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Cs₃ScCl₆

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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{Sc}-\text{Cl}) = 0.001$ Å; R factor = 0.023; wR factor = 0.050; data-to-parameter ratio = 68.6.

Crystals of tricaesium scandium(III) hexachloride were obtained as a side product from the reaction of U, SnCl₂, Sc, and S in a CsCl flux at 1073 K. Cs₃ScCl₆ crystallizes in the Rb₃YCl₆ structure type. The asymmetric unit comprises three Cs sites, two Sc sites, and six Cl sites, all of which have site symmetry 1, except for the two Sc sites that have site symmetries of 2 and $\bar{1}$, respectively. The structure is composed of isolated [ScCl₆]³⁻ octahedra that are surrounded by Cs⁺ cations. Two Cs⁺ cations have interactions with eight Cl⁻ anions, while the third has interactions with ten Cl⁻ anions.

Related literature

Cs₃ScCl₆ crystallizes in the Rb₃YCl₆ structure type (space group *C2/c*; Mattfeld & Meyer, 1992). Previously, a number of ternary scandium halides of the composition A₃ScX₆ were characterized by single-crystal X-ray diffraction or Rietveld refinements from powder data. These include Na₃ScF₆ (Dahlke & Babel, 1994), Na₃ScBr₆ (Bohnsack & Meyer, 1996), Li₃ScCl₆ (Bohnsack *et al.*, 1997), Li₃ScF₆ (Tyagi *et al.*, 2005), K₃ScCl₆ (Cerny *et al.*, 2010a), and Na₃ScCl₆ (Cerny *et al.*, 2010b). Except for Li₃ScCl₆, these compounds crystallize in one of two structure types: Na₃CrCl₆ (*P* $\bar{3}$ 1c; Friedrich *et al.*, 1987) or Na₃AlF₆ (*P*₂₁/*n*; Náray-Szabó & Sasvári, 1938). For other caesium scandium chloride compounds, see: Poeppelmeier *et al.* (1980). For standardization of structure data, see: Gelato & Parthé (1987).

Experimental

Crystal data

Cs₃ScCl₆ $M_r = 656.39$

Monoclinic, *C2/c*
 $a = 26.3310$ (5) Å
 $b = 7.9632$ (2) Å
 $c = 12.7085$ (3) Å
 $\beta = 100.006$ (1)°
 $V = 2624.17$ (10) Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 9.93$ mm⁻¹
 $T = 100$ K
 $0.05 \times 0.04 \times 0.03$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: numerical (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.341$, $T_{\max} = 0.438$

30195 measured reflections
 6379 independent reflections
 5631 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.050$
 $S = 1.33$
 6379 reflections

93 parameters
 $\Delta\rho_{\text{max}} = 0.98$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.26$ e Å⁻³

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014*; molecular graphics: *CrystalMaker* (Palmer, 2013); software used to prepare material for publication: *SHELXL2014*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5022).

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supporting information

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Cs₃ScCl₆

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S1. Comment

Ternary scandium halides of the composition A_3ScX_6 are known for $A = \text{Li, Na, K}$ and $X = \text{F, Cl, Br}$. These compounds crystallize in either the Na_3CrCl_6 ($P\bar{3}1c$) (Friedrich *et al.*, 1987) or the Na_3AlF_6 ($P2_1/n$) (Náray-Szabó & Sasvári, 1938) structure types, except for Li_3ScCl_6 which crystallizes in space group $C2/m$ (Bohnsack *et al.*, 1997). Single-crystal refinements have been carried out for Na_3ScF_6 (Dahlke & Babel, 1994), Na_3ScBr_6 (Bohnsack & Meyer, 1996), Li_3ScCl_6 (Bohnsack *et al.*, 1997), and Li_3ScF_6 (Tyagi *et al.*, 2005). The structures of K_3ScCl_6 (Cerny *et al.*, 2010a) and Na_3ScCl_6 (Cerny *et al.*, 2010b) were determined by Rietveld refinement of X-ray powder data. Cs_3ScCl_6 is the first Cs-containing compound of the A_3ScX_6 family. It crystallizes in the monoclinic space group $C2/c$ in the Rb_3YCl_6 structure type (Mattfeld & Meyer, 1992).

