Supporting Information

$Li_6Na_3Sr_{14}Al_{11}P_{22}O_{90}$: An Oxo-Centered Al_3 Cluster Based Phosphate Constructed from Two Types of (3,6)-Connected kgd Layers

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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 × 0.4 mm × 0.1 mm were carried out on a Bruker APEX-II CCD detector at 298 K using Mo Kα radiation (λ = 0.71073 Å). The collection of the intensity data, cell refinement, and data reduction were performed by the program CrysAlisPro[1]. The structures were solved by the direct method with the program SHELXS and refined by the full-matrix least-squares program SHELXL[2]. The structures were checked with the aid of the program PLATON[3]. 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 Kα radiation (λ = 1.5418 Å) at room temperature. The scanning step width of 0.02° and scanning rate of 0.05 °s^{-1} were applied to record the patterns in the 2θ 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 crystallographic 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^{-1} on a Nicolet Model 5DX spectrometer. The IR spectrum for **1** (Fig.S6) displays the absorption peaks at 465 cm^{-1} (due to Al-O structural units), 539 cm^{-1} (the deformation modes of P–O (PO_4^{3-}) groups), 713 cm^{-1} (the ν_s of P-O-P groups), 883 cm^{-1} (due to P–O–P asymmetric bending vibrations), and 1089 cm^{-1} (a normal vibrational mode in PO_4^{3-} group arising out of ν_3-symmetric stretching).[4] 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 $BaSO_4$ 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[5]: $F(R) = (1-R)^2/(2R) = K/S$, 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.[6]

8. Computational details

The periodic density functional theory (DFT) calculations were performed using the VASP within the MedeA software.[7] 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[8] were employed to describe the electron-ion interactions. The exchange-correlation energy was described by meta-GGA functional (revTPSS)[9], 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 2×3×1 Monkhorst-Pack[10] 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	$Li_6Na_3Sr_{14}Al_{11}P_{22}O_{90}$
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)
γ/°	90
Volume/$Å^3$	3483.39(11)
Z	2
$\rho_{calc}g/cm^3$	3.5802
μ/mm^{-1}	11.461
F(000)	3516.5
Crystal size/mm	0.3 × 0.4 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ 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^2	1.036
Final R indexes [I>=2σ (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 $Å^{-3}$	1.63/-1.17

[a] $R1=\sum||F_o|-|F_c||/\sum|F_o|$, and $wR2=[w(F_o^2-F_c^2)^2/w(F_o^2)^2]^{1/2}$

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

Atom	*x*	*y*	*z*	U(eq)

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)
P3	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)
P5	4562(3)	0	2480(2)	33.9(10)
P1	1138(3)	0	5862(2)	35.3(10)
Al3	2626(3)	0	5121(2)	30.9(11)
Al4	0	-2452(5)	5000	36.5(12)
Al2	1232(3)	0	1543(2)	32.4(11)
Al1	5000	0	0	30.1(15)
Al5	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)
O8	4439(7)	1210(9)	4336(5)	56(3)
O5	2066(5)	1319(8)	4494(4)	35.6(18)
O21	2122(5)	2565(9)	960(4)	39(2)
O12	2304(6)	2644(9)	3174(4)	48(2)
O17	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)

O9	3135(11)	0	3632(8)	77(5)
O2	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)
O11	5185(11)	-362(15)	2166(9)	44(5)
O4	920(6)	2435(9)	4749(5)	48(2)
O15	2788(6)	2414(11)	2245(5)	56(3)
O7	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)

Table S3. Bond lengths (Å) (a) and angles (deg.) (b)

(a)

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Al5	O15	1.820(10)	Na1	O5	2.321(12)
Al3[3]	O7	1.923(9)	Na2	O21	2.417(8)
Al1	O25	1.904(11)	Na1	O12	2.135(12)
Al2	O13	1.868(10)	Na2[16]	O26	2.640(3)

