

Title

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Abstract**Table 1**

Experimental details

| Crystal data | |
|--|--|
| Chemical formula | <chem>Ca4Li2O13Si4</chem> |
| M_r | 494.56 |
| Crystal system, space group | Triclinic, $P\bar{1}$ |
| Temperature (K) | 301 |
| a, b, c (Å) | 7.1593 (4), 8.2192 (4), 10.4182 (6) |
| α, β, γ (°) | 70.737 (5), 89.858 (4), 77.719 (5) |
| V (Å ³) | 563.96 (6) |
| Z | 2 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 2.42 |
| Crystal size (mm) | 0.04 × 0.03 × 0.02 |
| Data collection | |
| Diffractometer | ROD, Synergy Custom system, HyPix-Arc 150 |
| Absorption correction | Gaussian <i>CrysAlis PRO</i> 1.171.42.53a (Rigaku Oxford Diffraction, 2022) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. |
| T_{\min}, T_{\max} | 0.939, 0.995 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] | 18107, 3412, 3039 |
| reflections | |
| R_{int} | 0.052 |
| (sin θ/λ) _{max} (Å ⁻¹) | 0.714 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S | 0.045, 0.109, 1.20 |
| No. of reflections | 3412 |
| No. of parameters | 208 |
| $\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³) | 1.07, -0.67 |

Computer programs: *CrysAlis PRO* 1.171.42.53a (Rigaku OD, 2022), *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* 1.171.42.53a (Rigaku OD, 2022); cell refinement: *CrysAlis PRO* 1.171.42.53a (Rigaku OD, 2022); data reduction: *CrysAlis PRO* 1.171.42.53a (Rigaku OD, 2022); 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).

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Crystal data

$\text{Ca}_4\text{Li}_2\text{O}_{13}\text{Si}_4$
 $M_r = 494.56$
Triclinic, $P\bar{1}$
 $a = 7.1593 (4)$ Å
 $b = 8.2192 (4)$ Å
 $c = 10.4182 (6)$ Å
 $\alpha = 70.737 (5)^\circ$
 $\beta = 89.858 (4)^\circ$
 $\gamma = 77.719 (5)^\circ$
 $V = 563.96 (6)$ Å³

$Z = 2$
 $F(000) = 492$
 $D_x = 2.912 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7346 reflections
 $\theta = 2.7\text{--}52.2^\circ$
 $\mu = 2.42 \text{ mm}^{-1}$
 $T = 301$ K
Irregular, light brown
 $0.04 \times 0.03 \times 0.02$ 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: gaussian
CrysAlis PRO 1.171.42.53a (Rigaku Oxford
Diffraction, 2022) Numerical absorption correction
based on gaussian integration over a multifaceted
crystal model Empirical absorption correction using
spherical harmonics, implemented in SCALE3
ABSPACK scaling algorithm.
 $T_{\min} = 0.939$, $T_{\max} = 0.995$
18107 measured reflections
3412 independent reflections
3039 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$
 $\theta_{\max} = 30.5^\circ$, $\theta_{\min} = 2.7^\circ$
 $h = -10 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.109$
 $S = 1.20$
3412 reflections
208 parameters

0 restraints
Primary atom site location: dual
 $w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 1.1556P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.07 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.67 \text{ e } \text{\AA}^{-3}$

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.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|-------------|----------------------------------|
| Ca01 | 0.92881 (8) | 0.29223 (8) | 0.10560 (6) | 0.01033 (13) |
| Ca02 | 0.07009 (8) | 0.69707 (8) | 0.50534 (6) | 0.01015 (13) |
| Ca03 | 0.41678 (8) | 0.30573 (8) | 0.49700 (6) | 0.01070 (13) |
| Ca04 | 0.42446 (8) | 0.28960 (8) | 0.09733 (6) | 0.01048 (13) |
| Si01 | 0.57438 (12) | 0.58482 (11) | 0.22141 (8) | 0.00860 (16) |
| Si02 | 0.13667 (12) | 0.59303 (11) | 0.21937 (8) | 0.00882 (16) |
| Si03 | 0.21748 (12) | 0.11724 (11) | 0.80437 (8) | 0.00912 (16) |
| Si04 | 0.23332 (12) | 0.07255 (11) | 0.32133 (8) | 0.00987 (17) |
| Li01 | 0.2535 (13) | 0.9079 (9) | 0.0922 (7) | 0.0318 (16) |
| Li02 | 0.7275 (17) | 0.0749 (10) | 0.3856 (9) | 0.050 (3) |
| O01 | 0.0141 (3) | 0.1653 (3) | 0.3412 (2) | 0.0147 (4) |
| O02 | 0.7133 (3) | 0.1246 (3) | 0.5676 (2) | 0.0131 (4) |
| O03 | 0.4002 (3) | 0.1765 (3) | 0.3363 (2) | 0.0143 (4) |
| O04 | 0.3660 (3) | 0.5077 (3) | 0.6200 (2) | 0.0111 (4) |
| O05 | 0.1179 (3) | 0.5030 (3) | 0.3777 (2) | 0.0108 (4) |
| O06 | 0.1206 (3) | 0.4900 (3) | 0.1162 (2) | 0.0115 (4) |
| O07 | 0.6354 (3) | 0.4676 (3) | 0.1259 (2) | 0.0128 (4) |
| O08 | 0.2286 (3) | 0.0885 (3) | 0.1600 (2) | 0.0114 (4) |
| O09 | 0.0058 (3) | 0.2080 (3) | 0.8434 (2) | 0.0149 (4) |
| O10 | 0.3628 (3) | 0.2258 (3) | 0.8470 (2) | 0.0159 (5) |
| O11 | 0.7269 (3) | 0.0874 (3) | 0.1011 (2) | 0.0120 (4) |
| O12 | 0.2150 (3) | 0.1490 (3) | 0.6435 (2) | 0.0127 (4) |
| O13 | 0.3410 (3) | 0.6558 (3) | 0.1981 (2) | 0.0131 (4) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|-------------|-------------|-------------|
| Ca01 | 0.0095 (3) | 0.0077 (3) | 0.0129 (3) | -0.0017 (2) | 0.0001 (2) | -0.0025 (2) |
| Ca02 | 0.0094 (3) | 0.0102 (3) | 0.0121 (3) | -0.0028 (2) | 0.0024 (2) | -0.0052 (2) |
| Ca03 | 0.0096 (3) | 0.0101 (3) | 0.0130 (3) | -0.0020 (2) | 0.0013 (2) | -0.0046 (2) |
| Ca04 | 0.0100 (3) | 0.0080 (3) | 0.0129 (3) | -0.0025 (2) | 0.0018 (2) | -0.0025 (2) |
| Si01 | 0.0094 (4) | 0.0070 (4) | 0.0097 (3) | -0.0026 (3) | 0.0011 (3) | -0.0028 (3) |
| Si02 | 0.0102 (4) | 0.0070 (4) | 0.0095 (3) | -0.0021 (3) | 0.0012 (3) | -0.0031 (3) |
| Si03 | 0.0095 (4) | 0.0068 (4) | 0.0108 (4) | -0.0021 (3) | 0.0013 (3) | -0.0024 (3) |
| Si04 | 0.0119 (4) | 0.0068 (4) | 0.0105 (4) | -0.0016 (3) | 0.0011 (3) | -0.0027 (3) |
| Li01 | 0.061 (5) | 0.015 (3) | 0.021 (3) | -0.008 (3) | 0.006 (3) | -0.008 (3) |
| Li02 | 0.098 (8) | 0.012 (3) | 0.041 (5) | -0.004 (4) | 0.006 (5) | -0.015 (3) |
| O01 | 0.0178 (11) | 0.0125 (11) | 0.0130 (10) | -0.0003 (8) | 0.0031 (8) | -0.0051 (8) |
| O02 | 0.0117 (10) | 0.0078 (10) | 0.0169 (10) | -0.0005 (8) | 0.0004 (8) | -0.0016 (8) |
| O03 | 0.0194 (11) | 0.0123 (11) | 0.0139 (10) | -0.0071 (9) | 0.0018 (8) | -0.0057 (8) |
| O04 | 0.0118 (10) | 0.0083 (10) | 0.0119 (9) | -0.0016 (8) | -0.0001 (8) | -0.0023 (8) |
| O05 | 0.0120 (10) | 0.0091 (10) | 0.0110 (9) | -0.0022 (8) | 0.0022 (8) | -0.0029 (8) |
| O06 | 0.0155 (10) | 0.0108 (10) | 0.0101 (9) | -0.0043 (8) | 0.0021 (8) | -0.0051 (8) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| O07 | 0.0123 (10) | 0.0131 (10) | 0.0147 (10) | -0.0016 (8) | 0.0024 (8) | -0.0080 (8) |
| O08 | 0.0138 (10) | 0.0096 (10) | 0.0113 (9) | -0.0025 (8) | 0.0011 (8) | -0.0045 (8) |
| O09 | 0.0136 (10) | 0.0100 (10) | 0.0173 (10) | 0.0003 (8) | 0.0033 (8) | -0.0016 (8) |
| O10 | 0.0167 (11) | 0.0127 (11) | 0.0180 (11) | -0.0079 (9) | -0.0008 (9) | -0.0021 (9) |
| O11 | 0.0114 (10) | 0.0062 (9) | 0.0169 (10) | -0.0012 (8) | 0.0006 (8) | -0.0024 (8) |
| O12 | 0.0133 (10) | 0.0108 (10) | 0.0130 (10) | -0.0011 (8) | 0.0012 (8) | -0.0038 (8) |
| O13 | 0.0102 (10) | 0.0113 (10) | 0.0175 (10) | -0.0021 (8) | 0.0012 (8) | -0.0045 (8) |

