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Trisodium bis{1-[iminio(morpholino)-methyl]guanidinium} bis[hexahydrogen-hexamolybdoaluminate(III)] chloride icosahydrate

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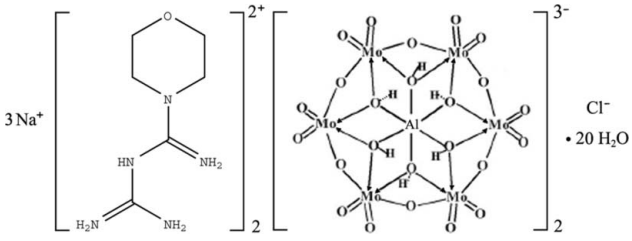
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.035; wR factor = 0.093; data-to-parameter ratio = 13.7.

In the title compound, $Na_3(C_6H_{15}N_5O)_2[Al(OH)_6Mo_6O_{18}]_2$-$Cl{\cdot}20H_2O$, the $[Al(OH)_6Mo_6O_{18}]^{3-}$ polyoxoanion has a B-type Anderson structure exhibiting approximate D_{3d} symmetry. There are two types of sodium cations: the Na^+ cations of type I have a distorted octahedral coordination geometry formed by six O atoms and are statistically distributed over two positions with equal occupancies, while the coordination polyhedra of the two Na^+ cations of type II share one Cl anion located on an inversion center. The latter fragment, containing a Cl anion and two sodium cations, links two polyoxoanions into centrosymmetric blocks. The diprotonated 1-[imino(morpholino)methyl]guanidinium cations and uncordinated water molecules contribute to extensive N—H···O and O—H···O hydrogen bonding, resulting in the formation a three-dimensional supramolecular structure.

Related literature

For related literature, see: Cao *et al.* (2007); Cheng *et al.* (2007); Lee *et al.* (1991); Li *et al.* (2005); Pope (1983); Shivaiah *et al.* (2003); Wang *et al.* (2007). For general background, see: Brown & Altermatt (1985).



Experimental

Crystal data

$Na_3(C_6H_{15}N_5O)_2[Al(OH)_6Mo_6O_{18}]_2Cl{\cdot}20H_2O$
M_r = 2796.54
Triclinic, $P\overline{1}$
a = 10.1070 (6) Å
b = 11.3869 (7) Å
c = 17.2548 (10) Å
α = 81.6980 (10)°
β = 75.3140 (10)°
γ = 77.0570 (10)°
V = 1864.03 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.15 mm^{-1}
T = 296 (2) K
0.31 × 0.25 × 0.22 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.528, T_{max} = 0.624
9902 measured reflections
6882 independent reflections
6108 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.06
6882 reflections
503 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.36 e Å^{-3}
$\Delta\rho_{min}$ = −1.29 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O8^{i}	0.90	2.00	2.855 (5)	158
N3—H3···O7^{ii}	0.90	1.86	2.750 (5)	173
N5—H6···O9^{iii}	0.90	1.92	2.821 (5)	179
O1—H8···O31	0.85	1.79	2.631 (5)	170
O3—H10···O32	0.85	1.87	2.715 (5)	169
O4—H11···O27^{iv}	0.85	1.90	2.736 (4)	170
O5—H12···O30^{v}	0.85	1.94	2.769 (5)	164
O6—H13···O28^{iv}	0.85	1.91	2.737 (4)	164
O26—H14···O19^{vi}	0.85	2.11	2.919 (5)	159
O26—H15···O35^{vii}	0.85	2.13	2.898 (5)	150
O27—H16···O34^{vii}	0.85	2.12	2.918 (5)	155
O27—H17···O35^{viii}	0.85	1.95	2.784 (5)	169
O28—H18···O17^{vii}	0.85	2.04	2.845 (5)	158
O28—H19···O16^{vii}	0.85	1.98	2.790 (5)	160
O29—H20···O20^{vi}	0.85	2.08	2.853 (5)	152
O29—H21···O12^{v}	0.84	1.90	2.735 (5)	168
O30—H22···O21^{vi}	0.85	2.11	2.890 (5)	152
O30—H23···O33^{v}	0.85	1.93	2.640 (7)	141
O31—H24···O32	0.86	2.09	2.889 (7)	154
O31—H25···O29	0.86	2.08	2.885 (6)	155
O32—H26···O33	0.85	2.00	2.632 (8)	130
O32—H27···O23^{ix}	0.85	2.03	2.843 (6)	160
O33—H29···O10	0.85	1.96	2.812 (6)	176
O34—H30···O14^{ii}	0.85	2.14	2.991 (5)	175
O34—H31···O11^{ix}	0.85	1.94	2.756 (5)	161
O35—H32···O34	0.85	2.03	2.768 (5)	145
O35—H33···O18	0.85	2.14	2.927 (5)	155

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2425).

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supporting information

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Trisodium bis{1-[iminio(morpholino)methyl]guanidinium} bis[hexahydrogenhexamolybdoaluminate(III)] chloride icosahydrate

Feng Wang, Rui-Ge Cao, Yi-Bing Pan and Shu-Xia Liu

S1. Comment

N-Amidino-4-morpholincarboxamidine (ABOB) is an effective antiviral agent to influenza, chickenpox, and measles. It is expected that the supramolecular interaction between ABOB and polyoxometalates (POMs) (Pope, 1983) may exhibit synergistic pharmaceutical activity. In our previous work, we have isolated a few compounds based on various polyoxoanions (Cheng *et al.*, 2007; Li *et al.*, 2005; Wang *et al.*, 2007). When investigating the reaction of B-type Anderson polyoxoanion $[Al(OH)_6Mo_6O_{18}]^{3-}$ and ABOB, a compound formulated as $Na_3(H_2ABOB)_2[Al(OH)_6Mo_6O_{18}]_2Cl{\cdot}20H_2O$ (I) was obtained.

