to an amorphous mass. The presence of the relics of the unaltered primary crystals are still visible (pink curve), but a newly crystallized overgrowth of extremely fine fibrous crystals could be attributed to a new strongly protonated Rb–Ga diarsenate with space group *P*321 (dark-red curve), which will be the subject of a future publication.

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Acta Cryst. (2018). E**74**, 1244-1249 [https://doi.org/10.1107/S2056989018011180]

Two new Rb–Ga arsenates: $RbGa(HAsO_4)_2$ and $RbGa_2As(HAsO_4)_6$

Karolina Schwendtner and Uwe Kolitsch

Computing details

For both structures, data collection: *COLLECT* (Nonius, 2003); cell refinement: *SCALEPACK* (Otwinowski *et al.*, 2003); data reduction: *DENZO* and *SCALEPACK* (Otwinowski *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2005). Software used to prepare material for publication: *publCIF* (Westrip, 2010) for RbGa2AsHAsO46.

Rubidium digallium arsenic(V) hexakis[hydrogen arsenate(V)] (RbGa2AsHAsO46)

Crystal data

$RbGa_2As(HAsO_4)_6$
M_r = 1139.40
Trigonal, $R\bar{3}c$:*H*
a = 8.491 (1) Å
c = 50.697 (11) Å
V = 3165.4 (10) Å^3
Z = 6
F(000) = 3168
D_x = 3.586 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2570 reflections
θ = 2.0–32.6°
μ = 15.85 mm^{-1}
T = 293 K
Large pseudo-octahedra, colourless
0.13 × 0.12 × 0.12 mm

Data collection

Nonius KappaCCD single-crystal four-circle diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SCALEPACK; Otwinowski *et al.*, 2003)
T_{min} = 0.232, T_{max} = 0.252
4684 measured reflections
1287 independent reflections
1196 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 32.5°, θ_{min} = 2.4°
h = −12→12
k = −10→10
l = −75→76

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.034
S = 1.13
1287 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
$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 10.4877P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000271 (17)

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)
Rb1A	0.000000	0.000000	0.750000	0.055 (3)	0.669 (3)
Rb1B	0.000000	−0.048 (2)	0.750000	0.0359 (11)	0.1103 (9)
Ga1	0.333333	0.666667	0.75604 (2)	0.00736 (6)	
As1	0.333333	0.666667	0.666667	0.00627 (7)	
As2	−0.44400 (2)	−0.40772 (2)	0.71144 (2)	0.00735 (5)	
O1	0.40249 (16)	−0.46597 (15)	0.68629 (2)	0.01016 (19)	
O2	−0.45254 (15)	−0.27043 (15)	0.73416 (2)	0.01025 (19)	
O3	−0.22887 (17)	−0.28592 (18)	0.69874 (3)	0.0194 (3)	
O4	0.48817 (15)	−0.12495 (15)	0.77869 (2)	0.0108 (2)	
H	−0.176 (4)	−0.337 (4)	0.7027 (6)	0.046 (9)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1A	0.050 (4)	0.050 (4)	0.066 (2)	0.0251 (18)	0.000	0.000
Rb1B	0.024 (4)	0.034 (4)	0.046 (4)	0.012 (2)	0.0044 (14)	0.0022 (7)
Ga1	0.00807 (8)	0.00807 (8)	0.00596 (12)	0.00403 (4)	0.000	0.000
As1	0.00747 (10)	0.00747 (10)	0.00389 (14)	0.00373 (5)	0.000	0.000
As2	0.00844 (7)	0.00803 (7)	0.00670 (7)	0.00495 (5)	0.00010 (5)	0.00053 (5)
O1	0.0138 (5)	0.0110 (5)	0.0078 (4)	0.0077 (4)	−0.0031 (4)	0.0000 (4)
O2	0.0109 (5)	0.0099 (5)	0.0098 (5)	0.0051 (4)	0.0005 (4)	−0.0022 (4)
O3	0.0121 (5)	0.0203 (6)	0.0264 (7)	0.0084 (5)	0.0076 (5)	0.0075 (5)
O4	0.0124 (5)	0.0095 (5)	0.0125 (5)	0.0070 (4)	−0.0030 (4)	−0.0042 (4)

Geometric parameters (Å, º)

Rb1A—Rb1B^{i}	0.41 (2)	Rb1B—O2	3.4234 (12)
Rb1A—Rb1B^{ii}	0.41 (2)	Rb1B—O2^{iv}	3.4234 (12)
Rb1A—O3^{iii}	3.4212 (16)	Rb1B—O3^{iii}	3.694 (14)
Rb1A—O3^{iv}	3.4212 (16)	Rb1B—O3^{ii}	3.694 (14)
Rb1A—O3^{ii}	3.4212 (15)	Rb1B—O2^{ii}	3.810 (18)
Rb1A—O3^{v}	3.4212 (16)	Rb1B—O2^{iii}	3.810 (18)
Rb1A—O3^{i}	3.4212 (15)	Rb1B—O4^{vi}	3.819 (18)
Rb1A—O3	3.4213 (16)	Rb1B—O4^{vii}	3.819 (18)
Rb1A—O2^{iv}	3.4438 (12)	Rb1B—As2^{v}	3.934 (8)
Rb1A—O2^{ii}	3.4438 (12)	Rb1B—As2^{i}	3.934 (8)
Rb1A—O2	3.4438 (12)	Ga1—O4^{viii}	1.9623 (12)
Rb1A—O2^{v}	3.4438 (12)	Ga1—O4^{i}	1.9623 (11)
Rb1A—O2^{iii}	3.4438 (12)	Ga1—O4^{ix}	1.9623 (11)

Rb1A—O2^{i}	3.4438 (12)	Ga1—O2^{x}	1.9625 (11)
Rb1A—As2^{iv}	4.1192 (5)	Ga1—O2^{ii}	1.9625 (11)
Rb1A—As2^{iii}	4.1192 (5)	Ga1—O2^{xi}	1.9625 (11)
Rb1A—As2^{v}	4.1192 (5)	As1—O1^{xii}	1.8067 (11)
Rb1A—As2^{ii}	4.1192 (4)	As1—O1^{xiii}	1.8068 (11)
Rb1B—Rb1B^{i}	0.70 (3)	As1—O1^{xiv}	1.8068 (11)
Rb1B—Rb1B^{ii}	0.70 (3)	As1—O1^{i}	1.8068 (11)
Rb1B—O2^{v}	3.136 (14)	As1—O1^{ix}	1.8068 (11)
Rb1B—O2^{i}	3.136 (14)	As1—O1^{viii}	1.8068 (11)
Rb1B—O3^{iv}	3.269 (6)	As2—O2	1.6658 (11)
Rb1B—O3	3.269 (6)	As2—O4^{iv}	1.6670 (11)
Rb1B—O3^{v}	3.358 (2)	As2—O1^{xv}	1.7100 (11)
Rb1B—O3^{i}	3.358 (2)	As2—O3	1.7122 (13)

Rb1B^{i}—Rb1A—Rb1B^{ii}	120.00 (7)	Rb1B^{ii}—Rb1B—O4^{vii}	153.31 (7)
Rb1B^{i}—Rb1A—O3^{iii}	64.81 (2)	O2^{v}—Rb1B—O4^{vii}	53.4 (3)
Rb1B^{ii}—Rb1A—O3^{iii}	77.69 (5)	O2^{i}—Rb1B—O4^{vii}	45.1 (2)
Rb1B^{i}—Rb1A—O3^{iv}	77.69 (2)	O3^{iv}—Rb1B—O4^{vii}	44.49 (19)
Rb1B^{ii}—Rb1A—O3^{iv}	129.70 (3)	O3—Rb1B—O4^{vii}	98.0 (5)
O3^{iii}—Rb1A—O3^{iv}	68.57 (4)	O3^{v}—Rb1B—O4^{vii}	76.7 (3)
Rb1B^{i}—Rb1A—O3^{ii}	77.69 (2)	O3^{i}—Rb1B—O4^{vii}	93.3 (3)
Rb1B^{ii}—Rb1A—O3^{ii}	64.81 (5)	O2—Rb1B—O4^{vii}	109.4 (4)
O3^{iii}—Rb1A—O3^{ii}	100.59 (5)	O2^{iv}—Rb1B—O4^{vii}	71.6 (2)
O3^{iv}—Rb1A—O3^{ii}	155.38 (5)	O3^{iii}—Rb1B—O4^{vii}	109.34 (9)
Rb1B^{i}—Rb1A—O3^{v}	129.70 (2)	O3^{ii}—Rb1B—O4^{vii}	157.2 (3)
Rb1B^{ii}—Rb1A—O3^{v}	64.81 (5)	O2^{ii}—Rb1B—O4^{vii}	144.11 (3)
O3^{iii}—Rb1A—O3^{v}	68.57 (4)	O2^{iii}—Rb1B—O4^{vii}	144.95 (3)
O3^{iv}—Rb1A—O3^{v}	68.57 (4)	O4^{vi}—Rb1B—O4^{vii}	53.5 (3)
O3^{ii}—Rb1A—O3^{v}	129.62 (5)	Rb1B^{i}—Rb1B—As2^{v}	137.8 (2)
Rb1B^{i}—Rb1A—O3^{i}	64.81 (2)	Rb1B^{ii}—Rb1B—As2^{v}	88.8 (3)
Rb1B^{ii}—Rb1A—O3^{i}	129.70 (3)	O2^{v}—Rb1B—As2^{v}	24.03 (3)
O3^{iii}—Rb1A—O3^{i}	129.62 (5)	O2^{i}—Rb1B—As2^{v}	107.9 (5)
O3^{iv}—Rb1A—O3^{i}	100.59 (5)	O3^{iv}—Rb1B—As2^{v}	82.2 (2)
O3^{ii}—Rb1A—O3^{i}	68.57 (4)	O3—Rb1B—As2^{v}	82.5 (2)
O3^{v}—Rb1A—O3^{i}	155.38 (4)	O3^{v}—Rb1B—As2^{v}	25.63 (7)
Rb1B^{i}—Rb1A—O3	129.70 (2)	O3^{i}—Rb1B—As2^{v}	145.3 (5)
Rb1B^{ii}—Rb1A—O3	77.69 (5)	O2—Rb1B—As2^{v}	51.65 (8)
O3^{iii}—Rb1A—O3	155.38 (4)	O2^{iv}—Rb1B—As2^{v}	128.9 (3)
O3^{iv}—Rb1A—O3	129.62 (5)	O3^{iii}—Rb1B—As2^{v}	91.62 (8)
O3^{ii}—Rb1A—O3	68.57 (4)	O3^{ii}—Rb1B—As2^{v}	123.66 (15)
O3^{v}—Rb1A—O3	100.59 (5)	O2^{ii}—Rb1B—As2^{v}	138.7 (4)
O3^{i}—Rb1A—O3	68.57 (4)	O2^{iii}—Rb1B—As2^{v}	90.34 (14)
Rb1B^{i}—Rb1A—O2^{iv}	38.519 (18)	O4^{vi}—Rb1B—As2^{v}	68.6 (3)
Rb1B^{ii}—Rb1A—O2^{iv}	153.03 (7)	O4^{vii}—Rb1B—As2^{v}	67.9 (3)
O3^{iii}—Rb1A—O2^{iv}	76.93 (3)	Rb1B^{i}—Rb1B—As2^{i}	88.8 (2)
O3^{iv}—Rb1A—O2^{iv}	45.66 (3)	Rb1B^{ii}—Rb1B—As2^{i}	137.8 (2)
O3^{ii}—Rb1A—O2^{iv}	111.42 (3)	O2^{v}—Rb1B—As2^{i}	107.9 (5)
O3^{v}—Rb1A—O2^{iv}	113.17 (3)	O2^{i}—Rb1B—As2^{i}	24.03 (3)

