Crystal structure of Tutton's salts, $Cs_2[M^{II}(H_2O)_6](SO_4)_2$, M^{II} = Mg, Mn, Fe, Co, Ni, Zn

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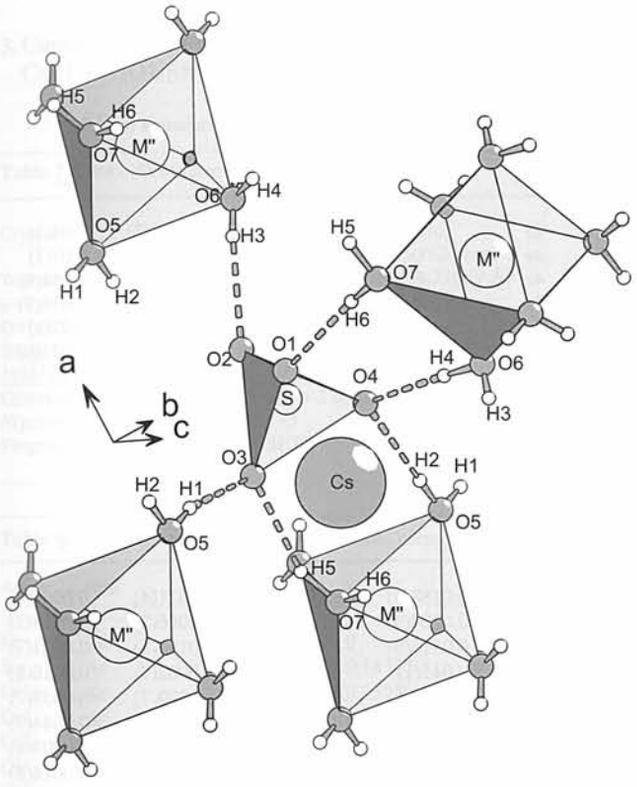

Abstract

$Cs_2H_{12}MgO_{14}S_2$, monoclinic, $P12_1/a1$ (No. 14), a = 9.338(2) Å, b = 12.849(4) Å, c = 6.361(2) Å, β = 107.07(2)°, V = 729.6 Å^3, Z = 2, $R_{gt}(F)$ = 0.017, $wR_{ref}(F^2)$ = 0.041, T = 293 K.

$Cs_2H_{12}MnO_{14}S_2$, monoclinic, $P12_1/a1$ (No. 14), a = 9.418(3) Å, b = 12.963(2) Å, c = 6.386(3) Å, β = 107.17(4)°, V = 744.9 Å^3, Z = 2, $R_{gt}(F)$ = 0.017, $wR_{ref}(F^2)$ = 0.030, T = 293 K.

$Cs_2FeO_{14}H_{12}S_2$, monoclinic, $P12_1/a1$ (No. 14), a = 9.357(2) Å, b = 12.886(2) Å, c = 6.381(1) Å, β = 106.94(1)°, V = 736.0 Å^3, Z = 2, $R_{gt}(F)$ = 0.015, $wR_{ref}(F^2)$ = 0.030, T = 293 K.

$CoCs_2H_{12}O_{14}S_2$, monoclinic, $P12_1/a1$ (No. 14), a = 9.318(1) Å, b = 12.826(3) Å, c = 6.3650(9) Å, β = 107.13(1)°, V = 727.0 Å^3, Z = 2, $R_{gt}(F)$ = 0.021, $wR_{ref}(F^2)$ = 0.049, T = 293 K.

$Cs_2H_{12}NiO_{14}S_2$, monoclinic, $P12_1/a1$ (No. 14), a = 9.259(2) Å, b = 12.767(2) Å, c = 6.358(1) Å, β = 107.00(2)°, V = 718.7 Å^3, Z = 2, $R_{gt}(F)$ = 0.014, $wR_{ref}(F^2)$ = 0.027, T = 293 K.

$Cs_2H_{12}O_{14}S_2Zn$, monoclinic, $P12_1/a1$ (No. 14), a = 9.314(2) Å, b = 12.817(2) Å, c = 6.369(2) Å, β = 106.94(2)°, V = 727.3 Å^3, Z = 2, $R_{gt}(F)$ = 0.015, $wR_{ref}(F^2)$ = 0.033, T = 293 K.

