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Hexasodium Trihydrogen Decatungstosamarate Octacosahydrate

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Abstract

The title compound, $Na_6H_3[SmW_{10}O_{36}].28H_2O$, consists of a decatungstosamarate anion, six fivefold- or sixfold-coordinated Na^+ cations and water molecules of crystallization. The decatungstosamarate anion is comprised of two $[W_5O_{18}]^{6-}$ moieties chelating to a central Sm^{3+} cation, which has tetragonal antiprismatic coordination with D_4 symmetry and Sm—O distances of 2.41–2.46 Å.

Comment

Photoluminescence of polyoxotungstolanthanoates and polyoxomolybdolanthanoates has been studied extensively for various kinds of polyoxoanions, which include $Na_7H_2[LnW_{10}O_{36}].xH_2O$ (Ln = Eu^{3+}, Pr^{3+} and Nd^{3+}) and $K_{13}[Eu(SiW_{11}O_{39})_2].xH_2O$ (Stillman & Thomson, 1976), $Na_9[LnW_{10}O_{36}].18H_2O$ (Ln = Sm^{3+}, Tb^{3+}, Dy^{3+} and Eu^{3+}) and $K_{17}[Eu(P_2W_{17}O_{61})_2].xH_2O$ (Blasse, Dirksen & Zonnevijlle, 1981), $K_{15}H_3[Eu_3(H_2O)_3(SbW_9O_{33})\text{-}(W_5O_{18})_3].25.5H_2O$ (Yamase, Naruke & Sasaki, 1990), $(NH_4)_{12}H_2[Eu_4(MoO_4)(H_2O)_{16}(Mo_7O_{24})_4].13H_2O$ (Naruke, Ozeki & Yamase, 1991; Naruke & Yamase, 1991), $Eu_2(H_2O)_{12}[Mo_8O_{27}].6H_2O$ (Yamase & Naruke, 1991), $K_3Na_4H_2[TbW_{10}O_{36}].20H_2O$ (Ozeki & Yamase, 1993*a*; Ozeki, Takahashi & Yamase, 1992), and $Na_9[EuW_{10}O_{36}]\text{-}.32H_2O$ (Sugeta & Yamase, 1993). In our previous study of the photoluminescence of decatungstoterbates, the counter cations of the polyoxometallate anions were found to influence the photoluminescence properties of the polyoxometallate solid (Ozeki & Yamase, 1993*a*). The crystal structure analysis of the title compound was undertaken in order to investigate the effect of the counter cations of the decatungstosamarate anion on its crystal and molecular structure. We are particularly interested in the coordination of the luminescent centre of the SmO_8 square antiprism, since this might indicate factors influencing its photoluminescence properties.

The title compound was obtained from an attempt to prepare the all-ammonium salt of the decatungstosamarate anion. The pH of a 40 ml aqueous solution containing 16.4 g $Na_2WO_4.2H_2O$ was brought to 7 by adding CH_3COOH. 2.00 g of $Sm(CH_3COO)_3.4H_2O$ in 30 ml H_2O and 0.80 g of NH_4Cl in 10 ml H_2O were added. Colourless crystals of sodium paratungstate precipitated after several hours and were filtered off. By keeping the filtrate at room temperature for two months, colourless crystals of the title compound were obtained.

Fig. 1 shows the structure of the $[SmW_{10}O_{36}]^{9-}$ anion. It consists of a central Sm^{3+} cation and two $[W_5O_{18}]^{6-}$ moieties. The latter may be regarded as derived by the removal of a WO_6 octahedron from a $[W_6O_{19}]^{2-}$ anion. It has a square array of O atoms at the lacunary site. Square arrays of O atoms from two $[W_5O_{18}]^{6-}$ moieties face each other, rotated by 41° to give a square antiprism of D_4 symmetry, at the centre of which is located the Sm^{3+} cation. Compared to the geometry of the SmO_8 square antiprism in the compound $K_3Na_4H_2[SmW_{10}O_{36}].22H_2O$ (Ozeki & Yamase, 1993*b*), the SmO_8 square antiprism in this compound is elongated along its fourfold axis. Also, the twist angle from the ideal D_{4d} value of 45° is 4°, which is 2° larger than the value found in the SmO_8 square antiprism in $K_3Na_4H_2[SmW_{10}O_{36}].22H_2O$. The Sm—O distances vary from 2.41 (1) to 2.46 (1) Å [average 2.43 (2) Å] and are shorter than the Sm—O distances in $K_3Na_4H_2[SmW_{10}O_{36}].22H_2O$ [2.42 (2)–2.49 (2), average 2.47 (3) Å]. As a result of the *trans* influence, the