O3^{i}—Rb1A—O2^{iv}	63.90 (3)	O3^{iv}—Rb1B—As2^{i}	82.5 (2)
O3—Rb1A—O2^{iv}	127.31 (3)	O3—Rb1B—As2^{i}	82.2 (2)
Rb1B^{i}—Rb1A—O2^{ii}	38.519 (18)	O3^{v}—Rb1B—As2^{i}	145.3 (5)
Rb1B^{ii}—Rb1A—O2^{ii}	83.75 (7)	O3^{i}—Rb1B—As2^{i}	25.63 (7)
O3^{iii}—Rb1A—O2^{ii}	63.90 (3)	O2—Rb1B—As2^{i}	128.9 (3)
O3^{iv}—Rb1A—O2^{ii}	111.42 (3)	O2^{iv}—Rb1B—As2^{i}	51.65 (8)
O3^{ii}—Rb1A—O2^{ii}	45.66 (3)	O3^{iii}—Rb1B—As2^{i}	123.66 (15)
O3^{v}—Rb1A—O2^{ii}	127.31 (3)	O3^{ii}—Rb1B—As2^{i}	91.62 (8)
O3^{i}—Rb1A—O2^{ii}	76.93 (3)	O2^{ii}—Rb1B—As2^{i}	90.34 (14)
O3—Rb1A—O2^{ii}	113.17 (3)	O2^{iii}—Rb1B—As2^{i}	138.7 (4)
O2^{iv}—Rb1A—O2^{ii}	77.04 (4)	O4^{vi}—Rb1B—As2^{i}	67.9 (3)
Rb1B^{i}—Rb1A—O2	153.035 (19)	O4^{vii}—Rb1B—As2^{i}	68.6 (3)
Rb1B^{ii}—Rb1A—O2	38.52 (7)	As2^{v}—Rb1B—As2^{i}	131.0 (5)
O3^{iii}—Rb1A—O2	111.42 (3)	O4^{viii}—Ga1—O4^{i}	89.24 (5)
O3^{iv}—Rb1A—O2	127.31 (3)	O4^{viii}—Ga1—O4^{ix}	89.24 (5)
O3^{ii}—Rb1A—O2	76.93 (3)	O4^{i}—Ga1—O4^{ix}	89.24 (5)
O3^{v}—Rb1A—O2	63.90 (3)	O4^{viii}—Ga1—O2^{x}	91.13 (5)
O3^{i}—Rb1A—O2	113.17 (3)	O4^{i}—Ga1—O2^{x}	88.49 (5)
O3—Rb1A—O2	45.67 (3)	O4^{ix}—Ga1—O2^{x}	177.69 (5)
O2^{iv}—Rb1A—O2	167.50 (4)	O4^{viii}—Ga1—O2^{ii}	177.69 (5)
O2^{ii}—Rb1A—O2	114.733 (13)	O4^{i}—Ga1—O2^{ii}	91.13 (5)
Rb1B^{i}—Rb1A—O2^{v}	153.03 (2)	O4^{ix}—Ga1—O2^{ii}	88.48 (5)
Rb1B^{ii}—Rb1A—O2^{v}	83.75 (8)	O2^{x}—Ga1—O2^{ii}	91.17 (5)
O3^{iii}—Rb1A—O2^{v}	113.17 (3)	O4^{viii}—Ga1—O2^{xi}	88.48 (5)
O3^{iv}—Rb1A—O2^{v}	76.93 (3)	O4^{i}—Ga1—O2^{xi}	177.69 (5)
O3^{ii}—Rb1A—O2^{v}	127.31 (3)	O4^{ix}—Ga1—O2^{xi}	91.12 (5)
O3^{v}—Rb1A—O2^{v}	45.66 (3)	O2^{x}—Ga1—O2^{xi}	91.16 (5)
O3^{i}—Rb1A—O2^{v}	111.42 (3)	O2^{ii}—Ga1—O2^{xi}	91.16 (5)
O3—Rb1A—O2^{v}	63.91 (3)	O4^{viii}—Ga1—Rb1B^{viii}	82.77 (12)
O2^{iv}—Rb1A—O2^{v}	114.733 (13)	O4^{i}—Ga1—Rb1B^{viii}	55.65 (8)
O2^{ii}—Rb1A—O2^{v}	167.50 (4)	O4^{ix}—Ga1—Rb1B^{viii}	143.89 (7)
O2—Rb1A—O2^{v}	53.93 (4)	O2^{x}—Ga1—Rb1B^{viii}	33.99 (5)
Rb1B^{i}—Rb1A—O2^{iii}	83.749 (19)	O2^{ii}—Ga1—Rb1B^{viii}	99.31 (13)
Rb1B^{ii}—Rb1A—O2^{iii}	38.52 (7)	O2^{xi}—Ga1—Rb1B^{viii}	123.61 (10)
O3^{iii}—Rb1A—O2^{iii}	45.66 (3)	O4^{viii}—Ga1—Rb1B^{i}	143.89 (6)
O3^{iv}—Rb1A—O2^{iii}	113.17 (3)	O4^{i}—Ga1—Rb1B^{i}	82.77 (12)
O3^{ii}—Rb1A—O2^{iii}	63.90 (3)	O4^{ix}—Ga1—Rb1B^{i}	55.65 (8)
O3^{v}—Rb1A—O2^{iii}	76.93 (3)	O2^{x}—Ga1—Rb1B^{i}	123.61 (9)
O3^{i}—Rb1A—O2^{iii}	127.31 (3)	O2^{ii}—Ga1—Rb1B^{i}	33.99 (5)
O3—Rb1A—O2^{iii}	111.42 (3)	O2^{xi}—Ga1—Rb1B^{i}	99.31 (12)
O2^{iv}—Rb1A—O2^{iii}	114.732 (14)	Rb1B^{viii}—Ga1—Rb1B^{i}	119.554 (12)
O2^{ii}—Rb1A—O2^{iii}	53.93 (4)	O4^{viii}—Ga1—Rb1B^{ix}	55.65 (10)
O2—Rb1A—O2^{iii}	77.04 (4)	O4^{i}—Ga1—Rb1B^{ix}	143.89 (7)
O2^{v}—Rb1A—O2^{iii}	114.731 (14)	O4^{ix}—Ga1—Rb1B^{ix}	82.77 (13)
Rb1B^{i}—Rb1A—O2^{i}	83.749 (19)	O2^{x}—Ga1—Rb1B^{ix}	99.31 (14)
Rb1B^{ii}—Rb1A—O2^{i}	153.03 (7)	O2^{ii}—Ga1—Rb1B^{ix}	123.61 (9)
O3^{iii}—Rb1A—O2^{i}	127.31 (3)	O2^{xi}—Ga1—Rb1B^{ix}	33.99 (6)
O3^{iv}—Rb1A—O2^{i}	63.90 (3)	Rb1B^{viii}—Ga1—Rb1B^{ix}	119.554 (7)