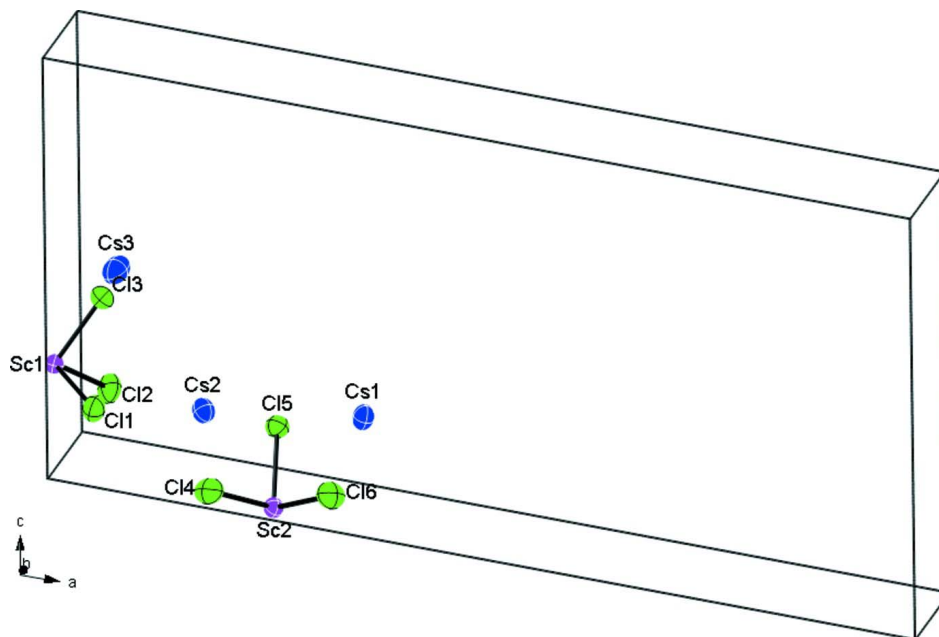
The structure of Cs_3ScCl_6 is composed of isolated $[\text{ScCl}_6]^{3-}$ octahedra that are surrounded by Cs^+ cations. The asymmetric unit, comprising three Cs, two Sc, and six Cl sites, is shown in Fig. 1, and a packing diagram is shown in Fig. 2. The composition achieves charge balance by assigning formal oxidation states of +1, +3, and -1 to Cs, Sc, and Cl, respectively. The Sc—Cl distances range from 2.4718 (5) Å to 2.5072 (6) Å at 100 K. These distances compare favorably with those of 2.601 Å at 298 K in $\text{Cs}_3\text{Sc}_2\text{Cl}_9$ (Poepelmeier *et al.*, 1980). Another caesium scandium chloride compound is CsScCl_3 (Poepelmeier *et al.*, 1980), which reportedly contains Sc(II).

S2. Experimental

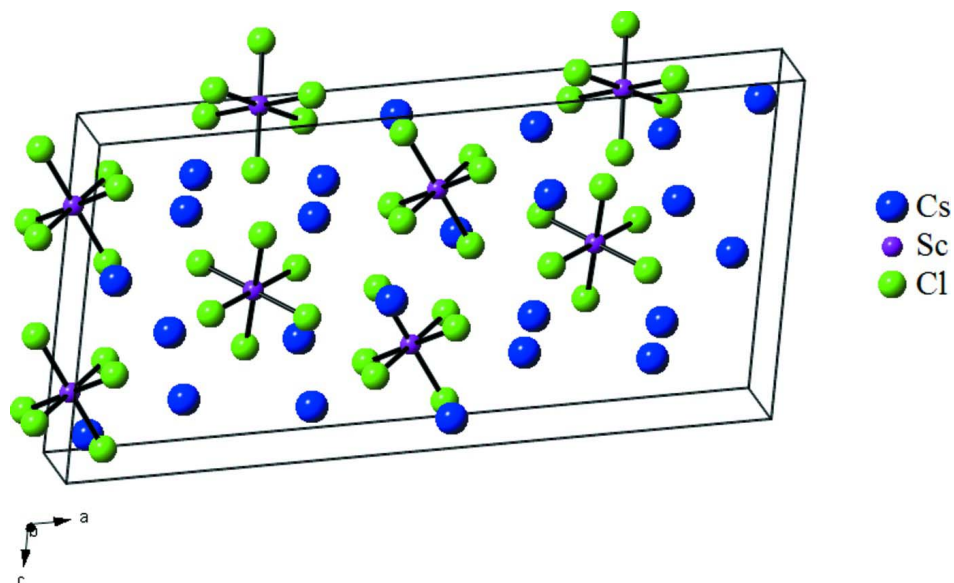
A reaction mixture containing U (0.126 mmol), SnCl_2 (0.126 mmol), Sc (1.290 mmol), S (0.378 mmol), and CsCl (0.594 mmol) was loaded into a carbon-coated fused-silica tube under an inert Ar atmosphere. The tube was then evacuated to 10^{-4} Torr, flame sealed, and placed in a computer-controlled furnace. The tube was heated to 1073 K in 12 h, held there for 96 h, cooled to 773 K at a rate of 2 K/h, and then cooled to 298 K over a further 48 h. The reaction yielded black rectangular prisms of $\text{ScU}_8\text{S}_{17}$, purple blocks of Cs_3ScCl_6 , and excess CsCl flux. Crystals of Cs_3ScCl_6 were also found as side products in other reactions that contained Sc and a CsCl flux. Crystals of Cs_3ScCl_6 are soluble in water.

