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## **Supporting Information**

# Li<sub>6</sub>Na<sub>3</sub>Sr<sub>14</sub>Al<sub>11</sub>P<sub>22</sub>O<sub>90</sub>: An Oxo-Centered Al<sub>3</sub> Cluster Based Phosphate

# Constructed from Two Types of (3,6)-Connected kgd Layers

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### Generals

#### **1. Synthetic Information**

Single crystals of  $Li_6Na_3Sr_{14}Al_{11}P_{22}O_{90}$  (1) were grown from high temperature solutions by using spontaneous crystallization. These solutions were prepared in platinum crucibles by melting mixtures of  $Na_2CO_3/SrF_2/LiF/Al_2O_3/NH_4H_2PO_4$  with molar ratio of 2:3:4:2:8. The mixtures were heated in programmable temperature electric furnaces at 950 °C and kept for 48 hours. The homogenized melt solutions were then cooled slowly (2 °C/h) to 650 °C, and then allowed to cool to room temperature at a rate of 10 °C/h. Pure, colorless and millimeter-sized crystals were then obtained after dissolving in water (Fig. S1).

#### 2. Single-Crystal X-ray Diffraction Structural Data Collections and Analysis

Single-Crystal X-ray Diffraction Data collections for 1 crystal with dimensions of 0.3 mm  $\times$  0.4 mm  $\times$  0.1 mm were carried out on a Bruker APEX-II CCD detector at 298 K using Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å). The collection of the intensity data, cell refinement, and data reduction were performed by the program CrysAlisPro<sup>1</sup>. The structures were solved by the direct method with the program SHELXS and refined by the full-matrix least-squares program SHELXL<sup>2</sup>. The structures were checked with the aid of the program PLATON<sup>3</sup>. Relevant crystallographic data are listed in Table S1 and S2. The selected bond distances and angles are shown in Tables S3.

#### 3. Polycrystalline Powder X-ray Diffraction Analysis

Its phase purity was confirmed by powder X-ray diffraction (XRD) diffraction analysis, which was performed on a Bruker Model D8 Avance powder diffractometer equipped with Cu K $\alpha$  radiation ( $\lambda = 1.5418$  Å) at room temperature. The scanning step width of 0.02° and scanning rate of 0.05 °s<sup>-1</sup> were applied to record the patterns in the 2 $\theta$  range of 4°–70°. The experimental powder X-ray diffraction patterns were found to be in good agreement with the calculated ones based on the single crystal lographic data (Fig.S2).

#### 4. Infrared (IR) Spectroscopy Analysis

The Fourier transform infrared (FTIR) spectra were recorded from KBr pellets in the range 4000–400 cm<sup>-1</sup> on a Nicolet Model 5DX spectrometer. The IR spectrum for **1** (Fig.S6) displays the absorption peaks at 465 cm<sup>-1</sup> (due to Al-O structural units), 539 cm<sup>-1</sup> (the deformation modes of P–O (PO<sub>4</sub><sup>3-</sup>) groups), 713 cm<sup>-1</sup> (the v<sub>s</sub> of P-O-P groups), 883 cm<sup>-1</sup> (due to P–O–P asymmetric bending vibrations), and 1089 cm<sup>-1</sup> (a normal vibrational mode in PO<sub>4</sub><sup>3-</sup> group arising out of  $v_3$ -symmetric stretching).<sup>4</sup> The IR spectrum further verifies the existence of Al-O and P-O groups.

### 5. UV-vis Diffuse Reflectance Spectroscopy Analysis

The UV-vis-NIR diffuse reflection data were recorded at room temperature using a powdered BaSO<sub>4</sub> sample as a standard (100% reflectance) on a Shimadzu uv2600 spectrophotometer. The scanning wavelength ranged from 230 nm to 1200 nm. Absorption (K/S) data were calculated by the following Kubelka–Munk function<sup>5</sup>:  $F(R) = (1-R)^2$  /(2R) = K/S, where R is the reflectance, K is the absorption, and S is the scattering (Fig.3b).

#### 6. Thermal Behavior Analysis

Investigation of the thermal behavior was performed on a simultaneous TGA/DSC 1 STARe System thermal analyzer instrument. The compound of about 15 mg was placed in platinum crucibles, heated with a heating rate of 10 K/m from 303 K to 1223 K. The measurements were carried out in an atmosphere of flowing  $N_2$  (Fig.3a).

### 7. Inductively Coupled Plasma (ICP) Analysis

Element analysis of the crystals was performed by using a Perkin Elmer Optima 8000 DV inductively coupled plasma optical emission spectrometer (ICP-OES). The crystal samples about 4 mg were first dried by DZG-6020

vacuum drying oven, and the digestion of the sample were afterwards processed using 1 ml perchloric acid. Following a cooling to room temperature, the digested samples were diluted with distilled water to a total volume of 100 ml.<sup>6</sup>

#### 8. Computational details

The periodic density functional theory (DFT) calculations were performed using the VASP within the MedeA software.<sup>7</sup> The primitive cell (151atoms in total) without any symmetry restrictions (space group P1) was employed in all the calculations. The projector augmented wave (PAW) pseudopotentials<sup>8</sup> were employed to describe the electron-ion interactions. The exchange-correlation energy was described by meta-GGA functional (revTPSS)<sup>9</sup>, which is found to improve the band gaps over the standard GGA band gaps. The plane-wave cutoff energy was set to 600 eV. The Brillouin zone integration was performed with a  $2\times3\times1$  Monkhorst-Pack<sup>10</sup> mesh of the primitive unit cell for the geometry optimization and total energy calculation. The self-consistent field (SCF) tolerance was  $10^{-6}$  eV and the forces on the ions were less than 0.005 eV/Å. The electron smearing was employed using the Gaussian smearing width of 0.2 eV. The electronic band structures and densities of states (DOS) were calculated at the same level used for the geometry optimization.

# **Tables and Figures**

Table S1. Crystal data and structure refinement

Empirical formula	Li <sub>6</sub> Na <sub>3</sub> Sr <sub>14</sub> Al <sub>11</sub> P <sub>22</sub> O <sub>90</sub>						
Parameter	1						
Formula weight	3755.41						
Temperature/K	298.0						
Crystal system	monoclinic						
Space group	C2/m						
a/Å	16.9643(3)						
b/Å	10.1943(1)						
c/Å	21.8245(4)						
α/°	90						
β/°	112.643(2)						
$\gamma/^{\circ}$	90						
Volume/Å <sup>3</sup>	3483.39(11)						
Ζ	2						
$\rho_{calc}g/cm^3$	3.5802						
$\mu/mm^{-1}$	11.461						
F(000)	3516.5						
Crystal size/mm	0.3  imes 0.4  imes 0.1						
Radiation	Mo K $\alpha$ ( $\lambda = 0.71073$ )						
$2\Theta$ range for data collection/°	5.56 to 50.02						
Index ranges	$-23 \le h \le 23, -14 \le k \le 14, -30 \le l \le 30$						
Reflections collected	36986						
Independent reflections	3224 [ $R_{int} = 0.0412$ , $R_{sigma} = 0.0278$ ]						
Data/restraints/parameters	3224/30/386						
Goodness-of-fit on F <sup>2</sup>	1.036						
Final R indexes [I>= $2\sigma$ (I)]	$R_1 = 0.0777, wR_2 = 0.1886$						
Final R indexes [all data]	$R_1 = 0.0783$ , $wR_2 = 0.1893$						
Largest diff. peak/hole / e Å <sup>-3</sup>	1.63/-1.17						
$^{a}R_{1}=\sum   F_{o} - F_{c}  /\sum  F_{o} $ , and wR	$aR_1 = \sum   F_o  -  F_c   / \sum  F_o $ , and wR2= $[w(F_o^2 - F_c^2)^2 / w(F_o^2)^2]^{1/2}$						

**Table S2.** Atomic coordinates (×10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup>×10<sup>3</sup>). $U_{eq}$  is defined as one-third of the trace of the orthogonalized  $U_{ij}$  tensor.

