catena-Poly[tetrasodium [[*cis*-dioxido-*trans*-bis(sulfato-κO)molybdate(VI)]-μ-sulfato-$\kappa^2 O{:}O'$]]

Susan J. Cline Schäffer[a]* and Rolf W. Berg[b]

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Single crystals of the title compound, $\{Na_4[Mo^{VI}O_2(SO_4)_3]\}_n$, were grown from a melt of MoO_3 and Na_2SO_4 in $Na_2S_2O_7$. In contrast to the structure of the isoformular K compound, $K_4[Mo^{VI}O_2(SO_4)_3]$, with its monomeric anion, this sodium analogue contains a polymeric anion of the type $\{[Mo^{VI}O_2(SO_4)_2\text{-}\mu\text{-}(SO_4)]^{4-}\}_n$. The Mo^{VI} cations, surrounded by two tightly bonded O atoms and four O atoms of one bridging and two terminal sulfato ligands, form zigzag chains parallel to [100]. All four Na^+ cations are situated between the anionic chains and have distorted octahedral coordination spheres.

Related literature

The structure of the title isoformular potassium compound, $K_4[Mo^{VI}O_2(SO_4)_3]$, was determined by Schäffer & Berg (2008). For related Mo-containing compounds, see Salles *et al.* (1996) and Nørbygaard *et al.* (1998). Related compounds with Mo replaced by W were discussed by Schäffer & Berg (2005) and Berg *et al.* (2006). Other sulfato complexes coordinated to late transition metal centers were reported by Berg & Thorup (2005), Borup *et al.* (1990), Nielsen *et al.* (1993) and Rasmussen *et al.* (2003).
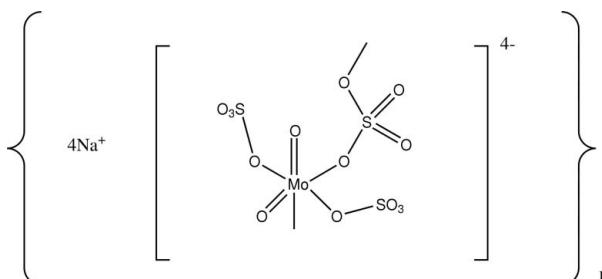
Experimental

Crystal data

$Na_4[MoO_2(SO_4)_3]$	$V = 1188.97$ (15) Å³
$M_r = 508.08$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.4739$ (6) Å	$\mu = 1.85$ mm⁻¹
$b = 9.2892$ (7) Å	$T = 120$ (2) K
$c = 15.1046$ (11) Å	$0.24 \times 0.18 \times 0.02$ mm

Data collection

Bruker SMART APEX CCD diffractometer	14125 measured reflections
Absorption correction: gaussian (*SHELXTL*; Sheldrick, 2008)	2861 independent reflections
	2817 reflections with $I > 2\sigma(I)$
$T_{min} = 0.665$, $T_{max} = 0.964$	$R_{int} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$	$\Delta\rho_{max} = 0.51$ e Å⁻³
$wR(F^2) = 0.042$	$\Delta\rho_{min} = -0.26$ e Å⁻³
$S = 1.10$	Absolute structure: Flack (1983),
2861 reflections	1205 Friedel pairs
199 parameters	Flack parameter: 0.01 (2)

Table 1
Selected bond lengths (Å).

Mo1—O2	1.6905 (16)	Mo1—O4	2.0102 (16)
Mo1—O1	1.7108 (16)	Mo1—O6^i	2.1661 (15)
Mo1—O5	1.9925 (16)	Mo1—O3	2.1907 (15)

Symmetry code: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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supporting information

catena-Poly[tetrasodium [[*cis*-dioxido-*trans*-bis(sulfato-*κO*)molybdate(VI)]-*μ*-sulfato-*κ²O:O′*]]

Susan J. Cline Schäffer and Rolf W. Berg

S1. Comment

Considerable amounts of molybdenum(VI) oxide, a solid well known for its insolubility in many acids, can be dissolved in sulfate melts at high temperatures, as was previously found for the chemically related tungsten(VI) oxide (Schäffer & Berg, 2005, Berg *et al.*, 2006). When varying molar amounts of MoO_3, Na_2SO_4, and hygroscopic $Na_2S_2O_7$ are placed in ampoules in a dry box, sealed, and heated to equilibration in a rocking furnace at 773 K for *ca.* 1 h, the resulting clear melts contain $[MoO_2]^{2+}$ moieties that are bonded to SO_4^{2-} units. The compositions of the reaction products have been determined to be in the stoichiometric ratio 1:1:1, or $MoO_3 + M_2SO_4 + M_2S_2O_7 \rightarrow M_4[Mo(SO_4)_3O_2]$. In the case where *M* = K, a monomeric anion is formed (Schäffer & Berg, 2008), while for *M* = Na the anion is in a polymeric form.

