

Title

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Abstract**Table 1**

Experimental details

Crystal data	
Chemical formula	GaLaO ₄ Sr
M_r	360.25
Crystal system, space group	Tetragonal, $I4/mmm$
Temperature (K)	301
a, c (Å)	3.8423 (1), 12.6752 (5)
V (Å ³)	187.13 (1)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	32.42
Crystal size (mm)	0.01 × 0.01 × 0.004
Data collection	
Diffractometer	ROD, Synergy Custom system, HyPix-Arc 150
Absorption correction	Multi-scan <i>CrysAlis PRO</i> 1.171.42.30a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{\min}, T_{\max}	0.887, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5418, 169, 162
R_{int}	0.027
(sin θ/λ) _{max} (Å ⁻¹)	0.831
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.007, 0.015, 1.33
No. of reflections	169
No. of parameters	13
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.54, -0.57

Computer programs: *CrysAlis PRO* 1.171.42.30a (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015), *SHELXL* 2018/3 (Sheldrick, 2015), Olex2 1.5-ac5-023 (Dolomanov *et al.*, 2009).

Acknowledgements

Funding information

References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* 42, 339-341.

Sheldrick, G. M. (2015). *Acta Cryst. A*71, 3-8.

Sheldrick, G. M. (2015). *Acta Cryst. C*71, 3-8.

Figure 1

supporting information

Title

Computing details

Data collection: *CrysAlis PRO* 1.171.42.30a (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* 1.171.42.30a (Rigaku OD, 2021); data reduction: *CrysAlis PRO* 1.171.42.30a (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015); program(s) used to refine structure: *SHELXL* 2018/3 (Sheldrick, 2015); molecular graphics: Olex2 1.5-ac5-023 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 1.5-ac5-023 (Dolomanov *et al.*, 2009).

(z00250120301r_pl_inc_mask_om75_bkg1)

Crystal data

GaLaO_4Sr
 $M_r = 360.25$
Tetragonal, $I4/mmm$
 $a = 3.8423 (1) \text{ \AA}$
 $c = 12.6752 (5) \text{ \AA}$
 $V = 187.13 (1) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 316$

$D_x = 6.394 \text{ Mg m}^{-3}$
 $\text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ \AA}$
Cell parameters from 3796 reflections
 $\theta = 3.2\text{--}41.7^\circ$
 $\mu = 32.42 \text{ mm}^{-1}$
 $T = 301 \text{ K}$
Irregular, colourless
 $0.01 \times 0.01 \times 0.004 \text{ mm}$

Data collection

ROD, Synergy Custom system, HyPix-Arc 150
diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku
(Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
 ω scans

Absorption correction: multi-scan
CrysAlis PRO 1.171.42.30a (Rigaku Oxford
Diffraction, 2021) Empirical absorption correction
using spherical harmonics, implemented in SCALE3
ABSPACK scaling algorithm.
 $T_{\min} = 0.887$, $T_{\max} = 1.000$
5418 measured reflections
169 independent reflections
162 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\max} = 36.2^\circ$, $\theta_{\min} = 3.2^\circ$
 $h = -6 \rightarrow 6$
 $k = -6 \rightarrow 6$
 $l = -20 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.007$
 $wR(F^2) = 0.015$
 $S = 1.33$
169 reflections
13 parameters
0 restraints
Primary atom site location: dual

$w = 1/[\sigma^2(F_o^2) + (0.003P)^2 + 0.2374P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.57 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL2018/3* (Sheldrick
2018), $\text{Fc}^* = k\text{Fc}[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{1/4}$
Extinction coefficient: 0.0011 (2)