Atom	x	У	Z	U(eq)
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Sr3	1654.6(11) 5000		3155.1(8)	34.8(5)
Sr4	1500.4(12)	0	3268.6(8)	42.9(5)
Sr1	4925.6(8)	2190.2(13)	1358.7(6)	37.6(4)
Sr2	2192.2(11)	5000	1364.8(8)	38.3(5)
Sr5	4210(4)	3022(10)	3121(4)	46.3(17)
Sr5'	4175(12)	2620(20)	3248(9)	77(4)
Р3	3878(3)	0	4277(2)	34.9(10)
P8	1168.5(19)	2370(3)	536.2(14)	31.8(7)
P7	3465(3)	0	549(2)	31.3(9)
P6	4359(3)	5000	1841(2)	35.5(10)
P2	1354(2)	2353(3)	4254.9(15)	33.7(7)
P4	2002(2)	2503(3)	2437.0(16)	34.6(7)
Р5	4562(3)	0	2480(2)	33.9(10)
P1	1138(3)	0	5862(2)	35.3(10)
A13	2626(3)	0	5121(2)	30.9(11)
Al4	0	-2452(5)	5000	36.5(12)
A12	1232(3)	0	1543(2)	32.4(11)
Al1	5000	0	0	30.1(15)
A15	2929(2)	1503(4)	1577.5(17)	32.6(8)
Na1	3049(6)	2499(10)	4214(4)	32(2)
Na2	2500	2500	0	61(4)
Li1	3629(12)	5000	460(9)	9(3)
Li2	5488(14)	0	4209(10)	19(5)
Li3	4665(12)	5000	222(9)	9(3)
O20	3381(6)	1204(9)	940(4)	41(2)
O29	3440(8)	5000	3377(6)	46(3)
08	4439(7)	1210(9)	4336(5)	56(3)
05	2066(5)	1319(8)	4494(4)	35.6(18)
O21	2122(5)	2565(9)	960(4)	39(2)
012	2304(6)	2644(9)	3174(4)	48(2)
017	5023(8)	5000	1511(6)	41(3)
O10	5005(9)	0	3217(7)	61(4)
O26	2202(8)	5000	144(6)	52(4)
O16	3999(7)	1196(12)	2229(6)	68(3)
O19	3797(7)	3781(12)	1598(6)	65(3)

09	3135(11)	0	3632(8)	77(5)
02	1842(8)	0	5577(6)	42(3)
O1	590(5)	-1220(10)	5662(4)	44(2)
O14	1485(8)	3666(11)	2086(5)	62(3)
O18	4777(9)	5000	2588(7)	68(5)
O3	3566(8)	0	4853(6)	40(3)
O6	750(6)	1974(10)	3567(5)	51(2)
O22	2337(7)	0	1516(5)	30(2)
011	5185(11)	-362(15)	2166(9)	44(5)
O4	920(6)	2435(9)	4749(5)	48(2)
015	2788(6)	2414(11)	2245(5)	56(3)
07	1757(5)	3707(9)	4230(4)	36.8(19)
O25	4391(8)	0	573(6)	34(3)
O13	1469(6)	1250(9)	2217(5)	47(2)
O24	738(5)	3687(8)	570(4)	32.8(18)
O28	3971(5)	3028(9)	155(4)	39(2)
O23	831(5)	1341(8)	884(4)	34.4(18)

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Table S3. Bond lengths  $(\text{\AA})$  (a) and angles (deg.) (b)

(a)											
Atom	Atom	Length/Å	Atom	Atom	Length/Å						
A15	015	1.820(10)	Na1	05	2.321(12)						
A13 <sup>3</sup>	O7	1.923(9)	Na2	O21	2.417(8)						
Al1	O25	1.904(11)	Na1	O12	2.135(12)						
Al2	O13	1.868(10)	Na216	O26	2.640(3)						

Al1 <sup>2</sup>	O24	1.925(8)	Na2	O26	2.640(3)
Al2	O23	1.910(9)	Na1 <sup>5</sup>	09	2.875(12)
A15	O20	1.853(9)	Na1	09	2.875(12)
Al4 <sup>15</sup>	08	1.951(11)	Na113	02	2.584(10)
A15	O21	1.855(9)	Na1 <sup>3</sup>	02	2.584(10)
Al2 <sup>15</sup>	O17	2.026(13)	Na113	01	2.574(12)
A15	O16	1.851(11)	Na1	O4 <sup>3</sup>	2.266(14)
Al4	01	1.885(10)	Na1	O2 <sup>3</sup>	2.584(10)
Al4	O4 <sup>14</sup>	1.842(9)	Na1	O1 <sup>8</sup>	2.574(12)
Al4	O4 <sup>5</sup>	1.842(9)	Na2	O28 <sup>10</sup>	2.446(8)
Al4	O8 <sup>13</sup>	1.951(11)	Na2	O20 <sup>10</sup>	2.415(9)
Al4	O8 <sup>6</sup>	1.951(11)	Na2	O21 <sup>10</sup>	2.417(8)
Al4	O1 <sup>17</sup>	1.885(10)	Na2	O26 <sup>10</sup>	2.640(3)
A12	O13 <sup>5</sup>	1.868(10)	Sr3	O71	2.638(8)
A12	O23 <sup>5</sup>	1.910(9)	Sr3	07	2.638(8)
A12	O17 <sup>6</sup>	2.026(13)	Sr3	O29	2.878(14)
A12	O22	1.898(12)	Sr3	O12 <sup>1</sup>	2.636(10)
All	O25 <sup>18</sup>	1.904(11)	Sr3	012	2.636(10)
All	O24 <sup>12</sup>	1.925(8)	Sr3	O10 <sup>2</sup>	2.853(15)
All	O24 <sup>10</sup>	1.925(8)	Sr3	O2 <sup>3</sup>	2.954(13)
Al1	O24 <sup>7</sup>	1.925(8)	Sr3	014	2.619(10)
All	O2411	1.925(8)	Sr3	O141	2.619(10)
A15	O22	1.809(7)	Sr3	O11 <sup>2</sup>	2.621(18)
A15 <sup>5</sup>	O22	1.809(7)	Sr3	O11 <sup>4</sup>	2.621(18)
A13	O7 <sup>3</sup>	1.923(9)	Sr4	013	2.609(9)
A13	O7 <sup>13</sup>	1.923(9)	Sr4	O13 <sup>5</sup>	2.609(9)
A13	O3	1.898(13)	Sr4	O6	2.595(10)
A13	05	1.893(9)	Sr4	O6 <sup>5</sup>	2.595(10)
A13	O5 <sup>5</sup>	1.893(9)	Sr4	05	2.811(8)
A13	02	1.944(13)	Sr4	O5 <sup>5</sup>	2.811(8)
Al4 <sup>14</sup>	O4	1.842(9)	Sr4	012	3.062(10)
Р3	03	1.540(13)	Sr4	O12 <sup>5</sup>	3.062(10)
Р3	O8 <sup>5</sup>	1.532(10)	Sr4	09	2.574(18)
Р3	08	1.532(10)	Sr4	O186	2.721(14)
Р3	09	1.485(17)	Sr1	O25	2.748(7)
P8	O24	1.545(9)	Sr1	O13 <sup>7</sup>	3.019(11)
P8	O28 <sup>10</sup>	1.489(9)	Sr1	O24 <sup>7</sup>	2.736(8)
P8	O23	1.529(9)	Sr1	O28	2.642(8)
P8	O21	1.536(9)	Sr1	O23 <sup>7</sup>	2.626(8)
P7	O25	1.552(12)	Sr1	O20	2.620(9)

