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A new quaternary rare earth borate, $CsLi_2Gd_4(BO_3)_5$

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Key indicators: single-crystal X-ray study; T = 295 K; mean σ(O–B) = 0.011 Å; R factor = 0.044; wR factor = 0.108; data-to-parameter ratio = 12.4.

Single crystals of caesium dilithium tetragadolinium pentaborate, $CsLi_2Gd_4(BO_3)_5$, were obtained by heating lithium and gadolinium in a caesium borate flux. The structure features chains of edge- and corner-sharing GdO_n polyhedra. These chains are interlocked to form $[Gd_8O_{16}(BO_3)_2]^{14-}$ layers, which are connected by borate groups in the third dimension. The Li and Cs atoms occupy O_5 pyramids and large cages in the framework, respectively.

Related literature

For related literature, see: Aka *et al.* (1997); Chaminade *et al.* (1999, 2001); Crumpton & Greaves (2004); Czirr *et al.* (1999); Darriet *et al.* (2005); Dorozhkin *et al.* (1981); Fouassier *et al.* (1981); Jubera *et al.* (2003); Jubera, Gravereau & Chaminade (2001); Jubera, Gravereau, Chaminade & Fouassier (2001); Mascetti *et al.* (1983); Muktha & Row (2006); Ren *et al.* (1999); Sablayrolles *et al.* (2005); Wu *et al.* (2001); van Eijk *et al.* (2001).

Experimental

Crystal data

$CsLi_2Gd_4(BO_3)_5$
M_r = 1069.84
Monoclinic, $P2/n$
a = 10.644 (2) Å
b = 6.4661 (15) Å
c = 20.093 (4) Å
β = 105.250 (16)°
V = 1334.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 22.40 mm^{-1}
T = 295 (2) K
0.16 × 0.12 × 0.08 mm

Data collection

Bruker P4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.042, T_{max} = 0.167
7381 measured reflections
3068 independent reflections
2829 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
3 standard reflections every 97 reflections intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.11
3068 reflections
248 parameters
$\Delta\rho_{max}$ = 4.05 e Å^{-3}
$\Delta\rho_{min}$ = −2.81 e Å^{-3}

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Version 1.0c; Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2036).

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supplementary materials

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A new quaternary rare earth borate, $CsLi_2Gd_4(BO_3)_5$

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Comment

Rare earth borates are promising luminescent materials (Jubera *et al.*, 2003; Sablayrolles *et al.*, 2005) and their applications are found in Plasma Displays Panels (PDP) and efficient light conversion bulbs (Fouassier *et al.*, 1981). Besides that, rare earth borates are good nonlinear optical materials, *e.g.* $YCa_4O(BO_3)_3$ (Aka *et al.*, 1997), $CaLa_2B_{10}O_{19}$ (Wu *et al.*, 2001), and self-frequency doubling laser crystals Nd^{3+}:$YAl_3(BO_3)$ (Dorozhkin *et al.*, 1981). Recently, $Li_6Gd(BO_3)_3$:Ce has received extensive attention as a new efficient thermal neutron detection material. (Czirr *et al.*, 1999; Chaminade *et al.*, 2001, van Eijk *et al.*, 2001)

In the Li_2O—Gd_2O_3—B_2O_3 system, there are four ternary compounds, $LiGd_6O_5(BO_3)_3$ (Chaminade *et al.*, 1999), $Li_6Gd(BO_3)_3$ (Mascetti *et al.*, 1983), $Li_3Gd(BO_3)_2$ and $LiGd_2O_2BO_3$ (Jubera, Gravereau & Chaminade, 2001). In an attempt to synthesize compounds in the system using caesium borate as the flux, we obtained a new quaternary compound $CsLi_2Gd_4(BO_3)_5$, which is, to our knowledge, the first rare-earth borate containing caesium.

The structure of $CsLi_2Gd_4(BO_3)_5$ is shown in figure 1. In the asymmetric unit, all six boron atoms are three-coordinated yielding planar BO_3 groups (B—O: 1.352 to 1.408 Å, average: 1.376 Å, which agrees with literature values). The site symmetry of B2 and B3 is 2.