The distorted octahedral coordination sphere of the Mo^{VI} cation contains two oxido ligands (*cis*), two terminally bound sulfato ligands (*trans*), and two O atoms of symmetry-related (*x* + 1/2, -*y* + 1/2, -*z* + 1) bridging sulfato ligands (*cis*), with O–Mo–O angles between any two *cis* oxygen atoms deviating as much as 15° from ideal values. The Mo–O bond distances to the tightly- bonded oxido ligands are similar (1.6905 (16) Å, 1.7108 (16) Å), which is expected as both bonds are *trans* to oxygen atoms in the bridging sulfato ligands. The Mo–O distances to the terminal sulfato ligands (Mo1–O4 and Mo1–O5) are slightly shorter than those to the brigding sulfato ligands, Mo1–03 and Mo1–O6A. The Mo–O distances compare well with previously reported values for related structures (Salles *et al.*, 1996; Nørbygaard *et al.*, 1998; Schäffer & Berg, 2008).

The coordination geometry of the sulfato ligands can be described as slightly distorted from tetrahedral, with angles ranging from 103.55 (9) to 113.77 (10)°. From the shortest to the longest, the S–O bond distances vary by type: S to terminal O atoms, 1.4516 (17)–1.4681 (17) Å; S to briding O atoms, 1.4941 (16) Å and 1.4953 (16) Å; S in the terminal sulfato ligands to the coordinating O atoms, 1.5589 (17) Å and 1.5346 (16) Å. This variation is typical for sulfato complexes of many different transition metal centers (Borup *et al.*, 1990; Nielsen *et al.*, 1993; Rasmussen *et al.*, 2003, and Berg & Thorup, 2005).

All four sodium cations are situated between the anionic chains and are six-coordinate with Na–O bond distances ranging from 2.2713 (18) to 2.7652 (18) Å.

S2. Experimental

Crystals were grown from a melt of equimolar amounts of MoO_3, Na_2SO_4, and $Na_2S_2O_7$, using a method described previously (Nørbygaard *et al.*, 1998).

S3. Refinement

On the basis of 1205 unmerged Friedel opposites, the fractional contribrution of the racemic twin was negligible (Flack, 1983). The two highest peaks in the final difference Fourier map were, respectively, 0.78 Å and 0.79 Å from Mo1, and

the deepest hole was 1.31 Å from S2.
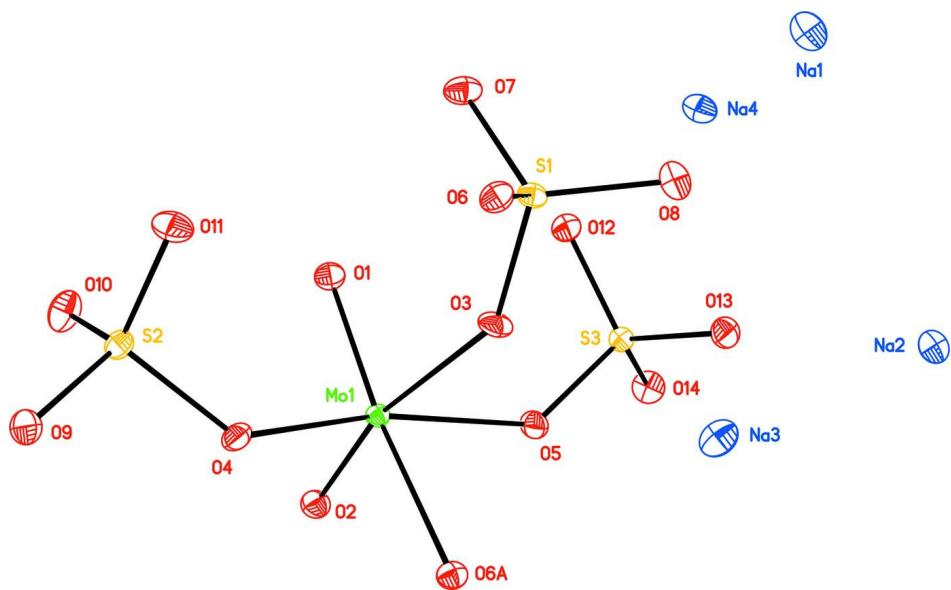
Figure 1