O3^{ii}—Rb1A—O2^{i}	113.17 (3)	Rb1B^{i}—Ga1—Rb1B^{ix}	119.554 (2)
O3^{v}—Rb1A—O2^{i}	111.42 (3)	O4^{viii}—Ga1—Rb1A^{viii}	80.57 (3)
O3^{i}—Rb1A—O2^{i}	45.66 (3)	O4^{i}—Ga1—Rb1A^{viii}	57.14 (3)
O3—Rb1A—O2^{i}	76.93 (3)	O4^{ix}—Ga1—Rb1A^{viii}	144.67 (3)
O2^{iv}—Rb1A—O2^{i}	53.93 (4)	O2^{x}—Ga1—Rb1A^{viii}	33.28 (3)
O2^{ii}—Rb1A—O2^{i}	114.732 (13)	O2^{ii}—Ga1—Rb1A^{viii}	101.54 (3)
O2—Rb1A—O2^{i}	114.732 (13)	O2^{xi}—Ga1—Rb1A^{viii}	122.02 (3)
O2^{v}—Rb1A—O2^{i}	77.04 (4)	Rb1B^{viii}—Ga1—Rb1A^{viii}	2.56 (14)
O2^{iii}—Rb1A—O2^{i}	167.50 (4)	Rb1B^{i}—Ga1—Rb1A^{viii}	122.12 (13)
Rb1B^{i}—Rb1A—As2^{iv}	60.329 (4)	Rb1B^{ix}—Ga1—Rb1A^{viii}	117.05 (14)
Rb1B^{ii}—Rb1A—As2^{iv}	151.382 (12)	O4^{viii}—Ga1—Rb1A	144.67 (3)
O3^{iii}—Rb1A—As2^{iv}	77.70 (2)	O4^{i}—Ga1—Rb1A	80.57 (3)
O3^{iv}—Rb1A—As2^{iv}	24.04 (2)	O4^{ix}—Ga1—Rb1A	57.14 (3)
O3^{ii}—Rb1A—As2^{iv}	134.60 (2)	O2^{x}—Ga1—Rb1A	122.02 (3)
O3^{v}—Rb1A—As2^{iv}	92.58 (3)	O2^{ii}—Ga1—Rb1A	33.28 (3)
O3^{i}—Rb1A—As2^{iv}	77.98 (3)	O2^{xi}—Ga1—Rb1A	101.53 (3)
O3—Rb1A—As2^{iv}	125.97 (2)	Rb1B^{viii}—Ga1—Rb1A	117.05 (14)
O2^{iv}—Rb1A—As2^{iv}	23.324 (18)	Rb1B^{i}—Ga1—Rb1A	2.56 (13)
O2^{ii}—Rb1A—As2^{iv}	98.261 (18)	Rb1B^{ix}—Ga1—Rb1A	122.12 (13)
O2—Rb1A—As2^{iv}	146.607 (19)	Rb1A^{viii}—Ga1—Rb1A	119.614 (1)
O2^{v}—Rb1A—As2^{iv}	92.721 (19)	O4^{viii}—Ga1—Rb1A^{xi}	57.14 (3)
O2^{iii}—Rb1A—As2^{iv}	122.596 (19)	O4^{i}—Ga1—Rb1A^{xi}	144.67 (4)
O2^{i}—Rb1A—As2^{iv}	49.72 (2)	O4^{ix}—Ga1—Rb1A^{xi}	80.57 (3)
Rb1B^{i}—Rb1A—As2^{iii}	67.492 (4)	O2^{x}—Ga1—Rb1A^{xi}	101.53 (3)
Rb1B^{ii}—Rb1A—As2^{iii}	60.33 (6)	O2^{ii}—Ga1—Rb1A^{xi}	122.02 (3)
O3^{iii}—Rb1A—As2^{iii}	24.04 (2)	O2^{xi}—Ga1—Rb1A^{xi}	33.28 (3)
O3^{iv}—Rb1A—As2^{iii}	92.58 (3)	Rb1B^{viii}—Ga1—Rb1A^{xi}	122.12 (14)
O3^{ii}—Rb1A—As2^{iii}	77.98 (3)	Rb1B^{i}—Ga1—Rb1A^{xi}	117.05 (13)
O3^{v}—Rb1A—As2^{iii}	77.70 (2)	Rb1B^{ix}—Ga1—Rb1A^{xi}	2.56 (14)
O3^{i}—Rb1A—As2^{iii}	125.97 (2)	Rb1A^{viii}—Ga1—Rb1A^{xi}	119.614 (1)
O3—Rb1A—As2^{iii}	134.60 (2)	Rb1A—Ga1—Rb1A^{xi}	119.614 (1)
O2^{iv}—Rb1A—As2^{iii}	92.720 (19)	O1^{xii}—As1—O1^{xiii}	92.59 (5)
O2^{ii}—Rb1A—As2^{iii}	49.72 (2)	O1^{xii}—As1—O1^{xiv}	92.59 (5)
O2—Rb1A—As2^{iii}	98.261 (18)	O1^{xiii}—As1—O1^{xiv}	92.59 (5)
O2^{v}—Rb1A—As2^{iii}	122.595 (19)	O1^{xii}—As1—O1^{i}	87.41 (5)
O2^{iii}—Rb1A—As2^{iii}	23.323 (18)	O1^{xiii}—As1—O1^{i}	180.00 (9)
O2^{i}—Rb1A—As2^{iii}	146.608 (19)	O1^{xiv}—As1—O1^{i}	87.41 (5)
As2^{iv}—Rb1A—As2^{iii}	99.334 (9)	O1^{xii}—As1—O1^{ix}	180.0
Rb1B^{i}—Rb1A—As2^{v}	151.382 (7)	O1^{xiii}—As1—O1^{ix}	87.41 (5)
Rb1B^{ii}—Rb1A—As2^{v}	67.49 (6)	O1^{xiv}—As1—O1^{ix}	87.41 (5)
O3^{iii}—Rb1A—As2^{v}	92.58 (3)	O1^{i}—As1—O1^{ix}	92.58 (5)
O3^{iv}—Rb1A—As2^{v}	77.70 (2)	O1^{xii}—As1—O1^{viii}	87.42 (5)
O3^{ii}—Rb1A—As2^{v}	125.97 (2)	O1^{xiii}—As1—O1^{viii}	87.42 (5)
O3^{v}—Rb1A—As2^{v}	24.04 (2)	O1^{xiv}—As1—O1^{viii}	180.00 (6)
O3^{i}—Rb1A—As2^{v}	134.60 (2)	O1^{i}—As1—O1^{viii}	92.58 (5)
O3—Rb1A—As2^{v}	77.98 (3)	O1^{ix}—As1—O1^{viii}	92.58 (5)
O2^{iv}—Rb1A—As2^{v}	122.596 (19)	O2—As2—O4^{iv}	117.31 (6)
O2^{ii}—Rb1A—As2^{v}	146.608 (19)	O2—As2—O1^{xv}	115.10 (6)

O2—Rb1A—As2^{v}	49.72 (2)	O4^{iv}—As2—O1^{xv}	100.43 (5)
O2^{v}—Rb1A—As2^{v}	23.323 (17)	O2—As2—O3	104.11 (6)
O2^{iii}—Rb1A—As2^{v}	92.72 (2)	O4^{iv}—As2—O3	111.03 (6)
O2^{i}—Rb1A—As2^{v}	98.261 (19)	O1^{xv}—As2—O3	108.86 (6)
As2^{iv}—Rb1A—As2^{v}	99.334 (9)	O2—As2—Rb1B^{ii}	50.1 (3)
As2^{iii}—Rb1A—As2^{v}	99.334 (9)	O4^{iv}—As2—Rb1B^{ii}	114.68 (16)
Rb1B^{i}—Rb1A—As2^{ii}	60.329 (3)	O1^{xv}—As2—Rb1B^{ii}	144.86 (16)
Rb1B^{ii}—Rb1A—As2^{ii}	67.49 (6)	O3—As2—Rb1B^{ii}	58.0 (2)
O3^{iii}—Rb1A—As2^{ii}	77.98 (3)	O2—As2—Rb1B	58.6 (2)
O3^{iv}—Rb1A—As2^{ii}	134.60 (2)	O4^{iv}—As2—Rb1B	106.7 (3)
O3^{ii}—Rb1A—As2^{ii}	24.04 (2)	O1^{xv}—As2—Rb1B	151.7 (2)
O3^{v}—Rb1A—As2^{ii}	125.97 (2)	O3—As2—Rb1B	53.57 (7)
O3^{i}—Rb1A—As2^{ii}	77.70 (2)	Rb1B^{ii}—As2—Rb1B	10.2 (5)
O3—Rb1A—As2^{ii}	92.58 (2)	O2—As2—Rb1A	54.94 (4)
O2^{iv}—Rb1A—As2^{ii}	98.261 (18)	O4^{iv}—As2—Rb1A	111.68 (4)
O2^{ii}—Rb1A—As2^{ii}	23.324 (18)	O1^{xv}—As2—Rb1A	147.34 (4)
O2—Rb1A—As2^{ii}	92.721 (19)	O3—As2—Rb1A	54.48 (5)
O2^{v}—Rb1A—As2^{ii}	146.607 (19)	Rb1B^{ii}—As2—Rb1A	5.1 (3)
O2^{iii}—Rb1A—As2^{ii}	49.72 (2)	Rb1B—As2—Rb1A	5.4 (3)
O2^{i}—Rb1A—As2^{ii}	122.596 (19)	O2—As2—Rb1B^{i}	56.09 (6)
As2^{iv}—Rb1A—As2^{ii}	120.658 (6)	O4^{iv}—As2—Rb1B^{i}	113.41 (9)
As2^{iii}—Rb1A—As2^{ii}	57.236 (12)	O1^{xv}—As2—Rb1B^{i}	145.26 (10)
As2^{v}—Rb1A—As2^{ii}	134.983 (5)	O3—As2—Rb1B^{i}	52.42 (10)
Rb1B^{i}—Rb1B—Rb1B^{ii}	60.00 (2)	Rb1B^{ii}—As2—Rb1B^{i}	6.1 (3)
Rb1B^{i}—Rb1B—O2^{v}	161.6 (2)	Rb1B—As2—Rb1B^{i}	6.7 (3)
Rb1B^{ii}—Rb1B—O2^{v}	108.4 (3)	Rb1A—As2—Rb1B^{i}	2.49 (11)
Rb1B^{i}—Rb1B—O2^{i}	108.4 (2)	O2—As2—Rb1B^{xvi}	93.36 (7)
Rb1B^{ii}—Rb1B—O2^{i}	161.60 (17)	O4^{iv}—As2—Rb1B^{xvi}	42.23 (4)
O2^{v}—Rb1B—O2^{i}	86.3 (5)	O1^{xv}—As2—Rb1B^{xvi}	80.78 (10)
Rb1B^{i}—Rb1B—O3^{iv}	91.2 (3)	O3—As2—Rb1B^{xvi}	153.23 (5)
Rb1B^{ii}—Rb1B—O3^{iv}	122.4 (3)	Rb1B^{ii}—As2—Rb1B^{xvi}	126.58 (16)
O2^{v}—Rb1B—O3^{iv}	83.6 (3)	Rb1B—As2—Rb1B^{xvi}	125.4 (2)
O2^{i}—Rb1B—O3^{iv}	69.1 (3)	Rb1A—As2—Rb1B^{xvi}	127.56 (9)
Rb1B^{i}—Rb1B—O3	122.4 (3)	Rb1B^{i}—As2—Rb1B^{xvi}	130.05 (2)
Rb1B^{ii}—Rb1B—O3	91.2 (3)	O2—As2—Rb1A^{xvii}	94.58 (4)
O2^{v}—Rb1B—O3	69.1 (3)	O4^{iv}—As2—Rb1A^{xvii}	42.53 (4)
O2^{i}—Rb1B—O3	83.6 (3)	O1^{xv}—As2—Rb1A^{xvii}	79.08 (4)
O3^{iv}—Rb1B—O3	142.5 (7)	O3—As2—Rb1A^{xvii}	153.36 (5)
Rb1B^{i}—Rb1B—O3^{v}	113.4 (3)	Rb1B^{ii}—As2—Rb1A^{xvii}	128.36 (6)
Rb1B^{ii}—Rb1B—O3^{v}	76.7 (3)	Rb1B—As2—Rb1A^{xvii}	127.17 (12)
O2^{v}—Rb1B—O3^{v}	48.28 (11)	Rb1A—As2—Rb1A^{xvii}	129.347 (10)
O2^{i}—Rb1B—O3^{v}	121.7 (5)	Rb1B^{i}—As2—Rb1A^{xvii}	131.84 (12)
O3^{iv}—Rb1B—O3^{v}	71.12 (11)	Rb1B^{xvi}—As2—Rb1A^{xvii}	1.79 (10)
O3—Rb1B—O3^{v}	105.18 (19)	O2—As2—Rb1B^{xviii}	92.74 (11)
Rb1B^{i}—Rb1B—O3^{i}	76.7 (3)	O4^{iv}—As2—Rb1B^{xviii}	46.4 (2)
Rb1B^{ii}—Rb1B—O3^{i}	113.4 (3)	O1^{xv}—As2—Rb1B^{xviii}	76.75 (13)
O2^{v}—Rb1B—O3^{i}	121.7 (5)	O3—As2—Rb1B^{xviii}	157.05 (19)
O2^{i}—Rb1B—O3^{i}	48.28 (11)	Rb1B^{ii}—As2—Rb1B^{xviii}	129.10 (5)