The Gd atoms occupy five different crystallographic sites, Gd2, Gd4 and Gd5 being coordinated by seven O atoms and Gd1 and Gd3 coordinated to eight and nine oxygen atoms, respectively. Gd2, Gd3 lie on twofold axes. The GdO_n polyhedra (Gd—O: 2.241 to 2.634 Å) share edges yielding two types of Gd—O chains. The chain containing Gd1, Gd3 and Gd5 atoms is terminated by two BO_3 groups (Fig. 2). The three-element Gd_3O_{17} chain (Fig. 3) joins other equivalent three-element chains to form an infinite zigzag chain. Both chains can be classified as fluorite-related ribbons, which are common in rare earth borate compounds (Ren *et al.*, 1999; Jubera, Gravereau, Chaminade & Fouassier, 2001). Similar Bi—O ribbons are reported in bismuth compounds (Crumpton & Greaves, 2004; Darriet *et al.*, 2005; Muktha & Row, 2006). The two chains in $CsLi_2Gd_4(BO_3)_5$ are interlocked by sharing the edges of Gd polyhedra to form a two dimensional $[Gd_8O_{16}(BO_3)_2]^{14-}$ layer in the *ac* plane. The layers are inter-linked by out of plane BO_3 groups in the *b* direction into a 3 dimensional network.

Both Li atoms are five-coordinated (distorted square pyramids, Li—O: 1.885 to 2.145 Å). The Cs atom is coordinated by seven O atoms and resides in a big basket-like cage.

Experimental

Single crystals of $CsLi_2Gd_4(BO_3)_5$ were obtained in a Pt crucible by melting a mixture of analytically pure Cs_2CO_3 (1.3028 g, 4 mmol, XinJiang Research Institute of Non-ferrous Metals), Li_2CO_3 (0.2217, 3 mmol, Beijing Chemical Reagents Company), Gd_2O_3 (0.7250 g, 2 mmol, CIAC), H_3BO_3 (0.9829, 16 mmol, Beijing Chemical Reagents Company). The melt was cooled slowly from 1023 to 873 K at a rate of 1 K h^{-1} and then at a rate of 20 K h^{-1} to the room temperature. Block-shaped colourless crystals were recovered and separated from the initial reaction product. The Rb analogue of the title compound can be synthesized by solid-state reaction, with the determined composition of $CsLi_2Gd_4(BO_3)_5$.

Refinement

Two space groups, Pn and P2/n, were proposed by the data preparation program. The noncentrosymmetric space group Pn was discarded for further consideration since detectable signal was not observed in a powder second harmonic generation test. Direct phase determination showed positions of 6 heavy atoms which were assigned to Gd. Subsequent difference Fourier syntheses revealed the positions of the oxygen atoms. Judging from its larger thermal parameters and much further coordination to the oxygen atoms one of the heavy atom was then assigned to Cs.

Figures

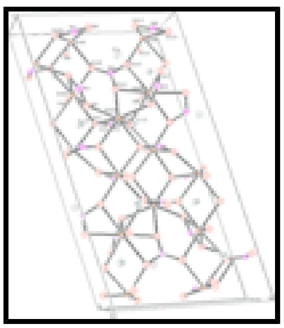


Fig. 1. The crystal structure of $CsLi_2Gd_4(BO_3)_5$ viewed along *a* axis.

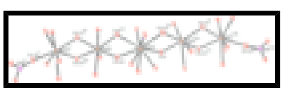


Fig. 2. G $d_5O_{29}(BO_3)_2$ chain in the $CsLi_2Gd_4(BO_3)_5$: [Symmetry code:(i) *x* + 1/2, −*y* + 1, *z* + 1/2;(ii) −*x* + 2, −*y* + 1,-*z* + 2; (iii) −*x* + 1, −*y* + 1, −*z* + 2; (iv) −*x* + 3/2, *y*, −*z* + 3/2; (v) *x* + 1/2, −*y* + 1, *z* − 1/2; (vi) *x* − 1/2, −*y* + 1, *z* − 1/2; (vii) −*x* + 1, −*y* + 1, −*z* + 1; (viii) −*x* + 1/2, *y*, −*z* + 3/2.]