The asymmetric unit of (I) is composed of a $[Al(OH)_6Mo_6O_{18}]^{3-}$ polyoxoanion, a protonated ABOB, one and a half Na^+ cation, half of a Cl^- ion, and ten water molecules (Fig. 1). The $[Al(OH)_6Mo_6O_{18}]^{3-}$ polyoxoanion has a B-type Anderson structure in which six $\{MoO_6\}$ octahedra arrange hexagonally around the central $\{Al(OH)_6\}$ octahedron with approximate D_{3d} symmetry; bond lengths and angles are within the normal ranges (Cao *et al*., 2007; Lee *et al.*, 1991; Shivaiah *et al.*, 2003). There are two types - **I** and **II**, respectively - of sodium cations: the Na^+ cations of type **I** have a distorted octahedral coordination geometry formed by six O atoms and are statistically distributed between two positions with equal occupancies, while coordination polyhedrons of two Na^+ cations of type **II** share one Cl anion located on an inversion center. The latter atomic fragment containig a Cl anion and two sodium cations link two polyoxoanions into centrosymmetric blocks. The diprotonated ABOB which acquires two protons from its two imine groups (N2, N4) were adopted to compensate for charge balance. Hydrogen-bonding interactions among the dimer, diprotonated ABOB, water molecules, and Cl^- ion result in a three-dimensional supramolecular structure (Fig. 2).

Bond valence sum calculations (Brown & Altermatt, 1985) indicated oxidation states of 5.94–6.01 for the Mo atoms and 2.85 for the Al atom in good agreement with the expected values of 6 and 3, respectively. Furthermore, bond valence sum calculations showed that the oxidation states of the O1–O6 atoms are in the range 1.14–1.22 and the O7–O24 atoms are in the range 1.70–1.91, which agrees with the results of X-ray single-crystal diffraction determination that there are six oxygen atoms protonated.

S2. Experimental

To a 30 ml aqueous solution of $AlCl_3.6H_2O$ (0.36 g, 1.5 mmol), the 10 ml aqueous solution of $Na_2MoO_4.2H_2O$ (0.90 g, 3.7 mmol) and 5 ml of glacial acetic acid were added, respectively, followed by addition of 10 ml ABOB (0.10 g, 0.6 mmol). The pH of the mixture was adjusted with dilute HCl to about 2.6 and it was stirred for half an hour. The filtrate was kept for one week under ambient condition and then block crystals of (I) were collected in about 71% yield based on Mo.

S3. Refinement

All H atoms (except H24 and H25) were placed in idealized positions and refined as riding model approximation with C–H = 0.97 Å, U_{iso}(H) = 1.2 U_{eq}(C), O–H = 0.85 Å, N–H = 0.90 Å and U_{iso}(H) = 1.2 U_{eq}(O,*N*). Atoms H24 and H25 (attached to O31) were geometrically positioned and not refined. Na2 atom was treated as disordered over two positions with equal occupancies equal to 0.5.

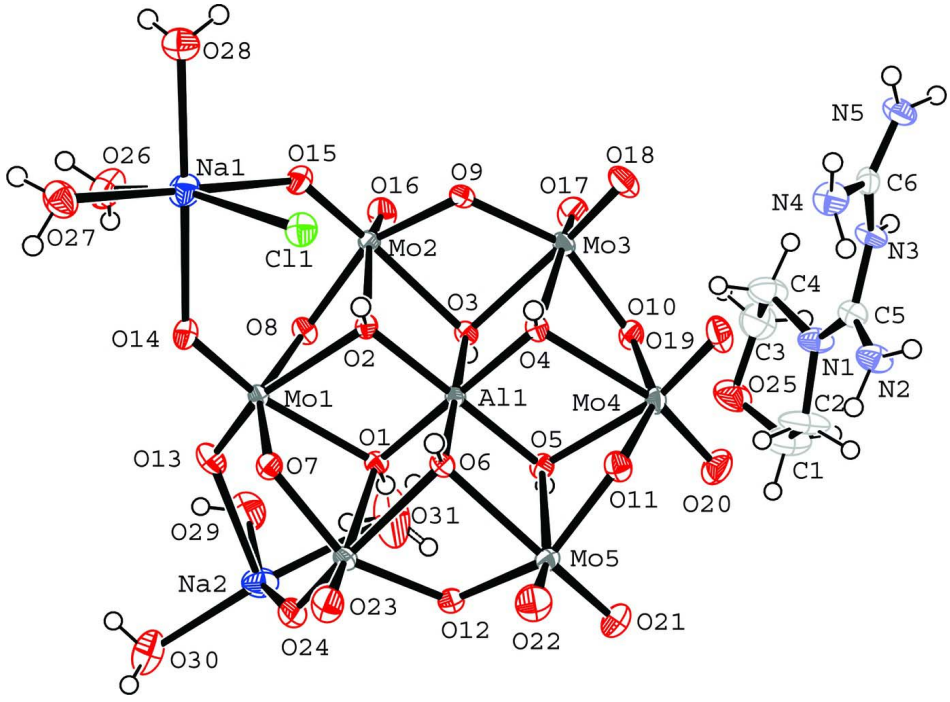

Figure 1

Asymmetric unit of (I), showing 30% probability displacement ellipsoids. Solvent waters have been omitted.