Geometric parameters (Å, °)

| | | | |
|---|-------------|---------------------------|-------------|
| Ca01—Ca04 ⁱ | 3.5450 (8) | Ca04—Si04 | 2.9626 (10) |
| Ca01—Si02 ⁱⁱ | 3.2069 (10) | Ca04—Li02 | 3.427 (10) |
| Ca01—Si04 ⁱ | 2.9558 (10) | Ca04—O03 | 2.373 (2) |
| Ca01—Li01 ⁱⁱ | 3.438 (7) | Ca04—O06 | 2.484 (2) |
| Ca01—Li02 | 3.379 (10) | Ca04—O07 ⁱⁱ | 2.481 (2) |
| Ca01—O01 ⁱ | 2.352 (2) | Ca04—O07 | 2.396 (2) |
| Ca01—O06 ⁱ | 2.369 (2) | Ca04—O08 | 2.322 (2) |
| Ca01—O06 ⁱⁱ | 2.382 (2) | Ca04—O10 ^{ix} | 2.877 (2) |
| Ca01—O07 | 2.334 (2) | Ca04—O11 | 2.425 (2) |
| Ca01—O08 ⁱ | 2.363 (2) | Si01—Li01 | 3.034 (8) |
| Ca01—O09 ⁱⁱⁱ | 3.053 (2) | Si01—O04 ^{vi} | 1.589 (2) |
| Ca01—O11 | 2.452 (2) | Si01—O07 | 1.600 (2) |
| Ca02—Ca03 ^{iv} | 3.4908 (8) | Si01—O10 ^{vi} | 1.642 (2) |
| Ca02—Si02 | 3.3668 (10) | Si01—O13 | 1.639 (2) |
| Ca02—Si04 ^v | 3.4906 (10) | Si02—Li01 | 2.794 (7) |
| Ca02—Si04 ^{iv} | 3.4716 (10) | Si02—O05 | 1.588 (2) |
| Ca02—Li02 ^{vi} | 3.078 (10) | Si02—O06 | 1.590 (2) |
| Ca02—Li02 ^{vii} | 3.382 (9) | Si02—O09 ^{iv} | 1.653 (2) |
| Ca02—O01 ^{iv} | 2.258 (2) | Si02—O13 | 1.643 (2) |
| Ca02—O02 ^{vi} | 2.315 (2) | Si03—Li01 ^x | 2.903 (7) |
| Ca02—O04 | 2.392 (2) | Si03—Li02 ^{viii} | 2.891 (8) |
| Ca02—O05 ^{iv} | 2.369 (2) | Si03—O09 | 1.654 (2) |
| Ca02—O05 | 2.365 (2) | Si03—O10 | 1.654 (2) |
| Ca02—O12 ^{iv} | 2.407 (2) | Si03—O11 ^{viii} | 1.607 (2) |
| Ca03—Si01 | 3.3939 (10) | Si03—O12 | 1.608 (2) |
| Ca03—Si01 ^{vi} | 3.3445 (10) | Si04—Li01 ^{xi} | 3.098 (7) |
| Ca03—Si02 | 3.3869 (10) | Si04—Li02 ^{viii} | 2.879 (9) |
| Ca03—Si04 | 3.4850 (10) | Si04—O01 | 1.637 (2) |
| Ca03—Li02 | 3.089 (10) | Si04—O02 ^{viii} | 1.616 (2) |
| Ca03—Li02 ^{viii} | 3.346 (9) | Si04—O03 | 1.645 (2) |
| Ca03—O02 | 2.281 (2) | Si04—O08 | 1.642 (2) |
| Ca03—O03 | 2.274 (2) | Li01—O08 ^v | 1.820 (7) |
| Ca03—O04 | 2.382 (2) | Li01—O09 ^{iv} | 2.264 (9) |
| Ca03—O04 ^{vi} | 2.455 (2) | Li01—O11 ⁱⁱ | 2.006 (7) |
| Ca03—O05 | 2.441 (2) | Li01—O13 | 1.961 (7) |
| Ca03—O12 | 2.358 (2) | Li02—O01 ⁱ | 2.322 (12) |
| Ca04—Si01 | 3.4489 (10) | Li02—O02 | 2.066 (9) |
| Ca04—Si01 ⁱⁱ | 3.1360 (10) | Li02—O03 | 2.311 (12) |
| Ca04—Si02 | 3.4604 (10) | Li02—O12 ^{viii} | 1.922 (8) |
| Si02 ⁱⁱ —Ca01—Ca04 ⁱ | 93.58 (2) | O05—Si02—Ca04 | 109.33 (9) |
| Si02 ⁱⁱ —Ca01—Li01 ⁱⁱ | 49.58 (12) | O05—Si02—Li01 | 127.21 (16) |

