

Crystal structure of CsCrAs₂O₇, a new member of the diarsenate family

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Caesium chromium(III) diarsenate(V), CsCrAs₂O₇, was prepared by solid-state reactions. The title structure consists of isolated CrO₆ octahedra and As₂O₇ diarsenate groups, sharing corners to build up a three-dimensional [CrAs₂O₇][−] anionic framework. In this framework, channels extending parallel to [001] are present in which the ten-coordinate Cs⁺ ions reside. CsCrAs₂O₇ is isotypic with the monoclinic *A*^I*M*^{III}*X*₂O₇ (*A*^I = alkali metal; *M*^{III} = Al, Cr, Fe; *X* = As, P) type I family of compounds crystallizing in the space group *P*2₁/*c*.

1. Chemical context

In recent years, inorganic metal phosphates and arsenates with formula *A*^I*M*^{III}*X*₂O₇ (*A*^I = alkali metal; *M*^{III} = Al, Cr, Fe; *X* = As, P) have been part of intensive research activities, with crystals grown either from high-temperature solid-state reactions or under aqueous solution conditions. The crystal chemistry of these compounds with *X*₂O₇ groups reveals a large structural variety accompanied in some cases by interesting magnetic, electric, optical, or thermal expansion properties. Focusing on compounds with *M*^{III} = Cr, it is noticeable that corresponding diphosphates have been studied extensively, in contrast to the scarcely studied chromium diarsenates. Herein the preparation and crystal structure of

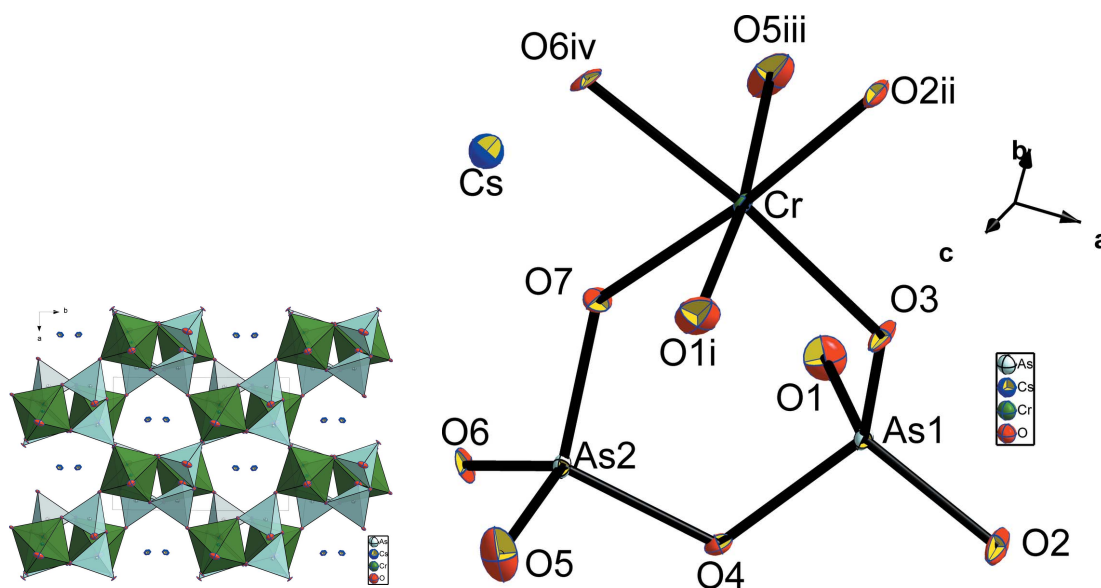


Figure 1
The coordination polyhedra around Cr and As atoms in the title structure. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $2 - x, \frac{1}{2} + y, \frac{3}{2} - z$; (iii) $x, \frac{1}{2} - y, -\frac{1}{2} + z$; (iv) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$.]