O3^{iv}—Rb1B—O3^{i}	105.18 (19)	Rb1B—As2—Rb1B^{xviii}	128.75 (3)
O3—Rb1B—O3^{i}	71.12 (11)	Rb1A—As2—Rb1B^{xviii}	130.52 (5)
O3^{v}—Rb1B—O3^{i}	169.0 (7)	Rb1B^{i}—As2—Rb1B^{xviii}	132.99 (17)
Rb1B^{i}—Rb1B—O2	118.6 (3)	Rb1B^{xvi}—As2—Rb1B^{xviii}	4.8 (2)
Rb1B^{ii}—Rb1B—O2	60.4 (4)	Rb1A^{xvii}—As2—Rb1B^{xviii}	3.88 (18)
O2^{v}—Rb1B—O2	56.66 (12)	O2—As2—Rb1B^{xvii}	97.48 (15)
O2^{i}—Rb1B—O2	124.3 (5)	O4^{iv}—As2—Rb1B^{xvii}	39.02 (18)
O3^{iv}—Rb1B—O2	133.6 (2)	O1^{xv}—As2—Rb1B^{xvii}	79.91 (7)
O3—Rb1B—O2	46.84 (5)	O3—As2—Rb1B^{xvii}	149.72 (18)
O3^{v}—Rb1B—O2	64.78 (4)	Rb1B^{ii}—As2—Rb1B^{xvii}	129.012 (18)
O3^{i}—Rb1B—O2	115.33 (5)	Rb1B—As2—Rb1B^{xvii}	127.02 (15)
Rb1B^{i}—Rb1B—O2^{iv}	60.4 (3)	Rb1A—As2—Rb1B^{xvii}	129.587 (13)
Rb1B^{ii}—Rb1B—O2^{iv}	118.6 (3)	Rb1B^{i}—As2—Rb1B^{xvii}	132.07 (12)
O2^{v}—Rb1B—O2^{iv}	124.3 (5)	Rb1B^{xvi}—As2—Rb1B^{xvii}	4.2 (2)
O2^{i}—Rb1B—O2^{iv}	56.66 (12)	Rb1A^{xvii}—As2—Rb1B^{xvii}	3.66 (17)
O3^{iv}—Rb1B—O2^{iv}	46.84 (5)	Rb1B^{xviii}—As2—Rb1B^{xvii}	7.4 (3)
O3—Rb1B—O2^{iv}	133.6 (2)	As2^{xix}—O1—As1^{xx}	131.96 (6)
O3^{v}—Rb1B—O2^{iv}	115.33 (5)	As2^{xix}—O1—Rb1B^{vii}	79.11 (18)
O3^{i}—Rb1B—O2^{iv}	64.78 (4)	As1^{xx}—O1—Rb1B^{vii}	129.23 (10)
O2—Rb1B—O2^{iv}	179.0 (7)	As2—O2—Ga1^{xvii}	123.99 (6)
Rb1B^{i}—Rb1B—O3^{iii}	48.36 (16)	As2—O2—Rb1B^{ii}	105.9 (2)
Rb1B^{ii}—Rb1B—O3^{iii}	56.58 (15)	Ga1^{xvii}—O2—Rb1B^{ii}	125.54 (18)
O2^{v}—Rb1B—O3^{iii}	113.81 (3)	As2—O2—Rb1B	96.8 (3)
O2^{i}—Rb1B—O3^{iii}	128.32 (3)	Ga1^{xvii}—O2—Rb1B	130.47 (10)
O3^{iv}—Rb1B—O3^{iii}	66.90 (12)	Rb1B^{ii}—O2—Rb1B	11.2 (6)
O3—Rb1B—O3^{iii}	147.5 (4)	As2—O2—Rb1A	101.74 (4)
O3^{v}—Rb1B—O3^{iii}	66.07 (15)	Ga1^{xvii}—O2—Rb1A	128.51 (4)
O3^{i}—Rb1B—O3^{iii}	122.7 (4)	Rb1B^{ii}—O2—Rb1A	4.6 (2)
O2—Rb1B—O3^{iii}	105.6 (3)	Rb1B—O2—Rb1A	6.8 (3)
O2^{iv}—Rb1B—O3^{iii}	73.63 (18)	As2—O2—Rb1B^{i}	102.64 (6)
Rb1B^{i}—Rb1B—O3^{ii}	56.58 (18)	Ga1^{xvii}—O2—Rb1B^{i}	128.80 (4)
Rb1B^{ii}—Rb1B—O3^{ii}	48.36 (15)	Rb1B^{ii}—O2—Rb1B^{i}	3.34 (18)
O2^{v}—Rb1B—O3^{ii}	128.32 (3)	Rb1B—O2—Rb1B^{i}	9.3 (4)
O2^{i}—Rb1B—O3^{ii}	113.81 (3)	Rb1A—O2—Rb1B^{i}	2.77 (12)
O3^{iv}—Rb1B—O3^{ii}	147.5 (4)	As2—O3—Rb1B	101.51 (6)
O3—Rb1B—O3^{ii}	66.90 (12)	As2—O3—Rb1B^{ii}	96.3 (3)
O3^{v}—Rb1B—O3^{ii}	122.7 (4)	Rb1B—O3—Rb1B^{ii}	12.1 (6)
O3^{i}—Rb1B—O3^{ii}	66.07 (15)	As2—O3—Rb1A	101.48 (6)
O2—Rb1B—O3^{ii}	73.63 (18)	Rb1B—O3—Rb1A	6.5 (3)
O2^{iv}—Rb1B—O3^{ii}	105.6 (3)	Rb1B^{ii}—O3—Rb1A	6.8 (3)
O3^{iii}—Rb1B—O3^{ii}	90.9 (4)	As2—O3—Rb1B^{i}	106.0 (2)
Rb1B^{i}—Rb1B—O2^{ii}	15.05 (2)	Rb1B—O3—Rb1B^{i}	9.3 (5)
Rb1B^{ii}—Rb1B—O2^{ii}	52.10 (7)	Rb1B^{ii}—O3—Rb1B^{i}	10.1 (5)
O2^{v}—Rb1B—O2^{ii}	160.5 (4)	Rb1A—O3—Rb1B^{i}	4.9 (2)
O2^{i}—Rb1B—O2^{ii}	112.87 (12)	As2^{iv}—O4—Ga1^{xx}	126.28 (6)
O3^{iv}—Rb1B—O2^{ii}	106.2 (3)	As2^{iv}—O4—Rb1B^{xxi}	120.71 (10)
O3—Rb1B—O2^{ii}	107.8 (3)	Ga1^{xx}—O4—Rb1B^{xxi}	99.25 (5)
O3^{v}—Rb1B—O2^{ii}	118.1 (4)	As2^{iv}—O4—Rb1A^{xix}	121.85 (5)

O3^{i}—Rb1B—O2^{ii}	72.8 (2)	Ga1^{xx}—O4—Rb1A^{xix}	99.67 (4)
O2—Rb1B—O2^{ii}	106.5 (4)	Rb1B^{xxi}—O4—Rb1A^{xix}	2.51 (13)
O2^{iv}—Rb1B—O2^{ii}	72.5 (2)	As2^{iv}—O4—Rb1B^{xix}	126.9 (3)
O3^{iii}—Rb1B—O2^{ii}	57.9 (3)	Ga1^{xx}—O4—Rb1B^{xix}	96.29 (16)
O3^{ii}—Rb1B—O2^{ii}	41.55 (19)	Rb1B^{xxi}—O4—Rb1B^{xix}	7.1 (3)
Rb1B^{i}—Rb1B—O2^{iii}	52.10 (12)	Rb1A^{xix}—O4—Rb1B^{xix}	5.2 (2)
Rb1B^{ii}—Rb1B—O2^{iii}	15.05 (5)	As2^{iv}—O4—Rb1B^{xxii}	117.91 (18)
O2^{v}—Rb1B—O2^{iii}	112.87 (12)	Ga1^{xx}—O4—Rb1B^{xxii}	103.25 (18)
O2^{i}—Rb1B—O2^{iii}	160.5 (4)	Rb1B^{xxi}—O4—Rb1B^{xxii}	4.1 (2)
O3^{iv}—Rb1B—O2^{iii}	107.8 (3)	Rb1A^{xix}—O4—Rb1B^{xxii}	3.99 (18)
O3—Rb1B—O2^{iii}	106.2 (3)	Rb1B^{xix}—O4—Rb1B^{xxii}	9.0 (4)
O3^{v}—Rb1B—O2^{iii}	72.8 (2)	As2^{iv}—O4—Rb1B	53.63 (19)
O3^{i}—Rb1B—O2^{iii}	118.1 (4)	Ga1^{xx}—O4—Rb1B	72.96 (19)
O2—Rb1B—O2^{iii}	72.5 (2)	Rb1B^{xxi}—O4—Rb1B	134.20 (8)
O2^{iv}—Rb1B—O2^{iii}	106.5 (4)	Rb1A^{xix}—O4—Rb1B	136.70 (6)
O3^{iii}—Rb1B—O2^{iii}	41.55 (19)	Rb1B^{xix}—O4—Rb1B	139.53 (16)
O3^{ii}—Rb1B—O2^{iii}	57.9 (3)	Rb1B^{xxii}—O4—Rb1B	135.79 (4)
O2^{ii}—Rb1B—O2^{iii}	48.4 (2)	As2^{iv}—O4—Rb1B^{i}	47.20 (15)
Rb1B^{i}—Rb1B—O4^{vi}	153.31 (5)	Ga1^{xx}—O4—Rb1B^{i}	80.09 (19)
Rb1B^{ii}—Rb1B—O4^{vi}	130.76 (15)	Rb1B^{xxi}—O4—Rb1B^{i}	130.0 (3)
O2^{v}—Rb1B—O4^{vi}	45.1 (2)	Rb1A^{xix}—O4—Rb1B^{i}	132.53 (17)
O2^{i}—Rb1B—O4^{vi}	53.4 (3)	Rb1B^{xix}—O4—Rb1B^{i}	136.12 (3)
O3^{iv}—Rb1B—O4^{vi}	98.0 (5)	Rb1B^{xxii}—O4—Rb1B^{i}	131.0 (3)
O3—Rb1B—O4^{vi}	44.50 (19)	Rb1B—O4—Rb1B^{i}	8.2 (4)
O3^{v}—Rb1B—O4^{vi}	93.3 (3)	As2^{iv}—O4—Rb1A	50.21 (3)
O3^{i}—Rb1B—O4^{vi}	76.7 (3)	Ga1^{xx}—O4—Rb1A	76.56 (3)
O2—Rb1B—O4^{vi}	71.6 (2)	Rb1B^{xxi}—O4—Rb1A	133.03 (14)
O2^{iv}—Rb1B—O4^{vi}	109.4 (4)	Rb1A^{xix}—O4—Rb1A	135.53 (3)
O3^{iii}—Rb1B—O4^{vi}	157.2 (3)	Rb1B^{xix}—O4—Rb1A	138.77 (15)
O3^{ii}—Rb1B—O4^{vi}	109.34 (9)	Rb1B^{xxii}—O4—Rb1A	134.28 (7)
O2^{ii}—Rb1B—O4^{vi}	144.95 (3)	Rb1B—O4—Rb1A	3.8 (2)
O2^{iii}—Rb1B—O4^{vi}	144.11 (3)	Rb1B^{i}—O4—Rb1A	4.5 (2)
Rb1B^{i}—Rb1B—O4^{vii}	130.76 (11)		

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) −*x*+*y*, −*x*, *z*; (iii) *x*−*y*, −*y*, −*z*+3/2; (iv) −*x*, −*x*+*y*, −*z*+3/2; (v) *y*, *x*, −*z*+3/2; (vi) *y*, *x*−1, −*z*+3/2; (vii) −*y*, *x*−*y*−1, *z*; (viii) *x*, *y*+1, *z*; (ix) −*x*+*y*+1, −*x*+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*−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}	0.80 (3)	1.98 (3)	2.7314 (17)	158 (3)