| | | | |
|--|-------------|---|-------------|
| Si02 ⁱⁱ —Ca01—Li02 | 138.26 (18) | O05—Si02—O06 | 120.64 (12) |
| Si04 ⁱ —Ca01—Ca04 ⁱ | 53.29 (2) | O05—Si02—O09 ^{iv} | 112.22 (12) |
| Si04 ⁱ —Ca01—Si02 ⁱⁱ | 137.80 (3) | O05—Si02—O13 | 108.97 (12) |
| Si04 ⁱ —Ca01—Li01 ⁱⁱ | 118.05 (13) | O06—Si02—Ca01 ^{xii} | 28.60 (8) |
| Si04 ⁱ —Ca01—Li02 | 70.64 (19) | O06—Si02—Ca01 ⁱⁱ | 45.58 (8) |
| Si04 ⁱ —Ca01—O09 ⁱⁱⁱ | 110.21 (5) | O06—Si02—Ca02 ^{iv} | 95.20 (8) |
| Li01 ⁱⁱ —Ca01—Ca04 ⁱ | 117.41 (14) | O06—Si02—Ca02 | 157.38 (9) |
| Li02—Ca01—Ca04 ⁱ | 123.52 (19) | O06—Si02—Ca03 | 107.51 (9) |
| Li02—Ca01—Li01 ⁱⁱ | 92.8 (2) | O06—Si02—Ca04 | 40.79 (8) |
| O01 ⁱ —Ca01—Ca04 ⁱ | 81.58 (6) | O06—Si02—Li01 | 111.48 (16) |
| O01 ⁱ —Ca01—Si02 ⁱⁱ | 170.17 (6) | O06—Si02—O09 ^{iv} | 108.08 (12) |
| O01 ⁱ —Ca01—Si04 ⁱ | 33.55 (6) | O06—Si02—O13 | 107.10 (12) |
| O01 ⁱ —Ca01—Li01 ⁱⁱ | 125.49 (13) | O09 ^{iv} —Si02—Ca01 ⁱⁱ | 69.61 (9) |
| O01 ⁱ —Ca01—Li02 | 43.4 (2) | O09 ^{iv} —Si02—Ca01 ^{xii} | 107.75 (9) |
| O01 ⁱ —Ca01—O06 ⁱⁱ | 158.30 (8) | O09 ^{iv} —Si02—Ca02 | 79.63 (9) |
| O01 ⁱ —Ca01—O06 ⁱ | 83.75 (8) | O09 ^{iv} —Si02—Ca02 ^{iv} | 111.68 (9) |
| O01 ⁱ —Ca01—O08 ⁱ | 66.48 (8) | O09 ^{iv} —Si02—Ca03 | 144.02 (9) |
| O01 ⁱ —Ca01—O09 ⁱⁱⁱ | 139.71 (7) | O09 ^{iv} —Si02—Ca04 | 137.84 (9) |
| O01 ⁱ —Ca01—O11 | 94.92 (8) | O09 ^{iv} —Si02—Li01 | 54.13 (19) |
| O06 ⁱⁱ —Ca01—Ca04 ⁱ | 88.62 (6) | O13—Si02—Ca01 ⁱⁱ | 88.52 (9) |
| O06 ⁱ —Ca01—Ca04 ⁱ | 44.37 (6) | O13—Si02—Ca01 ^{xii} | 133.93 (9) |
| O06 ⁱⁱ —Ca01—Si02 ⁱⁱ | 28.46 (5) | O13—Si02—Ca02 ^{iv} | 135.85 (9) |
| O06 ⁱ —Ca01—Si02 ⁱⁱ | 98.83 (6) | O13—Si02—Ca02 | 92.56 (9) |
| O06 ⁱⁱ —Ca01—Si04 ⁱ | 141.91 (6) | O13—Si02—Ca03 | 77.19 (8) |
| O06 ⁱ —Ca01—Si04 ⁱ | 76.10 (6) | O13—Si02—Ca04 | 75.54 (9) |
| O06 ⁱⁱ —Ca01—Li01 ⁱⁱ | 76.20 (13) | O13—Si02—Li01 | 43.5 (2) |
| O06 ⁱ —Ca01—Li01 ⁱⁱ | 146.62 (13) | O13—Si02—O09 ^{iv} | 97.16 (12) |
| O06 ⁱ —Ca01—Li02 | 120.58 (17) | Ca01 ^{viii} —Si03—Ca04 ^{viii} | 60.693 (19) |
| O06 ⁱⁱ —Ca01—Li02 | 147.0 (2) | Ca02 ^{iv} —Si03—Ca01 ^{viii} | 93.72 (2) |
| O06 ⁱ —Ca01—O06 ⁱⁱ | 75.78 (8) | Ca02 ^{iv} —Si03—Ca04 ^{viii} | 125.42 (3) |
| O06 ⁱ —Ca01—O09 ⁱⁱⁱ | 107.57 (7) | Ca03—Si03—Ca01 ^{viii} | 124.16 (3) |
| O06 ⁱⁱ —Ca01—O09 ⁱⁱⁱ | 56.12 (7) | Ca03—Si03—Ca02 ^{iv} | 59.479 (19) |
| O06 ⁱ —Ca01—O11 | 178.33 (8) | Ca03—Si03—Ca04 ^{viii} | 94.24 (2) |
| O06 ⁱⁱ —Ca01—O11 | 105.41 (8) | Li01 ^x —Si03—Ca01 ^{viii} | 63.23 (15) |
| O07—Ca01—Ca04 ⁱ | 141.18 (6) | Li01 ^x —Si03—Ca02 ^{iv} | 147.91 (17) |
| O07—Ca01—Si02 ⁱⁱ | 93.56 (6) | Li01 ^x —Si03—Ca03 | 151.70 (18) |
| O07—Ca01—Si04 ⁱ | 128.55 (6) | Li01 ^x —Si03—Ca04 ^{viii} | 64.48 (15) |
| O07—Ca01—Li01 ⁱⁱ | 95.84 (15) | Li02 ^{viii} —Si03—Ca01 ^{viii} | 62.06 (19) |
| O07—Ca01—Li02 | 70.18 (18) | Li02 ^{viii} —Si03—Ca02 ^{iv} | 62.7 (2) |
| O07—Ca01—O01 ⁱ | 95.55 (8) | Li02 ^{viii} —Si03—Ca03 | 62.10 (19) |
| O07—Ca01—O06 ⁱⁱ | 80.03 (8) | Li02 ^{viii} —Si03—Ca04 ^{viii} | 62.7 (2) |
| O07—Ca01—O06 ⁱ | 96.82 (8) | Li02 ^{viii} —Si03—Li01 ^x | 116.8 (2) |
| O07—Ca01—O08 ⁱ | 162.04 (8) | O09—Si03—Ca01 ^{viii} | 88.51 (9) |
| O07—Ca01—O09 ⁱⁱⁱ | 120.25 (7) | O09—Si03—Ca02 ^{iv} | 74.59 (9) |
| O07—Ca01—O11 | 82.29 (8) | O09—Si03—Ca03 | 122.84 (9) |
| O08 ⁱ —Ca01—Ca04 ⁱ | 40.40 (5) | O09—Si03—Ca04 ^{viii} | 141.90 (9) |
| O08 ⁱ —Ca01—Si02 ⁱⁱ | 104.35 (6) | O09—Si03—Li01 ^x | 82.38 (19) |
| O08 ⁱ —Ca01—Si04 ⁱ | 33.68 (5) | O09—Si03—Li02 ^{viii} | 124.4 (3) |
| O08 ⁱ —Ca01—Li01 ⁱⁱ | 94.82 (15) | O09—Si03—O10 | 103.22 (13) |
| O08 ⁱ —Ca01—Li02 | 94.92 (18) | O10—Si03—Ca01 ^{viii} | 145.09 (9) |
| O08 ⁱ —Ca01—O06 ⁱⁱ | 116.64 (8) | O10—Si03—Ca02 ^{iv} | 121.01 (9) |
| O08 ⁱ —Ca01—O06 ⁱ | 81.92 (8) | O10—Si03—Ca03 | 76.70 (9) |