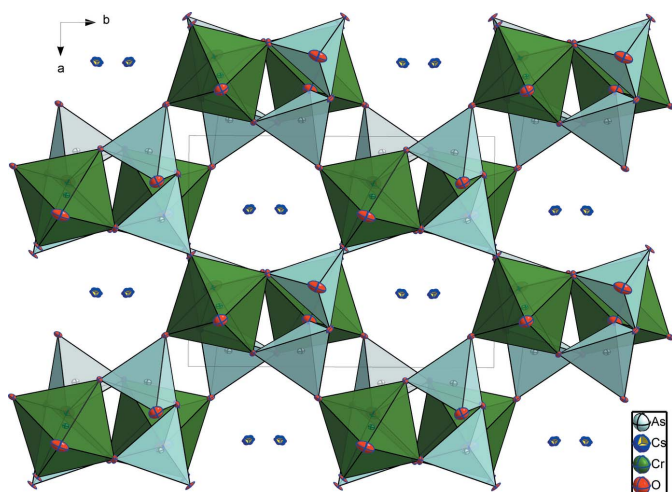


Figure 2
Projection of the $\text{CsCrAs}_2\text{O}_7$ structure showing the channels parallel to $[001]$ in which the Cs^+ cations are located.

$\text{CsCrAs}_2\text{O}_7$ is reported, one of a series of new cesium chromium(III) arsenate compounds recently isolated by our group.

2. Structural commentary

The structure of $\text{CsCrAs}_2\text{O}_7$ can be described as a three-dimensional $[\text{CrAs}_2\text{O}_7]^-$ anionic framework (Fig. 1) with channels extending parallel to $[001]$ that are occupied by ten-coordinate Cs^+ cations (Fig. 2).

The two independent arsenic atoms form AsO_4 tetrahedra and are connected *via* the bridging O4 atom into a diarsenate As_2O_7 anion. Like in the related structures of KAlAs_2O_7

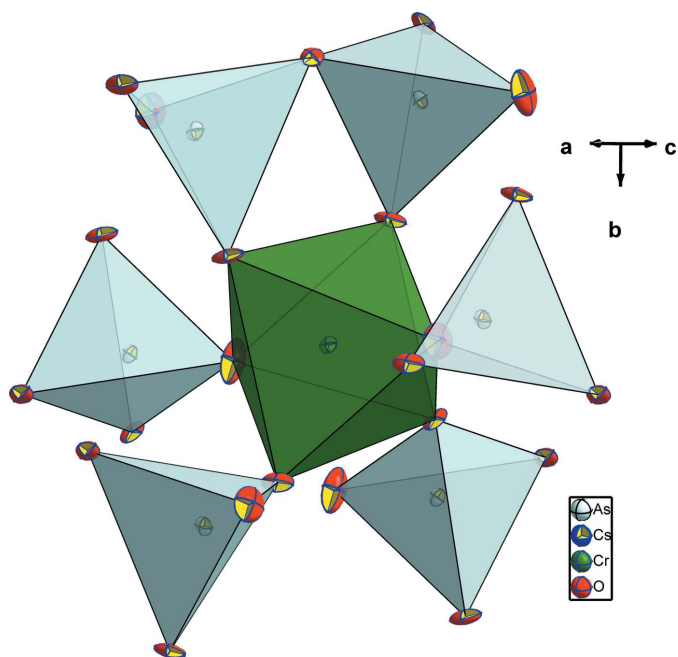


Figure 3
The environment of the CrO_6 octahedron in the structure of $\text{CsCrAs}_2\text{O}_7$.

Table 1
Selected bond lengths (\AA).

$\text{Cr}-\text{O}^{\text{I}}$	1.944 (4)	$\text{As1}-\text{O2}$	1.664 (4)
$\text{Cr}-\text{O7}$	1.954 (4)	$\text{As1}-\text{O3}$	1.681 (4)
$\text{Cr}-\text{O1}^{\text{II}}$	1.978 (4)	$\text{As1}-\text{O4}$	1.763 (4)
$\text{Cr}-\text{O3}$	1.982 (4)	$\text{As2}-\text{O5}$	1.641 (4)
$\text{Cr}-\text{O2}^{\text{III}}$	2.007 (4)	$\text{As2}-\text{O6}$	1.661 (4)
$\text{Cr}-\text{O6}^{\text{IV}}$	2.010 (4)	$\text{As2}-\text{O7}$	1.669 (4)
$\text{As1}-\text{O1}$	1.651 (4)	$\text{As2}-\text{O4}$	1.750 (4)

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (iii) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$; (iv) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