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

Rubidium gallium bis[hydrogen arsenate(V)] (RbGaHAsO42)

Crystal data

$RbGa(HAsO_4)_2$
M_r = 435.05

Trigonal, $R\bar{3}c$:*H*
a = 8.385 (1) Å

c = 53.880 (11) Å
V = 3280.7 (10) Å^3
Z = 18
F(000) = 3600
D_x = 3.964 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2663 reflections
θ = 2.3–30.0°
μ = 19.42 mm^{-1}
T = 293 K
Hexagonal plate, colourless
0.07 × 0.07 × 0.02 mm

Data collection

Nonius KappaCCD single-crystal four-circle diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SCALEPACK; Otwinowski *et al.*, 2003)
T_{min} = 0.343, T_{max} = 0.697
3896 measured reflections

1079 independent reflections
1027 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 30.0°, θ_{min} = 2.3°
h = −11→11
k = −9→9
l = −75→75

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.040
S = 1.11
1079 reflections
68 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
$w = 1/[\sigma^2(F_o^2) + (0.0168P)^2 + 20.8962P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.014
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000092 (13)

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)
Rb1A	0.000000	0.000000	0.750000	0.0297 (12)	0.909 (3)
Rb1B	0.000000	−0.050 (5)	0.750000	0.011 (3)	0.0304 (9)
Rb2	0.000000	0.000000	0.66714 (2)	0.02912 (12)	
Ga1	0.333333	0.666667	0.75374 (2)	0.00733 (9)	
Ga2	0.333333	0.666667	0.666667	0.00817 (11)	
As	−0.43059 (3)	−0.39514 (3)	0.71280 (2)	0.00799 (7)	
O1	0.4536 (2)	−0.4402 (2)	0.68636 (3)	0.0159 (3)	
O2	−0.4459 (2)	−0.2541 (2)	0.73338 (3)	0.0106 (3)	
O3	−0.1974 (2)	−0.2813 (2)	0.70523 (3)	0.0178 (3)	
O4	0.4789 (2)	−0.1223 (2)	0.77582 (3)	0.0103 (3)	
H	−0.161 (5)	−0.354 (5)	0.7099 (6)	0.035 (10)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1A	0.0333 (16)	0.0333 (16)	0.0225 (9)	0.0166 (8)	0.000	0.000
Rb1B	0.023 (11)	0.012 (7)	0.004 (7)	0.011 (5)	−0.002 (4)	−0.001 (2)
Rb2	0.03481 (17)	0.03481 (17)	0.0177 (2)	0.01740 (9)	0.000	0.000
Ga1	0.00785 (12)	0.00785 (12)	0.00629 (16)	0.00393 (6)	0.000	0.000
Ga2	0.00943 (15)	0.00943 (15)	0.0057 (2)	0.00472 (8)	0.000	0.000
As	0.00991 (11)	0.00839 (10)	0.00729 (10)	0.00580 (8)	0.00068 (7)	0.00083 (7)
O1	0.0246 (8)	0.0212 (8)	0.0087 (6)	0.0164 (7)	−0.0050 (6)	−0.0011 (6)
O2	0.0105 (7)	0.0106 (6)	0.0104 (6)	0.0049 (5)	0.0026 (5)	−0.0016 (5)
O3	0.0129 (7)	0.0173 (8)	0.0257 (9)	0.0093 (7)	0.0085 (6)	0.0093 (6)
O4	0.0116 (6)	0.0092 (6)	0.0120 (6)	0.0066 (6)	−0.0019 (5)	−0.0038 (5)

Geometric parameters (Å, º)

Rb1A—Rb1B^{i}	0.42 (4)	Rb2—O3^{ii}	2.9347 (17)
Rb1A—Rb1B^{ii}	0.42 (4)	Rb2—O1^{vi}	3.3714 (16)
Rb1A—O3^{iii}	3.197 (2)	Rb2—O1^{vii}	3.3715 (16)
Rb1A—O3^{iv}	3.197 (2)	Rb2—O1^{viii}	3.3715 (17)
Rb1A—O3^{ii}	3.197 (2)	Rb2—O4^{ix}	3.4960 (16)
Rb1A—O3^{i}	3.197 (2)	Rb2—O4^{x}	3.4960 (17)
Rb1A—O3^{v}	3.197 (2)	Rb2—O4^{xi}	3.4960 (16)
Rb1A—O3	3.197 (2)	Rb2—O3^{xii}	3.5327 (19)
Rb1A—O2^{iv}	3.3698 (16)	Rb2—O3^{xiii}	3.533 (2)
Rb1A—O2^{ii}	3.3698 (16)	Rb2—O3^{xiv}	3.5328 (19)
Rb1A—O2^{v}	3.3699 (16)	Rb2—As^{xiv}	3.7432 (5)
Rb1A—O2	3.3699 (16)	Rb2—As^{xii}	3.7432 (5)
Rb1A—O2^{iii}	3.3699 (15)	Rb2—As^{xiii}	3.7432 (5)
Rb1A—O2^{i}	3.3699 (15)	Ga1—O2^{xv}	1.9596 (14)
Rb1A—As^{iv}	4.0083 (5)	Ga1—O2^{ii}	1.9597 (15)
Rb1B—Rb1B^{i}	0.72 (7)	Ga1—O2^{xvi}	1.9597 (15)
Rb1B—Rb1B^{ii}	0.72 (7)	Ga1—O4^{xvii}	1.9690 (15)
Rb1B—O3^{iv}	3.019 (15)	Ga1—O4^{i}	1.9690 (15)
Rb1B—O3	3.019 (15)	Ga1—O4^{xviii}	1.9690 (15)
Rb1B—O2^{v}	3.05 (3)	Ga2—O1^{viii}	1.9625 (15)
Rb1B—O2^{i}	3.05 (3)	Ga2—O1^{xiv}	1.9625 (16)
Rb1B—O3^{i}	3.161 (2)	Ga2—O1^{xix}	1.9625 (15)
Rb1B—O3^{v}	3.161 (2)	Ga2—O1^{i}	1.9626 (15)
Rb1B—O2^{iv}	3.363 (2)	Ga2—O1^{xviii}	1.9626 (16)
Rb1B—O2	3.363 (2)	Ga2—O1^{xvii}	1.9626 (15)
Rb1B—O3^{iii}	3.47 (3)	As—O1^{xx}	1.6576 (15)
Rb1B—O3^{ii}	3.47 (3)	As—O2	1.6724 (15)
Rb2—O3	2.9346 (17)	As—O4^{iv}	1.6805 (15)
Rb2—O3^{i}	2.9347 (17)	As—O3	1.7417 (17)
Rb1B^{i}—Rb1A—Rb1B^{ii}	120.00 (15)	O1^{vi}—Rb2—As^{xii}	26.29 (3)
Rb1B^{i}—Rb1A—O3^{iii}	61.38 (3)	O1^{vii}—Rb2—As^{xii}	88.53 (3)

Rb1B^{ii}—Rb1A—O3^{iii}	81.43 (11)	O1^{viii}—Rb2—As^{xii}	105.88 (3)
Rb1B^{i}—Rb1A—O3^{iv}	81.43 (3)	O4^{ix}—Rb2—As^{xii}	26.56 (2)
Rb1B^{ii}—Rb1A—O3^{iv}	128.90 (5)	O4^{x}—Rb2—As^{xii}	54.15 (3)
O3^{iii}—Rb1A—O3^{iv}	69.26 (5)	O4^{xi}—Rb2—As^{xii}	71.43 (3)
Rb1B^{i}—Rb1A—O3^{ii}	81.43 (3)	O3^{xii}—Rb2—As^{xii}	27.50 (3)
Rb1B^{ii}—Rb1A—O3^{ii}	61.38 (9)	O3^{xiii}—Rb2—As^{xii}	63.12 (3)
O3^{iii}—Rb1A—O3^{ii}	102.21 (6)	O3^{xiv}—Rb2—As^{xii}	98.11 (3)
O3^{iv}—Rb1A—O3^{ii}	162.87 (7)	As^{xiv}—Rb2—As^{xii}	79.914 (13)
Rb1B^{i}—Rb1A—O3^{i}	61.38 (3)	O3—Rb2—As^{xiii}	177.27 (4)
Rb1B^{ii}—Rb1A—O3^{i}	128.90 (5)	O3^{i}—Rb2—As^{xiii}	100.79 (4)
O3^{iii}—Rb1A—O3^{i}	122.76 (7)	O3^{ii}—Rb2—As^{xiii}	102.80 (4)
O3^{iv}—Rb1A—O3^{i}	102.21 (6)	O1^{vi}—Rb2—As^{xiii}	88.53 (3)
O3^{ii}—Rb1A—O3^{i}	69.26 (5)	O1^{vii}—Rb2—As^{xiii}	105.88 (3)
Rb1B^{i}—Rb1A—O3^{v}	128.90 (3)	O1^{viii}—Rb2—As^{xiii}	26.29 (3)
Rb1B^{ii}—Rb1A—O3^{v}	61.38 (9)	O4^{ix}—Rb2—As^{xiii}	54.15 (3)
O3^{iii}—Rb1A—O3^{v}	69.26 (5)	O4^{x}—Rb2—As^{xiii}	71.43 (3)
O3^{iv}—Rb1A—O3^{v}	69.26 (5)	O4^{xi}—Rb2—As^{xiii}	26.56 (3)
O3^{ii}—Rb1A—O3^{v}	122.76 (6)	O3^{xii}—Rb2—As^{xiii}	98.11 (3)
O3^{i}—Rb1A—O3^{v}	162.87 (6)	O3^{xiii}—Rb2—As^{xiii}	27.50 (3)
Rb1B^{i}—Rb1A—O3	128.90 (3)	O3^{xiv}—Rb2—As^{xiii}	63.12 (3)
Rb1B^{ii}—Rb1A—O3	81.43 (11)	As^{xiv}—Rb2—As^{xiii}	79.914 (13)
O3^{iii}—Rb1A—O3	162.87 (6)	As^{xii}—Rb2—As^{xiii}	79.914 (13)
O3^{iv}—Rb1A—O3	122.76 (6)	O2^{xv}—Ga1—O2^{ii}	91.72 (6)
O3^{ii}—Rb1A—O3	69.26 (5)	O2^{xv}—Ga1—O2^{xvi}	91.72 (6)
O3^{i}—Rb1A—O3	69.26 (5)	O2^{ii}—Ga1—O2^{xvi}	91.72 (6)
O3^{v}—Rb1A—O3	102.21 (6)	O2^{xv}—Ga1—O4^{xvii}	92.25 (6)
Rb1B^{i}—Rb1A—O2^{iv}	37.49 (3)	O2^{ii}—Ga1—O4^{xvii}	175.98 (6)
Rb1B^{ii}—Rb1A—O2^{iv}	150.57 (13)	O2^{xvi}—Ga1—O4^{xvii}	88.72 (6)
O3^{iii}—Rb1A—O2^{iv}	70.43 (4)	O2^{xv}—Ga1—O4^{i}	88.72 (6)
O3^{iv}—Rb1A—O2^{iv}	48.04 (4)	O2^{ii}—Ga1—O4^{i}	92.25 (6)
O3^{ii}—Rb1A—O2^{iv}	115.61 (4)	O2^{xvi}—Ga1—O4^{i}	175.98 (7)
O3^{i}—Rb1A—O2^{iv}	64.84 (4)	O4^{xvii}—Ga1—O4^{i}	87.28 (6)
O3^{v}—Rb1A—O2^{iv}	113.71 (4)	O2^{xv}—Ga1—O4^{xviii}	175.98 (6)
O3—Rb1A—O2^{iv}	126.47 (4)	O2^{ii}—Ga1—O4^{xviii}	88.71 (6)
Rb1B^{i}—Rb1A—O2^{ii}	37.49 (3)	O2^{xvi}—Ga1—O4^{xviii}	92.25 (6)
Rb1B^{ii}—Rb1A—O2^{ii}	85.56 (15)	O4^{xvii}—Ga1—O4^{xviii}	87.28 (7)
O3^{iii}—Rb1A—O2^{ii}	64.84 (4)	O4^{i}—Ga1—O4^{xviii}	87.28 (7)
O3^{iv}—Rb1A—O2^{ii}	115.61 (4)	O2^{xv}—Ga1—Rb2^{xxi}	124.04 (4)
O3^{ii}—Rb1A—O2^{ii}	48.04 (4)	O2^{ii}—Ga1—Rb2^{xxi}	124.04 (4)
O3^{i}—Rb1A—O2^{ii}	70.43 (4)	O2^{xvi}—Ga1—Rb2^{xxi}	124.04 (4)
O3^{v}—Rb1A—O2^{ii}	126.47 (4)	O4^{xvii}—Ga1—Rb2^{xxi}	52.83 (5)
O3—Rb1A—O2^{ii}	113.71 (4)	O4^{i}—Ga1—Rb2^{xxi}	52.83 (5)
O2^{iv}—Rb1A—O2^{ii}	74.98 (5)	O4^{xviii}—Ga1—Rb2^{xxi}	52.83 (4)
Rb1B^{i}—Rb1A—O2^{v}	150.57 (3)	O2^{xv}—Ga1—Rb1A^{xvii}	32.81 (4)
Rb1B^{ii}—Rb1A—O2^{v}	85.56 (15)	O2^{ii}—Ga1—Rb1A^{xvii}	105.67 (4)
O3^{iii}—Rb1A—O2^{v}	113.71 (4)	O2^{xvi}—Ga1—Rb1A^{xvii}	120.04 (5)
O3^{iv}—Rb1A—O2^{v}	70.43 (4)	O4^{xvii}—Ga1—Rb1A^{xvii}	77.51 (4)
O3^{ii}—Rb1A—O2^{v}	126.47 (4)	O4^{i}—Ga1—Rb1A^{xvii}	59.26 (4)