P7         O20 $1.533(9)$ Sr1         O17 $2.8811(18)$ P7         O20 <sup>5</sup> $1.533(9)$ Sr1         O16 $3.067(13)$ Sr5         O29 $2.578(12)$ Sr1         O147 $2.654(12)$ P6         O17 $1.552(13)$ Sr1         O11 <sup>7</sup> $2.654(12)$ P6         O19 $1.531(11)$ Sr1         O11 <sup>3</sup> $2.485(16)$ P6         O19 $1.531(11)$ Sr2         O15 $3.189(12)$ P6         O18 $1.508(15)$ Sr2         O15 <sup>1</sup> $3.189(12)$ P2         O4 $1.525(9)$ Sr2         O24 <sup>1</sup> $2.755(8)$ P2         O6 $1.507(10)$ Sr2         O21 <sup>1</sup> $2.622(9)$ P4         O15 $1.546(10)$ Sr2         O19 $2.854(12)$ P4         O13 $1.511(10)$ Sr2         O14 $2.687(12)$ P4         O14 $1.499(11)$ Sr2         O14 <sup>14</sup> $2.687(12)$ P5         O16 $1.516(11)$ Sr5						
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P70.26101.499(14)Sr10.1472.654(12)P60171.552(13)Sr101152.485(16)P60191.531(11)Sr10113.077(17)P601911.531(11)Sr201513.189(12)P60181.508(15)Sr202412.755(8)P2041.525(9)Sr202412.622(9)P2061.507(10)Sr202112.622(9)P40151.546(10)Sr20262.672(13)P40151.546(10)Sr201912.854(12)P40131.531(10)Sr201412.687(12)P40131.516(11)Sr50142.687(12)P50101.490(14)Sr201412.687(12)P501651.516(11)Sr50672.511(11)P501651.516(11)Sr50672.411(11)P501611.511(16)Sr50123.030(11)P1302911.535(13)Sr50162.617(13)P140121.545(12)Sr50182.685(13)P140261.499(14)Sr50162.617(13)P1501151.513(10)Sr50162.617(13)P160261.499(14)Sr50162.617(13)P170261.499(14)Sr50162.617(13)P140211.535(13)Sr50162.530(15) <td>Sr5</td> <td>O29</td> <td>2.578(12)</td> <td>Sr1</td> <td>O19</td> <td>2.709(11)</td>	Sr5	O29	2.578(12)	Sr1	O19	2.709(11)
P6O171.552(13)Sr1O1152.485(16)P6O191.531(11)Sr2O113.077(17)P6O1911.531(11)Sr2O1513.189(12)P6O181.508(15)Sr2O242.755(8)P2O41.525(9)Sr2O2412.622(9)P2O51.507(10)Sr2O212.622(9)P2O51.534(9)Sr2O212.622(9)P4O151.546(10)Sr2O262.672(13)P4O151.546(10)Sr2O192.854(12)P4O121.496(9)Sr2O142.687(12)P4O141.499(11)Sr2O142.687(12)P5O101.490(14)Sr2O142.687(12)P5O161.516(11)Sr5O152.511(11)P5O161.511(16)Sr5O292.578(12)P5O1151.511(16)Sr5O162.617(13)P10O261.499(14)Sr5O162.617(13)P11O291.535(13)Sr5O162.617(13)P11O261.511(16)Sr5O182.658(10)P11O261.499(14)Sr5O162.617(13)P14O121.535(13)Sr5O162.617(13)P15O1151.511(16)Sr5O162.617(13)P16O261.499(14)Sr5O162.530(15)P1<	P7	O26 <sup>10</sup>	1.499(14)	Sr1	O14 <sup>7</sup>	2.654(12)
P6O191.531(11)Sr1O113.077(17)P6O1911.531(11)Sr2O1513.189(12)P6O181.508(15)Sr2O1513.189(12)P2O41.525(9)Sr2O2412.755(8)P2O61.507(10)Sr2O2112.622(9)P2O51.534(9)Sr2O2112.622(9)P4O151.546(10)Sr2O262.672(13)P4O131.531(10)Sr2O142.6854(12)P4O121.496(9)Sr2O142.687(12)P5O101.490(14)Sr2O142.687(12)P5O101.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O123.030(1)P5O111.511(16)Sr5O123.030(1)P11O281.489(9)Sr5O123.030(1)P13O291.535(13)Sr5O182.685(13)P14O11.513(10)Sr5O182.685(13)P1O261.499(14)Sr5O192.217(14)P1O291.535(13)Sr5O123.30(11)P13O291.535(13)Sr5O182.685(13)P1O151.513(10)Sr5'O162.530(15)P1O151.513(10)Sr5'O162.530(15)P1O151.513(10)Sr5'O162.530(15)P1	P6	O17	1.552(13)	Sr1	O11 <sup>5</sup>	2.485(16)
P6O1911.531(11)Sr2O153.189(12)P6O181.508(15)Sr2O1513.189(12)P2O41.525(9)Sr2O242.755(8)P2O71.551(9)Sr2O2412.622(9)P2O51.534(9)Sr2O212.622(9)P4O151.546(10)Sr2O262.672(13)P4O151.546(10)Sr2O192.854(12)P4O121.496(9)Sr2O142.687(12)P4O141.499(11)Sr2O142.687(12)P5O101.490(14)Sr2O142.687(12)P5O161.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O292.578(12)P5O161.516(11)Sr5O123.03(11)P5O111.511(16)Sr5O123.03(11)P5O111.511(16)Sr5O123.03(11)P13O291.535(13)Sr5O182.685(13)P14O11.513(10)Sr5'O182.685(13)P1O21.545(12)Sr5'O182.685(13)P1O151.513(10)Sr5'O162.510(1)P1O2812.51(2)Sr5'O182.66(3)L12O772.51(2)Sr5'O162.576(17)L13O2812.61(13)Sr5'O162.576(17)L12O3	P6	019	1.531(11)	Sr1	011	3.077(17)
P6O181.508(15)St2O1513.189(12)P2O41.525(9)St2O242.755(8)P2O71.551(9)St2O2412.622(9)P2O51.534(9)St2O2112.622(9)P4O151.546(10)St2O192.854(12)P4O151.531(10)St2O1912.854(12)P4O121.496(9)St2O1412.687(12)P4O141.499(11)St2O1412.687(12)P5O101.490(14)St2O1412.687(12)P5O1651.516(11)St5O152.511(11)P5O1651.516(11)St5O672.411(11)P5O1651.511(16)St5O83.130(14)P5O1151.511(16)St5O123.03(11)P13O291.535(13)St5O162.617(13)P14O21.545(12)St5O182.685(13)P1O261.499(14)St5O182.685(13)P1O271.535(13)St5O182.685(13)P1O281.535(13)St5O182.685(13)P1O151.513(10)St5'O182.685(13)P1O151.513(10)St5'O162.530(15)P1O152.51(2)St5'O182.685(13)P1O151.513(10)St5'O162.530(15)P1 </td <td>P6</td> <td>O19<sup>1</sup></td> <td>1.531(11)</td> <td>Sr2</td> <td>015</td> <td>3.189(12)</td>	P6	O19 <sup>1</sup>	1.531(11)	Sr2	015	3.189(12)
P2O41.525(9)Sr2O2412.755(8)P2O71.551(9)Sr2O2412.622(9)P2O51.534(9)Sr2O2112.622(9)P4O151.534(10)Sr2O122.672(13)P4O151.531(10)Sr2O192.854(12)P4O121.496(9)Sr2O1412.687(12)P4O141.499(11)Sr2O1412.687(12)P5O101.490(14)Sr2O1412.687(12)P5O1631.516(11)Sr5O672.411(11)P5O1641.516(11)Sr5O672.411(11)P5O1141.511(16)Sr5O672.411(11)P5O1151.516(11)Sr5O123.03(11)P5O1151.511(16)Sr5O123.03(11)P5O1151.511(16)Sr5O162.617(13)P710O261.499(14)Sr5O162.617(13)P110O271.535(13)Sr5O182.685(13)P1O2931.535(13)Sr5O182.685(13)P1O151.513(10)Sr5'O672.52(3)P1O151.513(10)Sr5'O162.578(14)Li2O772.51(2)Sr5'O162.67(17)Li2O7122.51(2)Sr5'O162.576(17)Li2O392.06(2)Sr5'O162.576(17)L	P6	018	1.508(15)	Sr2	O15 <sup>1</sup>	3.189(12)
P2O71.551(9)Sr2O2412.755(8)P2O61.507(10)Sr2O212.622(9)P4O151.534(9)Sr2O212.622(9)P4O151.546(10)Sr2O192.854(12)P4O131.531(10)Sr2O192.854(12)P4O121.496(9)Sr2O142.687(12)P4O141.499(11)Sr2O142.687(12)P5O101.490(14)Sr2O142.687(12)P5O1651.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O292.578(12)P5O161.511(16)Sr5O292.578(12)P5O111.511(16)Sr5O142.687(13)P5O1151.511(16)Sr5O123.03(11)P13O291.535(13)Sr5O162.617(13)P14O21.545(12)Sr5O182.685(13)P1O21.545(12)Sr5O182.685(13)P1O21.513(10)Sr5'O152.530(15)P1O151.513(10)Sr5'O672.52(3)Li2O772.51(2)Sr5'O162.576(17)Li2O392.06(2)Sr5'O162.576(17)Li2O392.06(2)Sr5'O162.576(17)Li2O392.06(2)Sr5'O162.576(17)Li3O	P2	04	1.525(9)	Sr2	O24	2.755(8)
P2061.507(10)Sr20212.622(9)P40151.534(9)Sr2021'2.622(9)P40151.546(10)Sr20192.854(12)P40131.531(10)Sr2019'2.854(12)P40121.496(9)Sr2014'2.687(12)P40141.499(11)Sr2014'2.687(12)P50101.490(14)Sr2014'2.687(12)P5016'1.516(11)Sr50152.511(11)P5016'1.516(11)Sr5067'2.411(11)P5011'1.511(16)Sr50292.578(12)P5011'1.511(16)Sr50123.303(11)P100281.489(9)Sr50123.303(11)P110291.535(13)Sr50182.685(13)P10261.545(12)Sr50182.685(13)P10271.535(13)Sr50182.685(13)P102811.513(10)Sr5'0182.663)P10151.513(10)Sr5'0123.12(3)Li207'2.51(2)Sr5'0162.530(15)Li207'2.51(2)Sr5'0162.66(3)Li203'2.60(2)Sr5'0162.576(17)Li203'2.615(18)Sr5'0183.18(4)Li203'2.615(18)Sr5'0183.18(4)Li3<	P2	07	1.551(9)	Sr2	O241	2.755(8)
P2O51.534(9)Sr2O2112.622(9)P4O151.546(10)Sr2O262.672(13)P4O131.531(10)Sr2O192.854(12)P4O121.496(9)Sr2O142.687(12)P4O141.499(11)Sr2O142.687(12)P5O101.490(14)Sr2O142.687(12)P5O161.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O292.578(12)P5O111.511(16)Sr5O292.578(12)P5O111.511(16)Sr5O163.03(11)P5O111.511(16)Sr5O162.617(13)P710O281.489(9)Sr5O162.617(13)P710O261.499(14)Sr5O182.685(13)P1O21.535(13)Sr5O182.685(13)P1O21.513(10)Sr5'O152.530(15)P1O151.513(10)Sr5'O162.578(14)Li2O772.51(2)Sr5'O123.12(3)Li2O7122.51(2)Sr5'O182.66(3)Li2O392.06(2)Sr5'O183.18(4)Li3O23162.615(18)Sr3 <sup>12</sup> O183.18(4)Li3O23162.615(18)Sr3 <sup>12</sup> O112.485(16)Li3O23162.381(17)Sr1 <sup>5</sup> O112.485(16) <t< td=""><td>P2</td><td>06</td><td>1.507(10)</td><td>Sr2</td><td>O21</td><td>2.622(9)</td></t<>	P2	06	1.507(10)	Sr2	O21	2.622(9)