(Boughzala & Jouini, 1995) and $\text{RbAlAs}_2\text{O}_7$ (Boughzala *et al.*, 1993), the $\text{As}-\text{O}$ distances involving the bridging O4 atom are the longest (Table 1). The $\text{As1}-\text{O4}-\text{As2}$ bridging angle of $118.7(2)^\circ$ in the title structure is somewhat smaller than that of $125.9(2)^\circ$ reported for the isotypic structure of CsCrP_2O_7 (Linde & Gorbunova, 1982). The $\text{O}-\text{As}-\text{O}$ bond angles span a range between $103.8(2)$ and $116.2(2)^\circ$ and $105.5(2)$ and $115.6(2)^\circ$, respectively, for As1 and As2, reflecting the distortion of each of the AsO_4 tetrahedra. The Cr^{III} cations are in a slightly distorted octahedral oxygen coordination with $\text{Cr}-\text{O}$ distances ranging from 1.944 (4) to 2.010 (4) \AA (Table 1), and with $\text{O}-\text{Cr}-\text{O}$ angles ranging from $82.96(18)$ to $95.94(17)^\circ$ and from $172.37(19)$ to $173.72(17)^\circ$. Each CrO_6 octahedron shares its corners with five As_2O_7 anions, one of which is chelating and the others belonging to four different As_2O_7 groups (Fig. 3). On the other hand, each As_2O_7 anion is surrounded by five CrO_6 octahedra as depicted in Fig. 4. The environment of the ten-coordinate Cs^+ cation situated in the cavities of the resulting $[\text{CrAs}_2\text{O}_7]^-$ framework is shown in Fig. 5.

It is worth mentioning that in the related aluminium diarsenate family $A^{\text{I}}\text{AlAs}_2\text{O}_7$ ($A^{\text{I}} = \text{K}, \text{Rb}, \text{Tl}, \text{Cs}$) (Boughzala & Jouini, 1992) that crystallizes isotypically in space group $P\bar{1}$ and is classified as type II, the diarsenate groups have a different conformational orientation as those of the title

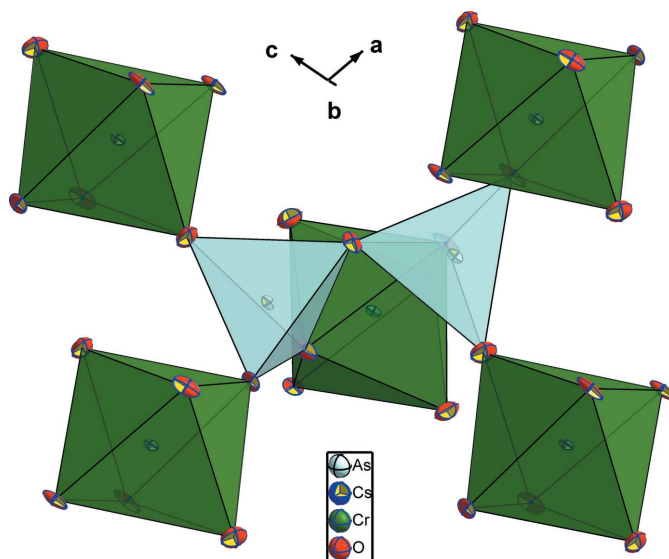


Figure 4
The environment of the diarsenate group in the structure of $\text{CsCrAs}_2\text{O}_7$.

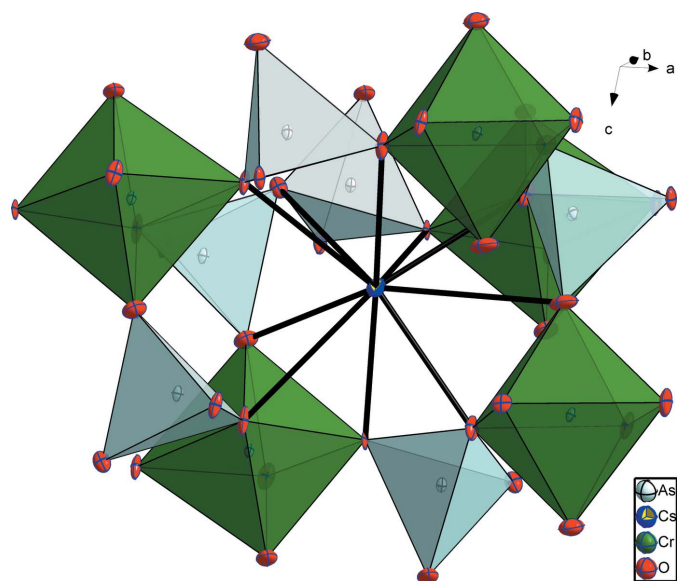


Figure 5
The surrounding of the ten-coordinated Cs^+ cation in the structure of $\text{CsCrAs}_2\text{O}_7$.

structure. In the title structure, belonging to the type I family of $A^{\text{I}}M^{\text{III}}X_2\text{O}_7$ diarsenates, the diarsenate tetrahedra are in a nearly eclipsed conformation with a torsion angle $\text{O}3-\text{As}1-\text{As}2-\text{O}7$ of $39.8(2)^\circ$, as shown in Fig. 6. The corresponding angle is $158.8(2)^\circ$ for KAlAs_2O_7 (Boughzala & Jouini, 1995).

