Supporting Information



Figure S1. Polyhedral the paradodecatungstate-B $[H_2W_{12}O_{42}]^{10-}$ anions, Colour codes: {WO₆} octahedra (pink), O (red).



Figure S2. Polyhedral and ball-and-stick representation of the 2D network structure of compound **1**, Na atoms and Lattice water molecules are omitted for clarity, Colour codes: {WO₆} octahedra (pink), Ca (blue), O (red).



Figure S3. 3-D packing arrangement of **1**. The polyanions, Ca atoms and Na atoms are represented with polyhedron; All the isolated water molecules are omitted for clarity.



Figure S4. The coordination polyhedrons around Ca atom in 1



Figure S5. Polyhedral and ball-and-stick representation of the 2D network structure of $[H_2W_{12}O_{42}]^{10-}$ polyanions coordinated with Sr1 atom in compound **2**, Lattice water molecules are omitted for clarity, Colour codes: {WO₆} octahedra (pink), Sr (green), O (red).



Figure S6. Polyhedral and ball-and-stick representation of the 2D network structure of $[H_2W_{12}O_{42}]^{10-}$ polyanions coordinated with Sr2 atom in compound **2**. Lattice water molecules are omitted for clarity, Colour codes: {WO₆} octahedra (pink), Sr (green), O (red).



Figure S7. 3-D packing arrangement of **2** with 1-D channels viewed along the b axis. The polyanions and Sr atoms are represented with polyhedron; The solvent water molecules are omitted for clarity.



Figure S8. The coordination polyhedrons around Sr1 atom in 2



Figure S9. (a)Polyhedral and ball-and-stick representation of the infinite 1D chain structure of $[H_2W_{12}O_{42}]^{10-}$ polyanions coordinated with Sr1 atom in compound **3**, Lattice water molecules are omitted for clarity, Colour codes: {WO₆} octahedra (pink), Sr (green), O (red).



Figure S10. Polyhedral and ball-and-stick representation of the 2D network structure of $[H_2W_{12}O_{42}]^{10-}$ polyanions coordinated with Sr2 atom in compound **3**. Lattice water molecules are omitted for clarity, Colour codes: {WO₆} octahedra (pink), Sr (green), O (red).



Figure S11. (a)Polyhedral and ball-and-stick representation of the infinite 1D chain structure of $[H_2W_{12}O_{42}]^{10-}$ polyanions coordinated with Na atom in compound **3**, Lattice water molecules are omitted for clarity, Colour codes: {WO₆} octahedra (pink), Na (yellow), O (red).



Figure S12. 3D packing arrangement of **3**. The polyanions, Sr atoms and Na atoms are represented with polyhedron; The solvent water molecules are omitted for clarity.



Figure S13. (a) The coordination polyhedrons around Sr1 atom in 3 (b) the adjacent Sr1 and Sr2 atoms in 3 were connected throught three μ_2 -O atoms.

FT-IR Spectroscopy

The IR spectrum of **1** (Figure S14) showed the characteristic peaks of the different W–O bonds of $[H_2W_{12}O_{42}]^{10-}$ at 600–1000 cm⁻¹. The bands at ca. 940, 870, 826 and 694 cm⁻¹ should be assigned to v(W–Ot), v(W–Ot'), v(W–Oc) and v(W–Ob), respectively.¹ A broad band at 3422 cm⁻¹ is due to the

aqua ligands. The peak at 1627 cm⁻¹ associates with the crystalline lattice water molecules. The IR spectra of complexes **2–4** (as shown in Figure S11) are similar to that of compound **1**.

References :

(1) L. Yuan, C. Qin, X. L Wang, E. B. Wang and Y. G. Li, Solid. State. Sci. 2008, 10, 967.



Figure S14. IR spectra of compounds 1, 2, 3 and 4.

Optical Band Gap

To explore conductivity potentials of compounds 1–4, the measurement of diffuse reflectivity for a powder sample was used to obtain band gap (E_g) (Figure S15), which was determined as the intersection point between the energy axis and the line extrapolated from the linear portion of the adsorption edge in a plot of Kubelka-Munk function F against energy E.¹⁻³ Kubelka–Munk function, $F = (1-R)^2/2R$, was converted from the recorded diffuse reflectance data, where R is the reflectance of an infinitely thick layer at a given wavelength. For compounds 1–4, the band gap can be assessed at 3.36, 3.56, 3.55, 3.39 eV, respectively. The reflectance spectra reveal the nature of

semiconductivities with a large energy gap for compounds 1–4.

References :

- (1) J. H. Liao, J. S. Juang and Y. C. Lai, Cryst. Growth Des. 2006, 6, 354;
- (2) Y. Xia, P. F. Wu, Y. G. Wei, Y. Wang and H. Y. Guo, Cryst. Growth Des. 2006, 6, 253;
- (3) L. J. Zhang, Y. G. Wei, C. C. Wang, H. Y. Guo and P. Wang, J. Solid State Chem. 2004, 177,

3433.



Figure S15. UV-Vis diffuse reflectance spectra of K-M functions versus energy (eV) of the compounds 1–4



Figure S16. SPS and EISPS of the compound $Na_{10}[H_2W_{12}O_{42}] \cdot 20H_2O$ under zero, positive and negative electric fields.

The $Na_{10}[H_2W_{12}O_{42}] \cdot 20H_2O$ was synthesized according to the literature¹ and characterized by IR spectrum.

Reference:

(1) H. T. Evans Jr, O. W. Rollins, Acta Crystallogr. Sect. B. 1976, 32 1565.

Thermogravimetric analysis

In order to analyse the thermal stability of the compounds **1-4**, The thermal gravimetric analysis(TGA) were carried out for below 600°C. The TGA curves of **1-4** (Figure S17-S20) show weight loss of 14.33%, 13.11%, 14.78% and 13.75% in the range of 29-422°C, 20-427°C, 42-428°C and 38-424°C, respectively, which are assigned to all the lattice water molecules. They are in good agreement with the calculated value of 14.86%, 12.66%, 14.15% and 13.26% for the compounds **1-4**, respectively. The results of the TGA of the compounds **1-4** agree with those of structural determination.



Figure S17. The TG curve of 1.



Figure S18. The TG curve of 2.



Figure S19. The TG curve of 3.



Figure S20. The TG curve of 4.

Table S1. Selected bond lengths [Å] and bond angles (°) for the compound 1.

O(1)-W(4)	1.742(11)	O(21)-W(5)	1.752(11)	
O(1)-Ca(1)	2.388(11)	O(22)-W(6)	1.876(12)	
O(2)-W(4)	1.857(11)	O(22)-W(4)#2	2.234(12)	
O(2)-W(2)	1.976(11)	O(22)-W(3)	2.315(11)	
O(3)-W(4)	1.761(11)	OW1-Na(2)	2.414(14)	
O(3)-Ca(1)#1	2.423(11)	OW1-Na(1)	2.434(14)	
O(3)-Na(1)	2.482(13)	OW2-Na(1)	2.349(15)	
O(4)-W(1)	1.788(11)	OW2-Na(2)	2.396(14)	
O(4)-W(4)	2.217(11)	OW3-Na(1)#1	2.355(13)	
O(5)-W(1)	1.936(10)	OW3-Ca(1)	2.400(12)	

O(5)-W(5)#2	2.184(11)	OW4-Na(3)	2.353(14)
O(5)-W(3)#2	2.218(12)	OW4-Na(2)#4	2.385(16)
O(6)-W(1)	1.926(11)	OW5-Na(3)	2.462(19)
O(6)-W(6)	1.962(11)	OW5-Na(3)#5	2.546(17)
O(7)-W(2)	1.717(12)	OW6-Na(3)	2.648(16)
O(7)-Na(1)#1	2.425(14)	OW7-Na(3)	2.391(16)
O(8)-W(2)	1.850(12)	OW8-Ca(1)	2.394(13)
O(8)-W(1)#2	2.100(12)	OW9-Ca(1)	2.408(12)
O(9)-W(2)	1.900(11)	OW10-Na(1)	2.433(15)
O(9)-W(6)#2	2.031(11)	OW11-Na(2)	2.558(16)
O(10)-W(5)	1.856(12)	OW12-Na(2)	2.405(15)
O(10)-W(2)	1.934(11)	OW12-Na(3)#6	2.499(17)
O(11)-W(2)#2	2.225(11)	OW14-Ca(1)	2.394(13)
O(11)-W(6)	2.246(10)	Na(1)-OW3#1	2.355(13)
O(11)-W(1)	2.271(11)	Na(1)-O(7)#1	2.425(14)
O(12)-W(5)	1.723(12)	Na(2)-OW4#6	2.385(16)
O(13)-W(6)	1.769(11)	Na(3)-OW12#4	2.499(17)
O(13)-W(5)	2.232(10)	Na(3)-OW5#5	2.546(17)
O(14)-W(3)	1.903(11)	Ca(1)-O(3)#1	2.423(11)
O(14)-W(4)#2	1.966(10)	Ca(1)-O(19)#7	2.442(11)
O(15)-W(3)	1.721(12)	W(1)-O(8)#2	2.100(12)
O(16)-W(3)	1.712(12)	W(2)-O(11)#2	2.225(11)
O(17)-W(3)	1.916(11)	W(3)-O(5)#2	2.218(12)
O(17)-W(5)	1.959(12)	W(4)-O(14)#2	1.966(10)
O(19)-W(6)	1.745(11)	W(4)-O(22)#2	2.234(12)
O(19)-Ca(1)#3	2.442(11)	W(5)-O(5)#2	2.184(11)
O(20)-W(1)	1.709(12)	W(6)-O(9)#2	2.031(11)
O(20)-Na(2)	2.446(14)	W(4)-O(1)-Ca(1)	159.7(6)
W(4)-O(2)-W(2)	148.0(7)	W(1)-O(4)-W(4)	140.5(6)
W(4)-O(3)-Ca(1)#1	132.2(6)	W(1)-O(5)-W(5)#2	138.1(7)
W(4)-O(3)-Na(1)	134.0(6)	W(1)-O(5)-W(3)#2	124.9(6)
Ca(1)#1-O(3)-Na(1)	93.8(4)	W(5)#2-O(5)-W(3)#2	95.9(4)
W(1)-O(6)-W(6)	121.2(5)	OW3#1-Na(1)-Ca(1)#1	41.6(3)
W(2)-O(7)-Na(1)#1	132.2(5)	O(7)#1-Na(1)-Ca(1)#1	108.1(3)
W(2)-O(8)-W(1)#2	115.0(5)	OW10-Na(1)-Ca(1)#1	121.8(4)
W(2)-O(9)-W(6)#2	117.0(5)	OW1-Na(1)-Ca(1)#1	65.6(3)
W(5)-O(10)-W(2)	149.5(7)	O(3)-Na(1)-Ca(1)#1	42.5(3)
W(2)#2-O(11)-W(6)	97.1(4)	Na(2)-Na(1)-Ca(1)#1	107.1(2)
W(2)#2-O(11)-W(1)	95.8(4)	OW4#6-Na(2)-OW2	158.3(6)
W(6)-O(11)-W(1)	97.2(4)	OW4#6-Na(2)-OW12	89.4(5)
W(6)-O(13)-W(5)	138.4(6)	OW2-Na(2)-OW12	94.9(5)
W(3)-O(14)-W(4)#2	118.2(5)	OW4#6-Na(2)-OW1	97.4(5)
W(3)-O(17)-W(5)	115.0(5)	OW2-Na(2)-OW1	85.2(5)
W(6)-O(19)-Ca(1)#3	150.8(7)	OW12-Na(2)-OW1	161.5(6)

