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Redetermination of tricalcium trilanthanum pentakis(orthoborate) from single-crystal data

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(La–B) = 0.004 Å; R factor = 0.012; wR factor = 0.031; data-to-parameter ratio = 10.1.

Single crystals of the title compound, $Ca_3La_3(BO_3)_5$, were obtained by spontaneous nucleation from a high-temperature melt. The crystal structure of $Ca_3La_3(BO_3)_5$ has been determined previously from X-ray powder data [Zhang, Liang, Chen, He & Xu (2001). *J. Alloys Compd*, **327**, 96–99]. The present refinement shows a significant improvement in terms of the precision of the geometric parameters and the correct determination of the absolute configuration in space group $P6_3mc$ with all atoms refined with anisotropic displacement parameters. The structure consists of isolated BO_3 triangles and distorted [CaO_8] and [LaO_{10}] polyhedra. Except for one O atom, all other atoms are situated on special positions: La, all O and one B atom on mirror planes, and two B atoms with site symmetry 3*m*.

Related literature

For phase equilibria in the system La_2O_3—CaO—B_2O_3, see: Zhang *et al.* (2001*a*). For a previous structure analysis of $Ca_3La_3(BO_3)_5$ based on X-ray powder diffraction data, see: Zhang *et al.* (2001*b*). For non-linear optical (NLO) applications of borate crystals containing triangular BO_3 anions, see: Chen *et al.* (1999). For a review of the geometry of the BO_3 group, see: Zobetz (1982). For the potential applications of $Ca_3La_3(BO_3)_5$ for photoluminescence, see: Zhang *et al.* (2005); Han *et al.* (2007).

Experimental

Crystal data

$Ca_3La_3(BO_3)_5$
M_r = 831.02
Hexagonal, $P6_3mc$
a = 10.530 (3) Å
c = 6.398 (2) Å
V = 614.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.59 mm^{-1}
T = 293 (2) K
0.22 × 0.12 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.206, T_{max} = 0.304
4065 measured reflections
534 independent reflections
534 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.012
$wR(F^2)$ = 0.030
S = 0.89
534 reflections
53 parameters
1 restraint
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack (1983), 236 Friedel pairs
Flack parameter: −0.03 (3)

Table 1
Selected geometric parameters (Å, °).

Ca1—O4^{i}	2.3139 (13)	La1—O3^{vii}	2.8112 (8)
Ca1—O1^{ii}	2.376 (3)	B1—O4	1.358 (6)
Ca1—O3	2.382 (4)	B1—O1^{i}	1.384 (3)
Ca1—O1^{iii}	2.662 (3)	B2—O2^{viii}	1.374 (3)
La1—O1^{iv}	2.501 (2)	B3—O3	1.389 (3)
La1—O4^{v}	2.516 (4)		
La1—O2^{vi}	2.6639 (15)		
O4—B1—O1^{i}	119.7 (2)	O2^{viii}—B2—O2^{xi}	120
O1^{i}—B1—O1^{x}	120.6 (4)	O3^{ix}—B3—O3	120

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2179).

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supplementary materials

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Redetermination of tricalcium trilanthanum pentakis(orthoborate) from single-crystal data

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Comment

Borate crystals containing parallel aligned BO_3 anions are predicted to have large nonlinear optical (NLO) coefficients, moderate birefringence and wide transparency in the UV-region. Therefore they are considered to be good candidates for NLO applications (Chen, 1999). The title compound $Ca_3La_3(BO_3)_5$, (I), has been investigated previously by Zhang *et al.* (2001a) during analysis of phase equilibria in the system La_2O_3—CaO—B_2O_3, and NLO and luminescent properties of this material have also been reported (Zhang, 2005; Han, 2007). The crystal structure of Ca_3La_3 $(BO_3)_5$ was originally determined from X-ray powder diffraction data in conjunction with IR spectroscopy (Zhang *et al.*, 2001b).