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Source of material

All compounds of the isomorphous series $Cs_2[M^{II}(H_2O)_6](SO_4)_2$ were prepared by dissolution of equimolar amounts of caesium sulphate Cs_2SO_4 and M^{II} sulphate hydrate $M^{II}SO_4 \cdot nH_2O$ in hot destilled water and ensuing evaporation of the solvent. The M^{II} sulphate hydrates contained different amounts of crystal water. For the syntheses of Tutton's salts with M^{II} = Mg, Fe, Co, Zn, the M^{II} sulphate heptahydrates were used, for M^{II} = Mn, the sulphate monohydrate, and for M^{II} = Ni, the sulphate hexahydrate. 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 caesium hexaaquacopper(II) sulphate [3]. The structure is characterized by the irregular CsO_8 polyhedra with d(Cs—O) = 3.054(2) Å – 3.480(2) Å and somewhat distorted $M^{II}(H_2O)_6$ octahedra with $d(M^{II}—O)$ = 2.061(2) Å – 2.183(2) Å, the latter being linked to the SO_4 tetrahedra by hydrogen bonds. Compared to the isotypic Rb sulphates [1], one finds:

1. For all the different M^{II} compounds, the lattice constants a, b, c increase on average by 1.2%, 3.2%, 2.1%, 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, in contrast to the Rb sulphates (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 sulphates.
2. The volumes of the $M^{II}O_6$ octahedra agree with those of the corresponding Rb sulphates.
3. The volumes of the CsO_8 coordination polyhedra increase on average by 15.2%. This is somewhat larger than the 3rd power of the mean Cs—O and Rb—O bond lengths, $[\overline{d}(Cs—O)/\overline{d}(Rb—O)]^3$ = 1.125.
4. While in agreement with chemical expectation, the sulphate 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 sulphate series, a, b and $V(CsO_8)$ of the Mg compound are significantly larger than expected from the linear lattice constant vs cation radius correlations observed for the other structures. This finding can be attributed to the smaller electro-

negativity of Mg, causing somewhat weaker shared Cs–O interactions, as reflected by increased distances d(Cs—O5) = 3.480(2) Å and d(Cs—O6) = 3.359(2) Å, compared to other M^{II} compounds of the same series.

6. The oxygen atoms of the SO_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, O3 and O4 are fixed by bifurcated bonds. For the individual Cs-sulphate compounds, the hydrogen bond lengths differ from those observed in the Rb analogues, but no significant difference is found for the mean distance $\bar{d}$(O–H···O) = 2.740 Å averaged over all donor-acceptor distances in the structure.

1. Caesium hexaaquamagnesium(II) sulphate, $Cs_2[Mg(H_2O)_6](SO_4)_2$

Table 1. Data collection and handling.

Crystal:	colorless ellipsoid, size 0.25 × 0.26 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	53.87 cm^{-1}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4932, 1267
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1206
$N(param)_{refined}$:	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*	0.207(4)	0.104(3)	0.279(7)	0.04(1)
H(2)	4*e*	0.217(5)	0.126(3)	0.105(7)	0.05(1)
H(3)	4*e*	–0.243(5)	0.100(3)	–0.049(6)	0.034(9)
H(4)	4*e*	–0.157(4)	0.172(3)	–0.017(6)	0.038(9)
H(5)	4*e*	–0.079(6)	–0.055(3)	0.340(8)	0.07(1)
H(6)	4*e*	0.011(4)	–0.125(3)	0.308(6)	0.031(9)