Al1[2]	O24	1.925(8)	Na2	O26	2.640(3)
Al2	O23	1.910(9)	Na1[5]	O9	2.875(12)
Al5	O20	1.853(9)	Na1	O9	2.875(12)
Al4[15]	O8	1.951(11)	Na1[13]	O2	2.584(10)
Al5	O21	1.855(9)	Na1[3]	O2	2.584(10)
Al2[15]	O17	2.026(13)	Na1[13]	O1	2.574(12)
Al5	O16	1.851(11)	Na1	O4[3]	2.266(14)
Al4	O1	1.885(10)	Na1	O2[3]	2.584(10)
Al4	O4[14]	1.842(9)	Na1	O1[8]	2.574(12)
Al4	O4[5]	1.842(9)	Na2	O28[10]	2.446(8)
Al4	O8[13]	1.951(11)	Na2	O20[10]	2.415(9)
Al4	O8[6]	1.951(11)	Na2	O21[10]	2.417(8)
Al4	O1[17]	1.885(10)	Na2	O26[10]	2.640(3)
Al2	O13[5]	1.868(10)	Sr3	O7[1]	2.638(8)
Al2	O23[5]	1.910(9)	Sr3	O7	2.638(8)
Al2	O17[6]	2.026(13)	Sr3	O29	2.878(14)
Al2	O22	1.898(12)	Sr3	O12[1]	2.636(10)
Al1	O25[18]	1.904(11)	Sr3	O12	2.636(10)
Al1	O24[12]	1.925(8)	Sr3	O10[2]	2.853(15)
Al1	O24[10]	1.925(8)	Sr3	O2[3]	2.954(13)
Al1	O24[7]	1.925(8)	Sr3	O14	2.619(10)
Al1	O24[11]	1.925(8)	Sr3	O14[1]	2.619(10)
Al5	O22	1.809(7)	Sr3	O11[2]	2.621(18)
Al5[5]	O22	1.809(7)	Sr3	O11[4]	2.621(18)
Al3	O7[3]	1.923(9)	Sr4	O13	2.609(9)
Al3	O7[13]	1.923(9)	Sr4	O13[5]	2.609(9)
Al3	O3	1.898(13)	Sr4	O6	2.595(10)
Al3	O5	1.893(9)	Sr4	O6[5]	2.595(10)
Al3	O5[5]	1.893(9)	Sr4	O5	2.811(8)
Al3	O2	1.944(13)	Sr4	O5[5]	2.811(8)
Al4[14]	O4	1.842(9)	Sr4	O12	3.062(10)
P3	O3	1.540(13)	Sr4	O12[5]	3.062(10)
P3	O8[5]	1.532(10)	Sr4	O9	2.574(18)
P3	O8	1.532(10)	Sr4	O18[6]	2.721(14)
P3	O9	1.485(17)	Sr1	O25	2.748(7)
P8	O24	1.545(9)	Sr1	O13[7]	3.019(11)
P8	O28[10]	1.489(9)	Sr1	O24[7]	2.736(8)
P8	O23	1.529(9)	Sr1	O28	2.642(8)
P8	O21	1.536(9)	Sr1	O23[7]	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[5]	1.533(9)	Sr1	O16	3.067(13)
Sr5	O29	2.578(12)	Sr1	O19	2.709(11)
P7	O26[10]	1.499(14)	Sr1	O14[7]	2.654(12)
P6	O17	1.552(13)	Sr1	O11[5]	2.485(16)
P6	O19	1.531(11)	Sr1	O11	3.077(17)
P6	O19[1]	1.531(11)	Sr2	O15	3.189(12)
P6	O18	1.508(15)	Sr2	O15[1]	3.189(12)
P2	O4	1.525(9)	Sr2	O24	2.755(8)
P2	O7	1.551(9)	Sr2	O24[1]	2.755(8)
P2	O6	1.507(10)	Sr2	O21	2.622(9)
P2	O5	1.534(9)	Sr2	O21[1]	2.622(9)
P4	O15	1.546(10)	Sr2	O26	2.672(13)
P4	O13	1.531(10)	Sr2	O19	2.854(12)
P4	O12	1.496(9)	Sr2	O19[1]	2.854(12)
P4	O14	1.499(11)	Sr2	O14	2.687(12)
P5	O10	1.490(14)	Sr2	O14[1]	2.687(12)
P5	O16[5]	1.516(11)	Sr5	O15	2.511(11)
P5	O16	1.516(11)	Sr5	O6[7]	2.411(11)
P5	O11	1.511(16)	Sr5	O29	2.578(12)
P5	O11[5]	1.511(16)	Sr5	O8	3.130(14)
P8[10]	O28	1.489(9)	Sr5	O12	3.303(11)
P1[3]	O29	1.535(13)	Sr5	O16	2.617(13)
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[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	O10	2.00(2)	Sr1[4]	O23	2.626(8)
Li1	O26	2.25(2)	Sr5[4]	O6	2.411(11)
Li2[2]	O7	2.51(2)	Sr5'[4]	O6	2.52(3)
Li1	O28	2.263(13)	Sr5[1]	O29	2.578(12)
Li3	O28	2.306(13)	Sr5'[1]	O29	2.789(14)
Li3[10]	O23	2.615(18)	Sr1[1]	O17	2.8810(18)
Li3[6]	O23	2.381(17)	Sr3[12]	O10	2.853(15)
Li1[9]	O3	2.06(2)	Sr5'[5]	O10	3.035(15)
Li2	O8	2.27(2)	Sr3[3]	O2	2.954(13)
Na1[3]	O4	2.266(14)	Sr5'[13]	O1	2.546(16)
Na1	O7	2.526(12)	Sr1[4]	O14	2.654(12)
Na1[5]	O3	2.874(11)	Sr4[15]	O18	2.721(14)
Na1	O3	2.874(11)	Sr5[1]	O18	2.685(13)
Na2	O28	2.446(8)	Sr5'[1]	O18	3.18(4)
Na2	O20	2.415(9)	Sr5[13]	O1	2.658(10)
Na1	O8	2.622(14)			