Plot of the asymmetric unit of $Na_4[Mo^{VI}(SO_4)_3O_2]$, showing atoms as ellipsoids at the 50% probability level. [Symmetry code A) $x+0.5$, $-y+0.5$, $-z+1$.]
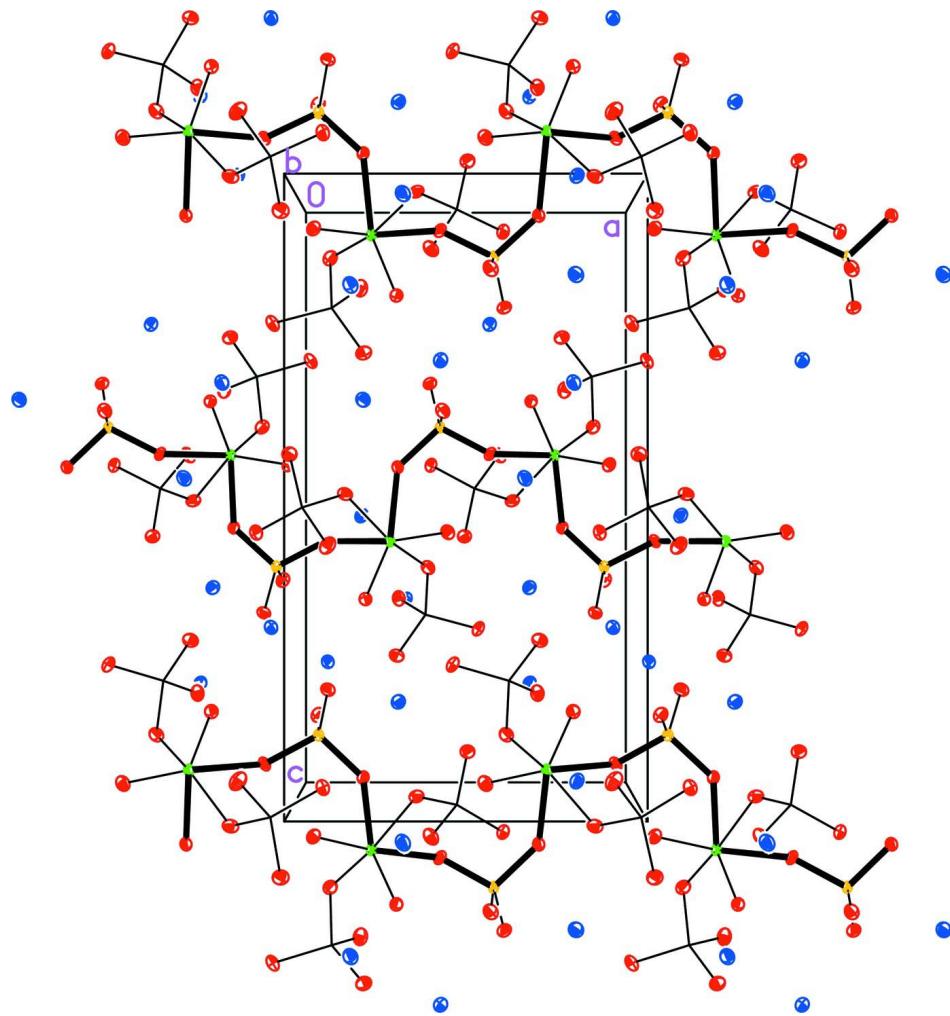
Figure 2
The crystal packing of $Na_4[Mo^{VI}(SO_4)_3O_2]$, viewed along the *b* axis, showing the chains (thick black lines). Ellipsoids are displayed at the 50% probability level.