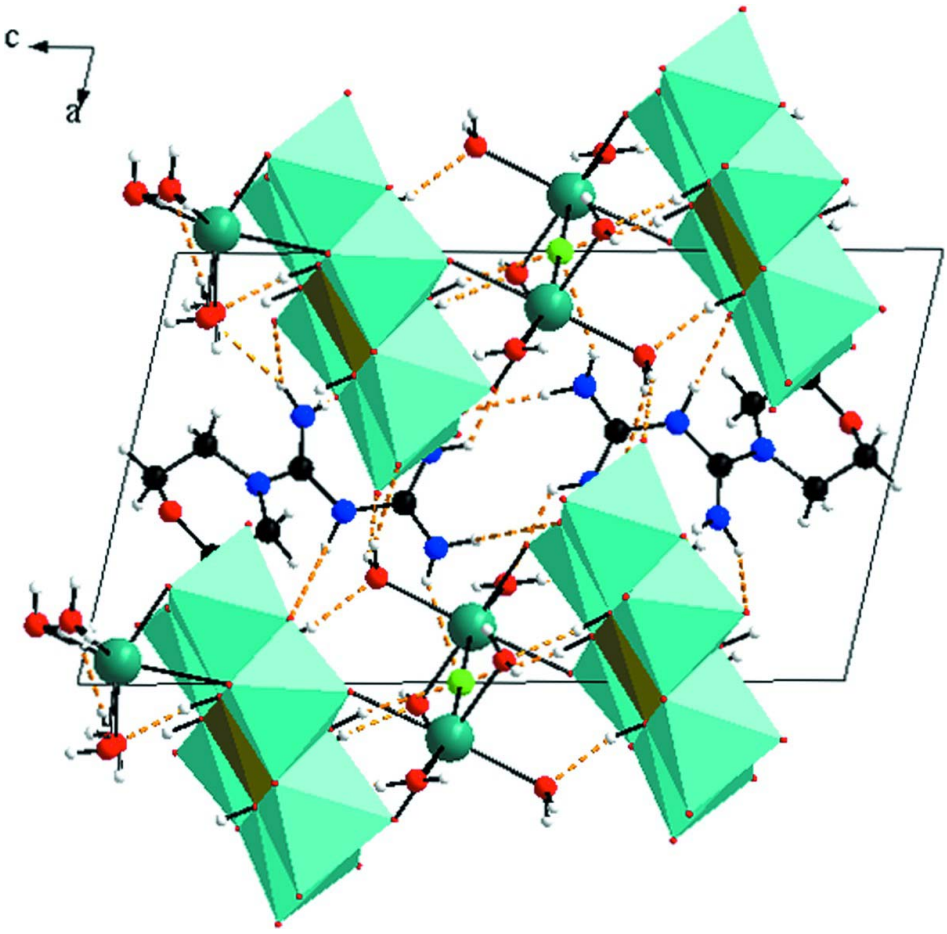

Figure 2

The crystal packing of (I) along *b* axis with hydrogen bonds drawn as dashed lines. Solvent waters have been omitted.

Trisodium bis{1-[iminio(morpholino)methyl]guanidinium} bis[hexahydrogenhexamolybdoaluminate(III)] chloride icosahydrate

Crystal data

$Na_3(C_6H_{15}N_5O)_2[Al(OH)_6Mo_6O_{18}]_2Cl\cdot 20H_2O$
$M_r = 2796.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.1070\ (6)$ Å
$b = 11.3869\ (7)$ Å
$c = 17.2548\ (10)$ Å
$\alpha = 81.698\ (1)°$
$\beta = 75.314\ (1)°$
$\gamma = 77.057\ (1)°$
$V = 1864.03\ (19)$ Å^3
$Z = 1$
$F(000) = 1364$
$D_x = 2.491$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6444 reflections
$\theta = 1.8–25.6°$
$\mu = 2.15$ mm^{-1}
$T = 296$ K
Block, colourless
0.31 × 0.25 × 0.22 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.528, T_{max} = 0.624
9902 measured reflections
6882 independent reflections
6108 reflections with $I > 2\sigma(I)$

R_{int} = 0.021
θ_{max} = 25.6°, θ_{min} = 1.8°
h = −12→12
k = −12→13
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.06
6882 reflections
503 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 4.9534P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.36 e Å^{-3}
$\Delta\rho_{min}$ = −1.29 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0137 (3)

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. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Al1	0.90661 (12)	0.18649 (10)	0.25816 (7)	0.0126 (3)	
Mo1	0.96744 (4)	−0.11386 (3)	0.27426 (2)	0.01484 (11)	
Mo2	0.66462 (4)	0.04088 (3)	0.37024 (2)	0.01508 (11)	
Mo3	0.60225 (4)	0.34140 (3)	0.34933 (2)	0.01652 (11)	
Mo4	0.84344 (4)	0.48692 (3)	0.23681 (2)	0.01781 (11)	
Mo5	1.14688 (4)	0.33344 (3)	0.14622 (2)	0.01812 (11)	
Mo6	1.20687 (4)	0.03452 (3)	0.16141 (2)	0.01669 (11)	
Na1	0.8711 (2)	−0.19733 (17)	0.50224 (11)	0.0280 (4)	
Na2	1.0528 (4)	−0.1445 (4)	0.0459 (2)	0.0327 (9)	0.50
Cl1	1.0000	0.0000	0.5000	0.0242 (3)	
C1	0.4802 (7)	0.6826 (7)	0.0390 (4)	0.0534 (17)	
H1A	0.4184	0.7562	0.0244	0.064*	
H1B	0.5480	0.6580	−0.0096	0.064*	
C2	0.5541 (6)	0.7090 (7)	0.0956 (3)	0.0472 (16)	
H2A	0.5920	0.7812	0.0744	0.057*	
H2B	0.6315	0.6425	0.1002	0.057*	
C3	0.2954 (7)	0.6335 (6)	0.1381 (4)	0.0460 (15)	
H3A	0.2348	0.5752	0.1573	0.055*	