Using the bond-valence method (Brown, 2002), the calculated bond-valence-sum values (in valence units) of 5.08, 4.97, 3.01 and 1.35, respectively, for As1, As2, Cr and Cs are in good agreement with the expected oxidation states.

3. Database survey

The structure of KAlP_2O_7 (Ng & Calvo, 1973) was the first published of the $A^{\text{I}}M^{\text{III}}X_2\text{O}_7$ family. Afterwards, based on different substitutions and combinations, a large number of

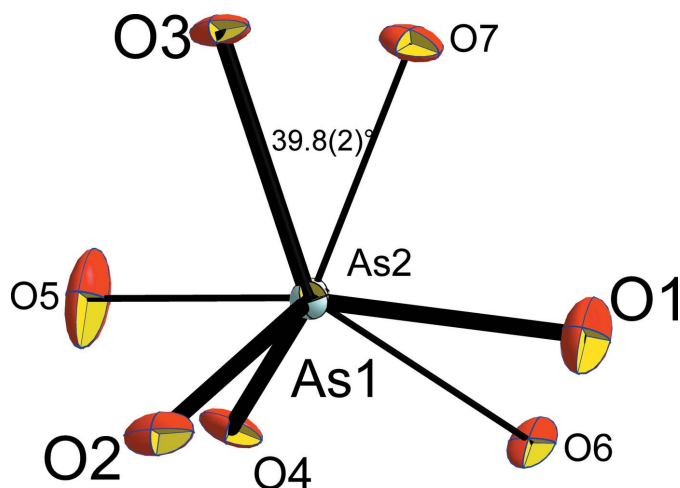


Figure 6
View parallel to the $\text{As}1-\text{As}2$ direction, emphasizing the nearly eclipsed conformation of the diarsenate anion.

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{CsCrAs}_2\text{O}_7$
M_r	446.75
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	7.908 (1), 10.0806 (10), 8.6371 (10)
β ($^\circ$)	105.841 (1)
V (Å ³)	662.38 (13)
Z	4
Radiation type	
	Mo $K\alpha$
μ (mm ⁻¹)	17.05
Crystal size (mm)	0.20 × 0.20 × 0.10
Data collection	
Diffractometer	Enraf–Nonius CAD-4
Absorption correction	ψ scan (North <i>et al.</i> , 1968)
$T_{\text{min}}, T_{\text{max}}$	0.132, 0.281
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1530, 1433, 1205
R_{int}	0.051
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.637
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.075, 1.13
No. of reflections	1433
No. of parameters	101
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.60, -1.23

Computer programs: *CAD-4 EXPRESS* (Enraf–Nonius, 1994), *XCAD4* (Harms & Wocadlo, 1995), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2008) and *pubCIF* (Westrip, 2010).

different phases were isolated and crystallographically characterized. Replacement of one of the cations can improve the structural and physical properties but also affects the coordination numbers, the degree of distortion of the coordination polyhedra and the conformation of the $X_2\text{O}_7$ groups. Also, the crystal symmetry can be affected. The structures are triclinic, in space group $P\bar{1}$ with two formula units, for the diarsenate compounds $A^{\text{I}}\text{AlAs}_2\text{O}_7$ ($A^{\text{I}} = \text{K, Rb, Tl, Cs}$) (Boughzala & Jouini, 1992; Boughzala *et al.*, 1993; Boughzala & Jouini, 1995), whereas diphosphates are generally monoclinic. The isotypic $A^{\text{I}}\text{CrP}_2\text{O}_7$ phases crystallize in space group $P2_1/c$ for $A^{\text{I}} = \text{Na}$ (Bohaty *et al.*, 1982), K (Gentil *et al.*, 1997), Rb (Zhao & Li, 2011) and Cs (Linde & Gorbunova, 1982). The same counts for the $A^{\text{I}}\text{FeP}_2\text{O}_7$ phases for $A^{\text{I}} = \text{Na}$ (Gabelica-Robert *et al.*, 1982) and K (Riou *et al.*, 1988). However, the two Li-containing phases LiMP_2O_7 show a symmetry reduction to space group $P2_1$ ($M = \text{Cr, Ivashkevich et al., 2007; M = Fe, Riou et al., 1990}$).