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Crystal data
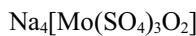
$Na_4[Mo(SO_4)_3O_2]$	$F(000) = 984$
$M_r = 508.08$	$D_x = 2.838$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 5457 reflections
$a = 8.4739$ (6) Å	$\theta = 2.6–27.9°$
$b = 9.2892$ (7) Å	$\mu = 1.86$ mm^{-1}
$c = 15.1046$ (11) Å	$T = 120$ K
$V = 1188.97$ (15) Å^3	Tabular, colorless
$Z = 4$	$0.24 \times 0.18 \times 0.02$ mm

Data collection

Bruker SMART APEX CCD diffractometer	14125 measured reflections
Radiation source: normal-focus sealed tube	2861 independent reflections
Graphite monochromator	2817 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.031$
Absorption correction: gaussian (*SHELXTL*; Sheldrick, 2008)	$\theta_{max} = 28.0°$, $\theta_{min} = 2.6°$
$T_{min} = 0.665$, $T_{max} = 0.964$	$h = -11 \rightarrow 11$
	$k = -12 \rightarrow 12$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.017$	$w = 1/[\sigma^2(F_o^2) + (0.0214P)^2 + 0.3747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.042$	
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
2861 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
0 restraints	Absolute structure: Flack (1983), 1205 Friedel pairs
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.01 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Five frame series were filtered for statistical outliers then corrected for absorption by integration using *SHELXTL*/*XPREP* (Bruker, 2001) before using *SAINT*/*SADABS* (Bruker, 2002) to sort, merge, and scale the combined data. A series of identical frames was collected twice during the experiment to monitor decay. No decay correction was applied. The systematic conditions suggested the uambiguous space group. The structure was solved by direct methods (Sheldrick, 2001). The final space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2. An extinction correction was not applied. The two highest peaks in the final difference Fourier map were, repectively, 0.78Å and 0.79Å from Mo1; the deepest hole was 1.31Å from S2. The final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Mo1	0.77389 (2)	0.108886 (19)	0.426923 (11)	0.00683 (5)
S1	0.42167 (6)	0.29669 (6)	0.38157 (3)	0.00770 (11)
S2	0.52730 (7)	−0.14389 (6)	0.48393 (3)	0.00870 (11)
S3	0.87553 (6)	0.37753 (6)	0.29746 (3)	0.00819 (10)
Na1	0.20072 (11)	0.58268 (10)	0.34042 (6)	0.01293 (19)
Na2	0.80653 (11)	0.75841 (10)	0.31656 (6)	0.01239 (19)
Na3	0.67303 (11)	0.51270 (10)	0.46834 (6)	0.0144 (2)
Na4	0.57005 (11)	0.46216 (10)	0.21305 (6)	0.01274 (19)
O1	0.70335 (19)	0.03236 (17)	0.33180 (10)	0.0107 (3)
O2	0.94651 (19)	0.02131 (17)	0.44263 (11)	0.0119 (3)
O3	0.57359 (18)	0.25797 (17)	0.42577 (11)	0.0107 (3)
O4	0.6456 (2)	−0.02040 (17)	0.50576 (10)	0.0116 (3)