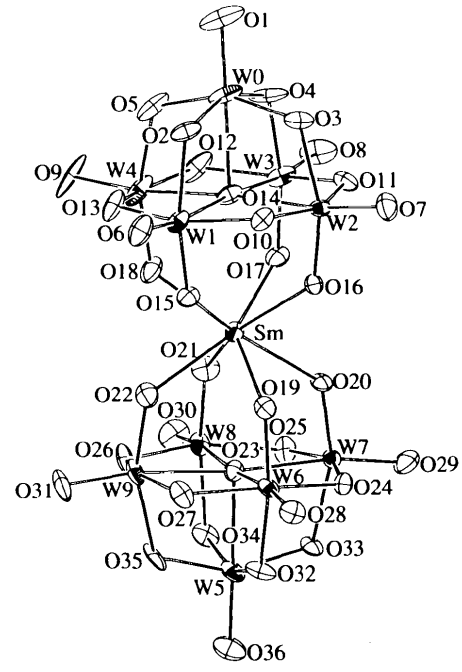

Fig. 1. *ORTEP*II (Johnson, 1976) drawing of the $[SmW_{10}O_{36}]^{9-}$ anion. Thermal ellipsoids are shown at 50% probability levels.

W—O bonds *trans* to the Sm—O bonds are 1.76 (1)-1.80 (1) Å [average 1.78 (1) Å], which are longer than the corresponding W—O distances in $K_3Na_4H_2[SmW_{10}O_{36}]$-$.22H_2O$ [1.72 (2)-1.77 (1), average 1.75 (2) Å]. The Sm—W distances are 3.815 (1)-3.842 (1) Å [average 3.832 (8) Å], which are shorter than the Sm—W distances in $K_3Na_4H_2[SmW_{10}O_{36}].22H_2O$ [3.820 (2)-3.889 (2), average 3.85 (2) Å]. Unlike in $K_3Na_4H_2[SmW_{10}O_{36}]$-$.22H_2O$, where K^+ cations are multiply coordinated to the O atoms of the $[SmW_{10}O_{36}]^{9-}$ anions and thus give rise to a distortion of the structure of the polyoxoanion (Ozeki & Yamase, 1993*b*), no counter cations are multiply coordinated to the $[SmW_{10}O_{36}]^{9-}$ anion in the crystal of the title compound, so the Sm—W distances are similar for the two $[W_5O_{18}]^{6-}$ moieties.

Fig. 2 shows a packing diagram of the crystal viewed down the c^* axis. Each of the six Na atoms is coordinated by either five or six O atoms with Na—O distances of 2.28 (2)-2.55 (2) Å [average 2.43 (7) Å]. The last ten O atoms of the water molecules of crystallization to be located (O60-O69) had large temperature factors and in some of them interatomic distances were unacceptably short [1.91 (4)-2.51 (4) Å]. It is convenient to divide the O atoms into three sets: set *A* comprises O1-O59, set *B* O60-O66 and set *C* O67-O69. There are no contacts of less than 2.67 Å between members of set *A* + *B* nor between members of set *A* + *C*. However, each member in set *B* has contacts less than 2.6 Å with one or more members in set *C*, and *vice versa*. Thus, a common site occupancy factor was applied to the members of set *B* and its complement was used as the site occupancy factor for the members of set *C*. After several least-squares refinements with various site occupancy factors for sets *B* and *C*, the value of 0.5 for both sets *B* and *C* was found to give the most reasonable temperature factors for all the O atoms in both sets.

