



$M\text{In}(\text{HAsO}_4)_2$ ($M = \text{K}, \text{Rb}, \text{Cs}$): three new hydrogenarsenates adopting two different structure types

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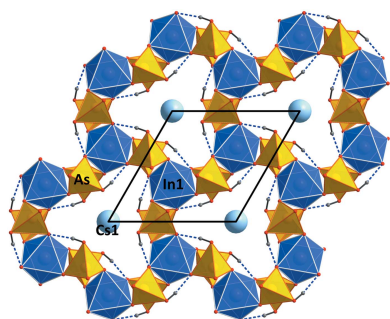
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Potassium indium bis[hydrogen arsenate(V)], $\text{KIn}(\text{HAsO}_4)_2$, rubidium indium bis[hydrogen arsenate(V)], $\text{RbIn}(\text{HAsO}_4)_2$, and caesium indium bis[hydrogen arsenate(V)], $\text{CsIn}(\text{HAsO}_4)_2$, were grown under mild hydrothermal conditions ($T = 493 \text{ K}$, 7–8 d). $\text{KIn}(\text{HAsO}_4)_2$ adopts the $\text{KSc}(\text{HAsO}_4)_2$ structure type (space group $C2/c$), while $\text{RbIn}(\text{HAsO}_4)_2$ and $\text{CsIn}(\text{HAsO}_4)_2$ crystallize in the space group $R\bar{3}c$ and are the first arsenate representatives of the $\text{RbFe}(\text{HPO}_4)_2$ structure type. All three compounds have tetrahedral–octahedral framework topologies. The M^+ cations, located in voids of the respective framework, are slightly disordered in $\text{RbIn}(\text{HAsO}_4)_2$. In $\text{KIn}(\text{HAsO}_4)_2$, there is a second K-atom position with a very low occupancy, which may suggest that the K atom can easily move in the channels extending along $[101]$.

1. Chemical context

Metal arsenates often form tetrahedral–octahedral framework structures that frequently show potentially interesting properties, such as ion conductivity, ion exchange and catalytic properties (Masquelier *et al.*, 1990, 1994*a,b*, 1995, 1996, 1998; Mesa *et al.*, 2000; Ouerfelli *et al.*, 2007*a,b*, 2008; Pintard-Scrépel *et al.*, 1983; Rouse *et al.*, 2013). In the course of a detailed study of the system $M^+-M^{3+}-\text{As}-\text{O}-(\text{H})$ by hydrothermal syntheses, a large variety of new arsenate(V) compounds and structure types were found (Kolitsch, 2004; Schwendtner, 2006; Schwendtner & Kolitsch, 2004*a,b*, 2005, 2007*a,b,c,d*, 2017*a,b,c*).

The three new title compounds belong to the family of hydrogenarsenate compounds with the general formula $M^+M^{3+}(\text{HAsO}_4)_2$. Including the three compounds reported here, nine compounds with this general formula are known. They crystallize in four different structure types. $\text{KIn}(\text{HAsO}_4)_2$ is a further representative of the $\text{KSc}(\text{HAsO}_4)_2$ structure type (Schwendtner & Kolitsch, 2004*a*), which is also adopted by $\text{AgGa}(\text{HAsO}_4)_2$ and $\text{AgAl}(\text{HAsO}_4)_2$ (Schwendtner & Kolitsch, 2017*c*). The $(\text{H}_3\text{O})\text{Fe}(\text{HPO}_4)_2$ structure type (Vencato *et al.*, 1989) is adopted by $\text{CsSc}(\text{HAsO}_4)_2$ (Schwendtner & Kolitsch, 2004*b*). Another modification of $\text{CsSc}(\text{HAsO}_4)_2$ crystallizes in the $(\text{NH}_4)\text{Fe}(\text{HPO}_4)_2$ type (Yakubovich, 1993), in which also $(\text{NH}_4)\text{Fe}(\text{HAsO}_4)_2$ crystallizes (Ouerfelli *et al.*, 2014). The two new title compounds $\text{RbIn}(\text{HAsO}_4)_2$ and $\text{CsIn}(\text{HAsO}_4)_2$ adopt a structure type hitherto unknown among arsenates which is, however, known from the phosphates $\text{RbFe}(\text{HPO}_4)_2$



(Lii & Wu, 1994) and $\text{RbM}^{3+}(\text{HPO}_4)_2$ ($M = \text{Al}, \text{Ga}$) (Lesage *et al.*, 2007). All of these compounds consist of frameworks of singly protonated AsO_4 tetrahedra and $M^{3+}\text{O}_6$ octahedra. The M^+ cations occupy channels that extend along one or more directions in the framework.

A number of M^+ –In–arsenates have been reported in the literature. Among these are several diarsenates: $\text{NaInAs}_2\text{O}_7$ (Belam *et al.*, 1997), KInAs_2O_7 (Schwendtner & Kolitsch, 2017*b*) and $\text{RbInAs}_2\text{O}_7$, $\text{TlInAs}_2\text{O}_7$ and $(\text{NH}_4)\text{InAs}_2\text{O}_7$ (Schwendtner, 2006), furthermore $\text{Na}_3\text{In}_2(\text{AsO}_4)_3$ (Lii & Ye, 1997; Khorari *et al.*, 1997) and $\text{KIn}(\text{H}_2\text{O})(\text{H}_{1.5}\text{AsO}_4)_2 \cdot (\text{H}_2\text{AsO}_4)$ (Schwendtner & Kolitsch, 2007*c*). There also exist indexed X-ray powder diffraction data of $\text{Li}_3\text{In}_2(\text{AsO}_4)_3$ (Winand *et al.*, 1990) and unindexed powder patterns of $\text{KIn}(\text{HAsO}_4)_2 \cdot x\text{H}_2\text{O}$, $\text{RbIn}(\text{HAsO}_4)_2 \cdot x\text{H}_2\text{O}$, $\text{CsIn}(\text{HAsO}_4)_2 \cdot x\text{H}_2\text{O}$ and $\text{CsInAs}_2\text{O}_7$ (Ezhova *et al.*, 1977).

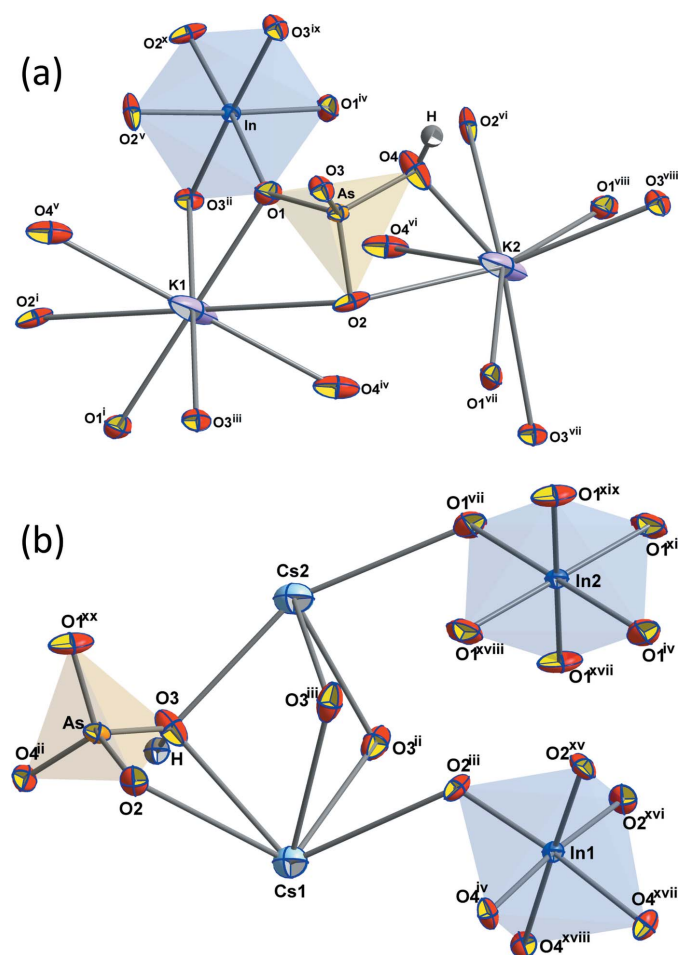


Figure 1

The principal building units of (a) $\text{KIn}(\text{HAsO}_4)_2$ and (b) $\text{CsIn}(\text{HAsO}_4)_2$, shown as displacement ellipsoids at the 70% probability level. Symmetry codes: $\text{KIn}(\text{HAsO}_4)_2$: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z$; (ii) $-x, -y + 1, -z$; (iii) $x + \frac{1}{2}, y - \frac{1}{2}, z$; (iv) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$; (v) $-x + 1, y, -z + \frac{1}{2}$; (vi) $x, -y + 1, z - \frac{1}{2}$; (vii) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (viii) $-x, y, -z + \frac{1}{2}$; (ix) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (x) $x - \frac{1}{2}, y + \frac{1}{2}, z$; $\text{CsIn}(\text{HAsO}_4)_2$: (ii) $-x, -y + 1, -z$; (iii) $-x + \frac{1}{2}, y - \frac{1}{2}, z$; (iv) $-y, x - y, z$; (vii) $y + \frac{2}{3}, -x + y + \frac{4}{3}, -z + \frac{4}{3}$; (xi) $x - y - \frac{1}{3}, x + \frac{1}{3}, -z + \frac{4}{3}$; (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) $-x + \frac{2}{3}, -y + \frac{1}{3}, -z + \frac{4}{3}$; (xx) $x - 1, y, z$.

Table 1

Selected bond lengths (Å) for $\text{KIn}(\text{HAsO}_4)_2$.

K1—O1 ⁱ	2.6488 (17)	K2—O3 ^{vii}	3.20 (3)
K1—O1	2.6488 (17)	K2—O2	3.33 (3)
K1—O3 ⁱⁱ	2.7788 (17)	K2—O2 ^{vi}	3.33 (3)
K1—O3 ⁱⁱⁱ	2.7788 (17)	In—O1	2.1104 (17)
K1—O4 ^{iv}	3.112 (2)	In—O1 ^{vi}	2.1104 (17)
K1—O4 ^v	3.112 (2)	In—O3 ⁱⁱ	2.1388 (16)
K1—O2	3.2553 (19)	In—O3 ^{ix}	2.1388 (16)
K1—O2 ⁱ	3.2553 (19)	In—O2 ^x	2.1473 (16)
K2—O4	2.74 (4)	In—O2 ^v	2.1473 (16)
K2—O4 ^{vi}	2.74 (4)	As—O1	1.6574 (17)
K2—O1 ^{vii}	2.792 (18)	As—O3	1.6721 (17)
K2—O1 ^{viii}	2.792 (18)	As—O2	1.6762 (16)
K2—O3 ^{viii}	3.20 (3)	As—O4	1.7231 (19)

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

The hydrogenphosphates $\text{KIn}(\text{HPO}_4)_2$ and $\text{RbIn}(\text{HPO}_4)_2$ (Filaretov *et al.*, 2002*b*), which are the phosphate analogues of two of the title compounds, crystallize in the $(\text{NH}_4)\text{In}(\text{HPO}_4)_2$ structure type ($P2_1/c$; Filaretov *et al.*, 2002*a*; Mao *et al.*, 2002), for which no arsenate members were known prior to the present work. $\text{CsIn}(\text{HPO}_4)_2$ (Huang *et al.*, 2004; Lesage *et al.*, 2007) is known as two modifications, the $(\text{NH}_4)\text{Fe}(\text{HPO}_4)_2$ -type ($P\bar{1}$; Yakubovich, 1993) and the $(\text{H}_3\text{O})\text{Fe}(\text{HPO}_4)_2$ -type ($P2_1/c$; Vencato *et al.*, 1989). Both structure types are common among hydrogenphosphates, with eleven and seven members, respectively, and both have one arsenate representative each, *viz.* α - and β - $\text{CsSc}(\text{HAsO}_4)_2$ (Schwendtner & Kolitsch, 2004). The $(\text{NH}_4)\text{Fe}(\text{HPO}_4)_2$ -type $\text{CsIn}(\text{HPO}_4)_2$ is closely related to and basically a distorted variety of the $\text{RbFe}(\text{HPO}_4)_2$ type in which $\text{CsIn}(\text{HAsO}_4)_2$ crystallizes (see discussion in Lesage *et al.*, 2007). According to Huang *et al.* (2004), a second variety of $\text{RbIn}(\text{HPO}_4)_2$ exists, which is also isotypic to $(\text{H}_3\text{O})\text{Fe}(\text{HPO}_4)_2$.

2. Structural commentary

$\text{KIn}(\text{HAsO}_4)_2$ crystallizes in space group $C2/c$ and is isotypic to $\text{KSc}(\text{HAsO}_4)_2$ (Schwendtner & Kolitsch, 2004*a*), $\text{AgGa}(\text{HAsO}_4)_2$ and $\text{AgAl}(\text{HAsO}_4)_2$ (Schwendtner & Kolitsch, 2017*c*). The asymmetric unit contains one K, one In, one As, one H and four O atoms (Fig. 1*a*). The slightly distorted InO_6 octahedra share corners with six HAsO_4 tetrahedra, thus forming a three-dimensional anionic framework with narrow channels parallel to $[110]$ and $[101]$ (Fig. 2*a,b*) which host the K atoms. There are two K-atom positions (K1 and K2), at a distance of 2.653 (15) Å from each other. The K1 position is located on an inversion centre and has a refined occupancy of 0.976 (2), while K2, which lies between two K1 positions, is located on a twofold axis (like the In atom) and has a refined occupancy of 0.024 (2). Both K-atom positions show a $[4 + 4]$ -coordination with average K—O bond lengths of 2.949 and 3.016 Å for K1 and K2, respectively (Table 1). This is slightly longer than the reported average K—O bond length for ^{81}K atoms of 2.85 Å (Baur, 1981). However, bond-valence calcu-

lations after Gagné & Hawthorne (2015) show bond-valence sums (BVSs) of 0.99 valence units (v.u.) for K1 and 0.85 v.u. for K2, indicating an ‘underbonded’ character of K2, and explaining the difference in site occupancies.

As expected, the protonated AsO_4 tetrahedron is strongly distorted as three vertices connect to neighbouring InO_6 octahedra, while O4 (OH) is a terminal vertex and only involved in a medium–strong hydrogen bond (Fig. 2*b* and 2*c*; Table 4).

Calculated BVSs (Gagné & Hawthorne, 2015) of the framework atoms amount to 3.06 v.u. for In, 5.07 v.u. for As and 2.11/1.83/1.96/1.20 v.u. for O1–O4, respectively. Although these sums appear slightly too high for In and As, the average In–O and As–O bond lengths fit very well to published

averages: the average As–O bond length in $\text{KIn}(\text{HAsO}_4)_2$ is 1.682 Å and the As–OH bond length is 1.723 Å, very close to the average of 704 analyzed AsO_4 groups in inorganic compounds [1.686 (10) Å; Schwendtner, 2008] and the average As–OH in 45 HAsO_4 groups [1.72 (3) Å; Schwendtner, 2008], respectively. The average In–O bond length (2.132 Å) is slightly shorter than the published average of 2.141 Å for inorganic compounds (Baur, 1981).

$\text{RbIn}(\text{HAsO}_4)_2$ and $\text{CsIn}(\text{HAsO}_4)_2$ crystallize in the space group $R\bar{3}c$ and are isotypic to $\text{RbFe}(\text{HPO}_4)_2$ (Lii & Wu, 1994) and $\text{RbM}^{3+}(\text{HPO}_4)_2$ ($M = \text{Al}, \text{Ga}$) (Lesage *et al.*, 2007). The asymmetric unit contains two M^+ , two In, one As, one H and four O positions and the structure is characterized by a long c axis in the hexagonal setting (Fig. 3). As in $\text{KIn}(\text{HAsO}_4)_2$, each InO_6 octahedron shares six vertices with six HAsO_4 tetrahedra, resulting in an $\text{InAs}_6\text{O}_{24}$ group. These groups are

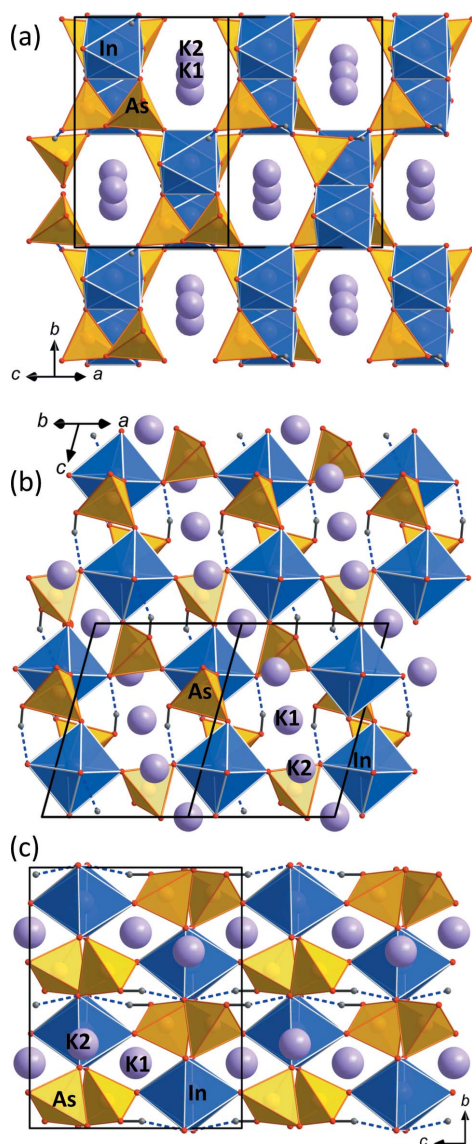


Figure 2
The framework structure of $\text{KIn}(\text{HAsO}_4)_2$ in views parallel to (a) [101], (b) [110] and (c) [100]. The K atoms are located in channels of the framework (note that the K2 position has an occupancy of only 0.024 (2)). Hydrogen bonds (dashed lines) reinforce the framework and extend roughly along c .

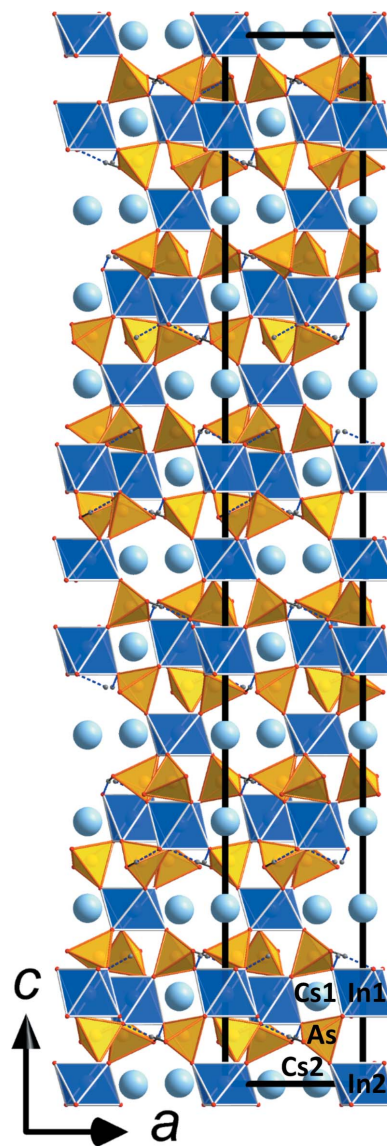


Figure 3
The framework structure of $\text{CsIn}(\text{HAsO}_4)_2$ in a view parallel to b . The unit cell (outlined) is characterized by a long c axis. Cs atoms occupy channels extending parallel to a and b . Hydrogen bonds are shown as dashed lines.

Table 2
Selected bond lengths (Å) for RbIn(HAsO₄).