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	0.0172(5)	0.0208(5)	0.0188(5)	–0.0021(4)	0.0071(4)	0.0005(4)
S	4*e*	0.39667(6)	0.14721(4)	0.74079(9)	0.0168(3)	0.0201(3)	0.0204(3)	–0.0015(2)	0.0066(2)	–0.0004(2)
O(1)	4*e*	0.4169(2)	0.2371(1)	0.6088(3)	0.042(1)	0.0248(9)	0.0316(9)	–0.0025(8)	0.0187(8)	0.0031(7)
O(2)	4*e*	0.5326(2)	0.0835(2)	0.8026(3)	0.0219(8)	0.036(1)	0.041(1)	0.0050(7)	0.0062(7)	0.0018(8)
O(3)	4*e*	0.2717(2)	0.0832(1)	0.6057(3)	0.0224(8)	0.034(1)	0.0264(8)	–0.0064(7)	0.0079(7)	–0.0059(7)
O(4)	4*e*	0.3602(2)	0.1837(1)	0.9397(3)	0.0356(9)	0.0301(9)	0.0233(8)	–0.0047(7)	0.0142(7)	–0.0044(7)
O(5)	4*e*	0.1618(2)	0.1068(2)	0.1607(4)	0.0276(9)	0.035(1)	0.023(1)	–0.0113(8)	0.0070(8)	–0.0007(8)
O(6)	4*e*	–0.1667(2)	0.1077(2)	0.0073(3)	0.0185(9)	0.028(1)	0.037(1)	0.0015(8)	0.0095(8)	0.0018(8)
O(7)	4*e*	–0.0066(2)	–0.0649(2)	0.2912(3)	0.0277(9)	0.025(1)	0.0267(8)	0.0029(7)	0.0141(7)	0.0035(7)
Cs	4*e*	0.12742(2)	0.35609(1)	0.35448(2)	0.0302(2)	0.0304(2)	0.0288(2)	0.00032(6)	0.01175(8)	0.00182(5)

2. Caesium hexaaquamanganese(II) sulphate, $Cs_2[Mn(H_2O)_6](SO_4)_2$

Table 4. Data collection and handling.

Crystal:	light pink ellipsoid, size 0.32 × 0.34 × 0.36 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	60.43 cm^{-1}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	49.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5000, 1279
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1255
$N(param)_{refined}$:	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*	0.204(4)	0.105(3)	0.269(6)	0.04(1)
H(2)	4*e*	0.234(4)	0.129(2)	0.100(5)	0.036(8)
H(3)	4*e*	–0.247(4)	0.104(3)	–0.064(5)	0.04(1)
H(4)	4*e*	–0.160(3)	0.172(3)	–0.018(5)	0.034(8)
H(5)	4*e*	–0.061(4)	–0.066(3)	0.329(6)	0.03(1)
H(6)	4*e*	0.016(4)	–0.136(3)	0.319(6)	0.043(9)

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	0.0197(2)	0.0230(2)	0.0227(2)	–0.0019(2)	0.0062(2)	0.0008(2)
S	4*e*	0.39830(6)	0.14535(4)	0.73996(9)	0.0193(3)	0.0226(3)	0.0226(3)	–0.0017(2)	0.0060(2)	–0.0007(2)
O(1)	4*e*	0.4178(2)	0.2341(1)	0.6074(3)	0.045(1)	0.0279(9)	0.0352(9)	–0.0043(8)	0.0182(8)	0.0026(7)
O(2)	4*e*	0.5324(2)	0.0816(2)	0.7999(3)	0.0236(9)	0.040(1)	0.047(1)	0.0055(8)	0.0053(8)	0.0015(8)
O(3)	4*e*	0.2731(2)	0.0827(1)	0.6065(3)	0.0240(8)	0.0365(9)	0.0297(8)	–0.0076(7)	0.0068(7)	–0.0067(7)
O(4)	4*e*	0.3640(2)	0.1824(1)	0.9384(3)	0.041(1)	0.0324(9)	0.0262(8)	–0.0034(8)	0.0141(7)	–0.0040(7)
O(5)	4*e*	0.1692(2)	0.1122(2)	0.1640(4)	0.030(1)	0.042(1)	0.024(1)	–0.0115(8)	0.0039(9)	–0.0008(8)
O(6)	4*e*	–0.1739(2)	0.1125(2)	0.0053(3)	0.023(1)	0.030(1)	0.045(1)	0.0015(8)	0.0111(9)	0.0016(8)
O(7)	4*e*	–0.0044(2)	–0.0697(2)	0.3035(3)	0.032(1)	0.031(1)	0.031(1)	0.0027(8)	0.0165(8)	0.0030(7)
Cs	4*e*	0.13029(2)	0.35642(1)	0.35607(3)	0.0328(1)	0.0332(1)	0.0321(1)	0.00042(6)	0.01162(7)	0.00165(6)

3. Caesium hexaaquairon(II) sulphate, $Cs_2[Fe(H_2O)_6](SO_4)_2$

Table 7. Data collection and handling.