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

(b)

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O4[5]	Al4	O4[14]	178.9(7)	O1[8]	Na1	O3	107.8(4)
O4[5]	Al4	O8[6]	90.7(4)	O1[8]	Na1	O8	60.6(4)
O4[14]	Al4	O8[6]	90.0(4)	O1[8]	Na1	O9	107.4(5)
O4[14]	Al4	O8[13]	90.7(4)	O1[8]	Na1	O2[3]	58.7(4)
O4[5]	Al4	O8[13]	90.0(4)	O4[3]	Na1	O7	108.2(4)
O4[5]	Al4	O1	87.8(4)	O4[3]	Na1	O3	64.4(4)
O4[5]	Al4	O1[17]	91.5(4)	O4[3]	Na1	O8	66.2(4)
O4[14]	Al4	O1[17]	87.8(4)	O4[3]	Na1	O5	96.3(4)
O8[6]	Al4	O8[13]	91.3(7)	O4[3]	Na1	O9	108.4(5)
O1	Al4	O8[6]	177.0(5)	O4[3]	Na1	O2[3]	79.6(5)
O1[17]	Al4	O8[6]	86.1(4)	O4[3]	Na1	O1[8]	64.2(4)
O1	Al4	O8[13]	86.1(4)	O7	Na1	O3	122.0(4)

