Supporting Information

$Li_2Na_2TiP_2O_9$: an ordered $Na_4TiP_2O_9$-Type Crystal with Ion-Exchange Properties

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CONTENTS

Single Crystal and Powder X-ray Diffraction

A colorless crystal with dimensions of 0.06×0.03×0.01mm^3 was selected for single-crystal X-ray diffraction. The diffraction data were collected on a Rigaku AFC10 single-crystal diffractometer equipped with graphite-monochromatic Mo Kα radiation (λ= 0.71073 Å) at 153.15 K and a Saturn CCD detector. CrystalClear program was used to record the intensity data and to conduct cell refinement and data reduction. The crystal structure was solved by the direct method with grogram SHELXS-97[1] and refined by full matrix least squares on F2 by SHELXL-97 programs. The structure was verified using the ADDSYM algorithm from the program PLATON, and no higher symmetry was found. The diffraction data of powder samples was collected by powder X-ray diffraction measurement on a Bruker D8 ADVANCE X-ray diffractometer using Cu Kα radiation (λ= 1.5418Å) at room temperature in the angular range of 2ϑ = 5-80º with a scan step width of 0.02º and a scan rate of 0.1.

UV-Vis diffuser reflectance

The reflection spectrum of LNTP crystal was performed with a Perkin-Elmer Lambda 900 UV–vis-NIR spectrometer in the range of 200–1100 nm.

Thermal Analysis

The differential scanning calorimetric (DSC) analysis (Fig.2) was performed on a NETZSCH STA–409CD apparatus using Al_2O_3 as reference material under N_2 flow with a sample heating rate of 10.0k/min from 50℃ to 1050℃. The crystal powders has melt at 850℃, after the melting, the sample was checked by powder XRD.

Ion exchange

The crystals of $Li_2Na_2TiP_2O_9$ (~10.0 mg) were added into 0.2 mol/L water solution (10 mL) of $AgNO_3$, $BaCl_2$, $CdCl_2$, $Pb(NO_3)_2$, $SrCl_2$, $ZnCl_2$ and $CoCl_2$, respectively. The mixture kept shaking for 24 h at RT and was then isolated by filtration and washed several times with water and acetone then dried in air. The ground powder of $Li_2Na_2TiP_2O_9$ (~100 mg) were added in 0.2 mol/L water solution (20 mL) of $CdCl_2$, $Pb(NO_3)_2$, $SrCl_2$, $ZnCl_2$ and $CoCl_2$, respectively. The mixture was kept under magnetic stirring for 24 h at RT. The solution was filtered and washed as previously mentioned.

Figure S1. (a) DSC curve for LNTP; (b) PXRD pattern for residuals DSC and calculated PXRD pattern for LNTP.

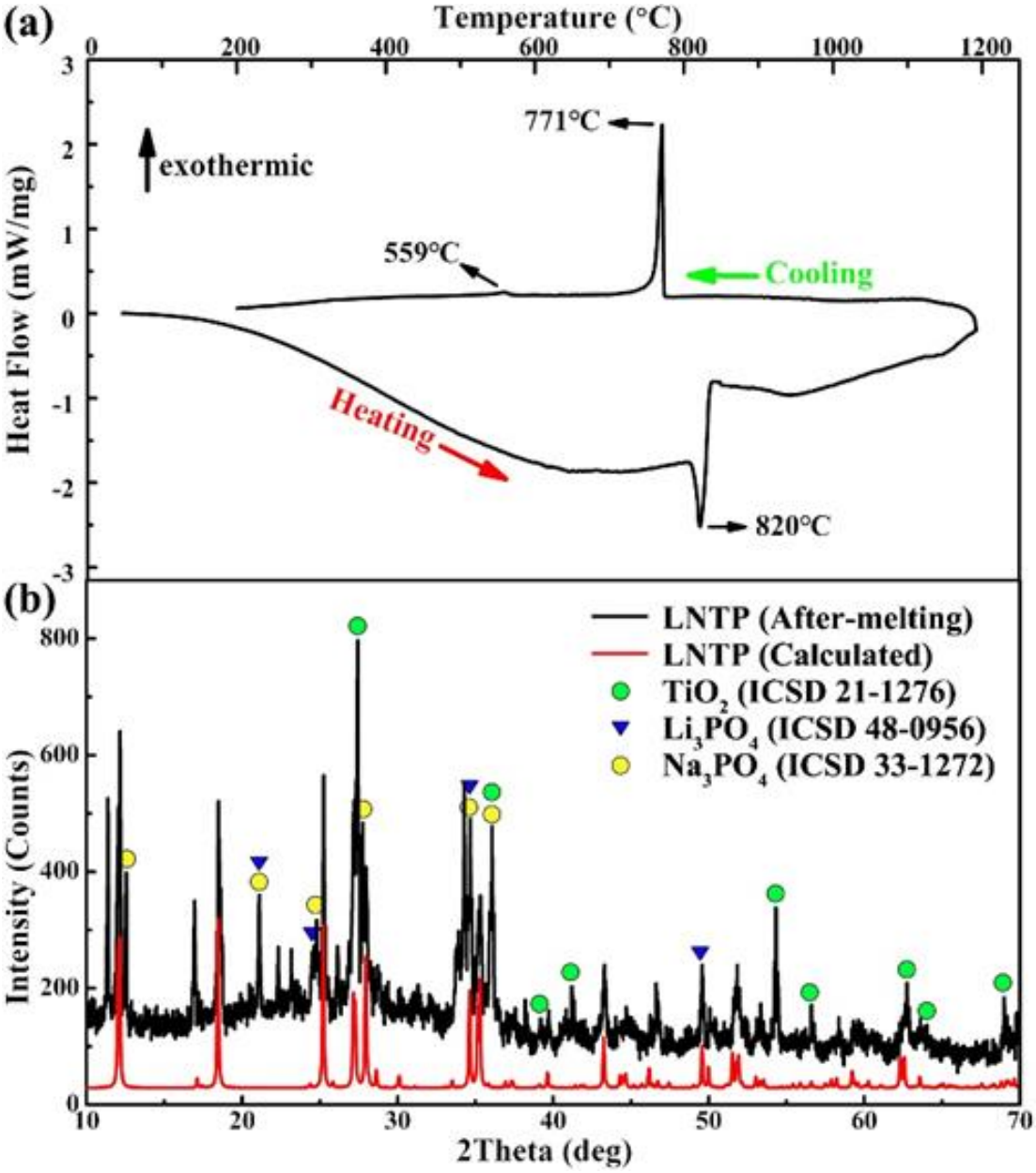
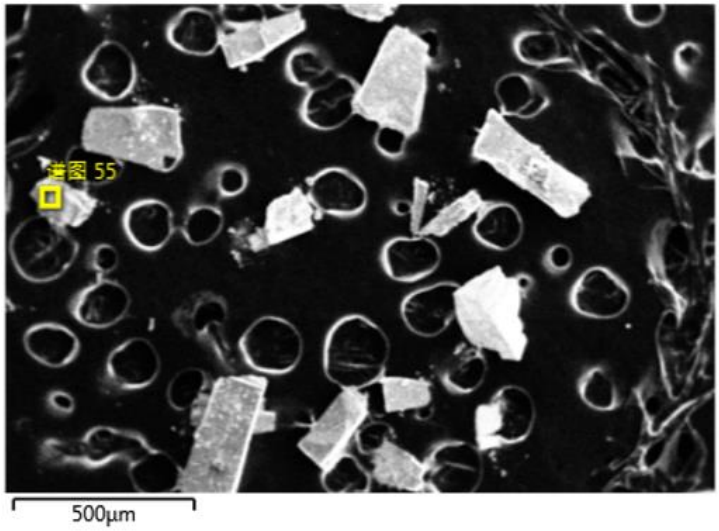