S3. Refinement

Atomic positions were standardized with the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak of 1.0 (2) $e/\text{Å}^3$ is 2.18 Å from atom Cs2 and the deepest hole of -1.3 (2) $e/\text{Å}^3$ is 0.92 Å from atom Cs3.


Figure 1

The asymmetric unit of Cs_3ScCl_6 . Displacement ellipsoids at the 99% probability level are shown. Caesium atoms are blue, scandium atoms are purple, and chlorine atoms are green.


Figure 2

Packing of Cs_3ScCl_6 viewed nearly along the b axis.

Tricaesium scandium(III) hexachloride

Crystal data

Cs_3ScCl_6

$M_r = 656.39$

Monoclinic, $C2/c$

$a = 26.3310 (5) \text{ \AA}$

$b = 7.9632 (2) \text{ \AA}$

$c = 12.7085 (3) \text{ \AA}$

$\beta = 100.006 (1)^\circ$
 $V = 2624.17 (10) \text{ \AA}^3$
 $Z = 8$
 $F(000) = 2304$
 $D_x = 3.323 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9931 reflections
 $\theta = 3.1\text{--}36.3^\circ$
 $\mu = 9.93 \text{ mm}^{-1}$
 $T = 100 \text{ K}$
 Block, purple
 $0.05 \times 0.04 \times 0.03 \text{ mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 φ and ω scans
 Absorption correction: numerical
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.341$, $T_{\max} = 0.438$
 30195 measured reflections

6379 independent reflections
 5631 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $\theta_{\max} = 36.4^\circ$, $\theta_{\min} = 1.6^\circ$
 $h = -39 \rightarrow 43$
 $k = -13 \rightarrow 12$
 $l = -20 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.050$
 $S = 1.33$
 6379 reflections

93 parameters
 0 restraints
 $w = 1/[\sigma^2(F_o^2) + (0.0114F_o^2)^2]$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.98 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.26 \text{ e \AA}^{-3}$

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cs1	0.16275 (2)	0.18961 (2)	0.30059 (2)	0.01108 (3)
Cs2	0.34717 (2)	0.18469 (2)	0.35501 (2)	0.01108 (3)
Cs3	0.44859 (2)	0.24984 (2)	0.06656 (2)	0.01686 (3)
Sc1	0.0000	0.22061 (6)	0.2500	0.00772 (8)
Sc2	0.2500	0.2500	0.0000	0.00814 (8)
Cl1	0.05410 (2)	0.00676 (6)	0.68924 (4)	0.01302 (9)
Cl2	0.05417 (2)	0.44314 (7)	0.18670 (4)	0.01398 (9)
Cl3	0.05588 (2)	0.22355 (7)	0.42769 (4)	0.01427 (9)
Cl4	0.18402 (2)	0.04527 (7)	0.03693 (4)	0.01557 (10)
Cl5	0.25017 (2)	0.38135 (6)	0.17777 (4)	0.01095 (8)
Cl6	0.32362 (2)	0.06505 (7)	0.07773 (4)	0.01453 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.00923 (5)	0.01059 (5)	0.01374 (6)	0.00077 (4)	0.00290 (4)	0.00089 (4)
Cs2	0.01074 (5)	0.01019 (5)	0.01199 (5)	0.00125 (4)	0.00105 (4)	-0.00113 (4)
Cs3	0.01421 (6)	0.02189 (7)	0.01509 (6)	-0.00445 (5)	0.00429 (5)	-0.00546 (5)

Sc1	0.0070 (2)	0.0084 (2)	0.0079 (2)	0.000	0.00144 (15)	0.000
Sc2	0.0078 (2)	0.0085 (2)	0.0081 (2)	-0.00052 (17)	0.00125 (16)	0.00062 (15)
Cl1	0.0106 (2)	0.0126 (2)	0.0162 (2)	-0.00042 (16)	0.00327 (16)	0.00394 (16)
Cl2	0.0123 (2)	0.0132 (2)	0.0167 (2)	-0.00298 (17)	0.00332 (16)	0.00265 (16)
Cl3	0.0103 (2)	0.0224 (2)	0.00960 (19)	0.00063 (17)	0.00039 (15)	-0.00036 (16)
Cl4	0.0193 (2)	0.0146 (2)	0.0138 (2)	-0.00819 (18)	0.00558 (17)	-0.00093 (16)
Cl5	0.0111 (2)	0.01172 (19)	0.01018 (18)	-0.00123 (16)	0.00216 (14)	-0.00105 (14)
Cl6	0.0148 (2)	0.0147 (2)	0.0134 (2)	0.00510 (18)	0.00040 (16)	0.00119 (16)

Geometric parameters (Å, °)