O3^{i}—Rb1A—O2^{v}	115.61 (4)	O4^{xviii}—Ga1—Rb1A^{xvii}	143.41 (5)
O3^{v}—Rb1A—O2^{v}	48.04 (4)	Rb2^{xxi}—Ga1—Rb1A^{xvii}	92.384 (4)
O3—Rb1A—O2^{v}	64.84 (4)	O2^{xv}—Ga1—Rb1A	120.04 (5)
O2^{iv}—Rb1A—O2^{v}	113.21 (2)	O2^{ii}—Ga1—Rb1A	32.81 (4)
O2^{ii}—Rb1A—O2^{v}	171.11 (5)	O2^{xvi}—Ga1—Rb1A	105.67 (4)
Rb1B^{i}—Rb1A—O2	150.57 (3)	O4^{xvii}—Ga1—Rb1A	143.41 (5)
Rb1B^{ii}—Rb1A—O2	37.49 (14)	O4^{i}—Ga1—Rb1A	77.51 (4)
O3^{iii}—Rb1A—O2	115.61 (4)	O4^{xviii}—Ga1—Rb1A	59.26 (5)
O3^{iv}—Rb1A—O2	126.47 (4)	Rb2^{xxi}—Ga1—Rb1A	92.384 (4)
O3^{ii}—Rb1A—O2	70.43 (4)	Rb1A^{xvii}—Ga1—Rb1A	119.828 (1)
O3^{i}—Rb1A—O2	113.71 (4)	O2^{xv}—Ga1—Rb1A^{xvi}	105.67 (5)
O3^{v}—Rb1A—O2	64.84 (4)	O2^{ii}—Ga1—Rb1A^{xvi}	120.04 (5)
O3—Rb1A—O2	48.04 (4)	O2^{xvi}—Ga1—Rb1A^{xvi}	32.81 (4)
O2^{iv}—Rb1A—O2	171.11 (5)	O4^{xvii}—Ga1—Rb1A^{xvi}	59.26 (4)
O2^{ii}—Rb1A—O2	113.21 (2)	O4^{i}—Ga1—Rb1A^{xvi}	143.41 (5)
O2^{v}—Rb1A—O2	58.86 (5)	O4^{xviii}—Ga1—Rb1A^{xvi}	77.51 (5)
Rb1B^{i}—Rb1A—O2^{iii}	85.56 (3)	Rb2^{xxi}—Ga1—Rb1A^{xvi}	92.384 (4)
Rb1B^{ii}—Rb1A—O2^{iii}	37.49 (14)	Rb1A^{xvii}—Ga1—Rb1A^{xvi}	119.828 (1)
O3^{iii}—Rb1A—O2^{iii}	48.04 (4)	Rb1A—Ga1—Rb1A^{xvi}	119.828 (1)
O3^{iv}—Rb1A—O2^{iii}	113.71 (4)	O1^{viii}—Ga2—O1^{xiv}	93.53 (6)
O3^{ii}—Rb1A—O2^{iii}	64.84 (4)	O1^{viii}—Ga2—O1^{xix}	93.53 (6)
O3^{i}—Rb1A—O2^{iii}	126.47 (4)	O1^{xiv}—Ga2—O1^{xix}	93.53 (6)
O3^{v}—Rb1A—O2^{iii}	70.43 (4)	O1^{viii}—Ga2—O1^{i}	180.0
O3—Rb1A—O2^{iii}	115.61 (4)	O1^{xiv}—Ga2—O1^{i}	86.48 (6)
O2^{iv}—Rb1A—O2^{iii}	113.21 (2)	O1^{xix}—Ga2—O1^{i}	86.48 (6)
O2^{ii}—Rb1A—O2^{iii}	58.87 (5)	O1^{viii}—Ga2—O1^{xviii}	86.48 (6)
O2^{v}—Rb1A—O2^{iii}	113.21 (2)	O1^{xiv}—Ga2—O1^{xviii}	180.0
O2—Rb1A—O2^{iii}	74.98 (5)	O1^{xix}—Ga2—O1^{xviii}	86.48 (6)
Rb1B^{i}—Rb1A—O2^{i}	85.56 (3)	O1^{i}—Ga2—O1^{xviii}	93.52 (6)
Rb1B^{ii}—Rb1A—O2^{i}	150.57 (14)	O1^{viii}—Ga2—O1^{xvii}	86.48 (6)
O3^{iii}—Rb1A—O2^{i}	126.47 (4)	O1^{xiv}—Ga2—O1^{xvii}	86.48 (6)
O3^{iv}—Rb1A—O2^{i}	64.84 (4)	O1^{xix}—Ga2—O1^{xvii}	180.0
O3^{ii}—Rb1A—O2^{i}	113.71 (4)	O1^{i}—Ga2—O1^{xvii}	93.52 (6)
O3^{i}—Rb1A—O2^{i}	48.04 (4)	O1^{xviii}—Ga2—O1^{xvii}	93.52 (6)
O3^{v}—Rb1A—O2^{i}	115.61 (4)	O1^{viii}—Ga2—Rb2^{xix}	63.39 (5)
O3—Rb1A—O2^{i}	70.43 (4)	O1^{xiv}—Ga2—Rb2^{xix}	66.53 (5)
O2^{iv}—Rb1A—O2^{i}	58.87 (5)	O1^{xix}—Ga2—Rb2^{xix}	146.92 (4)
O2^{ii}—Rb1A—O2^{i}	113.21 (2)	O1^{i}—Ga2—Rb2^{xix}	116.61 (5)
O2^{v}—Rb1A—O2^{i}	74.98 (5)	O1^{xviii}—Ga2—Rb2^{xix}	113.47 (5)
O2—Rb1A—O2^{i}	113.21 (2)	O1^{xvii}—Ga2—Rb2^{xix}	33.08 (4)
O2^{iii}—Rb1A—O2^{i}	171.11 (6)	O1^{viii}—Ga2—Rb2^{xvii}	116.62 (5)
Rb1B^{i}—Rb1A—As^{iv}	60.827 (6)	O1^{xiv}—Ga2—Rb2^{xvii}	113.48 (5)
Rb1B^{ii}—Rb1A—As^{iv}	149.73 (2)	O1^{xix}—Ga2—Rb2^{xvii}	33.08 (4)
O3^{iii}—Rb1A—As^{iv}	73.16 (3)	O1^{i}—Ga2—Rb2^{xvii}	63.38 (5)
O3^{iv}—Rb1A—As^{iv}	24.86 (3)	O1^{xviii}—Ga2—Rb2^{xvii}	66.52 (5)
O3^{ii}—Rb1A—As^{iv}	139.65 (3)	O1^{xvii}—Ga2—Rb2^{xvii}	146.92 (4)
O3^{i}—Rb1A—As^{iv}	79.79 (3)	Rb2^{xix}—Ga2—Rb2^{xvii}	180.0
O3^{v}—Rb1A—As^{iv}	93.74 (3)	O1^{viii}—Ga2—Rb2^{xvi}	113.48 (5)