O5	0.88450 (19)	0.28237 (18)	0.38036 (10)	0.0120 (3)
O6	0.29354 (19)	0.27689 (17)	0.44854 (9)	0.0096 (3)
O7	0.3902 (2)	0.20606 (18)	0.30489 (10)	0.0123 (3)
O8	0.4313 (2)	0.44896 (18)	0.35609 (11)	0.0124 (3)
O9	0.49519 (19)	−0.20813 (17)	0.56967 (11)	0.0130 (3)
O10	0.60611 (19)	−0.24259 (18)	0.42327 (12)	0.0147 (3)
O11	0.38958 (19)	−0.07781 (18)	0.44282 (11)	0.0139 (3)
O12	0.7888 (2)	0.29908 (17)	0.22934 (10)	0.0124 (3)
O13	0.7899 (2)	0.50790 (17)	0.32281 (10)	0.0126 (3)
O14	1.03833 (19)	0.40786 (18)	0.27218 (10)	0.0133 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.00576 (8)	0.00737 (9)	0.00738 (8)	0.00034 (7)	−0.00028 (6)	−0.00021 (7)
S1	0.0056 (2)	0.0096 (3)	0.0078 (2)	0.0014 (2)	−0.00017 (19)	−0.0001 (2)
S2	0.0073 (2)	0.0093 (2)	0.0095 (2)	−0.0009 (2)	0.0006 (2)	−0.00087 (19)
S3	0.0073 (2)	0.0087 (2)	0.0086 (2)	−0.0001 (2)	0.00067 (18)	0.0004 (2)
Na1	0.0125 (5)	0.0130 (5)	0.0133 (4)	0.0022 (4)	0.0012 (3)	0.0019 (3)
Na2	0.0111 (5)	0.0126 (4)	0.0135 (4)	0.0012 (4)	0.0018 (4)	0.0017 (3)
Na3	0.0123 (4)	0.0166 (5)	0.0145 (5)	−0.0034 (4)	0.0023 (4)	−0.0024 (4)
Na4	0.0107 (4)	0.0156 (5)	0.0120 (4)	0.0010 (4)	−0.0008 (4)	0.0020 (4)
O1	0.0097 (8)	0.0119 (8)	0.0104 (7)	0.0002 (6)	−0.0002 (6)	−0.0008 (6)
O2	0.0113 (8)	0.0112 (8)	0.0130 (8)	0.0020 (6)	−0.0021 (6)	−0.0007 (6)
O3	0.0086 (7)	0.0128 (7)	0.0107 (7)	0.0044 (6)	−0.0029 (7)	−0.0008 (7)
O4	0.0138 (8)	0.0116 (8)	0.0095 (7)	−0.0053 (7)	−0.0018 (6)	0.0001 (6)
O5	0.0116 (8)	0.0121 (8)	0.0122 (8)	−0.0036 (6)	−0.0020 (6)	0.0042 (6)
O6	0.0080 (7)	0.0110 (7)	0.0098 (7)	−0.0010 (6)	0.0006 (6)	−0.0012 (6)
O7	0.0116 (8)	0.0162 (9)	0.0092 (7)	0.0016 (7)	−0.0016 (6)	−0.0028 (6)
O8	0.0121 (8)	0.0111 (8)	0.0140 (8)	0.0018 (7)	0.0023 (7)	0.0023 (6)
O9	0.0141 (8)	0.0131 (8)	0.0119 (7)	−0.0042 (6)	−0.0001 (7)	0.0028 (7)
O10	0.0151 (8)	0.0119 (8)	0.0171 (8)	−0.0010 (7)	0.0051 (7)	−0.0045 (7)
O11	0.0093 (8)	0.0190 (9)	0.0133 (8)	0.0021 (7)	−0.0016 (6)	0.0017 (6)
O12	0.0141 (8)	0.0120 (8)	0.0109 (7)	−0.0002 (7)	−0.0015 (6)	−0.0011 (6)
O13	0.0106 (8)	0.0108 (8)	0.0163 (8)	0.0025 (7)	−0.0008 (7)	−0.0015 (6)
O14	0.0095 (8)	0.0167 (9)	0.0136 (7)	−0.0012 (7)	0.0042 (6)	0.0008 (7)

Geometric parameters (Å, º)

Mo1—O2	1.6905 (16)	Na1—O9ⁱᵛ	2.4972 (19)
Mo1—O1	1.7108 (16)	Na1—O1ⁱⁱ	2.7652 (18)
Mo1—O5	1.9925 (16)	Na2—O13	2.3333 (18)
Mo1—O4	2.0102 (16)	Na2—O14ᵛ	2.3350 (19)
Mo1—O6ⁱ	2.1661 (15)	Na2—O10ᵛⁱ	2.3415 (19)
Mo1—O3	2.1907 (15)	Na2—O9ⁱ	2.3932 (19)
S1—O7	1.4564 (16)	Na2—O7ⁱⁱ	2.5262 (18)
S1—O8	1.4681 (17)	Na2—O1ᵛⁱ	2.7006 (19)
S1—O3	1.4941 (16)	Na2—S3ᵛ	3.3837 (11)

