Crystal structure of Tutton's salts, $\text{Cs}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SeO}_4)_2$, $\text{M}^{\text{II}} = \text{Mg, Mn, Co, Ni, Zn}$

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Abstract

$\text{Cs}_2\text{H}_{12}\text{MgO}_{14}\text{Se}_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.513(1) \text{ \AA}$, $b = 13.037(1) \text{ \AA}$, $c = 6.4730(8) \text{ \AA}$, $\beta = 106.244(8)^\circ$, $V = 770.7 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.020$, $wR_{\text{ref}}(F^2) = 0.036$, $T = 293 \text{ K}$.

$\text{Cs}_2\text{H}_{12}\text{MnO}_{14}\text{Se}_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.591(1) \text{ \AA}$, $b = 13.141(2) \text{ \AA}$, $c = 6.5040(9) \text{ \AA}$, $\beta = 106.38(1)^\circ$, $V = 786.5 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.021$, $wR_{\text{ref}}(F^2) = 0.043$, $T = 293 \text{ K}$.

$\text{CoCs}_2\text{H}_{12}\text{O}_{14}\text{Se}_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.494(1) \text{ \AA}$, $b = 13.009(1) \text{ \AA}$, $c = 6.4833(8) \text{ \AA}$, $\beta = 106.239(9)^\circ$, $V = 768.8 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.016$, $wR_{\text{ref}}(F^2) = 0.032$, $T = 293 \text{ K}$.

$\text{Cs}_2\text{H}_{12}\text{NiO}_{14}\text{Se}_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.426(3) \text{ \AA}$, $b = 12.961(2) \text{ \AA}$, $c = 6.473(2) \text{ \AA}$, $\beta = 106.17(2)^\circ$, $V = 759.5 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.017$, $wR_{\text{ref}}(F^2) = 0.034$, $T = 293 \text{ K}$.

$\text{Cs}_2\text{H}_{12}\text{O}_{14}\text{Se}_2\text{Zn}$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.483(1) \text{ \AA}$, $b = 13.005(2) \text{ \AA}$, $c = 6.4850(8) \text{ \AA}$, $\beta = 106.16(1)^\circ$, $V = 768.2 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.019$, $wR_{\text{ref}}(F^2) = 0.037$, $T = 293 \text{ K}$.

Source of material

All compounds of the isomorphous series $\text{Cs}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SeO}_4)_2$ were prepared by dissolution of equimolar amounts of caesium selenate Cs_2SeO_4 and M^{II} selenate hydrate $\text{M}^{\text{II}}\text{SeO}_4 \cdot n\text{H}_2\text{O}$ in hot distilled water and ensuing evaporation of the solvent. The M^{II} selenate hydrates contained different amounts of crystal water. For the syntheses of the Tutton's salts with $\text{M}^{\text{II}} = \text{Mg, Co, Ni, Zn}$, the M^{II} selenate hexahydrates were used, for $\text{M}^{\text{II}} = \text{Mn}$, the M^{II} selenate pentahydrate. Differently coloured, mostly ideomorphic single crystals of dimensions up to 10 mm were obtained.

Discussion

All compounds are isotypic and crystallize similarly to the Rb sulphates [1], Rb selenates [2] and Cs sulphates [3]. The structure is characterized by irregular CsO_8 polyhedra, $d(\text{Cs—O}) = 3.065(3) \text{ \AA} - 3.483(3) \text{ \AA}$, and somewhat distorted $\text{M}^{\text{II}}(\text{H}_2\text{O})_6$ octahedra, $d(\text{M}^{\text{II}}\text{—O}) = 2.038(3) \text{ \AA} - 2.193(3) \text{ \AA}$, the latter being linked to the SeO_4 tetrahedra by hydrogen bonds. Compared to the Rb selenates [2], one finds:

