Crystal structure of Tutton's salts, $Cs_2[M^{II}(H_2O)_6](SeO_4)_2$, M^{II} = Mg, Mn, Co, Ni, Zn

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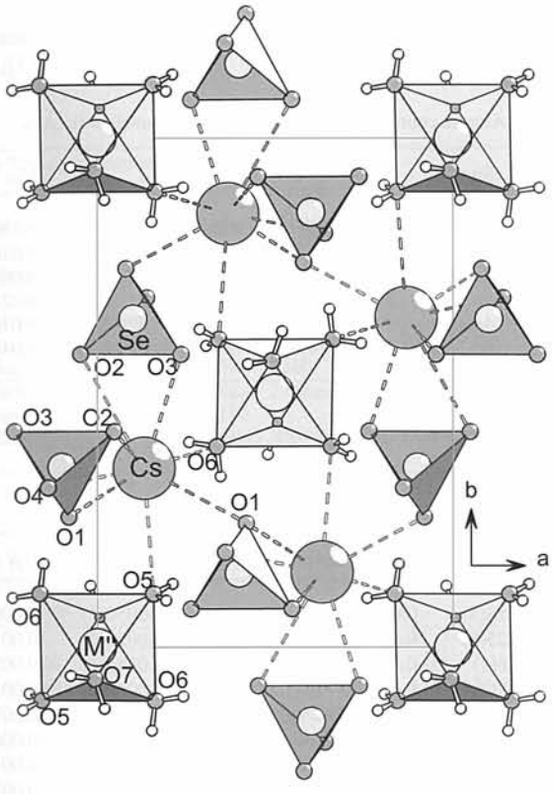

Abstract

$Cs_2H_{12}MgO_{14}Se_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.513(1)$ Å, $b = 13.037(1)$ Å, $c = 6.4730(8)$ Å, $\beta = 106.244(8)°$, $V = 770.7$ Å^3, $Z = 2$, $R_{gt}(F) = 0.020$, $wR_{ref}(F^2) = 0.036$, $T = 293$ K.

$Cs_2H_{12}MnO_{14}Se_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.591(1)$ Å, $b = 13.141(2)$ Å, $c = 6.5040(9)$ Å, $\beta = 106.38(1)°$, $V = 786.5$ Å^3, $Z = 2$, $R_{gt}(F) = 0.021$, $wR_{ref}(F^2) = 0.043$, $T = 293$ K.

$CoCs_2H_{12}O_{14}Se_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.494(1)$ Å, $b = 13.009(1)$ Å, $c = 6.4833(8)$ Å, $\beta = 106.239(9)°$, $V = 768.8$ Å^3, $Z = 2$, $R_{gt}(F) = 0.016$, $wR_{ref}(F^2) = 0.032$, $T = 293$ K.

$Cs_2H_{12}NiO_{14}Se_2$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.426(3)$ Å, $b = 12.961(2)$ Å, $c = 6.473(2)$ Å, $\beta = 106.17(2)°$, $V = 759.5$ Å^3, $Z = 2$, $R_{gt}(F) = 0.017$, $wR_{ref}(F^2) = 0.034$, $T = 293$ K.

$Cs_2H_{12}O_{14}Se_2Zn$, monoclinic, $P12_1/a1$ (No. 14), $a = 9.483(1)$ Å, $b = 13.005(2)$ Å, $c = 6.4850(8)$ Å, $\beta = 106.16(1)°$, $V = 768.2$ Å^3, $Z = 2$, $R_{gt}(F) = 0.019$, $wR_{ref}(F^2) = 0.037$, $T = 293$ K.

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Source of material

All compounds of the isomorphous series $Cs_2[M^{II}(H_2O)_6](SeO_4)_2$ were prepared by dissolution of equimolar amounts of caesium selenate Cs_2SeO_4 and M^{II} selenate hydrate $M^{II}SeO_4 \cdot nH_2O$ in hot destilled 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 M^{II} = Mg, Co, Ni, Zn, the M^{II} selenate hexahydrates were used, for M^{II} = Mn, the M^{II} selenate pentahydrate. Differently coloured, mostly ideomorphous 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(Cs—O) = 3.065(3) Å – 3.483(3) Å, and somewhat distorted $M^{II}(H_2O)_6$ octahedra, $d(M^{II}—O) = 2.038(3)$ Å – 2.193(3) Å, 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 $M^{II}O_6$ 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, $[\bar{d}(Cs—O)/\bar{d}(Rb—O)]^3 = 1.125$.
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 $M^{II}O_6$ and CsO_8 coordination polyhedra increase as the cation radii $R(M^{II})$ [5] increase. However, for $V(CsO_8)$, the rate of increase is about two times smaller than for $V(M^{II}O_6)$.
5. As in the Rb selenate series, the a, b axes and $V(CsO_8)$ 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(Cs—O5) = 3.483(3) Å and d(Cs—O6) = 3.372(3) Å, compared to other M^{II} compounds of the same series.

6. The oxygen atoms of the SeO_4 group are acceptors of 6 different hydrogen bonds, providing links to 4 different $M^{II}(H_2O)_6$ 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 $\overline{d}$(O–H···O) = 2.745 Å averaged over all donor-acceptor distances in the structure.

1. Caesium hexaaquamagnesium(II) selenate, $Cs_2[Mg(H_2O)_6](SeO_4)_2$

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}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5294, 1357
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1115
$N(param)_{refined}$:	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 2. Atomic coordinates and displacement parameters (in $Å^2$).

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

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mg	2*a*	0	0	0	0.0190(8)	0.0213(8)	0.0200(9)	–0.0022(6)	0.0058(7)	0.0003(6)
Se	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	–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)	4*e*	–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	4*e*	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, $Cs_2[Mn(H_2O)_6](SeO_4)_2$

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}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50.08°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5336, 1364
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1215
$N(param)_{refined}$:	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 5. Atomic coordinates and displacement parameters (in $Å^2$).

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

Table 6. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn	2*a*	0	0	0	0.0215(3)	0.0256(4)	0.0230(3)	–0.0017(3)	0.0058(3)	0.0009(3)
Se	4*e*	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*e*	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*e*	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*e*	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*e*	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*e*	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*e*	–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*e*	–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*e*	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, $Cs_2[Co(H_2O)_6](SeO_4)_2$

Table 7. Data collection and handling.

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

Table 8. Atomic coordinates and displacement parameters (in Å^2).

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

Table 9. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co	2*a*	0	0	0	0.0201(2)	0.0228(2)	0.0222(2)	–0.0016(2)	0.0069(2)	0.0008(2)
Se	4*e*	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*e*	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*e*	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*e*	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*e*	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*e*	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*e*	–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*e*	–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*e*	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, $Cs_2[Ni(H_2O)_6](SeO_4)_2$

Table 10. Data collection and handling.

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

Table 11. Atomic coordinates and displacement parameters (in Å^2).

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

Table 12. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni	2*a*	0	0	0	0.0169(2)	0.0204(3)	0.0187(2)	–0.0013(2)	0.0050(2)	0.0005(2)
Se	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	–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)	4*e*	–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	4*e*	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, $Cs_2[Zn(H_2O)_6](SeO_4)_2$

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}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50.16°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5269, 1355
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1223
$N(param)_{refined}$:	113
Programs:	SHELXS-97 [6], DIAMOND [7])

Table 14. Atomic coordinates and displacement parameters (in Å^2).

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

Table 15. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn	2*a*	0	0	0	0.0204(2)	0.0246(3)	0.0220(2)	–0.0019(2)	0.0061(2)	0.0011(2)
Se	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	–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)	4*e*	–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	4*e*	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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