O1[17]	Al4	O8[13]	177.0(5)	O7	Na1	O8	173.8(5)
O1[17]	Al4	O1	96.5(6)	O7	Na1	O9	129.0(5)
O13	Al2	O13[5]	86.0(6)	O7	Na1	O2[3]	61.3(4)
O13[5]	Al2	O23	170.8(5)	O7	Na1	O1[8]	119.9(5)
O13[5]	Al2	O23[5]	90.6(4)	O3	Na1	O9	51.0(4)
O13	Al2	O23	90.6(4)	O8	Na1	O3	54.0(4)
O13	Al2	O23[5]	170.8(5)	O8	Na1	O9	53.4(4)
O13	Al2	O17[6]	86.3(4)	O5	Na1	O7	62.2(4)
O13[5]	Al2	O17[6]	86.3(4)	O5	Na1	O3	61.9(4)
O13[5]	Al2	O22	96.2(4)	O5	Na1	O8	115.0(5)
O13	Al2	O22	96.2(4)	O5	Na1	O9	79.7(5)
O23	Al2	O23[5]	91.4(5)	O5	Na1	O2[3]	118.4(5)
O23	Al2	O17[6]	84.9(4)	O5	Na1	O1[8]	160.3(5)
O23[5]	Al2	O17[6]	84.9(4)	O12	Na1	O4[3]	166.6(6)
O22	Al2	O23	92.7(4)	O12	Na1	O7	79.6(4)
O22	Al2	O23[5]	92.7(4)	O12	Na1	O3	121.4(5)
O22	Al2	O17[6]	176.5(5)	O12	Na1	O8	106.5(5)
O25[18]	Al1	O25	180.0(5)	O12	Na1	O5	97.1(5)
O25[18]	Al1	O24[10]	87.6(3)	O12	Na1	O9	72.6(5)
O25	Al1	O24[10]	92.4(3)	O12	Na1	O2[3]	95.3(5)
O25[18]	Al1	O24[11]	87.6(3)	O12	Na1	O1[8]	102.5(5)
O25	Al1	O24[12]	87.6(3)	O2[3]	Na1	O3	143.3(5)
O25[18]	Al1	O24[12]	92.4(3)	O2[3]	Na1	O8	118.5(5)
O25	Al1	O24[7]	87.6(3)	O2[3]	Na1	O9	160.0(5)
O25[18]	Al1	O24[7]	92.4(3)	O28	Na2	O28[10]	180
O25	Al1	O24[11]	92.4(3)	O28[10]	Na2	O26[10]	90.2(3)
O24[7]	Al1	O24[11]	180.0(8)	O28[10]	Na2	O26	89.8(3)
O24[11]	Al1	O24[10]	88.1(5)	O28	Na2	O26	90.2(3)
O24[7]	Al1	O24[12]	88.1(5)	O28	Na2	O26[10]	89.8(3)
O24[10]	Al1	O24[12]	180.0(8)	O20[10]	Na2	O21	116.0(3)
O24[11]	Al1	O24[12]	91.9(5)	O20[10]	Na2	O26[10]	120.8(3)
O24[7]	Al1	O24[10]	91.9(5)	O26	Li1	O28	106.1(6)
O15	Al5	O20	154.8(5)	O26	Li1	O28[1]	106.1(6)
O15	Al5	O21	89.8(5)	O26	Li1	O17	141.4(10)
O15	Al5	O16	82.2(5)	O3[9]	Li2	O7[12]	69.3(7)
O22	Al5	O15	104.5(5)	O3[9]	Li2	O7[7]	69.3(7)
O22	Al5	O20	100.6(5)	O3[9]	Li2	O8	103.1(8)
O22	Al5	O21	101.9(4)	O39	Li2	O85	103.1(8)
O22	Al5	O16	105.4(5)	O8	Li2	O7[7]	114.9(3)
O7[3]	Al3	O7[13]	86.5(5)	O8[5]	Li2	O7[7]	172.4(10)