H3B	0.2391	0.7097	0.1222	0.055*
C4	0.3559 (6)	0.6502 (6)	0.2029 (3)	0.0402 (14)
H4A	0.3980	0.5716	0.2250	0.048*
H4B	0.2822	0.6871	0.2453	0.048*
C5	0.4993 (5)	0.7834 (4)	0.2270 (3)	0.0223 (9)
C6	0.4182 (5)	0.8042 (4)	0.3722 (3)	0.0197 (9)
N1	0.4633 (4)	0.7272 (4)	0.1760 (2)	0.0274 (9)
N2	0.6204 (4)	0.8142 (4)	0.2137 (2)	0.0284 (9)
H1	0.6948	0.7823	0.1765	0.034*
H2	0.6464	0.8679	0.2374	0.034*
N3	0.3989 (4)	0.8116 (3)	0.2962 (2)	0.0214 (8)
H3	0.3159	0.8429	0.2840	0.026*
N4	0.5371 (4)	0.7469 (4)	0.3894 (2)	0.0287 (9)
H4	0.6087	0.7685	0.3512	0.034*
H5	0.5516	0.7488	0.4385	0.034*
N5	0.3136 (4)	0.8525 (4)	0.4272 (2)	0.0285 (9)
H6	0.3317	0.8378	0.4765	0.034*
H7	0.2377	0.9106	0.4244	0.034*
O1	0.9705 (3)	0.0596 (3)	0.19008 (17)	0.0151 (6)
H8	0.9421	0.0643	0.1472	0.018*
O2	0.8941 (3)	0.0588 (2)	0.34240 (17)	0.0137 (6)
H9	0.9311	0.0607	0.3812	0.016*
O3	0.7143 (3)	0.1875 (2)	0.26901 (17)	0.0144 (6)
H10	0.6828	0.1832	0.2285	0.017*
O4	0.8404 (3)	0.3137 (3)	0.32567 (17)	0.0151 (6)
H11	0.8805	0.3146	0.3633	0.018*
O5	0.9193 (3)	0.3124 (3)	0.17301 (17)	0.0156 (6)
H12	0.8869	0.3112	0.1323	0.019*
O6	1.0986 (3)	0.1831 (3)	0.24666 (17)	0.0146 (6)
H13	1.1312	0.1796	0.2880	0.018*
O7	1.1509 (3)	−0.0732 (3)	0.25770 (18)	0.0186 (6)
O8	0.7693 (3)	−0.0652 (3)	0.28711 (18)	0.0181 (6)
O9	0.6296 (3)	0.1915 (3)	0.41825 (17)	0.0193 (6)
O10	0.6638 (3)	0.4432 (3)	0.25302 (19)	0.0210 (6)
O11	1.0414 (3)	0.4388 (3)	0.22920 (19)	0.0211 (7)
O12	1.1770 (3)	0.1847 (3)	0.09572 (18)	0.0211 (7)
O13	0.9982 (3)	−0.2022 (3)	0.1980 (2)	0.0272 (7)
O14	0.9798 (3)	−0.2103 (3)	0.35929 (19)	0.0252 (7)
O15	0.6820 (3)	−0.0552 (3)	0.45441 (19)	0.0254 (7)
O16	0.5052 (3)	0.0407 (3)	0.3533 (2)	0.0260 (7)
O17	0.4406 (3)	0.3449 (3)	0.3343 (2)	0.0291 (8)
O18	0.5761 (4)	0.4378 (3)	0.4208 (2)	0.0309 (8)
O19	0.8044 (4)	0.5837 (3)	0.3101 (2)	0.0292 (8)
O20	0.8410 (4)	0.5760 (3)	0.1485 (2)	0.0333 (8)
O21	1.1373 (4)	0.4294 (3)	0.0617 (2)	0.0332 (8)
O22	1.3079 (4)	0.3260 (3)	0.1628 (2)	0.0328 (8)
O23	1.3700 (3)	0.0303 (3)	0.1751 (2)	0.0293 (8)
O24	1.2263 (4)	−0.0587 (3)	0.08914 (19)	0.0282 (7)

O25	0.4015 (4)	0.5917 (4)	0.0695 (2)	0.0443 (10)
O26	0.7727 (4)	−0.3471 (3)	0.4712 (2)	0.0412 (9)
H14	0.7606	−0.3567	0.4257	0.049*
H15	0.7767	−0.4063	0.5072	0.049*
O27	1.0513 (4)	−0.3434 (3)	0.5500 (2)	0.0320 (8)
H16	1.0269	−0.4106	0.5687	0.038*
H17	1.1231	−0.3797	0.5185	0.038*
O28	0.7555 (3)	−0.1911 (3)	0.6411 (2)	0.0287 (7)
H18	0.7086	−0.2468	0.6578	0.034*
H19	0.6784	−0.1420	0.6539	0.034*
O29	0.8521 (5)	−0.1943 (4)	0.0585 (2)	0.0469 (10)
H20	0.8663	−0.2705	0.0695	0.056*
H21	0.8414	−0.2015	0.0126	0.056*
O30	1.1468 (5)	−0.3344 (4)	−0.0247 (3)	0.0468 (10)
H22	1.1144	−0.3929	0.0046	0.056*
H23	1.2350	−0.3517	−0.0313	0.056*
O31	0.8656 (6)	0.0541 (4)	0.0661 (3)	0.0680 (16)
H24	0.7963	0.1050	0.0906	0.082*
H25	0.8343	−0.0111	0.0688	0.082*
O32	0.5896 (5)	0.1589 (5)	0.1528 (3)	0.0566 (12)
H26	0.5532	0.2243	0.1292	0.068*
H27	0.5356	0.1083	0.1671	0.068*
O33	0.5983 (6)	0.3897 (5)	0.1147 (3)	0.0774 (16)
H28	0.5206	0.4255	0.1042	0.093*
H29	0.6148	0.4084	0.1568	0.093*
O34	0.1012 (4)	0.5252 (3)	0.3550 (2)	0.0393 (9)
H31	0.1008	0.4880	0.3158	0.047*
H30	0.0624	0.5995	0.3560	0.047*
O35	0.2881 (4)	0.5691 (4)	0.4350 (2)	0.0400 (9)
H32	0.2634	0.5508	0.3954	0.048*
H33	0.3707	0.5461	0.4418	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0114 (6)	0.0125 (6)	0.0131 (6)	0.0000 (5)	−0.0035 (5)	−0.0004 (5)
Mo1	0.01445 (19)	0.01288 (19)	0.01581 (19)	−0.00011 (14)	−0.00296 (14)	−0.00181 (14)
Mo2	0.01243 (19)	0.01500 (19)	0.01653 (19)	−0.00142 (14)	−0.00272 (14)	−0.00036 (14)
Mo3	0.0136 (2)	0.01542 (19)	0.0182 (2)	0.00193 (14)	−0.00290 (14)	−0.00296 (14)
Mo4	0.0185 (2)	0.01218 (19)	0.0213 (2)	0.00010 (14)	−0.00548 (15)	0.00012 (14)
Mo5	0.0164 (2)	0.0168 (2)	0.0192 (2)	−0.00425 (14)	−0.00140 (15)	0.00134 (15)
Mo6	0.0132 (2)	0.01648 (19)	0.0180 (2)	0.00022 (14)	−0.00215 (14)	−0.00154 (14)
Na1	0.0300 (10)	0.0288 (10)	0.0256 (10)	−0.0043 (8)	−0.0102 (8)	0.0007 (8)
Na2	0.034 (2)	0.040 (2)	0.026 (2)	−0.0118 (18)	−0.0036 (17)	−0.0084 (17)
Cl1	0.0264 (8)	0.0258 (8)	0.0232 (8)	−0.0042 (6)	−0.0117 (6)	−0.0015 (6)
C1	0.053 (4)	0.076 (5)	0.033 (3)	−0.020 (3)	0.001 (3)	−0.018 (3)
C2	0.034 (3)	0.086 (5)	0.026 (3)	−0.025 (3)	0.010 (2)	−0.025 (3)
C3	0.043 (3)	0.047 (4)	0.053 (4)	−0.018 (3)	−0.006 (3)	−0.014 (3)