Cs1—Cl5 ⁱ	3.3378 (5)	Cs3—Cl6	3.6297 (6)
Cs1—Cl1 ⁱⁱ	3.3504 (5)	Cs3—Cl1 ^v	3.6702 (6)
Cs1—Cl6 ⁱⁱⁱ	3.3564 (5)	Cs3—Cl3 ⁱⁱⁱ	3.7752 (6)
Cs1—Cl5	3.3637 (5)	Cs3—Cl2 ^{viii}	3.8144 (6)
Cs1—Cl3	3.4900 (6)	Cs3—Cl1 ⁱⁱⁱ	3.8312 (6)
Cs1—Cl4 ^{iv}	3.4998 (5)	Cs3—Cl4 ^{vii}	3.8714 (6)
Cs1—Cl2	3.5926 (5)	Cs3—Cl2 ⁱ	3.9852 (6)
Cs1—Cl4	3.6762 (6)	Sc1—Cl3 ^{ix}	2.4718 (5)
Cs2—Cl4 ⁱⁱⁱ	3.3463 (5)	Sc1—Cl3	2.4718 (5)
Cs2—Cl2 ⁱ	3.3479 (5)	Sc1—Cl2 ^{ix}	2.4940 (6)
Cs2—Cl5	3.4714 (5)	Sc1—Cl2	2.4941 (6)
Cs2—Cl5 ⁱ	3.4937 (5)	Sc1—Cl1 ^x	2.5072 (6)
Cs2—Cl3 ^v	3.4969 (5)	Sc1—Cl1 ⁱⁱ	2.5072 (6)
Cs2—Cl6	3.5986 (5)	Sc2—Cl4 ^{vii}	2.4859 (5)
Cs2—Cl6 ^{iv}	3.6000 (6)	Sc2—Cl4	2.4859 (5)
Cs2—Cl1 ^v	3.6904 (5)	Sc2—Cl5	2.4889 (5)
Cs3—Cl1 ^{vi}	3.5216 (5)	Sc2—Cl5 ^{vii}	2.4889 (5)
Cs3—Cl2 ^{vii}	3.5559 (6)	Sc2—Cl6	2.4975 (5)
Cs3—Cl3 ^{vi}	3.5878 (6)	Sc2—Cl6 ^{vii}	2.4976 (5)
Cl5 ⁱ —Cs1—Cl1 ⁱⁱ	102.445 (13)	Cl1 ^x —Sc1—Cs3 ^{xi}	58.901 (12)
Cl5 ⁱ —Cs1—Cl6 ⁱⁱⁱ	126.886 (13)	Cl1 ⁱⁱ —Sc1—Cs3 ^{xi}	126.341 (17)
Cl1 ⁱⁱ —Cs1—Cl6 ⁱⁱⁱ	128.714 (13)	Cs1—Sc1—Cs3 ^{xi}	108.888 (3)
Cl5 ⁱ —Cs1—Cl5	81.739 (7)	Cs1 ^{ix} —Sc1—Cs3 ^{xi}	71.484 (3)
Cl1 ⁱⁱ —Cs1—Cl5	128.226 (13)	Cl3 ^{ix} —Sc1—Cs3 ^{vii}	53.295 (13)
Cl6 ⁱⁱⁱ —Cs1—Cl5	77.438 (13)	Cl3—Sc1—Cs3 ^{vii}	126.632 (13)
Cl5 ⁱ —Cs1—Cl3	128.060 (13)	Cl2 ^{ix} —Sc1—Cs3 ^{vii}	122.186 (17)
Cl1 ⁱⁱ —Cs1—Cl3	62.204 (12)	Cl2—Sc1—Cs3 ^{vii}	52.590 (12)
Cl6 ⁱⁱⁱ —Cs1—Cl3	75.407 (14)	Cl1 ^x —Sc1—Cs3 ^{vii}	126.341 (17)
Cl5—Cs1—Cl3	148.367 (13)	Cl1 ⁱⁱ —Sc1—Cs3 ^{vii}	58.901 (12)
Cl5 ⁱ —Cs1—Cl4 ^{iv}	62.031 (12)	Cs1—Sc1—Cs3 ^{vii}	71.484 (3)
Cl1 ⁱⁱ —Cs1—Cl4 ^{iv}	96.352 (14)	Cs1 ^{ix} —Sc1—Cs3 ^{vii}	108.888 (3)
Cl6 ⁱⁱⁱ —Cs1—Cl4 ^{iv}	95.297 (13)	Cs3 ^{xi} —Sc1—Cs3 ^{vii}	173.961 (14)
Cl5—Cs1—Cl4 ^{iv}	128.348 (13)	Cl3 ^{ix} —Sc1—Cs3 ^{xii}	57.081 (16)
Cl3—Cs1—Cl4 ^{iv}	70.483 (13)	Cl3—Sc1—Cs3 ^{xii}	124.00 (2)
Cl5 ⁱ —Cs1—Cl2	159.024 (12)	Cl2 ^{ix} —Sc1—Cs3 ^{xii}	128.462 (13)
Cl1 ⁱⁱ —Cs1—Cl2	62.017 (12)	Cl2—Sc1—Cs3 ^{xii}	124.235 (13)