4. Synthesis and crystallization

The crystals of the title compound were obtained from heating a mixture of Cs_2CO_3 , Cr_2O_3 and $\text{NH}_4\text{H}_2\text{AsO}_4$, with a Cs:Cr:As molar ratio of 1:1:2. In order to eliminate volatile products, the sample was placed in a porcelain crucible and slowly heated under atmospheric conditions to 673 K and kept at that temperature for 24 h. In a second step, the crucible was progressively heated at 1023 K for 4 days and then slowly cooled down at a rate of 5 K/24 h to 923 K and finally

quenched to room temperature. The product was washed with water and rinsed with an aqueous solution of HCl. Two phases could be isolated. The major phase forms regular cube-shaped dark-green crystals of yet unknown composition. The second phase represents the title compound and was obtained in the form of pink crystals.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The maximum and minimum electron density in the final difference Fourier map is located at 0.95 Å, 0.87 Å, respectively, from the Cs atom.

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supporting information

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Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Caesium chromium (III) diarsenate

Crystal data

CsCrAs₂O₇

$M_r = 446.75$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.908$ (1) Å

$b = 10.0806$ (10) Å

$c = 8.6371$ (10) Å

$\beta = 105.841$ (1)°

$V = 662.38$ (13) Å³

$Z = 4$

$F(000) = 804$

$D_x = 4.480$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 3.8$ – 27°

$\mu = 17.05$ mm⁻¹

$T = 293$ K

Monoclinic, pink

$0.20 \times 0.20 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.132$, $T_{\max} = 0.281$

1530 measured reflections

1433 independent reflections

1205 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 26.9^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -10 \rightarrow 9$

$k = 0 \rightarrow 12$

$l = 0 \rightarrow 11$

2 standard reflections every 120 min

intensity decay: 1.1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.075$

$S = 1.13$

1433 reflections

101 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 1.1495P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.60$ e Å⁻³

$\Delta\rho_{\min} = -1.23$ e Å⁻³

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0018 (4)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
As1	0.93130 (7)	0.13138 (6)	0.68578 (6)	0.00527 (16)
As2	0.63567 (7)	0.08924 (5)	0.84021 (6)	0.00495 (16)
Cs	0.31839 (5)	0.19797 (4)	0.45751 (4)	0.01429 (15)
Cr	0.73911 (11)	0.39967 (8)	0.76602 (10)	0.0043 (2)
O1	0.8001 (6)	0.1049 (5)	0.5039 (5)	0.0168 (10)
O2	1.1355 (5)	0.0742 (4)	0.7202 (5)	0.0122 (9)
O3	0.9413 (5)	0.2889 (4)	0.7514 (5)	0.0099 (8)
O4	0.8363 (5)	0.0371 (4)	0.8122 (5)	0.0093 (8)
O5	0.6538 (6)	0.0802 (5)	1.0338 (5)	0.0199 (10)
O6	0.4833 (5)	−0.0082 (4)	0.7244 (5)	0.0085 (8)
O7	0.5967 (5)	0.2403 (4)	0.7594 (5)	0.0109 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.0033 (3)	0.0057 (3)	0.0069 (3)	0.0003 (2)	0.0014 (2)	−0.0003 (2)
As2	0.0034 (3)	0.0055 (3)	0.0059 (3)	−0.0009 (2)	0.0013 (2)	−0.0002 (2)
Cs	0.0106 (2)	0.0165 (2)	0.0136 (2)	−0.00201 (14)	−0.00033 (14)	0.00299 (14)
Cr	0.0026 (4)	0.0045 (4)	0.0055 (4)	0.0004 (3)	0.0005 (3)	−0.0002 (3)
O1	0.017 (2)	0.022 (2)	0.010 (2)	−0.0029 (19)	0.0010 (17)	−0.0022 (18)
O2	0.0044 (19)	0.007 (2)	0.025 (2)	−0.0020 (16)	0.0035 (16)	−0.0024 (17)
O3	0.0040 (18)	0.0045 (19)	0.020 (2)	0.0006 (15)	0.0012 (16)	−0.0032 (16)
O4	0.0077 (19)	0.0067 (19)	0.015 (2)	0.0038 (15)	0.0049 (15)	0.0035 (16)
O5	0.016 (2)	0.035 (3)	0.007 (2)	−0.009 (2)	0.0016 (17)	−0.0009 (18)
O6	0.0065 (19)	0.008 (2)	0.011 (2)	−0.0061 (16)	0.0024 (15)	−0.0007 (16)
O7	0.0074 (19)	0.0047 (19)	0.020 (2)	−0.0012 (16)	0.0018 (15)	0.0030 (17)