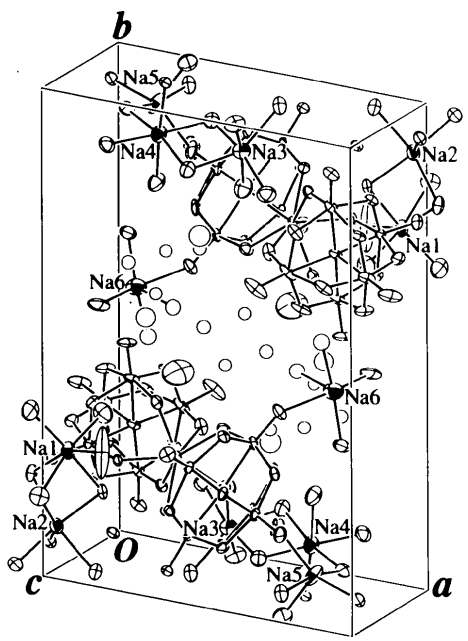

Fig. 2. Packing diagram of $Na_6H_3[SmW_{10}O_{36}].28H_2O$ viewed down the c^* axis. Thermal ellipsoids are shown at 50% probability levels. Na atoms are shown as ellipsoids with shaded octants.

Experimental

Crystal data

$Na_6H_3[SmW_{10}O_{36}].28H_2O$	$Z = 2$
$M_r = 3210.3$	$D_x = 3.36$ Mg m^{-3}
Triclinic	Mo $K\alpha$ radiation
$P\bar{1}$	$\lambda = 0.71069$ Å
$a = 12.945$ (2) Å	Cell parameters from 25 reflections
$b = 20.212$ (4) Å	$\theta = 10.0$-$12.5°$
$c = 12.882$ (3) Å	$\mu = 19.08$ mm^{-1}
$\alpha = 98.50$ (2)°	$T = 296$ K
$\beta = 102.19$ (2)°	0.35 × 0.25 × 0.20 mm
$\gamma = 101.11$ (2)°	Colourless
$V = 3170$ (2) Å^3	

Data collection

Rigaku AFC-5*S* diffractometer	11 833 observed reflections $[I > 3\sigma(I)]$
$\omega/2\theta$ scans	$\theta_{max} = 30.0°$
Absorption correction: empirical *via* ψ scans (North, Phillips & Mathews, 1968)	$h = -18 \rightarrow 17$
	$k = -28 \rightarrow 28$
$T_{min} = 0.76$, $T_{max} = 1.00$	$l = 0 \rightarrow 18$
19 219 measured reflections	3 standard reflections
18 463 independent reflections	monitored every 100 reflections
	intensity variation: −10.3%

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 0.01$
$R = 0.049$	$\Delta\rho_{max} = 3.82$ e Å^{-3}
$wR = 0.060$	$\Delta\rho_{min} = -4.74$ e Å^{-3}
$S = 1.76$	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)
11 833 reflections	
725 parameters	
Calculated weights $w = 1/[\sigma^2(F) + 0.000225F^2]$	

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}/U_{iso}
W0	0.03039 (7)	0.30155 (4)	0.33577 (6)	0.0325
W1	0.15445 (6)	0.17413 (3)	0.37121 (5)	0.0218
W2	0.03997 (5)	0.23318 (3)	0.55701 (5)	0.0183
W3	0.18460 (6)	0.38813 (3)	0.57827 (6)	0.0266
W4	0.30084 (7)	0.32928 (4)	0.39285 (6)	0.0356
W5	0.67418 (5)	0.20457 (4)	0.95088 (6)	0.0247
W6	0.42291 (5)	0.11998 (3)	0.81419 (5)	0.0197
W7	0.46230 (5)	0.27533 (3)	0.95552 (5)	0.0189
W8	0.63791 (5)	0.33400 (4)	0.82477 (6)	0.0233
W9	0.59897 (5)	0.17915 (4)	0.68051 (6)	0.0260