O3—Rb1A—As^{iv}	123.16 (3)	O1^{xiv}—Ga2—Rb2^{xvi}	33.08 (4)
O2^{iv}—Rb1A—As^{iv}	24.28 (2)	O1^{xix}—Ga2—Rb2^{xvi}	116.62 (6)
O2^{ii}—Rb1A—As^{iv}	97.93 (3)	O1^{i}—Ga2—Rb2^{xvi}	66.52 (5)
O2^{v}—Rb1A—As^{iv}	89.76 (3)	O1^{xviii}—Ga2—Rb2^{xvi}	146.92 (4)
O2—Rb1A—As^{iv}	148.57 (3)	O1^{xvii}—Ga2—Rb2^{xvi}	63.38 (6)
O2^{iii}—Rb1A—As^{iv}	121.15 (3)	Rb2^{xix}—Ga2—Rb2^{xvi}	60.0
O2^{i}—Rb1A—As^{iv}	53.64 (3)	Rb2^{xvii}—Ga2—Rb2^{xvi}	120.0
Rb1B^{i}—Rb1B—Rb1B^{ii}	60.00 (4)	O1^{viii}—Ga2—Rb2	33.08 (5)
Rb1B^{i}—Rb1B—O3^{iv}	94.7 (6)	O1^{xiv}—Ga2—Rb2	116.62 (5)
Rb1B^{ii}—Rb1B—O3^{iv}	123.8 (6)	O1^{xix}—Ga2—Rb2	113.48 (5)
Rb1B^{i}—Rb1B—O3	123.8 (6)	O1^{i}—Ga2—Rb2	146.92 (5)
Rb1B^{ii}—Rb1B—O3	94.7 (7)	O1^{xviii}—Ga2—Rb2	63.38 (5)
O3^{iv}—Rb1B—O3	136.7 (14)	O1^{xvii}—Ga2—Rb2	66.52 (5)
Rb1B^{i}—Rb1B—O2^{v}	160.6 (4)	Rb2^{xix}—Ga2—Rb2	60.0
Rb1B^{ii}—Rb1B—O2^{v}	109.8 (6)	Rb2^{xvii}—Ga2—Rb2	120.0
O3^{iv}—Rb1B—O2^{v}	77.3 (7)	Rb2^{xvi}—Ga2—Rb2	120.0
O3—Rb1B—O2^{v}	71.0 (6)	O1^{viii}—Ga2—Rb2^{xxii}	66.52 (5)
Rb1B^{i}—Rb1B—O2^{i}	109.8 (5)	O1^{xiv}—Ga2—Rb2^{xxii}	146.92 (4)
Rb1B^{ii}—Rb1B—O2^{i}	160.6 (3)	O1^{xix}—Ga2—Rb2^{xxii}	63.38 (6)
O3^{iv}—Rb1B—O2^{i}	71.0 (6)	O1^{i}—Ga2—Rb2^{xxii}	113.47 (5)
O3—Rb1B—O2^{i}	77.3 (7)	O1^{xviii}—Ga2—Rb2^{xxii}	33.08 (4)
O2^{v}—Rb1B—O2^{i}	84.6 (10)	O1^{xvii}—Ga2—Rb2^{xxii}	116.62 (6)
Rb1B^{i}—Rb1B—O3^{i}	72.1 (6)	Rb2^{xix}—Ga2—Rb2^{xxii}	120.0
Rb1B^{ii}—Rb1B—O3^{i}	109.8 (6)	Rb2^{xvii}—Ga2—Rb2^{xxii}	60.0
O3^{iv}—Rb1B—O3^{i}	107.2 (4)	Rb2^{xvi}—Ga2—Rb2^{xxii}	180.0
O3—Rb1B—O3^{i}	72.0 (2)	Rb2—Ga2—Rb2^{xxii}	60.0
O2^{v}—Rb1B—O3^{i}	127.0 (11)	O1^{viii}—Ga2—Rb2^{xxiii}	146.92 (5)
O2^{i}—Rb1B—O3^{i}	51.0 (2)	O1^{xiv}—Ga2—Rb2^{xxiii}	63.38 (5)
Rb1B^{i}—Rb1B—O3^{v}	109.8 (7)	O1^{xix}—Ga2—Rb2^{xxiii}	66.52 (5)
Rb1B^{ii}—Rb1B—O3^{v}	72.1 (7)	O1^{i}—Ga2—Rb2^{xxiii}	33.08 (5)
O3^{iv}—Rb1B—O3^{v}	72.0 (2)	O1^{xviii}—Ga2—Rb2^{xxiii}	116.61 (5)
O3—Rb1B—O3^{v}	107.2 (4)	O1^{xvii}—Ga2—Rb2^{xxiii}	113.47 (5)
O2^{v}—Rb1B—O3^{v}	51.0 (2)	Rb2^{xix}—Ga2—Rb2^{xxiii}	120.0
O2^{i}—Rb1B—O3^{v}	127.0 (11)	Rb2^{xvii}—Ga2—Rb2^{xxiii}	60.0
O3^{i}—Rb1B—O3^{v}	177.9 (14)	Rb2^{xvi}—Ga2—Rb2^{xxiii}	60.0
Rb1B^{i}—Rb1B—O2^{iv}	58.5 (7)	Rb2—Ga2—Rb2^{xxiii}	180.0
Rb1B^{ii}—Rb1B—O2^{iv}	116.2 (6)	Rb2^{xxii}—Ga2—Rb2^{xxiii}	119.997 (1)
O3^{iv}—Rb1B—O2^{iv}	49.25 (8)	O1^{xx}—As—O2	119.20 (8)
O3—Rb1B—O2^{iv}	133.4 (5)	O1^{xx}—As—O4^{iv}	105.45 (8)
O2^{v}—Rb1B—O2^{iv}	122.6 (9)	O2—As—O4^{iv}	114.88 (7)
O2^{i}—Rb1B—O2^{iv}	62.0 (3)	O1^{xx}—As—O3	107.00 (9)
O3^{i}—Rb1B—O2^{iv}	65.28 (4)	O2—As—O3	103.30 (8)
O3^{v}—Rb1B—O2^{iv}	114.83 (5)	O4^{iv}—As—O3	106.04 (8)
Rb1B^{i}—Rb1B—O2	116.2 (7)	O1^{xx}—As—Rb2^{xii}	64.25 (6)
Rb1B^{ii}—Rb1B—O2	58.5 (8)	O2—As—Rb2^{xii}	172.80 (5)
O3^{iv}—Rb1B—O2	133.4 (5)	O4^{iv}—As—Rb2^{xii}	68.49 (5)
O3—Rb1B—O2	49.25 (8)	O3—As—Rb2^{xii}	69.51 (6)
O2^{v}—Rb1B—O2	62.0 (3)	O1^{xx}—As—Rb1B^{ii}	142.0 (2)

O2^{i}—Rb1B—O2	122.6 (9)	O2—As—Rb1B^{ii}	50.6 (6)
O3^{i}—Rb1B—O2	114.83 (5)	O4^{iv}—As—Rb1B^{ii}	111.5 (3)
O3^{v}—Rb1B—O2	65.28 (4)	O3—As—Rb1B^{ii}	54.9 (5)
O2^{iv}—Rb1B—O2	174.7 (13)	Rb2^{xii}—As—Rb1B^{ii}	122.5 (5)
Rb1B^{i}—Rb1B—O3^{iii}	46.2 (3)	O1^{xx}—As—Rb1B	146.8 (4)
Rb1B^{ii}—Rb1B—O3^{iii}	58.9 (3)	O2—As—Rb1B	60.0 (4)
O3^{iv}—Rb1B—O3^{iii}	67.6 (2)	O4^{iv}—As—Rb1B	103.6 (5)
O3—Rb1B—O3^{iii}	153.6 (10)	O3—As—Rb1B	48.68 (19)
O2^{v}—Rb1B—O3^{iii}	114.75 (4)	Rb2^{xii}—As—Rb1B	113.4 (4)
O2^{i}—Rb1B—O3^{iii}	127.90 (5)	Rb1B^{ii}—As—Rb1B	10.8 (11)
O3^{i}—Rb1B—O3^{iii}	115.4 (7)	O1^{xx}—As—Rb1A	143.22 (6)
O3^{v}—Rb1B—O3^{iii}	66.2 (3)	O2—As—Rb1A	55.94 (5)
O2^{iv}—Rb1B—O3^{iii}	67.3 (3)	O4^{iv}—As—Rb1A	108.77 (5)
O2—Rb1B—O3^{iii}	108.7 (7)	O3—As—Rb1A	50.50 (6)
Rb1B^{i}—Rb1B—O3^{ii}	58.9 (4)	Rb2^{xii}—As—Rb1A	117.262 (8)
Rb1B^{ii}—Rb1B—O3^{ii}	46.2 (3)	Rb1B^{ii}—As—Rb1A	5.5 (5)
O3^{iv}—Rb1B—O3^{ii}	153.6 (10)	Rb1B—As—Rb1A	5.7 (6)
O3—Rb1B—O3^{ii}	67.6 (2)	O1^{xx}—As—Rb2	81.53 (7)
O2^{v}—Rb1B—O3^{ii}	127.90 (5)	O2—As—Rb2	99.68 (5)
O2^{i}—Rb1B—O3^{ii}	114.75 (4)	O4^{iv}—As—Rb2	133.31 (5)
O3^{i}—Rb1B—O3^{ii}	66.2 (3)	O3—As—Rb2	32.31 (6)
O3^{v}—Rb1B—O3^{ii}	115.4 (7)	Rb2^{xii}—As—Rb2	74.193 (8)
O2^{iv}—Rb1B—O3^{ii}	108.7 (7)	Rb1B^{ii}—As—Rb2	67.2 (2)
O2—Rb1B—O3^{ii}	67.3 (3)	Rb1B—As—Rb2	66.79 (16)
O3^{iii}—Rb1B—O3^{ii}	91.5 (9)	Rb1A—As—Rb2	65.327 (14)
O3—Rb2—O3^{i}	76.48 (6)	O1^{xx}—As—Rb1A^{xxiv}	87.84 (7)
O3—Rb2—O3^{ii}	76.48 (6)	O2—As—Rb1A^{xxiv}	94.28 (5)
O3^{i}—Rb2—O3^{ii}	76.48 (6)	O4^{iv}—As—Rb1A^{xxiv}	40.78 (5)
O3—Rb2—O1^{vi}	91.00 (4)	O3—As—Rb1A^{xxiv}	146.81 (6)
O3^{i}—Rb2—O1^{vi}	76.80 (4)	Rb2^{xii}—As—Rb1A^{xxiv}	92.146 (8)
O3^{ii}—Rb2—O1^{vi}	152.49 (5)	Rb1B^{ii}—As—Rb1A^{xxiv}	126.24 (14)
O3—Rb2—O1^{vii}	76.80 (5)	Rb1B—As—Rb1A^{xxiv}	125.1 (3)
O3^{i}—Rb2—O1^{vii}	152.49 (5)	Rb1A—As—Rb1A^{xxiv}	127.415 (12)
O3^{ii}—Rb2—O1^{vii}	91.00 (4)	Rb2—As—Rb1A^{xxiv}	165.357 (7)
O1^{vi}—Rb2—O1^{vii}	110.14 (3)	O1^{xx}—As—Rb2^{xxiv}	42.87 (6)
O3—Rb2—O1^{viii}	152.49 (5)	O2—As—Rb2^{xxiv}	127.54 (5)
O3^{i}—Rb2—O1^{viii}	91.00 (5)	O4^{iv}—As—Rb2^{xxiv}	64.16 (5)
O3^{ii}—Rb2—O1^{viii}	76.80 (5)	O3—As—Rb2^{xxiv}	128.20 (6)
O1^{vi}—Rb2—O1^{viii}	110.14 (3)	Rb2^{xii}—As—Rb2^{xxiv}	59.507 (5)
O1^{vii}—Rb2—O1^{viii}	110.13 (2)	Rb1B^{ii}—As—Rb2^{xxiv}	174.80 (5)
O3—Rb2—O4^{ix}	126.84 (4)	Rb1B—As—Rb2^{xxiv}	167.1 (6)
O3^{i}—Rb2—O4^{ix}	111.15 (5)	Rb1A—As—Rb2^{xxiv}	172.736 (5)
O3^{ii}—Rb2—O4^{ix}	156.15 (4)	Rb2—As—Rb2^{xxiv}	117.769 (15)
O1^{vi}—Rb2—O4^{ix}	45.47 (4)	Rb1A^{xxiv}—As—Rb2^{xxiv}	48.647 (11)
O1^{vii}—Rb2—O4^{ix}	90.21 (4)	As^{xxv}—O1—Ga2^{xxvi}	137.45 (10)
O1^{viii}—Rb2—O4^{ix}	80.43 (4)	As^{xxv}—O1—Rb2^{vi}	89.47 (6)
O3—Rb2—O4^{x}	111.15 (5)	Ga2^{xxvi}—O1—Rb2^{vi}	128.38 (6)
O3^{i}—Rb2—O4^{x}	156.15 (4)	As^{xxv}—O1—Rb2^{xxv}	76.24 (6)