Crystal:	dark yellow ellipsoid, size 0.22 × 0.23 × 0.24 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	62.44 cm^{-1}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5022, 1289
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 8. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.206(3)	0.101(2)	0.285(5)	0.039(9)
H(2)	4*e*	0.223(4)	0.125(2)	0.106(5)	0.036(9)
H(3)	4*e*	–0.252(4)	0.101(3)	–0.055(5)	0.05(1)
H(4)	4*e*	–0.156(3)	0.167(3)	–0.017(5)	0.035(9)
H(5)	4*e*	–0.070(4)	–0.063(3)	0.329(5)	0.04(1)
H(6)	4*e*	0.022(4)	–0.131(3)	0.315(6)	0.06(1)

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}
Fe	2*a*	0	0	0	0.0192(2)	0.0226(2)	0.0210(2)	–0.0017(2)	0.0058(2)	0.0008(2)
S	4*e*	0.39677(6)	0.14572(4)	0.74107(9)	0.0195(3)	0.0228(3)	0.0223(3)	–0.0016(2)	0.0059(2)	–0.0004(2)
O(1)	4*e*	0.4169(2)	0.2353(1)	0.6097(3)	0.044(1)	0.0281(9)	0.0333(9)	–0.0039(8)	0.0171(8)	0.0033(7)
O(2)	4*e*	0.5316(2)	0.0815(2)	0.8001(3)	0.0225(8)	0.039(1)	0.047(1)	0.0055(8)	0.0050(7)	0.0021(8)
O(3)	4*e*	0.2709(2)	0.0829(1)	0.6073(3)	0.0238(8)	0.037(1)	0.0281(8)	–0.0059(7)	0.0052(6)	–0.0059(7)
O(4)	4*e*	0.3620(2)	0.1823(1)	0.9406(3)	0.040(1)	0.0325(9)	0.0252(8)	–0.0038(8)	0.0131(7)	–0.0039(7)
O(5)	4*e*	0.1647(2)	0.1110(2)	0.1646(3)	0.0289(9)	0.041(1)	0.025(1)	–0.0121(8)	0.0054(8)	–0.0005(8)
O(6)	4*e*	–0.1717(2)	0.1099(2)	0.0075(3)	0.024(1)	0.030(1)	0.043(1)	0.0013(8)	0.0111(8)	0.0023(8)
O(7)	4*e*	–0.0035(2)	–0.0675(2)	0.2971(3)	0.031(1)	0.031(1)	0.0291(9)	0.0022(8)	0.0148(8)	0.0025(7)
Cs	4*e*	0.12886(2)	0.35576(1)	0.35553(2)	0.0324(1)	0.0326(1)	0.0309(1)	0.00076(6)	0.01116(6)	0.00183(6)

4. Caesium hexaaquacobalt(II) sulphate, $Cs_2[Co(H_2O)_6](SO_4)_2$

Table 10. Data collection and handling.