Cl6 ⁱⁱⁱ —Cs1—Cl2	72.479 (13)	Cl1 ^x —Sc1—Cs3 ^{xii}	54.672 (15)
Cl5—Cs1—Cl2	96.823 (12)	Cl1 ⁱⁱ —Sc1—Cs3 ^{xii}	51.268 (14)
Cl3—Cs1—Cl2	59.584 (12)	Cs1—Sc1—Cs3 ^{xii}	103.650 (8)
Cl4 ^{iv} —Cs1—Cl2	130.060 (13)	Cs1 ^{ix} —Sc1—Cs3 ^{xii}	70.532 (5)
Cl5 ⁱ —Cs1—Cl4	68.521 (12)	Cs3 ^{xi} —Sc1—Cs3 ^{xii}	113.557 (8)
Cl1 ⁱⁱ —Cs1—Cl4	73.931 (13)	Cs3 ^{vii} —Sc1—Cs3 ^{xii}	71.830 (5)
Cl6 ⁱⁱⁱ —Cs1—Cl4	132.642 (13)	Cl3 ^{ix} —Sc1—Cs3 ⁱ	124.00 (2)
Cl5—Cs1—Cl4	59.605 (12)	Cl3—Sc1—Cs3 ⁱ	57.082 (16)
Cl3—Cs1—Cl4	135.140 (12)	Cl2 ^{ix} —Sc1—Cs3 ⁱ	124.235 (13)
Cl4 ^{iv} —Cs1—Cl4	126.021 (7)	Cl2—Sc1—Cs3 ⁱ	128.461 (13)
Cl2—Cs1—Cl4	92.585 (13)	Cl1 ^x —Sc1—Cs3 ⁱ	51.268 (14)
Cl4 ⁱⁱⁱ —Cs2—Cl2 ⁱ	144.147 (14)	Cl1 ⁱⁱ —Sc1—Cs3 ⁱ	54.672 (15)
Cl4 ⁱⁱⁱ —Cs2—Cl5	70.962 (12)	Cs1—Sc1—Cs3 ⁱ	70.532 (5)
Cl2 ⁱ —Cs2—Cl5	131.312 (13)	Cs1 ^{ix} —Sc1—Cs3 ⁱ	103.650 (8)
Cl4 ⁱⁱⁱ —Cs2—Cl5 ⁱ	114.518 (14)	Cs3 ^{xi} —Sc1—Cs3 ⁱ	71.830 (5)
Cl2 ⁱ —Cs2—Cl5 ⁱ	99.045 (13)	Cs3 ^{vii} —Sc1—Cs3 ⁱ	113.557 (8)
Cl5—Cs2—Cl5 ⁱ	78.039 (6)	Cs3 ^{xii} —Sc1—Cs3 ⁱ	67.059 (8)
Cl4 ⁱⁱⁱ —Cs2—Cl3 ^v	72.190 (13)	Cl4 ^{vii} —Sc2—Cl4	179.999 (18)
Cl2 ⁱ —Cs2—Cl3 ^v	76.407 (13)	Cl4 ^{vii} —Sc2—Cl5	90.268 (17)
Cl5—Cs2—Cl3 ^v	140.539 (13)	Cl4—Sc2—Cl5	89.731 (17)
Cl5 ⁱ —Cs2—Cl3 ^v	131.180 (12)	Cl4 ^{vii} —Sc2—Cl5 ^{vii}	89.730 (17)
Cl4 ⁱⁱⁱ —Cs2—Cl6	128.042 (13)	Cl4—Sc2—Cl5 ^{vii}	90.271 (17)
Cl2 ⁱ —Cs2—Cl6	72.498 (12)	Cl5—Sc2—Cl5 ^{vii}	180.0
Cl5—Cs2—Cl6	60.126 (12)	Cl4 ^{vii} —Sc2—Cl6	86.646 (19)
Cl5 ⁱ —Cs2—Cl6	72.674 (12)	Cl4—Sc2—Cl6	93.354 (19)
Cl3 ^v —Cs2—Cl6	143.761 (13)	Cl5—Sc2—Cl6	90.573 (16)
Cl4 ⁱⁱⁱ —Cs2—Cl6 ^{iv}	93.629 (13)	Cl5 ^{vii} —Sc2—Cl6	89.427 (16)
Cl2 ⁱ —Cs2—Cl6 ^{iv}	92.949 (14)	Cl4 ^{vii} —Sc2—Cl6 ^{vii}	93.356 (19)
Cl5—Cs2—Cl6 ^{iv}	123.475 (13)	Cl4—Sc2—Cl6 ^{vii}	86.644 (19)
Cl5 ⁱ —Cs2—Cl6 ^{iv}	59.259 (11)	Cl5—Sc2—Cl6 ^{vii}	89.427 (16)
Cl3 ^v —Cs2—Cl6 ^{iv}	72.323 (12)	Cl5 ^{vii} —Sc2—Cl6 ^{vii}	90.574 (16)
Cl6—Cs2—Cl6 ^{iv}	126.850 (7)	Cl6—Sc2—Cl6 ^{vii}	180.0
Cl4 ⁱⁱⁱ —Cs2—Cl1 ^v	73.789 (14)	Cl4 ^{vii} —Sc2—Cs1 ⁱⁱ	132.946 (12)
Cl2 ⁱ —Cs2—Cl1 ^v	76.813 (13)	Cl4—Sc2—Cs1 ⁱⁱ	47.055 (12)
Cl5—Cs2—Cl1 ^v	93.390 (12)	Cl5—Sc2—Cs1 ⁱⁱ	136.773 (12)
Cl5 ⁱ —Cs2—Cl1 ^v	164.523 (12)	Cl5 ^{vii} —Sc2—Cs1 ⁱⁱ	43.228 (12)
Cl3 ^v —Cs2—Cl1 ^v	62.887 (12)	Cl6—Sc2—Cs1 ⁱⁱ	92.711 (13)
Cl6—Cs2—Cl1 ^v	91.899 (13)	Cl6 ^{vii} —Sc2—Cs1 ⁱⁱ	87.288 (13)
Cl6 ^{iv} —Cs2—Cl1 ^v	135.208 (12)	Cl4 ^{vii} —Sc2—Cs1 ⁱⁱⁱ	47.054 (12)
Cl1 ^{vi} —Cs3—Cl2 ^{vii}	121.939 (13)	Cl4—Sc2—Cs1 ⁱⁱⁱ	132.945 (12)
Cl1 ^{vi} —Cs3—Cl3 ^{vi}	63.717 (12)	Cl5—Sc2—Cs1 ⁱⁱⁱ	43.227 (12)
Cl2 ^{vii} —Cs3—Cl3 ^{vi}	58.283 (12)	Cl5 ^{vii} —Sc2—Cs1 ⁱⁱⁱ	136.772 (12)
Cl1 ^{vi} —Cs3—Cl6	148.943 (13)	Cl6—Sc2—Cs1 ⁱⁱⁱ	87.289 (13)
Cl2 ^{vii} —Cs3—Cl6	89.091 (12)	Cl6 ^{vii} —Sc2—Cs1 ⁱⁱⁱ	92.712 (13)
Cl3 ^{vi} —Cs3—Cl6	147.118 (12)	Cs1 ⁱⁱ —Sc2—Cs1 ⁱⁱⁱ	180.0
Cl1 ^{vi} —Cs3—Cl1 ^v	57.631 (15)	Sc1 ^x —Cl1—Cs1 ^{iv}	91.260 (16)
Cl2 ^{vii} —Cs3—Cl1 ^v	173.337 (13)	Sc1 ^x —Cl1—Cs3 ^{xi}	94.994 (16)
Cl3 ^{vi} —Cs3—Cl1 ^v	121.151 (12)	Cs1 ^{iv} —Cl1—Cs3 ^{xi}	173.698 (17)