1. For all the different M^{II} compounds, the lattice constants a, b, c increase on average by 1.3%, 3.0%, 2.2%, respectively, due to the bigger Cs ion and hence to the larger volume of the CsO_8 polyhedron [4,5]. The angle β increasing for all compounds by about 1.0° shows, contrary to the Rb selenates (slightly negative slope) a slightly positive slope in the linear correlation between β and the M^{II} cation radii. With respect to the exchange of M^{II} , the linear correlations between the lattice constants and the cation radii exhibit almost the same slopes as for the Rb-selenates.
2. The volumes of the $\text{M}^{\text{II}}\text{O}_6$ coordination octahedra agree with those of the corresponding Rb selenates, i.e., the Rb substitution by Cs has no effect on the hexahydrate complex.
3. The volumes of the CsO_8 coordination polyhedra increase on average by 14.9 %. This is somewhat more than the 3rd power of the mean Cs—O and Rb—O bond lengths ratio, $[\bar{d}(\text{Cs—O})/\bar{d}(\text{Rb—O})]^3 = 1.125$.
4. While in agreement with chemical expectation, the selenate group is practically invariant against the M^{II} cation exchange in the hexahydrate complex, the volumes of both the $\text{M}^{\text{II}}\text{O}_6$ and CsO_8 coordination polyhedra increase as the cation radii $R(\text{M}^{\text{II}})$ [5] increase. However, for $V(\text{CsO}_8)$, the rate of increase is about two times smaller than for $V(\text{M}^{\text{II}}\text{O}_6)$.
5. As in the Rb selenate series, the a, b axes and $V(\text{CsO}_8)$ of the Mg compound are significantly larger than expected from the linear lattice parameter vs cation radius correlations observed for the other structures. This finding can be attributed to the smaller electronegativity of Mg, causing less shared Cs—O interactions, as reflected by increased distances, $d(\text{Cs—O5}) = 3.483(3) \text{ \AA}$ and $d(\text{Cs—O6}) = 3.372(3) \text{ \AA}$, compared to other M^{II} compounds of the same series.

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6. The oxygen atoms of the SeO₄ group are acceptors of 6 different hydrogen bonds, providing links to 4 different M^{II}(H₂O)₆ octahedra. Contrary to O1 and O2, both O3 and O4 accept two hydrogen bonds each. For the individual Cs-selenate compounds, the hydrogen bond lengths differ from those observed in the Rb analogues, but no significant difference is found for the mean distance $\bar{d}(\text{O} \cdots \text{H} \cdots \text{O}) = 2.745 \text{ \AA}$ averaged over all donor-acceptor distances in the structure.

1. Caesium hexaaquamagnesium(II) selenate, Cs₂[Mg(H₂O)₆](SeO₄)₂

Table 1. Data collection and handling.

Crystal:	colorless ellipsoid, size 0.16 × 0.17 × 0.18 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	95.51 cm ⁻¹
Diffractionmeter, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\text{max}}$:	50.1°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	5294, 1357
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1115
$N(\text{param})_{\text{refined}}$:	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4e	0.194(5)	0.092(3)	0.265(7)	0.03(1)
H(2)	4e	0.212(5)	0.125(3)	0.109(7)	0.03(1)
H(3)	4e	-0.241(6)	0.097(4)	-0.044(8)	0.06(2)
H(4)	4e	-0.153(4)	0.164(3)	-0.014(6)	0.02(1)
H(5)	4e	-0.076(5)	-0.056(3)	0.310(7)	0.03(1)
H(6)	4e	0.020(4)	-0.121(3)	0.320(7)	0.04(1)

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Mg	2a	0	0	0	0.0190(8)	0.0213(8)	0.0200(9)	-0.0022(6)	0.0058(7)	0.0003(6)
Se	4e	0.39927(3)	0.14555(3)	0.74186(5)	0.0189(2)	0.0225(2)	0.0215(2)	-0.0021(1)	0.0052(1)	-0.0010(1)
O(1)	4e	0.4195(3)	0.2438(2)	0.5953(4)	0.047(2)	0.026(1)	0.034(2)	-0.004(1)	0.018(1)	0.005(1)
O(2)	4e	0.5477(3)	0.0761(2)	0.8038(4)	0.024(1)	0.038(2)	0.051(2)	0.007(1)	0.005(1)	0.001(1)
O(3)	4e	0.2639(3)	0.0753(2)	0.5981(4)	0.025(1)	0.035(1)	0.028(1)	-0.007(1)	0.006(1)	-0.007(1)
O(4)	4e	0.3607(3)	0.1865(2)	0.9600(4)	0.040(1)	0.031(1)	0.023(1)	-0.006(1)	0.015(1)	-0.006(1)
O(5)	4e	0.1580(3)	0.1049(2)	0.1606(5)	0.026(2)	0.040(2)	0.024(2)	-0.010(1)	0.005(1)	0.001(1)
O(6)	4e	-0.1634(3)	0.1053(2)	0.0101(5)	0.023(2)	0.025(2)	0.041(2)	0.002(1)	0.011(1)	0.002(1)
O(7)	4e	-0.0075(3)	-0.0629(2)	0.2849(4)	0.029(2)	0.030(2)	0.028(1)	0.005(1)	0.012(1)	0.004(1)
Cs	4e	0.13181(2)	0.35199(2)	0.35074(4)	0.0335(2)	0.0333(2)	0.0316(2)	0.0000(1)	0.0107(1)	0.0024(1)

2. Caesium hexaaquamanganese(II) selenate, Cs₂[Mn(H₂O)₆](SeO₄)₂

Table 4. Data collection and handling.