Rb1A—O3 ⁱ	3.042 (2)	Rb2A—O4 ^{xi}	3.668 (5)
Rb1A—O3 ⁱⁱ	3.042 (2)	Rb2A—O1 ^{xii}	3.830 (3)
Rb1A—O3 ⁱⁱⁱ	3.042 (2)	Rb2A—O1 ^{xiii}	3.830 (3)
Rb1A—O3 ^{iv}	3.042 (2)	Rb2A—O1 ^{xiv}	3.830 (3)
Rb1A—O3 ^v	3.042 (2)	In1—O2 ^{xv}	2.1306 (17)
Rb1A—O3	3.042 (2)	In1—O2 ^v	2.1306 (17)
Rb1A—O2	3.3114 (19)	In1—O2 ^{xvi}	2.1306 (17)
Rb1A—O2 ^{iv}	3.3115 (19)	In1—O4 ^{xvii}	2.1457 (17)
Rb1A—O2 ⁱⁱⁱ	3.3114 (19)	In1—O4 ⁱⁱ	2.1457 (16)
Rb1A—O2 ^v	3.3114 (19)	In1—O4 ^{xii}	2.1457 (16)
Rb1A—O2 ^l	3.3114 (18)	In2—O1 ^{vii}	2.1312 (19)
Rb1A—O2 ⁱⁱ	3.3114 (18)	In2—O1 ^{xviii}	2.131 (2)
Rb2A—O3	3.006 (5)	In2—O1 ^{li}	2.1312 (19)
Rb2A—O3 ⁱⁱ	3.006 (5)	In2—O1 ^{xii}	2.131 (2)
Rb2A—O3 ^v	3.006 (5)	In2—O1 ^{xvii}	2.1312 (19)
Rb2A—O1 ^{vi}	3.462 (3)	In2—O1 ^{xix}	2.1312 (19)
Rb2A—O1 ^{viii}	3.462 (3)	As—O1 ^{xiii}	1.6508 (18)
Rb2A—O1 ^{viii}	3.462 (3)	As—O2	1.6668 (17)
Rb2A—O4 ^{ix}	3.668 (5)	As—O4 ^{iv}	1.6736 (17)
Rb2A—O4 ^x	3.668 (5)	As—O3	1.7409 (19)

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

Table 3
Selected bond lengths (Å) for CsIn(HAsO₄).

Cs1—O3	3.280 (3)	Cs2—O3 ^{xi}	3.698 (3)
Cs1—O3 ⁱ	3.280 (3)	Cs2—O4 ^{xii}	3.703 (2)
Cs1—O3 ⁱⁱ	3.280 (3)	Cs2—O4 ^{xiii}	3.703 (2)
Cs1—O3 ⁱⁱⁱ	3.280 (3)	Cs2—O4 ^{xiv}	3.703 (2)
Cs1—O3 ^{iv}	3.280 (3)	In1—O2 ^{xv}	2.127 (2)
Cs1—O3 ^v	3.280 (3)	In1—O2 ⁱⁱⁱ	2.127 (2)
Cs1—O2	3.434 (2)	In1—O2 ^{xvi}	2.127 (2)
Cs1—O2 ⁱⁱ	3.434 (2)	In1—O4 ^{xvii}	2.150 (2)
Cs1—O2 ^v	3.434 (2)	In1—O4 ^{iv}	2.150 (2)
Cs1—O2 ⁱⁱⁱ	3.434 (2)	In1—O4 ^{xviii}	2.150 (2)
Cs1—O2 ^l	3.434 (2)	In2—O1 ^{vii}	2.133 (2)
Cs1—O2 ^{iv}	3.434 (2)	In2—O1 ^{xi}	2.133 (3)
Cs2—O3 ^{iv}	3.121 (3)	In2—O1 ^{xix}	2.133 (2)
Cs2—O3 ⁱⁱⁱ	3.121 (2)	In2—O1 ^{iv}	2.133 (2)
Cs2—O3	3.121 (3)	In2—O1 ^{xviii}	2.133 (3)
Cs2—O1 ^{vi}	3.419 (3)	In2—O1 ^{xvii}	2.133 (2)
Cs2—O1 ^{vii}	3.419 (3)	As—O1 ^{xx}	1.655 (2)
Cs2—O1 ^{viii}	3.419 (3)	As—O2	1.671 (2)
Cs2—O3 ^{ix}	3.698 (3)	As—O4 ⁱⁱ	1.679 (2)
Cs2—O3 ^x	3.698 (3)	As—O3	1.743 (3)

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) $y + \frac{2}{3}, -x + y + \frac{4}{3}, -z + \frac{4}{3}$; (viii) $x - y - \frac{4}{3}, x - \frac{2}{3}, -z + \frac{4}{3}$; (ix) $-x - \frac{1}{3}, -y - \frac{2}{3}, -z + \frac{4}{3}$; (x) $y + \frac{2}{3}, -x + y + \frac{4}{3}, -z + \frac{4}{3}$; (xi) $x - y - \frac{1}{3}, x + \frac{1}{3}, -z + \frac{4}{3}$; (xii) $x - \frac{1}{3}, x - y - \frac{2}{3}, z - \frac{1}{3}$; (xiii) $-y - \frac{1}{3}, -x + \frac{1}{3}, z - \frac{1}{3}$; (xiv) $-x + y + \frac{2}{3}, y + \frac{1}{3}, z - \frac{1}{3}$; (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) $-x + \frac{2}{3}, -y + \frac{1}{3}, -z + \frac{4}{3}$; (xx) $x - 1, y, z$.

in turn connected *via* three corners to other InO₆ octahedra. The protonated apices of the HAsO₄ tetrahedra form a strong hydrogen bond (O—H...O = 2.62–2.63 Å) to the neighbouring InAs₆O₂₄ group. The InAs₆O₂₄ groups in RbIn(HAsO₄)₂ and CsIn(HAsO₄)₂ are arranged in layers normal to *c*, and the groups within these layers are interconnected by strong hydrogen bonds extending in directions [100] and [110] (Fig. 4*a* and 4*b*). The 12-coordinated Cs atoms are located in channels which extend along *a* and *b*. As in KIn(HAsO₄)₂, the average In—O bond lengths (2.138/2.131 and 2.139/2.133 Å

for In1/In2 in the Rb and Cs compounds, respectively; Tables 2 and 3) are slightly smaller than the literature value (2.141 Å; Baur, 1981), while the average As—O bond lengths (1.683 and 1.687 Å) show good agreement with the literature value (see above). The calculated BVSS (Gagné & Hawthorne, 2015) amount to 1.05 (Rb1), 0.65 (Rb2), 3.02 (In1), 3.07 (In2), 5.07 (As) and 1.94/1.90/1.30/1.82 v.u. (O1–O4) for RbIn(HAsO₄)₂, and 0.92 (Cs1), 0.80 (Cs2), 3.02 (In1), 3.05 (In2), 5.01 (As) and 1.94/1.88/1.29/1.80 v.u. (O1–O4) for CsIn(HAsO₄)₂. These values are reasonably close to ideal valencies, although the fairly low value for Rb2 is noteworthy; apparently the Rb2-hosting cavity is too large for the Rb atom. In fact, both Rb atoms seem to ‘rattle’ somewhat in their cavities and are characterized by rather large anisotropic displacement ellipsoids; therefore, they were modeled by split positions involving an additional, low-occupancy Rb position (Rb1*B*, Rb2*B*) in each case. The severely underbonded O3 atom is donor of

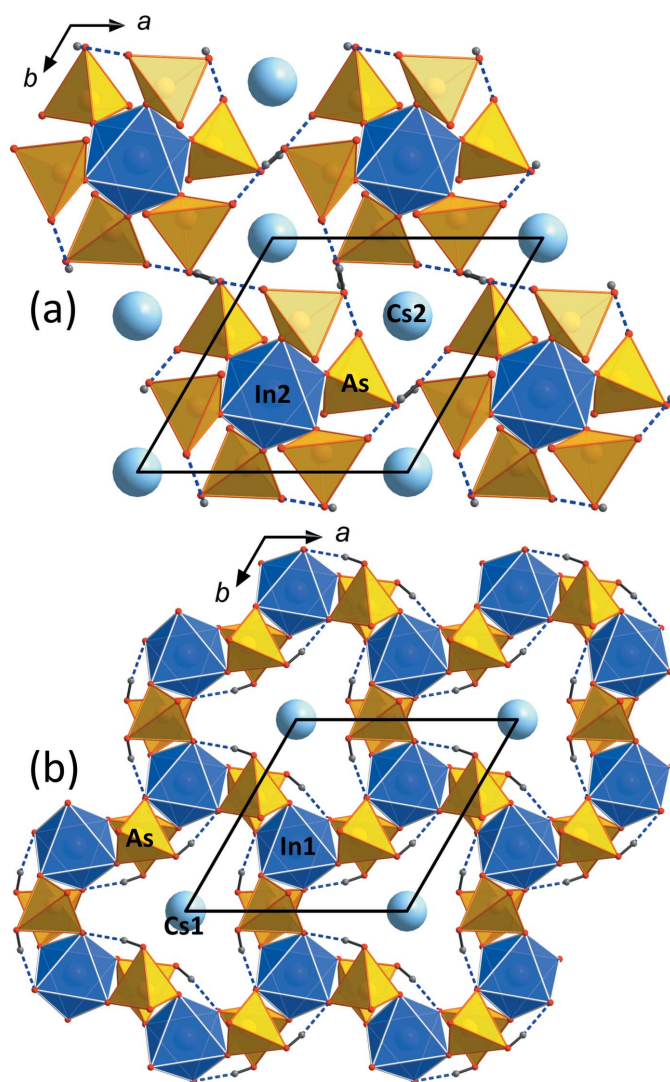


Figure 4
View along *c* of the two different layers involving the two different Cs atoms positions in the framework structure of CsIn(HAsO₄)₂. These layers are stacked along *c* (cf. Fig. 3). Hydrogen bonds are shown as dashed lines.

Table 4
Hydrogen-bond geometry ($\text{\AA}$, $^\circ$) for $\text{KIn}(\text{HAsO}_4)_2$.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O4}-\text{H}\cdots\text{O2}^{\text{xi}}$	0.88 (2)	1.89 (3)	2.690 (3)	151 (4)

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

Table 5
Hydrogen-bond geometry ($\text{\AA}$, $^\circ$) for $\text{RbIn}(\text{HAsO}_4)_2$.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H}\cdots\text{O4}^{\text{xx}}$	0.83 (3)	1.82 (3)	2.634 (2)	168 (4)

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

Table 6
Hydrogen-bond geometry ($\text{\AA}$, $^\circ$) for $\text{CsIn}(\text{HAsO}_4)_2$.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H}\cdots\text{O4}^{\text{xxi}}$	0.83 (3)	1.80 (3)	2.621 (3)	170 (4)

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

the strong hydrogen bonds (Tables 5 and 6). As expected, the unit-cell volume of the isotypic phosphates is about 20% smaller than that of the arsenates. The stronger condensation due to the smaller stronger-bonded phosphate also leads to even stronger hydrogen bonds, with $\text{O}-\text{H}\cdots\text{O}$ distances ranging from 2.58 to 2.59 $\text{\AA}$ (Lii & Wu, 1994; Lesage *et al.*, 2007).

3. Synthesis and crystallization

The compounds were grown by hydrothermal synthesis at 493 K (7–8 d, autogeneous pressure, slow furnace cooling) using Teflon-lined stainless steel autoclaves with an approximate filling volume of 2 cm^3 . Reagent-grade $\text{KOH}/\text{Rb}_2\text{CO}_3/\text{Cs}_2\text{CO}_3$, In_2O_3 , $\alpha\text{-Al}_2\text{O}_3$ (only in the case of the K–In–arsenate) and $\text{H}_3\text{AsO}_4\cdot 0.5\text{H}_2\text{O}$ were used as starting reagents in approximate volume ratios of $M^+ : M^{3+} : \text{As}$ of 1:1:2. In the synthesis of $\text{KIn}(\text{HAsO}_4)_2$, the $\text{In}_2\text{O}_3 : \alpha\text{-Al}_2\text{O}_3$ ratio was 1:1. The vessels were filled with distilled water to about 70% of their inner volumes which led to final pH values of < 1 for all synthesis batches except $\text{KIn}(\text{HAsO}_4)_2$ (initial pH 4.5, final pH 3). The reaction products were washed thoroughly with distilled water, filtered and dried at room temperature. They are stable in air.

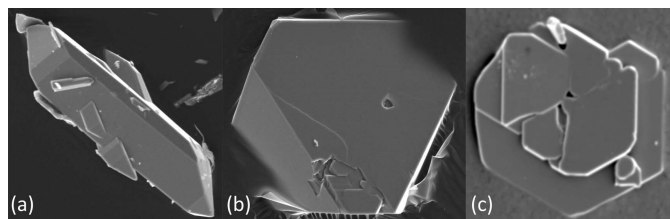


Figure 5
SEM micrographs of hydrothermally synthesized crystals of (a) $\text{KIn}(\text{HAsO}_4)_2$, (b) $\text{RbIn}(\text{HAsO}_4)_2$ and (c) $\text{CsIn}(\text{HAsO}_4)_2$.

$\text{KIn}(\text{HAsO}_4)_2$ formed prismatic-bipyramidal crystals (Fig. 5a) that were accompanied by cubic crystals of synthetic pharmacalumite $[\text{KAl}_4(\text{AsO}_4)_3(\text{OH})_4\cdot 6.5\text{H}_2\text{O}]$. Thus, the Al and In present in the synthesis of these phases seemingly fractionate completely between the two phases $\text{KIn}(\text{HAsO}_4)_2$ and $\text{KAl}_4(\text{AsO}_4)_3(\text{OH})_4\cdot 6.5\text{H}_2\text{O}$. $\text{RbIn}(\text{HAsO}_4)_2$ and $\text{CsIn}(\text{HAsO}_4)_2$ formed pseudo-octahedral crystals and platelets with pseudohexagonal outline (Fig. 5b and 5c, respectively). $\text{RbIn}(\text{HAsO}_4)_2$ was accompanied by crystals of $\text{RbInAs}_2\text{O}_7$ (Schwendtner, 2006), while the X-ray powder diffraction pattern of $\text{CsIn}(\text{HAsO}_4)_2$ showed a few peaks of an unidentified impurity.

Measured X-ray powder diffraction diagrams of $\text{RbIn}(\text{HAsO}_4)_2$ and $\text{CsIn}(\text{HAsO}_4)_2$ were deposited at the International Centre for Diffraction Data under PDF number 56–1371 (Prem *et al.*, 2005a) for $\text{RbIn}(\text{HAsO}_4)_2$ and 56–1372 (Prem *et al.*, 2005b) for $\text{CsIn}(\text{HAsO}_4)_2$.

The chemical composition of the title compounds was checked by standard SEM–EDX analysis of several crystals of each compound; no impurities could be detected.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 7.

For all three refinements, the atomic coordinates of the first description of the respective structure types $[\text{KSc}(\text{HAsO}_4)_2]$ (Schwendtner & Kolitsch, 2004a) and $\text{RbFe}(\text{HPO}_4)_2$ (Lii & Wu, 1994)] were used as initial parameters for better comparison. Hydrogen atoms and additional disordered positions were then located from difference-Fourier maps and added to the respective models.

The two K-atom positions in $\text{KIn}(\text{HAsO}_4)_2$ were restrained to give a total occupancy of one. Freely refined occupancies were 0.989 (4) (K1) and 0.029 (4) (K2), *i.e.* very close to the ideal bulk occupancy of 1.00. Also the anisotropic displacement parameters were restrained to the same values. The $\text{O}-\text{H}$ bond lengths were restrained to 0.90 (4) (K compound) and

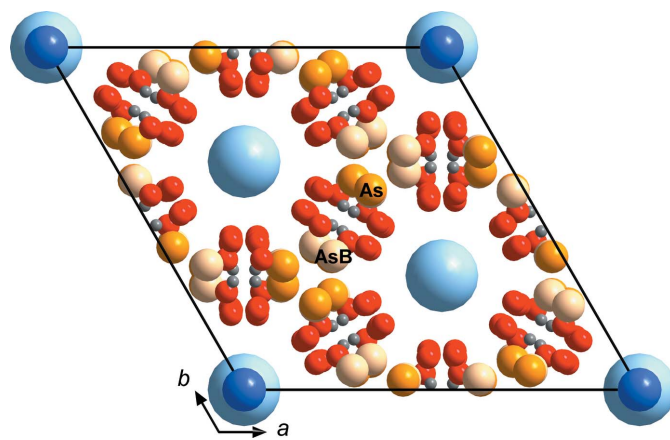


Figure 6
Possible second As position (AsB) in $\text{CsIn}(\text{HAsO}_4)_2$, which could explain the residual electron densities. The AsB position can roughly be generated by a mirror plane in (110). See text for discussion.

Table 7
Experimental details.

	KIn(HAsO ₄) ₂	RbIn(HAsO ₄) ₂	CsIn(HAsO ₄) ₂
Crystal data			
M_r	433.78	480.15	527.59
Crystal system, space group	Monoclinic, $C2/c$	Trigonal, $R\bar{3}c:H$	Trigonal, $R\bar{3}c:H$
Temperature (K)	293	293	293
a, b, c (Å)	8.340 (2), 10.657 (2), 9.197 (2)	8.512 (1), 8.512 (1), 56.434 (11)	8.629 (1), 8.629 (1), 56.986 (11)
α, β, γ (°)	90, 109.37 (3), 90	90, 90, 120	90, 90, 120
V (Å ³)	771.2 (3)	3541.1 (11)	3674.7 (11)
Z	4	18	18
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	12.13	17.50	15.34
Crystal size (mm)	0.19 × 0.02 × 0.02	0.05 × 0.05 × 0.02	0.06 × 0.06 × 0.04
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 (<i>SCALEPACK</i> ; Otwinowski <i>et al.</i> , 2003)	Multi-scan (<i>SCALEPACK</i> ; Otwinowski <i>et al.</i> , 2003)	Multi-scan (<i>SCALEPACK</i> ; Otwinowski <i>et al.</i> , 2003)
$T_{\min}, T_{\max}$	0.207, 0.794	0.475, 0.779	0.460, 0.579
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2743, 1406, 1295	5262, 1443, 1255	4350, 1199, 1039
R_{int}	0.015	0.024	0.019
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.758	0.757	0.704
Refinement			
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.019, 0.046, 1.09	0.018, 0.041, 1.12	0.022, 0.052, 1.07
No. of reflections	1406	1443	1199
No. of parameters	64	69	61
No. of restraints	1	3	1
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined	All H-atom parameters refined
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.18, -1.00	1.00, -0.86	2.09, -0.86

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).

0.90 (2) Å (Rb and Cs compounds). Residual electron-density peaks of 1.02 and 1.03 e Å⁻³ were encountered close to the Rb1 and Rb2 positions. It seems that the Rb atoms, similarly to what was found for isotypic RbAl(HPO₄)₂ (Lesage *et al.*, 2007), have irregular atomic displacement parameters; therefore, two further, low-occupancy Rb positions, Rb1*B* and Rb2*B*, were included in the refinement to model this positional disorder. The occupancies were accordingly restrained to give a total occupancy of 1.00 for Rb1 and Rb2 [$Rb1a = 0.949$ (3), $3 \times Rb1b = 0.0170$ (9), $Rb2a = 0.567$ (3), $3 \times Rb2b = 0.1442$ (9)]. The refined Rb1*A*—R1*B*, Rb1*B*—R1*B'*, Rb2*A*—R2*B'* and Rb2*B*—Rb2*B* distances are 0.44 (3), 0.76 (5), 0.249 (8) and 0.423 (14) Å, respectively. The anisotropic displacement parameters of Rb1*a* and Rb1*b*, as well as Rb2*a* and Rb2*b*, were restrained to give the same value.

The highest residual electron densities are 2.03 e Å⁻³ in CsIn(HAsO₄)₂. They are located about 1.65 Å from As at the same z coordinate value. At first, it seemed sensible that this position is a 'flipped' As position centring an alternative location of the AsO₄ tetrahedron. An unrestrained refinement of this position led to occupancy factors of 0.984 (2) for As and 0.015 (2) for the second position and $R1$ decreased from 2.17 to 1.99%. However, the isotropic displacement parameter of the second position refined to zero, which suggested that this position may be an artifact. The position can be generated by a mirror plane in (110) (Fig. 6). Since application of appropriate twin matrices to the original model did not improve the

refinement and since O ligands for this second possible As position could not be detected, the position was omitted from the model.