W(1)-O(20)-Na(2)	159.2(7)	OW4#6-Na(2)-O(20)	78.1(5)
W(6)-O(22)-W(4)#2	136.9(6)	OW2-Na(2)-O(20)	80.4(5)
W(6)-O(22)-W(3)	127.8(6)	OW12-Na(2)-O(20)	109.5(5)
W(4)#2-O(22)-W(3)	93.7(4)	OW1-Na(2)-O(20)	88.8(5)
Na(2)-OW1-Na(1)	90.3(5)	OW4#6-Na(2)-OW11	97.7(5)
Na(1)-OW2-Na(2)	92.9(5)	OW2-Na(2)-OW11	104.0(6)
Na(1)#1-OW3-Ca(1)	97.7(5)	OW12-Na(2)-OW11	79.3(5)
Na(3)-OW4-Na(2)#4	93.4(5)	OW1-Na(2)-OW11	82.8(5)
Na(3)-OW5-Na(3)#5	89.6(6)	O(20)-Na(2)-OW11	170.1(5)
Na(2)-OW12-Na(3)#6	89.3(5)	OW4#6-Na(2)-Na(1)	142.3(4)
OW2-Na(1)-OW3#1	167.8(6)	OW2-Na(2)-Na(1)	43.0(4)
OW2-Na(1)-O(7)#1	101.8(5)	OW12-Na(2)-Na(1)	127.2(5)
OW3#1-Na(1)-O(7)#1	90.4(5)	OW1-Na(2)-Na(1)	45.1(3)
OW2-Na(1)-OW10	95.9(5)	O(20)-Na(2)-Na(1)	95.1(4)
OW3#1-Na(1)-OW10	85.4(5)	OW11-Na(2)-Na(1)	82.7(4)
O(7)#1-Na(1)-OW10	90.1(5)	OW4#6-Na(2)-Na(3)#6	43.0(3)
OW2-Na(1)-OW1	85.8(5)	OW2-Na(2)-Na(3)#6	136.2(4)
OW3#1-Na(1)-OW1	82.1(5)	OW12-Na(2)-Na(3)#6	46.5(4)
O(7)#1-Na(1)-OW1	172.4(5)	OW1-Na(2)-Na(3)#6	138.3(4)
OW10-Na(1)-OW1	90.0(5)	O(20)-Na(2)-Na(3)#6	93.0(4)
OW2-Na(1)-O(3)	95.8(5)	OW11-Na(2)-Na(3)#6	89.8(4)
OW3#1-Na(1)-O(3)	80.9(4)	Na(1)-Na(2)-Na(3)#6	171.4(3)
O(7)#1-Na(1)-O(3)	98.2(4)	OW4-Na(3)-OW7	167.8(6)
OW10-Na(1)-O(3)	164.0(5)	OW4-Na(3)-OW5	83.8(6)
OW1-Na(1)-O(3)	80.0(4)	OW7-Na(3)-OW5	103.4(6)
OW2-Na(1)-Na(2)	44.1(3)	OW4-Na(3)-OW12#4	87.9(5)
OW3#1-Na(1)-Na(2)	124.6(4)	OW7-Na(3)-OW12#4	82.8(5)
O(7)#1-Na(1)-Na(2)	142.8(4)	OW5-Na(3)-OW12#4	165.0(6)
OW10-Na(1)-Na(2)	81.4(4)	OW4-Na(3)-OW5#5	78.4(5)
OW1-Na(1)-Na(2)	44.6(3)	OW7-Na(3)-OW5#5	111.0(5)
O(3)-Na(1)-Na(2)	99.6(4)	OW5-Na(3)-OW5#5	90.4(6)
OW2-Na(1)-Ca(1)#1	130.7(4)	OW12#4-Na(3)-OW5#5	100.2(6)
OW4-Na(3)-OW6	81.8(5)	O(3)#1-Ca(1)-Na(1)#1	43.7(3)
OW7-Na(3)-OW6	89.0(5)	O(19)#7-Ca(1)-Na(1)#1	97.6(3)
OW5-Na(3)-OW6	84.6(6)	O(1)-Ca(1)-W(4)#1	70.9(3)
OW12#4-Na(3)-OW6	81.8(5)	OW14-Ca(1)-W(4)#1	68.7(3)
OW5#5-Na(3)-OW6	160.0(5)	OW8-Ca(1)-W(4)#1	98.1(4)
OW4-Na(3)-Na(2)#4	43.7(4)	OW3-Ca(1)-W(4)#1	100.3(3)
OW7-Na(3)-Na(2)#4	126.3(5)	OW9-Ca(1)-W(4)#1	152.2(3)
OW5-Na(3)-Na(2)#4	125.9(5)	O(3)#1-Ca(1)-W(4)#1	19.9(3)
OW12#4-Na(3)-Na(2)#4	44.2(4)	O(19)#7-Ca(1)-W(4)#1	132.6(3)
OW5#5-Na(3)-Na(2)#4	90.4(4)	Na(1)#1-Ca(1)-W(4)#1	63.63(13)
OW6-Na(3)-Na(2)#4	77.1(4)	O(20)-W(1)-O(4)	103.1(6)
OW4-Na(3)-Na(3)#5	77.3(4)	O(20)-W(1)-O(6)	100.8(5)

OW7-Na(3)-Na(3)#5	114.8(5)	O(4)-W(1)-O(6)	92.4(5)
OW5-Na(3)-Na(3)#5	46.2(4)	O(20)-W(1)-O(5)	100.9(5)
OW12#4-Na(3)-Na(3)#5	143.3(6)	O(4)-W(1)-O(5)	93.9(5)
OW5#5-Na(3)-Na(3)#5	44.2(4)	O(6)-W(1)-O(5)	155.3(5)
OW6-Na(3)-Na(3)#5	127.7(5)	O(20)-W(1)-O(8)#2	95.8(5)
Na(2)#4-Na(3)-Na(3)#5	114.5(4)	O(4)-W(1)-O(8)#2	161.0(5)
O(1)-Ca(1)-OW14	131.7(4)	O(6)-W(1)-O(8)#2	83.0(5)
O(1)-Ca(1)-OW8	83.1(4)	O(5)-W(1)-O(8)#2	83.3(5)
OW14-Ca(1)-OW8	77.6(5)	O(20)-W(1)-O(11)	165.1(5)
O(1)-Ca(1)-OW3	90.4(4)	O(4)-W(1)-O(11)	89.4(4)
OW14-Ca(1)-OW3	121.7(4)	O(6)-W(1)-O(11)	70.2(4)
OW8-Ca(1)-OW3	157.2(5)	O(5)-W(1)-O(11)	86.0(4)
O(1)-Ca(1)-OW9	81.3(4)	O(8)#2-W(1)-O(11)	71.8(4)
OW14-Ca(1)-OW9	135.9(4)	O(7)-W(2)-O(8)	103.8(5)
OW8-Ca(1)-OW9	79.5(5)	O(7)-W(2)-O(9)	103.7(5)
OW3-Ca(1)-OW9	77.9(4)	O(8)-W(2)-O(9)	91.8(5)
O(1)-Ca(1)-O(3)#1	76.5(4)	O(7)-W(2)-O(10)	101.7(5)
OW14-Ca(1)-O(3)#1	74.6(4)	O(8)-W(2)-O(10)	86.7(5)
OW8-Ca(1)-O(3)#1	118.0(4)	O(9)-W(2)-O(10)	154.1(5)
OW3-Ca(1)-O(3)#1	81.2(4)	O(7)-W(2)-O(2)	99.2(5)
OW9-Ca(1)-O(3)#1	149.3(5)	O(8)-W(2)-O(2)	156.7(5)
O(1)-Ca(1)-O(19)#7	156.5(4)	O(9)-W(2)-O(2)	86.2(4)
OW14-Ca(1)-O(19)#7	68.5(4)	O(10)-W(2)-O(2)	85.1(4)
OW8-Ca(1)-O(19)#7	91.8(4)	O(7)-W(2)-O(11)#2	177.8(4)
OW3-Ca(1)-O(19)#7	85.4(4)	O(8)-W(2)-O(11)#2	77.4(4)
OW9-Ca(1)-O(19)#7	75.2(4)	O(9)-W(2)-O(11)#2	74.3(4)
O(3)#1-Ca(1)-O(19)#7	125.4(4)	O(10)-W(2)-O(11)#2	80.1(4)
O(1)-Ca(1)-Na(1)#1	94.2(3)	O(2)-W(2)-O(11)#2	79.7(5)
OW14-Ca(1)-Na(1)#1	90.8(4)	O(16)-W(3)-O(15)	101.8(6)
OW8-Ca(1)-Na(1)#1	161.2(4)	O(16)-W(3)-O(14)	97.8(5)
OW3-Ca(1)-Na(1)#1	40.7(3)	O(15)-W(3)-O(14)	99.1(5)
OW9-Ca(1)-Na(1)#1	118.5(3)	O(16)-W(3)-O(17)	95.6(5)
O(10)-W(5)-O(13)	83.6(4)	O(3)-W(4)-O(2)	99.0(5)
O(17)-W(5)-O(13)	78.7(4)	O(1)-W(4)-O(14)#2	94.9(5)
O(5)#2-W(5)-O(13)	76.9(4)	O(3)-W(4)-O(14)#2	94.7(5)
O(19)-W(6)-O(13)	102.7(5)	O(2)-W(4)-O(14)#2	156.7(5)
O(19)-W(6)-O(22)	103.2(5)	O(1)-W(4)-O(4)	164.8(5)
O(13)-W(6)-O(22)	94.9(5)	O(3)-W(4)-O(4)	90.6(5)
O(19)-W(6)-O(6)	96.4(5)	O(2)-W(4)-O(4)	84.2(5)
O(13)-W(6)-O(6)	92.4(5)	O(14)#2-W(4)-O(4)	77.0(4)
O(22)-W(6)-O(6)	157.0(5)	O(1)-W(4)-O(22)#2	89.8(5)
O(19)-W(6)-O(9)#2	94.8(5)	O(3)-W(4)-O(22)#2	163.7(5)
O(13)-W(6)-O(9)#2	162.0(4)	O(2)-W(4)-O(22)#2	88.5(5)
O(22)-W(6)-O(9)#2	84.9(5)	O(14)#2-W(4)-O(22)#2	73.8(4)

