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

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1. Except for Mg, the lattice parameters of all other M^{II} compounds increase on average by 0.4 % for *a*, but decrease on average by 0.1 %, 0.3 % for *b* and *c*, respectively. These subtle changes are due to the similar sizes of the Tl⁺ and Rb⁺ cations ($R(\text{Tl}^+) = 1.59 \text{ \AA}$, $R(\text{Rb}^+) = 1.61 \text{ \AA}$ [7]). The unit cell angle β increasing for all corresponding compounds by about 0.4° shows the same slope in the linear correlation between β and the M^{II} cation radius. The volume of the unit cells decrease only by about 0.2 %. With respect to the exchange of M^{II}, the linear correlations between the lattice constants and the cation radii exhibit for *a*, *b*, *c*, the same slopes, within error limits, as in the Rb sulfates.
2. The volumes of the various TlO₈ coordination polyhedra in the Tl sulfate salts show no significant deviations from the volumes of the RbO₈ coordination polyhedra in the Rb sulfates ($V(\text{TlO}_8) = 48.18(3) \text{ \AA}^3$ and $V(\text{RbO}_8) = 48.24(3) \text{ \AA}^3$ [7,8]). This result conforms with the equal mean Tl—O and Rb—O distances $\bar{d}$ of 3.067(6) Å.
3. Each of the volumes of the M^{II}O₆ coordination octahedra agrees with that of the corresponding Rb sulfates.
4. In agreement with chemical expectation, the sulfate group is practically invariant against the M^{II} cation exchange in the hexahydrate complexes, whereas the volumes of both the M^{II}O₆

and the TlO₈ coordination polyhedra increase as the cation radius $R(\text{M}^{\text{II}})$ [7,8] increases. For $V(\text{TlO}_8)$, the increase is more than three times smaller than that for $V(\text{M}^{\text{II}}\text{O}_6)$ similar to the Rb-sulfates.

5. As in the Rb sulfates, the *a* and *b* parameters of the Mg compound deviate significantly from the *a* vs $R(\text{M}^{\text{II}})$ relation $a[\text{\AA}] = 1.14(2) R(\text{M}^{\text{II}}) + 8.37(1)$. Again, this can be attributed to the larger M—O electronegativity difference causing somewhat weaker Tl—O interactions as reflected by the increased distances, $d(\text{Tl—O5}) = 3.363(4) \text{ \AA}$ and $d(\text{Tl—O6}) = 3.220(4) \text{ \AA}$, as compared to other M^{II} compounds of the same series, where $\bar{d}(\text{Tl—O5}) = 3.302(6) \text{ \AA}$ and $\bar{d}(\text{Tl—O6}) \geq 3.147(6) \text{ \AA}$.

6. The oxygen atoms of the SO₄ group are acceptors of 6 different hydrogen bonds, which provide links to 4 M^{II}(H₂O)₆ octahedra surrounding each sulfate anion. Contrary to O1 and O2, O3 and O4 are fixed by bifurcated bonds. Considering all structures of the here studied series, under the reservation that the H positions are derived rather than experimental ones, the hydrogen bond lengths differ negligibly ($\pm 0.011 \text{ \AA}$) from those observed in the Rb sulfates analogues, and also the averages over all donor-acceptor distances in the Tl salts structures $\bar{d}(\text{O—H}\cdots\text{O}) = 2.743(6) \text{ \AA}$ are equal to those in the Rb salts structures, $\bar{d}(\text{O—H}\cdots\text{O}) = 2.732(3) \text{ \AA}$.

1. Thallium hexaaquamagnesium(II) sulfate, Tl₂[Mg(H₂O)₆](SO₄)₂

Table 1. Data collection and handling.

Crystal:	colorless ellipsoid, size 0.27 × 0.26 × 0.25 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	238.34 cm ⁻¹
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\text{max}}$:	50.1°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4655, 1203
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1000
$N(\text{param})_{\text{refined}}$:	90
Programs:	SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11]

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	0.2030	0.0962	0.2740	0.029(7)
H(2)	4e	0.2287	0.1232	0.0963	0.029
H(3)	4e	-0.2457	0.1016	-0.0463	0.029
H(4)	4e	-0.1484	0.1716	-0.0076	0.029
H(5)	4e	-0.0749	-0.0611	0.3417	0.029
H(6)	4e	0.0195	-0.1275	0.3272	0.029