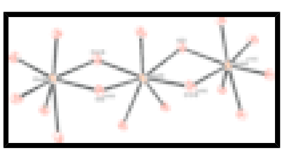


Fig. 3. G d_3O_{17} chain in the $CsLi_2Gd_4(BO_3)_5$: [Symmetry code: same as figure 2].

caesium dilithium tetragadolinium pentaborate

Crystal data

$CsLi_2Gd_4(BO_3)_5$	F_{000} = 1848
M_r = 1069.84	D_x = 5.326 Mg m^{-3}
Monoclinic, *P*2/*n*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yac	Cell parameters from 23 reflections
a = 10.644 (2) Å	θ = 6.5–11.7°
b = 6.4661 (15) Å	μ = 22.40 mm^{-1}
c = 20.093 (4) Å	*T* = 295 (2) K
β = 105.250 (16)°	Block, colourless
V = 1334.3 (5) $Å^3$	0.16 × 0.12 × 0.08 mm

$Z = 4$

Data collection

Bruker P4 diffractometer	$R_{int} = 0.060$
Radiation source: fine-focus sealed tube	$\theta_{max} = 27.5°$
Monochromator: graphite	$\theta_{min} = 2.0°$
$T = 295(2)$ K	$h = -13\rightarrow13$
ω scans	$k = -8\rightarrow8$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = -26\rightarrow25$
$T_{min} = 0.042$, $T_{max} = 0.167$	3 standard reflections
7381 measured reflections	every 97 reflections
3068 independent reflections	intensity decay: none
2829 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 1.5286P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.108$	$\Delta\rho_{max} = 4.05$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -2.81$ e Å^{-3}
3068 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
248 parameters	Extinction coefficient: 0.0133 (4)
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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*	$U_{iso}*/U_{eq}$
Gd1	0.45528 (3)	0.34144 (6)	0.649931 (16)	0.01704 (15)
Gd2	0.2500	0.59641 (9)	0.7500	0.02208 (16)

Gd3	0.7500	0.59044 (8)	0.7500	0.01776 (16)
Gd4	0.35686 (3)	0.64428 (6)	0.946524 (18)	0.01724 (14)
Gd5	0.84343 (3)	0.64848 (6)	0.953592 (16)	0.01731 (15)
Cs1	0.55501 (4)	0.09547 (9)	0.85836 (2)	0.02535 (16)
B1	0.4515 (6)	0.7837 (16)	0.6497 (4)	0.0190 (16)
B2	0.2500	0.1655 (18)	0.7500	0.020 (2)
B3	0.7500	0.1618 (19)	0.7500	0.023 (3)
B4	0.3429 (7)	0.1954 (19)	0.9500 (4)	0.0238 (19)
B5	0.8570 (8)	0.2030 (17)	0.9562 (4)	0.0216 (17)
B6	0.5418 (7)	0.5930 (13)	0.8231 (4)	0.0200 (15)
Li1	0.6372 (11)	0.978 (2)	0.6532 (7)	0.027 (3)
Li2	0.2786 (11)	0.987 (2)	0.6582 (6)	0.022 (2)
O1	0.4590 (4)	0.9903 (9)	0.6603 (3)	0.0231 (11)
O2	0.3386 (5)	0.6737 (8)	0.6485 (3)	0.0198 (11)
O3	0.5582 (5)	0.6740 (8)	0.6405 (3)	0.0189 (10)
O4	0.2500	−0.0436 (13)	0.7500	0.0252 (17)
O5	0.2777 (4)	0.2764 (8)	0.6974 (2)	0.0207 (10)
O6	0.7500	−0.0510 (13)	0.7500	0.0226 (17)
O7	0.8179 (4)	0.2672 (9)	0.8072 (2)	0.0206 (10)
O8	0.3404 (4)	−0.0048 (9)	0.9297 (3)	0.0190 (10)
O9	0.4550 (4)	0.3091 (9)	0.9728 (3)	0.0237 (11)
O10	0.2302 (4)	0.3107 (8)	0.9469 (3)	0.0202 (10)
O11	0.8424 (5)	−0.0004 (10)	0.9383 (3)	0.0203 (10)
O12	0.9664 (5)	0.3213 (8)	0.9531 (3)	0.0191 (10)
O13	0.7622 (4)	0.3197 (8)	0.9754 (3)	0.0220 (10)
O14	0.5248 (5)	0.4966 (10)	0.7606 (3)	0.0265 (11)
O15	0.6689 (4)	0.6496 (9)	0.8568 (3)	0.0219 (11)
O16	0.4352 (5)	0.6364 (9)	0.8473 (3)	0.0233 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.0196 (2)	0.0201 (2)	0.0127 (2)	0.00018 (11)	0.00648 (15)	0.00003 (12)
Gd2	0.0354 (3)	0.0193 (3)	0.0130 (3)	0.000	0.0089 (2)	0.000
Gd3	0.0211 (2)	0.0196 (3)	0.0133 (3)	0.000	0.00573 (18)	0.000
Gd4	0.0186 (2)	0.0209 (2)	0.0129 (2)	0.00014 (12)	0.00551 (14)	0.00020 (13)
Gd5	0.0198 (2)	0.0214 (3)	0.0120 (2)	−0.00005 (12)	0.00639 (15)	0.00026 (13)
Cs1	0.0253 (3)	0.0283 (3)	0.0243 (3)	−0.00007 (17)	0.00982 (19)	−0.00019 (19)
B1	0.021 (3)	0.024 (4)	0.013 (4)	0.003 (3)	0.004 (3)	0.006 (3)
B2	0.019 (5)	0.016 (6)	0.027 (6)	0.000	0.009 (4)	0.000
B3	0.022 (5)	0.021 (6)	0.027 (6)	0.000	0.009 (4)	0.000
B4	0.023 (3)	0.037 (5)	0.012 (4)	0.001 (3)	0.004 (3)	0.007 (3)
B5	0.026 (3)	0.030 (5)	0.009 (3)	0.003 (3)	0.005 (3)	−0.001 (3)
B6	0.020 (3)	0.025 (4)	0.016 (4)	−0.004 (3)	0.007 (3)	−0.003 (3)
Li1	0.026 (5)	0.033 (7)	0.023 (6)	−0.004 (5)	0.009 (5)	−0.010 (6)
Li2	0.028 (5)	0.024 (6)	0.015 (5)	−0.004 (5)	0.009 (4)	0.004 (5)
O1	0.023 (2)	0.021 (3)	0.028 (3)	0.001 (2)	0.013 (2)	0.001 (2)
O2	0.020 (2)	0.023 (3)	0.018 (2)	−0.0011 (19)	0.0078 (19)	0.000 (2)