Crystal:	light pink ellipsoid, size 0.27 × 0.28 × 0.29 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	100.86 cm ⁻¹
Diffractionmeter, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\text{max}}$:	50.08°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	5336, 1364
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1215
$N(\text{param})_{\text{refined}}$:	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 5. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4e	0.205(5)	0.106(4)	0.259(8)	0.04(2)
H(2)	4e	0.233(7)	0.131(4)	0.115(9)	0.07(2)
H(3)	4e	-0.254(6)	0.101(4)	-0.055(7)	0.05(1)
H(4)	4e	-0.159(7)	0.165(4)	-0.03(1)	0.08(2)
H(5)	4e	-0.086(6)	-0.063(4)	0.307(8)	0.05(2)
H(6)	4e	0.002(6)	-0.128(4)	0.307(9)	0.06(2)

Table 6. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Mn	2 <i>a</i>	0	0	0	0.0215(3)	0.0256(4)	0.0230(3)	−0.0017(3)	0.0058(3)	0.0009(3)
Se	4 <i>e</i>	0.40087(3)	0.14386(2)	0.74184(5)	0.0214(2)	0.0254(2)	0.0236(2)	−0.0019(1)	0.0057(1)	−0.0009(1)
O(1)	4 <i>e</i>	0.4207(3)	0.2409(2)	0.5948(4)	0.051(2)	0.032(1)	0.032(1)	−0.006(1)	0.016(1)	0.003(1)
O(2)	4 <i>e</i>	0.5469(3)	0.0742(2)	0.8012(5)	0.029(1)	0.044(2)	0.056(2)	0.007(1)	0.005(1)	0.001(1)
O(3)	4 <i>e</i>	0.2655(3)	0.0745(2)	0.6001(4)	0.027(1)	0.042(1)	0.032(1)	−0.007(1)	0.006(1)	−0.006(1)
O(4)	4 <i>e</i>	0.3647(3)	0.1849(2)	0.9593(4)	0.047(2)	0.035(1)	0.027(1)	−0.008(1)	0.015(1)	−0.005(1)
O(5)	4 <i>e</i>	0.1656(3)	0.1094(2)	0.1647(5)	0.032(2)	0.043(2)	0.027(2)	−0.011(1)	0.004(1)	−0.001(1)
O(6)	4 <i>e</i>	−0.1696(3)	0.1104(2)	0.0104(4)	0.027(1)	0.033(1)	0.044(2)	0.001(1)	0.011(1)	−0.000(1)
O(7)	4 <i>e</i>	−0.0066(3)	−0.0674(2)	0.2974(4)	0.036(2)	0.034(2)	0.031(1)	0.003(1)	0.015(1)	0.004(1)
Cs	4 <i>e</i>	0.13456(3)	0.35216(2)	0.35353(4)	0.0364(2)	0.0370(2)	0.0340(2)	0.0003(1)	0.0120(1)	0.0022(1)

3. Caesium hexaaquacobalt(II) selenate, Cs₂[Co(H₂O)₆](SeO₄)₂

Table 7. Data collection and handling.

Crystal:	dark red ellipsoid, size 0.25 × 0.26 × 0.27 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71069 Å)
<i>μ</i> :	105.76 cm ^{−1}
Diffractometer, scan mode:	RIGAKU AFC-6R, <i>ω</i>
2 θ _{max} :	50.1°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	5300, 1360
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1246
<i>N</i> (<i>param</i>) _{refined} :	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 8. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4 <i>e</i>	0.195(4)	0.091(3)	0.275(7)	0.05(1)
H(2)	4 <i>e</i>	0.218(4)	0.124(3)	0.116(6)	0.04(1)
H(3)	4 <i>e</i>	−0.238(4)	0.100(3)	−0.055(6)	0.05(1)
H(4)	4 <i>e</i>	−0.150(4)	0.173(3)	−0.011(6)	0.05(1)
H(5)	4 <i>e</i>	−0.074(5)	−0.059(4)	0.318(8)	0.08(2)
H(6)	4 <i>e</i>	0.015(4)	−0.126(3)	0.316(5)	0.033(9)