O(6)-W(6)-O(9)#2	81.6(5)	O(4)-W(4)-O(22)#2	75.7(4)	
O(19)-W(6)-O(11)	161.7(4)	O(1)-W(4)-Ca(1)#1	109.0(4)	
O(13)-W(6)-O(11)	90.5(4)	O(3)-W(4)-Ca(1)#1	27.9(3)	
O(22)-W(6)-O(11)	88.0(4)	O(2)-W(4)-Ca(1)#1	71.2(4)	
O(6)-W(6)-O(11)	70.1(4)	O(14)#2-W(4)-Ca(1)#1	120.3(3)	
O(9)#2-W(6)-O(11)	71.5(4)	O(4)-W(4)-Ca(1)#1	86.2(3)	
O(15)-W(3)-O(17)	101.8(5)	O(22)#2-W(4)-Ca(1)#1	154.2(3)	
O(14)-W(3)-O(17)	152.3(5)	O(12)-W(5)-O(21)	102.9(6)	
O(16)-W(3)-O(5)#2	163.6(5)	O(12)-W(5)-O(10)	98.6(5)	
O(15)-W(3)-O(5)#2	92.6(5)	O(21)-W(5)-O(10)	99.3(5)	
O(14)-W(3)-O(5)#2	87.4(4)	O(12)-W(5)-O(17)	96.3(5)	
O(17)-W(3)-O(5)#2	73.7(4)	O(21)-W(5)-O(17)	95.0(5)	
O(16)-W(3)-O(22)	89.4(5)	O(10)-W(5)-O(17)	156.5(5)	
O(15)-W(3)-O(22)	167.3(5)	O(12)-W(5)-O(5)#2	93.1(5)	
O(14)-W(3)-O(22)	73.1(4)	O(21)-W(5)-O(5)#2	161.5(5)	
O(17)-W(3)-O(22)	82.9(4)	O(10)-W(5)-O(5)#2	87.4(5)	
O(5)#2-W(3)-O(22)	77.2(4)	O(17)-W(5)-O(5)#2	73.7(4)	
O(1)-W(4)-O(3)	102.9(5)	O(12)-W(5)-O(13)	169.6(5)	
O(1)-W(4)-O(2)	100.1(5)	O(21)-W(5)-O(13)	86.7(5)	

Symmetry code for 1: #1 -x+2, -y+1, -z; #2 -x+2, -y, -z; #3 x+1/2, -y+1/2, z+1/2; #4 x+1/2, -y+1/2,

z-1/2; #5 -x+3, -y+1, -z; #6 x-1/2, -y+1/2, z+1/2; #7 x-1/2, -y+1/2, z-1/2.

W(1)-O(21)	1.735(9)	W(6)-O(9)	1.682(12)
W(1)-O(18)	1.791(8)	W(6)-O(15)	1.773(9)
W(1)-O(1)	1.927(10)	W(6)-O(7)	1.902(9)
W(1)-O(10)	1.954(9)	W(6)-O(10)	1.941(8)
W(1)-O(3)	2.105(9)	W(6)-O(11)	2.080(9)
W(1)-O(6)	2.236(8)	W(6)-O(6)	2.242(9)
W(2)-O(19)	1.709(12)	Sr(1)-O(17)	2.518(11)
W(2)-O(5)	1.745(9)	Sr(1)-O(2W)	2.567(13)
W(2)-O(16)	1.871(10)	Sr(1)-O(12)#2	2.569(10)
W(2)-O(8)	1.952(10)	Sr(1)-O(9)#3	2.573(12)
W(2)-O(15)#1	2.181(8)	Sr(1)-O(5W)	2.579(12)
W(2)-O(1)	2.230(10)	Sr(1)-O(4W)	2.620(12)
W(3)-O(20)	1.734(10)	Sr(1)-O(1W)	2.647(13)
W(3)-O(3)	1.858(9)	Sr(1)-O(3W)	2.728(12)
W(3)-O(11)	1.867(10)	Sr(2)-O(20)#4	2.568(10)
W(3)-O(14)#1	1.941(9)	Sr(2)-O(6W)	2.568(12)

Table S2. Selected bond lengths [Å] and bond angles (°) for the compound **2**.

W(3)-O(16)	1.960(11)	Sr(2)-O(7W)	2.576(14)
W(3)-O(6)	2.276(8)	Sr(2)-O(8W)	2.598(14)
W(4)-O(13)	1.716(10)	Sr(2)-O(5)	2.605(10)
W(4)-O(4)	1.723(10)	Sr(2)-O(10W)	2.630(11)
W(4)-O(2)	1.877(10)	Sr(2)-O(13)	2.641(11)
W(4)-O(8)	1.917(10)	Sr(2)-O(9W)	2.668(15)
W(4)-O(1)	2.259(10)	O(7)-W(5)#1	2.197(10)
W(4)-O(7)#1	2.283(8)	O(7)-W(4)#1	2.283(8)
W(5)-O(12)	1.718(11)	O(9)-Sr(1)#5	2.573(12)
W(5)-O(17)	1.747(10)	O(12)-Sr(1)#2	2.569(10)
W(5)-O(14)	1.888(9)	O(14)-W(3)#1	1.941(9)
W(5)-O(2)	2.017(8)	O(15)-W(2)#1	2.181(8)
W(5)-O(7)#1	2.197(10)	O(20)-Sr(2)#6	2.568(10)
W(5)-O(18)	2.226(9)	O(21)-W(1)-O(18)	102.1(4)
O(21)-W(1)-O(1)	101.7(5)	O(10)-W(1)-O(6)	70.5(3)
O(18)-W(1)-O(1)	96.2(4)	O(3)-W(1)-O(6)	72.8(3)
O(21)-W(1)-O(10)	98.7(5)	O(19)-W(2)-O(5)	102.4(5)
O(18)-W(1)-O(10)	91.4(4)	O(19)-W(2)-O(16)	98.8(5)
O(1)-W(1)-O(10)	156.1(4)	O(5)-W(2)-O(16)	97.6(4)
O(21)-W(1)-O(3)	95.2(4)	O(19)-W(2)-O(8)	97.3(5)
O(18)-W(1)-O(3)	162.4(4)	O(5)-W(2)-O(8)	94.6(4)
O(1)-W(1)-O(3)	83.4(4)	O(16)-W(2)-O(8)	157.2(4)
O(10)-W(1)-O(3)	82.6(4)	O(19)-W(2)-O(15)#1	90.6(4)
O(21)-W(1)-O(6)	164.5(4)	O(5)-W(2)-O(15)#1	165.8(4)
O(18)-W(1)-O(6)	89.6(3)	O(16)-W(2)-O(15)#1	86.1(4)
O(1)-W(1)-O(6)	86.9(3)	O(8)-W(2)-O(15)#1	77.8(3)
O(19)-W(2)-O(1)	166.2(4)	O(2)-W(5)-O(7)#1	73.0(3)
O(5)-W(2)-O(1)	88.9(4)	O(12)-W(5)-O(18)	166.1(4)
O(16)-W(2)-O(1)	87.4(4)	O(17)-W(5)-O(18)	88.9(4)
O(8)-W(2)-O(1)	73.6(4)	O(14)-W(5)-O(18)	84.9(4)
O(15)#1-W(2)-O(1)	77.5(3)	O(2)-W(5)-O(18)	78.2(3)
O(20)-W(3)-O(3)	100.1(4)	O(7)#1-W(5)-O(18)	77.0(3)
O(20)-W(3)-O(11)	104.3(4)	O(9)-W(6)-O(15)	104.2(5)
O(3)-W(3)-O(11)	93.2(4)	O(9)-W(6)-O(7)	101.8(4)
O(20)-W(3)-O(14)#1	102.0(4)	O(15)-W(6)-O(7)	94.9(4)
O(3)-W(3)-O(14)#1	157.0(4)	O(9)-W(6)-O(10)	97.9(4)
O(11)-W(3)-O(14)#1	87.6(4)	O(15)-W(6)-O(10)	93.0(4)
O(20)-W(3)-O(16)	99.0(5)	O(7)-W(6)-O(10)	156.3(4)
O(3)-W(3)-O(16)	86.1(4)	O(9)-W(6)-O(11)	93.0(4)
O(11)-W(3)-O(16)	156.5(4)	O(15)-W(6)-O(11)	162.7(5)
O(14)#1-W(3)-O(16)	84.2(4)	O(7)-W(6)-O(11)	83.2(4)
O(20)-W(3)-O(6)	176.5(4)	O(10)-W(6)-O(11)	82.7(3)
O(3)-W(3)-O(6)	76.4(3)	O(9)-W(6)-O(6)	162.7(3)
O(11)-W(3)-O(6)	76.2(4)	O(15)-W(6)-O(6)	89.7(4)