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sr01	0.000000	0.000000	0.35857 (2)	0.00628 (5)	0.5
La01	0.000000	0.000000	0.35857 (2)	0.00628 (5)	0.5
Ga01	0.000000	0.000000	0.000000	0.00719 (8)	
O01	0.000000	0.500000	0.000000	0.0078 (3)	
O02	0.000000	0.000000	0.16716 (17)	0.0149 (4)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr01	0.00674 (6)	0.00674 (6)	0.00537 (8)	0.000	0.000	0.000
La01	0.00674 (6)	0.00674 (6)	0.00537 (8)	0.000	0.000	0.000
Ga01	0.00338 (10)	0.00338 (10)	0.0148 (2)	0.000	0.000	0.000
O01	0.0081 (7)	0.0038 (7)	0.0114 (9)	0.000	0.000	0.000
O02	0.0175 (6)	0.0175 (6)	0.0097 (9)	0.000	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Sr01—Ga01 ⁱ	3.2551 (1)	Sr01—O02 ^{ix}	2.7364 (3)
Sr01—Ga01 ⁱⁱ	3.2551 (1)	Sr01—O02	2.426 (2)
Sr01—Ga01 ⁱⁱⁱ	3.2551 (1)	Sr01—O02 ^x	2.7364 (3)
Sr01—O01 ^{iv}	2.6277 (1)	Ga01—O01 ^{xi}	1.9212 (1)
Sr01—O01 ⁱⁱ	2.6277 (1)	Ga01—O01 ^{xii}	1.9212 (1)
Sr01—O01 ^v	2.6277 (1)	Ga01—O01 ^{xiii}	1.9212 (1)
Sr01—O01 ^{vi}	2.6277 (1)	Ga01—O01	1.9212 (1)
Sr01—O02 ^{vii}	2.7364 (3)	Ga01—O02 ^{xiv}	2.119 (2)
Sr01—O02 ^{viii}	2.7364 (3)	Ga01—O02	2.119 (2)
Ga01 ⁱⁱⁱ —Sr01—Ga01 ⁱ	72.343 (3)	O01—Ga01—Sr01 ^{viii}	126.171 (1)
Ga01 ⁱⁱ —Sr01—Ga01 ⁱ	72.343 (3)	O01 ^{xii} —Ga01—Sr01 ^{xv}	53.829 (2)
Ga01 ⁱⁱⁱ —Sr01—Ga01 ⁱⁱ	113.164 (6)	O01—Ga01—Sr01 ^{xvii}	126.171 (1)
O01 ⁱⁱ —Sr01—Ga01 ⁱⁱ	36.172 (2)	O01 ^{xii} —Ga01—Sr01 ^{xvi}	126.171 (2)
O01 ⁱⁱ —Sr01—Ga01 ⁱ	36.172 (2)	O01 ^{xi} —Ga01—Sr01 ^{xvii}	126.171 (1)
O01 ^{vi} —Sr01—Ga01 ⁱⁱ	36.172 (2)	O01 ^{xi} —Ga01—Sr01 ^x	53.829 (1)
O01 ^v —Sr01—Ga01 ⁱ	36.172 (2)	O01—Ga01—Sr01 ^{xv}	53.829 (2)
O01 ^v —Sr01—Ga01 ⁱⁱⁱ	36.172 (2)	O01 ^{xii} —Ga01—Sr01 ^{xvii}	53.829 (2)
O01 ^{iv} —Sr01—Ga01 ⁱⁱⁱ	36.172 (2)	O01 ^{xiii} —Ga01—Sr01 ^{xv}	126.171 (2)
O01 ^{vi} —Sr01—Ga01 ⁱⁱⁱ	93.198 (5)	O01—Ga01—Sr01 ^{xviii}	53.829 (2)
O01 ^v —Sr01—Ga01 ⁱⁱ	93.198 (5)	O01—Ga01—Sr01 ^x	53.829 (1)
O01 ^{iv} —Sr01—Ga01 ⁱ	93.198 (5)	O01 ^{xiii} —Ga01—Sr01 ^{viii}	53.829 (2)
O01 ⁱⁱ —Sr01—Ga01 ⁱⁱⁱ	93.198 (5)	O01 ^{xi} —Ga01—Sr01 ^{xv}	126.171 (1)
O01 ^{iv} —Sr01—Ga01 ⁱⁱ	93.198 (5)	O01 ^{xi} —Ga01—Sr01 ^{xvi}	53.829 (2)
O01 ^{vi} —Sr01—Ga01 ⁱ	93.198 (5)	O01 ^{xiii} —Ga01—Sr01 ^{xvi}	53.829 (2)
O01 ^v —Sr01—O01 ⁱⁱ	62.261 (4)	O01 ^{xiii} —Ga01—Sr01 ^x	126.171 (1)