C4	0.034 (3)	0.053 (4)	0.036 (3)	−0.022 (3)	0.005 (2)	−0.016 (3)
C5	0.021 (2)	0.026 (2)	0.019 (2)	0.0008 (18)	−0.0077 (18)	−0.0025 (18)
C6	0.025 (2)	0.015 (2)	0.020 (2)	−0.0021 (17)	−0.0081 (18)	−0.0012 (17)
N1	0.025 (2)	0.041 (2)	0.019 (2)	−0.0114 (18)	−0.0028 (16)	−0.0093 (18)
N2	0.022 (2)	0.038 (2)	0.027 (2)	−0.0077 (18)	−0.0031 (17)	−0.0125 (18)
N3	0.0178 (19)	0.029 (2)	0.0152 (18)	0.0043 (15)	−0.0063 (15)	−0.0052 (15)
N4	0.027 (2)	0.035 (2)	0.025 (2)	−0.0001 (18)	−0.0141 (17)	0.0013 (18)
N5	0.030 (2)	0.031 (2)	0.022 (2)	0.0012 (18)	−0.0032 (17)	−0.0094 (17)
O1	0.0162 (15)	0.0164 (14)	0.0132 (14)	−0.0020 (11)	−0.0045 (11)	−0.0027 (11)
O2	0.0129 (14)	0.0144 (14)	0.0142 (14)	−0.0005 (11)	−0.0067 (11)	0.0007 (11)
O3	0.0119 (14)	0.0165 (14)	0.0155 (14)	−0.0002 (11)	−0.0064 (11)	−0.0018 (11)
O4	0.0145 (15)	0.0146 (14)	0.0179 (14)	−0.0011 (11)	−0.0074 (11)	−0.0033 (11)
O5	0.0167 (15)	0.0171 (14)	0.0133 (14)	−0.0006 (11)	−0.0080 (11)	0.0017 (11)
O6	0.0115 (14)	0.0164 (14)	0.0166 (14)	−0.0014 (11)	−0.0051 (11)	−0.0025 (11)
O7	0.0129 (15)	0.0193 (15)	0.0225 (16)	−0.0011 (12)	−0.0055 (12)	0.0011 (12)
O8	0.0141 (15)	0.0182 (15)	0.0235 (16)	−0.0022 (12)	−0.0059 (12)	−0.0057 (12)
O9	0.0199 (16)	0.0187 (15)	0.0158 (15)	0.0000 (12)	−0.0006 (12)	−0.0029 (12)
O10	0.0157 (15)	0.0183 (15)	0.0269 (17)	0.0015 (12)	−0.0079 (13)	0.0026 (13)
O11	0.0159 (15)	0.0197 (15)	0.0281 (17)	−0.0025 (12)	−0.0059 (13)	−0.0041 (13)
O12	0.0244 (17)	0.0192 (15)	0.0160 (15)	−0.0022 (13)	−0.0007 (12)	0.0000 (12)
O13	0.0271 (18)	0.0250 (17)	0.0298 (18)	0.0005 (14)	−0.0063 (14)	−0.0129 (14)
O14	0.0274 (18)	0.0184 (16)	0.0260 (17)	−0.0006 (13)	−0.0060 (14)	0.0038 (13)
O15	0.0261 (18)	0.0222 (16)	0.0238 (17)	−0.0019 (13)	−0.0040 (14)	0.0043 (13)
O16	0.0163 (16)	0.0260 (17)	0.0361 (19)	−0.0034 (13)	−0.0073 (14)	−0.0027 (14)
O17	0.0187 (17)	0.0305 (18)	0.0363 (19)	−0.0011 (14)	−0.0097 (14)	0.0026 (15)
O18	0.033 (2)	0.0261 (18)	0.0303 (19)	0.0022 (15)	−0.0020 (15)	−0.0124 (15)
O19	0.0308 (19)	0.0184 (16)	0.039 (2)	−0.0014 (14)	−0.0072 (16)	−0.0097 (14)
O20	0.034 (2)	0.0271 (18)	0.035 (2)	−0.0041 (15)	−0.0101 (16)	0.0115 (15)
O21	0.041 (2)	0.0246 (18)	0.0289 (18)	−0.0069 (15)	−0.0048 (16)	0.0087 (15)
O22	0.0211 (18)	0.0329 (19)	0.046 (2)	−0.0099 (15)	−0.0063 (16)	−0.0031 (17)
O23	0.0155 (16)	0.0285 (18)	0.043 (2)	−0.0030 (13)	−0.0106 (15)	0.0038 (15)
O24	0.035 (2)	0.0224 (17)	0.0234 (17)	−0.0013 (14)	−0.0014 (14)	−0.0051 (14)
O25	0.049 (3)	0.049 (2)	0.037 (2)	−0.015 (2)	0.0010 (18)	−0.0233 (19)
O26	0.056 (3)	0.035 (2)	0.037 (2)	−0.0177 (19)	−0.0168 (19)	0.0055 (17)
O27	0.0309 (19)	0.0327 (19)	0.0318 (19)	0.0024 (15)	−0.0117 (15)	−0.0068 (15)
O28	0.0192 (17)	0.038 (2)	0.0297 (18)	−0.0064 (14)	−0.0061 (14)	−0.0035 (15)
O29	0.061 (3)	0.047 (2)	0.031 (2)	0.003 (2)	−0.0201 (19)	−0.0056 (18)
O30	0.057 (3)	0.035 (2)	0.053 (3)	−0.0123 (19)	−0.025 (2)	0.0108 (19)
O31	0.107 (4)	0.041 (2)	0.076 (3)	0.010 (3)	−0.070 (3)	−0.020 (2)
O32	0.049 (3)	0.078 (3)	0.050 (3)	−0.016 (2)	−0.024 (2)	0.002 (2)
O33	0.068 (4)	0.094 (4)	0.075 (4)	−0.002 (3)	−0.029 (3)	−0.021 (3)
O34	0.038 (2)	0.036 (2)	0.048 (2)	−0.0004 (17)	−0.0182 (18)	−0.0154 (18)
O35	0.029 (2)	0.044 (2)	0.048 (2)	0.0031 (17)	−0.0107 (17)	−0.0188 (19)