Cl6—Cs3—C11 ^v	91.731 (12)	Sc1 ^x —C11—Cs3 ^v	91.457 (16)
C11 ^{vi} —Cs3—Cl3 ⁱⁱⁱ	57.741 (11)	Cs1 ^{iv} —C11—Cs3 ^v	91.711 (12)
Cl2 ^{vii} —Cs3—Cl3 ⁱⁱⁱ	116.971 (12)	Cs3 ^{xi} —C11—Cs3 ^v	87.364 (13)
Cl3 ^{vi} —Cs3—Cl3 ⁱⁱⁱ	88.872 (13)	Sc1 ^x —C11—Cs2 ^v	168.727 (19)
Cl6—Cs3—Cl3 ⁱⁱⁱ	111.892 (12)	Cs1 ^{iv} —C11—Cs2 ^v	78.623 (11)
C11 ^v —Cs3—Cl3 ⁱⁱⁱ	56.679 (11)	Cs3 ^{xi} —C11—Cs2 ^v	95.079 (12)
C11 ^{vi} —Cs3—Cl2 ^{viii}	73.210 (12)	Cs3 ^v —C11—Cs2 ^v	83.964 (11)
Cl2 ^{vii} —Cs3—Cl2 ^{viii}	89.108 (12)	Sc1 ^x —C11—Cs3 ⁱ	87.017 (15)
Cl3 ^{vi} —Cs3—Cl2 ^{viii}	69.717 (12)	Cs1 ^{iv} —C11—Cs3 ⁱ	89.870 (13)
Cl6—Cs3—Cl2 ^{viii}	109.110 (12)	Cs3 ^{xi} —C11—Cs3 ⁱ	91.227 (12)
C11 ^v —Cs3—Cl2 ^{viii}	96.862 (12)	Cs3 ^v —C11—Cs3 ⁱ	177.828 (16)
Cl3 ⁱⁱⁱ —Cs3—Cl2 ^{viii}	130.920 (11)	Cs2 ^v —C11—Cs3 ⁱ	97.813 (13)
C11 ^{vi} —Cs3—C11 ⁱⁱⁱ	88.772 (12)	Sc1—Cl2—Cs2 ⁱⁱⁱ	164.21 (2)
Cl2 ^{vii} —Cs3—C11 ⁱⁱⁱ	57.881 (12)	Sc1—Cl2—Cs3 ^{vii}	93.554 (16)
Cl3 ^{vi} —Cs3—C11 ⁱⁱⁱ	56.711 (11)	Cs2 ⁱⁱⁱ —Cl2—Cs3 ^{vii}	89.963 (13)
Cl6—Cs3—C11 ⁱⁱⁱ	111.495 (11)	Sc1—Cl2—Cs1	86.012 (16)
C11 ^v —Cs3—C11 ⁱⁱⁱ	115.801 (4)	Cs2 ⁱⁱⁱ —Cl2—Cs1	78.554 (11)
Cl3 ⁱⁱⁱ —Cs3—C11 ⁱⁱⁱ	59.122 (11)	Cs3 ^{vii} —Cl2—Cs1	90.658 (13)
Cl2 ^{viii} —Cs3—C11 ⁱⁱⁱ	125.895 (12)	Sc1—Cl2—Cs3 ^{xiii}	99.566 (17)
C11 ^{vi} —Cs3—Cl4 ^{vii}	120.934 (12)	Cs2 ⁱⁱⁱ —Cl2—Cs3 ^{xiii}	95.760 (13)
Cl2 ^{vii} —Cs3—Cl4 ^{vii}	89.959 (12)	Cs3 ^{vii} —Cl2—Cs3 ^{xiii}	90.890 (12)
Cl3 ^{vi} —Cs3—Cl4 ^{vii}	123.282 (12)	Cs1—Cl2—Cs3 ^{xiii}	174.107 (16)
Cl6—Cs3—Cl4 ^{vii}	54.119 (11)	Sc1—Cl2—Cs3 ⁱⁱⁱ	95.280 (17)