S1—O6	1.4953 (16)	Na3—O11^i	2.3524 (19)
S2—O9	1.4516 (17)	Na3—O2^{iv}	2.3649 (19)
S2—O11	1.4575 (17)	Na3—O13	2.4115 (18)
S2—O10	1.4581 (17)	Na3—O10^{vi}	2.4398 (19)
S2—O4	1.5589 (17)	Na3—O3	2.5928 (19)
S3—O14	1.4590 (17)	Na3—O8	2.724 (2)
S3—O12	1.4595 (16)	Na4—O7^{ii}	2.3065 (19)
S3—O13	1.4627 (16)	Na4—O12	2.407 (2)
S3—O5	1.5346 (16)	Na4—O11^{ii}	2.4078 (19)
Na1—O12^{ii}	2.2713 (18)	Na4—O8	2.4629 (19)
Na1—O8	2.3273 (19)	Na4—O1^{ii}	2.5003 (19)
Na1—O14^{iii}	2.3649 (19)	Na4—O13	2.5297 (19)
Na1—O4^{iv}	2.4394 (18)		
O2—Mo1—O1	102.72 (8)	O11^i—Na3—O3	129.03 (7)
O2—Mo1—O5	91.81 (7)	O2^{iv}—Na3—O3	75.84 (6)
O1—Mo1—O5	101.77 (7)	O13—Na3—O3	83.71 (6)
O2—Mo1—O4	95.58 (7)	O10^{vi}—Na3—O3	134.87 (6)
O1—Mo1—O4	93.46 (7)	O11^i—Na3—O8	175.92 (7)
O5—Mo1—O4	161.18 (7)	O2^{iv}—Na3—O8	73.41 (6)
O2—Mo1—O6^i	92.71 (7)	O13—Na3—O8	74.78 (6)
O1—Mo1—O6^i	163.68 (7)	O10^{vi}—Na3—O8	81.61 (6)
O5—Mo1—O6^i	82.77 (6)	O3—Na3—O8	53.34 (5)
O4—Mo1—O6^i	79.62 (6)	O7^{ii}—Na4—O12	121.20 (7)
O2—Mo1—O3	167.36 (7)	O7^{ii}—Na4—O11^{ii}	90.91 (6)
O1—Mo1—O3	89.16 (7)	O12—Na4—O11^{ii}	83.88 (6)
O5—Mo1—O3	81.39 (6)	O7^{ii}—Na4—O8	102.80 (7)
O4—Mo1—O3	87.91 (6)	O12—Na4—O8	104.28 (6)
O6^i—Mo1—O3	75.92 (6)	O11^{ii}—Na4—O8	156.62 (7)
O7—S1—O8	111.01 (10)	O7^{ii}—Na4—O1^{ii}	81.21 (6)
O7—S1—O3	111.95 (9)	O12—Na4—O1^{ii}	154.90 (7)
O8—S1—O3	107.53 (10)	O11^{ii}—Na4—O1^{ii}	84.66 (6)
O7—S1—O6	109.52 (9)	O8—Na4—O1^{ii}	78.95 (6)
O8—S1—O6	109.65 (10)	O7^{ii}—Na4—O13	78.73 (6)
O3—S1—O6	107.08 (9)	O12—Na4—O13	58.10 (6)
O9—S2—O11	113.77 (10)	O11^{ii}—Na4—O13	124.20 (7)
O9—S2—O10	112.83 (10)	O8—Na4—O13	77.59 (6)
O11—S2—O10	111.33 (10)	O1^{ii}—Na4—O13	144.70 (7)
O9—S2—O4	103.55 (9)	Mo1—O1—Na4^{vii}	131.27 (9)
O11—S2—O4	107.18 (10)	Mo1—O1—Na2^{viii}	110.49 (7)
O10—S2—O4	107.52 (10)	Na4^{vii}—O1—Na2^{viii}	91.78 (6)
O14—S3—O12	112.83 (10)	Mo1—O1—Na1^{vii}	128.10 (8)
O14—S3—O13	112.19 (10)	Na4^{vii}—O1—Na1^{vii}	93.53 (5)
O12—S3—O13	110.37 (10)	Na2^{viii}—O1—Na1^{vii}	89.08 (5)
O14—S3—O5	106.14 (9)	Mo1—O2—Na3^i	147.82 (9)
O12—S3—O5	108.22 (9)	S1—O3—Mo1	145.42 (10)
O13—S3—O5	106.73 (10)	S1—O3—Na3	99.86 (8)
O12^{ii}—Na1—O8	119.12 (7)	Mo1—O3—Na3	108.85 (6)