Table 9. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Co	2 <i>a</i>	0	0	0	0.0201(2)	0.0228(2)	0.0222(2)	−0.0016(2)	0.0069(2)	0.0008(2)
Se	4 <i>e</i>	0.39977(3)	0.14451(2)	0.74259(4)	0.0210(1)	0.0238(2)	0.0237(1)	−0.0020(1)	0.0061(1)	−0.0010(1)
O(1)	4 <i>e</i>	0.4220(2)	0.2429(2)	0.5982(3)	0.049(1)	0.028(1)	0.036(1)	−0.0056(9)	0.0180(9)	0.0026(8)
O(2)	4 <i>e</i>	0.5471(2)	0.0736(2)	0.8024(4)	0.026(1)	0.042(1)	0.053(1)	0.0055(9)	0.0049(9)	−0.000(1)
O(3)	4 <i>e</i>	0.2631(2)	0.0756(2)	0.5981(3)	0.0264(9)	0.038(1)	0.0300(9)	−0.0072(8)	0.0068(8)	−0.0061(9)
O(4)	4 <i>e</i>	0.3620(2)	0.1856(2)	0.9604(3)	0.041(1)	0.033(1)	0.0270(9)	−0.0051(9)	0.0143(8)	−0.0047(8)
O(5)	4 <i>e</i>	0.1586(2)	0.1083(2)	0.1609(4)	0.029(1)	0.038(1)	0.027(1)	−0.0093(9)	0.007(1)	−0.0006(9)
O(6)	4 <i>e</i>	−0.1659(2)	0.1062(2)	0.0142(4)	0.025(1)	0.030(1)	0.041(1)	0.0028(9)	0.010(1)	0.0009(9)
O(7)	4 <i>e</i>	−0.0055(2)	−0.0633(2)	0.2890(3)	0.032(1)	0.029(1)	0.031(1)	0.0023(9)	0.0137(9)	0.0041(8)
Cs	4 <i>e</i>	0.13327(2)	0.35125(1)	0.35249(3)	0.0351(1)	0.0345(1)	0.0338(1)	0.00030(8)	0.01192(8)	0.00217(7)

4. Caesium hexaaquanickel(II) selenate, Cs₂[Ni(H₂O)₆](SeO₄)₂

Table 10. Data collection and handling.

Crystal:	greenish blue ellipsoid, size 0.31 × 0.32 × 0.33 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71069 Å)
<i>μ</i> :	108.52 cm ^{−1}
Diffractometer, scan mode:	RIGAKU AFC-6R, <i>ω</i>
2 θ _{max} :	50.1°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	5196, 1332
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1224
<i>N</i> (<i>param</i>) _{refined} :	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 11. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4 <i>e</i>	0.193(4)	0.093(3)	0.286(7)	0.05(1)
H(2)	4 <i>e</i>	0.219(4)	0.124(3)	0.115(6)	0.03(1)
H(3)	4 <i>e</i>	−0.252(6)	0.103(4)	−0.061(8)	0.08(2)
H(4)	4 <i>e</i>	−0.148(5)	0.162(3)	−0.006(7)	0.05(1)
H(5)	4 <i>e</i>	−0.078(5)	−0.056(3)	0.315(6)	0.04(1)
H(6)	4 <i>e</i>	0.016(4)	−0.124(3)	0.304(6)	0.04(1)