Geometric parameters (\AA , $^\circ$)

Cs—O7	2.948 (4)	Cr—O1 ^v	1.978 (4)
Cs—O3 ⁱ	3.030 (4)	Cr—O3	1.982 (4)
Cs—O6	3.113 (4)	Cr—O2 ^{vi}	2.007 (4)
Cs—O6 ⁱⁱ	3.152 (4)	Cr—O6 ^{vii}	2.010 (4)
Cs—O2 ⁱ	3.155 (4)	As1—O1	1.651 (4)
Cs—O7 ⁱⁱⁱ	3.196 (4)	As1—O2	1.664 (4)
Cs—O1 ⁱⁱ	3.237 (5)	As1—O3	1.681 (4)

Cs—O2 ^{iv}	3.253 (4)	As1—O4	1.763 (4)
Cs—O4 ⁱⁱ	3.314 (4)	As2—O5	1.641 (4)
Cs—O5 ⁱⁱⁱ	3.393 (5)	As2—O6	1.661 (4)
Cr—O5 ⁱⁱⁱ	1.944 (4)	As2—O7	1.669 (4)
Cr—O7	1.954 (4)	As2—O4	1.750 (4)
O1—As1—O2	116.2 (2)	O6 ⁱⁱ —Cs—O5 ⁱⁱⁱ	91.60 (11)
O1—As1—O3	115.7 (2)	O2 ⁱ —Cs—O5 ⁱⁱⁱ	80.89 (11)
O2—As1—O3	108.3 (2)	O7 ⁱⁱⁱ —Cs—O5 ⁱⁱⁱ	50.19 (10)
O1—As1—O4	103.8 (2)	O1 ⁱⁱ —Cs—O5 ⁱⁱⁱ	146.54 (11)
O2—As1—O4	105.1 (2)	O2 ^{iv} —Cs—O5 ⁱⁱⁱ	126.15 (10)
O3—As1—O4	106.8 (2)	O4 ⁱⁱ —Cs—O5 ⁱⁱⁱ	136.61 (10)
O5—As2—O6	115.3 (2)	O5 ⁱⁱⁱ —Cr—O7	91.2 (2)
O5—As2—O7	115.6 (2)	O5 ⁱⁱⁱ —Cr—O1 ^v	172.37 (19)
O6—As2—O7	105.5 (2)	O7—Cr—O1 ^v	89.22 (18)
O5—As2—O4	107.1 (2)	O5 ⁱⁱⁱ —Cr—O3	92.97 (19)
O6—As2—O4	105.98 (19)	O7—Cr—O3	90.21 (17)
O7—As2—O4	106.69 (19)	O1 ^v —Cr—O3	94.65 (19)
O7—Cs—O3 ⁱ	152.96 (12)	O5 ⁱⁱⁱ —Cr—O2 ^{vi}	89.8 (2)
O7—Cs—O6	51.76 (11)	O7—Cr—O2 ^{vi}	173.72 (17)
O3 ⁱ —Cs—O6	127.61 (10)	O1 ^v —Cr—O2 ^{vi}	88.99 (19)
O7—Cs—O6 ⁱⁱ	100.13 (11)	O3—Cr—O2 ^{vi}	95.94 (17)
O3 ⁱ —Cs—O6 ⁱⁱ	106.10 (11)	O5 ⁱⁱⁱ —Cr—O6 ^{vii}	86.15 (18)
O6—Cs—O6 ⁱⁱ	78.42 (11)	O7—Cr—O6 ^{vii}	82.96 (18)
O7—Cs—O2 ⁱ	124.64 (11)	O1 ^v —Cr—O6 ^{vii}	86.33 (18)
O3 ⁱ —Cs—O2 ⁱ	51.93 (11)	O3—Cr—O6 ^{vii}	173.08 (17)
O6—Cs—O2 ⁱ	172.88 (11)	O2 ^{vi} —Cr—O6 ^{vii}	90.92 (17)
O6 ⁱⁱ —Cs—O2 ⁱ	108.67 (11)	As1—O1—Cr ⁱⁱⁱ	154.6 (3)