C11 ^v —Cs3—Cl4 ^{vii}	85.176 (11)	Cs2 ⁱⁱⁱ —Cl2—Cs3 ⁱⁱⁱ	83.870 (12)
Cl3 ⁱⁱⁱ —Cs3—Cl4 ^{vii}	63.654 (11)	Cs3 ^{vii} —Cl2—Cs3 ⁱⁱⁱ	167.614 (16)
Cl2 ^{viii} —Cs3—Cl4 ^{vii}	163.219 (12)	Cs1—Cl2—Cs3 ⁱⁱⁱ	98.594 (12)
C11 ⁱⁱⁱ —Cs3—Cl4 ^{vii}	66.677 (11)	Cs3 ^{xiii} —Cl2—Cs3 ⁱⁱⁱ	79.100 (11)
C11 ^{vi} —Cs3—Cl2 ⁱ	96.304 (12)	Sc1—Cl3—Cs1	88.641 (15)
Cl2 ^{vii} —Cs3—Cl2 ⁱ	116.554 (5)	Sc1—Cl3—Cs2 ^v	163.83 (2)
Cl3 ^{vi} —Cs3—Cl2 ⁱ	123.146 (12)	Cs1—Cl3—Cs2 ^v	81.079 (11)
Cl6—Cs3—Cl2 ⁱ	65.179 (11)	Sc1—Cl3—Cs3 ^{xi}	93.175 (15)
C11 ^v —Cs3—Cl2 ⁱ	69.674 (11)	Cs1—Cl3—Cs3 ^{xi}	177.893 (16)
Cl3 ⁱⁱⁱ —Cs3—Cl2 ⁱ	126.317 (11)	Cs2 ^v —Cl3—Cs3 ^{xi}	97.376 (13)
Cl2 ^{viii} —Cs3—Cl2 ⁱ	53.436 (15)	Sc1—Cl3—Cs3 ⁱ	89.577 (19)
C11 ⁱⁱⁱ —Cs3—Cl2 ⁱ	174.105 (11)	Cs1—Cl3—Cs3 ⁱ	87.819 (13)
Cl4 ^{vii} —Cs3—Cl2 ⁱ	112.763 (11)	Cs2 ^v —Cl3—Cs3 ⁱ	102.381 (13)
Cl3 ^{ix} —Sc1—Cl3	178.91 (4)	Cs3 ^{xi} —Cl3—Cs3 ⁱ	91.125 (13)
Cl3 ^{ix} —Sc1—Cl2 ^{ix}	90.284 (19)	Sc2—Cl4—Cs2 ⁱ	150.42 (2)
Cl3—Sc1—Cl2 ^{ix}	88.945 (19)	Sc2—Cl4—Cs1 ⁱⁱ	101.617 (17)
Cl3 ^{ix} —Sc1—Cl2	88.945 (19)	Cs2 ⁱ —Cl4—Cs1 ⁱⁱ	83.078 (12)
Cl3—Sc1—Cl2	90.28 (2)	Sc2—Cl4—Cs1	100.906 (16)
Cl2 ^{ix} —Sc1—Cl2	89.45 (3)	Cs2 ⁱ —Cl4—Cs1	78.879 (11)
Cl3 ^{ix} —Sc1—C11 ^x	90.480 (19)	Cs1 ⁱⁱ —Cl4—Cs1	157.264 (17)
Cl3—Sc1—C11 ^x	90.306 (19)	Sc2—Cl4—Cs3 ^{vii}	106.150 (17)
Cl2 ^{ix} —Sc1—C11 ^x	91.511 (18)	Cs2 ⁱ —Cl4—Cs3 ^{vii}	103.290 (14)
Cl2—Sc1—C11 ^x	178.89 (2)	Cs1 ⁱⁱ —Cl4—Cs3 ^{vii}	86.175 (12)
Cl3 ^{ix} —Sc1—C11 ⁱⁱ	90.305 (19)	Cs1—Cl4—Cs3 ^{vii}	84.641 (13)
Cl3—Sc1—C11 ⁱⁱ	90.479 (19)	Sc2—Cl5—Cs1 ⁱⁱⁱ	106.063 (17)