Sm	0.34806 (7)	0.25510 (4)	0.64987 (7)	0.0190
Na1	0.0683 (6)	0.2609 (4)	0.9464 (6)	0.040
Na2	0.0123 (6)	0.0932 (4)	0.8753 (7)	0.038
Na3	0.4061 (8)	0.0765 (5)	0.2147 (8)	0.055
Na4	0.6922 (7)	0.0837 (5)	0.2892 (7)	0.047
Na5	0.7765 (8)	0.0598 (6)	0.6000 (8)	0.060
Na6	0.8844 (9)	0.4656 (5)	0.7639 (8)	0.061
O1	−0.070 (1)	0.3162 (7)	0.234 (1)	0.056
O2	0.0416 (10)	0.2109 (6)	0.2775 (9)	0.028
O3	−0.048 (1)	0.2602 (7)	0.427 (1)	0.033
O4	0.066 (1)	0.3829 (6)	0.444 (1)	0.039
O5	0.160 (1)	0.3347 (7)	0.2937 (10)	0.039
O6	0.132 (1)	0.0963 (6)	0.2843 (10)	0.035
O7	−0.066 (1)	0.2000 (7)	0.608 (1)	0.035
O8	0.185 (1)	0.4685 (6)	0.643 (1)	0.043
O9	0.387 (1)	0.3663 (8)	0.321 (1)	0.062
O10	0.0420 (9)	0.1547 (5)	0.4503 (9)	0.022
O11	0.0668 (9)	0.3304 (6)	0.6183 (9)	0.025
O12	0.280 (1)	0.4085 (6)	0.4825 (10)	0.040
O13	0.258 (1)	0.2337 (7)	0.3164 (9)	0.033
O14	0.1636 (10)	0.2814 (6)	0.4684 (9)	0.024
O15	0.2559 (9)	0.1685 (6)	0.4844 (9)	0.025
O16	0.1550 (9)	0.2233 (6)	0.6503 (9)	0.021
O17	0.2872 (9)	0.3614 (6)	0.6682 (9)	0.025
O18	0.390 (1)	0.3081 (7)	0.5034 (9)	0.033
O19	0.3284 (9)	0.1481 (6)	0.7168 (9)	0.023
O20	0.3637 (9)	0.2865 (6)	0.8438 (9)	0.023
O21	0.519 (1)	0.3393 (6)	0.729 (1)	0.032
O22	0.4881 (10)	0.2022 (7)	0.6013 (10)	0.031
O23	0.5359 (9)	0.2243 (6)	0.8249 (9)	0.022
O24	0.3933 (9)	0.1767 (6)	0.9351 (9)	0.022
O25	0.5726 (9)	0.3508 (6)	0.9439 (9)	0.026
O26	0.6820 (9)	0.2731 (7)	0.718 (1)	0.032
O27	0.5068 (9)	0.0993 (6)	0.709 (1)	0.028
O28	0.3557 (10)	0.0382 (6)	0.818 (1)	0.028
O29	0.421 (1)	0.3074 (7)	1.0692 (10)	0.036
O30	0.728 (1)	0.4118 (7)	0.839 (1)	0.041
O31	0.661 (1)	0.1408 (8)	0.589 (1)	0.043
O32	0.5622 (9)	0.1222 (6)	0.923 (1)	0.029
O33	0.5918 (9)	0.2454 (6)	1.0363 (9)	0.023
O34	0.7340 (9)	0.2928 (6)	0.932 (1)	0.029
O35	0.7019 (9)	0.1699 (7)	0.817 (1)	0.031
O36	0.778 (1)	0.1856 (7)	1.043 (1)	0.040
O37	0.1557 (9)	0.1786 (6)	0.8497 (10)	0.029
O38	0.831 (1)	0.0609 (7)	0.431 (1)	0.041
O39	−0.0826 (10)	0.1838 (7)	0.8150 (10)	0.034
O40	−0.057 (1)	0.0375 (6)	0.683 (1)	0.033
O41	−0.115 (1)	0.0025 (7)	0.903 (1)	0.043
O42	0.538 (1)	0.0434 (7)	0.358 (1)	0.050
O43	0.289 (1)	−0.0293 (8)	0.240 (1)	0.046
O44	0.840 (1)	0.1160 (7)	0.205 (1)	0.046
O45	−0.001 (1)	0.1682 (9)	1.043 (1)	0.058
O46	0.973 (1)	0.5005 (8)	0.632 (1)	0.059
O47	0.141 (1)	0.0161 (8)	0.887 (1)	0.055
O48	0.569 (1)	0.1301 (9)	0.166 (1)	0.061
O49	0.437 (1)	0.1710 (9)	0.363 (1)	0.060
O50	0.654 (1)	−0.0474 (8)	0.513 (1)	0.056
O51	0.386 (1)	0.0017 (8)	0.042 (1)	0.058
O52	0.902 (1)	0.3526 (7)	0.731 (2)	0.060
O53	0.300 (1)	0.1436 (8)	0.113 (1)	0.057
O54	0.161 (1)	0.3418 (9)	0.860 (1)	0.065
O55	0.731 (1)	0.1993 (9)	0.412 (1)	0.060
O56	−0.040 (1)	0.3362 (9)	1.002 (2)	0.093
O57	0.1272 (10)	0.0677 (6)	0.601 (1)	0.030
O58	0.215 (2)	0.288 (2)	1.092 (1)	0.187
O59	0.593 (2)	0.545 (1)	0.130 (2)	0.143
O60†	0.730 (2)	0.475 (1)	0.620 (2)	0.041 (7)
O61†	0.867 (2)	0.572 (2)	0.847 (2)	0.046 (7)
O62†	0.506 (2)	0.463 (1)	0.652 (2)	0.027 (5)
O63†	0.708 (2)	0.415 (1)	0.304 (2)	0.026 (5)
O64†	0.617 (2)	0.331 (1)	0.516 (2)	0.029 (5)
O65†	0.836 (2)	0.381 (1)	0.469 (2)	0.034 (6)
O66†	0.555 (3)	0.273 (2)	0.262 (3)	0.08 (1)
O67†	0.668 (2)	0.521 (1)	0.769 (2)	0.033 (6)
O68†	0.692 (2)	0.330 (1)	0.372 (2)	0.028 (5)
O69†	0.708 (3)	0.450 (2)	0.175 (3)	0.065 (10)