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|--|-------------|---|-------------|
| O08 ⁱ —Ca01—O09 ⁱⁱⁱ | 76.80 (7) | O10—Si03—Ca04 ^{viii} | 92.88 (9) |
| O08 ⁱ —Ca01—O11 | 98.49 (8) | O10—Si03—Li01 ^x | 85.56 (18) |
| O09 ⁱⁱⁱ —Ca01—Ca04 ⁱ | 80.99 (5) | O10—Si03—Li02 ^{viii} | 128.4 (3) |
| O09 ⁱⁱⁱ —Ca01—Si02 ⁱⁱ | 30.49 (5) | O11 ^{viii} —Si03—Ca01 ^{viii} | 35.88 (8) |
| O09 ⁱⁱⁱ —Ca01—Li01 ⁱⁱ | 40.29 (14) | O11 ^{viii} —Si03—Ca02 ^{iv} | 127.15 (9) |
| O09 ⁱⁱⁱ —Ca01—Li02 | 129.52 (15) | O11 ^{viii} —Si03—Ca03 | 125.67 (9) |
| O11—Ca01—Ca04 ⁱ | 136.49 (6) | O11 ^{viii} —Si03—Ca04 ^{viii} | 33.65 (8) |
| O11—Ca01—Si02 ⁱⁱ | 82.66 (6) | O11 ^{viii} —Si03—Li01 ^x | 41.52 (16) |
| O11—Ca01—Si04 ⁱ | 103.33 (6) | O11 ^{viii} —Si03—Li02 ^{viii} | 75.37 (19) |
| O11—Ca01—Li01 ⁱⁱ | 35.02 (13) | O11 ^{viii} —Si03—O09 | 108.38 (12) |
| O11—Ca01—Li02 | 57.79 (17) | O11 ^{viii} —Si03—O10 | 109.79 (12) |
| O11—Ca01—O09 ⁱⁱⁱ | 74.10 (7) | O11 ^{viii} —Si03—O12 | 114.10 (12) |
| Si02—Ca02—Ca03 ^{iv} | 94.30 (2) | O12—Si03—Ca01 ^{viii} | 95.32 (9) |
| Si02—Ca02—Si04 ^{iv} | 146.98 (3) | O12—Si03—Ca02 ^{iv} | 35.61 (8) |
| Si02—Ca02—Si04 ^v | 84.01 (2) | O12—Si03—Ca03 | 34.03 (8) |
| Si02—Ca02—Li02 ^{vii} | 100.28 (15) | O12—Si03—Ca04 ^{viii} | 95.50 (9) |
| Si04 ^v —Ca02—Ca03 ^{iv} | 121.60 (2) | O12—Si03—Li01 ^x | 155.53 (16) |
| Si04 ^{iv} —Ca02—Ca03 ^{iv} | 60.07 (2) | O12—Si03—Li02 ^{viii} | 38.75 (19) |
| Si04 ^{iv} —Ca02—Si04 ^v | 92.15 (2) | O12—Si03—O09 | 110.19 (12) |
| Li02 ^{vii} —Ca02—Ca03 ^{iv} | 58.23 (19) | O12—Si03—O10 | 110.58 (12) |
| Li02 ^{vi} —Ca02—Ca03 ^{iv} | 127.6 (2) | Ca01 ^{xii} —Si04—Ca02 ^{xi} | 106.47 (3) |
| Li02 ^{vi} —Ca02—Si02 | 129.15 (19) | Ca01 ^{xii} —Si04—Ca02 ^{iv} | 78.43 (3) |
| Li02 ^{vi} —Ca02—Si04 ^{iv} | 68.0 (2) | Ca01 ^{xii} —Si04—Ca03 ^{viii} | 156.36 (3) |
| Li02 ^{vii} —Ca02—Si04 ^v | 64.70 (18) | Ca01 ^{xii} —Si04—Ca03 | 114.36 (3) |
| Li02 ^{vi} —Ca02—Si04 ^v | 51.52 (17) | Ca01 ^{xii} —Si04—Ca04 | 73.59 (3) |
| Li02 ^{vii} —Ca02—Si04 ^{iv} | 49.66 (15) | Ca01 ^{xii} —Si04—Li01 ^{xi} | 71.65 (15) |
| Li02 ^{vi} —Ca02—Li02 ^{vii} | 83.3 (3) | Ca02 ^{iv} —Si04—Ca02 ^{xi} | 87.85 (2) |
| O01 ^{iv} —Ca02—Ca03 ^{iv} | 81.51 (6) | Ca02 ^{iv} —Si04—Ca03 | 60.24 (2) |
| O01 ^{iv} —Ca02—Si02 | 165.23 (7) | Ca02 ^{iv} —Si04—Ca03 ^{viii} | 120.19 (3) |
| O01 ^{iv} —Ca02—Si04 ^v | 86.16 (6) | Ca02 ^{xi} —Si04—Ca03 ^{viii} | 63.17 (2) |
| O01 ^{iv} —Ca02—Si04 ^{iv} | 22.64 (6) | Ca03—Si04—Ca02 ^{xi} | 119.17 (3) |
| O01 ^{iv} —Ca02—Li02 ^{vii} | 48.7 (2) | Ca03—Si04—Ca03 ^{viii} | 88.67 (2) |
| O01 ^{iv} —Ca02—Li02 ^{vii} | 65.45 (16) | Ca04—Si04—Ca02 ^{iv} | 115.69 (3) |
| O01 ^{iv} —Ca02—O02 ^{vi} | 87.92 (9) | Ca04—Si04—Ca02 ^{xi} | 155.40 (3) |
| O01 ^{iv} —Ca02—O04 | 98.37 (8) | Ca04—Si04—Ca03 ^{viii} | 106.69 (3) |
| O01 ^{iv} —Ca02—O05 | 166.10 (9) | Ca04—Si04—Ca03 | 81.07 (3) |
| O01 ^{iv} —Ca02—O05 ^{iv} | 86.08 (8) | Ca04—Si04—Li01 ^{xi} | 73.26 (14) |
| O01 ^{iv} —Ca02—O12 ^{iv} | 94.11 (8) | Li01 ^{xi} —Si04—Ca02 ^{iv} | 144.79 (17) |
| O02 ^{vi} —Ca02—Ca03 ^{iv} | 143.74 (6) | Li01 ^{xi} —Si04—Ca02 ^{xi} | 83.34 (13) |
| O02 ^{vi} —Ca02—Si02 | 87.21 (6) | Li01 ^{xi} —Si04—Ca03 | 150.81 (16) |
| O02 ^{vi} —Ca02—Si04 ^{iv} | 101.56 (6) | Li01 ^{xi} —Si04—Ca03 ^{viii} | 85.66 (15) |
| O02 ^{vi} —Ca02—Si04 ^v | 22.49 (6) | Li02 ^{viii} —Si04—Ca01 ^{xii} | 137.7 (2) |
| O02 ^{vi} —Ca02—Li02 ^{vii} | 42.15 (19) | Li02 ^{viii} —Si04—Ca02 ^{iv} | 63.55 (19) |
| O02 ^{vi} —Ca02—Li02 ^{vii} | 85.80 (19) | Li02 ^{viii} —Si04—Ca02 ^{xi} | 56.82 (19) |
| O02 ^{vi} —Ca02—O04 | 77.35 (8) | Li02 ^{viii} —Si04—Ca03 ^{viii} | 56.73 (19) |
| O02 ^{vi} —Ca02—O05 ^{iv} | 168.72 (8) | Li02 ^{viii} —Si04—Ca03 | 62.58 (18) |
| O02 ^{vi} —Ca02—O05 | 105.52 (8) | Li02 ^{viii} —Si04—Ca04 | 138.7 (2) |
| O02 ^{vi} —Ca02—O12 ^{iv} | 104.77 (8) | Li02 ^{viii} —Si04—Li01 ^{xi} | 133.5 (2) |
| O04—Ca02—Ca03 ^{iv} | 138.38 (6) | O01—Si04—Ca01 ^{xii} | 52.54 (8) |
| O04—Ca02—Si02 | 94.16 (6) | O01—Si04—Ca02 ^{xi} | 80.10 (9) |
| O04—Ca02—Si04 ^{iv} | 118.77 (6) | O01—Si04—Ca02 ^{iv} | 32.07 (8) |
| O04—Ca02—Si04 ^v | 99.79 (6) | O01—Si04—Ca03 | 90.66 (9) |