Cl2 ^{ix} —Sc1—Cl1 ⁱⁱ	178.89 (2)	Sc2—Cl5—Cs1	109.697 (16)
Cl2—Sc1—Cl1 ⁱⁱ	91.510 (18)	Cs1 ⁱⁱⁱ —Cl5—Cs1	144.225 (16)
Cl1 ^x —Sc1—Cl1 ⁱⁱ	87.54 (3)	Sc2—Cl5—Cs2	106.525 (16)
Cl3 ^{ix} —Sc1—Cs1	124.476 (13)	Cs1 ⁱⁱⁱ —Cl5—Cs2	82.000 (11)
Cl3—Sc1—Cs1	55.599 (13)	Cs1—Cl5—Cs2	88.842 (12)
Cl2 ^{ix} —Sc1—Cs1	127.855 (17)	Sc2—Cl5—Cs2 ⁱⁱⁱ	107.265 (15)
Cl2—Sc1—Cs1	57.945 (12)	Cs1 ⁱⁱⁱ —Cl5—Cs2 ⁱⁱⁱ	88.886 (12)
Cl1 ^x —Sc1—Cs1	121.740 (17)	Cs1—Cl5—Cs2 ⁱⁱⁱ	79.759 (11)
Cl1 ⁱⁱ —Sc1—Cs1	52.385 (11)	Cs2—Cl5—Cs2 ⁱⁱⁱ	146.210 (15)
Cl3 ^{ix} —Sc1—Cs1 ^{ix}	55.600 (13)	Sc2—Cl6—Cs1 ⁱ	136.14 (2)
Cl3—Sc1—Cs1 ^{ix}	124.478 (13)	Sc2—Cl6—Cs2	102.768 (17)
Cl2 ^{ix} —Sc1—Cs1 ^{ix}	57.945 (12)	Cs1 ⁱ —Cl6—Cs2	78.359 (11)
Cl2—Sc1—Cs1 ^{ix}	127.855 (17)	Sc2—Cl6—Cs2 ⁱⁱ	104.044 (16)
Cl1 ^x —Sc1—Cs1 ^{ix}	52.385 (11)	Cs1 ⁱ —Cl6—Cs2 ⁱⁱ	81.426 (12)
Cl1 ⁱⁱ —Sc1—Cs1 ^{ix}	121.740 (17)	Cs2—Cl6—Cs2 ⁱⁱ	153.152 (16)
Cs1—Sc1—Cs1 ^{ix}	173.309 (14)	Sc2—Cl6—Cs3	113.085 (18)
Cl3 ^{ix} —Sc1—Cs3 ^{xi}	126.634 (13)	Cs1 ⁱ —Cl6—Cs3	110.735 (14)
Cl3—Sc1—Cs3 ^{xi}	53.296 (13)	Cs2—Cl6—Cs3	85.863 (12)
Cl2 ^{ix} —Sc1—Cs3 ^{xi}	52.590 (13)	Cs2 ⁱⁱ —Cl6—Cs3	84.957 (13)
Cl2—Sc1—Cs3 ^{xi}	122.185 (17)		

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