P4O151.546(10)Sr2O262.672(13)P4O131.531(10)Sr2O192.854(12)P4O121.496(9)Sr2O142.687(12)P4O141.499(11)Sr2O142.687(12)P5O101.490(14)Sr2O142.687(12)P5O16 <sup>5</sup> 1.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O672.411(11)P5O1111.511(16)Sr5O292.578(12)P5O1151.511(16)Sr5O123.03(11)P13O281.489(9)Sr5O162.617(13)P7 <sup>10</sup> O261.499(14)Sr5O182.685(13)P1O291.535(13)Sr5O182.685(13)P1O211.513(10)Sr5'O162.530(15)P1O151.513(10)Sr5'O162.530(15)P1O151.513(10)Sr5'O123.12(3)Li1O28 <sup>1</sup> 2.51(2)Sr5'O123.12(3)Li2O7 <sup>7</sup> 2.51(2)Sr5'O123.12(3)Li2O7 <sup>12</sup> 2.51(2)Sr5'O182.66(3)Li2O3 <sup>9</sup> 2.06(2)Sr5'O183.18(4)Li2O3 <sup>9</sup> 2.306(13)Sr5'O183.18(4)Li3O23 <sup>16</sup> 2.615(18)Sr3 <sup>12</sup> O112.485(16)Li3O23 <sup>15</sup> 2.381(17)Sr1 <sup>5</sup> O112.48	P2	05	1.534(9)	Sr2	O21 <sup>1</sup>	2.622(9)
P4O131.531(10)Sr2O192.854(12)P4O121.496(9)Sr2O19'2.854(12)P4O141.499(11)Sr2O142.687(12)P5O101.490(14)Sr2O14'2.687(12)P5O16'1.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O292.578(12)P5O1111.511(16)Sr5O292.578(12)P5O1151.511(16)Sr5O163.030(11)P13O291.535(13)Sr5O162.617(13)P10O261.499(14)Sr5O182.658(10)P1O261.499(14)Sr5O182.658(10)P1O261.535(13)Sr5O182.658(13)P1O211.545(12)Sr5O182.658(13)P1O131.513(10)Sr5'O672.52(3)P1O151.513(10)Sr5'O672.52(3)Li1O2812.263(13)Sr5'O123.12(3)Li2O772.51(2)Sr5'O162.576(17)Li3O23162.615(18)Sr5'O183.035(15)Li3O23162.615(18)Sr5'O183.18(4)Li3O23162.615(18)Sr5'O183.18(4)Li3O23162.615(18)Sr5'O112.485(16)Li3O23162.381(17)Sr15O112.485(16) <td>P4</td> <td>015</td> <td>1.546(10)</td> <td>Sr2</td> <td>O26</td> <td>2.672(13)</td>	P4	015	1.546(10)	Sr2	O26	2.672(13)
P4         O12         1.496(9)         Sr2         O19 <sup>1</sup> 2.854(12)           P4         O14         1.499(11)         Sr2         O14         2.687(12)           P5         O10         1.490(14)         Sr2         O14 <sup>1</sup> 2.687(12)           P5         O16         1.516(11)         Sr5         O15         2.511(11)           P5         O16         1.516(11)         Sr5         O29         2.578(12)           P5         O11         1.511(16)         Sr5         O29         2.578(12)           P5         O11 <sup>5</sup> 1.511(16)         Sr5         O12         3.303(11)           P8 <sup>10</sup> O28         1.489(9)         Sr5         O12         3.303(11)           P1 <sup>3</sup> O29         1.535(13)         Sr5         O16         2.617(13)           P1 <sup>10</sup> O2         1.545(12)         Sr5         O18         2.658(10)           P1         O2         1.545(12)         Sr5         O18         2.658(13)           P1         O1         1.513(10)         Sr5'         O15         2.530(15)           Li1         O28 <sup>1</sup> 2.51(2)         Sr5'         O29         2.789(14) <td>P4</td> <td>013</td> <td>1.531(10)</td> <td>Sr2</td> <td>O19</td> <td>2.854(12)</td>	P4	013	1.531(10)	Sr2	O19	2.854(12)
P4         O14         1.499(11)         Sr2         O14         2.687(12)           P5         O10         1.490(14)         Sr2         O14 <sup>1</sup> 2.687(12)           P5         O16 <sup>5</sup> 1.516(11)         Sr5         O15         2.511(11)           P5         O16         1.516(11)         Sr5         O67         2.411(11)           P5         O11         1.511(16)         Sr5         O29         2.578(12)           P5         O11 <sup>5</sup> 1.511(16)         Sr5         O29         2.578(12)           P5         O11 <sup>5</sup> 1.511(16)         Sr5         O12         3.303(11)           P1         O28         1.489(9)         Sr5         O16         2.617(13)           P1 <sup>10</sup> O29         1.535(13)         Sr5         O18         2.685(13)           P1         O2         1.545(12)         Sr5         O18         2.685(13)           P1         O2         1.513(10)         Sr5'         O18         2.685(13)           P1         O1 <sup>5</sup> 1.513(10)         Sr5'         O16         2.530(15)           P1         O1 <sup>5</sup> 1.513(10)         Sr5'         O29         2.789(14) </td <td>P4</td> <td>012</td> <td>1.496(9)</td> <td>Sr2</td> <td>O191</td> <td>2.854(12)</td>	P4	012	1.496(9)	Sr2	O191	2.854(12)
P5O101.490(14)Sr2O1412.687(12)P5O1651.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O672.411(11)P5O111.511(16)Sr5O292.578(12)P5O1151.511(16)Sr5O83.130(14)P810O281.489(9)Sr5O162.617(13)P713O291.535(13)Sr5O162.617(13)P710O261.499(14)Sr5O182.658(10)P1O21.545(12)Sr5O182.685(13)P1O21.535(13)Sr5O182.685(13)P1O11.513(10)Sr5'O152.530(15)P1O151.513(10)Sr5'O672.52(3)Li1O2812.263(13)Sr5'O123.12(3)Li2O772.51(2)Sr5'O162.576(17)Li2O392.06(2)Sr5'O162.576(17)Li3O23162.615(18)Sr5'O183.18(4)Li3O23162.615(18)Sr312O112.621(18)Li3O23152.381(17)Sr15O112.485(16)Li3O2372.381(17)Sr14O133.019(10)Li3O172.64(2)Sr14O133.019(10)	P4	O14	1.499(11)	Sr2	O14	2.687(12)
P5O1651.516(11)Sr5O152.511(11)P5O161.516(11)Sr5O672.411(11)P5O111.511(16)Sr5O292.578(12)P5O1151.511(16)Sr5O83.130(14)P8 <sup>10</sup> O281.489(9)Sr5O123.303(11)P13O291.535(13)Sr5O162.617(13)P7 <sup>10</sup> O261.499(14)Sr5O193.217(14)P1O21.545(12)Sr5O182.658(10)P1O231.535(13)Sr5O182.658(13)P1O11.513(10)Sr5'O152.530(15)P1O151.513(10)Sr5'O672.52(3)Li1O28 <sup>1</sup> 2.263(13)Sr5'O292.789(14)Li2O772.51(2)Sr5'O123.12(3)Li2O772.51(2)Sr5'O162.576(17)Li2O392.06(2)Sr5'O162.576(17)Li3O23 <sup>10</sup> 2.615(18)Sr5'O183.18(4)Li3O23 <sup>16</sup> 2.615(18)Sr3 <sup>12</sup> O112.621(18)Li3O23 <sup>15</sup> 2.381(17)Sr1 <sup>5</sup> O252.748(7)Li1O172.58(2)Sr1 <sup>4</sup> O133.019(10)Li3O172.64(2)Sr1 <sup>4</sup> O242.736(8)	P5	O10	1.490(14)	Sr2	O14 <sup>1</sup>	2.687(12)
P5O161.516(11)Sr5O672.411(11)P5O111.511(16)Sr5O292.578(12)P5O11 <sup>5</sup> 1.511(16)Sr5O83.130(14)P8 <sup>10</sup> O281.489(9)Sr5O123.303(11)P1 <sup>3</sup> O291.535(13)Sr5O162.617(13)P7 <sup>10</sup> O261.499(14)Sr5O193.217(14)P1O21.545(12)Sr5O182.658(10)P1O21.535(13)Sr5O182.658(13)P1O11.513(10)Sr5'O152.530(15)P1O1 <sup>5</sup> 1.513(10)Sr5'O672.52(3)Li1O28 <sup>1</sup> 2.263(13)Sr5'O292.789(14)Li2O7 <sup>7</sup> 2.51(2)Sr5'O103.035(15)Li2O7 <sup>7</sup> 2.51(2)Sr5'O103.035(15)Li2O3 <sup>9</sup> 2.06(2)Sr5'O162.576(17)Li3O23 <sup>16</sup> 2.615(18)Sr5'O183.18(4)Li3O23 <sup>16</sup> 2.615(18)Sr3 <sup>12</sup> O112.621(18)Li3O23 <sup>15</sup> 2.381(17)Sr1 <sup>5</sup> O112.485(16)Li3O23 <sup>7</sup> 2.381(17)Sr1 <sup>5</sup> O252.748(7)Li1O172.58(2)Sr1 <sup>4</sup> O133.019(10)Li3O172.64(2)Sr1 <sup>4</sup> O242.736(8)	Р5	O16 <sup>5</sup>	1.516(11)	Sr5	015	2.511(11)
P5O111.511(16)Sr5O292.578(12)P5O11 <sup>5</sup> 1.511(16)Sr5O83.130(14)P8 <sup>10</sup> O281.489(9)Sr5O123.303(11)P1 <sup>3</sup> O291.535(13)Sr5O162.617(13)P7 <sup>10</sup> O261.499(14)Sr5O193.217(14)P1O21.545(12)Sr5O182.658(10)P1O21.545(12)Sr5O182.658(13)P1O11.513(10)Sr5'O152.530(15)P1O1 <sup>5</sup> 1.513(10)Sr5'O672.52(3)Li1O28 <sup>1</sup> 2.263(13)Sr5'O292.789(14)Li2O7 <sup>7</sup> 2.51(2)Sr5'O182.66(3)Li2O7 <sup>12</sup> 2.51(2)Sr5'O103.035(15)Li2O3 <sup>9</sup> 2.06(2)Sr5'O103.035(15)Li3O23 <sup>16</sup> 2.27(2)Sr5'O182.546(16)Li3O23 <sup>16</sup> 2.615(18)Sr5'O183.18(4)Li3O23 <sup>16</sup> 2.615(18)Sr1 <sup>2</sup> O112.621(18)Li3O23 <sup>15</sup> 2.381(17)Sr1 <sup>5</sup> O112.485(16)Li3O23 <sup>7</sup> 2.381(17)Sr1 <sup>5</sup> O122.748(7)Li1O172.58(2)Sr1 <sup>4</sup> O133.019(10)Li3O172.64(2)Sr1 <sup>4</sup> O242.736(8)	P5	O16	1.516(11)	Sr5	O6 <sup>7</sup>	2.411(11)