O3	0.023 (2)	0.020 (2)	0.016 (2)	0.0020 (19)	0.0085 (18)	0.000 (2)
O4	0.040 (4)	0.021 (4)	0.019 (4)	0.000	0.015 (3)	0.000
O5	0.028 (2)	0.021 (2)	0.016 (2)	0.000 (2)	0.0109 (18)	0.000 (2)
O6	0.025 (3)	0.028 (4)	0.015 (3)	0.000	0.005 (3)	0.000
O7	0.0218 (19)	0.027 (3)	0.013 (2)	−0.002 (2)	0.0046 (17)	0.001 (2)
O8	0.023 (2)	0.015 (2)	0.018 (2)	0.0030 (19)	0.0021 (18)	−0.001 (2)
O9	0.022 (2)	0.026 (3)	0.023 (3)	−0.002 (2)	0.0060 (19)	−0.001 (2)
O10	0.022 (2)	0.024 (2)	0.017 (2)	0.003 (2)	0.0088 (18)	0.001 (2)
O11	0.028 (2)	0.016 (2)	0.019 (2)	0.000 (2)	0.0092 (19)	0.001 (2)
O12	0.020 (2)	0.023 (3)	0.015 (2)	−0.0036 (19)	0.0058 (18)	0.000 (2)
O13	0.023 (2)	0.021 (2)	0.025 (3)	−0.001 (2)	0.013 (2)	0.000 (2)
O14	0.034 (2)	0.032 (3)	0.016 (2)	0.000 (3)	0.011 (2)	−0.002 (2)
O15	0.018 (2)	0.029 (3)	0.019 (3)	−0.0022 (19)	0.0048 (19)	−0.004 (2)
O16	0.021 (2)	0.029 (3)	0.023 (3)	0.000 (2)	0.012 (2)	−0.002 (2)

Geometric parameters (Å, °)