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| O04—Ca02—Li02 ^{vii} | 157.23 (18) | O01—Si04—Ca03 ^{viii} | 137.00 (9) |
| O04—Ca02—Li02 ^{vi} | 73.90 (19) | O01—Si04—Ca04 | 115.65 (9) |
| O04—Ca02—O12 ^{iv} | 167.43 (8) | O01—Si04—Li01 ^{xi} | 112.72 (19) |
| O05 ^{iv} —Ca02—Ca03 ^{iv} | 44.29 (5) | O01—Si04—Li02 ^{viii} | 85.3 (2) |
| O05—Ca02—Ca03 ^{iv} | 89.36 (6) | O01—Si04—O03 | 116.13 (13) |
| O05—Ca02—Si02 | 25.24 (5) | O01—Si04—O08 | 104.00 (12) |
| O05 ^{iv} —Ca02—Si02 | 100.87 (6) | O02 ^{viii} —Si04—Ca01 ^{xii} | 138.52 (9) |
| O05 ^{iv} —Ca02—Si04 ^{iv} | 75.95 (6) | O02 ^{viii} —Si04—Ca02 ^{xi} | 33.22 (8) |
| O05 ^{iv} —Ca02—Si04 ^v | 164.95 (6) | O02 ^{viii} —Si04—Ca02 ^{iv} | 101.88 (9) |
| O05—Ca02—Si04 ^v | 107.60 (6) | O02 ^{viii} —Si04—Ca03 | 100.48 (9) |
| O05—Ca02—Si04 ^{iv} | 149.32 (6) | O02 ^{viii} —Si04—Ca03 ^{viii} | 30.78 (8) |
| O05—Ca02—Li02 ^{vi} | 142.6 (2) | O02 ^{viii} —Si04—Ca04 | 136.33 (9) |
| O05—Ca02—Li02 ^{vii} | 118.16 (16) | O02 ^{viii} —Si04—Li01 ^{xi} | 89.03 (15) |
| O05 ^{iv} —Ca02—Li02 ^{vi} | 128.65 (19) | O02 ^{viii} —Si04—Li02 ^{viii} | 44.53 (17) |
| O05 ^{iv} —Ca02—Li02 ^{vii} | 100.31 (19) | O02 ^{viii} —Si04—O01 | 107.99 (12) |
| O05—Ca02—O04 | 81.51 (8) | O02 ^{viii} —Si04—O03 | 108.50 (12) |
| O05 ^{iv} —Ca02—O04 | 94.08 (8) | O02 ^{viii} —Si04—O08 | 116.90 (12) |
| O05—Ca02—O05 ^{iv} | 80.08 (8) | O03—Si04—Ca01 ^{xii} | 112.98 (9) |
| O05—Ca02—O12 ^{iv} | 86.00 (8) | O03—Si04—Ca02 ^{iv} | 89.98 (9) |
| O05 ^{iv} —Ca02—O12 ^{iv} | 85.20 (8) | O03—Si04—Ca02 ^{xi} | 139.17 (9) |
| O12 ^{iv} —Ca02—Ca03 ^{iv} | 42.35 (5) | O03—Si04—Ca03 | 32.42 (8) |
| O12 ^{iv} —Ca02—Si02 | 73.71 (6) | O03—Si04—Ca03 ^{viii} | 83.28 (9) |
| O12 ^{iv} —Ca02—Si04 ^v | 82.53 (6) | O03—Si04—Ca04 | 53.11 (8) |
| O12 ^{iv} —Ca02—Si04 ^{iv} | 73.27 (6) | O03—Si04—Li01 ^{xi} | 118.40 (18) |
| O12 ^{iv} —Ca02—Li02 ^{vi} | 116.18 (19) | O03—Si04—Li02 ^{viii} | 86.0 (2) |
| O12 ^{iv} —Ca02—Li02 ^{vii} | 33.75 (17) | O08—Si04—Ca01 ^{xii} | 52.93 (8) |
| Si01 ^{vi} —Ca03—Si01 | 114.27 (2) | O08—Si04—Ca02 ^{iv} | 131.14 (9) |
| Si01 ^{vi} —Ca03—Si02 | 118.63 (3) | O08—Si04—Ca02 ^{xi} | 108.30 (8) |
| Si01—Ca03—Si04 | 96.26 (2) | O08—Si04—Ca03 | 132.08 (9) |
| Si01 ^{vi} —Ca03—Si04 | 147.79 (3) | O08—Si04—Ca03 ^{viii} | 108.03 (9) |
| Si01 ^{vi} —Ca03—Li02 ^{viii} | 101.36 (15) | O08—Si04—Ca04 | 51.32 (8) |
| Si02—Ca03—Si01 | 54.79 (2) | O08—Si04—Li01 ^{xi} | 28.03 (15) |
| Si02—Ca03—Si04 | 70.29 (2) | O08—Si04—Li02 ^{viii} | 161.43 (18) |
| Li02—Ca03—Si01 | 73.26 (16) | O08—Si04—O03 | 103.60 (12) |
| Li02 ^{viii} —Ca03—Si01 | 144.19 (15) | Ca01 ⁱⁱ —Li01—Ca01 ^{vii} | 112.8 (2) |
| Li02—Ca03—Si01 ^{vi} | 130.7 (2) | Ca01 ^{vii} —Li01—Ca04 ^v | 59.32 (11) |
| Li02 ^{viii} —Ca03—Si02 | 111.21 (19) | Ca01 ⁱⁱ —Li01—Ca04 ^v | 146.2 (2) |
| Li02—Ca03—Si02 | 105.30 (18) | Ca01 ⁱⁱ —Li01—Ca04 ⁱⁱ | 62.69 (12) |
| Li02 ^{viii} —Ca03—Si04 | 49.80 (16) | Ca04 ⁱⁱ —Li01—Ca01 ^{vii} | 147.7 (2) |
| Li02—Ca03—Si04 | 66.2 (2) | Ca04 ⁱⁱ —Li01—Ca04 ^v | 105.2 (2) |
| Li02—Ca03—Li02 ^{viii} | 81.1 (3) | Si01—Li01—Ca01 ^{vii} | 151.0 (2) |
| O02—Ca03—Si01 ^{vi} | 89.00 (6) | Si01—Li01—Ca01 ⁱⁱ | 92.27 (18) |
| O02—Ca03—Si01 | 93.71 (6) | Si01—Li01—Ca04 ^v | 107.2 (2) |
| O02—Ca03—Si02 | 143.67 (6) | Si01—Li01—Ca04 ⁱⁱ | 56.66 (13) |
| O02—Ca03—Si04 | 99.48 (6) | Si01—Li01—Si04 ^v | 98.8 (2) |
| O02—Ca03—Li02 ^{viii} | 83.0 (2) | Si02—Li01—Ca01 ^{vii} | 114.3 (3) |
| O02—Ca03—Li02 | 42.0 (2) | Si02—Li01—Ca01 ⁱⁱ | 60.91 (14) |
| O02—Ca03—O04 | 107.74 (8) | Si02—Li01—Ca04 ^v | 152.6 (2) |
| O02—Ca03—O04 ^{vi} | 76.70 (8) | Si02—Li01—Ca04 ⁱⁱ | 91.96 (18) |
| O02—Ca03—O05 | 169.02 (8) | Si02—Li01—Si01 | 64.59 (15) |
| O02—Ca03—O12 | 102.96 (8) | Si02—Li01—Si03 ^{xiii} | 128.6 (3) |
| O03—Ca03—Si01 ^{vi} | 167.89 (6) | Si02—Li01—Si04 ^v | 102.2 (2) |