Crystal:	dark red ellipsoid, size 0.28 × 0.29 × 0.31 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	64.64 cm^{-1}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4958, 1273
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1219
$N(param)_{refined}$:	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*	0.200(5)	0.098(4)	0.266(8)	0.05(1)
H(2)	4*e*	0.220(5)	0.123(3)	0.097(7)	0.03(1)
H(3)	4*e*	–0.242(5)	0.100(3)	–0.047(7)	0.04(1)
H(4)	4*e*	–0.157(5)	0.169(4)	–0.007(7)	0.05(1)
H(5)	4*e*	–0.082(7)	–0.062(4)	0.331(9)	0.07(2)
H(6)	4*e*	0.025(8)	–0.114(5)	0.29(1)	0.08(2)

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}
Co	2*a*	0	0	0	0.0177(3)	0.0205(3)	0.0185(3)	–0.0016(2)	0.0052(2)	0.0004(2)
S	4*e*	0.39716(8)	0.14607(4)	0.7410(1)	0.0192(4)	0.0210(4)	0.0209(5)	–0.0014(2)	0.0048(3)	–0.0003(2)
O(1)	4*e*	0.4188(2)	0.2360(2)	0.6107(3)	0.042(1)	0.026(1)	0.032(1)	–0.0039(8)	0.0158(9)	0.0029(8)
O(2)	4*e*	0.5325(2)	0.0814(2)	0.8023(4)	0.0227(9)	0.036(1)	0.044(1)	0.0031(8)	0.0040(8)	–0.0004(9)
O(3)	4*e*	0.2708(2)	0.0833(2)	0.6049(3)	0.0234(9)	0.036(1)	0.0258(9)	–0.0065(8)	0.0044(7)	–0.0055(8)
O(4)	4*e*	0.3613(2)	0.1827(2)	0.9396(3)	0.039(1)	0.030(1)	0.0243(9)	–0.0037(8)	0.0112(8)	–0.0040(8)
O(5)	4*e*	0.1621(2)	0.1107(2)	0.1604(4)	0.028(1)	0.039(1)	0.022(1)	–0.0109(9)	0.005(1)	–0.0018(9)
O(6)	4*e*	–0.1692(3)	0.1085(2)	0.0111(4)	0.021(1)	0.030(1)	0.038(1)	0.0005(9)	0.0077(9)	0.0005(9)
O(7)	4*e*	–0.0041(2)	–0.0654(2)	0.2951(3)	0.030(1)	0.028(1)	0.0267(9)	0.0025(8)	0.0132(8)	0.0023(8)
Cs	4*e*	0.12887(2)	0.35536(1)	0.35586(3)	0.0318(2)	0.0309(2)	0.0293(2)	0.00051(6)	0.0102(1)	0.00168(5)

5. Caesium hexaaquanickel(II) sulphate, $Cs_2[Ni(H_2O)_6](SO_4)_2$

Table 13. Data collection and handling.

Crystal:	greenish blue ellipsoid, size 0.265 × 0.275 × 0.285 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	66.94 cm^{-1}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4808, 1234
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1193
$N(param)_{refined}$:	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*	0.196(3)	0.102(2)	0.274(5)	0.031(8)
H(2)	4*e*	0.220(4)	0.122(2)	0.100(5)	0.028(8)
H(3)	4*e*	–0.240(4)	0.099(3)	–0.056(5)	0.04(1)
H(4)	4*e*	–0.152(4)	0.165(3)	–0.013(5)	0.036(9)
H(5)	4*e*	–0.073(4)	–0.058(3)	0.325(5)	0.042(9)
H(6)	4*e*	0.020(4)	–0.125(3)	0.315(5)	0.038(8)