P5O1151.511(16)Sr5O83.130(14)P810O281.489(9)Sr5O123.303(11)P13O291.535(13)Sr5O162.617(13)P710O261.499(14)Sr5O193.217(14)P1O21.545(12)Sr5O182.658(10)P1O2931.535(13)Sr5O182.685(13)P1O11.513(10)Sr5'O152.530(15)P1O151.513(10)Sr5'O672.52(3)Li1O2812.263(13)Sr5'O292.789(14)Li2O772.51(2)Sr5'O123.12(3)Li2O772.51(2)Sr5'O162.576(17)Li3O2812.306(13)Sr5'O182.546(16)Li3O23162.615(18)Sr5'O183.18(4)Li3O23152.381(17)Sr15O112.621(18)Li3O2372.381(17)Sr15O252.748(7)Li1O172.58(2)Sr14O133.019(10)Li3O172.64(2)Sr14O242.736(8)	P5	011	1.511(16)	Sr5	O29	2.578(12)
P810O281.489(9)Sr5O123.303(11)P13O291.535(13)Sr5O162.617(13)P710O261.499(14)Sr5O193.217(14)P1O21.545(12)Sr5O182.658(10)P1O2931.535(13)Sr5O182.685(13)P1O11.513(10)Sr5'O152.530(15)P1O11.513(10)Sr5'O672.52(3)Li1O2812.263(13)Sr5'O672.52(3)Li2O772.51(2)Sr5'O82.66(3)Li2O772.51(2)Sr5'O103.035(15)Li2O392.06(2)Sr5'O162.576(17)Li3O2812.306(13)Sr5'O183.18(4)Li3O23162.615(18)Sr312O112.621(18)Li3O23152.381(17)Sr15O112.485(16)Li3O2372.381(17)Sr15O252.748(7)Li1O172.58(2)Sr14O133.019(10)Li3O172.64(2)Sr14O242.736(8)	Р5	O11 <sup>5</sup>	1.511(16)	Sr5	08	3.130(14)
P13O291.535(13)Sr5O162.617(13)P7 <sup>10</sup> O261.499(14)Sr5O193.217(14)P1O21.545(12)Sr5O182.658(10)P1O29 <sup>3</sup> 1.535(13)Sr5O182.685(13)P1O11.513(10)Sr5'O152.530(15)P1O1 <sup>5</sup> 1.513(10)Sr5'O6 <sup>7</sup> 2.52(3)Li1O28 <sup>1</sup> 2.263(13)Sr5'O292.789(14)Li2O7 <sup>7</sup> 2.51(2)Sr5'O123.12(3)Li2O7 <sup>12</sup> 2.51(2)Sr5'O162.576(17)Li2O3 <sup>9</sup> 2.06(2)Sr5'O162.576(17)Li3O28 <sup>1</sup> 2.306(13)Sr5'O183.035(15)Li3O23 <sup>16</sup> 2.615(18)Sr5'O183.18(4)Li3O23 <sup>16</sup> 2.615(18)Sr3 <sup>12</sup> O112.621(18)Li3O23 <sup>15</sup> 2.381(17)Sr1 <sup>5</sup> O112.485(16)Li3O23 <sup>7</sup> 2.381(17)Sr1 <sup>5</sup> O252.748(7)Li1O172.58(2)Sr1 <sup>4</sup> O133.019(10)Li3O172.64(2)Sr1 <sup>4</sup> O242.736(8)	P8 <sup>10</sup>	O28	1.489(9)	Sr5	012	3.303(11)
$P7^{10}$ $O26$ $1.499(14)$ $Sr5$ $O19$ $3.217(14)$ P1 $O2$ $1.545(12)$ $Sr5$ $O1^8$ $2.658(10)$ P1 $O29^3$ $1.535(13)$ $Sr5$ $O18$ $2.685(13)$ P1 $O1$ $1.513(10)$ $Sr5'$ $O15$ $2.530(15)$ P1 $O1^5$ $1.513(10)$ $Sr5'$ $O6^7$ $2.52(3)$ Li1 $O28^1$ $2.263(13)$ $Sr5'$ $O29$ $2.789(14)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O8$ $2.66(3)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.621(18)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	P1 <sup>3</sup>	O29	1.535(13)	Sr5	016	2.617(13)
P1 $O2$ $1.545(12)$ $Sr5$ $O1^8$ $2.658(10)$ P1 $O29^3$ $1.535(13)$ $Sr5$ $O18$ $2.685(13)$ P1 $O1$ $1.513(10)$ $Sr5'$ $O15$ $2.530(15)$ P1 $O1^5$ $1.513(10)$ $Sr5'$ $O6^7$ $2.52(3)$ Li1 $O28^1$ $2.263(13)$ $Sr5'$ $O29$ $2.789(14)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O12$ $3.12(3)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O16$ $2.576(17)$ Li2 $O8^5$ $2.27(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{16}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{7}$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	P7 <sup>10</sup>	O26	1.499(14)	Sr5	019	3.217(14)
P1 $O29^3$ $1.535(13)$ $Sr5$ $O18$ $2.685(13)$ P1 $O1$ $1.513(10)$ $Sr5'$ $O15$ $2.530(15)$ P1 $O1^5$ $1.513(10)$ $Sr5'$ $O6^7$ $2.52(3)$ Li1 $O28^1$ $2.263(13)$ $Sr5'$ $O29$ $2.789(14)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O8$ $2.66(3)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O12$ $3.12(3)$ Li2 $O7^{12}$ $2.51(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	P1	02	1.545(12)	Sr5	O1 <sup>8</sup>	2.658(10)
P1O1 $1.513(10)$ Sr5'O15 $2.530(15)$ P1O1 <sup>5</sup> $1.513(10)$ Sr5'O6 <sup>7</sup> $2.52(3)$ Li1O28 <sup>1</sup> $2.263(13)$ Sr5'O29 $2.789(14)$ Li2O7 <sup>7</sup> $2.51(2)$ Sr5'O8 $2.66(3)$ Li2O7 <sup>12</sup> $2.51(2)$ Sr5'O12 $3.12(3)$ Li2O3 <sup>9</sup> $2.06(2)$ Sr5'O10 $3.035(15)$ Li2O8 <sup>5</sup> $2.27(2)$ Sr5'O16 $2.576(17)$ Li3O28 <sup>1</sup> $2.306(13)$ Sr5'O18 $3.18(4)$ Li3O23 <sup>16</sup> $2.615(18)$ Sr5'O11 $2.621(18)$ Li3O23 <sup>15</sup> $2.381(17)$ Sr1 <sup>5</sup> O11 $2.485(16)$ Li3O23 <sup>7</sup> $2.381(17)$ Sr1 <sup>5</sup> O25 $2.748(7)$ Li1O17 $2.58(2)$ Sr1 <sup>4</sup> O13 $3.019(10)$ Li3O17 $2.64(2)$ Sr1 <sup>4</sup> O24 $2.736(8)$	P1	O29 <sup>3</sup>	1.535(13)	Sr5	018	2.685(13)
P1 $O1^5$ $1.513(10)$ $Sr5'$ $O6^7$ $2.52(3)$ Li1 $O28^1$ $2.263(13)$ $Sr5'$ $O29$ $2.789(14)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O8$ $2.66(3)$ Li2 $O7^{12}$ $2.51(2)$ $Sr5'$ $O12$ $3.12(3)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O8^5$ $2.27(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{16}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	P1	01	1.513(10)	Sr5'	015	2.530(15)
Li1 $O28^1$ $2.263(13)$ $Sr5'$ $O29$ $2.789(14)$ Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O8$ $2.66(3)$ Li2 $O7^{12}$ $2.51(2)$ $Sr5'$ $O12$ $3.12(3)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O8^5$ $2.27(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O18$ $2.546(16)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	P1	O1 <sup>5</sup>	1.513(10)	Sr5'	O6 <sup>7</sup>	2.52(3)
Li2 $O7^7$ $2.51(2)$ $Sr5'$ $O8$ $2.66(3)$ Li2 $O7^{12}$ $2.51(2)$ $Sr5'$ $O12$ $3.12(3)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O8^5$ $2.27(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O18$ $2.546(16)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	Li1	O281	2.263(13)	Sr5'	O29	2.789(14)
Li2 $O7^{12}$ $2.51(2)$ $Sr5'$ $O12$ $3.12(3)$ Li2 $O3^9$ $2.06(2)$ $Sr5'$ $O10$ $3.035(15)$ Li2 $O8^5$ $2.27(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O1^8$ $2.546(16)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	Li2	O7 <sup>7</sup>	2.51(2)	Sr5'	08	2.66(3)
Li2 $O3^9$ 2.06(2)Sr5'O103.035(15)Li2 $O8^5$ 2.27(2)Sr5'O162.576(17)Li3 $O28^1$ 2.306(13)Sr5'O182.546(16)Li3 $O23^{16}$ 2.615(18)Sr5'O183.18(4)Li3 $O23^{10}$ 2.615(18)Sr3^{12}O112.621(18)Li3 $O23^{15}$ 2.381(17)Sr1^5O112.485(16)Li3 $O23^7$ 2.381(17)Sr1^5O252.748(7)Li1O172.58(2)Sr1^4O133.019(10)Li3O172.64(2)Sr1^4O242.736(8)	Li2	O7 <sup>12</sup>	2.51(2)	Sr5'	012	3.12(3)
Li2 $O8^5$ $2.27(2)$ $Sr5'$ $O16$ $2.576(17)$ Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O1^8$ $2.546(16)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	Li2	O39	2.06(2)	Sr5'	O10	3.035(15)
Li3 $O28^1$ $2.306(13)$ $Sr5'$ $O1^8$ $2.546(16)$ Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	Li2	O8 <sup>5</sup>	2.27(2)	Sr5'	016	2.576(17)
Li3 $O23^{16}$ $2.615(18)$ $Sr5'$ $O18$ $3.18(4)$ Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	Li3	O28 <sup>1</sup>	2.306(13)	Sr5'	O18	2.546(16)
Li3 $O23^{10}$ $2.615(18)$ $Sr3^{12}$ $O11$ $2.621(18)$ Li3 $O23^{15}$ $2.381(17)$ $Sr1^5$ $O11$ $2.485(16)$ Li3 $O23^7$ $2.381(17)$ $Sr1^5$ $O25$ $2.748(7)$ Li1 $O17$ $2.58(2)$ $Sr1^4$ $O13$ $3.019(10)$ Li3 $O17$ $2.64(2)$ $Sr1^4$ $O24$ $2.736(8)$	Li3	O23 <sup>16</sup>	2.615(18)	Sr5'	O18	3.18(4)
Li3O23152.381(17)Sr15O112.485(16)Li3O2372.381(17)Sr15O252.748(7)Li1O172.58(2)Sr14O133.019(10)Li3O172.64(2)Sr14O242.736(8)	Li3	O23 <sup>10</sup>	2.615(18)	Sr312	011	2.621(18)
Li3O2372.381(17)Sr15O252.748(7)Li1O172.58(2)Sr14O133.019(10)Li3O172.64(2)Sr14O242.736(8)	Li3	O23 <sup>15</sup>	2.381(17)	Sr1 <sup>5</sup>	011	2.485(16)
Li1O172.58(2)Sr14O133.019(10)Li3O172.64(2)Sr14O242.736(8)	Li3	O23 <sup>7</sup>	2.381(17)	Sr1 <sup>5</sup>	O25	2.748(7)
Li3 O17 2.64(2) Sr1 <sup>4</sup> O24 2.736(8)	Li1	017	2.58(2)	Sr1 <sup>4</sup>	013	3.019(10)
	Li3	O17	2.64(2)	Sr1 <sup>4</sup>	O24	2.736(8)