O(14)#1-W(3)-O(6)	81.5(3)	O(7)-W(6)-O(6)	87.1(4)
O(16)-W(3)-O(6)	80.8(3)	O(10)-W(6)-O(6)	70.6(3)
O(13)-W(4)-O(4)	102.6(5)	O(11)-W(6)-O(6)	73.1(4)
O(13)-W(4)-O(2)	96.7(5)	O(17)-Sr(1)-O(2W)	145.8(3)
O(4)-W(4)-O(2)	100.3(5)	O(17)-Sr(1)-O(12)#2	75.4(3)
O(13)-W(4)-O(8)	100.8(4)	O(2W)-Sr(1)-O(12)#2	75.5(4)
O(4)-W(4)-O(8)	96.6(4)	O(17)-Sr(1)-O(9)#3	141.2(3)
O(2)-W(4)-O(8)	152.4(4)	O(2W)-Sr(1)-O(9)#3	68.9(3)
O(13)-W(4)-O(1)	88.1(4)	O(12)#2-Sr(1)-O(9)#3	143.3(3)
O(4)-W(4)-O(1)	166.8(4)	O(17)-Sr(1)-O(5W)	112.0(6)
O(2)-W(4)-O(1)	85.9(4)	O(2W)-Sr(1)-O(5W)	81.0(7)
O(8)-W(4)-O(1)	73.5(4)	O(12)#2-Sr(1)-O(5W)	82.0(4)
O(13)-W(4)-O(7)#1	162.7(5)	O(9)#3-Sr(1)-O(5W)	83.9(5)
O(4)-W(4)-O(7)#1	93.3(4)	O(17)-Sr(1)-O(4W)	83.2(4)
O(2)-W(4)-O(7)#1	73.5(4)	O(2W)-Sr(1)-O(4W)	73.7(5)
O(8)-W(4)-O(7)#1	83.9(3)	O(12)#2-Sr(1)-O(4W)	78.3(4)
O(1)-W(4)-O(7)#1	77.2(3)	O(9)#3-Sr(1)-O(4W)	99.5(4)
O(12)-W(5)-O(17)	103.7(5)	O(5W)-Sr(1)-O(4W)	151.1(6)
O(12)-W(5)-O(14)	98.4(4)	O(17)-Sr(1)-O(1W)	75.7(4)
O(17)-W(5)-O(14)	100.5(4)	O(2W)-Sr(1)-O(1W)	118.2(5)
O(12)-W(5)-O(2)	94.8(4)	O(12)#2-Sr(1)-O(1W)	139.8(4)
O(17)-W(5)-O(2)	93.7(4)	O(9)#3-Sr(1)-O(1W)	68.9(4)
O(14)-W(5)-O(2)	157.6(4)	O(5W)-Sr(1)-O(1W)	135.1(5)
O(12)-W(5)-O(7)#1	89.5(4)	O(4W)-Sr(1)-O(1W)	71.1(4)
O(17)-W(5)-O(7)#1	162.2(3)	O(17)-Sr(1)-O(3W)	81.7(4)
O(14)-W(5)-O(7)#1	89.1(4)	O(2W)-Sr(1)-O(3W)	132.2(5)
O(12)#2-Sr(1)-O(3W)	135.2(4)	O(8W)-Sr(2)-O(9W)	85.0(5)
O(9)#3-Sr(1)-O(3W)	69.8(4)	O(5)-Sr(2)-O(9W)	126.6(3)
O(5W)-Sr(1)-O(3W)	71.7(6)	O(10W)-Sr(2)-O(9W)	72.6(4)
O(4W)-Sr(1)-O(3W)	136.5(5)	O(13)-Sr(2)-O(9W)	72.8(4)
O(1W)-Sr(1)-O(3W)	65.7(5)	W(1)-O(1)-W(2)	137.2(5)
O(20)#4-Sr(2)-O(6W)	101.7(4)	W(1)-O(1)-W(4)	126.1(4)
O(20)#4-Sr(2)-O(7W)	68.9(4)	W(2)-O(1)-W(4)	94.5(4)
O(6W)-Sr(2)-O(7W)	73.1(5)	W(4)-O(2)-W(5)	116.7(4)
O(20)#4-Sr(2)-O(8W)	137.4(4)	W(3)-O(3)-W(1)	115.1(4)
O(6W)-Sr(2)-O(8W)	74.4(4)	W(2)-O(5)-Sr(2)	139.1(6)
O(7W)-Sr(2)-O(8W)	142.1(5)	W(1)-O(6)-W(6)	97.7(3)
O(20)#4-Sr(2)-O(5)	147.7(3)	W(1)-O(6)-W(3)	95.8(3)
O(6W)-Sr(2)-O(5)	76.1(3)	W(6)-O(6)-W(3)	95.3(3)
O(7W)-Sr(2)-O(5)	79.8(4)	W(6)-O(7)-W(5)#1	138.3(5)
O(8W)-Sr(2)-O(5)	73.9(4)	W(6)-O(7)-W(4)#1	125.4(5)
O(20)#4-Sr(2)-O(10W)	71.3(4)	W(5)#1-O(7)-W(4)#1	95.5(3)
O(6W)-Sr(2)-O(10W)	72.0(4)	W(4)-O(8)-W(2)	116.9(5)
O(7W)-Sr(2)-O(10W)	119.0(5)	W(6)-O(9)-Sr(1)#5	155.5(5)

O(8W)-Sr(2)-O(10W)	67.2(4)	W(6)-O(10)-W(1)	120.0(4)	
O(5)-Sr(2)-O(10W)	134.7(4)	W(3)-O(11)-W(6)	115.4(5)	
O(20)#4-Sr(2)-O(13)	89.3(3)	W(5)-O(12)-Sr(1)#2	161.8(5)	
O(6W)-Sr(2)-O(13)	143.4(4)	W(4)-O(13)-Sr(2)	137.8(5)	
O(7W)-Sr(2)-O(13)	78.8(4)	W(5)-O(14)-W(3)#1	145.5(6)	
O(8W)-Sr(2)-O(13)	119.5(3)	W(6)-O(15)-W(2)#1	139.1(5)	
O(5)-Sr(2)-O(13)	76.3(3)	W(2)-O(16)-W(3)	149.1(6)	
O(10W)-Sr(2)-O(13)	143.9(4)	W(5)-O(17)-Sr(1)	147.7(4)	
O(20)#4-Sr(2)-O(9W)	73.8(4)	W(1)-O(18)-W(5)	139.1(5)	
O(6W)-Sr(2)-O(9W)	143.8(4)	W(3)-O(20)-Sr(2)#6	165.3(6)	
O(7W)-Sr(2)-O(9W)	132.8(5)			

Symmetry code for **2**: #1 -x+1, -y, -z; #2 -x+1, -y+1, -z; #3 -x+1/2, y+1/2, -z-1/2; #4 -x+1/2, y+1/2,

-z+1/2; #5 -x+1/2, y-1/2, -z-1/2; #6 -x+1/2, y-1/2, -z+1/2.

O(1)-W(1)	1.813(10)	O(11)-W(5)	1.863(11)	
O(1)-W(6)	2.156(10)	O(11)-W(2)	2.098(11)	
O(2)-W(4)	1.757(13)	O(10W)-Sr(2)	2.725(14)	
O(2)-Na(1)	2.442(15)	O(10W)-Sr(1)	2.803(14)	
O(1W)-Na(1)#1	2.433(15)	O(12)-W(4)	1.717(11)	
O(1W)-Sr(1)	2.709(13)	O(13)-W(6)	1.882(11)	
O(3)-W(2)	1.796(11)	O(13)-W(5)	1.960(11)	
O(3)-W(3)	2.209(11)	O(14)-W(3)	1.915(10)	
O(2W)-Na(1)#1	2.478(17)	O(14)-W(5)#3	1.933(10)	
O(2W)-Sr(1)	2.631(13)	O(15)-W(6)	1.740(12)	
O(4)-W(1)	1.899(11)	O(15)-Na(1)	2.388(13)	
O(4)-W(3)	2.209(12)	O(16)-W(5)	1.858(10)	
O(4)-W(4)	2.279(10)	O(16)-W(1)#3	2.067(10)	
O(3W)-Sr(1)	2.671(16)	O(17)-W(2)	1.730(12)	
O(5)-W(3)	1.730(12)	O(17)-Na(1)#1	2.266(14)	
O(5)-Sr(2)#2	2.551(13)	O(18)-W(2)	1.932(11)	
O(4W)-Sr(1)	2.594(14)	O(18)-W(1)#3	1.960(10)	
O(6)-W(5)	2.232(12)	O(19)-W(3)	1.726(12)	
O(6)-W(1)#3	2.249(12)	O(19)-Sr(1)	2.610(12)	
O(6)-W(2)	2.284(11)	O(20)-W(5)	1.731(11)	
O(5W)-Sr(1)	2.599(12)	O(21)-W(2)	1.919(11)	
O(5W)-Sr(2)	2.600(13)	O(21)-W(6)	2.241(11)	
O(7)-W(1)	1.748(12)	O(21)-W(4)	2.292(11)	
O(7)-Sr(2)#4	2.484(13)	O(21)-Na(1)	2.773(13)	
O(6W)-Sr(1)	2.674(14)	Sr(1)-O(9)#5	2.701(13)	

Table S3. Selected bond lengths [Å] and bond angles (°) for the compound **3**.