† Occupancy factor 0.5; U_{iso} given.

Table 2. *Selected bond lengths* (Å)

W0—O1	1.75 (1)	W5—O32	1.92 (1)
W0—O3	1.89 (1)	W5—O23	2.29 (1)
W0—O5	1.90 (1)	W6—O28	1.72 (1)
W0—O4	1.90 (1)	W6—O19	1.80 (1)
W0—O2	1.92 (1)	W6—O24	1.94 (1)
W0—O14	2.30 (1)	W6—O27	1.95 (1)
W1—O6	1.73 (1)	W6—O32	2.03 (1)
W1—O15	1.78 (1)	W6—O23	2.29 (1)
W1—O13	1.94 (1)	W7—O29	1.74 (1)
W1—O10	1.96 (1)	W7—O20	1.78 (1)
W1—O2	2.02 (1)	W7—O25	1.93 (1)
W1—O14	2.31 (1)	W7—O24	1.98 (1)
W2—O7	1.71 (1)	W7—O33	2.03 (1)
W2—O16	1.77 (1)	W7—O23	2.31 (1)
W2—O11	1.94 (1)	W8—O30	1.73 (1)
W2—O10	1.95 (1)	W8—O21	1.79 (1)
W2—O3	2.03 (1)	W8—O25	1.92 (1)
W2—O14	2.31 (1)	W8—O26	1.96 (1)
W3—O8	1.71 (1)	W8—O34	2.04 (1)
W3—O17	1.79 (1)	W8—O23	2.35 (1)
W3—O11	1.94 (1)	W9—O31	1.74 (1)
W3—O12	1.96 (1)	W9—O22	1.76 (1)
W3—O4	2.03 (1)	W9—O26	1.93 (1)
W3—O14	2.33 (1)	W9—O27	1.95 (1)
W4—O9	1.73 (1)	W9—O35	2.03 (1)
W4—O18	1.79 (1)	W9—O23	2.32 (1)
W4—O12	1.93 (1)	Sm—O18	2.41 (1)
W4—O13	1.95 (1)	Sm—O22	2.42 (1)
W4—O5	2.03 (1)	Sm—O17	2.42 (1)
W4—O14	2.32 (1)	Sm—O21	2.43 (1)
W5—O36	1.74 (1)	Sm—O19	2.43 (1)
W5—O34	1.87 (1)	Sm—O20	2.44 (1)
W5—O33	1.90 (1)	Sm—O15	2.46 (1)
W5—O35	1.90 (1)	Sm—O16	2.46 (1)

Data collection: *RCRYSTAN* (Rigaku Corporation, 1985). Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1989). Program(s) used to solve structure: *MITHRIL* (Gilmore, 1984). Program(s) used to refine structure: *TEXSAN LS*. Molecular graphics: *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71648 (33 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1081]

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$K_3H(SeO_4)_2$ at 297 and 30 K

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Abstract

In tripotassium hydrogen bis(selenate), $K_3H(SeO_4)_2$, two selenate groups form a dimer through a hydrogen bond of 2.496 (2) Å, at 30 K (10 K above the low-temperature transition point). This is the shortest hydrogen bond among the members of the $M_3H(SeO_4)_2$-type crystals exhibiting the low-temperature phase transition.