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Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4 <sup>5</sup>	Al4	O4 <sup>14</sup>	178.9(7)	O18	Na1	03	107.8(4)
O4 <sup>5</sup>	Al4	O86	90.7(4)	O18	Na1	08	60.6(4)
O4 <sup>14</sup>	Al4	O8 <sup>6</sup>	90.0(4)	O1 <sup>8</sup>	Na1	09	107.4(5)
O4 <sup>14</sup>	Al4	O813	90.7(4)	O18	Na1	O2 <sup>3</sup>	58.7(4)
O4 <sup>5</sup>	Al4	O813	90.0(4)	O4 <sup>3</sup>	Na1	07	108.2(4)
O4 <sup>5</sup>	Al4	01	87.8(4)	O4 <sup>3</sup>	Na1	03	64.4(4)
O4 <sup>5</sup>	Al4	O1 <sup>17</sup>	91.5(4)	O4 <sup>3</sup>	Na1	08	66.2(4)
O4 <sup>14</sup>	Al4	O1 <sup>17</sup>	87.8(4)	O4 <sup>3</sup>	Na1	05	96.3(4)
O86	Al4	O813	91.3(7)	O4 <sup>3</sup>	Na1	09	108.4(5)
01	Al4	O86	177.0(5)	O4 <sup>3</sup>	Na1	O2 <sup>3</sup>	79.6(5)
O1 <sup>17</sup>	Al4	O86	86.1(4)	O4 <sup>3</sup>	Na1	O1 <sup>8</sup>	64.2(4)
01	Al4	O813	86.1(4)	07	Na1	O3	122.0(4)