O(6W)-Sr(2)	2.735(13)	Sr(2)-O(7)#5	2.484(13)
O(8)-W(4)	1.886(12)	Sr(2)-O(5)#6	2.551(13)
O(8)-W(6)	1.982(11)	W(1)-O(18)#3	1.960(10)
O(7W)-Sr(2)	2.719(18)	W(1)-O(16)#3	2.067(10)
O(9)-W(6)	1.729(13)	W(1)-O(6)#3	2.249(12)
O(9)-Sr(1)#4	2.701(13)	W(5)-O(14)#3	1.933(10)
O(8W)-Sr(2)	2.650(17)	Na(1)-O(17)#1	2.266(14)
O(10)-W(4)	1.918(12)	Na(1)-O(1W)#1	2.433(15)
O(10)-W(3)	1.958(11)	Na(1)-O(2W)#1	2.478(17)
O(9W)-Sr(2)	2.560(16)	W(1)-O(1)-W(6)	138.2(6)
W(4)-O(2)-Na(1)	115.7(7)	W(3)-O(5)-Sr(2)#2	151.2(6)
Na(1)#1-O(1W)-Sr(1)	101.0(5)	W(5)-O(6)-W(1)#3	96.1(5)
W(2)-O(3)-W(3)	139.3(6)	W(5)-O(6)-W(2)	95.6(4)
Na(1)#1-O(2W)-Sr(1)	102.1(5)	W(1)#3-O(6)-W(2)	96.4(5)
W(1)-O(4)-W(3)	138.2(6)	Sr(1)-O(5W)-Sr(2)	103.0(4)
W(1)-O(4)-W(4)	126.0(6)	W(1)-O(7)-Sr(2)#4	152.5(7)
W(3)-O(4)-W(4)	94.9(4)	Sr(1)-O(6W)-Sr(2)	97.6(4)
W(4)-O(8)-W(6)	117.9(5)	O(6W)-Sr(1)-O(1W)	137.0(4)
W(6)-O(9)-Sr(1)#4	149.0(6)	O(9)#5-Sr(1)-O(1W)	66.4(4)
W(4)-O(10)-W(3)	117.1(6)	O(4W)-Sr(1)-O(10W)	135.4(4)
W(5)-O(11)-W(2)	115.2(5)	O(5W)-Sr(1)-O(10W)	67.8(4)
Sr(2)-O(10W)-Sr(1)	94.8(4)	O(19)-Sr(1)-O(10W)	67.0(4)
W(6)-O(13)-W(5)	146.6(7)	O(2W)-Sr(1)-O(10W)	109.8(4)
W(3)-O(14)-W(5)#3	146.3(6)	O(3W)-Sr(1)-O(10W)	69.6(4)
W(6)-O(15)-Na(1)	117.2(6)	O(6W)-Sr(1)-O(10W)	65.4(4)
W(5)-O(16)-W(1)#3	116.2(5)	O(9)#5-Sr(1)-O(10W)	124.7(4)
W(2)-O(17)-Na(1)#1	153.9(7)	O(1W)-Sr(1)-O(10W)	136.5(4)
W(2)-O(18)-W(1)#3	120.5(6)	O(4W)-Sr(1)-Na(1)#1	68.3(4)
W(3)-O(19)-Sr(1)	153.2(6)	O(5W)-Sr(1)-Na(1)#1	120.1(3)
W(2)-O(21)-W(6)	138.7(5)	O(19)-Sr(1)-Na(1)#1	80.7(3)
W(2)-O(21)-W(4)	124.9(5)	O(2W)-Sr(1)-Na(1)#1	37.6(3)
W(6)-O(21)-W(4)	94.0(4)	O(3W)-Sr(1)-Na(1)#1	103.4(3)
W(2)-O(21)-Na(1)	103.2(5)	O(6W)-Sr(1)-Na(1)#1	151.2(3)
W(6)-O(21)-Na(1)	89.1(4)	O(9)#5-Sr(1)-Na(1)#1	88.9(3)
W(4)-O(21)-Na(1)	89.2(4)	O(1W)-Sr(1)-Na(1)#1	36.9(3)
O(4W)-Sr(1)-O(5W)	135.1(5)	O(10W)-Sr(1)-Na(1)#1	142.2(3)
O(4W)-Sr(1)-O(19)	146.9(5)	O(4W)-Sr(1)-Sr(2)	125.8(4)
O(5W)-Sr(1)-O(19)	70.6(4)	O(5W)-Sr(1)-Sr(2)	38.5(3)
O(4W)-Sr(1)-O(2W)	77.5(5)	O(19)-Sr(1)-Sr(2)	87.3(3)
O(5W)-Sr(1)-O(2W)	138.4(4)	O(2W)-Sr(1)-Sr(2)	150.8(3)
O(19)-Sr(1)-O(2W)	70.8(4)	O(3W)-Sr(1)-Sr(2)	97.0(3)
O(4W)-Sr(1)-O(3W)	71.5(4)	O(6W)-Sr(1)-Sr(2)	41.8(3)
O(5W)-Sr(1)-O(3W)	134.4(4)	O(9)#5-Sr(1)-Sr(2)	82.9(3)
O(19)-Sr(1)-O(3W)	106.4(5)	O(1W)-Sr(1)-Sr(2)	122.2(3)

O(2W)-Sr(1)-O(3W)	72.2(5)	O(10W)-Sr(1)-Sr(2)	41.9(3)
O(4W)-Sr(1)-O(6W)	84.8(5)	Na(1)#1-Sr(1)-Sr(2)	158.48(13)
O(5W)-Sr(1)-O(6W)	72.3(4)	O(7)#5-Sr(2)-O(5)#6	95.2(4)
O(19)-Sr(1)-O(6W)	127.6(4)	O(7)#5-Sr(2)-O(9W)	145.8(5)
O(2W)-Sr(1)-O(6W)	147.1(4)	O(5)#6-Sr(2)-O(9W)	104.3(5)
O(3W)-Sr(1)-O(6W)	76.0(5)	O(7)#5-Sr(2)-O(5W)	87.0(4)
O(4W)-Sr(1)-O(9)#5	68.8(4)	O(5)#6-Sr(2)-O(5W)	144.3(4)
O(5W)-Sr(1)-O(9)#5	67.4(4)	O(9W)-Sr(2)-O(5W)	92.8(5)
O(19)-Sr(1)-O(9)#5	123.4(4)	O(7)#5-Sr(2)-O(8W)	74.1(5)
O(2W)-Sr(1)-O(9)#5	125.1(4)	O(5)#6-Sr(2)-O(8W)	79.0(5)
O(3W)-Sr(1)-O(9)#5	130.1(5)	O(9W)-Sr(2)-O(8W)	82.4(5)
O(6W)-Sr(1)-O(9)#5	71.4(4)	O(5W)-Sr(2)-O(8W)	135.0(5)
O(4W)-Sr(1)-O(1W)	88.0(4)	O(7)#5-Sr(2)-O(7W)	75.6(5)
O(5W)-Sr(1)-O(1W)	83.9(4)	O(5)#6-Sr(2)-O(7W)	147.9(5)
O(19)-Sr(1)-O(1W)	72.9(4)	O(9W)-Sr(2)-O(7W)	73.0(5)
O(2W)-Sr(1)-O(1W)	70.4(4)	O(5W)-Sr(2)-O(7W)	66.9(5)
O(3W)-Sr(1)-O(1W)	140.4(4)	O(8W)-Sr(2)-O(7W)	69.0(6)
O(21)-W(2)-O(11)	82.3(5)	O(7)#5-Sr(2)-O(10W)	135.5(4)
O(18)-W(2)-O(11)	81.9(5)	O(5)#6-Sr(2)-O(10W)	85.5(4)
O(17)-W(2)-O(6)	161.8(5)	O(9W)-Sr(2)-O(10W)	74.7(5)
O(3)-W(2)-O(6)	89.9(4)	O(5W)-Sr(2)-O(10W)	69.0(4)
O(21)-W(2)-O(6)	86.3(5)	O(8W)-Sr(2)-O(10W)	148.1(5)
O(18)-W(2)-O(6)	70.7(4)	O(7W)-Sr(2)-O(10W)	122.7(5)
O(11)-W(2)-O(6)	71.8(4)	O(7)#5-Sr(2)-O(6W)	71.5(4)
O(17)-W(2)-Na(1)	64.0(4)	O(5)#6-Sr(2)-O(6W)	75.7(4)
O(3)-W(2)-Na(1)	127.8(4)	O(9W)-Sr(2)-O(6W)	140.2(5)
O(21)-W(2)-Na(1)	46.6(4)	O(5W)-Sr(2)-O(6W)	71.3(4)
O(18)-W(2)-Na(1)	136.5(3)	O(8W)-Sr(2)-O(6W)	134.6(5)
O(11)-W(2)-Na(1)	62.2(3)	O(7W)-Sr(2)-O(6W)	127.3(5)
O(6)-W(2)-Na(1)	115.5(3)	O(10W)-Sr(2)-O(6W)	65.6(4)
O(19)-W(3)-O(5)	101.9(6)	O(7)#5-Sr(2)-Sr(1)	95.0(3)
O(19)-W(3)-O(14)	100.1(5)	O(5)#6-Sr(2)-Sr(1)	106.0(3)
O(5)-W(3)-O(14)	97.4(5)	O(9W)-Sr(2)-Sr(1)	105.8(4)
O(19)-W(3)-O(10)	93.8(5)	O(5W)-Sr(2)-Sr(1)	38.5(3)
O(5)-W(3)-O(10)	97.4(5)	O(8W)-Sr(2)-Sr(1)	168.5(4)
O(14)-W(3)-O(10)	157.2(5)	O(7W)-Sr(2)-Sr(1)	105.4(4)
O(19)-W(3)-O(4)	162.2(5)	O(10W)-Sr(2)-Sr(1)	43.3(3)
O(5)-W(3)-O(4)	92.5(5)	O(6W)-Sr(2)-Sr(1)	40.6(3)
O(14)-W(3)-O(4)	88.3(4)	O(7)-W(1)-O(1)	103.1(5)
O(10)-W(3)-O(4)	73.8(4)	O(7)-W(1)-O(4)	102.5(5)
O(19)-W(3)-O(3)	90.1(5)	O(1)-W(1)-O(4)	94.0(5)
O(5)-W(3)-O(3)	167.7(5)	O(7)-W(1)-O(18)#3	98.7(5)
O(14)-W(3)-O(3)	82.9(4)	O(1)-W(1)-O(18)#3	92.0(5)
O(10)-W(3)-O(3)	79.0(4)	O(4)-W(1)-O(18)#3	156.0(5)