Geometric parameters (Å, º)

Al1—O4	1.887 (3)	Na2—H25	2.3601
Al1—O1	1.890 (3)	Cl1—Na1^{ii}	2.8298 (19)

Al1—O6	1.892 (3)	C1—O25	1.408 (7)
Al1—O5	1.900 (3)	C1—C2	1.468 (8)
Al1—O3	1.902 (3)	C1—H1A	0.9700
Al1—O2	1.903 (3)	C1—H1B	0.9700
Mo1—O13	1.696 (3)	C2—N1	1.471 (6)
Mo1—O14	1.715 (3)	C2—H2A	0.9700
Mo1—O8	1.918 (3)	C2—H2B	0.9700
Mo1—O7	1.953 (3)	C3—O25	1.439 (7)
Mo1—O1	2.277 (3)	C3—C4	1.455 (8)
Mo1—O2	2.317 (3)	C3—H3A	0.9700
Mo2—O15	1.709 (3)	C3—H3B	0.9700
Mo2—O16	1.709 (3)	C4—N1	1.488 (6)
Mo2—O9	1.934 (3)	C4—H4A	0.9700
Mo2—O8	1.948 (3)	C4—H4B	0.9700
Mo2—O3	2.276 (3)	C5—N2	1.304 (6)
Mo2—O2	2.296 (3)	C5—N1	1.321 (6)
Mo3—O18	1.700 (3)	C5—N3	1.383 (6)
Mo3—O17	1.709 (3)	C6—N5	1.304 (6)
Mo3—O10	1.932 (3)	C6—N4	1.316 (6)
Mo3—O9	1.943 (3)	C6—N3	1.361 (5)
Mo3—O4	2.293 (3)	N2—H1	0.9000
Mo3—O3	2.300 (3)	N2—H2	0.8998
Mo4—O20	1.706 (3)	N3—H3	0.8999
Mo4—O19	1.710 (3)	N4—H4	0.9000
Mo4—O11	1.928 (3)	N4—H5	0.9000
Mo4—O10	1.931 (3)	N5—H6	0.8999
Mo4—O5	2.296 (3)	N5—H7	0.8999
Mo4—O4	2.318 (3)	O1—H8	0.8500
Mo5—O21	1.701 (3)	O2—H9	0.8500
Mo5—O22	1.704 (3)	O3—H10	0.8501
Mo5—O11	1.943 (3)	O4—H11	0.8499
Mo5—O12	1.945 (3)	O5—H12	0.8500
Mo5—O5	2.288 (3)	O6—H13	0.8499
Mo5—O6	2.293 (3)	O26—H14	0.8499
Mo6—O24	1.698 (3)	O26—H15	0.8501
Mo6—O23	1.713 (3)	O27—H16	0.8500
Mo6—O12	1.919 (3)	O27—H17	0.8500
Mo6—O7	1.957 (3)	O28—H18	0.8500
Mo6—O1	2.274 (3)	O28—H19	0.8500
Mo6—O6	2.301 (3)	O29—H20	0.8486
Na1—O26	2.340 (4)	O29—H21	0.8441
Na1—O28	2.388 (4)	O30—H22	0.8500
Na1—O27	2.402 (4)	O30—H23	0.8501
Na1—O14	2.444 (4)	O31—Na2^{i}	2.116 (7)
Na1—O15	2.446 (4)	O31—H24	0.8624
Na1—Cl1	2.8298 (19)	O31—H25	0.8617
Na2—O31^{i}	2.116 (7)	O32—H26	0.8501
Na2—O29	2.177 (6)	O32—H27	0.8500

Na2—O24	2.496 (5)	O33—H28	0.8500
Na2—O30	2.513 (6)	O33—H29	0.8500
Na2—O13	2.559 (5)	O34—H31	0.8499
Na2—O31	2.607 (6)	O34—H30	0.8500
Na2—Na2^{i}	3.502 (9)	O35—H32	0.8500
Na2—H20	2.5362	O35—H33	0.8500
Na2—H21	2.5822		

O4—Al1—O1	179.20 (13)	O29—Na2—H20	18.8
O4—Al1—O6	96.29 (13)	O24—Na2—H20	153.3
O1—Al1—O6	84.45 (13)	O30—Na2—H20	69.5
O4—Al1—O5	84.77 (13)	O13—Na2—H20	75.6
O1—Al1—O5	94.99 (13)	O31—Na2—H20	91.6
O6—Al1—O5	84.48 (13)	Na2^{i}—Na2—H20	111.3
O4—Al1—O3	84.60 (13)	O31^{i}—Na2—H21	99.6
O1—Al1—O3	94.66 (13)	O29—Na2—H21	18.0
O6—Al1—O3	179.09 (13)	O24—Na2—H21	169.8
O5—Al1—O3	95.81 (13)	O30—Na2—H21	74.0
O4—Al1—O2	96.00 (13)	O13—Na2—H21	99.1
O1—Al1—O2	84.23 (13)	O31—Na2—H21	77.7
O6—Al1—O2	95.63 (13)	Na2^{i}—Na2—H21	86.7
O5—Al1—O2	179.20 (13)	H20—Na2—H21	27.3
O3—Al1—O2	84.06 (13)	O31^{i}—Na2—H25	95.2
O13—Mo1—O14	106.44 (16)	O29—Na2—H25	54.5
O13—Mo1—O8	97.66 (14)	O24—Na2—H25	109.9
O14—Mo1—O8	101.93 (14)	O30—Na2—H25	133.5
O13—Mo1—O7	100.20 (15)	O13—Na2—H25	86.1
O14—Mo1—O7	95.41 (14)	O31—Na2—H25	19.2
O8—Mo1—O7	150.41 (12)	Na2^{i}—Na2—H25	49.6
O13—Mo1—O1	93.31 (14)	H20—Na2—H25	72.4
O14—Mo1—O1	158.53 (13)	H21—Na2—H25	60.0
O8—Mo1—O1	83.25 (12)	Na1—Cl1—Na1^{ii}	180.00 (4)
O7—Mo1—O1	72.38 (11)	O25—C1—C2	114.0 (5)
O13—Mo1—O2	158.48 (14)	O25—C1—H1A	108.8
O14—Mo1—O2	94.31 (13)	C2—C1—H1A	108.8
O8—Mo1—O2	71.94 (11)	O25—C1—H1B	108.8
O7—Mo1—O2	83.10 (11)	C2—C1—H1B	108.8
O1—Mo1—O2	67.22 (10)	H1A—C1—H1B	107.7
O15—Mo2—O16	107.36 (16)	C1—C2—N1	112.6 (5)
O15—Mo2—O9	97.76 (14)	C1—C2—H2A	109.1
O16—Mo2—O9	101.84 (14)	N1—C2—H2A	109.1
O15—Mo2—O8	100.08 (14)	C1—C2—H2B	109.1
O16—Mo2—O8	94.96 (14)	N1—C2—H2B	109.1
O9—Mo2—O8	150.56 (12)	H2A—C2—H2B	107.8
O15—Mo2—O3	157.71 (14)	O25—C3—C4	111.5 (5)
O16—Mo2—O3	94.40 (13)	O25—C3—H3A	109.3
O9—Mo2—O3	72.44 (11)	C4—C3—H3A	109.3
O8—Mo2—O3	82.39 (12)	O25—C3—H3B	109.3