Gd1—O1^{i}	2.279 (6)	B1—Li1	2.329 (15)
Gd1—O5	2.368 (4)	B2—O4	1.352 (14)
Gd1—O14	2.373 (5)	B2—O5^{ii}	1.372 (8)
Gd1—O10^{ii}	2.389 (5)	B2—O5	1.372 (8)
Gd1—O7^{iii}	2.389 (4)	B2—Li2^{viii}	2.265 (14)
Gd1—O12^{iii}	2.431 (5)	B2—Li2^{i}	2.265 (14)
Gd1—O3	2.443 (5)	B2—Cs1^{ii}	3.4305 (18)
Gd1—O2	2.478 (5)	B3—O7^{iii}	1.367 (8)
Gd1—B1	2.860 (11)	B3—O7	1.368 (8)
Gd1—Li2^{i}	2.999 (12)	B3—O6	1.375 (15)
Gd1—Li1^{i}	3.033 (14)	B3—Li1^{ix}	2.323 (14)
Gd1—Gd3	3.6274 (8)	B3—Li1^{i}	2.323 (14)
Gd2—O4^{iv}	2.328 (8)	B3—Cs1^{iii}	3.4075 (17)
Gd2—O5	2.377 (5)	B4—O8	1.355 (13)
Gd2—O5^{ii}	2.377 (5)	B4—O9	1.374 (10)
Gd2—O16^{ii}	2.398 (5)	B4—O10	1.400 (10)
Gd2—O16	2.398 (5)	B4—Li2^{viii}	2.597 (15)
Gd2—O2	2.511 (5)	B5—O11	1.362 (12)
Gd2—O2^{ii}	2.511 (5)	B5—O13	1.393 (10)
Gd2—B2	2.786 (12)	B5—O12	1.408 (10)
Gd2—B6^{ii}	3.067 (7)	B5—Li1^{ix}	2.650 (17)
Gd2—B6	3.067 (7)	B6—O14	1.372 (9)
Gd3—O6^{iv}	2.319 (8)	B6—O16	1.376 (9)
Gd3—O7	2.403 (5)	B6—O15	1.393 (8)
Gd3—O7^{iii}	2.403 (5)	B6—Cs1^{iv}	3.320 (8)
Gd3—O14	2.535 (5)	Li1—O11^{x}	1.913 (14)
Gd3—O14^{iii}	2.535 (5)	Li1—O1	1.941 (13)
Gd3—O15^{iii}	2.544 (5)	Li1—O6^{iv}	2.007 (13)