The structure of compound (I) can be described in terms of BO_3 triangles and complex irregular [CaO_8] and [LaO_{10}] polyhedra. Each of the three crystallographically different B atoms is coordinated to three O atoms to form planar BO_3 triangles. The B—O bond lengths range from 1.384 (3) to 1.389 (3) Å, which is in good agreement with the results of geometric studies of the BO_3 unit (Zobetz, 1982). Two of the three BO_3 groups exhibit 3*m* symmetry, and the third BO_3 group has *m* symmetry with O–B–O angles very close to 120°. The La^{3+} cations are 10-fold coordinated by oxygen atoms with La—O bond lengths ranging from 2.501 (2) to 2.812 (2) Å. The [LaO_{10}] polyhedra are connected to each other and to the borate groups by sharing corners and edges forming a three-dimensional network with channels running parallel to [001]. In these channels the Ca^{2+} cations are situated and are surrounded by eight oxygen atoms with Ca—O bond lengths ranging from 2.3139 (13) to 2.662 (3) Å (Table 1).

Experimental

Single crystals of compound (I) were grown using a $LiBO_2$-containing flux. The composition of the mixture for crystal growth was 1:1:4:3 of $CaCO_3$ (Sinopharm Regent, AR), La_2O_3 (Materials, 99.8%), H_3BO_3 (Sinopharm Regent, 99.99%), and Li_2CO_3 (Sinopharm Reagent, AR). The mixture was heated in a platinum crucible to 1373 K, held at this temperature for several hours, and then cooled at a rate of 10 K/h from 1373 to 873 K. The remaining solified flux attached to the crystals was readily dissolved in water. Crystals with an average size of 0.5 mm and mostly rod shaped habit were obtained.

Refinement

The present study confirms the basic structural features determined from the previous investigation by Zhang *et al.* (2001*b*) with a much higher precesion and with all displacement parameters refined anisotropically.

Figures

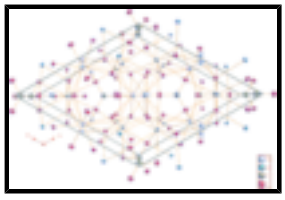

Fig. 1. The structure of (I) in a projection approximatly along the [001] direction with displacement ellipsoids drawn at the 85% probability level.

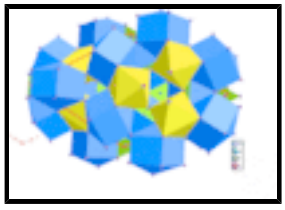

Fig. 2. Packing diagram of the structure of (I). [CaO_8] polyhedra are yellow, [LaO_{10}] polyhedra are blue and [BO_3] units are green.

tricalcium trilanthanum pentakis(orthoborate)