O15—Mo2—O2	91.79 (13)	C4—C3—H3B	109.3
O16—Mo2—O2	158.68 (13)	H3A—C3—H3B	108.0
O9—Mo2—O2	84.31 (12)	C3—C4—N1	112.9 (5)
O8—Mo2—O2	71.95 (11)	C3—C4—H4A	109.0
O3—Mo2—O2	67.73 (10)	N1—C4—H4A	109.0
O18—Mo3—O17	105.49 (17)	C3—C4—H4B	109.0
O18—Mo3—O10	100.65 (15)	N1—C4—H4B	109.0
O17—Mo3—O10	96.30 (15)	H4A—C4—H4B	107.8
O18—Mo3—O9	97.33 (15)	N2—C5—N1	123.4 (4)
O17—Mo3—O9	101.13 (15)	N2—C5—N3	120.5 (4)
O10—Mo3—O9	150.56 (12)	N1—C5—N3	116.0 (4)
O18—Mo3—O4	93.17 (14)	N5—C6—N4	121.7 (4)
O17—Mo3—O4	159.96 (14)	N5—C6—N3	117.6 (4)
O10—Mo3—O4	72.67 (11)	N4—C6—N3	120.7 (4)
O9—Mo3—O4	83.28 (12)	C5—N1—C2	120.3 (4)
O18—Mo3—O3	158.31 (14)	C5—N1—C4	122.1 (4)
O17—Mo3—O3	95.15 (14)	C2—N1—C4	115.3 (4)
O10—Mo3—O3	83.29 (12)	C5—N2—H1	122.8
O9—Mo3—O3	71.74 (11)	C5—N2—H2	129.3
O4—Mo3—O3	67.44 (10)	H1—N2—H2	107.9
O20—Mo4—O19	106.06 (17)	C6—N3—C5	127.3 (4)
O20—Mo4—O11	100.82 (16)	C6—N3—H3	122.6
O19—Mo4—O11	98.43 (15)	C5—N3—H3	109.9
O20—Mo4—O10	97.79 (15)	C6—N4—H4	109.8
O19—Mo4—O10	99.41 (15)	C6—N4—H5	119.8
O11—Mo4—O10	149.46 (13)	H4—N4—H5	109.9
O20—Mo4—O5	92.72 (14)	C6—N5—H6	112.3
O19—Mo4—O5	160.56 (14)	C6—N5—H7	132.5
O11—Mo4—O5	72.58 (11)	H6—N5—H7	113.4
O10—Mo4—O5	82.59 (12)	Al1—O1—Mo6	104.56 (13)
O20—Mo4—O4	158.16 (14)	Al1—O1—Mo1	105.23 (13)
O19—Mo4—O4	94.86 (14)	Mo6—O1—Mo1	93.54 (11)
O11—Mo4—O4	81.85 (12)	Al1—O1—H8	120.5
O10—Mo4—O4	72.12 (11)	Mo6—O1—H8	110.4
O5—Mo4—O4	67.18 (10)	Mo1—O1—H8	118.5
O21—Mo5—O22	106.29 (18)	Al1—O2—Mo2	103.71 (12)
O21—Mo5—O11	100.95 (15)	Al1—O2—Mo1	103.31 (12)
O22—Mo5—O11	97.37 (15)	Mo2—O2—Mo1	92.32 (10)
O21—Mo5—O12	96.44 (15)	Al1—O2—H9	117.7
O22—Mo5—O12	100.96 (15)	Mo2—O2—H9	119.0
O11—Mo5—O12	150.02 (13)	Mo1—O2—H9	116.9
O21—Mo5—O5	94.55 (15)	Al1—O3—Mo2	104.49 (12)
O22—Mo5—O5	158.37 (14)	Al1—O3—Mo3	103.59 (12)
O11—Mo5—O5	72.51 (11)	Mo2—O3—Mo3	93.06 (10)
O12—Mo5—O5	81.98 (12)	Al1—O3—H10	121.1
O21—Mo5—O6	159.79 (14)	Mo2—O3—H10	112.8
O22—Mo5—O6	92.62 (14)	Mo3—O3—H10	117.6
O11—Mo5—O6	83.22 (12)	Al1—O4—Mo3	104.35 (13)