Gd3—O15	2.544 (5)	Li1—O7^{x}	2.036 (15)
Gd3—O3^{iii}	2.634 (5)	Li1—O3	2.130 (15)
Gd3—O3	2.634 (5)	Li1—B3^{iv}	2.323 (14)
Gd3—B3	2.772 (13)	Li1—B5^{x}	2.650 (17)
Gd3—B6	2.963 (7)	Li1—Gd1^{iv}	3.033 (14)
Gd3—B6^{iii}	2.963 (7)	Li1—Gd5^{iii}	3.072 (13)
Gd4—O9^{v}	2.241 (5)	Li1—Cs1^{x}	3.429 (12)
Gd4—O13^{v}	2.273 (5)	Li2—O8^{xi}	1.885 (13)
Gd4—O8^{iv}	2.294 (6)	Li2—O1	1.909 (12)
Gd4—O16	2.356 (6)	Li2—O4^{iv}	1.957 (12)
Gd4—O9	2.404 (5)	Li2—O5^{iv}	2.034 (14)
Gd4—O2^{ii}	2.433 (5)	Li2—O2	2.145 (14)
Gd4—O10	2.545 (5)	Li2—B2^{iv}	2.265 (14)
Gd4—B4	2.908 (12)	Li2—B4^{xi}	2.597 (15)
Gd4—Li2^{ii}	3.132 (13)	Li2—Gd1^{iv}	2.999 (12)
Gd4—Gd4^{v}	3.7337 (10)	Li2—Gd4^{ii}	3.132 (13)
Gd4—Gd5^{v}	3.7958 (8)	Li2—Cs1^{xi}	3.549 (12)
Gd5—O11^{iv}	2.291 (6)	O1—Gd1^{iv}	2.279 (6)
Gd5—O15	2.309 (5)	O2—Gd4^{ii}	2.433 (5)
Gd5—O12^{vi}	2.378 (5)	O3—Gd5^{iii}	2.396 (5)
Gd5—O13	2.379 (5)	O4—Li2^{viii}	1.957 (12)
Gd5—O3^{iii}	2.396 (5)	O4—Li2^{i}	1.957 (12)
Gd5—O12	2.489 (5)	O4—Gd2^{i}	2.328 (8)
Gd5—B5	2.884 (11)	O4—Cs1^{ii}	3.517 (2)
Gd5—Li1^{iii}	3.072 (13)	O5—Li2^{i}	2.034 (14)
Gd5—Gd4^{v}	3.7957 (7)	O5—Cs1^{ii}	3.616 (5)
Gd5—Gd1^{vii}	3.8099 (9)	O6—Li1^{ix}	2.007 (13)
Gd5—Gd5^{vi}	3.8737 (10)	O6—Li1^{i}	2.007 (13)
Cs1—O8	3.069 (5)	O6—Gd3^{i}	2.319 (8)
Cs1—O9	3.101 (5)	O6—Cs1^{iii}	3.510 (2)
Cs1—O11	3.121 (5)	O7—Li1^{ix}	2.036 (15)
Cs1—O13	3.126 (5)	O7—Gd1^{iii}	2.389 (4)
Cs1—O15^{i}	3.131 (5)	O8—Li2^{viii}	1.885 (13)
Cs1—O16^{i}	3.215 (6)	O8—Gd4^{i}	2.294 (6)
Cs1—O14	3.219 (6)	O9—Gd4^{v}	2.241 (5)
Cs1—B6	3.289 (9)	O10—Gd5^{v}	2.346 (5)
Cs1—B6^{i}	3.320 (9)	O10—Gd1^{ii}	2.389 (5)
Cs1—B4	3.331 (9)	O11—Li1^{ix}	1.913 (14)
Cs1—B5	3.370 (8)	O11—Gd5^{i}	2.291 (6)
Cs1—B3	3.4074 (19)	O12—Gd5^{vi}	2.378 (5)
B1—O1	1.352 (12)	O12—Gd1^{iii}	2.431 (5)