Crystal data

$Ca_3La_3(BO_3)_5$	$Z = 2$
$M_r = 831.02$	$F_{000} = 752$
Hexagonal, $P6_3mc$	$D_x = 4.492$ Mg m^{-3}
Hall symbol: P 6c -2c	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.530$ (3) Å	Cell parameters from 1909 reflections
$b = 10.530$ (3) Å	$\theta = 2.2$–27.5º
$c = 6.398$ (2) Å	$\mu = 11.59$ mm^{-1}
$\alpha = 90$º	$T = 293$ (2) K
$\beta = 90$º	Rod, colourless
$\gamma = 120$º	0.22 × 0.12 × 0.10 mm
$V = 614.4$ (3) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	534 independent reflections
Radiation source: Sealed Tube	534 reflections with $I > 2\sigma(I)$
Monochromator: Graphite Monochromator	$R_{int} = 0.035$
Detector resolution: 14.6306 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 293(1)$ K	$\theta_{min} = 2.2$º
CCD_Profile_fitting scans	$h = -13\rightarrow13$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	$k = -13\rightarrow13$
$T_{min} = 0.206$, $T_{max} = 0.304$	$l = -8\rightarrow7$
4065 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 1.5843P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.012$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.030$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
$S = 0.89$	$\Delta\rho_{min} = -0.59$ e Å^{-3}
534 reflections	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
53 parameters	Extinction coefficient: 0.0632 (12)
1 restraint	Absolute structure: Flack (1983), 236 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.03 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.47334 (5)	0.52666 (5)	0.76261 (15)	0.00673 (19)
La1	0.156065 (12)	0.843935 (12)	0.08229 (8)	0.00493 (11)
B1	0.1989 (3)	0.8011 (3)	0.5473 (8)	0.0049 (10)
B2	0	0	0.2435 (15)	0.0086 (17)
B3	0.6667	0.3333	0.598 (3)	0.0092 (19)
O1	0.6272 (3)	0.9278 (2)	0.4462 (4)	0.0067 (5)
O2	0.07534 (16)	0.92466 (16)	0.7399 (6)	0.0097 (7)
O3	0.59052 (16)	0.40948 (16)	0.5984 (8)	0.0083 (6)
O4	0.22657 (17)	0.77343 (17)	0.7443 (5)	0.0066 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0060 (3)	0.0060 (3)	0.0073 (4)	0.0023 (3)	−0.0001 (2)	0.0001 (2)
La1	0.00442 (12)	0.00442 (12)	0.00474 (14)	0.00129 (9)	0.00003 (8)	−0.00003 (8)
B1	0.0052 (15)	0.0052 (15)	0.007 (3)	0.0044 (18)	−0.0006 (10)	0.0006 (10)

B2	0.011 (3)	0.011 (3)	0.003 (4)	0.0057 (13)	0	0
B3	0.009 (2)	0.009 (2)	0.009 (6)	0.0046 (11)	0	0
O1	0.0069 (10)	0.0056 (10)	0.0073 (11)	0.0029 (9)	−0.0014 (10)	0.0016 (9)
O2	0.0090 (12)	0.0090 (12)	0.0124 (16)	0.0055 (14)	−0.0005 (7)	0.0005 (7)
O3	0.0101 (10)	0.0101 (10)	0.0067 (17)	0.0065 (11)	0.0005 (9)	−0.0005 (9)
O4	0.0067 (11)	0.0067 (11)	0.0055 (16)	0.0026 (13)	−0.0014 (7)	0.0014 (7)

Geometric parameters (Å, °)