The highest residual electron densities of RbIn(HAsO₄)₂ are at or below 1 e Å⁻³ and 1.43 Å from atom O4. The highest residual electron densities of KIn(HAsO₄)₂ are 1.18 e Å⁻³ and close to the As position.

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supporting information

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MIn(HAsO₄)₂ (M = K, Rb, Cs): three new hydrogenarsenates adopting two different structure types

Karolina Schwendtner and Uwe Kolitsch

Computing details

For all 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).

Potassium indium bis[hydrogen arsenate(V)] (KInHAsO₄2)

Crystal data

KIn(HAsO ₄) ₂	$F(000) = 800$
$M_r = 433.78$	$D_x = 3.736 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.340 (2) \text{ \AA}$	Cell parameters from 1474 reflections
$b = 10.657 (2) \text{ \AA}$	$\theta = 3.4\text{--}32.6^\circ$
$c = 9.197 (2) \text{ \AA}$	$\mu = 12.13 \text{ mm}^{-1}$
$\beta = 109.37 (3)^\circ$	$T = 293 \text{ K}$
$V = 771.2 (3) \text{ \AA}^3$	Small prisms, colourless
$Z = 4$	$0.19 \times 0.02 \times 0.02 \text{ mm}$

Data collection

Nonius KappaCCD single-crystal four-circle diffractometer	1406 independent reflections
Radiation source: fine-focus sealed tube	1295 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.015$
Absorption correction: multi-scan (SCALEPACK; Otwinowski <i>et al.</i> , 2003)	$\theta_{\text{max}} = 32.6^\circ$, $\theta_{\text{min}} = 3.4^\circ$
$T_{\text{min}} = 0.207$, $T_{\text{max}} = 0.794$	$h = -12 \rightarrow 12$
2743 measured reflections	$k = -16 \rightarrow 16$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.019$	All H-atom parameters refined
$wR(F^2) = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 1.2908P]$
$S = 1.09$	where $P = (F_o^2 + 2F_c^2)/3$
1406 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
64 parameters	$\Delta\rho_{\text{max}} = 1.18 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -1.00 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Extinction correction: SHELXL2016
 (Sheldrick, 2015),
 $F_c^* = k F_c [1 + 0.001 x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00181 (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 ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
K1	0.250000	0.250000	0.000000	0.0437 (3)	0.976 (2)
K2	0.000000	0.678 (5)	0.250000	0.0437 (3)	0.024 (2)
In	0.000000	0.13427 (2)	0.250000	0.00852 (7)	
As	0.27607 (3)	0.39725 (2)	0.36013 (2)	0.00952 (7)	
O1	0.1914 (2)	0.26806 (16)	0.26523 (19)	0.0186 (3)	
O2	0.3114 (2)	0.49181 (17)	0.22827 (18)	0.0177 (3)	
O3	0.4522 (2)	0.36289 (15)	0.50672 (18)	0.0139 (3)	
O4	0.1329 (2)	0.4729 (2)	0.4285 (2)	0.0254 (4)	
H	0.159 (6)	0.473 (5)	0.529 (2)	0.076 (16)*	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0550 (7)	0.0588 (7)	0.0301 (5)	−0.0355 (6)	0.0312 (5)	−0.0195 (5)
K2	0.0550 (7)	0.0588 (7)	0.0301 (5)	−0.0355 (6)	0.0312 (5)	−0.0195 (5)
In	0.00910 (10)	0.00802 (11)	0.00799 (10)	0.000	0.00224 (7)	0.000
As	0.01099 (11)	0.00995 (12)	0.00731 (10)	−0.00206 (7)	0.00262 (8)	−0.00008 (7)
O1	0.0243 (9)	0.0157 (8)	0.0181 (8)	−0.0108 (7)	0.0103 (7)	−0.0055 (6)
O2	0.0199 (8)	0.0178 (8)	0.0114 (7)	−0.0096 (6)	−0.0003 (6)	0.0062 (6)
O3	0.0138 (7)	0.0176 (8)	0.0087 (7)	0.0024 (6)	0.0015 (6)	−0.0005 (5)
O4	0.0192 (9)	0.0402 (12)	0.0152 (8)	0.0122 (8)	0.0035 (7)	−0.0053 (8)

Geometric parameters ($\text{\AA}$, $^\circ$)

K1—O1 ⁱ	2.6488 (17)	K2—O3 ^{ix}	3.20 (3)
K1—O1	2.6488 (17)	K2—O2	3.33 (3)
K1—K2 ⁱⁱ	2.653 (15)	K2—O2 ^{viii}	3.33 (3)
K1—K2 ⁱⁱⁱ	2.653 (15)	K2—As ^{ix}	3.35 (4)
K1—O3 ^{iv}	2.7788 (17)	K2—As ^x	3.35 (4)
K1—O3 ^v	2.7788 (17)	In—O1	2.1104 (17)
K1—O4 ^{vi}	3.112 (2)	In—O1 ^{viii}	2.1104 (17)
K1—O4 ^{vii}	3.112 (2)	In—O3 ^{iv}	2.1388 (16)
K1—O2	3.2553 (19)	In—O3 ^{xi}	2.1388 (16)
K1—O2 ⁱ	3.2553 (19)	In—O2 ^{xii}	2.1473 (16)
K1—As	3.6059 (7)	In—O2 ^{vii}	2.1473 (16)

K1—As ⁱ	3.6059 (7)	As—O1	1.6574 (17)
K2—O4	2.74 (4)	As—O3	1.6721 (17)
K2—O4 ^{viii}	2.74 (4)	As—O2	1.6762 (16)
K2—O1 ^{ix}	2.792 (18)	As—O4	1.7231 (19)
K2—O1 ^x	2.792 (18)	O4—H	0.876 (19)
K2—O3 ^x	3.20 (3)		
O1 ⁱ —K1—O1	180.0	K1 ^{ix} —K2—As ^{ix}	72.8 (8)
O1 ⁱ —K1—K2 ⁱⁱ	63.6 (3)	K1 ^x —K2—As ^{ix}	83.9 (10)
O1—K1—K2 ⁱⁱ	116.4 (3)	O4—K2—As ^{ix}	125.63 (13)
O1 ⁱ —K1—K2 ⁱⁱⁱ	116.4 (3)	O4 ^{viii} —K2—As ^{ix}	122.06 (11)
O1—K1—K2 ⁱⁱⁱ	63.6 (3)	O1 ^{ix} —K2—As ^{ix}	29.6 (4)
K2 ⁱⁱ —K1—K2 ⁱⁱⁱ	180 (2)	O1 ^x —K2—As ^{ix}	113.1 (16)
O1 ⁱ —K1—O3 ^{iv}	115.35 (5)	O3 ^x —K2—As ^{ix}	90.8 (12)
O1—K1—O3 ^{iv}	64.65 (5)	O3 ^{ix} —K2—As ^{ix}	29.5 (3)
K2 ⁱⁱ —K1—O3 ^{iv}	72.1 (6)	O2—K2—As ^{ix}	82.73 (9)
K2 ⁱⁱⁱ —K1—O3 ^{iv}	107.9 (6)	O2 ^{viii} —K2—As ^{ix}	163.5 (6)
O1 ⁱ —K1—O3 ^v	64.65 (5)	K1 ^{ix} —K2—As ^x	83.9 (10)
O1—K1—O3 ^v	115.35 (5)	K1 ^x —K2—As ^x	72.8 (8)
K2 ⁱⁱ —K1—O3 ^v	107.9 (6)	O4—K2—As ^x	122.06 (11)
K2 ⁱⁱⁱ —K1—O3 ^v	72.1 (6)	O4 ^{viii} —K2—As ^x	125.63 (13)
O3 ^{iv} —K1—O3 ^v	180.00 (6)	O1 ^{ix} —K2—As ^x	113.1 (16)
O1 ⁱ —K1—O4 ^{vi}	90.87 (5)	O1 ^x —K2—As ^x	29.6 (4)
O1—K1—O4 ^{vi}	89.13 (5)	O3 ^x —K2—As ^x	29.5 (3)
K2 ⁱⁱ —K1—O4 ^{vi}	56.1 (11)	O3 ^{ix} —K2—As ^x	90.8 (12)
K2 ⁱⁱⁱ —K1—O4 ^{vi}	123.9 (11)	O2—K2—As ^x	163.5 (6)
O3 ^{iv} —K1—O4 ^{vi}	101.27 (5)	O2 ^{viii} —K2—As ^x	82.73 (9)
O3 ^v —K1—O4 ^{vi}	78.73 (5)	As ^{ix} —K2—As ^x	91.7 (13)
O1 ⁱ —K1—O4 ^{vii}	89.13 (5)	O1—In—O1 ^{viii}	94.99 (10)
O1—K1—O4 ^{vii}	90.87 (5)	O1—In—O3 ^{iv}	86.23 (7)
K2 ⁱⁱ —K1—O4 ^{vii}	123.9 (11)	O1 ^{viii} —In—O3 ^{iv}	92.67 (7)
K2 ⁱⁱⁱ —K1—O4 ^{vii}	56.1 (11)	O1—In—O3 ^{xi}	92.67 (7)
O3 ^{iv} —K1—O4 ^{vii}	78.73 (5)	O1 ^{viii} —In—O3 ^{xi}	86.23 (7)
O3 ^v —K1—O4 ^{vii}	101.27 (5)	O3 ^{iv} —In—O3 ^{xi}	178.38 (9)
O4 ^{vi} —K1—O4 ^{vii}	180.0	O1—In—O2 ^{xii}	177.02 (7)
O1 ⁱ —K1—O2	127.87 (5)	O1 ^{viii} —In—O2 ^{xii}	87.52 (7)
O1—K1—O2	52.13 (5)	O3 ^{iv} —In—O2 ^{xii}	92.07 (6)
K2 ⁱⁱ —K1—O2	104.0 (10)	O3 ^{xi} —In—O2 ^{xii}	89.08 (7)
K2 ⁱⁱⁱ —K1—O2	76.0 (10)	O1—In—O2 ^{vii}	87.52 (7)
O3 ^{iv} —K1—O2	106.19 (5)	O1 ^{viii} —In—O2 ^{vii}	177.02 (7)
O3 ^v —K1—O2	73.81 (5)	O3 ^{iv} —In—O2 ^{vii}	89.08 (7)
O4 ^{vi} —K1—O2	49.92 (5)	O3 ^{xi} —In—O2 ^{vii}	92.07 (6)
O4 ^{vii} —K1—O2	130.08 (5)	O2 ^{xii} —In—O2 ^{vii}	90.01 (10)
O1 ⁱ —K1—O2 ⁱ	52.13 (5)	O1—In—K1 ^{viii}	107.25 (5)
O1—K1—O2 ⁱ	127.87 (5)	O1 ^{viii} —In—K1 ^{viii}	42.55 (5)
K2 ⁱⁱ —K1—O2 ⁱ	76.0 (10)	O3 ^{iv} —In—K1 ^{viii}	132.97 (5)
K2 ⁱⁱⁱ —K1—O2 ⁱ	104.0 (10)	O3 ^{xi} —In—K1 ^{viii}	46.31 (5)
O3 ^{iv} —K1—O2 ⁱ	73.80 (5)	O2 ^{xii} —In—K1 ^{viii}	75.69 (5)

O3 ^v —K1—O2 ⁱ	106.20 (5)	O2 ^{vii} —In—K1 ^{viii}	135.06 (5)
O4 ^{vi} —K1—O2 ⁱ	130.08 (5)	O1—In—K1	42.55 (5)
O4 ^{vii} —K1—O2 ⁱ	49.92 (5)	O1 ^{viii} —In—K1	107.25 (5)
O2—K1—O2 ⁱ	180.0	O3 ^{iv} —In—K1	46.31 (5)
O1 ⁱ —K1—As	154.71 (4)	O3 ^{xi} —In—K1	132.97 (5)
O1—K1—As	25.29 (4)	O2 ^{xii} —In—K1	135.06 (5)
K2 ⁱⁱ —K1—As	117.5 (7)	O2 ^{vii} —In—K1	75.69 (5)
K2 ⁱⁱⁱ —K1—As	62.5 (7)	K1 ^{viii} —In—K1	141.977 (12)
O3 ^{iv} —K1—As	87.14 (4)	O1—In—K2 ⁱⁱⁱ	36.3 (7)
O3 ^v —K1—As	92.86 (4)	O1 ^{viii} —In—K2 ⁱⁱⁱ	130.9 (7)
O4 ^{vi} —K1—As	72.55 (4)	O3 ^{iv} —In—K2 ⁱⁱⁱ	80.73 (5)
O4 ^{vii} —K1—As	107.45 (4)	O3 ^{xi} —In—K2 ⁱⁱⁱ	99.09 (6)
O2—K1—As	27.68 (3)	O2 ^{xii} —In—K2 ⁱⁱⁱ	140.9 (7)
O2 ⁱ —K1—As	152.32 (3)	O2 ^{vii} —In—K2 ⁱⁱⁱ	51.8 (7)
O1 ⁱ —K1—As ⁱ	25.29 (4)	K1 ^{viii} —In—K2 ⁱⁱⁱ	135.3 (4)
O1—K1—As ⁱ	154.71 (4)	K1—In—K2 ⁱⁱⁱ	38.4 (3)
K2 ⁱⁱ —K1—As ⁱ	62.5 (7)	O1—In—K2 ^{xii}	130.9 (7)
K2 ⁱⁱⁱ —K1—As ⁱ	117.5 (7)	O1 ^{viii} —In—K2 ^{xii}	36.3 (7)
O3 ^{iv} —K1—As ⁱ	92.86 (4)	O3 ^{iv} —In—K2 ^{xii}	99.09 (6)
O3 ^v —K1—As ⁱ	87.14 (4)	O3 ^{xi} —In—K2 ^{xii}	80.73 (5)
O4 ^{vi} —K1—As ⁱ	107.45 (4)	O2 ^{xii} —In—K2 ^{xii}	51.8 (7)
O4 ^{vii} —K1—As ⁱ	72.55 (4)	O2 ^{vii} —In—K2 ^{xii}	140.9 (7)
O2—K1—As ⁱ	152.32 (3)	K1 ^{viii} —In—K2 ^{xii}	38.4 (3)
O2 ⁱ —K1—As ⁱ	27.68 (3)	K1—In—K2 ^{xii}	135.3 (4)
As—K1—As ⁱ	180.0	K2 ⁱⁱⁱ —In—K2 ^{xii}	167.1 (14)
K1 ^{ix} —K2—K1 ^x	147 (2)	O1—As—O3	110.45 (9)
K1 ^{ix} —K2—O4	70.4 (4)	O1—As—O2	105.35 (8)
K1 ^x —K2—O4	142.6 (17)	O3—As—O2	113.38 (8)
K1 ^{ix} —K2—O4 ^{viii}	142.6 (17)	O1—As—O4	110.80 (10)
K1 ^x —K2—O4 ^{viii}	70.4 (4)	O3—As—O4	109.76 (8)
O4—K2—O4 ^{viii}	73.9 (13)	O2—As—O4	106.99 (10)
K1 ^{ix} —K2—O1 ^{ix}	58.2 (4)	O1—As—K2 ⁱⁱⁱ	56.3 (5)
K1 ^x —K2—O1 ^{ix}	109.3 (10)	O3—As—K2 ⁱⁱⁱ	70.26 (6)
O4—K2—O1 ^{ix}	96.2 (5)	O2—As—K2 ⁱⁱⁱ	87.2 (6)
O4 ^{viii} —K2—O1 ^{ix}	116.1 (8)	O4—As—K2 ⁱⁱⁱ	163.7 (7)
K1 ^{ix} —K2—O1 ^x	109.3 (10)	O1—As—K1	43.06 (6)
K1 ^x —K2—O1 ^x	58.2 (4)	O3—As—K1	114.49 (6)
O4—K2—O1 ^x	116.1 (8)	O2—As—K1	64.44 (6)
O4 ^{viii} —K2—O1 ^x	96.2 (5)	O4—As—K1	134.49 (6)
O1 ^{ix} —K2—O1 ^x	140 (2)	K2 ⁱⁱⁱ —As—K1	44.66 (8)
K1 ^{ix} —K2—O3 ^x	55.8 (6)	O1—As—K2	114.2 (5)
K1 ^x —K2—O3 ^x	102.0 (12)	O3—As—K2	134.2 (4)
O4—K2—O3 ^x	100.01 (14)	O2—As—K2	63.8 (2)
O4 ^{viii} —K2—O3 ^x	144.0 (5)	O4—As—K2	43.88 (15)
O1 ^{ix} —K2—O3 ^x	99.8 (12)	K2 ⁱⁱⁱ —As—K2	146.9 (3)
O1 ^x —K2—O3 ^x	53.8 (5)	K1—As—K2	104.94 (19)
K1 ^{ix} —K2—O3 ^{ix}	102.0 (12)	As—O1—In	140.97 (10)
K1 ^x —K2—O3 ^{ix}	55.8 (6)	As—O1—K1	111.65 (8)

O4—K2—O3 ^{ix}	144.0 (5)	In—O1—K1	104.85 (7)
O4 ^{viii} —K2—O3 ^{ix}	100.01 (14)	As—O1—K2 ⁱⁱⁱ	94.1 (9)
O1 ^{ix} —K2—O3 ^{ix}	53.8 (5)	In—O1—K2 ⁱⁱⁱ	117.1 (10)
O1 ^x —K2—O3 ^{ix}	99.8 (12)	K1—O1—K2 ⁱⁱⁱ	58.29 (14)
O3 ^x —K2—O3 ^{ix}	104.1 (15)	As—O2—In ^{xiii}	131.05 (9)
K1 ^{ix} —K2—O2	79.6 (4)	As—O2—K1	87.88 (7)
K1 ^x —K2—O2	121.6 (6)	In ^{xiii} —O2—K1	124.98 (7)
O4—K2—O2	52.4 (7)	As—O2—K2	89.3 (6)
O4 ^{viii} —K2—O2	69.8 (10)	In ^{xiii} —O2—K2	97.7 (7)
O1 ^{ix} —K2—O2	56.7 (3)	K1—O2—K2	123.5 (5)
O1 ^x —K2—O2	163.3 (17)	As—O3—In ^{xi}	130.50 (9)
O3 ^x —K2—O2	134.62 (5)	As—O3—K1 ^v	129.02 (8)
O3 ^{ix} —K2—O2	91.84 (5)	In ^{xi} —O3—K1 ^v	99.88 (6)
K1 ^{ix} —K2—O2 ^{viii}	121.6 (6)	As—O3—K2 ⁱⁱⁱ	80.2 (3)
K1 ^x —K2—O2 ^{viii}	79.6 (4)	In ^{xi} —O3—K2 ⁱⁱⁱ	139.1 (7)
O4—K2—O2 ^{viii}	69.8 (10)	K1 ^v —O3—K2 ⁱⁱⁱ	52.13 (8)
O4 ^{viii} —K2—O2 ^{viii}	52.4 (7)	As—O4—K2	110.3 (2)
O1 ^{ix} —K2—O2 ^{viii}	163.3 (17)	As—O4—K1 ^{ix}	108.30 (10)
O1 ^x —K2—O2 ^{viii}	56.7 (3)	K2—O4—K1 ^{ix}	53.4 (7)
O3 ^x —K2—O2 ^{viii}	91.84 (5)	As—O4—H	115 (3)
O3 ^{ix} —K2—O2 ^{viii}	134.62 (5)	K2—O4—H	123 (3)
O2—K2—O2 ^{viii}	106.6 (15)	K1 ^{ix} —O4—H	80 (3)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H $\cdots$ O2 ^{xiv}	0.88 (2)	1.89 (3)	2.690 (3)	151 (4)

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

Rubidium indium bis[hydrogen arsenate(V)] (RbInHAsO₄2)

Crystal data

RbIn(HAsO₄)₂
 $M_r = 480.15$
 Trigonal, $R\bar{3}c:H$
 $a = 8.512$ (1) $\text{\AA}$
 $c = 56.434$ (11) $\text{\AA}$
 $V = 3541.1$ (11) $\text{\AA}^3$
 $Z = 18$
 $F(000) = 3924$