B1—O2	1.391 (9)	O13—Gd4^{v}	2.273 (5)
B1—O3	1.392 (9)	O15—Cs1^{iv}	3.131 (5)
B1—Li2	2.302 (15)	O16—Cs1^{iv}	3.215 (6)
O1^{i}—Gd1—O5	77.44 (17)	B5—Cs1—B3	72.48 (14)
O1^{i}—Gd1—O14	110.0 (2)	O1—B1—O2	121.5 (6)
O5—Gd1—O14	77.49 (17)	O1—B1—O3	120.6 (7)
O1^{i}—Gd1—O10^{ii}	88.99 (18)	O2—B1—O3	117.9 (8)
O5—Gd1—O10^{ii}	74.75 (16)	O1—B1—Li2	56.0 (5)
O14—Gd1—O10^{ii}	141.81 (18)	O2—B1—Li2	65.7 (5)
O1^{i}—Gd1—O7^{iii}	77.01 (18)	O3—B1—Li2	174.9 (7)
O5—Gd1—O7^{iii}	131.07 (17)	O1—B1—Li1	56.4 (5)
O14—Gd1—O7^{iii}	73.17 (17)	O2—B1—Li1	177.9 (7)
O10^{ii}—Gd1—O7^{iii}	144.84 (17)	O3—B1—Li1	64.2 (5)
O1^{i}—Gd1—O12^{iii}	91.33 (18)	Li2—B1—Li1	112.2 (7)
O5—Gd1—O12^{iii}	145.34 (17)	O1—B1—Gd1	171.0 (5)
O14—Gd1—O12^{iii}	136.74 (18)	O2—B1—Gd1	60.0 (4)
O10^{ii}—Gd1—O12^{iii}	72.34 (17)	O3—B1—Gd1	58.6 (4)
O7^{iii}—Gd1—O12^{iii}	75.88 (16)	Li2—B1—Gd1	125.5 (4)
O1^{i}—Gd1—O3	152.44 (16)	Li1—B1—Gd1	121.9 (5)
O5—Gd1—O3	127.53 (17)	O4—B2—O5^{ii}	121.5 (5)
O14—Gd1—O3	70.40 (19)	O4—B2—O5	121.5 (5)
O10^{ii}—Gd1—O3	107.56 (17)	O5^{ii}—B2—O5	117.0 (9)
O7^{iii}—Gd1—O3	76.93 (18)	O4—B2—Li2^{viii}	59.3 (4)
O12^{iii}—Gd1—O3	73.74 (17)	O5^{ii}—B2—Li2^{viii}	62.4 (4)
O1^{i}—Gd1—O2	149.44 (16)	O5—B2—Li2^{viii}	175.3 (4)
O5—Gd1—O2	73.01 (17)	O4—B2—Li2^{i}	59.3 (4)
O14—Gd1—O2	71.09 (19)	O5^{ii}—B2—Li2^{i}	175.3 (4)
O10^{ii}—Gd1—O2	76.03 (18)	O5—B2—Li2^{i}	62.4 (4)
O7^{iii}—Gd1—O2	129.38 (17)	Li2^{viii}—B2—Li2^{i}	118.6 (8)
O12^{iii}—Gd1—O2	108.66 (17)	O4—B2—Gd2	180.000 (3)
O3—Gd1—O2	57.97 (17)	O5^{ii}—B2—Gd2	58.5 (5)
O1^{i}—Gd1—B1	174.87 (19)	O5—B2—Gd2	58.5 (5)
O5—Gd1—B1	99.54 (19)	Li2^{viii}—B2—Gd2	120.7 (4)
O14—Gd1—B1	65.1 (2)	Li2^{i}—B2—Gd2	120.7 (4)
O10^{ii}—Gd1—B1	94.24 (19)	O4—B2—Cs1	82.41 (19)
O7^{iii}—Gd1—B1	102.36 (19)	O5^{ii}—B2—Cs1	86.51 (19)
O12^{iii}—Gd1—B1	93.45 (19)	O5—B2—Cs1	101.5 (2)
O3—Gd1—B1	29.10 (17)	Li2^{viii}—B2—Cs1	73.9 (3)
O2—Gd1—B1	29.11 (17)	Li2^{i}—B2—Cs1	98.2 (3)
O1^{i}—Gd1—Li2^{i}	39.5 (3)	Gd2—B2—Cs1	97.59 (19)
O5—Gd1—Li2^{i}	42.5 (3)	O4—B2—Cs1^{ii}	82.41 (19)