Figure S2. EDS result for the ion-exchange experiment of Ag+ in LNTP.



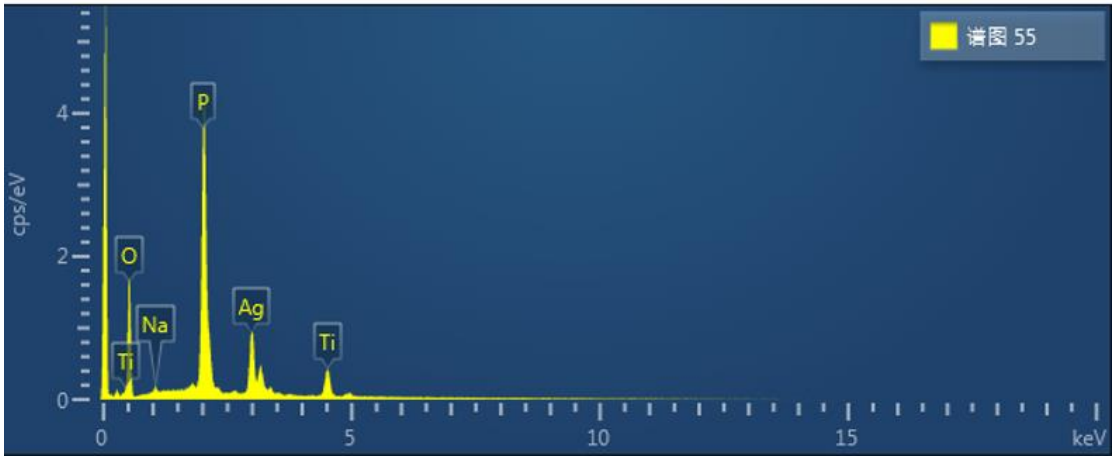


Figure S3. EDS result for the ion-exchange experiment of Cd^{2+} in LNTP.

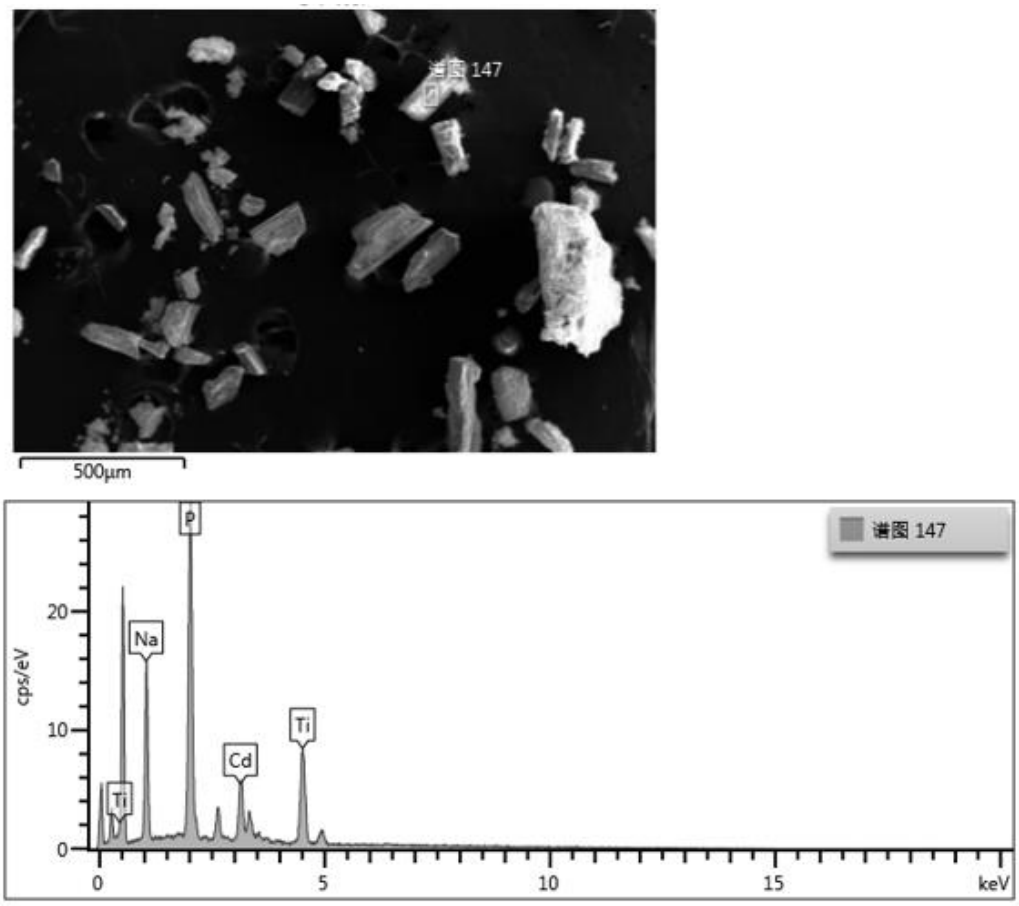
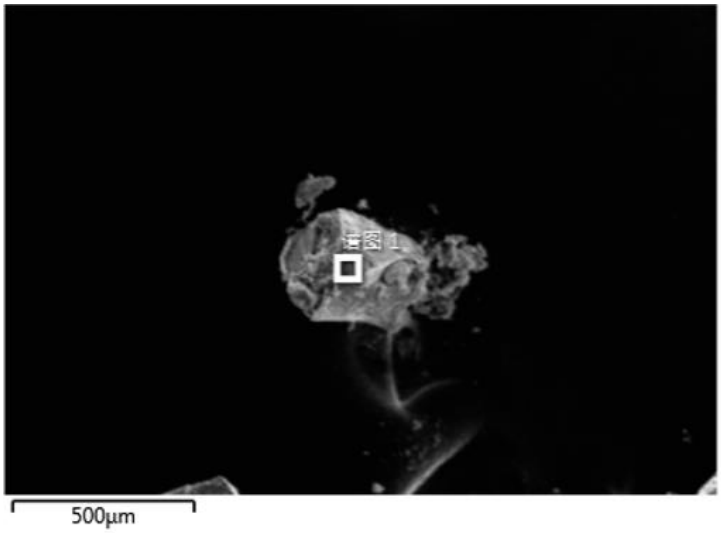