Ca1—O4^{i}	2.3139 (13)	La1—O1^{i}	2.678 (3)
Ca1—O4^{ii}	2.3139 (13)	La1—O3^{xiv}	2.8112 (8)
Ca1—O1^{iii}	2.376 (3)	La1—O3^{xv}	2.8112 (8)
Ca1—O1^{iv}	2.376 (3)	La1—B2^{xvi}	3.028 (3)
Ca1—O3	2.382 (4)	La1—B1	3.076 (5)
Ca1—O3^{v}	2.444 (5)	B1—O4	1.358 (6)
Ca1—O1^{ii}	2.662 (3)	B1—O1^{i}	1.384 (3)
Ca1—O1^{vi}	2.662 (3)	B1—O1^{xiii}	1.384 (3)
Ca1—B1^{i}	2.858 (4)	B1—Ca1^{i}	2.858 (4)
Ca1—B1^{ii}	2.858 (4)	B1—Ca1^{ii}	2.858 (4)
Ca1—Ca1^{v}	3.3435 (11)	B2—O2^{xvii}	1.374 (3)
Ca1—Ca1^{vii}	3.3435 (11)	B2—O2^{xviii}	1.374 (3)
La1—O1^{viii}	2.501 (2)	B2—O2^{xix}	1.374 (3)
La1—O1^{ix}	2.501 (2)	B2—La1^{xx}	3.028 (3)
La1—O4^{x}	2.516 (4)	B2—La1^{i}	3.028 (3)
La1—O2^{x}	2.639 (3)	B2—La1^{xxi}	3.028 (3)
La1—O2^{xi}	2.6639 (15)	B3—O3^{xxii}	1.389 (3)
La1—O2^{xii}	2.6639 (15)	B3—O3^{xxiii}	1.389 (3)
La1—O1^{xiii}	2.678 (3)	B3—O3	1.389 (3)
O4^{i}—Ca1—O4^{ii}	93.58 (15)	O1^{ix}—La1—O3^{xiv}	116.83 (10)
O4^{i}—Ca1—O1^{iii}	151.80 (11)	O4^{x}—La1—O3^{xiv}	64.52 (12)
O4^{ii}—Ca1—O1^{iii}	80.01 (9)	O2^{x}—La1—O3^{xiv}	122.29 (12)
O4^{i}—Ca1—O1^{iv}	80.01 (9)	O2^{xi}—La1—O3^{xiv}	155.42 (13)
O4^{ii}—Ca1—O1^{iv}	151.80 (11)	O2^{xii}—La1—O3^{xiv}	121.81 (10)
O1^{iii}—Ca1—O1^{iv}	92.72 (12)	O1^{xiii}—La1—O3^{xiv}	88.50 (10)
O4^{i}—Ca1—O3	126.18 (10)	O1^{i}—La1—O3^{xiv}	65.77 (12)
O4^{ii}—Ca1—O3	126.18 (10)	O1^{viii}—La1—O3^{xv}	116.83 (9)
O1^{iii}—Ca1—O3	77.64 (10)	O1^{ix}—La1—O3^{xv}	69.51 (8)
O1^{iv}—Ca1—O3	77.64 (10)	O4^{x}—La1—O3^{xv}	64.52 (12)
O4^{i}—Ca1—O3^{v}	73.69 (10)	O2^{x}—La1—O3^{xv}	122.29 (12)
O4^{ii}—Ca1—O3^{v}	73.69 (10)	O2^{xi}—La1—O3^{xv}	121.81 (10)
O1^{iii}—Ca1—O3^{v}	78.17 (9)	O2^{xii}—La1—O3^{xv}	155.42 (13)
O1^{iv}—Ca1—O3^{v}	78.17 (9)	O1^{xiii}—La1—O3^{xv}	65.77 (12)