(b)

<sup>1</sup>+X,1-Y,+Z; <sup>2</sup>-1/2+X,1/2+Y,+Z; <sup>3</sup>1/2-X,1/2-Y,1-Z; <sup>4</sup>-1/2+X,1/2-Y,+Z; <sup>5</sup>+X,-Y,+Z; <sup>6</sup>-1/2+X,-1/2+Y,+Z; <sup>7</sup>1/2+X,1/2-Y,+Z; <sup>8</sup>1/2-X,1/2+Y,1-Z; <sup>9</sup>1-X,-Y,1-Z; <sup>10</sup>1/2-X,1/2-Y,-Z; <sup>11</sup>1/2-X,-1/2+Y,-Z; <sup>12</sup>1/2+X,-1/2+Y,+Z; <sup>13</sup>1/2-X,-1/2+Y,1-Z; <sup>14</sup>-X,-Y,1-Z; <sup>15</sup>1/2+X,1/2+Y,+Z; <sup>16</sup>1/2-X,1/2+Y,-Z; <sup>17</sup>-X,+Y,1-Z; <sup>18</sup>1-X,-Y,-Z

Li2	O10	2.00(2)	Sr1 <sup>4</sup>	O23	2.626(8)
Li1	O26	2.25(2)	Sr5 <sup>4</sup>	O6	2.411(11)
Li2 <sup>2</sup>	07	2.51(2)	Sr5 <sup>'4</sup>	O6	2.52(3)
Li1	O28	2.263(13)	Sr5 <sup>1</sup>	O29	2.578(12)
Li3	O28	2.306(13)	Sr5 <sup>1</sup>	O29	2.789(14)
Li310	O23	2.615(18)	$Sr1^1$	017	2.8810(18)
Li36	O23	2.381(17)	Sr3 <sup>12</sup>	O10	2.853(15)
Li19	03	2.06(2)	Sr5 <sup>'5</sup>	O10	3.035(15)
Li2	08	2.27(2)	Sr3 <sup>3</sup>	02	2.954(13)
Na1 <sup>3</sup>	04	2.266(14)	Sr5'13	01	2.546(16)
Nal	07	2.526(12)	Sr1 <sup>4</sup>	014	2.654(12)
Na1 <sup>5</sup>	03	2.874(11)	Sr415	O18	2.721(14)
Nal	03	2.874(11)	Sr51	018	2.685(13)
Na2	O28	2.446(8)	Sr5'1	O18	3.18(4)
Na2	O20	2.415(9)	Sr513	01	2.658(10)
Na1	08	2.622(14)			

		0.012		~ -			
0117	Al4	0813	177.0(5)	07	Nal	08	173.8(5)
011/	Al4	01	96.5(6)	07	Nal	09	129.0(5)
013	Al2	0135	86.0(6)	07	Nal	023	61.3(4)
0135	Al2	023	170.8(5)	07	Nal	018	119.9(5)
O135	Al2	O235	90.6(4)	03	Na1	09	51.0(4)
013	Al2	023	90.6(4)	08	Na1	03	54.0(4)
013	A12	O23 <sup>5</sup>	170.8(5)	08	Na1	09	53.4(4)
013	A12	O17 <sup>6</sup>	86.3(4)	05	Na1	07	62.2(4)
O13 <sup>5</sup>	A12	O17 <sup>6</sup>	86.3(4)	05	Na1	03	61.9(4)
O13 <sup>5</sup>	Al2	O22	96.2(4)	05	Na1	08	115.0(5)
013	Al2	O22	96.2(4)	05	Na1	09	79.7(5)
O23	A12	O23 <sup>5</sup>	91.4(5)	05	Na1	O2 <sup>3</sup>	118.4(5)
O23	Al2	O17 <sup>6</sup>	84.9(4)	05	Na1	O18	160.3(5)
O23 <sup>5</sup>	Al2	O17 <sup>6</sup>	84.9(4)	012	Na1	O4 <sup>3</sup>	166.6(6)
O22	Al2	O23	92.7(4)	012	Na1	07	79.6(4)
O22	A12	O23 <sup>5</sup>	92.7(4)	012	Na1	O3	121.4(5)
O22	Al2	O17 <sup>6</sup>	176.5(5)	O12	Na1	08	106.5(5)
O25 <sup>18</sup>	Al1	O25	180.0(5)	O12	Na1	05	97.1(5)
O25 <sup>18</sup>	Al1	O24 <sup>10</sup>	87.6(3)	O12	Na1	09	72.6(5)
O25	Al1	O24 <sup>10</sup>	92.4(3)	012	Na1	O2 <sup>3</sup>	95.3(5)
O25 <sup>18</sup>	Al1	O2411	87.6(3)	012	Na1	O18	102.5(5)
O25	Al1	O24 <sup>12</sup>	87.6(3)	O2 <sup>3</sup>	Na1	03	143.3(5)
O25 <sup>18</sup>	Al1	O24 <sup>12</sup>	92.4(3)	O2 <sup>3</sup>	Na1	08	118.5(5)
O25	Al1	O24 <sup>7</sup>	87.6(3)	O2 <sup>3</sup>	Na1	09	160.0(5)
O25 <sup>18</sup>	Al1	O24 <sup>7</sup>	92.4(3)	O28	Na2	O28 <sup>10</sup>	180
O25	Al1	O2411	92.4(3)	O28 <sup>10</sup>	Na2	O26 <sup>10</sup>	90.2(3)
O24 <sup>7</sup>	Al1	O2411	180.0(8)	O28 <sup>10</sup>	Na2	O26	89.8(3)
O24 <sup>11</sup>	Al1	O24 <sup>10</sup>	88.1(5)	O28	Na2	O26	90.2(3)
O24 <sup>7</sup>	Al1	O24 <sup>12</sup>	88.1(5)	O28	Na2	O26 <sup>10</sup>	89.8(3)
O24 <sup>10</sup>	Al1	O24 <sup>12</sup>	180.0(8)	O20 <sup>10</sup>	Na2	O21	116.0(3)
O24 <sup>11</sup>	Al1	O24 <sup>12</sup>	91.9(5)	O20 <sup>10</sup>	Na2	O26 <sup>10</sup>	120.8(3)
O24 <sup>7</sup>	Al1	O24 <sup>10</sup>	91.9(5)	O26	Lil	O28	106.1(6)
O15	A15	O20	154.8(5)	O26	Lil	O28 <sup>1</sup>	106.1(6)
015	A15	O21	89.8(5)	O26	Li1	017	141.4(10)
015	A15	016	82.2(5)	O3 <sup>9</sup>	Li2	O7 <sup>12</sup>	69.3(7)
022	A15	015	104.5(5)	O3 <sup>9</sup>	Li2	O7 <sup>7</sup>	69.3(7)
022	A15	O20	100.6(5)	O3 <sup>9</sup>	Li2	08	103.1(8)
022	A15	021	101 9(4)	039	Li2	085	103 1(8)
022	A15	016	105 4(5)	08	Li2	077	114 9(3)
073	Δ13	0713	86 5(5)	085	Li2	$07^{7}$	172 4(10)
015	AD	07.5	00.3(3)	005	LIZ	07	1/2.4(10)