Figure S4. EDS result for the ion-exchange experiment of Pb^{2+} in LNTP.



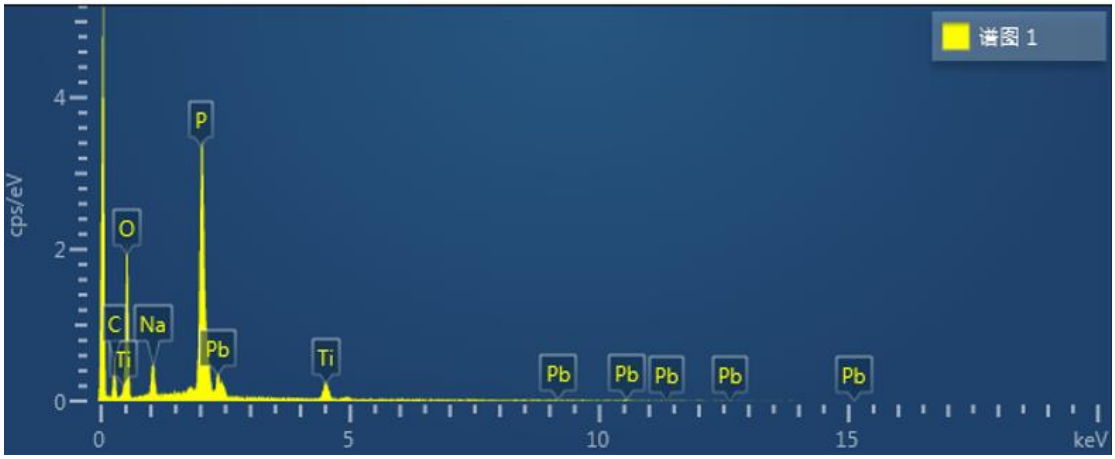


Figure S5. EDS result for the ion-exchange experiment of Sr^{2+} in LNTP.