$D_x = 4.053$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ $\text{\AA}$
 Cell parameters from 2882 reflections
 $\theta = 2.9\text{--}32.6^\circ$
 $\mu = 17.50$ mm⁻¹
 $T = 293$ K
 Small hexagonal platelets, colourless
 $0.05 \times 0.05 \times 0.02$ 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)
 $T_{\min} = 0.475, T_{\max} = 0.779$
 5262 measured reflections
 1443 independent reflections

1255 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.024$ $\theta_{\text{max}} = 32.6^\circ$, $\theta_{\text{min}} = 2.9^\circ$ $h = -12 \rightarrow 12$ $k = -10 \rightarrow 10$ $l = -85 \rightarrow 85$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.018$ $wR(F^2) = 0.041$ $S = 1.12$

1443 reflections

69 parameters

3 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

All H-atom parameters refined

 $w = 1/[\sigma^2(F_o^2) + (0.014P)^2 + 16.3085P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.006$ $\Delta\rho_{\text{max}} = 1.00 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.86 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL2016

(Sheldrick, 2015),

 $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.000313 (12)

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Rb1A	0.000000	0.000000	0.750000	0.0236 (2)	0.949 (3)
Rb1B	0.000000	−0.051 (4)	0.750000	0.0236 (2)	0.0170 (9)
Rb2A	0.000000	0.000000	0.66882 (10)	0.0423 (6)	0.567 (3)
Rb2B	−0.0304 (11)	−0.0266 (11)	0.66795 (15)	0.0423 (6)	0.1442 (9)
In1	0.333333	0.666667	0.75297 (2)	0.01028 (7)	
In2	0.333333	0.666667	0.666667	0.01217 (8)	
As	−0.39741 (3)	−0.36940 (3)	0.71279 (2)	0.01097 (7)	
O1	0.5235 (3)	−0.3776 (3)	0.68584 (3)	0.0298 (5)	
O2	−0.4271 (2)	−0.2389 (2)	0.73221 (3)	0.0171 (3)	
O3	−0.1635 (2)	−0.2654 (3)	0.70899 (3)	0.0201 (4)	
O4	0.4679 (2)	−0.1119 (2)	0.77738 (3)	0.0155 (3)	
H	−0.131 (6)	−0.339 (5)	0.7128 (7)	0.051 (13)*	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1A	0.0267 (3)	0.0267 (3)	0.0175 (3)	0.01335 (15)	0.000	0.000
Rb1B	0.0267 (3)	0.0267 (3)	0.0175 (3)	0.01335 (15)	0.000	0.000
Rb2A	0.0509 (8)	0.0509 (8)	0.0250 (4)	0.0254 (4)	0.000	0.000
Rb2B	0.0509 (8)	0.0509 (8)	0.0250 (4)	0.0254 (4)	0.000	0.000
In1	0.01052 (8)	0.01052 (8)	0.00981 (12)	0.00526 (4)	0.000	0.000
In2	0.01472 (11)	0.01472 (11)	0.00707 (16)	0.00736 (6)	0.000	0.000
As	0.01290 (11)	0.01207 (11)	0.01030 (10)	0.00802 (9)	0.00056 (8)	0.00086 (8)
O1	0.0399 (12)	0.0513 (14)	0.0129 (8)	0.0337 (12)	−0.0062 (8)	−0.0002 (8)

O2	0.0170 (8)	0.0122 (8)	0.0203 (8)	0.0060 (7)	0.0076 (7)	−0.0012 (6)
O3	0.0145 (8)	0.0163 (9)	0.0308 (10)	0.0087 (7)	0.0061 (7)	0.0072 (7)
O4	0.0137 (8)	0.0133 (8)	0.0217 (8)	0.0084 (6)	−0.0038 (6)	−0.0056 (6)

Geometric parameters (Å, °)

Rb1A—Rb1B ⁱ	0.44 (3)	Rb2A—O1 ^{vi}	3.462 (3)
Rb1A—Rb1B ⁱⁱ	0.44 (3)	Rb2A—O1 ^{vii}	3.462 (3)
Rb1A—O3 ⁱⁱⁱ	3.042 (2)	Rb2A—O1 ^{viii}	3.462 (3)
Rb1A—O3 ⁱ	3.042 (2)	Rb2A—O4 ^{ix}	3.668 (5)
Rb1A—O3 ^{iv}	3.042 (2)	Rb2A—O4 ^x	3.668 (5)
Rb1A—O3 ^v	3.042 (2)	Rb2A—O4 ^{xi}	3.668 (5)
Rb1A—O3 ⁱⁱ	3.042 (2)	Rb2A—O1 ^{xii}	3.830 (3)
Rb1A—O3	3.042 (2)	Rb2A—O1 ^{xiii}	3.830 (3)
Rb1A—O2	3.3114 (19)	Rb2A—O1 ^{xiv}	3.830 (3)
Rb1A—O2 ^v	3.3115 (19)	Rb2A—O3 ^{xv}	3.888 (4)
Rb1A—O2 ^{iv}	3.3114 (19)	Rb2B—Rb2B ⁱ	0.423 (14)
Rb1A—O2 ⁱⁱ	3.3114 (19)	Rb2B—Rb2B ⁱⁱ	0.423 (14)
Rb1A—O2 ⁱⁱⁱ	3.3114 (18)	Rb2B—O3	2.911 (9)
Rb1A—O2 ⁱ	3.3114 (18)	Rb2B—O3 ⁱⁱ	3.056 (9)
Rb1A—As ⁱⁱⁱ	3.8862 (5)	Rb2B—O3 ⁱ	3.185 (8)
Rb1A—H	3.28 (4)	Rb2B—O1 ^{viii}	3.259 (8)
Rb1A—H ⁱ	3.28 (4)	Rb2B—O1 ^{vi}	3.436 (9)
Rb1A—H ⁱⁱ	3.28 (4)	Rb2B—O4 ^x	3.525 (8)
Rb1A—H ^{iv}	3.28 (4)	Rb2B—O1 ^{xiii}	3.608 (9)
Rb1A—H ⁱⁱⁱ	3.28 (4)	Rb2B—As ^{xvi}	3.781 (8)
Rb1A—H ^v	3.28 (4)	Rb2B—As ^{xv}	3.869 (8)
Rb1B—Rb1B ⁱ	0.76 (6)	Rb2B—As	3.945 (9)
Rb1B—Rb1B ⁱⁱ	0.76 (5)	In1—O2 ^{xvii}	2.1306 (17)
Rb1B—O3 ^v	2.842 (12)	In1—O2 ⁱⁱ	2.1306 (17)
Rb1B—O3	2.842 (12)	In1—O2 ^{xviii}	2.1306 (17)
Rb1B—O2 ^{iv}	2.98 (2)	In1—O4 ^{xix}	2.1457 (17)
Rb1B—O2 ⁱ	2.98 (2)	In1—O4 ⁱ	2.1457 (16)
Rb1B—O3 ^{iv}	3.035 (3)	In1—O4 ^{xii}	2.1457 (16)
Rb1B—O3 ⁱ	3.035 (3)	In2—O1 ^{vii}	2.1312 (19)
Rb1B—O2	3.312 (3)	In2—O1 ^{xvi}	2.131 (2)
Rb1B—O2 ^v	3.312 (3)	In2—O1 ⁱ	2.1312 (19)
Rb1B—O3 ⁱⁱⁱ	3.32 (2)	In2—O1 ^{xii}	2.131 (2)
Rb1B—O3 ⁱⁱ	3.32 (2)	In2—O1 ^{xix}	2.1312 (19)
Rb1B—H	2.99 (4)	In2—O1 ^{xx}	2.1312 (19)
Rb1B—H ^v	2.99 (4)	As—O1 ^{xiii}	1.6508 (18)
Rb2A—Rb2B ⁱⁱ	0.249 (8)	As—O2	1.6668 (17)
Rb2A—Rb2B ⁱ	0.249 (8)	As—O4 ^v	1.6736 (17)
Rb2A—O3	3.006 (5)	As—O3	1.7409 (19)
Rb2A—O3 ⁱ	3.006 (5)	O3—H	0.83 (3)
Rb2A—O3 ⁱⁱ	3.006 (5)		
Rb1B ⁱ —Rb1A—Rb1B ⁱⁱ	120.00 (12)	O3—Rb2A—O1 ^{xiv}	76.69 (8)

Rb1B ⁱ —Rb1A—O3 ⁱⁱⁱ	59.08 (4)	O3 ⁱ —Rb2A—O1 ^{xiv}	44.11 (5)
Rb1B ⁱⁱ —Rb1A—O3 ⁱⁱⁱ	85.05 (9)	O3 ⁱⁱ —Rb2A—O1 ^{xiv}	112.37 (15)
Rb1B ⁱ —Rb1A—O3 ⁱ	59.08 (4)	O1 ^{vi} —Rb2A—O1 ^{xiv}	45.46 (6)
Rb1B ⁱⁱ —Rb1A—O3 ⁱ	126.88 (5)	O1 ^{vii} —Rb2A—O1 ^{xiv}	95.29 (5)
O3 ⁱⁱⁱ —Rb1A—O3 ⁱ	118.16 (8)	O1 ^{viii} —Rb2A—O1 ^{xiv}	150.55 (6)
Rb1B ⁱ —Rb1A—O3 ^{iv}	126.88 (4)	O4 ^{ix} —Rb2A—O1 ^{xiv}	78.40 (6)
Rb1B ⁱⁱ —Rb1A—O3 ^{iv}	59.08 (7)	O4 ^x —Rb2A—O1 ^{xiv}	120.81 (10)
O3 ⁱⁱⁱ —Rb1A—O3 ^{iv}	68.39 (6)	O4 ^{xi} —Rb2A—O1 ^{xiv}	111.19 (9)
O3 ⁱ —Rb1A—O3 ^{iv}	170.10 (7)	O1 ^{xii} —Rb2A—O1 ^{xiv}	113.93 (7)
Rb1B ⁱ —Rb1A—O3 ^v	85.05 (4)	O1 ^{xiii} —Rb2A—O1 ^{xiv}	113.93 (7)
Rb1B ⁱⁱ —Rb1A—O3 ^v	126.88 (5)	Rb2B ⁱⁱ —Rb2A—O3 ^{xv}	126 (3)
O3 ⁱⁱⁱ —Rb1A—O3 ^v	68.39 (6)	Rb2B ⁱ —Rb2A—O3 ^{xv}	74 (3)
O3 ⁱ —Rb1A—O3 ^v	106.24 (7)	O3—Rb2A—O3 ^{xv}	89.86 (5)
O3 ^{iv} —Rb1A—O3 ^v	68.39 (6)	O3 ⁱ —Rb2A—O3 ^{xv}	129.48 (6)
Rb1B ⁱ —Rb1A—O3 ⁱⁱ	85.05 (4)	O3 ⁱⁱ —Rb2A—O3 ^{xv}	145.79 (7)
Rb1B ⁱⁱ —Rb1A—O3 ⁱⁱ	59.08 (7)	O1 ^{vi} —Rb2A—O3 ^{xv}	42.24 (6)
O3 ⁱⁱⁱ —Rb1A—O3 ⁱⁱ	106.24 (7)	O1 ^{vii} —Rb2A—O3 ^{xv}	117.63 (15)
O3 ⁱ —Rb1A—O3 ⁱⁱ	68.39 (6)	O1 ^{viii} —Rb2A—O3 ^{xv}	66.65 (8)
O3 ^{iv} —Rb1A—O3 ⁱⁱ	118.16 (7)	O4 ^{ix} —Rb2A—O3 ^{xv}	42.47 (6)
O3 ^v —Rb1A—O3 ⁱⁱ	170.10 (8)	O4 ^x —Rb2A—O3 ^{xv}	40.66 (6)
Rb1B ⁱ —Rb1A—O3	126.88 (4)	O4 ^{xi} —Rb2A—O3 ^{xv}	76.43 (11)
Rb1B ⁱⁱ —Rb1A—O3	85.05 (9)	O1 ^{xii} —Rb2A—O3 ^{xv}	151.71 (14)
O3 ⁱⁱⁱ —Rb1A—O3	170.10 (7)	O1 ^{xiii} —Rb2A—O3 ^{xv}	69.64 (5)
O3 ⁱ —Rb1A—O3	68.38 (6)	O1 ^{xiv} —Rb2A—O3 ^{xv}	87.30 (5)
O3 ^{iv} —Rb1A—O3	106.24 (7)	Rb2B ⁱ —Rb2B—Rb2B ⁱⁱ	60.00 (6)
O3 ^v —Rb1A—O3	118.16 (7)	Rb2B ⁱ —Rb2B—O3	106.1 (12)
O3 ⁱⁱ —Rb1A—O3	68.38 (6)	Rb2B ⁱⁱ —Rb2B—O3	127.22 (14)
Rb1B ⁱ —Rb1A—O2	148.87 (3)	Rb2B ⁱ —Rb2B—O3 ⁱⁱ	104.1 (12)
Rb1B ⁱⁱ —Rb1A—O2	37.75 (11)	Rb2B ⁱⁱ —Rb2B—O3 ⁱⁱ	66.3 (12)
O3 ⁱⁱⁱ —Rb1A—O2	120.30 (5)	O3—Rb2B—O3 ⁱⁱ	69.9 (2)
O3 ⁱ —Rb1A—O2	112.03 (5)	Rb2B ⁱ —Rb2B—O3 ⁱ	46.66 (16)
O3 ^{iv} —Rb1A—O2	67.27 (5)	Rb2B ⁱⁱ —Rb2B—O3 ⁱ	68.5 (12)
O3 ^v —Rb1A—O2	125.02 (5)	O3—Rb2B—O3 ⁱ	68.05 (19)
O3 ⁱⁱ —Rb1A—O2	64.77 (5)	O3 ⁱⁱ —Rb2B—O3 ⁱ	66.39 (17)
O3—Rb1A—O2	50.13 (4)	Rb2B ⁱ —Rb2B—O1 ^{viii}	158.2 (7)
Rb1B ⁱ —Rb1A—O2 ^v	37.75 (3)	Rb2B ⁱⁱ —Rb2B—O1 ^{viii}	111 (2)
Rb1B ⁱⁱ —Rb1A—O2 ^v	148.87 (10)	O3—Rb2B—O1 ^{viii}	94.9 (2)
O3 ⁱⁱⁱ —Rb1A—O2 ^v	64.77 (5)	O3 ⁱⁱ —Rb2B—O1 ^{viii}	88.5 (2)
O3 ⁱ —Rb1A—O2 ^v	67.27 (5)	O3 ⁱ —Rb2B—O1 ^{viii}	153.0 (3)
O3 ^{iv} —Rb1A—O2 ^v	112.03 (5)	Rb2B ⁱ —Rb2B—O1 ^{vi}	62.0 (19)
O3 ^v —Rb1A—O2 ^v	50.13 (5)	Rb2B ⁱⁱ —Rb2B—O1 ^{vi}	118.2 (19)
O3 ⁱⁱ —Rb1A—O2 ^v	120.30 (5)	O3—Rb2B—O1 ^{vi}	87.5 (2)
O3—Rb1A—O2 ^v	125.02 (5)	O3 ⁱⁱ —Rb2B—O1 ^{vi}	149.7 (3)
O2—Rb1A—O2 ^v	172.51 (6)	O3 ⁱ —Rb2B—O1 ^{vi}	86.8 (2)
Rb1B ⁱ —Rb1A—O2 ^{iv}	148.87 (3)	O1 ^{viii} —Rb2B—O1 ^{vi}	114.2 (2)
Rb1B ⁱⁱ —Rb1A—O2 ^{iv}	86.26 (12)	Rb2B ⁱ —Rb2B—O4 ^x	113.2 (3)
O3 ⁱⁱⁱ —Rb1A—O2 ^{iv}	112.03 (5)	Rb2B ⁱⁱ —Rb2B—O4 ^x	105.2 (7)
O3 ⁱ —Rb1A—O2 ^{iv}	120.30 (5)	O3—Rb2B—O4 ^x	125.4 (3)

O3 ^{iv} —Rb1A—O2 ^{iv}	50.13 (4)	O3 ⁱⁱ —Rb2B—O4 ^x	130.1 (3)
O3 ^v —Rb1A—O2 ^{iv}	64.77 (5)	O3 ⁱ —Rb2B—O4 ^x	159.7 (3)
O3 ⁱⁱ —Rb1A—O2 ^{iv}	125.02 (5)	O1 ^{viii} —Rb2B—O4 ^x	47.08 (11)
O3—Rb1A—O2 ^{iv}	67.27 (5)	O1 ^{vi} —Rb2B—O4 ^x	79.33 (17)
O2—Rb1A—O2 ^{iv}	62.27 (6)	Rb2B ⁱ —Rb2B—O1 ^{xiii}	150.5 (18)
O2 ^v —Rb1A—O2 ^{iv}	111.23 (3)	Rb2B ⁱⁱ —Rb2B—O1 ^{xiii}	141.8 (19)
Rb1B ⁱ —Rb1A—O2 ⁱⁱ	37.75 (3)	O3—Rb2B—O1 ^{xiii}	47.02 (14)
Rb1B ⁱⁱ —Rb1A—O2 ⁱⁱ	86.26 (12)	O3 ⁱⁱ —Rb2B—O1 ^{xiii}	79.7 (2)
O3 ⁱⁱⁱ —Rb1A—O2 ⁱⁱ	67.27 (5)	O3 ⁱ —Rb2B—O1 ^{xiii}	113.9 (3)
O3 ⁱ —Rb1A—O2 ⁱⁱ	64.77 (5)	O1 ^{viii} —Rb2B—O1 ^{xiii}	48.49 (13)
O3 ^{iv} —Rb1A—O2 ⁱⁱ	125.02 (5)	O1 ^{vi} —Rb2B—O1 ^{xiii}	99.9 (2)
O3 ^v —Rb1A—O2 ⁱⁱ	120.30 (5)	O4 ^x —Rb2B—O1 ^{xiii}	83.29 (17)
O3 ⁱⁱ —Rb1A—O2 ⁱⁱ	50.13 (5)	Rb2B ⁱ —Rb2B—As ^{xvi}	132.4 (6)
O3—Rb1A—O2 ⁱⁱ	112.03 (5)	Rb2B ⁱⁱ —Rb2B—As ^{xvi}	98.8 (15)
O2—Rb1A—O2 ⁱⁱ	111.23 (3)	O3—Rb2B—As ^{xvi}	119.4 (2)
O2 ^v —Rb1A—O2 ⁱⁱ	75.50 (6)	O3 ⁱⁱ —Rb2B—As ^{xvi}	104.1 (2)
O2 ^{iv} —Rb1A—O2 ⁱⁱ	172.51 (6)	O3 ⁱ —Rb2B—As ^{xvi}	166.2 (3)
Rb1B ⁱ —Rb1A—O2 ⁱⁱⁱ	86.26 (3)	O1 ^{viii} —Rb2B—As ^{xvi}	25.78 (7)
Rb1B ⁱⁱ —Rb1A—O2 ⁱⁱⁱ	37.75 (11)	O1 ^{vi} —Rb2B—As ^{xvi}	104.6 (2)
O3 ⁱⁱⁱ —Rb1A—O2 ⁱⁱⁱ	50.13 (4)	O4 ^x —Rb2B—As ^{xvi}	26.18 (6)
O3 ⁱ —Rb1A—O2 ⁱⁱⁱ	125.02 (5)	O1 ^{xiii} —Rb2B—As ^{xvi}	72.35 (15)
O3 ^{iv} —Rb1A—O2 ⁱⁱⁱ	64.77 (5)	Rb2B ⁱ —Rb2B—As ^{xv}	75.0 (15)
O3 ^v —Rb1A—O2 ⁱⁱⁱ	112.03 (5)	Rb2B ⁱⁱ —Rb2B—As ^{xv}	117.0 (13)
O3 ⁱⁱ —Rb1A—O2 ⁱⁱⁱ	67.27 (5)	O3—Rb2B—As ^{xv}	105.0 (2)
O3—Rb1A—O2 ⁱⁱⁱ	120.30 (5)	O3 ⁱⁱ —Rb2B—As ^{xv}	174.4 (3)
O2—Rb1A—O2 ⁱⁱⁱ	75.50 (6)	O3 ⁱ —Rb2B—As ^{xv}	110.1 (2)
O2 ^v —Rb1A—O2 ⁱⁱⁱ	111.23 (3)	O1 ^{viii} —Rb2B—As ^{xv}	94.17 (18)
O2 ^{iv} —Rb1A—O2 ⁱⁱⁱ	111.23 (3)	O1 ^{vi} —Rb2B—As ^{xv}	25.24 (7)
O2 ⁱⁱ —Rb1A—O2 ⁱⁱⁱ	62.27 (6)	O4 ^x —Rb2B—As ^{xv}	54.35 (12)
Rb1B ⁱ —Rb1A—O2 ⁱ	86.26 (3)	O1 ^{xiii} —Rb2B—As ^{xv}	98.42 (18)
Rb1B ⁱⁱ —Rb1A—O2 ⁱ	148.87 (11)	As ^{xvi} —Rb2B—As ^{xv}	80.12 (15)
O3 ⁱⁱⁱ —Rb1A—O2 ⁱ	125.02 (5)	Rb2B ⁱ —Rb2B—As	129.9 (12)
O3 ⁱ —Rb1A—O2 ⁱ	50.13 (4)	Rb2B ⁱⁱ —Rb2B—As	133.2 (10)
O3 ^{iv} —Rb1A—O2 ⁱ	120.30 (5)	O3—Rb2B—As	23.86 (9)
O3 ^v —Rb1A—O2 ⁱ	67.27 (5)	O3 ⁱⁱ —Rb2B—As	67.16 (17)
O3 ⁱⁱ —Rb1A—O2 ⁱ	112.03 (5)	O3 ⁱ —Rb2B—As	89.1 (2)
O3—Rb1A—O2 ⁱ	64.77 (5)	O1 ^{viii} —Rb2B—As	71.31 (17)
O2—Rb1A—O2 ⁱ	111.23 (3)	O1 ^{vi} —Rb2B—As	100.0 (2)
O2 ^v —Rb1A—O2 ⁱ	62.27 (6)	O4 ^x —Rb2B—As	107.7 (2)
O2 ^{iv} —Rb1A—O2 ⁱ	75.50 (6)	O1 ^{xiii} —Rb2B—As	24.73 (7)
O2 ⁱⁱ —Rb1A—O2 ⁱ	111.23 (3)	As ^{xvi} —Rb2B—As	96.34 (18)
O2 ⁱⁱⁱ —Rb1A—O2 ⁱ	172.51 (7)	As ^{xv} —Rb2B—As	109.1 (2)
Rb1B ⁱ —Rb1A—As ⁱⁱⁱ	68.045 (6)	O2 ^{xvii} —In1—O2 ⁱⁱ	92.65 (7)
Rb1B ⁱⁱ —Rb1A—As ⁱⁱⁱ	62.23 (10)	O2 ^{xvii} —In1—O2 ^{xviii}	92.65 (7)
O3 ⁱⁱⁱ —Rb1A—As ⁱⁱⁱ	25.58 (3)	O2 ⁱⁱ —In1—O2 ^{xviii}	92.65 (7)
O3 ⁱ —Rb1A—As ⁱⁱⁱ	121.18 (4)	O2 ^{xvii} —In1—O4 ^{xix}	91.95 (7)
O3 ^{iv} —Rb1A—As ⁱⁱⁱ	68.11 (4)	O2 ⁱⁱ —In1—O4 ^{xix}	173.42 (7)
O3 ^v —Rb1A—As ⁱⁱⁱ	92.38 (4)	O2 ^{xviii} —In1—O4 ^{xix}	91.82 (7)