O12—Mo5—O6	72.48 (11)	Al1—O4—Mo4	103.82 (13)
O5—Mo5—O6	67.61 (10)	Mo3—O4—Mo4	91.65 (10)
O24—Mo6—O23	107.00 (17)	Al1—O4—H11	119.0
O24—Mo6—O12	97.20 (14)	Mo3—O4—H11	121.2
O23—Mo6—O12	101.23 (15)	Mo4—O4—H11	112.5
O24—Mo6—O7	99.93 (14)	Al1—O5—Mo5	103.92 (12)
O23—Mo6—O7	95.46 (15)	Al1—O5—Mo4	104.23 (13)
O12—Mo6—O7	151.39 (12)	Mo5—O5—Mo4	91.93 (10)
O24—Mo6—O1	92.32 (14)	Al1—O5—H12	120.6
O23—Mo6—O1	158.90 (14)	Mo5—O5—H12	116.0
O12—Mo6—O1	84.23 (12)	Mo4—O5—H12	115.8
O7—Mo6—O1	72.38 (11)	Al1—O6—Mo5	103.97 (13)
O24—Mo6—O6	157.89 (14)	Al1—O6—Mo6	103.45 (12)
O23—Mo6—O6	94.42 (14)	Mo5—O6—Mo6	91.97 (10)
O12—Mo6—O6	72.74 (11)	Al1—O6—H13	120.2
O7—Mo6—O6	83.02 (11)	Mo5—O6—H13	117.2
O1—Mo6—O6	67.51 (10)	Mo6—O6—H13	115.6
O26—Na1—O28	98.76 (15)	Mo1—O7—Mo6	116.00 (15)
O26—Na1—O27	92.75 (15)	Mo1—O8—Mo2	118.76 (15)
O28—Na1—O27	85.13 (13)	Mo2—O9—Mo3	117.88 (15)
O26—Na1—O14	78.03 (14)	Mo4—O10—Mo3	117.74 (15)
O28—Na1—O14	176.70 (14)	Mo4—O11—Mo5	116.73 (15)
O27—Na1—O14	95.76 (13)	Mo6—O12—Mo5	117.58 (15)
O26—Na1—O15	85.00 (14)	Mo1—O13—Na2	129.4 (2)
O28—Na1—O15	94.41 (13)	Mo1—O14—Na1	133.86 (17)
O27—Na1—O15	177.61 (15)	Mo2—O15—Na1	136.74 (18)
O14—Na1—O15	84.57 (12)	Mo6—O24—Na2	131.4 (2)
O26—Na1—Cl1	166.36 (12)	C1—O25—C3	107.9 (4)
O28—Na1—Cl1	93.76 (10)	Na1—O26—H14	127.7
O27—Na1—Cl1	93.69 (11)	Na1—O26—H15	109.1
O14—Na1—Cl1	89.35 (10)	H14—O26—H15	120.0
O15—Na1—Cl1	88.69 (10)	Na1—O27—H16	113.0
O31^{i}—Na2—O29	116.0 (2)	Na1—O27—H17	122.8
O31^{i}—Na2—O24	82.05 (19)	H16—O27—H17	90.5
O29—Na2—O24	155.2 (2)	Na1—O28—H18	112.3
O31^{i}—Na2—O30	85.3 (2)	Na1—O28—H19	118.8
O29—Na2—O30	83.64 (19)	H18—O28—H19	86.1
O24—Na2—O30	116.1 (2)	Na2—O29—H20	105.3
O31^{i}—Na2—O13	159.2 (2)	Na2—O29—H21	109.3
O29—Na2—O13	81.59 (18)	H20—O29—H21	91.0
O24—Na2—O13	77.99 (15)	Na2—O30—H22	109.5
O30—Na2—O13	108.83 (19)	Na2—O30—H23	109.4
O31^{i}—Na2—O31	84.8 (3)	H22—O30—H23	107.5
O29—Na2—O31	73.6 (2)	Na2^{i}—O31—Na2	95.2 (3)
O24—Na2—O31	92.50 (18)	Na2^{i}—O31—H24	106.6
O30—Na2—O31	148.0 (2)	Na2—O31—H24	158.0
O13—Na2—O31	90.10 (18)	Na2^{i}—O31—H25	121.3
O31^{i}—Na2—Na2^{i}	47.84 (16)	Na2—O31—H25	64.0

O29—Na2—Na2^{i}	93.1 (2)	H24—O31—H25	105.3
O24—Na2—Na2^{i}	87.08 (17)	H26—O32—H27	112.7
O30—Na2—Na2^{i}	125.6 (2)	H28—O33—H29	115.7
O13—Na2—Na2^{i}	124.5 (2)	H31—O34—H30	118.8
O31—Na2—Na2^{i}	36.99 (15)	H32—O35—H33	122.5
O31^{i}—Na2—H20	124.6		

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+2, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O8^{iii}	0.90	2.00	2.855 (5)	158
N3—H3···O7^{iv}	0.90	1.86	2.750 (5)	173
N5—H6···O9^{v}	0.90	1.92	2.821 (5)	179
O1—H8···O31	0.85	1.79	2.631 (5)	170
O3—H10···O32	0.85	1.87	2.715 (5)	169
O4—H11···O27^{ii}	0.85	1.90	2.736 (4)	170
O5—H12···O30^{i}	0.85	1.94	2.769 (5)	164
O6—H13···O28^{ii}	0.85	1.91	2.737 (4)	164
O26—H14···O19^{vi}	0.85	2.11	2.919 (5)	159
O26—H15···O35^{vii}	0.85	2.13	2.898 (5)	150
O27—H16···O34^{vii}	0.85	2.12	2.918 (5)	155
O27—H17···O35^{viii}	0.85	1.95	2.784 (5)	169
O28—H18···O17^{vii}	0.85	2.04	2.845 (5)	158
O28—H19···O16^{vii}	0.85	1.98	2.790 (5)	160
O29—H20···O20^{vi}	0.85	2.08	2.853 (5)	152
O29—H21···O12^{i}	0.84	1.90	2.735 (5)	168
O30—H22···O21^{vi}	0.85	2.11	2.890 (5)	152
O30—H23···O33^{i}	0.85	1.93	2.640 (7)	141
O31—H24···O32	0.86	2.09	2.889 (7)	154
O31—H25···O29	0.86	2.08	2.885 (6)	155
O32—H26···O33	0.85	2.00	2.632 (8)	130
O32—H27···O23^{ix}	0.85	2.03	2.843 (6)	160
O33—H29···O10	0.85	1.96	2.812 (6)	176
O34—H30···O14^{iv}	0.85	2.14	2.991 (5)	175
O34—H31···O11^{ix}	0.85	1.94	2.756 (5)	161
O35—H32···O34	0.85	2.03	2.768 (5)	145
O35—H33···O18	0.85	2.14	2.927 (5)	155

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