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	0.019(1)	0.019(1)	0.022(2)	-0.001(1)	0.004(1)	-0.000(1)
S	4e	0.4065(1)	0.1376(1)	0.7367(2)	0.0181(6)	0.0229(7)	0.0248(7)	-0.0027(6)	0.0049(5)	-0.0023(6)
O(1)	4e	0.4155(5)	0.2292(3)	0.5915(7)	0.052(3)	0.030(2)	0.035(3)	-0.010(2)	0.019(2)	0.003(2)
O(2)	4e	0.5445(5)	0.0739(4)	0.7865(8)	0.021(2)	0.044(3)	0.059(3)	0.007(2)	0.003(2)	-0.004(2)
O(3)	4e	0.2802(4)	0.0687(3)	0.6152(7)	0.025(2)	0.034(2)	0.036(2)	-0.007(2)	0.008(2)	-0.007(2)
O(4)	4e	0.3797(5)	0.1757(3)	0.9462(7)	0.042(2)	0.031(2)	0.023(2)	-0.005(2)	0.012(2)	-0.005(2)
O(5)	4e	0.1659(4)	0.1064(3)	0.1623(7)	0.026(2)	0.036(2)	0.028(2)	-0.007(2)	0.006(2)	-0.001(2)
O(6)	4e	-0.1642(4)	0.1108(3)	0.0209(7)	0.020(2)	0.026(2)	0.040(3)	0.002(2)	0.009(2)	-0.001(2)
O(7)	4e	-0.0048(4)	-0.0673(3)	0.2974(7)	0.029(2)	0.026(2)	0.032(2)	0.005(2)	0.016(2)	0.003(2)
Tl	4e	0.12634(3)	0.35470(2)	0.35039(4)	0.0358(2)	0.0352(2)	0.0374(2)	-0.0018(1)	0.0131(1)	0.0006(1)

2. Thallium hexaaquamanganese(II) sulfate, $\text{Th}_2[\text{Mn}(\text{H}_2\text{O})_6](\text{SO}_4)_2$

Table 4. Data collection and handling.

Crystal:	light pink ellipsoid, size $0.30 \times 0.29 \times 0.28$ mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ :	241.87 cm ⁻¹
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\text{max}}$:	50.1°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4816, 1238
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1041
$N(\text{param})_{\text{refined}}$:	89
Programs:	SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11]

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

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.2120	0.0960	0.2843	0.09(2)
H(2)	4e	0.2293	0.1285	0.1138	0.09
H(3)	4e	-0.2456	0.1052	-0.0456	0.09
H(4)	4e	-0.1555	0.1763	-0.0079	0.09
H(5)	4e	-0.0699	-0.0679	0.3527	0.09
H(6)	4e	0.0190	-0.1275	0.3448	0.09

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn	2a	0	0	0	0.0294(7)	0.0297(8)	0.0294(8)	-0.0003(6)	0.0075(6)	0.0008(6)
S	4e	0.4081(2)	0.1357(1)	0.7367(3)	0.0292(8)	0.0313(9)	0.0328(9)	-0.0025(7)	0.0085(7)	-0.0020(7)
O(1)	4e	0.4191(7)	0.2255(4)	0.5919(9)	0.063(4)	0.035(3)	0.044(3)	-0.009(3)	0.019(3)	0.003(2)
O(2)	4e	0.5437(6)	0.0711(5)	0.782(1)	0.037(3)	0.053(4)	0.069(4)	0.013(3)	0.006(3)	-0.001(3)
O(3)	4e	0.2816(6)	0.0686(4)	0.6167(9)	0.036(3)	0.043(3)	0.040(3)	-0.008(2)	0.010(2)	-0.006(3)
O(4)	4e	0.3841(6)	0.1750(4)	0.9457(9)	0.055(3)	0.040(3)	0.033(3)	-0.005(2)	0.013(3)	-0.004(2)
O(5)	4e	0.1742(6)	0.1119(4)	0.1676(9)	0.036(3)	0.046(3)	0.032(3)	-0.010(2)	0.001(2)	0.000(2)
O(6)	4e	-0.1713(6)	0.1157(4)	0.0226(9)	0.030(3)	0.041(3)	0.043(3)	0.003(2)	0.009(2)	0.001(2)
O(7)	4e	-0.0041(6)	-0.0719(4)	0.3095(9)	0.047(3)	0.038(3)	0.038(3)	0.004(2)	0.018(2)	0.002(2)
Tl	4e	0.13002(3)	0.35561(3)	0.35045(5)	0.0468(2)	0.0446(2)	0.0437(2)	-0.0026(2)	0.0161(1)	0.0005(2)

3. Thallium hexaaquairon(II) sulfate, $\text{Th}_2[\text{Fe}(\text{H}_2\text{O})_6](\text{SO}_4)_2$

Table 7. Data collection and handling.