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}
Ni	2*a*	0	0	0	0.0142(2)	0.0169(2)	0.0159(2)	–0.0014(1)	0.0052(1)	0.0004(1)
S	4*e*	0.39663(6)	0.14648(4)	0.74097(8)	0.0154(2)	0.0179(2)	0.0182(2)	–0.0015(2)	0.0049(2)	–0.0003(2)
O(1)	4*e*	0.4191(2)	0.2375(1)	0.6118(3)	0.0385(9)	0.0226(8)	0.0302(8)	–0.0037(7)	0.0163(7)	0.0029(7)
O(2)	4*e*	0.5326(2)	0.0814(1)	0.8020(3)	0.0189(8)	0.0321(9)	0.0402(9)	0.0047(7)	0.0042(7)	0.0010(8)
O(3)	4*e*	0.2696(2)	0.0838(1)	0.6039(2)	0.0195(7)	0.0312(9)	0.0236(7)	–0.0056(7)	0.0046(6)	–0.0046(7)
O(4)	4*e*	0.3597(2)	0.1832(1)	0.9404(2)	0.0328(9)	0.0280(8)	0.0210(7)	–0.0041(7)	0.0115(6)	–0.0036(6)
O(5)	4*e*	0.1585(2)	0.1093(1)	0.1577(3)	0.0232(8)	0.0314(9)	0.0189(9)	–0.0085(7)	0.0046(7)	–0.0002(7)
O(6)	4*e*	–0.1670(2)	0.1062(1)	0.0139(3)	0.0177(9)	0.0231(9)	0.0328(9)	0.0013(7)	0.0082(8)	0.0014(7)
O(7)	4*e*	–0.0012(2)	–0.0628(1)	0.2937(2)	0.0234(8)	0.0224(9)	0.0229(8)	0.0019(7)	0.0113(7)	0.0024(6)
Cs	4*e*	0.12839(2)	0.35492(1)	0.35470(2)	0.0279(1)	0.0274(1)	0.0265(1)	0.00041(6)	0.00989(6)	0.00161(5)

6. Caesium hexaaquazink(II) sulphate, $Cs_2[Zn(H_2O)_6](SO_4)_2$

Table 16. Data collection and handling.

Crystal:	colorless ellipsoid, size 0.18 × 0.19 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	69.70 cm^{-1}
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{max}$:	49.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4798, 1230
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1122
$N(param)_{refined}$:	113
Programs:	SHELXS-97 [6], DIAMOND [7]

Table 17. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.192(4)	0.101(3)	0.261(7)	0.03(1)
H(2)	4*e*	0.227(5)	0.124(3)	0.097(6)	0.037(9)
H(3)	4*e*	–0.246(4)	0.098(3)	–0.044(6)	0.03(1)
H(4)	4*e*	–0.156(5)	0.172(4)	–0.009(7)	0.06(1)
H(5)	4*e*	–0.081(5)	–0.060(3)	0.325(6)	0.04(1)
H(6)	4*e*	0.019(6)	–0.125(4)	0.298(8)	0.06(1)

Table 18. 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	0.0186(2)	0.0206(2)	0.0192(2)	–0.0024(1)	0.0055(2)	0.0005(2)
S	4*e*	0.39618(7)	0.14631(4)	0.7415(1)	0.0169(3)	0.0188(3)	0.0199(3)	–0.0014(2)	0.0049(2)	–0.0004(2)
O(1)	4*e*	0.4175(2)	0.2369(2)	0.6126(3)	0.041(1)	0.023(1)	0.031(1)	–0.0019(8)	0.0164(9)	0.0039(7)
O(2)	4*e*	0.5319(2)	0.0816(2)	0.8007(3)	0.0213(9)	0.033(1)	0.042(1)	0.0039(8)	0.0037(8)	0.0013(9)
O(3)	4*e*	0.2701(2)	0.0832(2)	0.6056(3)	0.0220(9)	0.033(1)	0.0243(9)	–0.0053(8)	0.0051(7)	–0.0044(8)
O(4)	4*e*	0.3605(2)	0.1826(2)	0.9409(3)	0.036(1)	0.030(1)	0.0232(9)	–0.0038(8)	0.0112(8)	–0.0024(8)
O(5)	4*e*	0.1607(2)	0.1106(2)	0.1606(4)	0.028(1)	0.035(1)	0.021(1)	–0.0112(9)	0.005(1)	0.0000(9)
O(6)	4*e*	–0.1702(3)	0.1083(2)	0.0125(3)	0.020(1)	0.025(1)	0.039(1)	–0.0001(8)	0.0099(9)	0.0009(9)
O(7)	4*e*	–0.0027(2)	–0.0645(2)	0.2944(3)	0.026(1)	0.024(1)	0.0251(9)	0.0013(8)	0.0114(8)	0.0019(8)
Cs	4*e*	0.12786(2)	0.35535(1)	0.35590(3)	0.0296(1)	0.0285(1)	0.0281(1)	0.00057(6)	0.01029(8)	0.00164(6)

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