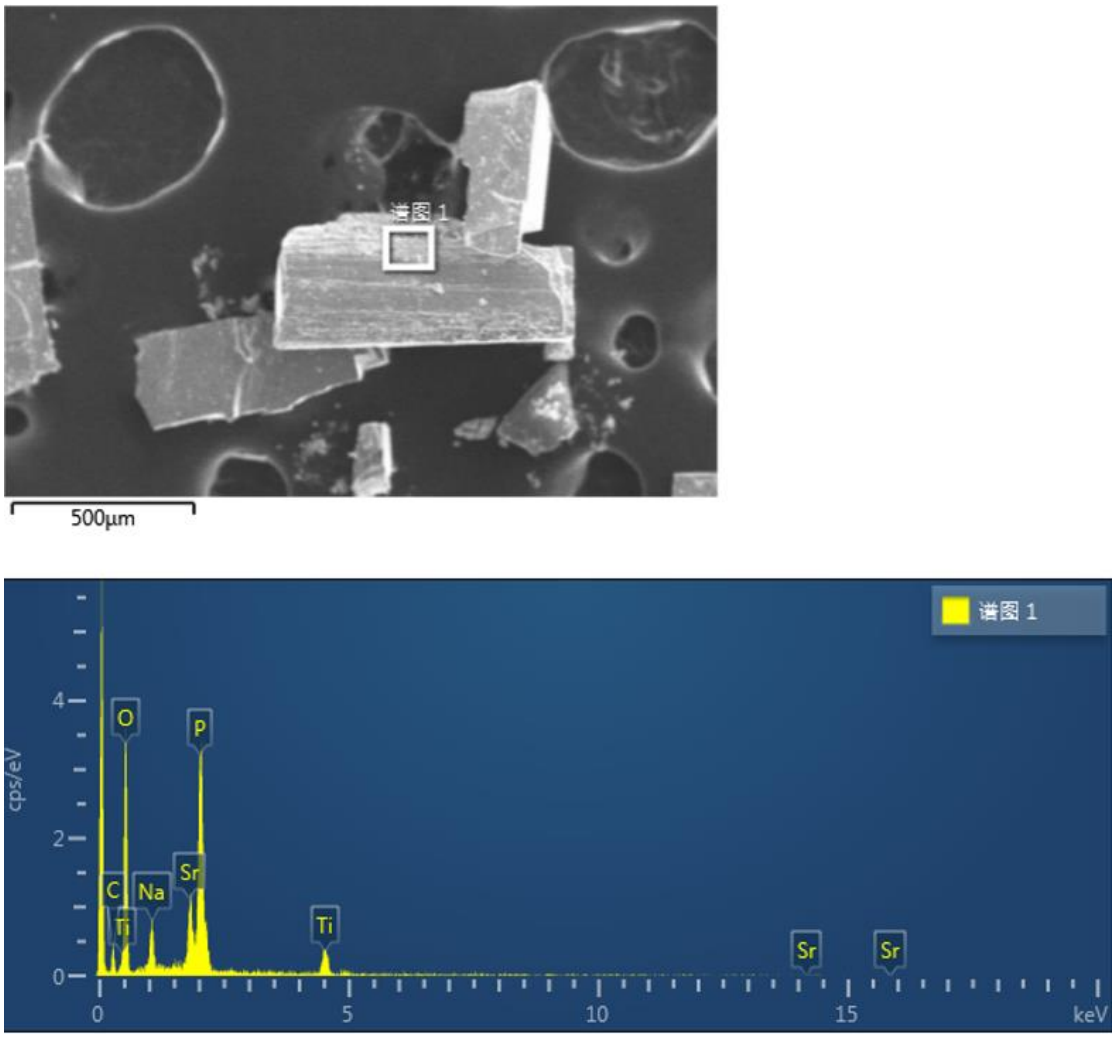
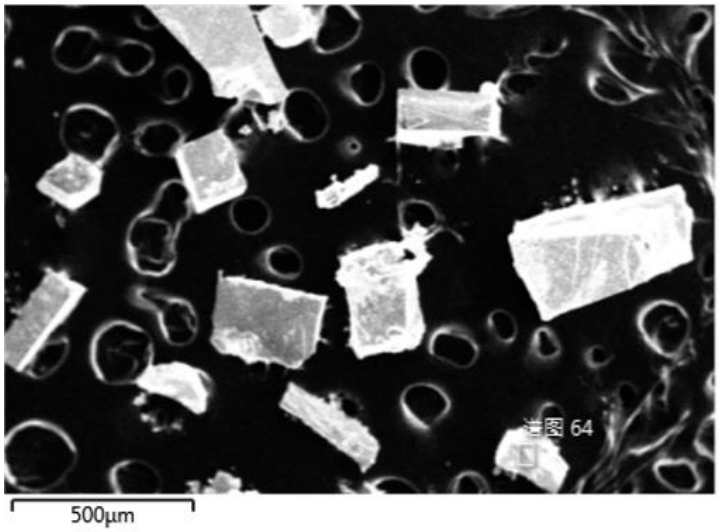


Figure S6. EDS result for the ion-exchange experiment of Zn^{2+} in LNTP.



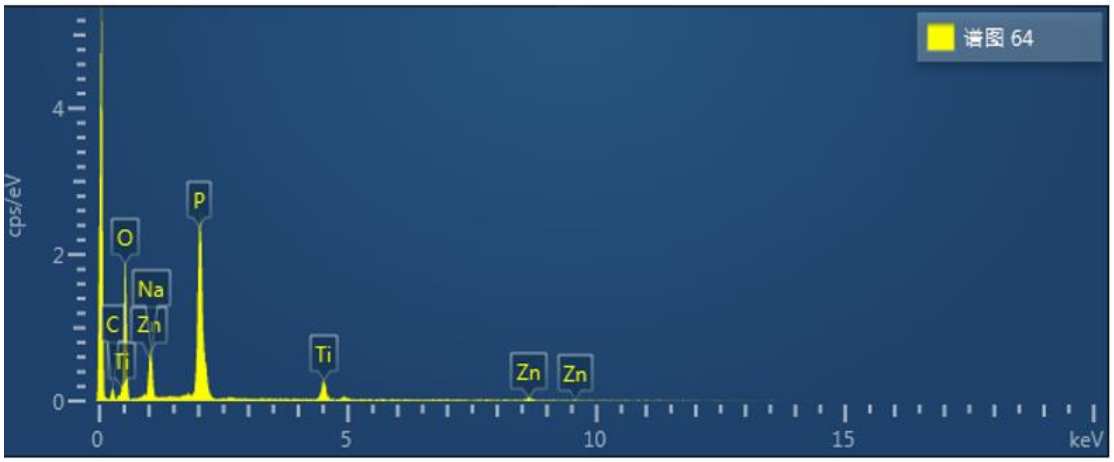


Table S1. Crystal data and structure refinement for LNTP.

Formula	$Li_2Na_2TiP_2O_9$
formula mass(amu)	313.70
crystal system	othorhombic
space group	*Pbcm* (57)
a(Å)	7.2930(15)
b(Å)	7.0892(14)
c(Å)	14.699(3)
α	90
β	90
γ	90
V(Å^3)	760.0(3)
Z	4
T(K)	153.15
ρ*(calcd)(g/cm^3)*	2.742
λ (Å)	0.71073
F(000)	608
θ*(deg)*	2.7715-27.4584
Cryst size (mm^3)	0.06×0.03×0.01
μ(mm^{-1})	1.689
R(F) [a]	0.0835
$R_w(F_o^2)$ [b]	0.1739

[a] $R(F) = \sum \| \|F_o\| - \|F_c\| \| / \sum |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$.

[b] $R_w(F_o^2) = \{(\sum [w(F_o^2 - F_c^2)^2] / \sum wF_o^4\}^{1/2}$ for all data.

$w^{-1} = \sigma^2(F_o^2) + (zP)^2$, where $P = (_{Max}(F_o^2, 0) + 2F_c^2)/3$.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for LNTP.