Crystal:	light green ellipsoid, size $0.18 \times 0.17 \times 0.16$ mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ :	245.86 cm ⁻¹
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\text{max}}$:	50.08°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4740, 121
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 946
$N(\text{param})_{\text{refined}}$:	90
Programs:	SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11]

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

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.2060	0.0960	0.2840	0.05(2)
H(2)	4e	0.2346	0.1242	0.1007	0.05
H(3)	4e	-0.2510	0.1051	-0.0518	0.05
H(4)	4e	-0.1504	0.1743	-0.0059	0.05
H(5)	4e	-0.0749	-0.0656	0.3386	0.05
H(6)	4e	0.0232	-0.1363	0.3318	0.05

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe	2a	0	0	0	0.0194(9)	0.0206(8)	0.0207(8)	0.0001(7)	0.0050(7)	0.0001(7)
S	4e	0.4070(2)	0.1363(2)	0.7365(3)	0.021(1)	0.023(1)	0.0253(9)	-0.001(1)	0.0051(7)	-0.0040(9)
O(1)	4e	0.4185(8)	0.2269(5)	0.594(1)	0.046(4)	0.030(4)	0.038(3)	-0.010(3)	0.014(3)	0.001(3)
O(2)	4e	0.5438(8)	0.0712(7)	0.784(1)	0.017(4)	0.054(5)	0.069(5)	0.002(4)	0.008(3)	-0.010(4)
O(3)	4e	0.2784(7)	0.0695(5)	0.616(1)	0.025(4)	0.030(3)	0.038(3)	-0.010(3)	0.008(3)	-0.011(3)
O(4)	4e	0.3813(9)	0.1747(5)	0.946(1)	0.052(5)	0.030(4)	0.033(3)	-0.006(3)	0.017(3)	-0.009(3)
O(5)	4e	0.1697(7)	0.1119(5)	0.167(1)	0.026(3)	0.038(4)	0.029(3)	-0.008(3)	0.007(3)	0.001(3)
O(6)	4e	-0.1702(7)	0.1138(5)	0.022(1)	0.024(3)	0.027(3)	0.044(4)	0.008(3)	0.009(3)	0.003(3)
O(7)	4e	0.0003(7)	-0.0703(5)	0.3044(9)	0.036(4)	0.029(3)	0.029(3)	-0.002(3)	0.015(3)	0.003(3)
Tl	4e	0.12926(4)	0.35444(3)	0.35035(6)	0.0369(3)	0.0356(2)	0.0371(2)	-0.0018(2)	0.0136(2)	0.0008(2)

4. Thallium hexaaquacobalte(II) sulfate, Tl₂[Co(H₂O)₆](SO₄)₂

Table 10. Data collection and handling.

Crystal:	light red ellipsoid, size 0.20 × 0.19 × 0.18 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	250.43 cm ⁻¹
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\max}$:	50.1°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4622, 118
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 988
$N(\text{param})_{\text{refined}}$:	90
Programs:	SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11]

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)	4e	0.2029	0.0965	0.2775	0.06(1)
H(2)	4e	0.2339	0.1242	0.0999	0.06
H(3)	4e	-0.2467	0.1031	-0.0460	0.06
H(4)	4e	-0.1508	0.1753	-0.0025	0.06
H(5)	4e	-0.0758	-0.0646	0.3378	0.06
H(6)	4e	0.0237	-0.1308	0.3251	0.06

Table 12. 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	2a	0	0	0	0.0166(5)	0.0165(5)	0.0184(5)	-0.0012(4)	0.0047(4)	0.0004(4)
S	4e	0.4069(1)	0.1367(1)	0.7362(2)	0.0179(6)	0.0199(6)	0.0222(6)	-0.0021(5)	0.0052(5)	-0.0016(5)
O(1)	4e	0.4186(5)	0.2286(3)	0.5933(7)	0.053(3)	0.027(2)	0.033(2)	-0.010(2)	0.020(2)	-0.003(2)
O(2)	4e	0.5440(5)	0.0716(4)	0.7851(9)	0.021(2)	0.043(3)	0.060(3)	0.007(2)	0.005(2)	-0.003(2)
O(3)	4e	0.2785(4)	0.0694(3)	0.6135(7)	0.023(2)	0.029(2)	0.032(2)	-0.007(2)	0.005(2)	-0.008(2)
O(4)	4e	0.3813(5)	0.1761(3)	0.9465(7)	0.041(2)	0.028(2)	0.025(2)	-0.007(2)	0.010(2)	-0.005(2)
O(5)	4e	0.1672(4)	0.1102(3)	0.1620(7)	0.026(2)	0.028(2)	0.027(2)	-0.003(2)	0.006(2)	0.004(2)
O(6)	4e	-0.1675(4)	0.1115(3)	0.0271(7)	0.021(2)	0.023(2)	0.042(2)	0.005(2)	0.011(2)	0.002(2)
O(7)	4e	-0.0023(4)	-0.0671(3)	0.3004(6)	0.026(2)	0.026(2)	0.027(2)	0.003(2)	0.012(2)	0.003(2)
Tl	4e	0.12921(3)	0.35370(2)	0.35096(4)	0.0343(2)	0.0322(2)	0.0345(2)	-0.0013(1)	0.0128(1)	0.0007(1)