O01 ^{iv} —Sr01—O01 ⁱⁱ	93.962 (7)	O01 ^{xi} —Ga01—Sr01 ^{viii}	126.171 (1)
O01 ^v —Sr01—O01 ^{iv}	62.261 (4)	O01 ^{xii} —Ga01—Sr01 ^x	126.171 (1)
O01 ^{iv} —Sr01—O01 ^{vi}	62.261 (4)	O01 ^{xii} —Ga01—Sr01 ^{xviii}	126.171 (1)
O01 ^{vi} —Sr01—O01 ⁱⁱ	62.261 (4)	O01 ^{xii} —Ga01—Sr01 ^{xvii}	53.829 (1)
O01 ^v —Sr01—O01 ^{vi}	93.962 (7)	O01 ^{xiii} —Ga01—Sr01 ^{xviii}	126.171 (1)
O01 ^{vi} —Sr01—O02 ^{vii}	126.48 (3)	O01 ^{xiii} —Ga01—Sr01 ^{xvii}	53.829 (1)
O01 ^{iv} —Sr01—O02 ^{viii}	126.48 (3)	O01 ^{xi} —Ga01—Sr01 ^{xviii}	53.829 (2)
O01 ^{iv} —Sr01—O02 ^{ix}	64.41 (4)	O01—Ga01—Sr01 ^{xvi}	126.171 (1)
O01 ⁱⁱ —Sr01—O02 ^x	126.48 (3)	O01 ^{xi} —Ga01—O01	90.0
O01 ^v —Sr01—O02 ^{ix}	126.48 (3)	O01 ^{xi} —Ga01—O01 ^{xiii}	90.0
O01 ^{vi} —Sr01—O02 ^x	126.48 (3)	O01—Ga01—O01 ^{xiii}	180.0
O01 ⁱⁱ —Sr01—O02 ^{viii}	64.41 (4)	O01 ^{xii} —Ga01—O01 ^{xiii}	90.0
O01 ⁱⁱ —Sr01—O02 ^{vii}	64.41 (4)	O01—Ga01—O01 ^{xii}	90.0
O01 ⁱⁱ —Sr01—O02 ^{ix}	126.48 (3)	O01 ^{xi} —Ga01—O01 ^{xii}	180.0
O01 ^v —Sr01—O02 ^x	64.41 (4)	O01 ^{xiii} —Ga01—O02	90.0
O01 ^v —Sr01—O02 ^{viii}	126.48 (3)	O01—Ga01—O02	90.0
O01 ^{vi} —Sr01—O02 ^{viii}	64.41 (4)	O01 ^{xiii} —Ga01—O02 ^{xiv}	90.0
O01 ^{vi} —Sr01—O02 ^{ix}	64.41 (4)	O01 ^{xi} —Ga01—O02	90.0
O01 ^{iv} —Sr01—O02 ^x	64.41 (4)	O01 ^{xii} —Ga01—O02 ^{xiv}	90.0
O01 ^v —Sr01—O02 ^{vii}	64.41 (4)	O01 ^{xii} —Ga01—O02	90.0
O01 ^{iv} —Sr01—O02 ^{vii}	126.48 (3)	O01 ^{xi} —Ga01—O02 ^{xiv}	90.0
O02 ^x —Sr01—Ga01 ⁱⁱ	153.43 (4)	O01—Ga01—O02 ^{xiv}	90.0
O02—Sr01—Ga01 ⁱ	123.418 (3)	O02—Ga01—Sr01 ^{xv}	123.419 (3)
O02 ^{ix} —Sr01—Ga01 ⁱⁱⁱ	93.76 (2)	O02—Ga01—Sr01 ^{viii}	56.581 (3)
O02 ^x —Sr01—Ga01 ⁱ	93.76 (2)	O02 ^{xiv} —Ga01—Sr01 ^{xv}	56.581 (3)
O02—Sr01—Ga01 ⁱⁱⁱ	123.418 (3)	O02 ^{xiv} —Ga01—Sr01 ^{xviii}	56.581 (3)