O7[13]	Al3	O2	84.7(4)	O8	Li2	O7[12]	172.4(10)
O7[3]	Al3	O2	84.7(4)	O8[5]	Li2	O7[12]	114.9(3)
O3	Al3	O7[3]	86.8(4)	O8	Li2	O8[5]	65.8(8)
O3	Al3	O7[13]	86.8(4)	O10	Li2	O7[12]	90.7(8)
O3	Al3	O2	168.3(6)	O10	Li2	O7[7]	90.7(8)
O5	Al3	O7[13]	177.3(4)	O10	Li2	O3[9]	156.3(13)
O5	Al3	O7[3]	91.4(4)	O10	Li2	O8	96.8(9)
O5[5]	Al3	O7[13]	91.4(4)	O10	Li2	O8[5]	96.8(9)
O5[5]	Al3	O7[3]	177.3(4)	O28[1]	Li3	O28	121.4(9)
O5	Al3	O3	91.4(4)	O28[1]	Li3	O23[16]	60.7(4)
O5[5]	Al3	O3	91.4(4)	O28	Li3	O23[16]	115.0(7)
O5[5]	Al3	O5	90.6(5)	O28[1]	Li3	O23[15]	79.8(3)
O5[5]	Al3	O2	96.8(4)	O28[1]	Li3	O23[10]	115.0(7)
O5	Al3	O2	96.8(4)	O28	Li3	O23[15]	145.4(8)
O28[10]	P8	O24	113.0(5)	O28	Li3	O23[10]	60.7(4)
O28[10]	P8	O23	111.9(5)	O28[1]	Li3	O23[7]	145.4(8)
O28[10]	P8	O21	111.5(5)	O28	Li3	O23[7]	79.8(3)
O28[10]	P8	Na2	56.8(3)	O28	Li3	O17	88.3(6)
O9	P3	O3	109.9(8)	O28[1]	Li3	O17	88.3(6)
O9	P3	O8	110.6(6)	O23[10]	Li3	O23[16]	63.0(5)
O9	P3	O8[5]	110.6(6)	O23[15]	Li3	O23[10]	139.3(8)
O8[5]	P3	O3	109.2(5)	O23[15]	Li3	O23[16]	99.1(5)
O8	P3	O3	109.2(5)	O23[15]	Li3	O23[7]	70.1(6)
O8[5]	P3	O8	107.2(9)	O23[7]	Li3	O23[16]	139.3(8)
O23	P8	O24	107.3(4)	O23[7]	Li3	O23[10]	99.1(5)
O23	P8	O21	107.3(5)	O23[10]	Li3	O17	147.5(3)
O21	P8	O24	105.4(5)	O23[7]	Li3	O17	63.7(5)
O20	P7	O25	106.9(4)	O23[16]	Li3	O17	147.5(3)
O20[5]	P7	O25	106.9(4)	O23[15]	Li3	O17	63.7(5)
O20	P7	O20[5]	106.4(7)	O26	Li1	O28	106.1(6)
O26[10]	P7	O25	113.3(7)	Al5	O22	Al2	121.6(3)
O26[10]	P7	O20	111.5(5)	Al5[5]	O22	Al2	121.6(3)
O26[10]	P7	O20[5]	111.5(5)	Al5	O22	Al5[5]	115.8(6)
O19[1]	P6	O17	107.8(5)	O14	P4	O15	107.7(7)
O19	P6	O17	107.8(5)	O14	P4	O13	109.9(6)
O18	P6	O17	112.2(8)	O10	P5	O16	112.1(6)
O18	P6	O19[1]	110.2(6)	O10	P5	O16[5]	112.1(6)
O18	P6	O19	110.2(6)	O10	P5	O11[5]	109.9(9)
O4	P2	O7	108.4(5)	O10	P5	O11	109.9(9)
O4	P2	O5	109.2(5)	O11	P5	O16[5]	95.3(8)

O6	P2	O4	112.9(6)	O11^{5}	P5	O16	95.3(8)
O6	P2	O7	109.5(5)	O11^{5}	P5	O16^{5}	119.0(9)
O6	P2	O5	107.9(5)	O11	P5	O11^{5}	28.2(12)
O5	P2	O7	108.9(5)				