Atom	Wyck.	Site	x/a	y/b	z/c
Ti1	4d	..m	0.0169(3)	0.7875(3)	1/4
P1	8e	1	0.2693(3)	0.5096(3)	0.38778(14)
Na1	4c	2..	0.0171(6)	1/4	1/2
Na2	4d	..m	0.5449(7)	0.7338(6)	1/4
O5	4d	..m	0.1088(10)	1.0138(10)	1/4
O3	8e	1	0.4679(7)	0.4978(7)	0.3603(4)
O2	8e	1	0.2250(7)	0.5102(8)	0.4888(4)
O4	8e	1	0.1872(8)	0.6970(7)	0.3465(4)
O1	8e	1	0.1682(8)	0.3354(7)	0.3453(4)
Li1	8e	1	0.288(2)	0.547(3)	0.6089(11)

Table S3. Anisotropic displacement parameters, in $Å^2$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0139(10)	0.0091(9)	0.0122(10)	0.0018(8)	0.00000	0.00000
P1	0.0138(10)	0.0065(9)	0.0125(11)	-0.0007(8)	-0.0008(9)	0.0006(8)
Na1	0.016(2)	0.010(2)	0.020(2)	0.00000	0.00000	0.0023(16)
Na2	0.029(3)	0.011(2)	0.019(2)	-0.0047(19)	0.00000	0.00000
O5	0.015(4)	0.008(4)	0.018(4)	0.001(3)	0.00000	0.00000
O3	0.014(3)	0.013(3)	0.015(3)	0.002(2)	-0.001(2)	0.002(2)
O2	0.015(3)	0.010(3)	0.016(3)	0.000(2)	-0.001(2)	0.003(2)
O4	0.021(3)	0.006(3)	0.022(3)	0.003(2)	-0.006(3)	-0.002(2)
O1	0.022(3)	0.011(3)	0.015(3)	-0.005(2)	-0.006(3)	0.000(2)
Li1	0.027(8)	0.052(11)	0.021(8)	0.013(8)	-0.008(7)	-0.018(8)

Table S4. Selected geometric information for LNTP

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
Ti1—Na1^{i}	3.6927(8)	Na2—O5^{x}	18.0225(81)
Ti1—Na1^{ii}	3.6927(8)	Na2—O3^{xiii}	11.3758(66)
Ti1—Na2^{iii}	3.4633(56)	Na2—O3^{v}	13.1962(65)
Ti1—O5	1.7387(74)	Na2—O3	2.3965(63)
Ti1—O5^{iv}	17.9060(74)	Na2—O3^{xiv}	12.3567(66)
Ti1—O4^{v}	13.3539(65)	Na2—O4^{v}	13.5368(65)
Ti1—O4	1.9915(60)	Na2—O4	2.9808(74)
Ti1—O1^{vi}	9.2159(61)	Na2—O1^{xiv}	10.6543(65)
Ti1—O1^{vii}	9.8633(60)	Na2—O1^{xiii}	10.3227(65)
Ti1—Li1^{viii}	13.1709(188)	Na2—Li1^{xv}	3.1224(185)
Ti1—Li1^{ix}	17.0104(210)	Na2—Li1^{xvi}	3.1224(185)
P1—Na1	3.0807(34)	O5—Ti1^{vii}	11.8139(60)
P1—Na1^{i}	3.1604(36)	O5—Na2^{xiv}	15.5542(79)
P1—Na2^{x}	18.0882(50)	O5—Li1^{ix}	15.6193(218)
P1—Na2	3.2661(43)	O5—Li1^{viii}	12.2811(187)
P1—O3	1.5060(56)	O3—Na2^{x}	17.1132(69)
P1—O2	1.5196(62)	O3—Li1^{xvi}	1.8641(158)
P1—O4	1.5785(57)	O2—Na1^{i}	2.4565(62)
P1—O1	1.5680(57)	O2—Li1	1.8427(172)
Na1—P1^{xi}	10.6931(28)	O4—Na1^{i}	2.7298(63)
Na1—O2^{i}	2.4565(62)	O4—Li1^{viii}	12.9493(199)
Na1—O2^{xi}	9.414(6)	O1—Ti1^{iv}	14.4966(60)
Na1—O2^{xii}	7.5713(61)	O1—Na2^{x}	17.3530(71)
Na1—O2	2.3934(61)	Li1—Ti1^{xvii}	21.7070(207)
Na1—O4^{xii}	6.1255(58)	Li1—Na1^{i}	3.0959(170)
Na1—O4^{i}	2.7298(63)	Li1—Na2^{xvii}	22.1020(206)

Na1—O1^{xi}	10.5669(61)	Li1—Na2^{xvi}	3.1224(185)
Na1—O1	2.5984(61)	Li1—O5^{xvii}	23.2278(218)
Na1—Li1^{i}	3.0959(170)	Li1—O3^{xvi}	1.8641(158)
Na1—Li1^{xii}	9.4044(165)	Li1—O4^{viii}	14.5916(203)
Na2—P1^{xiii}	10.9135(37)		