O3—Ca1—O3^{v}	144.65 (19)	O1^{i}—La1—O3^{xv}	88.50 (10)
O4^{i}—Ca1—O1^{ii}	56.39 (9)	O3^{xiv}—La1—O3^{xv}	50.66 (12)
O4^{ii}—Ca1—O1^{ii}	112.85 (10)	O4—B1—O1^{i}	119.7 (2)
O1^{iii}—Ca1—O1^{ii}	151.00 (8)	O4—B1—O1^{xiii}	119.7 (2)
O1^{iv}—Ca1—O1^{ii}	86.53 (8)	O1^{i}—B1—O1^{xiii}	120.6 (4)
O3—Ca1—O1^{ii}	73.88 (10)	O2^{xvii}—B2—O2^{xviii}	120.00 (0)
O3^{v}—Ca1—O1^{ii}	129.62 (7)	O2^{xvii}—B2—O2^{xix}	120.00 (0)
O4^{i}—Ca1—O1^{vi}	112.85 (10)	O2^{xviii}—B2—O2^{xix}	120.00 (0)
O4^{ii}—Ca1—O1^{vi}	56.39 (9)	O3^{xxii}—B3—O3^{xxiii}	120.00 (0)
O1^{iii}—Ca1—O1^{vi}	86.53 (8)	O3^{xxii}—B3—O3	120.00 (0)
O1^{iv}—Ca1—O1^{vi}	151.00 (8)	O3^{xxiii}—B3—O3	120.00 (0)
O3—Ca1—O1^{vi}	73.88 (10)	B1^{ii}—O1—Ca1^{xv}	147.6 (3)
O3^{v}—Ca1—O1^{vi}	129.62 (7)	B1^{ii}—O1—La1^{xxiv}	114.0 (3)
O1^{ii}—Ca1—O1^{vi}	80.50 (11)	Ca1^{xv}—O1—La1^{xxiv}	94.81 (8)
O1^{viii}—La1—O1^{ix}	138.96 (12)	B1^{ii}—O1—Ca1^{i}	83.5 (2)
O1^{viii}—La1—O4^{x}	73.88 (6)	Ca1^{xv}—O1—Ca1^{i}	82.95 (8)
O1^{ix}—La1—O4^{x}	73.88 (6)	La1^{xxiv}—O1—Ca1^{i}	87.75 (8)
O1^{viii}—La1—O2^{x}	71.80 (6)	B1^{ii}—O1—La1^{ii}	92.9 (2)
O1^{ix}—La1—O2^{x}	71.80 (6)	Ca1^{xv}—O1—La1^{ii}	89.98 (9)
O4^{x}—La1—O2^{x}	64.64 (11)	La1^{xxiv}—O1—La1^{ii}	111.47 (9)
O1^{viii}—La1—O2^{xi}	121.07 (8)	Ca1^{i}—O1—La1^{ii}	160.08 (10)
O1^{ix}—La1—O2^{xi}	71.30 (9)	B2^{xxv}—O2—La1^{xxvi}	123.0 (5)
O4^{x}—La1—O2^{xi}	137.71 (9)	B2^{xxv}—O2—La1^{xxvii}	91.42 (19)
O2^{x}—La1—O2^{xi}	82.07 (7)	La1^{xxvi}—O2—La1^{xxvii}	107.69 (7)
O1^{viii}—La1—O2^{xii}	71.30 (9)	B2^{xxv}—O2—La1^{xxviii}	91.42 (19)
O1^{ix}—La1—O2^{xii}	121.07 (8)	La1^{xxvi}—O2—La1^{xxviii}	107.69 (7)
O4^{x}—La1—O2^{xii}	137.71 (9)	La1^{xxvii}—O2—La1^{xxviii}	135.45 (14)
O2^{x}—La1—O2^{xii}	82.07 (7)	B3—O3—Ca1	154.0 (8)
O2^{xi}—La1—O2^{xii}	53.07 (13)	B3—O3—Ca1^{vii}	118.3 (8)
O1^{viii}—La1—O1^{xiii}	137.03 (9)	Ca1—O3—Ca1^{vii}	87.71 (10)
O1^{ix}—La1—O1^{xiii}	83.72 (6)	B3—O3—La1^{xxix}	94.64 (7)
O4^{x}—La1—O1^{xiii}	129.92 (8)	Ca1—O3—La1^{xxix}	86.76 (7)
O2^{x}—La1—O1^{xiii}	146.79 (6)	Ca1^{vii}—O3—La1^{xxix}	85.94 (9)
O2^{xi}—La1—O1^{xiii}	68.76 (8)	B3—O3—La1^{iii}	94.64 (7)
O2^{xii}—La1—O1^{xiii}	92.23 (9)	Ca1—O3—La1^{iii}	86.76 (7)
O1^{viii}—La1—O1^{i}	83.72 (6)	Ca1^{vii}—O3—La1^{iii}	85.94 (9)
O1^{ix}—La1—O1^{i}	137.03 (9)	La1^{xxix}—O3—La1^{iii}	169.80 (13)
O4^{x}—La1—O1^{i}	129.92 (8)	B1—O4—Ca1^{ii}	98.91 (12)
O2^{x}—La1—O1^{i}	146.79 (6)	B1—O4—Ca1^{i}	98.91 (12)
O2^{xi}—La1—O1^{i}	92.23 (9)	Ca1^{ii}—O4—Ca1^{i}	145.78 (15)
O2^{xii}—La1—O1^{i}	68.76 (8)	B1—O4—La1^{xxvi}	127.4 (3)

O1^{xiii}—La1—O1^{i}	53.37 (10)	Ca1^{ii}—O4—La1^{xxvi}	96.00 (9)
O1^{viii}—La1—O3^{xiv}	69.51 (8)	Ca1^{i}—O4—La1^{xxvi}	96.00 (9)