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

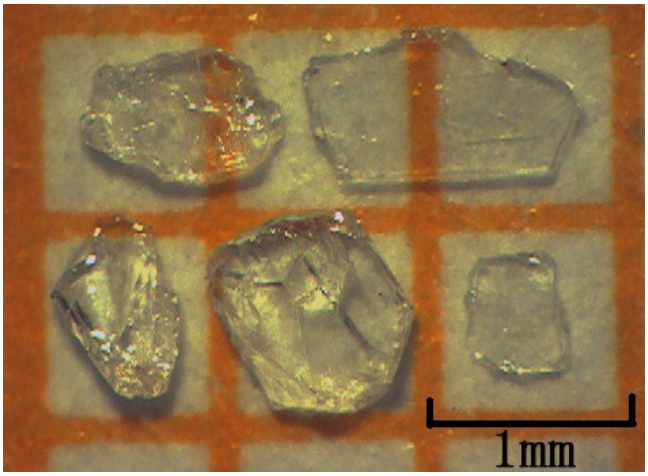


Fig. S1 The photograph of **1** crystal

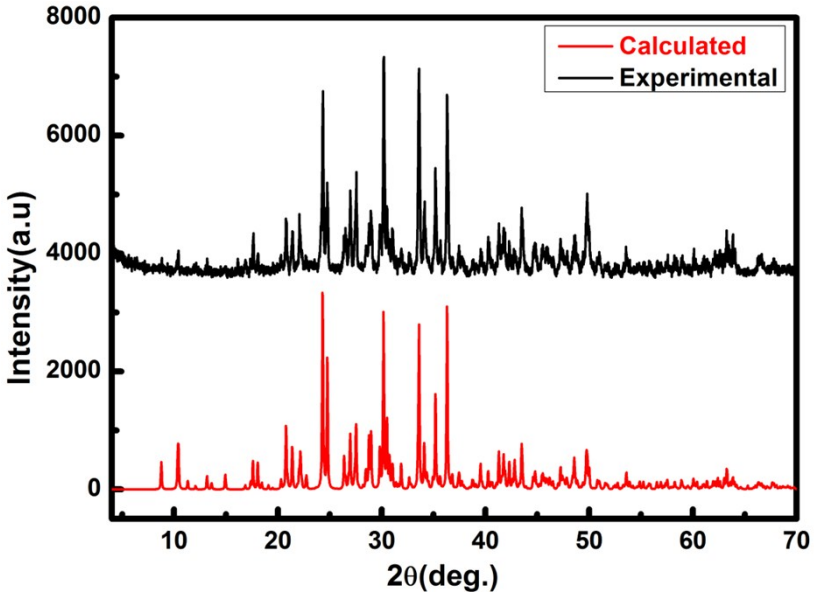


Fig.S2 Experimental and simulated powder X-ray diffraction patterns for **1**.