Atoms 1,2,3	**Angle 1,2,3 [°]**	**Atoms 1,2,3**	**Angle 1,2,3 [°]**
Na1^{ii}—Ti1—Na1^{i}	168.700(4)	O1^{xi}—Na1—Li1^{i}	101.327(306)
Na2^{iii}—Ti1—Na1^{ii}	85.719(11)	O1—Na1—Li1^{xii}	142.744(162)
Na2^{iii}—Ti1—Na1^{i}	85.719(11)	O1—Na1—Li1^{i}	75.168(329)
O5^{iv}—Ti1—Na1^{ii}	61.866(3)	Li1^{i}—Na1—Li1^{xii}	138.343(316)
O5—Ti1—Na1^{i}	95.297(6)	O5^{x}—Na2—P1^{xiii}	112.780(11)
O5—Ti1—Na1^{ii}	95.297(6)	O5^{x}—Na2—O4	108.444(102)
O5^{iv}—Ti1—Na1^{i}	110.205(3)	O5^{x}—Na2—O4^{v}	115.278(23)
O5^{iv}—Ti1—Na2^{iii}	86.391(13)	O5^{x}—Na2—Li1^{xvi}	67.553(368)
O5—Ti1—Na2^{iii}	118.985(268)	O5^{x}—Na2—Li1^{xv}	22.545(339)
O5—Ti1—O5^{iv}	145.717(21)	O3^{xiv}—Na2—P1^{xiii}	115.460(29)
O5—Ti1—O4	93.259(146)	O3^{xiii}—Na2—P1^{xiii}	7.375(30)
O5—Ti1—O4^{v}	90.486(22)	O3—Na2—P1^{xiii}	69.430(138)
O5—Ti1—O1^{vii}	111.714(30)	O3^{v}—Na2—P1^{xiii}	35.948(27)
O5—Ti1—O1^{vi}	71.711(32)	O3^{v}—Na2—O5^{x}	107.563(23)
O5^{iv}—Ti1—Li1^{viii}	156.586(83)	O3^{xiv}—Na2—O5^{x}	37.679(24)
O5—Ti1—Li1^{viii}	55.913(88)	O3^{xiii}—Na2—O5^{x}	109.538(26)
O5—Ti1—Li1^{ix}	35.066(74)	O3—Na2—O5^{x}	73.27(12)
O5^{iv}—Ti1—Li1^{ix}	171.951(68)	O3^{v}—Na2—O3	39.741(138)
O4—Ti1—Na1^{ii}	136.675(169)	O3—Na2—O3^{xiii}	73.854(139)
O4^{v}—Ti1—Na1^{i}	9.289(25)	O3^{v}—Na2—O3^{xiii}	42.683(39)
O4—Ti1—Na1^{i}	46.362(168)	O3^{v}—Na2—O3^{xiv}	133.585(37)
O4^{v}—Ti1—Na1^{ii}	172.960(25)	O3^{xiii}—Na2—O3^{xiv}	108.685(39)

O4^{v}—Ti1—Na2^{iii}	95.000(25)	O3—Na2—O3^{xiv}	109.013(136)
O4—Ti1—Na2^{iii}	125.764(168)	O3^{xiii}—Na2—O4	99.047(115)
O4—Ti1—O5^{iv}	88.595(146)	O3^{xiii}—Na2—O4^{v}	48.974(39)
O4^{v}—Ti1—O5^{iv}	111.158(23)	O3^{v}—Na2—O4	58.673(115)
O4—Ti1—O4^{v}	38.573(170)	O3—Na2—O4	53.977(167)
O4^{v}—Ti1—Li1^{viii}	48.450(75)	O3^{xiv}—Na2—O4^{v}	144.012(36)
O4—Ti1—Li1^{viii}	79.285(173)	O3—Na2—O4^{v}	43.752(139)
O4^{v}—Ti1—Li1^{ix}	75.462(59)	O3^{v}—Na2—O4^{v}	10.612(36)
O4—Ti1—Li1^{ix}	99.439(157)	O3^{xiv}—Na2—O4	141.766(114)
O1^{vii}—Ti1—Na1^{i}	149.107(34)	O3—Na2—O1^{xiv}	113.03(14)
O1^{vi}—Ti1—Na1^{ii}	166.854(36)	O3^{v}—Na2—O1^{xiv}	141.633(40)
O1^{vii}—Ti1—Na1^{ii}	24.829(34)	O3^{xiii}—Na2—O1^{xiii}	11.894(43)
O1^{vi}—Ti1—Na1^{i}	23.659(37)	O3^{xiv}—Na2—O1^{xiii}	119.979(41)
O1^{vi}—Ti1—Na2^{iii}	98.679(36)	O3—Na2—O1^{xiii}	74.707(141)
O1^{vii}—Ti1—Na2^{iii}	93.554(34)	O3^{xiii}—Na2—O1^{xiv}	117.293(42)
O1^{vii}—Ti1—O5^{iv}	39.083(31)	O3^{v}—Na2—O1^{xiii}	38.389(41)
O1^{vi}—Ti1—O5^{iv}	130.506(33)	O3^{xiv}—Na2—O1^{xiv}	9.016(40)
O1^{vii}—Ti1—O4^{v}	148.252(42)	O3—Na2—Li1^{xvi}	36.581(358)
O1^{vi}—Ti1—O4	48.892(173)	O3^{v}—Na2—Li1^{xv}	126.445(298)
O1^{vi}—Ti1—O4^{v}	19.701(44)	O3—Na2—Li1^{xv}	95.495(347)
O1^{vii}—Ti1—O4	114.70(17)	O3^{xiv}—Na2—Li1^{xvi}	90.116(299)
O1^{vii}—Ti1—O1^{vi}	163.499(49)	O3^{v}—Na2—Li1^{xvi}	43.739(306)
O1^{vi}—Ti1—Li1^{ix}	56.498(67)	O3^{xiv}—Na2—Li1^{xv}	15.752(308)
O1^{vii}—Ti1—Li1^{ix}	135.345(68)	O3^{xiii}—Na2—Li1^{xvi}	49.599(289)
O1^{vii}—Ti1—Li1^{viii}	163.165(82)	O3^{xiii}—Na2—Li1^{xv}	113.547(301)
O1^{vi}—Ti1—Li1^{viii}	31.154(82)	O4—Na2—P1^{xiii}	91.689(113)
Li1^{ix}—Ti1—Na1^{ii}	111.570(56)	O4^{v}—Na2—P1^{xiii}	41.735(27)
Li1^{viii}—Ti1—Na1^{i}	47.582(71)	O4^{v}—Na2—O4	50.418(115)
Li1^{ix}—Ti1—Na1^{i}	75.545(55)	O4—Na2—Li1^{xv}	127.003(301)
Li1^{viii}—Ti1—Na1^{ii}	138.545(72)	O4^{v}—Na2—Li1^{xvi}	53.933(303)