O3 ⁱⁱ —Rb1A—As ⁱⁱⁱ	83.92 (4)	O2 ^{xvii} —In1—O4 ⁱ	91.82 (7)
O3—Rb1A—As ⁱⁱⁱ	145.24 (3)	O2 ⁱⁱ —In1—O4 ⁱ	91.95 (7)
O2—Rb1A—As ⁱⁱⁱ	99.68 (3)	O2 ^{xviii} —In1—O4 ⁱ	173.42 (7)
O2 ^v —Rb1A—As ⁱⁱⁱ	86.65 (3)	O4 ^{xix} —In1—O4 ⁱ	83.21 (7)
O2 ^{iv} —Rb1A—As ⁱⁱⁱ	118.16 (3)	O2 ^{xvii} —In1—O4 ^{xii}	173.42 (7)
O2 ⁱⁱ —Rb1A—As ⁱⁱⁱ	57.81 (3)	O2 ⁱⁱ —In1—O4 ^{xii}	91.82 (7)
O2 ⁱⁱⁱ —Rb1A—As ⁱⁱⁱ	25.19 (3)	O2 ^{xviii} —In1—O4 ^{xii}	91.95 (7)
O2 ⁱ —Rb1A—As ⁱⁱⁱ	148.88 (3)	O4 ^{xix} —In1—O4 ^{xii}	83.21 (7)
Rb1B ⁱ —Rb1A—H	127.6 (7)	O4 ⁱ —In1—O4 ^{xii}	83.21 (7)
Rb1B ⁱⁱ —Rb1A—H	95.7 (8)	O2 ^{xvii} —In1—Rb2A ^{xxi}	123.37 (5)
O3 ⁱⁱⁱ —Rb1A—H	170.2 (6)	O2 ⁱⁱ —In1—Rb2A ^{xxi}	123.36 (5)
O3 ⁱ —Rb1A—H	69.0 (7)	O2 ^{xviii} —In1—Rb2A ^{xxi}	123.36 (5)
O3 ^{iv} —Rb1A—H	103.6 (7)	O4 ^{xix} —In1—Rb2A ^{xxi}	50.06 (5)
O3 ^v —Rb1A—H	103.8 (6)	O4 ⁱ —In1—Rb2A ^{xxi}	50.06 (5)
O3 ⁱⁱ —Rb1A—H	82.3 (6)	O4 ^{xii} —In1—Rb2A ^{xxi}	50.06 (5)
O3—Rb1A—H	14.5 (6)	O2 ^{xvii} —In1—Rb1A ^{xix}	32.08 (5)
O2—Rb1A—H	58.6 (7)	O2 ⁱⁱ —In1—Rb1A ^{xix}	107.92 (5)
O2 ^v —Rb1A—H	115.4 (7)	O2 ^{xviii} —In1—Rb1A ^{xix}	118.90 (5)
O2 ^{iv} —Rb1A—H	58.4 (6)	O4 ^{xix} —In1—Rb1A ^{xix}	73.96 (4)
O2 ⁱⁱ —Rb1A—H	122.5 (6)	O4 ⁱ —In1—Rb1A ^{xix}	63.88 (4)
O2 ⁱⁱⁱ —Rb1A—H	132.7 (7)	O4 ^{xii} —In1—Rb1A ^{xix}	141.47 (5)
O2 ⁱ —Rb1A—H	53.3 (7)	Rb2A ^{xxi} —In1—Rb1A ^{xix}	91.955 (3)
As ⁱⁱⁱ —Rb1A—H	157.8 (7)	O2 ^{xvii} —In1—Rb1A	118.90 (5)
Rb1B ⁱ —Rb1A—H ⁱ	44.8 (6)	O2 ⁱⁱ —In1—Rb1A	32.08 (5)
Rb1B ⁱⁱ —Rb1A—H ⁱ	127.6 (8)	O2 ^{xviii} —In1—Rb1A	107.92 (5)
O3 ⁱⁱⁱ —Rb1A—H ⁱ	103.8 (6)	O4 ^{xix} —In1—Rb1A	141.47 (5)
O3 ⁱ —Rb1A—H ⁱ	14.5 (6)	O4 ⁱ —In1—Rb1A	73.96 (4)
O3 ^{iv} —Rb1A—H ⁱ	170.2 (6)	O4 ^{xii} —In1—Rb1A	63.88 (5)
O3 ^v —Rb1A—H ⁱ	103.6 (7)	Rb2A ^{xxi} —In1—Rb1A	91.954 (3)
O3 ⁱⁱ —Rb1A—H ⁱ	69.0 (7)	Rb1A ^{xix} —In1—Rb1A	119.9
O3—Rb1A—H ⁱ	82.3 (6)	O2 ^{xvii} —In1—Rb1A ^{xviii}	107.92 (5)
O2—Rb1A—H ⁱ	122.5 (6)	O2 ⁱⁱ —In1—Rb1A ^{xviii}	118.90 (5)
O2 ^v —Rb1A—H ⁱ	58.4 (6)	O2 ^{xviii} —In1—Rb1A ^{xviii}	32.08 (5)
O2 ^{iv} —Rb1A—H ⁱ	132.7 (7)	O4 ^{xix} —In1—Rb1A ^{xviii}	63.88 (5)
O2 ⁱⁱ —Rb1A—H ⁱ	53.3 (7)	O4 ⁱ —In1—Rb1A ^{xviii}	141.47 (5)
O2 ⁱⁱⁱ —Rb1A—H ⁱ	115.4 (7)	O4 ^{xii} —In1—Rb1A ^{xviii}	73.96 (5)
O2 ⁱ —Rb1A—H ⁱ	58.6 (7)	Rb2A ^{xxi} —In1—Rb1A ^{xviii}	91.954 (3)
As ⁱⁱⁱ —Rb1A—H ⁱ	107.6 (7)	Rb1A ^{xix} —In1—Rb1A ^{xviii}	119.9
H—Rb1A—H ⁱ	83.5 (9)	Rb1A—In1—Rb1A ^{xviii}	119.9
Rb1B ⁱ —Rb1A—H ⁱⁱ	95.7 (7)	O1 ^{vii} —In2—O1 ^{xvi}	96.52 (7)
Rb1B ⁱⁱ —Rb1A—H ⁱⁱ	44.8 (6)	O1 ^{vii} —In2—O1 ⁱ	180.0
O3 ⁱⁱⁱ —Rb1A—H ⁱⁱ	103.6 (7)	O1 ^{xvi} —In2—O1 ⁱ	83.48 (7)
O3 ⁱ —Rb1A—H ⁱⁱ	82.3 (6)	O1 ^{vii} —In2—O1 ^{xii}	83.48 (7)
O3 ^{iv} —Rb1A—H ⁱⁱ	103.8 (6)	O1 ^{xvi} —In2—O1 ^{xii}	180.0
O3 ^v —Rb1A—H ⁱⁱ	170.2 (6)	O1 ⁱ —In2—O1 ^{xii}	96.52 (7)
O3 ⁱⁱ —Rb1A—H ⁱⁱ	14.5 (6)	O1 ^{vii} —In2—O1 ^{xix}	83.48 (7)
O3—Rb1A—H ⁱⁱ	69.0 (7)	O1 ^{xvi} —In2—O1 ^{xix}	83.48 (7)
O2—Rb1A—H ⁱⁱ	53.3 (7)	O1 ⁱ —In2—O1 ^{xix}	96.52 (7)

O2 ^v —Rb1A—H ⁱⁱ	132.7 (7)	O1 ^{xii} —In2—O1 ^{xix}	96.52 (7)
O2 ^{iv} —Rb1A—H ⁱⁱ	115.4 (8)	O1 ^{vii} —In2—O1 ^{xx}	96.52 (7)
O2 ⁱⁱ —Rb1A—H ⁱⁱ	58.6 (7)	O1 ^{xvi} —In2—O1 ^{xx}	96.52 (7)
O2 ⁱⁱⁱ —Rb1A—H ⁱⁱ	58.4 (6)	O1 ⁱ —In2—O1 ^{xx}	83.48 (7)
O2 ⁱ —Rb1A—H ⁱⁱ	122.5 (6)	O1 ^{xii} —In2—O1 ^{xx}	83.48 (7)
As ⁱⁱⁱ —Rb1A—H ⁱⁱ	78.9 (7)	O1 ^{xix} —In2—O1 ^{xx}	180.0
H—Rb1A—H ⁱⁱ	83.5 (9)	O1 ^{vii} —In2—Rb2A ^{xx}	47.93 (8)
H ⁱ —Rb1A—H ⁱⁱ	83.5 (9)	O1 ^{xvi} —In2—Rb2A ^{xx}	80.47 (7)
Rb1B ⁱ —Rb1A—H ^{iv}	127.6 (7)	O1 ⁱ —In2—Rb2A ^{xx}	132.07 (8)
Rb1B ⁱⁱ —Rb1A—H ^{iv}	44.8 (6)	O1 ^{xii} —In2—Rb2A ^{xx}	99.53 (7)
O3 ⁱⁱⁱ —Rb1A—H ^{iv}	69.0 (7)	O1 ^{xix} —In2—Rb2A ^{xx}	37.05 (8)
O3 ⁱ —Rb1A—H ^{iv}	170.2 (6)	O1 ^{xx} —In2—Rb2A ^{xx}	142.95 (8)
O3 ^{iv} —Rb1A—H ^{iv}	14.5 (6)	O1 ^{vii} —In2—Rb2A ^{xix}	132.07 (8)
O3 ^v —Rb1A—H ^{iv}	82.3 (6)	O1 ^{xvi} —In2—Rb2A ^{xix}	99.53 (7)
O3 ⁱⁱ —Rb1A—H ^{iv}	103.8 (6)	O1 ⁱ —In2—Rb2A ^{xix}	47.93 (8)
O3—Rb1A—H ^{iv}	103.6 (7)	O1 ^{xii} —In2—Rb2A ^{xix}	80.47 (7)
O2—Rb1A—H ^{iv}	58.4 (6)	O1 ^{xix} —In2—Rb2A ^{xix}	142.95 (8)
O2 ^v —Rb1A—H ^{iv}	122.5 (6)	O1 ^{xx} —In2—Rb2A ^{xix}	37.05 (8)
O2 ^{iv} —Rb1A—H ^{iv}	58.6 (7)	Rb2A ^{xx} —In2—Rb2A ^{xix}	180.0
O2 ⁱⁱ —Rb1A—H ^{iv}	115.4 (7)	O1 ^{vii} —In2—Rb2A	37.05 (8)
O2 ⁱⁱⁱ —Rb1A—H ^{iv}	53.3 (7)	O1 ^{xvi} —In2—Rb2A	132.07 (8)
O2 ⁱ —Rb1A—H ^{iv}	132.7 (7)	O1 ⁱ —In2—Rb2A	142.95 (8)
As ⁱⁱⁱ —Rb1A—H ^{iv}	62.0 (7)	O1 ^{xii} —In2—Rb2A	47.93 (8)
H—Rb1A—H ^{iv}	104.8 (15)	O1 ^{xix} —In2—Rb2A	80.47 (7)
H ⁱ —Rb1A—H ^{iv}	168.6 (14)	O1 ^{xx} —In2—Rb2A	99.53 (7)
H ⁱⁱ —Rb1A—H ^{iv}	89.6 (11)	Rb2A ^{xx} —In2—Rb2A	60.060 (6)
Rb1B ⁱ —Rb1A—H ⁱⁱⁱ	44.8 (6)	Rb2A ^{xix} —In2—Rb2A	119.940 (6)
Rb1B ⁱⁱ —Rb1A—H ⁱⁱⁱ	95.7 (8)	O1 ^{vii} —In2—Rb2A ^{xviii}	99.53 (7)
O3 ⁱⁱⁱ —Rb1A—H ⁱⁱⁱ	14.5 (6)	O1 ^{xvi} —In2—Rb2A ^{xviii}	37.05 (8)
O3 ⁱ —Rb1A—H ⁱⁱⁱ	103.8 (6)	O1 ⁱ —In2—Rb2A ^{xviii}	80.47 (7)
O3 ^{iv} —Rb1A—H ⁱⁱⁱ	82.3 (6)	O1 ^{xii} —In2—Rb2A ^{xviii}	142.95 (8)
O3 ^v —Rb1A—H ⁱⁱⁱ	69.0 (7)	O1 ^{xix} —In2—Rb2A ^{xviii}	47.93 (8)
O3 ⁱⁱ —Rb1A—H ⁱⁱⁱ	103.6 (7)	O1 ^{xx} —In2—Rb2A ^{xviii}	132.07 (8)
O3—Rb1A—H ⁱⁱⁱ	170.2 (6)	Rb2A ^{xx} —In2—Rb2A ^{xviii}	60.060 (6)
O2—Rb1A—H ⁱⁱⁱ	132.7 (7)	Rb2A ^{xix} —In2—Rb2A ^{xviii}	119.940 (7)
O2 ^v —Rb1A—H ⁱⁱⁱ	53.3 (7)	Rb2A—In2—Rb2A ^{xviii}	119.940 (6)
O2 ^{iv} —Rb1A—H ⁱⁱⁱ	122.5 (6)	O1 ^{vii} —In2—Rb2A ^{xxii}	80.47 (7)
O2 ⁱⁱ —Rb1A—H ⁱⁱⁱ	58.4 (6)	O1 ^{xvi} —In2—Rb2A ^{xxii}	142.95 (8)
O2 ⁱⁱⁱ —Rb1A—H ⁱⁱⁱ	58.6 (7)	O1 ⁱ —In2—Rb2A ^{xxii}	99.53 (7)
O2 ⁱ —Rb1A—H ⁱⁱⁱ	115.4 (7)	O1 ^{xii} —In2—Rb2A ^{xxii}	37.05 (8)
As ⁱⁱⁱ —Rb1A—H ⁱⁱⁱ	33.5 (7)	O1 ^{xix} —In2—Rb2A ^{xxii}	132.07 (8)
H—Rb1A—H ⁱⁱⁱ	168.6 (14)	O1 ^{xx} —In2—Rb2A ^{xxii}	47.93 (8)
H ⁱ —Rb1A—H ⁱⁱⁱ	89.6 (12)	Rb2A ^{xx} —In2—Rb2A ^{xxii}	119.940 (6)
H ⁱⁱ —Rb1A—H ⁱⁱⁱ	104.8 (15)	Rb2A ^{xix} —In2—Rb2A ^{xxii}	60.060 (6)
H ^{iv} —Rb1A—H ⁱⁱⁱ	83.5 (9)	Rb2A—In2—Rb2A ^{xxii}	60.061 (6)
Rb1B ⁱ —Rb1A—H ^v	95.7 (7)	Rb2A ^{xviii} —In2—Rb2A ^{xxii}	180.0
Rb1B ⁱⁱ —Rb1A—H ^v	127.6 (8)	O1 ^{vii} —In2—Rb2A ^{xxiii}	142.95 (8)
O3 ⁱⁱⁱ —Rb1A—H ^v	82.3 (6)	O1 ^{xvi} —In2—Rb2A ^{xxiii}	47.93 (8)