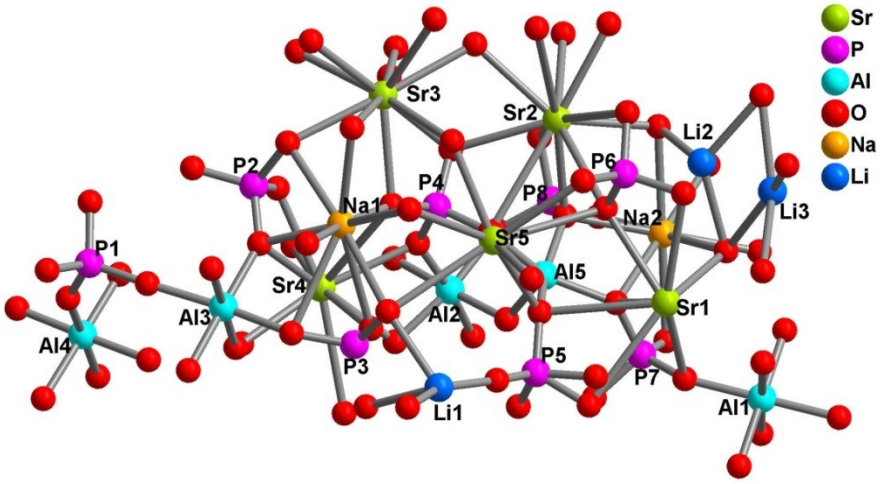


Fig.S3 The symmetric unit of **1** crystal

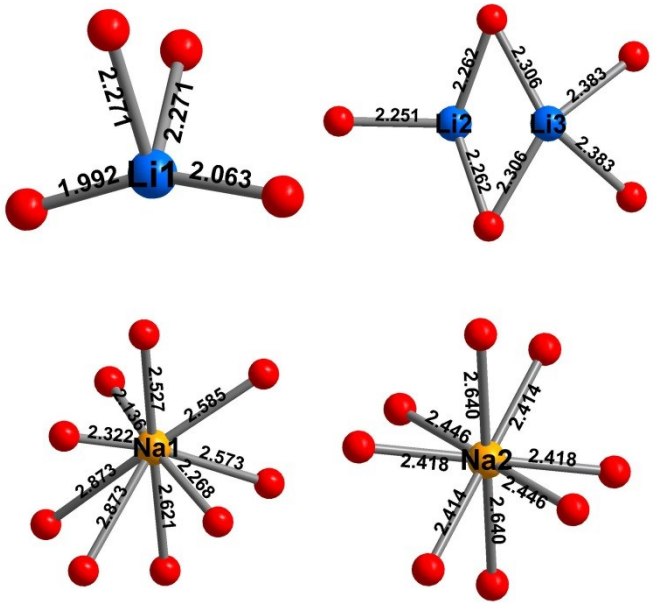
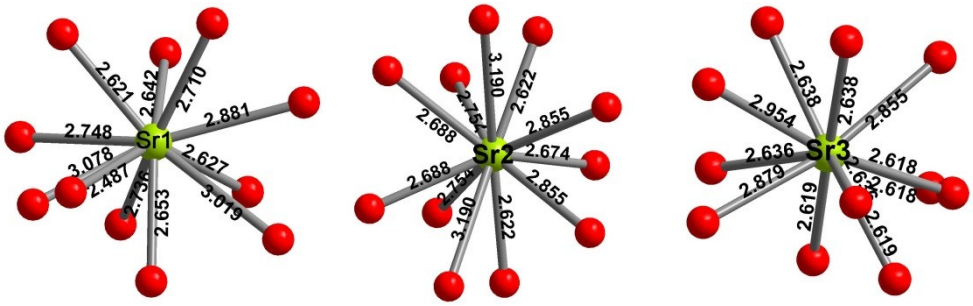