$Li1^{viii}$—Ti1—$Na2^{iii}$	84.647(64)	$O4^{v}$—Na2—$Li1^{xv}$	135.610(299)
$Li1^{ix}$—Ti1—$Na2^{iii}$	88.486(50)	O4—Na2—$Li1^{xvi}$	88.263(295)
$Li1^{viii}$—Ti1—$Li1^{ix}$	28.074(106)	$O1^{xiv}$—Na2—$P1^{xiii}$	124.200(33)
Na1—P1—$Na1^{i}$	69.396(45)	$O1^{xiii}$—Na2—$P1^{xiii}$	7.847(34)
Na1—P1—$Na2^{x}$	100.159(41)	$O1^{xiii}$—Na2—$O5^{x}$	120.448(29)
$Na1^{i}$—P1—Na2	117.900(65)	$O1^{xiv}$—Na2—$O5^{x}$	39.904(29)
Na1—P1—Na2	171.938(77)	$O1^{xiv}$—Na2—O4	136.976(116)
$Na2^{x}$—P1—$Na1^{i}$	168.202(45)	$O1^{xiii}$—Na2—O4	90.453(116)
$Na2^{x}$—P1—Na2	72.220(36)	$O1^{xiv}$—Na2—$O4^{v}$	151.723(40)
O3—P1—$Na1^{i}$	143.666(230)	$O1^{xiii}$—Na2—$O4^{v}$	42.178(41)
O3—P1—Na1	133.207(229)	$O1^{xiii}$—Na2—$O1^{xiv}$	128.342(44)
O3—P1—Na2	43.018(209)	$O1^{xiv}$—Na2—$Li1^{xvi}$	97.906(299)
O3—P1—$Na2^{x}$	47.809(213)	$O1^{xiii}$—Na2—$Li1^{xvi}$	56.886(291)
O3—P1—O2	117.821(324)	$O1^{xiii}$—Na2—$Li1^{xv}$	125.437(312)
O3—P1—O4	107.967(313)	$O1^{xiv}$—Na2—$Li1^{xv}$	17.538(309)
O3—P1—O1	107.559(316)	$Li1^{xv}$—Na2—$P1^{xiii}$	119.204(304)
O2—P1—$Na1^{i}$	49.306(220)	$Li1^{xvi}$—Na2—$P1^{xiii}$	49.213(291)
O2—P1—Na1	49.575(221)	$Li1^{xv}$—Na2—$Li1^{xvi}$	83.248(459)
O2—P1—Na2	137.338(239)	Ti1—O5—$Ti1^{vii}$	42.064(12)
O2—P1—$Na2^{x}$	128.147(229)	Ti1—O5—$Na2^{xiv}$	74.627(11)
O2—P1—O4	107.014(326)	$Ti1^{vii}$—O5—$Na2^{xiv}$	45.591(1)
O2—P1—O1	106.939(326)	$Ti1^{vii}$—O5—$Li1^{viii}$	158.389(85)
O4—P1—Na1	118.825(217)	Ti1—O5—$Li1^{viii}$	117.354(95)
O4—P1—$Na1^{i}$	59.741(205)	Ti1—O5—$Li1^{ix}$	141.268(80)
O4—P1—Na2	65.513(208)	$Ti1^{vii}$—O5—$Li1^{ix}$	156.957(72)
O4—P1—$Na2^{x}$	124.815(206)	$Li1^{viii}$—O5—$Na2^{xiv}$	149.357(79)
O1—P1—Na1	57.452(204)	$Li1^{ix}$—O5—$Na2^{xiv}$	144.006(66)
O1—P1—$Na1^{i}$	108.770(219)	$Li1^{viii}$—O5—$Li1^{ix}$	31.439(111)
O1—P1—$Na2^{x}$	59.822(205)	P1—O3—$Na2^{x}$	128.453(225)
O1—P1—Na2	115.196(222)	P1—O3—Na2	111.595(287)

O1—P1—O4	109.355(289)	P1—O3—Li1^{xvi}	149.631(569)
P1—Na1—P1^{xi}	105.45(4)	Na2—O3—Na2^{x}	92.212(124)
P1—Na1—Li1^{xii}	121.191(110)	Li1^{xvi}—O3—Na2^{x}	64.328(534)
P1^{xi}—Na1—Li1^{xii}	49.673(100)	Li1^{xvi}—O3—Na2	93.409(596)
P1^{xi}—Na1—Li1^{i}	93.477(314)	P1—O2—Na1^{i}	102.723(278)
P1—Na1—Li1^{i}	82.794(322)	P1—O2—Na1	101.521(280)
O2^{xi}—Na1—P1	101.383(51)	P1—O2—Li1	152.067(643)
O2^{xii}—Na1—P1^{xi}	50.445(46)	Na1—O2—Na1^{i}	94.210(196)
O2—Na1—P1^{xi}	78.083(139)	Li1—O2—Na1^{i}	90.976(566)
O2^{xi}—Na1—P1^{xi}	4.687(37)	Li1—O2—Na1	101.605(593)
O2^{i}—Na1—P1	92.958(134)	Ti1—O4—Na1^{i}	101.769(229)
O2^{i}—Na1—P1^{xi}	56.955(132)	Ti1—O4—Na2	100.292(218)
O2^{xii}—Na1—P1	122.282(58)	Ti1—O4—Li1^{viii}	92.023(173)
O2—Na1—P1	28.903(136)	P1—O4—Ti1	141.396(345)
O2^{xi}—Na1—O2^{i}	54.235(135)	P1—O4—Na1^{i}	90.295(245)
O2^{xi}—Na1—O2^{xii}	54.520(57)	P1—O4—Na2	85.677(238)
O2^{xii}—Na1—O2^{i}	104.415(140)	P1—O4—Li1^{viii}	119.072(229)
O2—Na1—O2^{xii}	97.249(146)	Na1^{i}—O4—Na2	149.197(227)
O2—Na1—O2^{i}	85.790(184)	Li1^{viii}—O4—Na1^{i}	40.646(123)
O2—Na1—O2^{xi}	74.486(142)	Li1^{viii}—O4—Na2	117.626(139)
O2^{xi}—Na1—O4^{i}	32.766(125)	Ti1^{iv}—O1—Na1	108.122(131)
O2^{xii}—Na1—O4^{xii}	17.129(69)	Ti1^{iv}—O1—Na2^{x}	39.726(14)
O2—Na1—O4^{i}	107.250(174)	P1—O1—Ti1^{iv}	154.320(223)
O2^{i}—Na1—O4^{i}	57.116(172)	P1—O1—Na1	91.973(249)
O2^{xi}—Na1—O4^{xii}	70.759(64)	P1—O1—Na2^{x}	115.698(214)
O2—Na1—O4^{xii}	109.123(147)	Na1—O1—Na2^{x}	122.500(138)
O2^{i}—Na1—O4^{xii}	116.605(141)	Ti1^{xvii}—Li1—Na1	136.055(371)
O2^{xii}—Na1—O4^{i}	50.095(131)	Ti1^{xvii}—Li1—Na2^{xvi}	108.797(399)
O2^{xii}—Na1—O1^{xi}	42.017(55)	Ti1^{xvii}—Li1—Na2^{xvii}	10.082(9)
O2^{xii}—Na1—O1	143.351(135)	Na1^{i}—Li1—Ti1^{xvii}	74.621(360)