O7—Cs—O7 ⁱⁱⁱ	89.34 (11)	As1—O1—Cs ⁱⁱ	100.29 (19)
O3 ⁱ —Cs—O7 ⁱⁱⁱ	112.83 (12)	Cr ⁱⁱⁱ —O1—Cs ⁱⁱ	95.14 (16)
O6—Cs—O7 ⁱⁱⁱ	108.42 (11)	As1—O2—Cr ^{viii}	139.0 (2)
O6 ⁱⁱ —Cs—O7 ⁱⁱⁱ	48.86 (11)	As1—O2—Cs ^{ix}	96.55 (17)
O2 ⁱ —Cs—O7 ⁱⁱⁱ	76.75 (11)	Cr ^{viii} —O2—Cs ^{ix}	117.92 (17)
O7—Cs—O1 ⁱⁱ	102.27 (11)	As1—O2—Cs ^x	109.71 (19)
O3 ⁱ —Cs—O1 ⁱⁱ	80.54 (11)	Cr ^{viii} —O2—Cs ^x	94.09 (15)
O6—Cs—O1 ⁱⁱ	50.85 (11)	Cs ^{ix} —O2—Cs ^x	87.81 (10)
O6 ⁱⁱ —Cs—O1 ⁱⁱ	71.11 (11)	As1—O3—Cr	126.1 (2)
O2 ⁱ —Cs—O1 ⁱⁱ	131.26 (11)	As1—O3—Cs ^{ix}	100.80 (17)
O7 ⁱⁱⁱ —Cs—O1 ⁱⁱ	119.98 (11)	Cr—O3—Cs ^{ix}	128.28 (18)
O7—Cs—O2 ^{iv}	78.78 (11)	As2—O4—As1	118.7 (2)
O3 ⁱ —Cs—O2 ^{iv}	82.70 (11)	As2—O4—Cs ⁱⁱ	97.91 (16)
O6—Cs—O2 ^{iv}	53.39 (11)	As1—O4—Cs ⁱⁱ	95.06 (16)
O6 ⁱⁱ —Cs—O2 ^{iv}	119.42 (10)	As2—O5—Cr ^v	162.6 (3)
O2 ⁱ —Cs—O2 ^{iv}	121.35 (13)	As2—O5—Cs ^v	85.37 (19)
O7 ⁱⁱⁱ —Cs—O2 ^{iv}	161.82 (10)	Cr ^v —O5—Cs ^v	99.46 (18)
O1 ⁱⁱ —Cs—O2 ^{iv}	50.97 (11)	As2—O6—Cr ^{xi}	138.4 (2)
O7—Cs—O4 ⁱⁱ	140.21 (11)	As2—O6—Cs	98.02 (17)
O3 ⁱ —Cs—O4 ⁱⁱ	60.20 (10)	Cr ^{xi} —O6—Cs	98.31 (15)

O6—Cs—O4 ⁱⁱ	92.45 (11)	As2—O6—Cs ⁱⁱ	106.32 (18)
O6 ⁱⁱ —Cs—O4 ⁱⁱ	49.76 (10)	Cr ^{xi} —O6—Cs ⁱⁱ	107.45 (16)
O2 ⁱ —Cs—O4 ⁱⁱ	92.76 (11)	Cs—O6—Cs ⁱⁱ	101.58 (11)
O7 ⁱⁱⁱ —Cs—O4 ⁱⁱ	86.49 (10)	As2—O7—Cr	134.3 (2)
O1 ⁱⁱ —Cs—O4 ⁱⁱ	48.42 (10)	As2—O7—Cs	104.25 (18)
O2 ^{iv} —Cs—O4 ⁱⁱ	93.83 (10)	Cr—O7—Cs	115.48 (17)
O7—Cs—O5 ⁱⁱⁱ	51.51 (11)	As2—O7—Cs ^v	91.67 (16)
O3 ⁱ —Cs—O5 ⁱⁱⁱ	132.61 (11)	Cr—O7—Cs ^v	107.45 (17)
O6—Cs—O5 ⁱⁱⁱ	98.57 (11)	Cs—O7—Cs ^v	92.57 (11)

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