Table 12. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Ni	2a	0	0	0	0.0169(2)	0.0204(3)	0.0187(2)	−0.0013(2)	0.0050(2)	0.0005(2)
Se	4e	0.39953(3)	0.14484(2)	0.74242(4)	0.0184(2)	0.0215(2)	0.0214(2)	−0.0018(1)	0.0048(1)	−0.0009(1)
O(1)	4e	0.4228(2)	0.2441(2)	0.5991(3)	0.045(1)	0.027(1)	0.032(1)	−0.006(1)	0.016(1)	0.0043(9)
O(2)	4e	0.5472(2)	0.0733(2)	0.8025(4)	0.022(1)	0.036(1)	0.051(1)	0.0054(9)	0.0033(9)	−0.000(1)
O(3)	4e	0.2617(2)	0.0759(2)	0.5966(3)	0.023(1)	0.034(1)	0.028(1)	−0.0079(9)	0.0045(8)	−0.0062(9)
O(4)	4e	0.3607(2)	0.1860(2)	0.9606(3)	0.040(1)	0.031(1)	0.025(1)	−0.005(1)	0.0131(9)	−0.0041(9)
O(5)	4e	0.1551(2)	0.1069(2)	0.1580(4)	0.026(1)	0.033(1)	0.025(1)	−0.008(1)	0.0065(9)	0.0003(9)
O(6)	4e	−0.1637(2)	0.1040(2)	0.0164(3)	0.022(1)	0.026(1)	0.036(1)	0.0021(9)	0.0096(9)	0.0017(9)
O(7)	4e	−0.0026(3)	−0.0607(2)	0.2879(3)	0.027(1)	0.028(1)	0.025(1)	0.0005(9)	0.0108(9)	0.0024(9)
Cs	4e	0.13338(2)	0.35103(2)	0.35126(3)	0.0322(1)	0.0319(1)	0.0312(1)	0.00012(8)	0.01026(8)	0.00196(8)

5. Caesium hexaaquazink(II) selenate, Cs₂[Zn(H₂O)₆](SeO₄)₂

Table 13. Data collection and handling.

Crystal:	colorless ellipsoid, size 0.23 × 0.25 × 0.27 mm
Wavelength:	Mo K _α radiation (0.71069 Å)
μ:	110.66 cm ^{−1}
Diffraction, scan mode:	RIGAKU AFC-6R, ω
2θ _{max} :	50.16°
N(hkl) _{measured} , N(hkl) _{unique} :	5269, 1355
Criterion for I _{obs} , N(hkl) _{gt} :	I _{obs} > 2 σ(I _{obs}), 1223
N(param) _{refined} :	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 14. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U _{iso}
H(1)	4e	0.191(4)	0.089(3)	0.280(7)	0.03(1)
H(2)	4e	0.216(5)	0.123(4)	0.117(8)	0.04(1)
H(3)	4e	−0.249(7)	0.106(5)	−0.08(1)	0.09(2)
H(4)	4e	−0.148(6)	0.158(4)	−0.001(9)	0.06(2)
H(5)	4e	−0.066(5)	−0.065(3)	0.316(6)	0.03(1)
H(6)	4e	0.020(5)	−0.136(4)	0.306(7)	0.05(1)

Table 15. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Zn	2a	0	0	0	0.0204(2)	0.0246(3)	0.0220(2)	−0.0019(2)	0.0061(2)	0.0011(2)
Se	4e	0.39922(3)	0.14478(2)	0.74298(5)	0.0182(2)	0.0227(2)	0.0218(2)	−0.0020(1)	0.0049(1)	−0.0010(1)
O(1)	4e	0.4211(3)	0.2437(2)	0.5993(4)	0.046(1)	0.028(1)	0.031(1)	−0.004(1)	0.015(1)	0.005(1)
O(2)	4e	0.5462(2)	0.0740(2)	0.8020(4)	0.022(1)	0.040(1)	0.053(2)	0.006(1)	0.002(1)	−0.001(1)
O(3)	4e	0.2624(2)	0.0760(2)	0.5990(3)	0.022(1)	0.039(1)	0.028(1)	−0.008(1)	0.0036(9)	−0.007(1)
O(4)	4e	0.3615(3)	0.1855(2)	0.9615(3)	0.039(1)	0.033(1)	0.025(1)	−0.005(1)	0.014(1)	−0.005(1)
O(5)	4e	0.1581(3)	0.1083(2)	0.1612(4)	0.027(1)	0.038(1)	0.024(1)	−0.009(1)	0.005(1)	−0.001(1)
O(6)	4e	−0.1669(3)	0.1057(2)	0.0151(4)	0.024(1)	0.029(1)	0.039(1)	0.002(1)	0.010(1)	0.001(1)
O(7)	4e	−0.0037(3)	−0.0626(2)	0.2883(4)	0.028(1)	0.032(2)	0.026(1)	0.001(1)	0.013(1)	0.003(1)
Cs	4e	0.13267(2)	0.35145(2)	0.35274(3)	0.0322(1)	0.0333(2)	0.0316(1)	0.00021(9)	0.01047(9)	0.00206(9)

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