Symmetry codes: (i) −*y*+1, *x*−*y*+1, *z*; (ii) −*x*+*y*, −*x*+1, *z*; (iii) *x*−*y*+1, *x*, *z*+1/2; (iv) −*x*+1, −*x*+*y*, *z*+1/2; (v) −*x*+1, −*y*+1, *z*+1/2; (vi) *x*, *x*−*y*+1, *z*; (vii) −*x*+1, −*y*+1, *z*−1/2; (viii) *y*−1, *x*, *z*−1/2; (ix) −*x*+1, −*y*+2, *z*−1/2; (x) *x*, *y*, *z*−1; (xi) *x*−*y*+1, *x*+1, *z*−1/2; (xii) *y*−1, −*x*+*y*, *z*−1/2; (xiii) −*x*+*y*, *y*, *z*; (xiv) *x*−*y*, *x*, *z*−1/2; (xv) *y*, −*x*+*y*+1, *z*−1/2; (xvi) *x*, *y*+1, *z*; (xvii) *y*−1, −*x*+*y*−1, *z*−1/2; (xviii) *x*−*y*+1, *x*, *z*−1/2; (xix) −*x*, −*y*+1, *z*−1/2; (xx) −*x*+*y*−1, −*x*, *z*; (xxi) *x*, *y*−1, *z*; (xxii) −*x*+*y*+1, −*x*+1, *z*; (xxiii) −*y*+1, *x*−*y*, *z*; (xxiv) −*x*+1, −*y*+2, *z*+1/2; (xxv) −*x*, −*y*+1, *z*+1/2; (xxvi) *x*, *y*, *z*+1; (xxvii) *y*−1, −*x*+*y*, *z*+1/2; (xxviii) *x*−*y*+1, *x*+1, *z*+1/2; (xxix) *y*, −*x*+*y*, *z*+1/2.

Fig. 1

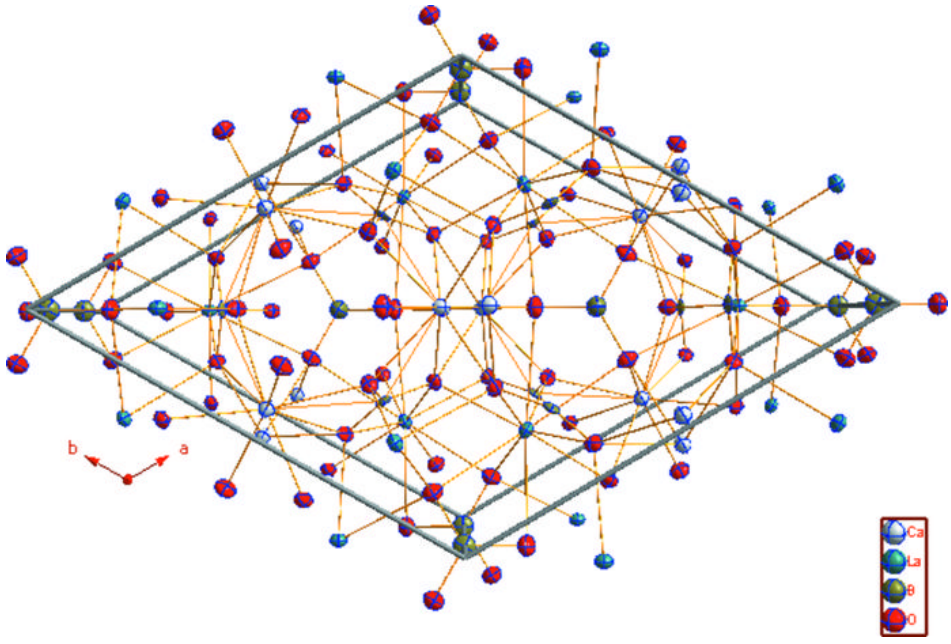

Fig. 2