O3 ⁱ —Rb1A—H ^v	103.6 (7)	O1 ⁱ —In2—Rb2A ^{xxiii}	37.05 (8)
O3 ^{iv} —Rb1A—H ^v	69.0 (7)	O1 ^{xii} —In2—Rb2A ^{xxiii}	132.07 (8)
O3 ^v —Rb1A—H ^v	14.5 (6)	O1 ^{xix} —In2—Rb2A ^{xxiii}	99.53 (7)
O3 ⁱⁱ —Rb1A—H ^v	170.2 (6)	O1 ^{xx} —In2—Rb2A ^{xxiii}	80.47 (7)
O3—Rb1A—H ^v	103.8 (6)	Rb2A ^{xx} —In2—Rb2A ^{xxiii}	119.940 (7)
O2—Rb1A—H ^v	115.4 (8)	Rb2A ^{xix} —In2—Rb2A ^{xxiii}	60.060 (6)
O2 ^v —Rb1A—H ^v	58.6 (7)	Rb2A—In2—Rb2A ^{xxiii}	180.0
O2 ^{iv} —Rb1A—H ^v	53.3 (7)	Rb2A ^{xviii} —In2—Rb2A ^{xxiii}	60.061 (6)
O2 ⁱⁱ —Rb1A—H ^v	132.7 (7)	Rb2A ^{xxii} —In2—Rb2A ^{xxiii}	119.939 (6)
O2 ⁱⁱⁱ —Rb1A—H ^v	122.5 (6)	O1 ^{xiii} —As—O2	116.08 (10)
O2 ⁱ —Rb1A—H ^v	58.4 (6)	O1 ^{xiii} —As—O4 ^v	109.85 (10)
As ⁱⁱⁱ —Rb1A—H ^v	105.4 (6)	O2—As—O4 ^v	113.73 (8)
H—Rb1A—H ^v	89.6 (11)	O1 ^{xiii} —As—O3	104.27 (10)
H ⁱ —Rb1A—H ^v	104.8 (14)	O2—As—O3	104.94 (9)
H ⁱⁱ —Rb1A—H ^v	168.6 (15)	O4 ^v —As—O3	106.99 (8)
H ^{iv} —Rb1A—H ^v	83.5 (9)	O1 ^{xiii} —As—Rb1B ⁱⁱ	133.87 (15)
H ⁱⁱⁱ —Rb1A—H ^v	83.5 (9)	O2—As—Rb1B ⁱⁱ	51.9 (5)
Rb1B ⁱ —Rb1B—Rb1B ⁱⁱ	60.00 (3)	O4 ^v —As—Rb1B ⁱⁱ	115.4 (2)
Rb1B ⁱ —Rb1B—O3 ^v	97.5 (5)	O3—As—Rb1B ⁱⁱ	54.3 (4)
Rb1B ⁱⁱ —Rb1B—O3 ^v	123.7 (5)	O1 ^{xiii} —As—Rb1B	138.5 (3)
Rb1B ⁱ —Rb1B—O3	123.7 (5)	O2—As—Rb1B	62.1 (4)
Rb1B ⁱⁱ —Rb1B—O3	97.5 (6)	O4 ^v —As—Rb1B	107.4 (4)
O3 ^v —Rb1B—O3	133.3 (11)	O3—As—Rb1B	46.49 (19)
Rb1B ⁱ —Rb1B—O2 ^{iv}	158.5 (3)	Rb1B ⁱⁱ —As—Rb1B	11.6 (9)
Rb1B ⁱⁱ —Rb1B—O2 ^{iv}	109.8 (5)	O1 ^{xiii} —As—Rb2B ^{xxiv}	59.16 (16)
O3 ^v —Rb1B—O2 ^{iv}	71.7 (5)	O2—As—Rb2B ^{xxiv}	175.06 (16)
O3—Rb1B—O2 ^{iv}	74.5 (5)	O4 ^v —As—Rb2B ^{xxiv}	68.35 (14)
Rb1B ⁱ —Rb1B—O2 ⁱ	109.8 (4)	O3—As—Rb2B ^{xxiv}	78.23 (14)
Rb1B ⁱⁱ —Rb1B—O2 ⁱ	158.5 (3)	Rb1B ⁱⁱ —As—Rb2B ^{xxiv}	131.9 (5)
O3 ^v —Rb1B—O2 ⁱ	74.5 (5)	Rb1B—As—Rb2B ^{xxiv}	122.0 (3)
O3—Rb1B—O2 ⁱ	71.7 (5)	O1 ^{xiii} —As—Rb2B ^{xv}	62.57 (15)
O2 ^{iv} —Rb1B—O2 ⁱ	85.8 (8)	O2—As—Rb2B ^{xv}	175.80 (17)
Rb1B ⁱ —Rb1B—O3 ^{iv}	105.8 (5)	O4 ^v —As—Rb2B ^{xv}	70.24 (15)
Rb1B ⁱⁱ —Rb1B—O3 ^{iv}	68.2 (6)	O3—As—Rb2B ^{xv}	72.08 (14)
O3 ^v —Rb1B—O3 ^{iv}	71.05 (15)	Rb1B ⁱⁱ —As—Rb2B ^{xv}	125.7 (4)
O3—Rb1B—O3 ^{iv}	111.7 (3)	Rb1B—As—Rb2B ^{xv}	115.9 (3)
O2 ^{iv} —Rb1B—O3 ^{iv}	53.4 (2)	Rb2B ^{xxiv} —As—Rb2B ^{xv}	6.2 (2)
O2 ⁱ —Rb1B—O3 ^{iv}	132.8 (9)	O1 ^{xiii} —As—Rb1A	134.73 (9)
Rb1B ⁱ —Rb1B—O3 ⁱ	68.2 (5)	O2—As—Rb1A	57.74 (6)
Rb1B ⁱⁱ —Rb1B—O3 ⁱ	105.8 (5)	O4 ^v —As—Rb1A	112.84 (6)
O3 ^v —Rb1B—O3 ⁱ	111.7 (3)	O3—As—Rb1A	48.98 (7)
O3—Rb1B—O3 ⁱ	71.04 (15)	Rb1B ⁱⁱ —As—Rb1A	6.0 (4)
O2 ^{iv} —Rb1B—O3 ⁱ	132.8 (9)	Rb1B—As—Rb1A	6.2 (5)
O2 ⁱ —Rb1B—O3 ⁱ	53.4 (2)	Rb2B ^{xxiv} —As—Rb1A	126.16 (13)
O3 ^{iv} —Rb1B—O3 ⁱ	173.4 (12)	Rb2B ^{xv} —As—Rb1A	119.97 (12)
Rb1B ⁱ —Rb1B—O2	114.7 (5)	O1 ^{xiii} —As—Rb2A ^{xv}	61.31 (9)
Rb1B ⁱⁱ —Rb1B—O2	57.8 (6)	O2—As—Rb2A ^{xv}	177.30 (9)
O3 ^v —Rb1B—O2	132.6 (4)	O4 ^v —As—Rb2A ^{xv}	68.43 (8)

O3—Rb1B—O2	51.41 (7)	O3—As—Rb2A ^{xv}	75.58 (7)
O2 ^{iv} —Rb1B—O2	65.7 (2)	Rb1B ⁱⁱ —As—Rb2A ^{xv}	129.1 (4)
O2 ⁱ —Rb1B—O2	120.6 (6)	Rb1B—As—Rb2A ^{xv}	119.2 (3)
O3 ^{iv} —Rb1B—O2	67.34 (7)	Rb2B ^{xxiv} —As—Rb2A ^{xv}	2.88 (15)
O3 ⁱ —Rb1B—O2	112.19 (11)	Rb2B ^{xv} —As—Rb2A ^{xv}	3.52 (13)
Rb1B ⁱ —Rb1B—O2 ^v	57.8 (5)	Rb1A—As—Rb2A ^{xv}	123.340 (18)
Rb1B ⁱⁱ —Rb1B—O2 ^v	114.7 (4)	O1 ^{xiii} —As—Rb2B	66.15 (14)
O3 ^v —Rb1B—O2 ^v	51.41 (7)	O2—As—Rb2B	104.87 (14)
O3—Rb1B—O2 ^v	132.6 (4)	O4 ^v —As—Rb2B	137.04 (14)
O2 ^{iv} —Rb1B—O2 ^v	120.6 (6)	O3—As—Rb2B	42.56 (14)
O2 ⁱ —Rb1B—O2 ^v	65.7 (2)	Rb1B ⁱⁱ —As—Rb2B	74.7 (2)
O3 ^{iv} —Rb1B—O2 ^v	112.19 (11)	Rb1B—As—Rb2B	74.33 (18)
O3 ⁱ —Rb1B—O2 ^v	67.34 (7)	Rb2B ^{xxiv} —As—Rb2B	74.78 (3)
O2—Rb1B—O2 ^v	172.4 (11)	Rb2B ^{xv} —As—Rb2B	70.9 (2)
Rb1B ⁱ —Rb1B—O3 ⁱⁱⁱ	45.4 (3)	Rb1A—As—Rb2B	72.61 (11)
Rb1B ⁱⁱ —Rb1B—O3 ⁱⁱⁱ	61.5 (3)	Rb2A ^{xv} —As—Rb2B	73.66 (14)
O3 ^v —Rb1B—O3 ⁱⁱⁱ	66.84 (19)	O1 ^{xiii} —As—Rb2B ^{xxv}	63.55 (13)
O3—Rb1B—O3 ⁱⁱⁱ	158.9 (9)	O2—As—Rb2B ^{xxv}	178.70 (16)
O2 ^{iv} —Rb1B—O3 ⁱⁱⁱ	113.43 (5)	O4 ^v —As—Rb2B ^{xxv}	65.54 (13)
O2 ⁱ —Rb1B—O3 ⁱⁱⁱ	126.87 (6)	O3—As—Rb2B ^{xxv}	76.36 (14)
O3 ^{iv} —Rb1B—O3 ⁱⁱⁱ	64.9 (3)	Rb1B ⁱⁱ —As—Rb2B ^{xxv}	129.3 (5)
O3 ⁱ —Rb1B—O3 ⁱⁱⁱ	110.3 (6)	Rb1B—As—Rb2B ^{xxv}	119.0 (4)
O2—Rb1B—O3 ⁱⁱⁱ	112.4 (6)	Rb2B ^{xxiv} —As—Rb2B ^{xxv}	4.39 (15)
O2 ^v —Rb1B—O3 ⁱⁱⁱ	61.9 (2)	Rb2B ^{xv} —As—Rb2B ^{xxv}	5.30 (19)
Rb1B ⁱ —Rb1B—O3 ⁱⁱ	61.5 (3)	Rb1A—As—Rb2B ^{xxv}	123.48 (12)
Rb1B ⁱⁱ —Rb1B—O3 ⁱⁱ	45.4 (3)	Rb2A ^{xv} —As—Rb2B ^{xxv}	2.94 (15)
O3 ^v —Rb1B—O3 ⁱⁱ	158.9 (9)	Rb2B—As—Rb2B ^{xxv}	76.18 (18)
O3—Rb1B—O3 ⁱⁱ	66.84 (19)	As ^{xxvi} —O1—In2 ^{xxvii}	142.20 (12)
O2 ^{iv} —Rb1B—O3 ⁱⁱ	126.87 (6)	As ^{xxvi} —O1—Rb2B ^{xxviii}	95.06 (18)
O2 ⁱ —Rb1B—O3 ⁱⁱ	113.43 (5)	In2 ^{xxvii} —O1—Rb2B ^{xxviii}	119.53 (18)
O3 ^{iv} —Rb1B—O3 ⁱⁱ	110.3 (6)	As ^{xxvi} —O1—Rb2B ^{vi}	92.19 (16)
O3 ⁱ —Rb1B—O3 ⁱⁱ	64.9 (3)	In2 ^{xxvii} —O1—Rb2B ^{vi}	123.76 (15)
O2—Rb1B—O3 ⁱⁱ	61.9 (2)	Rb2B ^{xxviii} —O1—Rb2B ^{vi}	6.6 (3)
O2 ^v —Rb1B—O3 ⁱⁱ	112.4 (6)	As ^{xxvi} —O1—Rb2A ^{vi}	93.97 (12)
O3 ⁱⁱⁱ —Rb1B—O3 ⁱⁱ	94.2 (8)	In2 ^{xxvii} —O1—Rb2A ^{vi}	121.16 (11)
Rb1B ⁱ —Rb1B—H	135.3 (8)	Rb2B ^{xxviii} —O1—Rb2A ^{vi}	2.47 (17)
Rb1B ⁱⁱ —Rb1B—H	112.7 (9)	Rb2B ^{vi} —O1—Rb2A ^{vi}	4.12 (14)
O3 ^v —Rb1B—H	117.3 (12)	As ^{xxvi} —O1—Rb2B ^{xxvi}	89.12 (16)
O3—Rb1B—H	16.1 (6)	In2 ^{xxvii} —O1—Rb2B ^{xxvi}	106.82 (16)
O2 ^{iv} —Rb1B—H	65.2 (9)	Rb2B ^{xxviii} —O1—Rb2B ^{xxvi}	86.07 (7)
O2 ⁱ —Rb1B—H	59.4 (9)	Rb2B ^{vi} —O1—Rb2B ^{xxvi}	80.1 (2)
O3 ^{iv} —Rb1B—H	111.3 (10)	Rb2A ^{vi} —O1—Rb2B ^{xxvi}	83.83 (15)
O3 ⁱ —Rb1B—H	73.1 (8)	As ^{xxvi} —O1—Rb2A ^{xxvi}	87.55 (12)
O2—Rb1B—H	61.4 (8)	In2 ^{xxvii} —O1—Rb2A ^{xxvi}	107.67 (9)
O2 ^v —Rb1B—H	124.3 (10)	Rb2B ^{xxviii} —O1—Rb2A ^{xxvi}	86.97 (17)
O3 ⁱⁱⁱ —Rb1B—H	173.7 (9)	Rb2B ^{vi} —O1—Rb2A ^{xxvi}	80.92 (17)
O3 ⁱⁱ —Rb1B—H	82.4 (6)	Rb2A ^{vi} —O1—Rb2A ^{xxvi}	84.71 (5)
Rb1B ⁱ —Rb1B—H ^v	112.7 (9)	Rb2B ^{xxvi} —O1—Rb2A ^{xxvi}	1.7 (2)

Rb1B ⁱⁱ —Rb1B—H ^v	135.3 (7)	As ^{xxvi} —O1—Rb2A ^{xxvii}	110.41 (11)
O3 ^v —Rb1B—H ^v	16.1 (6)	In2 ^{xxvii} —O1—Rb2A ^{xxvii}	74.80 (7)
O3—Rb1B—H ^v	117.3 (12)	Rb2B ^{xxviii} —O1—Rb2A ^{xxvii}	65.58 (17)
O2 ^{iv} —Rb1B—H ^v	59.4 (9)	Rb2B ^{vi} —O1—Rb2A ^{xxvii}	72.13 (14)
O2 ⁱ —Rb1B—H ^v	65.2 (9)	Rb2A ^{vi} —O1—Rb2A ^{xxvii}	68.03 (4)
O3 ^{iv} —Rb1B—H ^v	73.1 (8)	Rb2B ^{xxvi} —O1—Rb2A ^{xxvii}	146.21 (11)
O3 ⁱ —Rb1B—H ^v	111.3 (9)	Rb2A ^{xxvi} —O1—Rb2A ^{xxvii}	147.76 (12)
O2—Rb1B—H ^v	124.3 (11)	As—O2—In1 ^{xxix}	123.06 (9)
O2 ^v —Rb1B—H ^v	61.4 (8)	As—O2—Rb1B ⁱⁱ	102.0 (4)
O3 ⁱⁱⁱ —Rb1B—H ^v	82.4 (6)	In1 ^{xxix} —O2—Rb1B ⁱⁱ	124.8 (3)
O3 ⁱⁱ —Rb1B—H ^v	173.7 (10)	As—O2—Rb1A	97.07 (7)
H—Rb1B—H ^v	101.4 (15)	In1 ^{xxix} —O2—Rb1A	127.94 (7)
Rb2B ⁱⁱ —Rb2A—Rb2B ⁱ	116 (2)	Rb1B ⁱⁱ —O2—Rb1A	5.1 (4)
Rb2B ⁱⁱ —Rb2A—O3	134 (3)	As—O2—Rb1B	91.5 (4)
Rb2B ⁱ —Rb2A—O3	99 (3)	In1 ^{xxix} —O2—Rb1B	128.91 (9)
Rb2B ⁱⁱ —Rb2A—O3 ⁱ	99 (3)	Rb1B ⁱⁱ —O2—Rb1B	12.4 (9)
Rb2B ⁱ —Rb2A—O3 ⁱ	65 (3)	Rb1A—O2—Rb1B	7.5 (5)
O3—Rb2A—O3 ⁱ	69.31 (13)	As—O2—Rb2A	56.91 (5)
Rb2B ⁱⁱ —Rb2A—O3 ⁱⁱ	65 (3)	In1 ^{xxix} —O2—Rb2A	162.73 (8)
Rb2B ⁱ —Rb2A—O3 ⁱⁱ	134 (3)	Rb1B ⁱⁱ —O2—Rb2A	68.43 (19)
O3—Rb2A—O3 ⁱⁱ	69.31 (13)	Rb1A—O2—Rb2A	66.24 (6)
O3 ⁱ —Rb2A—O3 ⁱⁱ	69.31 (13)	Rb1B—O2—Rb2A	66.61 (7)
Rb2B ⁱⁱ —Rb2A—O1 ^{vi}	140 (3)	As—O3—Rb1B	107.13 (15)
Rb2B ⁱ —Rb2A—O1 ^{vi}	34 (2)	As—O3—Rb2B	113.58 (18)
O3—Rb2A—O1 ^{vi}	85.60 (6)	Rb1B—O3—Rb2B	107.8 (5)
O3 ⁱ —Rb2A—O1 ^{vi}	89.21 (6)	As—O3—Rb2A	117.21 (9)
O3 ⁱⁱ —Rb2A—O1 ^{vi}	151.25 (17)	Rb1B—O3—Rb2A	103.8 (4)
Rb2B ⁱⁱ —Rb2A—O1 ^{vii}	34 (2)	Rb2B—O3—Rb2A	4.46 (18)
Rb2B ⁱ —Rb2A—O1 ^{vii}	82 (2)	As—O3—Rb1B ⁱⁱ	98.0 (5)
O3—Rb2A—O1 ^{vii}	151.25 (17)	Rb1B—O3—Rb1B ⁱⁱ	14.3 (10)
O3 ⁱ —Rb2A—O1 ^{vii}	85.60 (6)	Rb2B—O3—Rb1B ⁱⁱ	102.66 (17)
O3 ⁱⁱ —Rb2A—O1 ^{vii}	89.21 (6)	Rb2A—O3—Rb1B ⁱⁱ	99.24 (11)
O1 ^{vi} —Rb2A—O1 ^{vii}	108.60 (10)	As—O3—Rb1A	105.44 (8)
Rb2B ⁱⁱ —Rb2A—O1 ^{viii}	82 (2)	Rb1B—O3—Rb1A	7.6 (6)
Rb2B ⁱ —Rb2A—O1 ^{viii}	140 (3)	Rb2B—O3—Rb1A	102.30 (16)
O3—Rb2A—O1 ^{viii}	89.21 (6)	Rb2A—O3—Rb1A	98.50 (9)
O3 ⁱ —Rb2A—O1 ^{viii}	151.25 (17)	Rb1B ⁱⁱ —O3—Rb1A	8.2 (6)
O3 ⁱⁱ —Rb2A—O1 ^{viii}	85.60 (6)	As—O3—Rb2B ⁱ	121.23 (19)
O1 ^{vi} —Rb2A—O1 ^{viii}	108.60 (10)	Rb1B—O3—Rb2B ⁱ	103.8 (4)
O1 ^{vii} —Rb2A—O1 ^{viii}	108.59 (10)	Rb2B—O3—Rb2B ⁱ	7.6 (3)
Rb2B ⁱⁱ —Rb2A—O4 ^{ix}	98 (3)	Rb2A—O3—Rb2B ⁱ	4.62 (15)
Rb2B ⁱ —Rb2A—O4 ^{ix}	53 (3)	Rb1B ⁱⁱ —O3—Rb2B ⁱ	100.4 (2)
O3—Rb2A—O4 ^{ix}	126.63 (6)	Rb1A—O3—Rb2B ⁱ	99.01 (18)
O3 ⁱ —Rb2A—O4 ^{ix}	117.83 (6)	As—O3—Rb2B ⁱⁱ	115.94 (17)
O3 ⁱⁱ —Rb2A—O4 ^{ix}	163.52 (11)	Rb1B—O3—Rb2B ⁱⁱ	101.7 (5)
O1 ^{vi} —Rb2A—O4 ^{ix}	44.75 (6)	Rb2B—O3—Rb2B ⁱⁱ	6.1 (2)
O1 ^{vii} —Rb2A—O4 ^{ix}	77.05 (10)	Rb2A—O3—Rb2B ⁱⁱ	3.2 (2)
O1 ^{viii} —Rb2A—O4 ^{ix}	90.14 (12)	Rb1B ⁱⁱ —O3—Rb2B ⁱⁱ	96.67 (18)