$O2^{i}$—Na1—$O1^{xi}$	64.866(136)	$Na1^{i}$—Li1—Na1	67.396(423)
$O2^{xi}$—Na1—$O1^{xi}$	12.647(47)	$Na1^{i}$—Li1—$Na2^{xvi}$	156.973(602)
$O2^{i}$—Na1—O1	101.667(178)	$Na1^{i}$—Li1—$Na2^{xvii}$	67.810(338)
$O2^{xi}$—Na1—O1	130.141(132)	$Na2^{xvi}$—Li1—Na1	98.571(418)
O2—Na1—$O1^{xi}$	80.850(142)	$Na2^{xvii}$—Li1—Na1	126.291(370)
O2—Na1—O1	59.441(179)	$Na2^{xvi}$—Li1—$Na2^{xvii}$	111.930(385)
$O2^{xi}$—Na1—$Li1^{i}$	90.676(322)	$O5^{xvii}$—Li1—$Ti1^{xvii}$	2.150(4)
O2—Na1—$Li1^{i}$	93.525(345)	$O5^{xvii}$—Li1—Na1	134.398(370)
$O2^{i}$—Na1—$Li1^{i}$	36.522(329)	$O5^{xvii}$—Li1—$Na1^{i}$	72.501(359)
$O2^{xii}$—Na1—$Li1^{xii}$	1.273(109)	$O5^{xvii}$—Li1—$Na2^{xvii}$	9.052(8)
O2—Na1—$Li1^{xii}$	96.023(177)	$O5^{xvii}$—Li1—$Na2^{xvi}$	110.880(398)
$O2^{xi}$—Na1—$Li1^{xii}$	53.696(107)	$O3^{xvi}$—Li1—$Ti1^{xvii}$	98.330(627)
$O2^{i}$—Na1—$Li1^{xii}$	104.013(169)	$O3^{xvi}$—Li1—Na1	125.493(676)
$O2^{xii}$—Na1—$Li1^{i}$	138.404(304)	$O3^{xvi}$—Li1—$Na1^{i}$	153.017(749)
$O4^{xii}$—Na1—P1	129.296(64)	$O3^{xvi}$—Li1—$Na2^{xvii}$	107.802(591)
$O4^{i}$—Na1—P1	133.330(127)	$O3^{xvi}$—Li1—$Na2^{xvi}$	50.009(437)
$O4^{xii}$—Na1—$P1^{xi}$	66.443(55)	$O3^{xvi}$—Li1—$O5^{xvii}$	100.062(625)
$O4^{i}$—Na1—$P1^{xi}$	29.365(121)	$O3^{xvi}$—Li1—$O4^{viii}$	103.306(593)
$O4^{xii}$—Na1—$O4^{i}$	59.635(133)	O2—Li1—$Ti1^{xvii}$	121.136(618)
$O4^{i}$—Na1—$Li1^{xii}$	50.123(157)	O2—Li1—Na1	45.249(416)
$O4^{xii}$—Na1—$Li1^{xii}$	18.252(114)	O2—Li1—$Na1^{i}$	52.502(429)
$O4^{i}$—Na1—$Li1^{i}$	88.343(313)	O2—Li1—$Na2^{xvi}$	130.046(754)
$O4^{xii}$—Na1—$Li1^{i}$	144.682(314)	O2—Li1—$Na2^{xvii}$	117.513(615)
O1—Na1—$P1^{xi}$	134.587(129)	O2—Li1—$O5^{xvii}$	119.064(620)
O1—Na1—P1	30.575(131)	O2—Li1—$O3^{xvi}$	116.529(840)
$O1^{xi}$—Na1—$P1^{xi}$	8.432(33)	O2—Li1—$O4^{viii}$	125.440(616)
$O1^{xi}$—Na1—P1	109.230(49)	$O4^{viii}$—Li1—$Ti1^{xvii}$	11.488(34)
$O1^{xi}$—Na1—$O4^{i}$	28.766(125)	$O4^{viii}$—Li1—Na1	129.430(381)
O1—Na1—$O4^{i}$	157.328(179)	$O4^{viii}$—Li1—$Na1^{i}$	74.949(338)
O1—Na1—$O4^{xii}$	139.667(136)	$O4^{viii}$—Li1—$Na2^{xvii}$	8.100(34)

$O1^{xi}$—Na1—$O4^{xii}$	58.118(63)	$O4^{viii}$—Li1—$Na2^{xvi}$	103.849(387)
$O1^{xi}$—Na1—O1	139.440(133)	$O4^{viii}$—Li1—$O5^{xvii}$	12.035(37)
$O1^{xi}$—Na1—$Li1^{xii}$	41.241(104)		

(i) -x, 1-y, 1-z; (ii) -x, 1-y, -0.5+z; (iii) -1+x, y, z; (iv) x, -0.5-y, -z;

(v) x, y, 1.5-z; (vi) x, 1.5-y, 0.5+z; (vii) x, 0.5-y, -z; (viii) -x, 1.5+y, 1.5-z;

(ix) -x, 2.5+y, z; (x) 1+x, -0.5-y, -z; (xi) -x, 0.5+y, 1.5-z; (xii) x, 0.5-y, 0.5+z;

(xiii) 1+x, 1.5-y, 0.5+z; (xiv) 1+x, 0.5-y, -z; (xv) 1-x, 1-y, -0.5+z; (xvi) 1-x, 1-y, 1-z;

(xvii) -x, 2.5+y, 1+z.

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