O02 ^{vii} —Sr01—Ga01 ⁱⁱ	93.76 (2)	O02—Ga01—Sr01 ^{xviii}	123.419 (3)
O02 ^{vii} —Sr01—Ga01 ⁱ	40.26 (4)	O02 ^{xiv} —Ga01—Sr01 ^{viii}	123.419 (3)
O02 ^{ix} —Sr01—Ga01 ⁱ	153.43 (4)	O02—Ga01—Sr01 ^x	56.581 (3)
O02 ^x —Sr01—Ga01 ⁱⁱⁱ	40.26 (4)	O02 ^{xiv} —Ga01—Sr01 ^{xvi}	56.581 (3)
O02 ^{ix} —Sr01—Ga01 ⁱⁱ	93.76 (2)	O02 ^{xiv} —Ga01—Sr01 ^x	123.419 (3)
O02—Sr01—Ga01 ⁱⁱ	123.418 (3)	O02—Ga01—Sr01 ^{xvii}	123.419 (3)
O02 ^{viii} —Sr01—Ga01 ⁱⁱⁱ	153.43 (4)	O02 ^{xiv} —Ga01—Sr01 ^{xviii}	56.581 (3)
O02 ^{viii} —Sr01—Ga01 ⁱ	93.76 (2)	O02—Ga01—Sr01 ^{xvi}	123.419 (3)
O02 ^{vii} —Sr01—Ga01 ⁱⁱⁱ	93.76 (2)	O02 ^{xiv} —Ga01—O02	180.0
O02 ^{viii} —Sr01—Ga01 ⁱⁱ	40.26 (4)	Sr01 ^x —O01—Sr01 ^{xviii}	86.039 (7)
O02—Sr01—O01 ⁱⁱ	133.019 (3)	Sr01 ^x —O01—Sr01 ^{vii}	93.961 (7)
O02—Sr01—O01 ^{iv}	133.019 (3)	Sr01 ^{xv} —O01—Sr01 ^{vii}	86.039 (7)
O02—Sr01—O01 ^{vi}	133.019 (3)	Sr01 ^{xv} —O01—Sr01 ^x	180.0
O02—Sr01—O01 ^v	133.019 (3)	Sr01 ^{xviii} —O01—Sr01 ^{vii}	180.0
O02 ^{vii} —Sr01—O02 ^{ix}	166.31 (9)	Sr01 ^{xv} —O01—Sr01 ^{xviii}	93.961 (7)
O02 ^{viii} —Sr01—O02 ^{ix}	89.186 (11)	Ga01 ^{xix} —O01—Sr01 ^{xv}	90.0
O02—Sr01—O02 ^{ix}	83.16 (4)	Ga01 ^{xix} —O01—Sr01 ^{vii}	90.0
O02—Sr01—O02 ^{vii}	83.16 (4)	Ga01—O01—Sr01 ^{xviii}	90.0
O02 ^{viii} —Sr01—O02 ^x	166.31 (9)	Ga01—O01—Sr01 ^{xv}	90.0
O02 ^{viii} —Sr01—O02 ^{vii}	89.186 (11)	Ga01—O01—Sr01 ^x	90.0
O02—Sr01—O02 ^{viii}	83.16 (4)	Ga01—O01—Sr01 ^{vii}	90.0
O02 ^x —Sr01—O02 ^{ix}	89.186 (11)	Ga01 ^{xix} —O01—Sr01 ^{xviii}	90.0
O02—Sr01—O02 ^x	83.16 (4)	Ga01 ^{xix} —O01—Sr01 ^x	90.0
O02 ^x —Sr01—O02 ^{vii}	89.186 (11)	Ga01 ^{xix} —O01—Ga01	180.0
Sr01 ^{xv} —Ga01—Sr01 ^{xvi}	113.163 (6)	Sr01—O02—Sr01 ^{vii}	96.84 (4)
Sr01 ^{xvii} —Ga01—Sr01 ^{xv}	72.343 (3)	Sr01 ^{ix} —O02—Sr01 ^{vii}	166.31 (9)