Rb2B ⁱⁱ —Rb2A—O4 ^x	86 (3)	Rb1A—O3—Rb2B ⁱⁱ	96.23 (18)
Rb2B ⁱ —Rb2A—O4 ^x	98 (3)	Rb2B ⁱ —O3—Rb2B ⁱⁱ	7.4 (2)
O3—Rb2A—O4 ^x	117.83 (6)	As—O3—Rb1B ⁱ	110.6 (3)
O3 ⁱ —Rb2A—O4 ^x	163.52 (11)	Rb1B—O3—Rb1B ⁱ	10.9 (8)
O3 ⁱⁱ —Rb2A—O4 ^x	126.63 (6)	Rb2B—O3—Rb1B ⁱ	97.1 (4)
O1 ^{vi} —Rb2A—O4 ^x	77.05 (10)	Rb2A—O3—Rb1B ⁱ	93.2 (4)
O1 ^{vii} —Rb2A—O4 ^x	90.14 (12)	Rb1B ⁱⁱ —O3—Rb1B ⁱ	12.6 (9)
O1 ^{viii} —Rb2A—O4 ^x	44.75 (6)	Rb1A—O3—Rb1B ⁱ	6.0 (4)
O4 ^{ix} —Rb2A—O4 ^x	45.71 (8)	Rb2B ⁱ —O3—Rb1B ⁱ	93.5 (4)
Rb2B ⁱⁱ —Rb2A—O4 ^{xi}	53 (3)	Rb2B ⁱⁱ —O3—Rb1B ⁱ	91.0 (4)
Rb2B ⁱ —Rb2A—O4 ^{xi}	86 (3)	As—O3—Rb2A ^{xv}	78.72 (7)
O3—Rb2A—O4 ^{xi}	163.52 (11)	Rb1B—O3—Rb2A ^{xv}	159.5 (6)
O3 ⁱ —Rb2A—O4 ^{xi}	126.63 (6)	Rb2B—O3—Rb2A ^{xv}	86.8 (2)
O3 ⁱⁱ —Rb2A—O4 ^{xi}	117.83 (6)	Rb2A—O3—Rb2A ^{xv}	90.14 (5)
O1 ^{vi} —Rb2A—O4 ^{xi}	90.14 (12)	Rb1B ⁱⁱ —O3—Rb2A ^{xv}	170.52 (10)
O1 ^{vii} —Rb2A—O4 ^{xi}	44.75 (6)	Rb1A—O3—Rb2A ^{xv}	167.05 (8)
O1 ^{viii} —Rb2A—O4 ^{xi}	77.05 (10)	Rb2B ⁱ —O3—Rb2A ^{xv}	88.8 (2)
O4 ^{ix} —Rb2A—O4 ^{xi}	45.71 (8)	Rb2B ⁱⁱ —O3—Rb2A ^{xv}	92.8 (2)
O4 ^x —Rb2A—O4 ^{xi}	45.71 (8)	Rb1B ⁱ —O3—Rb2A ^{xv}	167.03 (11)
Rb2B ⁱⁱ —Rb2A—O1 ^{xii}	26 (3)	As—O3—H	108 (3)
Rb2B ⁱ —Rb2A—O1 ^{xii}	117 (2)	Rb1B—O3—H	92 (3)
O3—Rb2A—O1 ^{xii}	112.37 (15)	Rb2B—O3—H	125 (3)
O3 ⁱ —Rb2A—O1 ^{xii}	76.69 (8)	Rb2A—O3—H	124 (3)
O3 ⁱⁱ —Rb2A—O1 ^{xii}	44.11 (5)	Rb1B ⁱⁱ —O3—H	105 (3)
O1 ^{vi} —Rb2A—O1 ^{xii}	150.55 (6)	Rb1A—O3—H	99 (3)
O1 ^{vii} —Rb2A—O1 ^{xii}	45.46 (6)	Rb2B ⁱ —O3—H	120 (3)
O1 ^{viii} —Rb2A—O1 ^{xii}	95.29 (5)	Rb2B ⁱⁱ —O3—H	127 (3)
O4 ^{ix} —Rb2A—O1 ^{xii}	120.81 (10)	Rb1B ⁱ —O3—H	100 (3)
O4 ^x —Rb2A—O1 ^{xii}	111.19 (9)	Rb2A ^{xv} —O3—H	68 (3)
O4 ^{xi} —Rb2A—O1 ^{xii}	78.40 (6)	As ^v —O4—In1 ^{xxvii}	127.87 (9)
Rb2B ⁱⁱ —Rb2A—O1 ^{xiii}	117 (2)	As ^v —O4—Rb2B ^{xxx}	85.47 (16)
Rb2B ⁱ —Rb2A—O1 ^{xiii}	126 (2)	In1 ^{xxvii} —O4—Rb2B ^{xxx}	106.35 (17)
O3—Rb2A—O1 ^{xiii}	44.11 (5)	As ^v —O4—Rb2A ^{xxx}	86.47 (7)
O3 ⁱ —Rb2A—O1 ^{xiii}	112.37 (15)	In1 ^{xxvii} —O4—Rb2A ^{xxx}	103.30 (7)
O3 ⁱⁱ —Rb2A—O1 ^{xiii}	76.69 (8)	Rb2B ^{xxx} —O4—Rb2A ^{xxx}	3.25 (18)
O1 ^{vi} —Rb2A—O1 ^{xiii}	95.29 (5)	As ^v —O4—Rb1A ^{xxvi}	131.05 (7)
O1 ^{vii} —Rb2A—O1 ^{xiii}	150.54 (6)	In1 ^{xxvii} —O4—Rb1A ^{xxvi}	90.25 (5)
O1 ^{viii} —Rb2A—O1 ^{xiii}	45.46 (6)	Rb2B ^{xxx} —O4—Rb1A ^{xxvi}	115.02 (15)
O4 ^{ix} —Rb2A—O1 ^{xiii}	111.19 (9)	Rb2A ^{xxx} —O4—Rb1A ^{xxvi}	116.54 (4)
O4 ^x —Rb2A—O1 ^{xiii}	78.40 (6)	As ^v —O4—Rb1A	48.38 (5)
O4 ^{xi} —Rb2A—O1 ^{xiii}	120.81 (10)	In1 ^{xxvii} —O4—Rb1A	80.54 (5)
O1 ^{xii} —Rb2A—O1 ^{xiii}	113.93 (7)	Rb2B ^{xxx} —O4—Rb1A	109.65 (15)

Rb2B ⁱⁱ —Rb2A—O1 ^{xiv}	126 (2)	Rb2A ^{xxx} —O4—Rb1A	108.26 (4)
Rb2B ⁱ —Rb2A—O1 ^{xiv}	26 (3)	Rb1A ^{xxvi} —O4—Rb1A	135.18 (4)

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) $-x+2/3, -y-2/3, -z+4/3$; (vii) $y+2/3, -x+y+4/3, -z+4/3$; (viii) $x-y-4/3, x-2/3, -z+4/3$; (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) $-x+y+1, -x+1, z$; (xiii) $x-1, y, z$; (xiv) $-y, x-y-1, z$; (xv) $-x-1/3, -y-2/3, -z+4/3$; (xvi) $x-y-1/3, x+1/3, -z+4/3$; (xvii) $-y, x-y+1, z$; (xviii) $x+1, y+1, z$; (xix) $x, y+1, z$; (xx) $-x+2/3, -y+1/3, -z+4/3$; (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) $y-1/3, -x+y-2/3, -z+4/3$; (xxv) $x-y-1/3, x-2/3, -z+4/3$; (xxvi) $x+1, y, z$; (xxvii) $x, y-1, z$; (xxviii) $y+2/3, -x+y-2/3, -z+4/3$; (xxix) $x-1, y-1, z$; (xxx) $-y+1/3, -x-1/3, z+1/6$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O3—H $\cdots$ O4 ^{xxxi}	0.83 (3)	1.82 (3)	2.634 (2)	168 (4)

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

Caesium indium bis[hydrogen arsenate(V)] (CsInHASO₄2)

Crystal data

CsIn(HAsO₄)₂
 $M_r = 527.59$
 Trigonal, $R\bar{3}c:H$
 $a = 8.629$ (1) $\text{\AA}$
 $c = 56.986$ (11) $\text{\AA}$
 $V = 3674.7$ (11) $\text{\AA}^3$
 $Z = 18$
 $F(000) = 4248$

$D_x = 4.291$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ $\text{\AA}$
 Cell parameters from 2985 reflections
 $\theta = 3.1\text{--}30.0^\circ$
 $\mu = 15.34$ mm⁻¹
 $T = 293$ K
 Small pseudooctahedra, colourless
 $0.06 \times 0.06 \times 0.04$ 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)
 $T_{\min} = 0.460, T_{\max} = 0.579$
 4350 measured reflections

1199 independent reflections
 1039 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\max} = 30.0^\circ, \theta_{\min} = 3.1^\circ$
 $h = -12 \rightarrow 12$
 $k = -9 \rightarrow 9$
 $l = -79 \rightarrow 79$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.052$
 $S = 1.07$
 1199 reflections
 61 parameters
 1 restraint
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0234P)^2 + 28.1228P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 2.09$ e $\text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.86$ e $\text{\AA}^{-3}$
 Extinction correction: SHELXL2016 (Sheldrick, 2015),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.000028 (7)

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cs1	0.000000	0.000000	0.750000	0.02557 (14)
Cs2	0.000000	0.000000	0.66740 (2)	0.02940 (12)
In1	0.333333	0.666667	0.75230 (2)	0.00967 (10)
In2	0.333333	0.666667	0.666667	0.01033 (12)
As	−0.41576 (4)	−0.38822 (4)	0.71249 (2)	0.01182 (10)
O1	0.4878 (4)	−0.4176 (4)	0.68649 (4)	0.0247 (6)
O2	−0.4350 (3)	−0.2496 (3)	0.73117 (4)	0.0154 (5)
O3	−0.1870 (3)	−0.2856 (3)	0.70680 (5)	0.0217 (5)
O4	0.4768 (3)	−0.1133 (3)	0.77606 (4)	0.0147 (5)
H	−0.152 (5)	−0.354 (4)	0.7115 (6)	0.013 (10)*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.0283 (2)	0.0283 (2)	0.0201 (3)	0.01415 (10)	0.000	0.000
Cs2	0.03461 (17)	0.03461 (17)	0.0190 (2)	0.01730 (8)	0.000	0.000
In1	0.01027 (13)	0.01027 (13)	0.00848 (17)	0.00513 (6)	0.000	0.000
In2	0.01173 (16)	0.01173 (16)	0.0075 (2)	0.00587 (8)	0.000	0.000
As	0.01466 (17)	0.01309 (17)	0.01022 (15)	0.00882 (14)	0.00082 (12)	0.00125 (11)
O1	0.0366 (15)	0.0361 (15)	0.0126 (11)	0.0265 (13)	−0.0067 (11)	−0.0014 (10)
O2	0.0155 (11)	0.0154 (11)	0.0157 (11)	0.0079 (9)	0.0056 (9)	−0.0020 (9)
O3	0.0174 (12)	0.0216 (13)	0.0290 (13)	0.0120 (11)	0.0083 (10)	0.0115 (11)
O4	0.0154 (11)	0.0126 (11)	0.0183 (11)	0.0086 (9)	−0.0032 (9)	−0.0057 (9)

Geometric parameters ($\text{\AA}$, $^\circ$)

Cs1—O3	3.280 (3)	Cs2—O4 ^{xii}	3.703 (2)
Cs1—O3 ⁱ	3.280 (3)	Cs2—O4 ^{xiii}	3.703 (2)
Cs1—O3 ⁱⁱ	3.280 (3)	Cs2—O4 ^{xiv}	3.703 (2)
Cs1—O3 ⁱⁱⁱ	3.280 (3)	Cs2—As ^{xi}	3.8762 (6)
Cs1—O3 ^{iv}	3.280 (3)	Cs2—As ^{ix}	3.8762 (6)
Cs1—O3 ^v	3.280 (3)	Cs2—As ^x	3.8762 (6)
Cs1—O2	3.434 (2)	In1—O2 ^{xv}	2.127 (2)
Cs1—O2 ⁱⁱ	3.434 (2)	In1—O2 ⁱⁱⁱ	2.127 (2)
Cs1—O2 ^v	3.434 (2)	In1—O2 ^{xvi}	2.127 (2)
Cs1—O2 ⁱⁱⁱ	3.434 (2)	In1—O4 ^{xvii}	2.150 (2)
Cs1—O2 ⁱ	3.434 (2)	In1—O4 ^{iv}	2.150 (2)
Cs1—O2 ^{iv}	3.434 (2)	In1—O4 ^{xviii}	2.150 (2)
Cs1—H	3.44 (4)	In2—O1 ^{vii}	2.133 (2)

Cs1—H ^{iv}	3.44 (4)	In2—O1 ^{xi}	2.133 (3)
Cs1—H ⁱⁱⁱ	3.44 (4)	In2—O1 ^{xix}	2.133 (2)
Cs2—O3 ^{iv}	3.121 (3)	In2—O1 ^{iv}	2.133 (2)
Cs2—O3 ⁱⁱⁱ	3.121 (2)	In2—O1 ^{xviii}	2.133 (3)
Cs2—O3	3.121 (3)	In2—O1 ^{xvii}	2.133 (2)
Cs2—O1 ^{vi}	3.419 (3)	As—O1 ^{xx}	1.655 (2)
Cs2—O1 ^{vii}	3.419 (3)	As—O2	1.671 (2)
Cs2—O1 ^{viii}	3.419 (3)	As—O4 ⁱⁱ	1.679 (2)
Cs2—O3 ^{ix}	3.698 (3)	As—O3	1.743 (3)
Cs2—O3 ^x	3.698 (3)	O3—H	0.83 (3)
Cs2—O3 ^{xi}	3.698 (3)		
O3—Cs1—O3 ⁱ	166.65 (9)	O1 ^{vi} —Cs2—As ^{xi}	102.94 (4)
O3—Cs1—O3 ⁱⁱ	119.30 (9)	O1 ^{vii} —Cs2—As ^{xi}	88.69 (5)
O3 ⁱ —Cs1—O3 ⁱⁱ	69.82 (7)	O1 ^{viii} —Cs2—As ^{xi}	25.24 (4)
O3—Cs1—O3 ⁱⁱⁱ	69.82 (7)	O3 ^{ix} —Cs2—As ^{xi}	61.32 (4)
O3 ⁱ —Cs1—O3 ⁱⁱⁱ	103.15 (9)	O3 ^x —Cs2—As ^{xi}	94.72 (4)
O3 ⁱⁱ —Cs1—O3 ⁱⁱⁱ	166.65 (10)	O3 ^{xi} —Cs2—As ^{xi}	26.48 (4)
O3—Cs1—O3 ^{iv}	69.82 (7)	O4 ^{xii} —Cs2—As ^{xi}	70.49 (4)
O3 ⁱ —Cs1—O3 ^{iv}	119.30 (10)	O4 ^{xiii} —Cs2—As ^{xi}	25.47 (3)
O3 ⁱⁱ —Cs1—O3 ^{iv}	103.15 (9)	O4 ^{xiv} —Cs2—As ^{xi}	53.44 (4)
O3 ⁱⁱⁱ —Cs1—O3 ^{iv}	69.82 (7)	O3 ^{iv} —Cs2—As ^{ix}	107.26 (5)
O3—Cs1—O3 ^v	103.15 (9)	O3 ⁱⁱⁱ —Cs2—As ^{ix}	174.10 (5)
O3 ⁱ —Cs1—O3 ^v	69.82 (7)	O3—Cs2—As ^{ix}	100.69 (5)
O3 ⁱⁱ —Cs1—O3 ^v	69.82 (7)	O1 ^{vi} —Cs2—As ^{ix}	25.24 (4)
O3 ⁱⁱⁱ —Cs1—O3 ^v	119.30 (9)	O1 ^{vii} —Cs2—As ^{ix}	102.94 (4)
O3 ^{iv} —Cs1—O3 ^v	166.65 (9)	O1 ^{viii} —Cs2—As ^{ix}	88.69 (5)
O3—Cs1—O2	47.28 (6)	O3 ^{ix} —Cs2—As ^{ix}	26.48 (4)
O3 ⁱ —Cs1—O2	119.81 (6)	O3 ^x —Cs2—As ^{ix}	61.32 (4)
O3 ⁱⁱ —Cs1—O2	126.64 (6)	O3 ^{xi} —Cs2—As ^{ix}	94.72 (4)
O3 ⁱⁱⁱ —Cs1—O2	66.62 (6)	O4 ^{xii} —Cs2—As ^{ix}	25.47 (3)
O3 ^{iv} —Cs1—O2	111.83 (6)	O4 ^{xiii} —Cs2—As ^{ix}	53.44 (4)
O3 ^v —Cs1—O2	67.00 (6)	O4 ^{xiv} —Cs2—As ^{ix}	70.49 (4)
O3—Cs1—O2 ⁱⁱ	126.65 (6)	As ^{xi} —Cs2—As ^{ix}	78.314 (13)
O3 ⁱ —Cs1—O2 ⁱⁱ	66.61 (6)	O3 ^{iv} —Cs2—As ^x	100.69 (5)
O3 ⁱⁱ —Cs1—O2 ⁱⁱ	47.28 (6)	O3 ⁱⁱⁱ —Cs2—As ^x	107.26 (5)
O3 ⁱⁱⁱ —Cs1—O2 ⁱⁱ	119.81 (6)	O3—Cs2—As ^x	174.10 (5)
O3 ^{iv} —Cs1—O2 ⁱⁱ	67.01 (6)	O1 ^{vi} —Cs2—As ^x	88.69 (5)
O3 ^v —Cs1—O2 ⁱⁱ	111.83 (6)	O1 ^{vii} —Cs2—As ^x	25.24 (4)
O2—Cs1—O2 ⁱⁱ	170.75 (8)	O1 ^{viii} —Cs2—As ^x	102.94 (4)
O3—Cs1—O2 ^v	67.01 (6)	O3 ^{ix} —Cs2—As ^x	94.72 (4)
O3 ⁱ —Cs1—O2 ^v	111.83 (6)	O3 ^x —Cs2—As ^x	26.48 (4)
O3 ⁱⁱ —Cs1—O2 ^v	66.61 (6)	O3 ^{xi} —Cs2—As ^x	61.32 (4)
O3 ⁱⁱⁱ —Cs1—O2 ^v	126.65 (6)	O4 ^{xii} —Cs2—As ^x	53.44 (4)
O3 ^{iv} —Cs1—O2 ^v	119.81 (6)	O4 ^{xiii} —Cs2—As ^x	70.49 (4)
O3 ^v —Cs1—O2 ^v	47.28 (6)	O4 ^{xiv} —Cs2—As ^x	25.47 (4)
O2—Cs1—O2 ^v	61.36 (8)	As ^{xi} —Cs2—As ^x	78.314 (13)
O2 ⁱⁱ —Cs1—O2 ^v	110.71 (3)	As ^{ix} —Cs2—As ^x	78.314 (13)