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| O03—Ca03—Si01 | 77.58 (6) | Si03 ^{xiii} —Li01—Ca01 ^{vii} | 81.26 (17) |
| O03—Ca03—Si02 | 69.61 (6) | Si03 ^{xiii} —Li01—Ca01 ⁱⁱ | 67.83 (15) |
| O03—Ca03—Si04 | 22.82 (6) | Si03 ^{xiii} —Li01—Ca04 ^v | 78.38 (16) |
| O03—Ca03—Li02 ^{viii} | 66.68 (16) | Si03 ^{xiii} —Li01—Ca04 ⁱⁱ | 67.32 (14) |
| O03—Ca03—Li02 | 48.2 (2) | Si03 ^{xiii} —Li01—Si01 | 123.3 (3) |
| O03—Ca03—O02 | 87.67 (9) | Si03 ^{xiii} —Li01—Si04 ^v | 123.0 (2) |
| O03—Ca03—O04 ^{vi} | 96.03 (8) | Si04 ^v —Li01—Ca01 ⁱⁱ | 153.2 (3) |
| O03—Ca03—O04 | 163.32 (9) | Si04 ^v —Li01—Ca01 ^{vii} | 52.31 (11) |
| O03—Ca03—O05 | 83.75 (8) | Si04 ^v —Li01—Ca04 ^v | 51.65 (11) |
| O03—Ca03—O12 | 95.09 (8) | Si04 ^v —Li01—Ca04 ⁱⁱ | 142.8 (3) |
| O04—Ca03—Si01 ^{vi} | 25.90 (5) | O08 ^v —Li01—Ca01 ^{vii} | 37.06 (19) |
| O04 ^{vi} —Ca03—Si01 | 25.67 (5) | O08 ^v —Li01—Ca01 ⁱⁱ | 149.8 (4) |
| O04 ^{vi} —Ca03—Si01 ^{vi} | 94.52 (6) | O08 ^v —Li01—Ca04 ⁱⁱ | 138.2 (4) |
| O04—Ca03—Si01 | 94.66 (6) | O08 ^v —Li01—Ca04 ^v | 33.30 (17) |
| O04—Ca03—Si02 | 93.82 (6) | O08 ^v —Li01—Si01 | 117.3 (4) |
| O04 ^{vi} —Ca03—Si02 | 77.94 (5) | O08 ^v —Li01—Si02 | 124.5 (3) |
| O04 ^{vi} —Ca03—Si04 | 117.65 (6) | O08 ^v —Li01—Si03 ^{xiii} | 97.9 (3) |
| O04—Ca03—Si04 | 149.87 (6) | O08 ^v —Li01—Si04 ^v | 25.09 (13) |
| O04 ^{vi} —Ca03—Li02 ^{viii} | 153.97 (18) | O08 ^v —Li01—O09 ^{iv} | 104.8 (4) |
| O04 ^{vi} —Ca03—Li02 | 72.92 (18) | O08 ^v —Li01—O11 ⁱⁱ | 129.5 (4) |
| O04—Ca03—Li02 ^{viii} | 120.38 (16) | O08 ^v —Li01—O13 | 125.5 (4) |
| O04—Ca03—Li02 | 143.9 (2) | O09 ^{iv} —Li01—Ca01 ⁱⁱ | 60.69 (18) |
| O04—Ca03—O04 ^{vi} | 81.79 (8) | O09 ^{iv} —Li01—Ca01 ^{vii} | 80.9 (2) |
| O04—Ca03—O05 | 80.15 (8) | O09 ^{iv} —Li01—Ca04 ^v | 137.4 (3) |
| O05—Ca03—Si01 ^{vi} | 100.77 (6) | O09 ^{iv} —Li01—Ca04 ⁱⁱ | 117.0 (3) |
| O05—Ca03—Si01 | 77.78 (5) | O09 ^{iv} —Li01—Si01 | 100.6 (2) |
| O05—Ca03—Si02 | 25.64 (5) | O09 ^{iv} —Li01—Si02 | 36.27 (12) |
| O05—Ca03—Si04 | 74.89 (6) | O09 ^{iv} —Li01—Si03 ^{xiii} | 112.0 (3) |
| O05—Ca03—Li02 | 127.65 (19) | O09 ^{iv} —Li01—Si04 ^v | 93.1 (2) |
| O05—Ca03—Li02 ^{viii} | 99.7 (2) | O11 ⁱⁱ —Li01—Ca01 ⁱⁱ | 44.54 (17) |
| O05—Ca03—O04 ^{vi} | 97.36 (7) | O11 ⁱⁱ —Li01—Ca01 ^{vii} | 110.5 (3) |
| O12—Ca03—Si01 | 161.57 (6) | O11 ⁱⁱ —Li01—Ca04 ⁱⁱ | 41.90 (17) |
| O12—Ca03—Si01 ^{vi} | 74.33 (6) | O11 ⁱⁱ —Li01—Ca04 ^v | 104.4 (3) |
| O12—Ca03—Si02 | 106.85 (6) | O11 ⁱⁱ —Li01—Si01 | 97.4 (3) |
| O12—Ca03—Si04 | 73.49 (6) | O11 ⁱⁱ —Li01—Si02 | 102.7 (3) |
| O12—Ca03—Li02 | 114.48 (18) | O11 ⁱⁱ —Li01—Si03 ^{xiii} | 32.07 (12) |
| O12—Ca03—Li02 ^{viii} | 34.14 (17) | O11 ⁱⁱ —Li01—Si04 ^v | 154.3 (3) |
| O12—Ca03—O04 ^{vi} | 168.84 (8) | O11 ⁱⁱ —Li01—O09 ^{iv} | 103.2 (3) |
| O12—Ca03—O04 | 87.78 (8) | O13—Li01—Ca01 ⁱⁱ | 77.4 (2) |
| O12—Ca03—O05 | 84.67 (8) | O13—Li01—Ca01 ^{vii} | 140.4 (3) |
| Si01 ⁱⁱ —Ca04—Si01 | 110.38 (2) | O13—Li01—Ca04 ^v | 131.3 (3) |
| Si01 ⁱⁱ —Ca04—Si02 | 113.89 (3) | O13—Li01—Ca04 ⁱⁱ | 71.8 (2) |
| Si01—Ca04—Si02 | 53.69 (2) | O13—Li01—Si01 | 29.42 (15) |
| Si01 ⁱⁱ —Ca04—Li02 | 141.11 (18) | O13—Li01—Si02 | 35.22 (14) |
| Si04—Ca04—Si01 ⁱⁱ | 140.27 (3) | O13—Li01—Si03 ^{xiii} | 134.9 (3) |
| Si04—Ca04—Si01 | 105.82 (3) | O13—Li01—Si04 ^v | 100.9 (3) |
| Si04—Ca04—Si02 | 75.60 (3) | O13—Li01—O09 ^{iv} | 71.2 (2) |
| Si04—Ca04—Li02 | 68.30 (18) | O13—Li01—O11 ⁱⁱ | 103.0 (3) |
| Li02—Ca04—Si01 | 68.61 (13) | Ca01—Li02—Ca02 ^{xiv} | 99.9 (3) |
| Li02—Ca04—Si02 | 96.81 (15) | Ca01—Li02—Ca04 | 64.20 (16) |
| O03—Ca04—Si01 | 75.29 (6) | Ca02 ^{vi} —Li02—Ca01 | 78.3 (2) |
| O03—Ca04—Si01 ⁱⁱ | 173.92 (6) | Ca02 ^{vi} —Li02—Ca02 ^{xiv} | 96.7 (3) |