O3^{ii}—Rb2—O4^{x}	126.84 (4)	Ga2^{xxvi}—O1—Rb2^{xxv}	92.73 (6)
O1^{vi}—Rb2—O4^{x}	80.43 (4)	Rb2^{vi}—O1—Rb2^{xxv}	76.74 (3)
O1^{vii}—Rb2—O4^{x}	45.46 (4)	As^{xxv}—O1—Rb2^{xxvi}	122.41 (7)
O1^{viii}—Rb2—O4^{x}	90.21 (4)	Ga2^{xxvi}—O1—Rb2^{xxvi}	89.56 (6)
O4^{ix}—Rb2—O4^{x}	45.74 (4)	Rb2^{vi}—O1—Rb2^{xxvi}	75.20 (3)
O3—Rb2—O4^{xi}	156.15 (5)	Rb2^{xxv}—O1—Rb2^{xxvi}	145.76 (4)
O3^{i}—Rb2—O4^{xi}	126.84 (5)	As—O2—Ga1^{xxiv}	121.66 (8)
O3^{ii}—Rb2—O4^{xi}	111.15 (5)	As—O2—Rb1B^{ii}	104.3 (5)
O1^{vi}—Rb2—O4^{xi}	90.21 (4)	Ga1^{xxiv}—O2—Rb1B^{ii}	125.9 (3)
O1^{vii}—Rb2—O4^{xi}	80.43 (4)	As—O2—Rb1B	94.4 (5)
O1^{viii}—Rb2—O4^{xi}	45.46 (4)	Ga1^{xxiv}—O2—Rb1B	130.14 (12)
O4^{ix}—Rb2—O4^{xi}	45.74 (4)	Rb1B^{ii}—O2—Rb1B	11.7 (11)
O4^{x}—Rb2—O4^{xi}	45.74 (4)	As—O2—Rb1A	99.78 (6)
O3—Rb2—O3^{xii}	83.50 (5)	Ga1^{xxiv}—O2—Rb1A	128.83 (6)
O3^{i}—Rb2—O3^{xii}	119.25 (6)	Rb1B^{ii}—O2—Rb1A	4.8 (5)
O3^{ii}—Rb2—O3^{xii}	150.88 (6)	Rb1B—O2—Rb1A	7.1 (7)
O1^{vi}—Rb2—O3^{xii}	46.57 (4)	As—O2—Rb2	60.35 (4)
O1^{vii}—Rb2—O3^{xii}	63.66 (4)	Ga1^{xxiv}—O2—Rb2	162.84 (6)
O1^{viii}—Rb2—O3^{xii}	123.76 (4)	Rb1B^{ii}—O2—Rb2	64.9 (2)
O4^{ix}—Rb2—O3^{xii}	45.78 (4)	Rb1B—O2—Rb2	63.47 (7)
O4^{x}—Rb2—O3^{xii}	43.39 (4)	Rb1A—O2—Rb2	63.10 (2)
O4^{xi}—Rb2—O3^{xii}	80.11 (4)	As—O3—Rb2	129.19 (8)
O3—Rb2—O3^{xiii}	150.89 (6)	As—O3—Rb1B	105.64 (12)
O3^{i}—Rb2—O3^{xiii}	83.50 (5)	Rb2—O3—Rb1B	97.7 (5)
O3^{ii}—Rb2—O3^{xiii}	119.25 (6)	As—O3—Rb1B^{ii}	98.2 (6)
O1^{vi}—Rb2—O3^{xiii}	63.66 (4)	Rb2—O3—Rb1B^{ii}	94.64 (16)
O1^{vii}—Rb2—O3^{xiii}	123.75 (4)	Rb1B—O3—Rb1B^{ii}	13.2 (13)
O1^{viii}—Rb2—O3^{xiii}	46.57 (4)	As—O3—Rb1A	104.65 (8)
O4^{ix}—Rb2—O3^{xiii}	43.39 (4)	Rb2—O3—Rb1A	93.37 (5)
O4^{x}—Rb2—O3^{xiii}	80.11 (4)	Rb1B—O3—Rb1A	7.0 (7)
O4^{xi}—Rb2—O3^{xiii}	45.78 (4)	Rb1B^{ii}—O3—Rb1A	7.5 (7)
O3^{xii}—Rb2—O3^{xiii}	88.19 (4)	As—O3—Rb1B^{i}	109.5 (4)
O3—Rb2—O3^{xiv}	119.25 (6)	Rb2—O3—Rb1B^{i}	88.4 (5)
O3^{i}—Rb2—O3^{xiv}	150.88 (6)	Rb1B—O3—Rb1B^{i}	10.0 (9)
O3^{ii}—Rb2—O3^{xiv}	83.50 (5)	Rb1B^{ii}—O3—Rb1B^{i}	11.3 (10)
O1^{vi}—Rb2—O3^{xiv}	123.76 (4)	Rb1A—O3—Rb1B^{i}	5.4 (5)
O1^{vii}—Rb2—O3^{xiv}	46.57 (4)	As—O3—Rb2^{xii}	82.99 (7)
O1^{viii}—Rb2—O3^{xiv}	63.66 (4)	Rb2—O3—Rb2^{xii}	96.50 (5)
O4^{ix}—Rb2—O3^{xiv}	80.11 (4)	Rb1B—O3—Rb2^{xii}	152.4 (7)
O4^{x}—Rb2—O3^{xiv}	45.78 (4)	Rb1B^{ii}—O3—Rb2^{xii}	164.5 (4)
O4^{xi}—Rb2—O3^{xiv}	43.38 (4)	Rb1A—O3—Rb2^{xii}	159.28 (6)
O3^{xii}—Rb2—O3^{xiv}	88.19 (4)	Rb1B^{i}—O3—Rb2^{xii}	159.23 (8)
O3^{xiii}—Rb2—O3^{xiv}	88.19 (4)	As^{iv}—O4—Ga1^{xxvi}	130.00 (8)
O3—Rb2—As^{xiv}	102.80 (4)	As^{iv}—O4—Rb2^{xxvii}	84.95 (5)
O3^{i}—Rb2—As^{xiv}	177.27 (4)	Ga1^{xxvi}—O4—Rb2^{xxvii}	100.50 (6)
O3^{ii}—Rb2—As^{xiv}	100.79 (4)	As^{iv}—O4—Rb1A^{xxv}	124.06 (6)
O1^{vi}—Rb2—As^{xiv}	105.88 (3)	Ga1^{xxvi}—O4—Rb1A^{xxv}	96.95 (5)
O1^{vii}—Rb2—As^{xiv}	26.29 (3)	Rb2^{xxvii}—O4—Rb1A^{xxv}	118.51 (4)

O1^{viii}—Rb2—As^{xiv}	88.53 (3)	As^{iv}—O4—Rb1A	51.95 (4)
O4^{ix}—Rb2—As^{xiv}	71.43 (3)	Ga1^{xxvi}—O4—Rb1A	78.99 (4)
O4^{x}—Rb2—As^{xiv}	26.56 (2)	Rb2^{xxvii}—O4—Rb1A	104.39 (3)
O4^{xi}—Rb2—As^{xiv}	54.15 (3)	Rb1A^{xxv}—O4—Rb1A	136.81 (4)
O3^{xii}—Rb2—As^{xiv}	63.12 (3)	As^{iv}—O4—Rb2^{xxviii}	98.27 (5)
O3^{xiii}—Rb2—As^{xiv}	98.10 (3)	Ga1^{xxvi}—O4—Rb2^{xxviii}	129.76 (6)
O3^{xiv}—Rb2—As^{xiv}	27.50 (3)	Rb2^{xxvii}—O4—Rb2^{xxviii}	66.64 (2)
O3—Rb2—As^{xii}	100.79 (4)	Rb1A^{xxv}—O4—Rb2^{xxviii}	57.20 (2)
O3^{i}—Rb2—As^{xii}	102.80 (4)	Rb1A—O4—Rb2^{xxviii}	150.18 (3)
O3^{ii}—Rb2—As^{xii}	177.27 (4)		

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) −*x*+*y*, −*x*, *z*; (iii) *x*−*y*, −*y*, −*z*+3/2; (iv) −*x*, −*x*+*y*, −*z*+3/2; (v) *y*, *x*, −*z*+3/2; (vi) −*x*+2/3, −*y*−2/3, −*z*+4/3; (vii) *x*−*y*−4/3, *x*−2/3, −*z*+4/3; (viii) *y*+2/3, −*x*+*y*+4/3, −*z*+4/3; (ix) *x*−1/3, *x*−*y*−2/3, *z*−1/6; (x) −*y*−1/3, −*x*+1/3, *z*−1/6; (xi) −*x*+*y*+2/3, *y*+1/3, *z*−1/6; (xii) −*x*−1/3, −*y*−2/3, −*z*+4/3; (xiii) *y*+2/3, −*x*+*y*+1/3, −*z*+4/3; (xiv) *x*−*y*−1/3, *x*+1/3, −*z*+4/3; (xv) −*y*, *x*−*y*+1, *z*; (xvi) *x*+1, *y*+1, *z*; (xvii) *x*, *y*+1, *z*; (xviii) −*x*+*y*+1, −*x*+1, *z*; (xix) −*x*+2/3, −*y*+1/3, −*z*+4/3; (xx) *x*−1, *y*, *z*; (xxi) −*y*+1/3, −*x*+2/3, *z*+1/6; (xxii) −*x*−1/3, −*y*+1/3, −*z*+4/3; (xxiii) −*x*+2/3, −*y*+4/3, −*z*+4/3; (xxiv) *x*−1, *y*−1, *z*; (xxv) *x*+1, *y*, *z*; (xxvi) *x*, *y*−1, *z*; (xxvii) −*y*+1/3, −*x*−1/3, *z*+1/6; (xxviii) *y*+1, *x*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H···O4^{xxix}	0.85 (3)	1.76 (3)	2.598 (2)	168 (4)

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