Fig.S4 The coordinate environments of the Li^+ and Na^+ cations



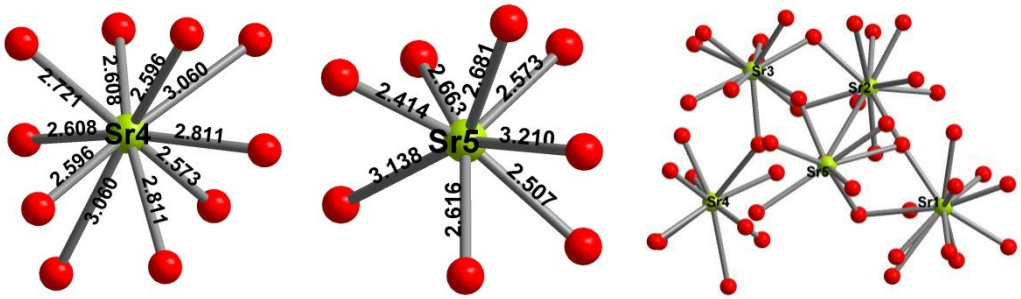


Fig.S5 The coordinate environments of the Sr^{2+} cations

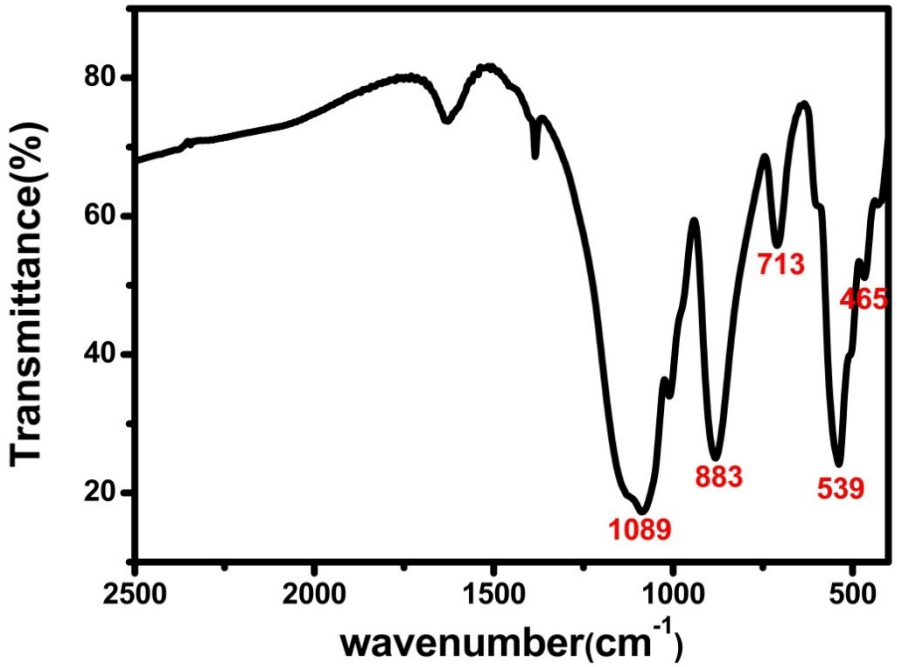


Fig.S6 IR spectra

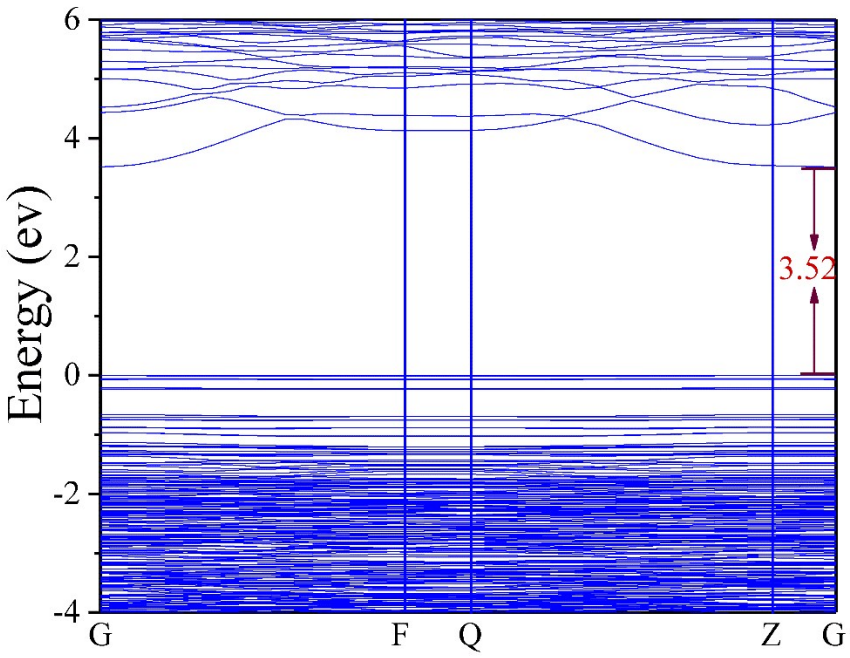


Fig.S7 Band structure

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