O(4)-W(3)-O(3)	75.2(4)	O(7)-W(1)-O(16)#3	96.5(5)
O(12)-W(4)-O(2)	103.0(6)	O(1)-W(1)-O(16)#3	160.3(4)
O(12)-W(4)-O(8)	97.5(5)	O(4)-W(1)-O(16)#3	84.1(5)
O(2)-W(4)-O(8)	101.2(5)	O(18)#3-W(1)-O(16)#3	82.5(4)
O(12)-W(4)-O(10)	98.2(5)	O(7)-W(1)-O(6)#3	164.9(5)
O(2)-W(4)-O(10)	98.1(5)	O(1)-W(1)-O(6)#3	88.5(5)
O(8)-W(4)-O(10)	151.6(5)	O(4)-W(1)-O(6)#3	86.0(4)
O(12)-W(4)-O(4)	92.3(5)	O(18)#3-W(1)-O(6)#3	71.0(4)
O(2)-W(4)-O(4)	163.4(5)	O(16)#3-W(1)-O(6)#3	71.7(4)
O(8)-W(4)-O(4)	83.0(5)	O(17)-W(2)-O(3)	104.5(5)
O(10)-W(4)-O(4)	72.9(4)	O(17)-W(2)-O(21)	102.9(5)
O(12)-W(4)-O(21)	166.6(5)	O(3)-W(2)-O(21)	95.3(5)
O(2)-W(4)-O(21)	88.7(5)	O(17)-W(2)-O(18)	97.0(5)
O(8)-W(4)-O(21)	73.5(4)	O(3)-W(2)-O(18)	93.8(5)
O(10)-W(4)-O(21)	86.4(4)	O(21)-W(2)-O(18)	155.2(5)
O(4)-W(4)-O(21)	77.0(4)	O(17)-W(2)-O(11)	93.7(5)
O(12)-W(4)-Na(1)	139.8(4)	O(3)-W(2)-O(11)	161.7(4)
O(2)-W(4)-Na(1)	38.0(5)	O(15)-Na(1)-O(1W)#1	87.3(5)
O(8)-W(4)-Na(1)	85.5(4)	O(17)#1-Na(1)-O(2)	88.1(5)
O(10)-W(4)-Na(1)	97.4(4)	O(15)-Na(1)-O(2)	84.4(5)
O(4)-W(4)-Na(1)	127.7(3)	O(1W)#1-Na(1)-O(2)	116.8(5)
O(21)-W(4)-Na(1)	50.9(3)	O(17)#1-Na(1)-O(2W)#1	83.4(5)
O(20)-W(5)-O(16)	101.9(5)	O(15)-Na(1)-O(2W)#1	104.2(5)
O(20)-W(5)-O(11)	101.8(5)	O(1W)#1-Na(1)-O(2W)#1	77.6(5)
O(16)-W(5)-O(11)	92.3(5)	O(2)-Na(1)-O(2W)#1	164.0(6)
O(20)-W(5)-O(14)#3	100.7(5)	O(17)#1-Na(1)-O(21)	112.5(5)
O(16)-W(5)-O(14)#3	87.3(5)	O(15)-Na(1)-O(21)	65.1(4)
O(11)-W(5)-O(14)#3	157.1(4)	O(1W)#1-Na(1)-O(21)	152.2(5)
O(20)-W(5)-O(13)	101.0(5)	O(2)-Na(1)-O(21)	66.1(4)
O(16)-W(5)-O(13)	156.4(5)	O(2W)#1-Na(1)-O(21)	104.8(5)
O(11)-W(5)-O(13)	88.8(5)	O(17)#1-Na(1)-W(6)	151.5(4)
O(14)#3-W(5)-O(13)	82.7(5)	O(15)-Na(1)-W(6)	25.9(3)
O(20)-W(5)-O(6)	177.5(5)	O(1W)#1-Na(1)-W(6)	113.0(4)
O(16)-W(5)-O(6)	75.9(5)	O(2)-Na(1)-W(6)	76.1(3)
O(11)-W(5)-O(6)	77.3(4)	O(2W)#1-Na(1)-W(6)	105.6(4)
O(14)#3-W(5)-O(6)	80.4(4)	O(21)-Na(1)-W(6)	39.3(2)
O(13)-W(5)-O(6)	81.3(5)	O(17)#1-Na(1)-W(4)	101.3(4)
O(9)-W(6)-O(15)	103.0(5)	O(15)-Na(1)-W(4)	72.2(3)
O(9)-W(6)-O(13)	100.3(5)	O(1W)#1-Na(1)-W(4)	136.5(4)
O(15)-W(6)-O(13)	99.0(5)	O(2)-Na(1)-W(4)	26.3(3)
O(9)-W(6)-O(8)	96.0(5)	O(2W)#1-Na(1)-W(4)	143.7(4)
O(15)-W(6)-O(8)	93.9(5)	O(21)-Na(1)-W(4)	39.9(2)
O(13)-W(6)-O(8)	156.4(5)	W(6)-Na(1)-W(4)	55.57(11)
O(9)-W(6)-O(1)	91.1(5)	O(17)#1-Na(1)-W(2)	90.3(4)

O(15)-W(6)-O(1)	164.5(5)	O(15)-Na(1)-W(2)	89.9(4)
O(13)-W(6)-O(1)	84.5(4)	O(1W)#1-Na(1)-W(2)	158.6(4)
O(8)-W(6)-O(1)	78.1(4)	O(2)-Na(1)-W(2)	84.0(4)
O(9)-W(6)-O(21)	164.8(5)	O(2W)#1-Na(1)-W(2)	82.5(3)
O(15)-W(6)-O(21)	88.3(5)	O(21)-Na(1)-W(2)	30.2(2)
O(13)-W(6)-O(21)	87.6(5)	W(6)-Na(1)-W(2)	64.88(13)
O(8)-W(6)-O(21)	73.0(4)	W(4)-Na(1)-W(2)	61.64(12)
O(1)-W(6)-O(21)	76.7(4)	O(17)#1-Na(1)-Sr(1)#1	103.7(4)
O(9)-W(6)-Na(1)	139.5(4)	O(15)-Na(1)-Sr(1)#1	82.9(3)
O(15)-W(6)-Na(1)	36.9(4)	O(1W)#1-Na(1)-Sr(1)#1	42.0(3)
O(13)-W(6)-Na(1)	93.3(4)	O(2)-Na(1)-Sr(1)#1	155.7(4)
O(8)-W(6)-Na(1)	85.2(3)	O(2W)#1-Na(1)-Sr(1)#1	40.4(3)
O(1)-W(6)-Na(1)	128.2(3)	O(21)-Na(1)-Sr(1)#1	125.5(3)
O(21)-W(6)-Na(1)	51.6(3)	W(6)-Na(1)-Sr(1)#1	100.10(18)
O(17)#1-Na(1)-O(15)	172.4(5)	W(4)-Na(1)-Sr(1)#1	155.0(2)
O(17)#1-Na(1)-O(1W)#1	95.2(5)	W(2)-Na(1)-Sr(1)#1	116.6(2)

Symmetry code for **3**: #1 -x+1, -y, -z+1; #2 x, -y+1/2, z-1/2; #3 -x+2, -y, -z+1; #4 x, y, z-1; #5 x, y,

z+1; #6 x, -y+1/2, z+1/2.