5. Thallium hexaaquanickel(II) sulfate, Tl₂[Ni(H₂O)₆](SO₄)₂

Table 13. Data collection and handling.

Crystal:	greenish blue ellipsoid, size 0.18 × 0.17 × 0.16 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	255.20 cm ⁻¹
Diffractometer, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\max}$:	49.98°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4574, 117
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 996
$N(\text{param})_{\text{refined}}$:	90
Programs:	SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11]

Table 14. 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	0.1982	0.0943	0.2709	0.041(9)
H(2)	4e	0.2309	0.1236	0.0978	0.041
H(3)	4e	-0.2466	0.1015	-0.0484	0.041
H(4)	4e	-0.1465	0.1696	-0.0019	0.041
H(5)	4e	-0.0712	-0.0600	0.3357	0.041
H(6)	4e	0.0254	-0.1289	0.3273	0.041

Table 15. 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
Ni	2a	0	0	0	0.0124(4)	0.0159(4)	0.0156(4)	-0.0012(3)	0.0040(3)	-0.0004(3)
S	4e	0.4069(1)	0.1372(1)	0.7360(2)	0.0148(6)	0.0192(6)	0.0198(5)	-0.0029(5)	0.0045(4)	-0.0013(5)
O(1)	4e	0.4194(5)	0.2290(3)	0.5931(7)	0.043(2)	0.026(2)	0.033(2)	-0.010(2)	0.015(2)	-0.001(2)
O(2)	4e	0.5446(4)	0.0719(4)	0.7829(8)	0.015(2)	0.042(2)	0.053(3)	0.008(2)	0.002(2)	-0.005(2)
O(3)	4e	0.2771(4)	0.0697(3)	0.6123(6)	0.015(2)	0.033(2)	0.028(2)	-0.009(2)	0.005(1)	-0.009(2)
O(4)	4e	0.3798(5)	0.1762(3)	0.9468(6)	0.041(2)	0.027(2)	0.022(2)	-0.006(2)	0.013(2)	-0.006(2)
O(5)	4e	0.1639(4)	0.1102(3)	0.1593(6)	0.016(2)	0.030(2)	0.020(2)	-0.005(2)	0.001(1)	0.001(2)
O(6)	4e	-0.1645(4)	0.1095(3)	0.0271(6)	0.020(2)	0.023(2)	0.032(2)	0.001(2)	0.009(2)	-0.002(2)
O(7)	4e	0.0011(4)	-0.0653(3)	0.2999(6)	0.024(2)	0.021(2)	0.025(2)	0.002(2)	0.012(2)	0.001(2)
Tl	4e	0.12950(3)	0.35327(2)	0.35071(4)	0.0306(2)	0.0312(2)	0.0315(2)	-0.0012(1)	0.01179(9)	0.0004(1)

6. Thallium hexaaquazinc(II) sulfate, $\text{Ti}_2[\text{Zn}(\text{H}_2\text{O})_6](\text{SO}_4)_2$

Table 16. Data collection and handling.

Crystal:	colorless ellipsoid, size $0.18 \times 0.17 \times 0.16$ mm
Wavelength:	Mo K_α radiation ($0.71069 \text{ \AA}$)
μ :	255.88 cm^{-1}
Diffractionmeter, scan mode:	RIGAKU AFC-6R, ω
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4613, 118
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 967
$N(\text{param})_{\text{refined}}$:	90
Programs:	SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11]

Table 17. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.2045	0.0967	0.2771	0.046(8)
H(2)	4e	0.2358	0.1258	0.0985	0.046
H(3)	4e	-0.2496	0.1040	-0.0433	0.046
H(4)	4e	-0.1487	0.1748	0.0020	0.046
H(5)	4e	-0.0738	-0.0619	0.3359	0.046
H(6)	4e	0.0238	-0.1309	0.3226	0.046