O7 <sup>13</sup>	A13	02	84.7(4)	08	Li2	O7 <sup>12</sup>	172.4(10)
O7 <sup>3</sup>	A13	02	84.7(4)	O8 <sup>5</sup>	Li2	O7 <sup>12</sup>	114.9(3)
O3	A13	O7 <sup>3</sup>	86.8(4)	08	Li2	O8 <sup>5</sup>	65.8(8)
O3	A13	O7 <sup>13</sup>	86.8(4)	O10	Li2	O7 <sup>12</sup>	90.7(8)
O3	A13	02	168.3(6)	O10	Li2	O7 <sup>7</sup>	90.7(8)
O5	A13	O7 <sup>13</sup>	177.3(4)	O10	Li2	O39	156.3(13)
05	A13	O7 <sup>3</sup>	91.4(4)	O10	Li2	08	96.8(9)
O5 <sup>5</sup>	A13	O7 <sup>13</sup>	91.4(4)	O10	Li2	O8 <sup>5</sup>	96.8(9)
O5 <sup>5</sup>	A13	O7 <sup>3</sup>	177.3(4)	O28 <sup>1</sup>	Li3	O28	121.4(9)
05	A13	03	91.4(4)	O28 <sup>1</sup>	Li3	O23 <sup>16</sup>	60.7(4)
O5 <sup>5</sup>	A13	03	91.4(4)	O28	Li3	O23 <sup>16</sup>	115.0(7)
O5 <sup>5</sup>	A13	05	90.6(5)	O28 <sup>1</sup>	Li3	O23 <sup>15</sup>	79.8(3)
O5 <sup>5</sup>	A13	02	96.8(4)	O281	Li3	O23 <sup>10</sup>	115.0(7)
05	Al3	02	96.8(4)	O28	Li3	O23 <sup>15</sup>	145.4(8)
O28 <sup>10</sup>	P8	O24	113.0(5)	O28	Li3	O23 <sup>10</sup>	60.7(4)
O28 <sup>10</sup>	P8	O23	111.9(5)	O281	Li3	O23 <sup>7</sup>	145.4(8)
O28 <sup>10</sup>	P8	O21	111.5(5)	O28	Li3	O23 <sup>7</sup>	79.8(3)
O28 <sup>10</sup>	P8	Na2	56.8(3)	O28	Li3	O17	88.3(6)
09	P3	03	109.9(8)	O28 <sup>1</sup>	Li3	017	88.3(6)
09	Р3	08	110.6(6)	O23 <sup>10</sup>	Li3	O23 <sup>16</sup>	63.0(5)
09	P3	O8 <sup>5</sup>	110.6(6)	O23 <sup>15</sup>	Li3	O23 <sup>10</sup>	139.3(8)
O8 <sup>5</sup>	P3	03	109.2(5)	O23 <sup>15</sup>	Li3	O23 <sup>16</sup>	99.1(5)
08	P3	03	109.2(5)	O23 <sup>15</sup>	Li3	O23 <sup>7</sup>	70.1(6)
O8 <sup>5</sup>	P3	08	107.2(9)	O23 <sup>7</sup>	Li3	O23 <sup>16</sup>	139.3(8)
O23	P8	O24	107.3(4)	O23 <sup>7</sup>	Li3	O23 <sup>10</sup>	99.1(5)
O23	P8	O21	107.3(5)	O23 <sup>10</sup>	Li3	O17	147.5(3)
O21	P8	O24	105.4(5)	O23 <sup>7</sup>	Li3	017	63.7(5)
O20	P7	O25	106.9(4)	O23 <sup>16</sup>	Li3	O17	147.5(3)
O20 <sup>5</sup>	P7	O25	106.9(4)	O23 <sup>15</sup>	Li3	O17	63.7(5)
O20	P7	O20 <sup>5</sup>	106.4(7)	O26	Li1	O28	106.1(6)
O26 <sup>10</sup>	P7	O25	113.3(7)	A15	022	A12	121.6(3)
O26 <sup>10</sup>	P7	O20	111.5(5)	A15 <sup>5</sup>	O22	Al2	121.6(3)
O26 <sup>10</sup>	P7	O20 <sup>5</sup>	111.5(5)	A15	022	A15 <sup>5</sup>	115.8(6)
O191	P6	O17	107.8(5)	O14	P4	015	107.7(7)
O19	P6	O17	107.8(5)	O14	P4	013	109.9(6)
O18	P6	017	112.2(8)	O10	P5	O16	112.1(6)
O18	P6	O19 <sup>1</sup>	110.2(6)	O10	Р5	O16 <sup>5</sup>	112.1(6)
O18	P6	019	110.2(6)	O10	P5	O11 <sup>5</sup>	109.9(9)
O4	P2	07	108.4(5)	O10	P5	011	109.9(9)
O4	P2	05	109.2(5)	011	P5	O16 <sup>5</sup>	95.3(8)
			. /				

O6	P2	O4	112.9(6)	O11 <sup>5</sup>	Р5	O16	95.3(8)
O6	P2	07	109.5(5)	O11 <sup>5</sup>	Р5	O16 <sup>5</sup>	119.0(9)
06	P2	05	107.9(5)	O11	Р5	O11 <sup>5</sup>	28.2(12)
05	P2	07	108.9(5)				

<sup>1</sup>+X,1-Y,+Z;+Z; <sup>3</sup>1/2-X,1/2+Y,1-Z; <sup>5</sup>+X,-Y,+Z; <sup>6</sup>-1/2+X,-1/2+Y,+Z; <sup>7</sup>1/2+X,1/2-Y,+Z; <sup>8</sup>1/2-X,1/2-Y,1-Z; <sup>9</sup>1/2-X,1/2+Y,-Z; <sup>10</sup>1/2-X,-1/2+Y,-Z; <sup>11</sup>1/2+X,-1/2+Y,+Z; <sup>12</sup>1/2-X,-1/2+Y,1-Z; <sup>13</sup>1-X,+Y,1-Z; <sup>14</sup>-X,-Y,1-Z; <sup>15</sup>1/2+X,1/2+Y,+Z; <sup>16</sup>1/2-X,1/2+Y,-Z; <sup>17</sup>-X,+Y,1-Z; <sup>18</sup>1-X,+Y,-Z



Fig. S1 The photograph of 1 crystal



Fig.S2 Experimental and simulated powder X-ray diffraction patterns for 1.



Fig.S3 The symmetric unit of 1 crystal



 $\mbox{Fig.S4}$  The coordinate environments of the  $\mbox{Li}^+$  and  $\mbox{Na}^+$  cations





Fig.S5 The coordinate environments of the  $Sr^{2+}$  cations



Fig.S6 IR spectra



Fig.S7 Band structure

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