O12ii—Na1—O14iii	115.36 (7)	S2—O4—Mo1	131.46 (9)
O8—Na1—O14iii	99.58 (7)	S2—O4—Na1i	98.63 (8)
O12ii—Na1—O4iv	131.24 (7)	Mo1—O4—Na1i	127.05 (8)
O8—Na1—O4iv	86.40 (6)	S3—O5—Mo1	136.93 (10)
O14iii—Na1—O4iv	98.10 (6)	S1—O6—Mo1iv	125.67 (9)
O12ii—Na1—O9iv	82.33 (6)	S1—O7—Na4vii	129.39 (10)
O8—Na1—O9iv	141.19 (7)	S1—O7—Na2vii	125.94 (10)
O14iii—Na1—O9iv	98.72 (7)	Na4vii—O7—Na2vii	101.54 (7)
O4iv—Na1—O9iv	57.26 (6)	S1—O8—Na1	119.62 (10)
O12ii—Na1—O1ii	72.64 (6)	S1—O8—Na4	107.73 (9)
O8—Na1—O1ii	76.04 (6)	Na1—O8—Na4	106.56 (7)
O14iii—Na1—O1ii	69.21 (5)	S1—O8—Na3	95.05 (8)
O4iv—Na1—O1ii	155.81 (6)	Na1—O8—Na3	125.35 (7)
O9iv—Na1—O1ii	142.71 (6)	Na4—O8—Na3	100.15 (7)
O13—Na2—O14v	130.56 (7)	S2—O9—Na2iv	147.79 (11)
O13—Na2—O10vi	85.66 (6)	S2—O9—Na1i	99.36 (8)
O14v—Na2—O10vi	143.70 (7)	Na2iv—O9—Na1i	99.58 (7)
O13—Na2—O9i	79.43 (6)	S2—O10—Na2viii	139.66 (10)
O14v—Na2—O9i	98.75 (7)	S2—O10—Na3viii	121.13 (10)
O10vi—Na2—O9i	89.40 (7)	Na2viii—O10—Na3viii	91.56 (6)
O13—Na2—O7ii	78.32 (6)	S2—O11—Na3iv	119.33 (9)
O14v—Na2—O7ii	93.97 (6)	S2—O11—Na4vii	111.58 (9)
O10vi—Na2—O7ii	91.17 (7)	Na3iv—O11—Na4vii	128.97 (8)
O9i—Na2—O7ii	157.64 (7)	S3—O12—Na1vii	138.53 (11)
O13—Na2—O1vi	156.46 (7)	S3—O12—Na4	98.37 (8)
O14v—Na2—O1vi	70.79 (6)	Na1vii—O12—Na4	122.67 (8)
O10vi—Na2—O1vi	73.15 (6)	S3—O13—Na2	141.74 (10)
O9i—Na2—O1vi	109.81 (6)	S3—O13—Na3	117.23 (9)
O7ii—Na2—O1vi	91.70 (6)	Na2—O13—Na3	92.48 (6)
O11i—Na3—O2iv	110.07 (7)	S3—O13—Na4	93.14 (8)
O11i—Na3—O13	101.80 (6)	Na2—O13—Na4	100.69 (7)
O2iv—Na3—O13	148.13 (7)	Na3—O13—Na4	107.34 (7)
O11i—Na3—O10vi	95.79 (7)	S3—O14—Na2ix	124.60 (10)
O2iv—Na3—O10vi	95.42 (7)	S3—O14—Na1x	124.66 (10)
O13—Na3—O10vi	81.85 (6)	Na2ix—O14—Na1x	109.32 (7)

Symmetry codes: (i) $x+1/2$, $-y+1/2$, $-z+1$; (ii) $-x+1$, $y+1/2$, $-z+1/2$; (iii) $x-1$, y, z; (iv) $x-1/2$, $-y+1/2$, $-z+1$; (v) $-x+2$, $y+1/2$, $-z+1/2$; (vi) x, $y+1$, z; (vii) $-x+1$, $y-1/2$, $-z+1/2$; (viii) x, $y-1$, z; (ix) $-x+2$, $y-1/2$, $-z+1/2$; (x) $x+1$, y, z.