Sr01 ^{xvii} —Ga01—Sr01 ^{xvi}	72.343 (3)	Sr01 ^{viii} —O02—Sr01 ^x	166.31 (9)
Sr01 ^{xviii} —Ga01—Sr01 ^{viii}	180.0	Sr01 ^{viii} —O02—Sr01 ^{ix}	89.187 (11)
Sr01 ^{viii} —Ga01—Sr01 ^{xv}	107.657 (3)	Sr01 ^x —O02—Sr01 ^{ix}	89.187 (11)
Sr01 ^{xvii} —Ga01—Sr01 ^{viii}	66.837 (6)	Sr01—O02—Sr01 ^{vii}	96.84 (4)
Sr01 ^{xviii} —Ga01—Sr01 ^{xv}	72.343 (3)	Sr01 ^x —O02—Sr01 ^{vii}	89.187 (11)
Sr01 ^{xvii} —Ga01—Sr01 ^x	180.0	Sr01—O02—Sr01 ^{ix}	96.84 (4)
Sr01 ^{xvii} —Ga01—Sr01 ^{xviii}	113.163 (6)	Sr01—O02—Sr01 ^x	96.84 (4)
Sr01 ^x —Ga01—Sr01 ^{xv}	107.657 (3)	Sr01 ^{viii} —O02—Sr01 ^{vii}	89.187 (11)
Sr01 ^x —Ga01—Sr01 ^{xviii}	66.837 (6)	Ga01—O02—Sr01 ^{vii}	83.16 (4)
Sr01 ^x —Ga01—Sr01 ^{vii}	107.657 (3)	Ga01—O02—Sr01 ^{ix}	83.16 (4)
Sr01 ^{viii} —Ga01—Sr01 ^{xvi}	107.657 (3)	Ga01—O02—Sr01 ^{viii}	83.16 (4)
Sr01 ^x —Ga01—Sr01 ^{viii}	113.163 (6)	Ga01—O02—Sr01	180.0
Sr01 ^{xviii} —Ga01—Sr01 ^{xvi}	72.343 (3)	Ga01—O02—Sr01 ^x	83.16 (4)

Symmetry codes: (i) $x-1/2, y+1/2, z+1/2$; (ii) $x-1/2, y-1/2, z+1/2$; (iii) $x+1/2, y+1/2, z+1/2$; (iv) $x+1/2, y-1/2, z+1/2$; (v) $-y+1/2, x+1/2, z+1/2$; (vi) $-y+1/2, x-1/2, z+1/2$; (vii) $-x-1/2, -y+1/2, -z+1/2$; (viii) $-x-1/2, -y-1/2, -z+1/2$; (ix) $-x+1/2, -y-1/2, -z+1/2$; (x) $-x+1/2, -y+1/2, -z+1/2$; (xi) $-y+1, x, z$; (xii) $-y, x, z$; (xiii) $x, y-1, z$; (xiv) $-x, -y, -z$; (xv) $x-1/2, y+1/2, z-1/2$; (xvi) $x+1/2, y-1/2, z-1/2$; (xvii) $x-1/2, y-1/2, z-1/2$; (xviii) $x+1/2, y+1/2, z-1/2$; (xix) $x, y+1, z$.