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| O03—Ca04—Si02 | 67.33 (6) | Ca02 ^{vi} —Li02—Ca03 ^{viii} | 138.9 (3) |
| O03—Ca04—Si04 | 33.67 (6) | Ca02 ^{vi} —Li02—Ca03 | 73.02 (17) |
| O03—Ca04—Li02 | 42.27 (19) | Ca02 ^{vi} —Li02—Ca04 | 117.0 (2) |
| O03—Ca04—O06 | 80.38 (8) | Ca02 ^{xiv} —Li02—Ca04 | 136.6 (3) |
| O03—Ca04—O07 ⁱⁱ | 152.23 (8) | Ca03 ^{viii} —Li02—Ca01 | 136.9 (3) |
| O03—Ca04—O07 | 91.14 (8) | Ca03—Li02—Ca01 | 116.1 (2) |
| O03—Ca04—O10 ^{ix} | 143.04 (7) | Ca03 ^{viii} —Li02—Ca02 ^{xiv} | 62.52 (14) |
| O03—Ca04—O11 | 94.63 (8) | Ca03—Li02—Ca02 ^{xiv} | 138.7 (3) |
| O06—Ca04—Si01 ⁱⁱ | 98.61 (5) | Ca03—Li02—Ca03 ^{viii} | 98.9 (3) |
| O06—Ca04—Si01 | 76.34 (5) | Ca03 ^{viii} —Li02—Ca04 | 100.5 (3) |
| O06—Ca04—Si02 | 24.71 (5) | Ca03—Li02—Ca04 | 80.3 (2) |
| O06—Ca04—Si04 | 74.37 (5) | Si03 ^{viii} —Li02—Ca01 | 68.8 (2) |
| O06—Ca04—Li02 | 117.68 (17) | Si03 ^{viii} —Li02—Ca02 ^{vi} | 139.7 (4) |
| O06—Ca04—O10 ^{ix} | 104.31 (7) | Si03 ^{viii} —Li02—Ca02 ^{xiv} | 67.86 (17) |
| O07—Ca04—Si01 ⁱⁱ | 94.94 (6) | Si03 ^{viii} —Li02—Ca03 | 142.6 (4) |
| O07 ⁱⁱ —Ca04—Si01 | 86.04 (6) | Si03 ^{viii} —Li02—Ca03 ^{viii} | 68.09 (17) |
| O07 ⁱⁱ —Ca04—Si01 ⁱⁱ | 30.34 (5) | Si03 ^{viii} —Li02—Ca04 | 68.7 (2) |
| O07—Ca04—Si01 | 24.19 (5) | Si04 ^{viii} —Li02—Ca01 | 144.9 (4) |
| O07—Ca04—Si02 | 76.48 (6) | Si04 ^{viii} —Li02—Ca02 ^{vi} | 71.7 (2) |
| O07 ⁱⁱ —Ca04—Si02 | 85.09 (5) | Si04 ^{viii} —Li02—Ca02 ^{xiv} | 66.80 (19) |
| O07—Ca04—Si04 | 124.51 (6) | Si04 ^{viii} —Li02—Ca03 | 72.1 (2) |
| O07 ⁱⁱ —Ca04—Si04 | 143.51 (6) | Si04 ^{viii} —Li02—Ca03 ^{viii} | 67.62 (18) |
| O07 ⁱⁱ —Ca04—Li02 | 145.89 (18) | Si04 ^{viii} —Li02—Ca04 | 147.2 (4) |
| O07—Ca04—Li02 | 68.67 (17) | Si04 ^{viii} —Li02—Si03 ^{viii} | 127.0 (3) |
| O07—Ca04—O06 | 96.84 (8) | O01 ⁱ —Li02—Ca01 | 44.06 (18) |
| O07 ⁱⁱ —Ca04—O06 | 75.28 (7) | O01 ⁱ —Li02—Ca02 ^{vi} | 46.91 (19) |
| O07—Ca04—O07 ⁱⁱ | 78.84 (8) | O01 ⁱ —Li02—Ca02 ^{xiv} | 75.5 (3) |
| O07—Ca04—O10 ^{ix} | 123.82 (7) | O01 ⁱ —Li02—Ca03 | 116.6 (3) |
| O07 ⁱⁱ —Ca04—O10 ^{ix} | 58.21 (7) | O01 ⁱ —Li02—Ca03 ^{viii} | 137.8 (4) |
| O07—Ca04—O11 | 81.60 (8) | O01 ⁱ —Li02—Ca04 | 107.1 (3) |
| O08—Ca04—Si01 ⁱⁱ | 107.18 (6) | O01 ⁱ —Li02—Si03 ^{viii} | 92.8 (3) |
| O08—Ca04—Si01 | 138.06 (6) | O01 ⁱ —Li02—Si04 ^{viii} | 101.0 (4) |
| O08—Ca04—Si02 | 94.18 (6) | O02—Li02—Ca01 | 126.3 (4) |
| O08—Ca04—Si04 | 33.51 (5) | O02—Li02—Ca02 ^{xiv} | 95.2 (3) |
| O08—Ca04—Li02 | 93.07 (18) | O02—Li02—Ca02 ^{vi} | 48.8 (2) |
| O08—Ca04—O03 | 66.75 (8) | O02—Li02—Ca03 | 47.6 (2) |
| O08—Ca04—O06 | 80.29 (8) | O02—Li02—Ca03 ^{viii} | 95.6 (3) |
| O08—Ca04—O07 | 157.88 (8) | O02—Li02—Ca04 | 127.3 (4) |
| O08—Ca04—O07 ⁱⁱ | 120.84 (8) | O02—Li02—Si03 ^{viii} | 160.3 (4) |
| O08—Ca04—O10 ^{ix} | 77.80 (7) | O02—Li02—Si04 ^{viii} | 33.27 (15) |
| O08—Ca04—O11 | 99.26 (8) | O02—Li02—O01 ⁱ | 92.5 (4) |
| O10 ^{ix} —Ca04—Si01 ⁱⁱ | 31.32 (5) | O02—Li02—O03 | 92.1 (4) |
| O10 ^{ix} —Ca04—Si01 | 141.67 (5) | O03—Li02—Ca01 | 105.7 (3) |
| O10 ^{ix} —Ca04—Si02 | 127.58 (5) | O03—Li02—Ca02 ^{vi} | 115.9 (3) |
| O10 ^{ix} —Ca04—Si04 | 111.25 (5) | O03—Li02—Ca02 ^{xiv} | 141.8 (4) |
| O10 ^{ix} —Ca04—Li02 | 134.89 (15) | O03—Li02—Ca03 ^{viii} | 79.5 (3) |
| O11—Ca04—Si01 ⁱⁱ | 86.52 (6) | O03—Li02—Ca03 | 47.16 (19) |
| O11—Ca04—Si01 | 100.96 (6) | O03—Li02—Ca04 | 43.69 (18) |
| O11—Ca04—Si02 | 150.99 (6) | O03—Li02—Si03 ^{viii} | 95.5 (3) |
| O11—Ca04—Si04 | 102.35 (6) | O03—Li02—Si04 ^{viii} | 103.5 (4) |
| O11—Ca04—Li02 | 57.09 (17) | O03—Li02—O01 ⁱ | 141.6 (4) |
| O11—Ca04—O06 | 174.77 (8) | O12 ^{viii} —Li02—Ca01 | 95.5 (3) |

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| O11—Ca04—O07 ⁱⁱ | 109.18 (8) | O12 ^{viii} —Li02—Ca02 ^{vi} | 139.2 (5) |
| O11—Ca04—O10 ^{ix} | 80.62 (7) | O12 ^{viii} —Li02—Ca02 ^{xiv} | 44.1 (2) |
| Ca01—Si01—Ca02 ^{vi} | 68.82 (2) | O12 ^{viii} —Li02—Ca03 ^{viii} | 43.5 (2) |
| Ca03—Si01—Ca01 | 103.31 (3) | O12 ^{viii} —Li02—Ca03 | 141.0 (5) |
| Ca03 ^{vi} —Si01—Ca01 | 130.07 (3) | O12 ^{viii} —Li02—Ca04 | 95.1 (4) |
| Ca03 ^{vi} —Si01—Ca02 ^{vi} | 62.98 (2) | O12 ^{viii} —Li02—Si03 ^{viii} | 31.58 (16) |
| Ca03—Si01—Ca02 ^{vi} | 62.95 (2) | O12 ^{viii} —Li02—Si04 ^{viii} | 95.5 (3) |
| Ca03 ^{vi} —Si01—Ca03 | 65.73 (2) | O12 ^{viii} —Li02—O01 ⁱ | 101.8 (5) |
| Ca03 ^{vi} —Si01—Ca04 | 141.45 (3) | O12 ^{viii} —Li02—O02 | 128.7 (5) |
| Ca03—Si01—Ca04 | 75.92 (2) | O12 ^{viii} —Li02—O03 | 104.7 (5) |
| Ca04—Si01—Ca01 | 61.667 (19) | Ca02 ^{iv} —O01—Ca01 ^{xii} | 124.67 (10) |
| Ca04 ⁱⁱ —Si01—Ca01 | 67.63 (2) | Ca02 ^{iv} —O01—Li02 ^{xii} | 84.4 (2) |
| Ca04 ⁱⁱ —Si01—Ca02 ^{vi} | 133.23 (3) | Si04—O01—Ca01 ^{xii} | 93.91 (10) |
| Ca04—Si01—Ca02 ^{vi} | 103.33 (3) | Si04—O01—Ca02 ^{iv} | 125.28 (13) |
| Ca04 ⁱⁱ —Si01—Ca03 ^{vi} | 146.88 (3) | Si04—O01—Li02 ^{xii} | 135.9 (2) |
| Ca04 ⁱⁱ —Si01—Ca03 | 144.49 (3) | Li02 ^{xii} —O01—Ca01 ^{xii} | 92.6 (2) |
| Ca04 ⁱⁱ —Si01—Ca04 | 69.62 (2) | Ca03—O02—Ca02 ^{vi} | 105.93 (9) |
| Li01—Si01—Ca01 | 136.84 (13) | Si04 ^{viii} —O02—Ca02 ^{vi} | 124.29 (12) |
| Li01—Si01—Ca02 ^{vi} | 152.67 (13) | Si04 ^{viii} —O02—Ca03 | 127.96 (12) |
| Li01—Si01—Ca03 | 109.05 (14) | Si04 ^{viii} —O02—Li02 | 102.2 (3) |
| Li01—Si01—Ca03 ^{vi} | 89.75 (13) | Li02—O02—Ca02 ^{vi} | 89.1 (3) |
| Li01—Si01—Ca04 | 99.36 (14) | Li02—O02—Ca03 | 90.4 (3) |
| Li01—Si01—Ca04 ⁱⁱ | 69.42 (13) | Ca03—O03—Ca04 | 129.83 (10) |
| O04 ^{vi} —Si01—Ca01 | 97.11 (9) | Ca03—O03—Li02 | 84.7 (2) |
| O04 ^{vi} —Si01—Ca02 ^{vi} | 30.42 (8) | Si04—O03—Ca03 | 124.76 (13) |
| O04 ^{vi} —Si01—Ca03 ^{vi} | 40.90 (8) | Si04—O03—Ca04 | 93.22 (10) |
| O04 ^{vi} —Si01—Ca03 | 42.00 (8) | Si04—O03—Li02 | 130.8 (2) |
| O04 ^{vi} —Si01—Ca04 ⁱⁱ | 163.65 (9) | Li02—O03—Ca04 | 94.0 (2) |
| O04 ^{vi} —Si01—Ca04 | 109.15 (9) | Ca02—O04—Ca03 ^{vi} | 98.39 (8) |
| O04 ^{vi} —Si01—Li01 | 126.05 (15) | Ca03—O04—Ca02 | 99.62 (8) |
| O04 ^{vi} —Si01—O07 | 117.06 (13) | Ca03—O04—Ca03 ^{vi} | 98.21 (8) |
| O04 ^{vi} —Si01—O10 ^{vi} | 114.28 (12) | Si01 ^{vi} —O04—Ca02 | 129.92 (12) |
| O04 ^{vi} —Si01—O13 | 109.35 (12) | Si01 ^{vi} —O04—Ca03 ^{vi} | 112.33 (11) |
| O07—Si01—Ca01 | 28.87 (8) | Si01 ^{vi} —O04—Ca03 | 113.20 (11) |
| O07—Si01—Ca02 ^{vi} | 93.68 (9) | Ca02—O05—Ca02 ^{iv} | 99.92 (8) |
| O07—Si01—Ca03 | 103.58 (9) | Ca02 ^{iv} —O05—Ca03 | 93.05 (8) |
| O07—Si01—Ca03 ^{vi} | 156.61 (9) | Ca02—O05—Ca03 | 98.70 (8) |
| O07—Si01—Ca04 ⁱⁱ | 51.55 (9) | Si02—O05—Ca02 ^{iv} | 131.00 (12) |
| O07—Si01—Ca04 | 37.85 (8) | Si02—O05—Ca02 | 115.35 (12) |
| O07—Si01—Li01 | 113.62 (16) | Si02—O05—Ca03 | 112.67 (11) |
| O07—Si01—O10 ^{vi} | 108.35 (13) | Ca01 ^{xii} —O06—Ca01 ⁱⁱ | 104.22 (8) |
| O07—Si01—O13 | 106.96 (12) | Ca01 ^{xii} —O06—Ca04 | 93.82 (8) |
| O10 ^{vi} —Si01—Ca01 | 101.62 (9) | Ca01 ⁱⁱ —O06—Ca04 | 101.53 (8) |
| O10 ^{vi} —Si01—Ca02 ^{vi} | 108.27 (9) | Si02—O06—Ca01 ⁱⁱ | 105.96 (11) |
| O10 ^{vi} —Si01—Ca03 | 147.46 (10) | Si02—O06—Ca01 ^{xii} | 132.66 (12) |
| O10 ^{vi} —Si01—Ca03 ^{vi} | 82.24 (9) | Si02—O06—Ca04 | 114.50 (12) |
| O10 ^{vi} —Si01—Ca04 ⁱⁱ | 65.59 (9) | Ca01—O07—Ca04 ⁱⁱ | 103.04 (8) |
| O10 ^{vi} —Si01—Ca04 | 135.18 (9) | Ca01—O07—Ca04 | 99.76 (9) |
| O10 ^{vi} —Si01—Li01 | 63.27 (17) | Ca04—O07—Ca04 ⁱⁱ | 101.16 (8) |
| O13—Si01—Ca01 | 135.58 (9) | Si01—O07—Ca01 | 131.79 (13) |
| O13—Si01—Ca02 ^{vi} | 138.35 (9) | Si01—O07—Ca04 | 117.96 (12) |
| O13—Si01—Ca03 ^{vi} | 91.30 (9) | Si01—O07—Ca04 ⁱⁱ | 98.11 (11) |