O3—Cs1—O2 ⁱⁱⁱ	111.83 (6)	O2 ^{xv} —In1—O2 ⁱⁱⁱ	91.11 (9)
O3 ⁱ —Cs1—O2 ⁱⁱⁱ	67.01 (6)	O2 ^{xv} —In1—O2 ^{xvi}	91.11 (9)
O3 ⁱⁱ —Cs1—O2 ⁱⁱⁱ	119.81 (6)	O2 ⁱⁱⁱ —In1—O2 ^{xvi}	91.11 (9)
O3 ⁱⁱⁱ —Cs1—O2 ⁱⁱⁱ	47.28 (6)	O2 ^{xv} —In1—O4 ^{xvii}	92.57 (9)
O3 ^{iv} —Cs1—O2 ⁱⁱⁱ	66.61 (6)	O2 ⁱⁱⁱ —In1—O4 ^{xvii}	175.38 (9)
O3 ^v —Cs1—O2 ⁱⁱⁱ	126.65 (6)	O2 ^{xvi} —In1—O4 ^{xvii}	91.61 (9)
O2—Cs1—O2 ⁱⁱⁱ	110.71 (3)	O2 ^{xv} —In1—O4 ^{iv}	91.61 (8)
O2 ⁱⁱ —Cs1—O2 ⁱⁱⁱ	77.59 (7)	O2 ⁱⁱⁱ —In1—O4 ^{iv}	92.57 (9)
O2 ^v —Cs1—O2 ⁱⁱⁱ	170.75 (8)	O2 ^{xvi} —In1—O4 ^{iv}	175.38 (9)
O3—Cs1—O2 ⁱ	119.82 (6)	O4 ^{xvii} —In1—O4 ^{iv}	84.54 (9)
O3 ⁱ —Cs1—O2 ⁱ	47.28 (6)	O2 ^{xv} —In1—O4 ^{xviii}	175.38 (9)
O3 ⁱⁱ —Cs1—O2 ⁱ	111.83 (6)	O2 ⁱⁱⁱ —In1—O4 ^{xviii}	91.61 (9)
O3 ⁱⁱⁱ —Cs1—O2 ⁱ	67.01 (6)	O2 ^{xvi} —In1—O4 ^{xviii}	92.57 (9)
O3 ^{iv} —Cs1—O2 ⁱ	126.65 (6)	O4 ^{xvii} —In1—O4 ^{xviii}	84.54 (9)
O3 ^v —Cs1—O2 ⁱ	66.61 (6)	O4 ^{iv} —In1—O4 ^{xviii}	84.54 (9)
O2—Cs1—O2 ⁱ	77.59 (7)	O2 ^{xv} —In1—Cs2 ^{xxi}	124.48 (6)
O2 ⁱⁱ —Cs1—O2 ⁱ	110.71 (3)	O2 ⁱⁱⁱ —In1—Cs2 ^{xxi}	124.48 (6)
O2 ^v —Cs1—O2 ⁱ	110.71 (3)	O2 ^{xvi} —In1—Cs2 ^{xxi}	124.48 (6)
O2 ⁱⁱⁱ —Cs1—O2 ⁱ	61.36 (8)	O4 ^{xvii} —In1—Cs2 ^{xxi}	50.96 (6)
O3—Cs1—O2 ^{iv}	66.61 (6)	O4 ^{iv} —In1—Cs2 ^{xxi}	50.96 (6)
O3 ⁱ —Cs1—O2 ^{iv}	126.65 (6)	O4 ^{xviii} —In1—Cs2 ^{xxi}	50.96 (6)
O3 ⁱⁱ —Cs1—O2 ^{iv}	67.01 (6)	O1 ^{vii} —In2—O1 ^{xi}	94.56 (9)
O3 ⁱⁱⁱ —Cs1—O2 ^{iv}	111.83 (6)	O1 ^{vii} —In2—O1 ^{xix}	94.55 (9)
O3 ^{iv} —Cs1—O2 ^{iv}	47.28 (6)	O1 ^{xi} —In2—O1 ^{xix}	94.55 (9)
O3 ^v —Cs1—O2 ^{iv}	119.81 (6)	O1 ^{vii} —In2—O1 ^{iv}	180.0
O2—Cs1—O2 ^{iv}	110.71 (3)	O1 ^{xi} —In2—O1 ^{iv}	85.45 (9)
O2 ⁱⁱ —Cs1—O2 ^{iv}	61.36 (8)	O1 ^{xix} —In2—O1 ^{iv}	85.45 (9)
O2 ^v —Cs1—O2 ^{iv}	77.59 (7)	O1 ^{vii} —In2—O1 ^{xviii}	85.45 (9)
O2 ⁱⁱⁱ —Cs1—O2 ^{iv}	110.71 (3)	O1 ^{xi} —In2—O1 ^{xviii}	180.0
O2 ⁱ —Cs1—O2 ^{iv}	170.75 (8)	O1 ^{xix} —In2—O1 ^{xviii}	85.45 (9)
O3—Cs1—H	13.9 (5)	O1 ^{iv} —In2—O1 ^{xviii}	94.55 (9)
O3 ⁱ —Cs1—H	170.1 (7)	O1 ^{vii} —In2—O1 ^{xvii}	85.45 (9)
O3 ⁱⁱ —Cs1—H	105.5 (5)	O1 ^{xi} —In2—O1 ^{xvii}	85.45 (9)
O3 ⁱⁱⁱ —Cs1—H	83.1 (5)	O1 ^{xix} —In2—O1 ^{xvii}	180.0
O3 ^{iv} —Cs1—H	69.8 (6)	O1 ^{iv} —In2—O1 ^{xvii}	94.55 (9)
O3 ^v —Cs1—H	100.5 (7)	O1 ^{xviii} —In2—O1 ^{xvii}	94.55 (9)
O2—Cs1—H	55.4 (6)	O1 ^{vii} —In2—Cs2 ^{xix}	56.94 (8)
O2 ⁱⁱ —Cs1—H	117.1 (6)	O1 ^{xi} —In2—Cs2 ^{xix}	72.56 (8)
O2 ^v —Cs1—H	58.5 (6)	O1 ^{xix} —In2—Cs2 ^{xix}	146.29 (7)
O2 ⁱⁱⁱ —Cs1—H	122.2 (6)	O1 ^{iv} —In2—Cs2 ^{xix}	123.06 (8)
O2 ⁱ —Cs1—H	131.7 (6)	O1 ^{xviii} —In2—Cs2 ^{xix}	107.44 (8)
O2 ^{iv} —Cs1—H	55.8 (6)	O1 ^{xvii} —In2—Cs2 ^{xix}	33.71 (7)
O3—Cs1—H ^{iv}	83.1 (5)	O1 ^{vii} —In2—Cs2 ^{xvii}	123.06 (8)
O3 ⁱ —Cs1—H ^{iv}	105.5 (6)	O1 ^{xi} —In2—Cs2 ^{xvii}	107.44 (8)
O3 ⁱⁱ —Cs1—H ^{iv}	100.5 (6)	O1 ^{xix} —In2—Cs2 ^{xvii}	33.71 (7)
O3 ⁱⁱⁱ —Cs1—H ^{iv}	69.8 (6)	O1 ^{iv} —In2—Cs2 ^{xvii}	56.94 (8)
O3 ^{iv} —Cs1—H ^{iv}	13.9 (5)	O1 ^{xviii} —In2—Cs2 ^{xvii}	72.56 (8)
O3 ^v —Cs1—H ^{iv}	170.2 (6)	O1 ^{xvii} —In2—Cs2 ^{xvii}	146.29 (7)

O2—Cs1—H ^{iv}	122.2 (6)	Cs2 ^{xix} —In2—Cs2 ^{xvii}	180.0
O2 ⁱⁱ —Cs1—H ^{iv}	58.5 (6)	O1 ^{vii} —In2—Cs2	33.71 (7)
O2 ^v —Cs1—H ^{iv}	131.7 (6)	O1 ^{xi} —In2—Cs2	123.06 (8)
O2 ⁱⁱⁱ —Cs1—H ^{iv}	55.8 (6)	O1 ^{xix} —In2—Cs2	107.44 (8)
O2 ⁱ —Cs1—H ^{iv}	117.1 (6)	O1 ^{iv} —In2—Cs2	146.29 (7)
O2 ^{iv} —Cs1—H ^{iv}	55.4 (6)	O1 ^{xviii} —In2—Cs2	56.94 (8)
H—Cs1—H ^{iv}	83.7 (8)	O1 ^{xvii} —In2—Cs2	72.56 (8)
O3—Cs1—H ⁱⁱⁱ	69.8 (6)	Cs2 ^{xix} —In2—Cs2	60.0
O3 ⁱ —Cs1—H ⁱⁱⁱ	100.5 (6)	Cs2 ^{xvii} —In2—Cs2	120.0
O3 ⁱⁱ —Cs1—H ⁱⁱⁱ	170.2 (6)	O1 ^{vii} —In2—Cs2 ^{xvi}	107.44 (8)
O3 ⁱⁱⁱ —Cs1—H ⁱⁱⁱ	13.9 (5)	O1 ^{xi} —In2—Cs2 ^{xvi}	33.71 (7)
O3 ^{iv} —Cs1—H ⁱⁱⁱ	83.1 (5)	O1 ^{xix} —In2—Cs2 ^{xvi}	123.06 (8)
O3 ^v —Cs1—H ⁱⁱⁱ	105.5 (5)	O1 ^{iv} —In2—Cs2 ^{xvi}	72.56 (8)
O2—Cs1—H ⁱⁱⁱ	55.8 (6)	O1 ^{xviii} —In2—Cs2 ^{xvi}	146.29 (7)
O2 ⁱⁱ —Cs1—H ⁱⁱⁱ	131.7 (6)	O1 ^{xvii} —In2—Cs2 ^{xvi}	56.94 (8)
O2 ^v —Cs1—H ⁱⁱⁱ	117.1 (7)	Cs2 ^{xix} —In2—Cs2 ^{xvi}	60.0
O2 ⁱⁱⁱ —Cs1—H ⁱⁱⁱ	55.4 (6)	Cs2 ^{xvii} —In2—Cs2 ^{xvi}	120.0
O2 ⁱ —Cs1—H ⁱⁱⁱ	58.5 (6)	Cs2—In2—Cs2 ^{xvi}	120.0
O2 ^{iv} —Cs1—H ⁱⁱⁱ	122.2 (6)	O1 ^{vii} —In2—Cs2 ^{xxii}	72.56 (8)
H—Cs1—H ⁱⁱⁱ	83.7 (8)	O1 ^{xi} —In2—Cs2 ^{xxii}	146.29 (7)
H ^{iv} —Cs1—H ⁱⁱⁱ	83.7 (8)	O1 ^{xix} —In2—Cs2 ^{xxii}	56.94 (8)
O3 ^{iv} —Cs2—O3 ⁱⁱⁱ	73.97 (8)	O1 ^{iv} —In2—Cs2 ^{xxii}	107.44 (8)
O3 ^{iv} —Cs2—O3	73.97 (8)	O1 ^{xviii} —In2—Cs2 ^{xxii}	33.71 (7)
O3 ⁱⁱⁱ —Cs2—O3	73.97 (8)	O1 ^{xvii} —In2—Cs2 ^{xxii}	123.06 (8)
O3 ^{iv} —Cs2—O1 ^{vi}	82.81 (6)	Cs2 ^{xix} —In2—Cs2 ^{xxii}	120.0
O3 ⁱⁱⁱ —Cs2—O1 ^{vi}	153.75 (6)	Cs2 ^{xvii} —In2—Cs2 ^{xxii}	60.0
O3—Cs2—O1 ^{vi}	88.16 (7)	Cs2—In2—Cs2 ^{xxii}	60.0
O3 ^{iv} —Cs2—O1 ^{vii}	88.16 (7)	Cs2 ^{xvi} —In2—Cs2 ^{xxii}	180.0
O3 ⁱⁱⁱ —Cs2—O1 ^{vii}	82.80 (7)	O1 ^{vii} —In2—Cs2 ^{xxiii}	146.29 (7)
O3—Cs2—O1 ^{vii}	153.75 (7)	O1 ^{xi} —In2—Cs2 ^{xxiii}	56.94 (8)
O1 ^{vi} —Cs2—O1 ^{vii}	108.90 (4)	O1 ^{xix} —In2—Cs2 ^{xxiii}	72.56 (8)
O3 ^{iv} —Cs2—O1 ^{viii}	153.75 (7)	O1 ^{iv} —In2—Cs2 ^{xxiii}	33.71 (7)
O3 ⁱⁱⁱ —Cs2—O1 ^{viii}	88.16 (7)	O1 ^{xviii} —In2—Cs2 ^{xxiii}	123.06 (8)
O3—Cs2—O1 ^{viii}	82.81 (6)	O1 ^{xvii} —In2—Cs2 ^{xxiii}	107.44 (8)
O1 ^{vi} —Cs2—O1 ^{viii}	108.90 (4)	Cs2 ^{xix} —In2—Cs2 ^{xxiii}	120.0
O1 ^{vii} —Cs2—O1 ^{viii}	108.90 (4)	Cs2 ^{xvii} —In2—Cs2 ^{xxiii}	60.0
O3 ^{iv} —Cs2—O3 ^{ix}	124.57 (9)	Cs2—In2—Cs2 ^{xxiii}	180.0
O3 ⁱⁱⁱ —Cs2—O3 ^{ix}	148.48 (9)	Cs2 ^{xvi} —In2—Cs2 ^{xxiii}	60.0
O3—Cs2—O3 ^{ix}	86.50 (7)	Cs2 ^{xxii} —In2—Cs2 ^{xxiii}	120.0
O1 ^{vi} —Cs2—O3 ^{ix}	44.45 (6)	O1 ^{xx} —As—O2	117.25 (12)
O1 ^{vii} —Cs2—O3 ^{ix}	119.69 (6)	O1 ^{xx} —As—O4 ⁱⁱ	108.41 (12)
O1 ^{viii} —Cs2—O3 ^{ix}	64.61 (6)	O2—As—O4 ⁱⁱ	113.77 (11)
O3 ^{iv} —Cs2—O3 ^x	86.50 (7)	O1 ^{xx} —As—O3	105.44 (13)
O3 ⁱⁱⁱ —Cs2—O3 ^x	124.56 (9)	O2—As—O3	104.33 (12)
O3—Cs2—O3 ^x	148.48 (8)	O4 ⁱⁱ —As—O3	106.72 (11)
O1 ^{vi} —Cs2—O3 ^x	64.61 (6)	O1 ^{xx} —As—Cs2 ^{ix}	61.74 (9)
O1 ^{vii} —Cs2—O3 ^x	44.45 (6)	O2—As—Cs2 ^{ix}	174.14 (8)
O1 ^{viii} —Cs2—O3 ^x	119.69 (6)	O4 ⁱⁱ —As—Cs2 ^{ix}	71.50 (8)

O3 ^{ix} —Cs2—O3 ^x	84.57 (6)	O3—As—Cs2 ^{ix}	71.06 (9)
O3 ^{iv} —Cs2—O3 ^{xi}	148.48 (9)	O1 ^{xx} —As—Cs1	139.73 (11)
O3 ⁱⁱⁱ —Cs2—O3 ^{xi}	86.50 (7)	O2—As—Cs1	55.91 (8)
O3—Cs2—O3 ^{xi}	124.57 (9)	O4 ⁱⁱ —As—Cs1	109.82 (8)
O1 ^{vi} —Cs2—O3 ^{xi}	119.69 (6)	O3—As—Cs1	51.15 (9)
O1 ^{vii} —Cs2—O3 ^{xi}	64.61 (6)	Cs2 ^{ix} —As—Cs1	120.598 (10)
O1 ^{viii} —Cs2—O3 ^{xi}	44.45 (6)	O1 ^{xx} —As—Cs2	75.26 (11)
O3 ^{ix} —Cs2—O3 ^{xi}	84.57 (6)	O2—As—Cs2	99.50 (8)
O3 ^x —Cs2—O3 ^{xi}	84.57 (6)	O4 ⁱⁱ —As—Cs2	138.02 (8)
O3 ^{iv} —Cs2—O4 ^{xii}	113.69 (6)	O3—As—Cs2	37.36 (8)
O3 ⁱⁱⁱ —Cs2—O4 ^{xii}	159.43 (6)	Cs2 ^{ix} —As—Cs2	74.638 (9)
O3—Cs2—O4 ^{xii}	126.02 (6)	Cs1—As—Cs2	68.078 (14)
O1 ^{vi} —Cs2—O4 ^{xii}	44.41 (5)	As ^{xxiv} —O1—In2 ^{xxv}	140.67 (15)
O1 ^{vii} —Cs2—O4 ^{xii}	78.54 (5)	As ^{xxiv} —O1—Cs2 ^{vi}	93.02 (10)
O1 ^{viii} —Cs2—O4 ^{xii}	89.74 (5)	In2 ^{xxv} —O1—Cs2 ^{vi}	126.03 (9)
O3 ^{ix} —Cs2—O4 ^{xii}	43.56 (5)	As ^{xxiv} —O1—Cs2 ^{xxiv}	82.42 (10)
O3 ^x —Cs2—O4 ^{xii}	41.47 (5)	In2 ^{xxv} —O1—Cs2 ^{xxiv}	97.96 (9)
O3 ^{xi} —Cs2—O4 ^{xii}	77.76 (5)	Cs2 ^{vi} —O1—Cs2 ^{xxiv}	80.74 (5)
O3 ^{iv} —Cs2—O4 ^{xiii}	159.43 (6)	As ^{xxiv} —O1—Cs2 ^{xxv}	118.31 (12)
O3 ⁱⁱⁱ —Cs2—O4 ^{xiii}	126.02 (6)	In2 ^{xxv} —O1—Cs2 ^{xxv}	82.33 (8)
O3—Cs2—O4 ^{xiii}	113.70 (7)	Cs2 ^{vi} —O1—Cs2 ^{xxv}	72.50 (5)
O1 ^{vi} —Cs2—O4 ^{xiii}	78.54 (5)	Cs2 ^{xxiv} —O1—Cs2 ^{xxv}	146.39 (6)
O1 ^{vii} —Cs2—O4 ^{xiii}	89.74 (6)	As—O2—In1 ^{xxvi}	122.05 (12)
O1 ^{viii} —Cs2—O4 ^{xiii}	44.41 (5)	As—O2—Cs1	100.33 (9)
O3 ^{ix} —Cs2—O4 ^{xiii}	41.47 (5)	In1 ^{xxvi} —O2—Cs1	125.68 (9)
O3 ^x —Cs2—O4 ^{xiii}	77.76 (5)	As—O2—Cs2	60.78 (7)
O3 ^{xi} —Cs2—O4 ^{xiii}	43.56 (5)	In1 ^{xxvi} —O2—Cs2	162.87 (9)
O4 ^{xii} —Cs2—O4 ^{xiii}	45.97 (6)	Cs1—O2—Cs2	66.29 (4)
O3 ^{iv} —Cs2—O4 ^{xiv}	126.02 (6)	As—O3—Cs2	122.83 (12)
O3 ⁱⁱⁱ —Cs2—O4 ^{xiv}	113.69 (6)	As—O3—Cs1	104.40 (11)
O3—Cs2—O4 ^{xiv}	159.43 (6)	Cs2—O3—Cs1	94.64 (7)
O1 ^{vi} —Cs2—O4 ^{xiv}	89.74 (5)	As—O3—Cs2 ^{ix}	82.46 (10)
O1 ^{vii} —Cs2—O4 ^{xiv}	44.41 (5)	Cs2—O3—Cs2 ^{ix}	93.50 (7)
O1 ^{viii} —Cs2—O4 ^{xiv}	78.53 (5)	Cs1—O3—Cs2 ^{ix}	164.05 (8)
O3 ^{ix} —Cs2—O4 ^{xiv}	77.76 (5)	As—O3—H	107 (3)
O3 ^x —Cs2—O4 ^{xiv}	43.56 (5)	Cs2—O3—H	124 (3)
O3 ^{xi} —Cs2—O4 ^{xiv}	41.47 (5)	Cs1—O3—H	94 (3)
O4 ^{xii} —Cs2—O4 ^{xiv}	45.97 (6)	Cs2 ^{ix} —O3—H	70 (3)
O4 ^{xiii} —Cs2—O4 ^{xiv}	45.97 (6)	As ⁱⁱ —O4—In1 ^{xxv}	129.32 (12)
O3 ^{iv} —Cs2—As ^{xi}	174.10 (5)	As ⁱⁱ —O4—Cs2 ^{xxvii}	83.03 (8)
O3 ⁱⁱⁱ —Cs2—As ^{xi}	100.69 (5)	In1 ^{xxv} —O4—Cs2 ^{xxvii}	102.24 (8)
O3—Cs2—As ^{xi}	107.26 (5)		

Symmetry codes: (i) $x-y, -y, -z+3/2$; (ii) $-x, -x+y, -z+3/2$; (iii) $-x+y, -x, z$; (iv) $-y, x-y, z$; (v) $y, x, -z+3/2$; (vi) $-x+2/3, -y-2/3, -z+4/3$; (vii) $y+2/3, -x+y+4/3, -z+4/3$; (viii) $x-y-4/3, x-2/3, -z+4/3$; (ix) $-x-1/3, -y-2/3, -z+4/3$; (x) $y+2/3, -x+y+1/3, -z+4/3$; (xi) $x-y-1/3, x+1/3, -z+4/3$; (xii) $x-1/3, x-y-2/3, z-1/6$; (xiii) $-y-1/3, -x+1/3, z-1/6$; (xiv) $-x+y+2/3, y+1/3, z-1/6$; (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) $x+1, y, z$; (xxv) $x, y-1, z$; (xxvi) $x-1, y-1, z$; (xxvii) $-y+1/3, -x-1/3, z+1/6$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H $\cdots$ O4 ^{xxviii}	0.83 (3)	1.80 (3)	2.621 (3)	170 (4)

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