Comment

Among the members of the $M_3H(XO_4)_2$-type crystals (M = K, Rb, Cs; X = S, Se) which exhibit a low-temperature (possibly antiferroelectric) phase transition, $K_3H(SeO_4)_2$ has the lowest transition temperature (T_c) of 20 K (Endo, Kaneko, Osaka & Makita, 1983).

In view of the low T_c of the title compound, the hydrogen-bond distance just above T_c is needed in order to examine the correlation between the transition temperature and hydrogen-bonding distances in the $M_3H(SeO_4)_2$-type crystals. Thus the structure determination at 30 K was undertaken. The data at 297 K were collected so that comparison may be made with previous work performed with a spherical shaped specimen (Ichikawa, Sato, Komukae & Osaka, 1992). An as-grown crystal was used in this work which had a hexagonal plate shape and was obtained by evaporation of a saturated solution.

The bond lengths and angles at 297 K agree with the previous results at 299 K (Ichikawa *et al.*, 1992) within 3σ, except for O(2)—Se—O(4) (4σ). The hydrogen-bond distance R [2.496 (2) Å] in $K_3H(SeO_4)_2$ at 30 K is the shortest among the members of the $M_3H(XO_4)_2$-type crystals exhibiting the low-temperature phase transition. By including the present results, the validity of a linear correlation between T_c and R is also established for $M_3H(SeO_4)_2$-type crystals with zero-dimensional hydrogen-bond networks (Ichikawa, Gustafsson & Olovsson, 1993).

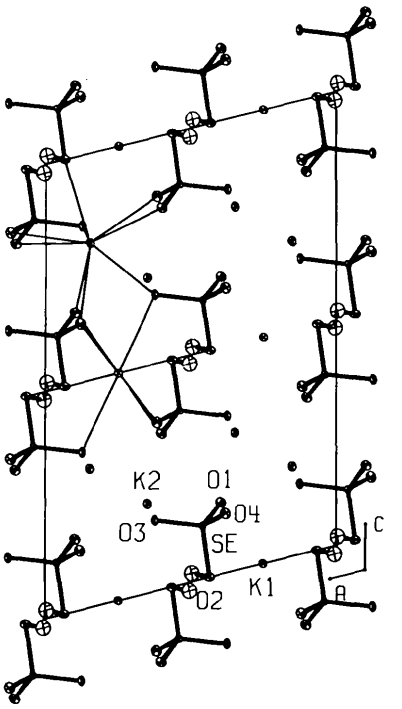

Fig. 1. The *b*-axis projection of the structure of $K_3H(SeO_4)_2$ at 30 K. Thermal ellipsoids are scaled to include 50% probability. The B value of the H atoms is set to 2.0 Å^2. Thick lines denote covalent bonds, thin lines indicate short K···O distances.

Experimental

At 30 K

Crystal data

$K_3H(SeO_4)_2$
M_r = 404.2
Monoclinic
$A2/a$
a = 10.0464 (8) Å
b = 5.8561 (4) Å
c = 14.8215 (13) Å
β = 103.629 (12)°
V = 847.44 (10) Å^3
Z = 4
D_x = 3.168 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 30 reflections
θ = 25.9-29.9°
μ = 9.86 mm^{-1}
Hexagonal plate
0.250 × 0.233 × 0.067 mm
Colourless

Data collection

Huber/Stoe/Aracor diffractometer
$\omega/2\theta$ scans
Absorption correction: *ABSSTOE* (Lundgren, 1983)
T_{min} = 0.287, T_{max} = 0.466
2543 observed reflections [All $I>0$ and those $I<0$ with $|I|<15\sigma(I)$]
R_{int} = 0.017
θ_{max} = 40.00°
h = −18 → 13
k = −10 → 10
l = 0 → 26