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| O13—Si01—Ca03 | 77.01 (8) | Ca04—O08—Ca01 ^{xii} | 98.34 (8) |
| O13—Si01—Ca04 ⁱⁱ | 86.42 (9) | Si04—O08—Ca01 ^{xii} | 93.38 (10) |
| O13—Si01—Ca04 | 75.95 (9) | Si04—O08—Ca04 | 95.17 (10) |
| O13—Si01—Li01 | 36.01 (17) | Si04—O08—Li01 ^{xi} | 126.9 (3) |
| O13—Si01—O10 ^{vi} | 99.12 (12) | Li01 ^{xi} —O08—Ca01 ^{xii} | 115.3 (3) |
| Ca01 ⁱⁱ —Si02—Ca01 ^{xii} | 66.07 (2) | Li01 ^{xi} —O08—Ca04 | 121.2 (3) |
| Ca01 ⁱⁱ —Si02—Ca02 ^{iv} | 132.01 (3) | Si02 ^{iv} —O09—Ca01 ^{xv} | 79.90 (9) |
| Ca01 ⁱⁱ —Si02—Ca02 | 149.11 (3) | Si02 ^{iv} —O09—Si03 | 133.18 (15) |
| Ca01 ⁱⁱ —Si02—Ca03 | 144.16 (3) | Si02 ^{iv} —O09—Li01 ^{iv} | 89.6 (2) |
| Ca01 ⁱⁱ —Si02—Ca04 | 68.75 (2) | Si03—O09—Ca01 ^{xv} | 125.13 (12) |
| Ca02 ^{iv} —Si02—Ca01 ^{xii} | 68.51 (2) | Si03—O09—Li01 ^{iv} | 130.3 (2) |
| Ca02—Si02—Ca01 ^{xii} | 129.13 (3) | Li01 ^{iv} —O09—Ca01 ^{xv} | 79.03 (18) |
| Ca02—Si02—Ca02 ^{iv} | 62.42 (2) | Si01 ^{vi} —O10—Ca04 ^{xvi} | 83.09 (10) |
| Ca02—Si02—Ca03 | 65.37 (2) | Si01 ^{vi} —O10—Si03 | 137.01 (16) |
| Ca02—Si02—Ca04 | 141.11 (3) | Si03—O10—Ca04 ^{xvi} | 131.24 (12) |
| Ca03—Si02—Ca01 ^{xii} | 100.92 (3) | Ca04—O11—Ca01 | 95.75 (8) |
| Ca03—Si02—Ca02 ^{iv} | 59.700 (19) | Si03 ^{viii} —O11—Ca01 | 121.53 (12) |
| Ca03—Si02—Ca04 | 75.86 (2) | Si03 ^{viii} —O11—Ca04 | 124.80 (12) |
| Ca04—Si02—Ca01 ^{xii} | 59.853 (19) | Si03 ^{viii} —O11—Li01 ⁱⁱ | 106.4 (2) |
| Ca04—Si02—Ca02 ^{iv} | 100.83 (2) | Li01 ⁱⁱ —O11—Ca01 | 100.4 (2) |
| Li01—Si02—Ca01 ⁱⁱ | 69.51 (15) | Li01 ⁱⁱ —O11—Ca04 | 104.6 (3) |
| Li01—Si02—Ca01 ^{xii} | 135.58 (15) | Ca03—O12—Ca02 ^{iv} | 94.20 (8) |
| Li01—Si02—Ca02 ^{iv} | 152.34 (14) | Si03—O12—Ca02 ^{iv} | 121.51 (12) |
| Li01—Si02—Ca02 | 90.40 (14) | Si03—O12—Ca03 | 123.53 (12) |
| Li01—Si02—Ca03 | 115.55 (17) | Si03—O12—Li02 ^{viii} | 109.7 (3) |
| Li01—Si02—Ca04 | 104.13 (16) | Li02 ^{viii} —O12—Ca02 ^{iv} | 102.1 (3) |
| O05—Si02—Ca01 ^{xii} | 96.78 (9) | Li02 ^{viii} —O12—Ca03 | 102.4 (3) |
| O05—Si02—Ca01 ⁱⁱ | 161.63 (9) | Si01—O13—Si02 | 143.90 (16) |
| O05—Si02—Ca02 | 39.41 (8) | Si01—O13—Li01 | 114.6 (3) |
| O05—Si02—Ca02 ^{iv} | 29.63 (8) | Si02—O13—Li01 | 101.3 (3) |
| O05—Si02—Ca03 | 41.69 (8) | | |

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