O(1)-W(2)	1.767(17)	O(18)-W(2)	1.876(15)	
O(1)-Ba(2)#1	2.512(17)	O(18)-W(5)#2	1.986(15)	
O(2)-W(5)	1.851(17)	O(19)-W(4)	1.763(17)	
O(2)-W(3)	2.123(18)	O(19)-Na(1)#3	2.41(2)	
O(3)-W(1)#2	1.789(16)	O(20)-W(6)	1.731(17)	
O(3)-W(6)	2.184(16)	O(20)-Na(1)#3	2.43(2)	
O(4)-W(5)	1.866(17)	O(21)-W(3)	1.779(16)	
O(4)-W(1)	2.073(16)	O(21)-W(2)	2.215(16)	
O(5)-W(3)	1.892(16)	OW1-Ba(2)	2.71(2)	
O(5)-W(4)	2.274(16)	OW2-Ba(2)	2.56(2)	
O(5)-W(6)	2.292(15)	OW4-Na(1)	2.51(2)	
O(5)-Na(1)#3	2.76(2)	OW4-Ba(1)#3	2.641(18)	
O(6)-W(1)	1.737(16)	OW7-Ba(2)	2.60(2)	
O(6)-Ba(2)#4	2.480(16)	OW11-Ba(1)	2.595(18)	
O(7)-W(6)	1.756(17)	OW11-Ba(2)	2.620(19)	
O(7)-Ba(1)#5	2.698(18)	OW12-Ba(1)	2.688(19)	
O(8)-W(2)	1.732(17)	OW12-Ba(2)	2.742(17)	
O(8)-Ba(1)#3	2.605(17)	OW13-Ba(2)	2.701(18)	
O(9)-W(3)	1.941(16)	OW13-Ba(1)	2.81(2)	
O(9)-W(1)	1.968(16)	OW14-Na(1)#3	2.48(2)	

Table S4. Selected bond lengths [Å] and bond angles (°) for the compound 4.

O(10)-W(6)	1.911(17)	OW14-Ba(1)	2.676(19)
O(10)-W(5)	1.921(16)	OW15-Ba(1)	2.517(19)
O(11)-W(3)	1.716(17)	OW16-Ba(1)	2.63(2)
O(11)-Na(1)	2.27(2)	Ba(1)-O(8)#3	2.605(17)
O(12)-W(1)	1.881(15)	Ba(1)-OW4#3	2.641(18)
O(12)-W(2)#2	2.215(15)	Ba(1)-O(7)#5	2.698(18)
O(12)-W(4)#2	2.285(15)	Ba(2)-O(6)#6	2.480(16)
O(13)-W(4)	1.926(17)	Ba(2)-O(1)#7	2.512(17)
O(13)-W(2)	1.974(16)	W(1)-O(3)#2	1.789(16)
O(14)-W(4)	1.767(19)	W(2)-O(12)#2	2.215(15)
O(15)-W(4)	1.912(16)	W(4)-O(12)#2	2.285(15)
O(15)-W(6)	1.955(16)	W(5)-O(18)#2	1.986(15)
O(16)-W(5)	1.740(17)	Na(1)-O(19)#3	2.41(2)
O(17)-W(5)	2.244(16)	Na(1)-O(20)#3	2.43(2)
O(17)-W(1)	2.249(16)	Na(1)-OW14#3	2.48(2)
O(17)-W(3)	2.257(15)	Na(1)-O(5)#3	2.76(2)
W(2)-O(1)-Ba(2)#1	153.3(10)	W(4)-O(5)-W(6)	92.9(6)
W(5)-O(2)-W(3)	114.2(8)	W(3)-O(5)-Na(1)#3	103.4(7)
W(1)#2-O(3)-W(6)	138.0(8)	W(4)-O(5)-Na(1)#3	89.9(6)
W(5)-O(4)-W(1)	115.7(8)	W(6)-O(5)-Na(1)#3	89.3(6)
W(3)-O(5)-W(4)	127.1(8)	W(1)-O(6)-Ba(2)#4	153.9(9)
W(3)-O(5)-W(6)	137.3(8)	W(6)-O(7)-Ba(1)#5	149.8(9)
W(2)-O(8)-Ba(1)#3	153.6(10)	O(8)#3-Ba(1)-O(7)#5	124.0(6)
W(3)-O(9)-W(1)	119.7(8)	OW16-Ba(1)-O(7)#5	127.7(7)
W(6)-O(10)-W(5)	146.4(9)	OW4#3-Ba(1)-O(7)#5	124.7(5)
W(3)-O(11)-Na(1)	154.7(10)	OW14-Ba(1)-O(7)#5	65.8(5)
W(1)-O(12)-W(2)#2	138.2(8)	OW12-Ba(1)-O(7)#5	71.0(5)
W(1)-O(12)-W(4)#2	126.4(8)	OW15-Ba(1)-OW13	136.5(6)
W(2)#2-O(12)-W(4)#2	94.6(6)	OW11-Ba(1)-OW13	67.8(6)
W(4)-O(13)-W(2)	116.1(8)	O(8)#3-Ba(1)-OW13	66.6(5)
W(4)-O(15)-W(6)	117.7(8)	OW16-Ba(1)-OW13	70.5(7)
W(5)-O(17)-W(1)	95.9(6)	OW4#3-Ba(1)-OW13	110.6(5)
W(5)-O(17)-W(3)	95.8(6)	OW14-Ba(1)-OW13	137.0(6)
W(1)-O(17)-W(3)	97.2(6)	OW12-Ba(1)-OW13	65.3(5)
W(2)-O(18)-W(5)#2	145.7(9)	O(7)#5-Ba(1)-OW13	124.4(5)
W(4)-O(19)-Na(1)#3	116.6(9)	OW15-Ba(1)-Na(1)#3	66.4(5)
W(6)-O(20)-Na(1)#3	117.1(9)	OW11-Ba(1)-Na(1)#3	120.1(5)
W(3)-O(21)-W(2)	140.4(9)	O(8)#3-Ba(1)-Na(1)#3	81.9(4)
Na(1)-OW4-Ba(1)#3	102.1(7)	OW16-Ba(1)-Na(1)#3	104.0(6)
Ba(1)-OW11-Ba(2)	102.7(6)	OW4#3-Ba(1)-Na(1)#3	37.7(5)
Ba(1)-OW12-Ba(2)	97.2(6)	OW14-Ba(1)-Na(1)#3	37.3(5)
Ba(2)-OW13-Ba(1)	95.2(6)	OW12-Ba(1)-Na(1)#3	150.2(4)
Na(1)#3-OW14-Ba(1)	101.9(7)	O(7)#5-Ba(1)-Na(1)#3	88.4(4)
OW15-Ba(1)-OW11	135.1(6)	OW13-Ba(1)-Na(1)#3	143.3(4)

OW15-Ba(1)-O(8)#3	146.1(7)	OW15-Ba(1)-Ba(2)	126.9(5)
OW11-Ba(1)-O(8)#3	70.8(6)	OW11-Ba(1)-Ba(2)	38.9(4)
OW15-Ba(1)-OW16	70.7(7)	O(8)#3-Ba(1)-Ba(2)	86.9(4)
OW11-Ba(1)-OW16	134.6(7)	OW16-Ba(1)-Ba(2)	96.4(5)
O(8)#3-Ba(1)-OW16	108.1(7)	OW4#3-Ba(1)-Ba(2)	151.2(4)
OW15-Ba(1)-OW4#3	76.0(6)	OW14-Ba(1)-Ba(2)	122.2(4)
OW11-Ba(1)-OW4#3	138.9(6)	OW12-Ba(1)-Ba(2)	41.9(4)
O(8)#3-Ba(1)-OW4#3	71.6(5)	O(7)#5-Ba(1)-Ba(2)	83.1(4)
OW16-Ba(1)-OW4#3	73.4(7)	OW13-Ba(1)-Ba(2)	41.3(4)
OW15-Ba(1)-OW14	86.4(6)	Na(1)#3-Ba(1)-Ba(2)	158.9(2)
OW11-Ba(1)-OW14	83.5(6)	O(6)#6-Ba(2)-O(1)#7	97.8(5)
O(8)#3-Ba(1)-OW14	74.2(6)	O(6)#6-Ba(2)-OW2	145.3(7)
OW16-Ba(1)-OW14	141.3(7)	O(1)#7-Ba(2)-OW2	101.5(7)
OW4#3-Ba(1)-OW14	71.0(6)	O(6)#6-Ba(2)-OW7	73.7(6)
OW15-Ba(1)-OW12	85.7(6)	O(1)#7-Ba(2)-OW7	78.0(6)
OW11-Ba(1)-OW12	72.4(6)	OW2-Ba(2)-OW7	82.5(7)
O(8)#3-Ba(1)-OW12	127.4(5)	O(6)#6-Ba(2)-OW11	86.5(6)
OW16-Ba(1)-OW12	74.5(7)	O(1)#7-Ba(2)-OW11	143.5(6)
OW4#3-Ba(1)-OW12	146.8(6)	OW2-Ba(2)-OW11	94.4(7)
OW14-Ba(1)-OW12	136.0(6)	OW7-Ba(2)-OW11	137.1(6)
OW15-Ba(1)-O(7)#5	68.7(6)	O(6)#6-Ba(2)-OW13	136.0(5)
OW11-Ba(1)-O(7)#5	67.3(6)	O(1)#7-Ba(2)-OW13	83.4(6)
OW2-Ba(2)-OW13	75.1(7)	O(18)-W(2)-O(13)	157.9(7)
OW7-Ba(2)-OW13	147.3(6)	O(8)-W(2)-O(12)#2	162.8(7)
OW11-Ba(2)-OW13	69.2(6)	O(1)-W(2)-O(12)#2	91.5(7)
O(6)#6-Ba(2)-OW1	73.8(6)	O(18)-W(2)-O(12)#2	89.1(6)
O(1)#7-Ba(2)-OW1	148.5(7)	O(13)-W(2)-O(12)#2	74.2(6)
OW2-Ba(2)-OW1	74.6(7)	O(8)-W(2)-O(21)	89.9(7)
OW7-Ba(2)-OW1	70.5(7)	O(1)-W(2)-O(21)	167.1(7)
OW11-Ba(2)-OW1	67.5(7)	O(18)-W(2)-O(21)	84.2(6)
OW13-Ba(2)-OW1	124.0(6)	O(13)-W(2)-O(21)	77.7(6)
O(6)#6-Ba(2)-OW12	71.5(5)	O(12)#2-W(2)-O(21)	75.6(6)
O(1)#7-Ba(2)-OW12	76.0(6)	O(11)-W(3)-O(21)	103.4(7)
OW2-Ba(2)-OW12	141.2(7)	O(11)-W(3)-O(5)	101.5(7)
OW7-Ba(2)-OW12	132.6(6)	O(21)-W(3)-O(5)	95.2(7)
OW11-Ba(2)-OW12	71.1(6)	O(11)-W(3)-O(9)	97.2(7)
OW13-Ba(2)-OW12	66.1(5)	O(21)-W(3)-O(9)	93.9(7)
OW1-Ba(2)-OW12	126.7(6)	O(5)-W(3)-O(9)	156.7(7)
O(6)#6-Ba(2)-Ba(1)	95.3(4)	O(11)-W(3)-O(2)	93.5(7)
O(1)#7-Ba(2)-Ba(1)	105.1(4)	O(21)-W(3)-O(2)	163.0(7)
OW2-Ba(2)-Ba(1)	106.9(6)	O(5)-W(3)-O(2)	83.3(7)
OW7-Ba(2)-Ba(1)	169.0(5)	O(9)-W(3)-O(2)	81.8(7)
OW11-Ba(2)-Ba(1)	38.4(4)	O(11)-W(3)-O(17)	162.3(7)
OW13-Ba(2)-Ba(1)	43.4(4)	O(21)-W(3)-O(17)	90.8(6)