Table 18. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn	2a	0	0	0	0.0188(4)	0.0215(4)	0.0207(4)	-0.0013(3)	0.0058(3)	0.0002(3)
S	4e	0.4066(1)	0.1370(1)	0.7362(2)	0.0190(6)	0.0225(7)	0.0241(6)	-0.0026(5)	0.0064(5)	-0.0019(5)
O(1)	4e	0.4171(5)	0.2292(3)	0.5946(6)	0.052(3)	0.029(2)	0.034(2)	-0.010(2)	0.017(2)	0.000(2)
O(2)	4e	0.5447(4)	0.0717(4)	0.7815(7)	0.022(2)	0.045(3)	0.055(3)	0.010(2)	0.003(2)	-0.004(2)
O(3)	4e	0.2782(4)	0.0695(3)	0.6135(6)	0.024(2)	0.034(2)	0.032(2)	-0.005(2)	0.007(2)	-0.007(2)
O(4)	4e	0.3813(4)	0.1754(3)	0.9468(6)	0.045(2)	0.031(2)	0.028(2)	-0.005(2)	0.014(2)	-0.005(2)
O(5)	4e	0.1664(4)	0.1108(3)	0.1623(6)	0.023(2)	0.035(2)	0.023(2)	-0.006(2)	0.000(2)	0.001(2)
O(6)	4e	-0.1681(4)	0.1118(3)	0.0266(7)	0.024(2)	0.029(2)	0.038(2)	0.003(2)	0.010(2)	0.001(2)
O(7)	4e	-0.0006(4)	-0.0663(3)	0.3009(5)	0.029(2)	0.024(2)	0.027(2)	0.002(2)	0.013(2)	0.001(2)
Tl	4e	0.12899(2)	0.35377(2)	0.35107(4)	0.0356(1)	0.0352(2)	0.0354(1)	-0.0016(1)	0.01383(9)	0.0003(1)

References

- Euler, H.; Barbier, B.; Klumpp, S.; Kirfel, A.: Crystal structure of Tutton's salts, $\text{Rb}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SO}_4)_2$, $\text{M}^{\text{II}} = \text{Mg, Mn, Fe, Co, Ni, Zn}$. *Z. Kristallogr. NCS* **215** (2000) 473-476.
- Euler, H.; Barbier, B.; Meents, A.; Kirfel, A.: Crystal structure of Tutton's salts, $\text{Rb}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SeO}_4)_2$, $\text{M}^{\text{II}} = \text{Mg, Mn, Co, Zn}$. *Z. Kristallogr. NCS* **218** (2003) 265-268.
- Euler, H.; Barbier, B.; Meents, A.; Kirfel, A.: Crystal structure of Tutton's salts, $\text{Cs}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SO}_4)_2$, $\text{M}^{\text{II}} = \text{Mg, Mn, Fe, Co, Ni, Zn}$. *Z. Kristallogr. NCS* **218** (2003) 405-408.
- Euler, H.; Barbier, B.; Meents, A.; Kirfel, A.: Crystal structure of Tutton's salts, $\text{Cs}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SeO}_4)_2$, $\text{M}^{\text{II}} = \text{Mg, Mn, Fe, Co, Ni, Zn}$. *Z. Kristallogr. NCS* **218** (2003) 409-413.
- Euler, H.; Barbier, B.; Meents, A.; Kirfel, A.: Refinement of the crystal structure of potassium hexaaquairon(II) sulfate, $\text{K}_2[\text{Fe}(\text{H}_2\text{O})_6](\text{SO}_4)_2$ and potassium hexaaquazinc(II) sulfate, $\text{K}_2[\text{Zn}(\text{H}_2\text{O})_6](\text{SO}_4)_2$. *Z. Kristallogr. NCS* **224** (2009) 171-173.
- Euler, H.; Barbier, B.; Meents, A.; Kirfel, A.: Crystal structure of Tutton's salts, $\text{K}_2[\text{M}^{\text{II}}(\text{H}_2\text{O})_6](\text{SeO}_4)_2$, $\text{M}^{\text{II}} = \text{Co, Ni, Zn}$ and refinement of the crystal structure of potassium hexaaquamagnesium(II) selenate, $\text{K}_2[\text{Mg}(\text{H}_2\text{O})_6](\text{SeO}_4)_2$. *Z. Kristallogr.* **224** (2009) 351-354.
- Shannon, R. D.: Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides. *Acta Crystallogr. A* **32** (1976) 751-767.
- Zunic, T. B.; Vickovic, I.: IVTON-program for the calculation of geometrical aspects of crystal structures and some crystal chemical applications. *J. Appl. Crystallogr.* **29** (1996) 305-306.
- Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
- Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
- Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 3.1. Crystal Impact, Bonn, Germany 1998.