OW1-Ba(2)-Ba(1)	105.9(5)	O(5)-W(3)-O(17)	87.5(6)
OW12-Ba(2)-Ba(1)	40.9(4)	O(9)-W(3)-O(17)	71.0(6)
O(6)-W(1)-O(3)#2	103.2(7)	O(2)-W(3)-O(17)	72.3(6)
O(6)-W(1)-O(12)	102.5(7)	O(11)-W(3)-Na(1)#3	63.1(6)
O(3)#2-W(1)-O(12)	94.4(7)	O(21)-W(3)-Na(1)#3	127.5(6)
O(6)-W(1)-O(9)	98.0(7)	O(5)-W(3)-Na(1)#3	46.6(5)
O(3)#2-W(1)-O(9)	91.5(7)	O(9)-W(3)-Na(1)#3	136.1(5)
O(12)-W(1)-O(9)	156.7(7)	O(2)-W(3)-Na(1)#3	62.4(5)
O(6)-W(1)-O(4)	96.1(7)	O(17)-W(3)-Na(1)#3	116.1(4)
O(3)#2-W(1)-O(4)	160.5(7)	O(19)-W(4)-O(14)	103.6(9)
O(12)-W(1)-O(4)	84.4(7)	O(19)-W(4)-O(15)	100.1(8)
O(9)-W(1)-O(4)	82.7(7)	O(14)-W(4)-O(15)	97.0(8)
O(6)-W(1)-O(17)	164.4(6)	O(19)-W(4)-O(13)	97.2(8)
O(3)#2-W(1)-O(17)	88.2(6)	O(14)-W(4)-O(13)	99.6(8)
O(12)-W(1)-O(17)	86.9(6)	O(15)-W(4)-O(13)	152.5(7)
O(9)-W(1)-O(17)	70.8(6)	O(19)-W(4)-O(5)	87.5(7)
O(4)-W(1)-O(17)	72.3(6)	O(14)-W(4)-O(5)	167.3(7)
O(8)-W(2)-O(1)	102.6(8)	O(15)-W(4)-O(5)	74.7(6)
O(8)-W(2)-O(18)	98.8(8)	O(13)-W(4)-O(5)	84.9(6)
O(1)-W(2)-O(18)	96.8(8)	O(19)-W(4)-O(12)#2	162.3(7)
O(8)-W(2)-O(13)	93.9(8)	O(14)-W(4)-O(12)#2	92.8(7)
O(1)-W(2)-O(13)	98.0(8)	O(15)-W(4)-O(12)#2	84.0(6)
O(13)-W(4)-O(12)#2	73.5(6)	O(11)-Na(1)-O(19)#3	90.1(7)
O(5)-W(4)-O(12)#2	77.0(6)	O(11)-Na(1)-O(20)#3	174.1(8)
O(19)-W(4)-Na(1)#3	37.2(7)	O(19)#3-Na(1)-O(20)#3	84.3(7)
O(14)-W(4)-Na(1)#3	139.6(6)	O(11)-Na(1)-OW14#3	94.0(7)
O(15)-W(4)-Na(1)#3	85.3(5)	O(19)#3-Na(1)-OW14#3	116.6(8)
O(13)-W(4)-Na(1)#3	95.9(5)	O(20)#3-Na(1)-OW14#3	86.7(7)
O(5)-W(4)-Na(1)#3	50.5(4)	O(11)-Na(1)-OW4	82.9(7)
O(12)#2-W(4)-Na(1)#3	127.4(5)	O(19)#3-Na(1)-OW4	165.7(9)
O(16)-W(5)-O(2)	102.7(8)	O(20)#3-Na(1)-OW4	103.0(7)
O(16)-W(5)-O(4)	101.7(8)	OW14#3-Na(1)-OW4	76.5(7)
O(2)-W(5)-O(4)	92.2(7)	O(11)-Na(1)-O(5)#3	113.8(7)
O(16)-W(5)-O(10)	100.2(7)	O(19)#3-Na(1)-O(5)#3	65.6(6)
O(2)-W(5)-O(10)	90.0(7)	O(20)#3-Na(1)-O(5)#3	65.6(6)
O(4)-W(5)-O(10)	156.9(7)	OW14#3-Na(1)-O(5)#3	152.2(7)
O(16)-W(5)-O(18)#2	98.4(7)	OW4-Na(1)-O(5)#3	105.9(7)
O(2)-W(5)-O(18)#2	158.7(7)	O(11)-Na(1)-W(6)#3	153.5(6)
O(4)-W(5)-O(18)#2	86.5(7)	O(19)#3-Na(1)-W(6)#3	75.6(5)
O(10)-W(5)-O(18)#2	83.2(7)	O(20)#3-Na(1)-W(6)#3	25.6(4)
O(16)-W(5)-O(17)	177.9(7)	OW14#3-Na(1)-W(6)#3	112.2(5)
O(2)-W(5)-O(17)	77.6(6)	OW4-Na(1)-W(6)#3	105.7(5)
O(4)-W(5)-O(17)	76.2(6)	O(5)#3-Na(1)-W(6)#3	40.0(4)
O(10)-W(5)-O(17)	81.8(6)	O(11)-Na(1)-W(4)#3	103.4(5)

O(18)#2-W(5)-O(17)	81.4(6)	O(19)#3-Na(1)-W(4)#3	26.2(4)
O(20)-W(6)-O(7)	102.3(8)	O(20)#3-Na(1)-W(4)#3	72.2(5)
O(20)-W(6)-O(10)	97.5(8)	OW14#3-Na(1)-W(4)#3	136.1(7)
O(7)-W(6)-O(10)	101.7(8)	OW4-Na(1)-W(4)#3	144.7(6)
O(20)-W(6)-O(15)	94.2(8)	O(5)#3-Na(1)-W(4)#3	39.6(4)
O(7)-W(6)-O(15)	94.6(7)	W(6)#3-Na(1)-W(4)#3	55.28(16)
O(10)-W(6)-O(15)	157.4(7)	O(11)-Na(1)-W(3)#3	91.8(6)
O(20)-W(6)-O(3)	164.6(7)	O(19)#3-Na(1)-W(3)#3	84.3(5)
O(7)-W(6)-O(3)	92.2(7)	O(20)#3-Na(1)-W(3)#3	89.6(5)
O(10)-W(6)-O(3)	84.7(6)	OW14#3-Na(1)-W(3)#3	158.2(6)
O(15)-W(6)-O(3)	79.1(6)	OW4-Na(1)-W(3)#3	83.5(6)
O(20)-W(6)-O(5)	87.9(7)	O(5)#3-Na(1)-W(3)#3	29.9(4)
O(7)-W(6)-O(5)	165.0(7)	W(6)#3-Na(1)-W(3)#3	65.0(2)
O(10)-W(6)-O(5)	87.6(6)	W(4)#3-Na(1)-W(3)#3	61.9(2)
O(15)-W(6)-O(5)	73.5(6)	O(11)-Na(1)-Ba(1)#3	102.3(5)
O(3)-W(6)-O(5)	76.9(6)	O(19)#3-Na(1)-Ba(1)#3	154.2(7)
O(20)-W(6)-Na(1)#3	37.3(6)	O(20)#3-Na(1)-Ba(1)#3	82.1(5)
O(7)-W(6)-Na(1)#3	139.0(6)	OW14#3-Na(1)-Ba(1)#3	40.8(5)
O(10)-W(6)-Na(1)#3	92.7(5)	OW4-Na(1)-Ba(1)#3	40.2(4)
O(15)-W(6)-Na(1)#3	84.9(5)	O(5)#3-Na(1)-Ba(1)#3	126.5(5)
O(3)-W(6)-Na(1)#3	127.5(4)	W(6)#3-Na(1)-Ba(1)#3	99.9(3)
O(5)-W(6)-Na(1)#3	50.6(4)	W(4)#3-Na(1)-Ba(1)#3	154.3(3)
W(3)#3-Na(1)-Ba(1)#3	117.4(3)		

Symmetry code for **4**: #1 -x, y-1/2, -z+3/2; #2 -x+1, -y, -z+2; #3 -x, -y, -z+2; #4 x+1, y, z+1; #5 -x,

-y, -z+1; #6 x-1, y, z-1; #7 -x, y+1/2, -z+3/2.