O14—Gd1—Li2^{i}	108.5 (3)
O10^{ii}—Gd1—Li2^{i}	65.5 (3)
O7^{iii}—Gd1—Li2^{i}	114.5 (3)
O12^{iii}—Gd1—Li2^{i}	111.5 (3)
O3—Gd1—Li2^{i}	168.0 (3)
O2—Gd1—Li2^{i}	110.1 (3)
B1—Gd1—Li2^{i}	139.1 (3)
O1^{i}—Gd1—Li1^{i}	39.8 (3)
O5—Gd1—Li1^{i}	115.2 (3)
O14—Gd1—Li1^{i}	105.5 (3)
O10^{ii}—Gd1—Li1^{i}	109.9 (3)
O7^{iii}—Gd1—Li1^{i}	42.1 (3)
O12^{iii}—Gd1—Li1^{i}	67.5 (3)
O3—Gd1—Li1^{i}	112.7 (3)
O2—Gd1—Li1^{i}	170.6 (3)
B1—Gd1—Li1^{i}	141.5 (3)
Li2^{i}—Gd1—Li1^{i}	79.2 (4)
O1^{i}—Gd1—Gd3	113.56 (12)
O5—Gd1—Gd3	121.42 (12)
O14—Gd1—Gd3	44.10 (12)
O10^{ii}—Gd1—Gd3	153.86 (13)
O7^{iii}—Gd1—Gd3	40.95 (13)
O12^{iii}—Gd1—Gd3	93.18 (12)
O3—Gd1—Gd3	46.54 (11)
O2—Gd1—Gd3	88.82 (12)
B1—Gd1—Gd3	64.33 (13)
Li2^{i}—Gd1—Gd3	140.6 (2)
Li1^{i}—Gd1—Gd3	82.9 (2)
O4^{iv}—Gd2—O5	150.52 (11)
O4^{iv}—Gd2—O5^{ii}	150.52 (11)
O5—Gd2—O5^{ii}	59.0 (2)
O4^{iv}—Gd2—O16^{ii}	83.80 (14)
O5—Gd2—O16^{ii}	84.42 (18)
O5^{ii}—Gd2—O16^{ii}	106.56 (18)
O4^{iv}—Gd2—O16	83.80 (14)
O5—Gd2—O16	106.56 (17)
O5^{ii}—Gd2—O16	84.42 (18)
O16^{ii}—Gd2—O16	167.6 (3)
O4^{iv}—Gd2—O2	78.52 (12)
O5—Gd2—O2	72.26 (16)
O5^{ii}—Gd2—O2	130.64 (17)
O5^{ii}—B2—Cs1^{ii}	101.5 (2)
O5—B2—Cs1^{ii}	86.51 (19)
Li2^{viii}—B2—Cs1^{ii}	98.2 (3)
Li2^{i}—B2—Cs1^{ii}	73.9 (3)
Gd2—B2—Cs1^{ii}	97.59 (19)
Cs1—B2—Cs1^{ii}	164.8 (4)
O7^{iii}—B3—O7	120.2 (10)
O7^{iii}—B3—O6	119.9 (5)
O7—B3—O6	119.9 (5)
O7^{iii}—B3—Li1^{ix}	179.0 (7)
O7—B3—Li1^{ix}	60.6 (5)
O6—B3—Li1^{ix}	59.3 (5)
O7^{iii}—B3—Li1^{i}	60.6 (5)
O7—B3—Li1^{i}	179.1 (7)
O6—B3—Li1^{i}	59.3 (5)
Li1^{ix}—B3—Li1^{i}	118.7 (9)
O7^{iii}—B3—Gd3	60.1 (5)
O7—B3—Gd3	60.1 (5)
O6—B3—Gd3	180.000 (3)
Li1^{ix}—B3—Gd3	120.7 (5)
Li1^{i}—B3—Gd3	120.7 (5)
O7^{iii}—B3—Cs1	108.9 (2)
O7—B3—Cs1	78.59 (19)
O6—B3—Cs1	82.8 (2)
Li1^{ix}—B3—Cs1	70.6 (3)
Li1^{i}—B3—Cs1	101.7 (4)
Gd3—B3—Cs1	97.2 (2)
O7^{iii}—B3—Cs1^{iii}	78.59 (18)
O7—B3—Cs1^{iii}	108.9 (2)
O6—B3—Cs1^{iii}	82.8 (2)
Li1^{ix}—B3—Cs1^{iii}	101.7 (4)
Li1^{i}—B3—Cs1^{iii}	70.6 (3)
Gd3—B3—Cs1^{iii}	97.2 (2)
Cs1—B3—Cs1^{iii}	165.5 (4)
O8—B4—O9	123.9 (7)
O8—B4—O10	123.1 (7)
O9—B4—O10	112.9 (9)
O9—B4—Li2^{viii}	139.0 (6)
O10—B4—Li2^{viii}	90.4 (5)
O8—B4—Gd4	160.6 (5)
O9—B4—Gd4	55.1 (5)

O16^{ii}—Gd2—O2	73.76 (17)	O10—B4—Gd4	61.1 (5)
O16—Gd2—O2	103.69 (17)	Li2^{viii}—B4—Gd4	121.1 (4)
O4^{iv}—Gd2—O2^{ii}	78.52 (12)	O8—B4—Cs1	67.1 (4)
O5—Gd2—O2^{ii}	130.64 (17)	O9—B4—Cs1	68.4 (4)
O5^{ii}—Gd2—O2^{ii}	72.26 (16)	O10—B4—Cs1	140.9 (5)
O16^{ii}—Gd2—O2^{ii}	103.69 (17)	Li2^{viii}—B4—Cs1	72.4 (3)
O16—Gd2—O2^{ii}	73.76 (17)	Gd4—B4—Cs1	97.7 (3)
O2—Gd2—O2^{ii}	157.0 (2)	O11—B5—O13	123.8 (7)
O4^{iv}—Gd2—B2	180.000 (4)	O11—B5—O12	123.4 (7)
O5—Gd2—B2	29.48 (11)	O13—B5—O12	112.7 (8)
O5^{ii}—Gd2—B2	29.48 (11)	O13—B5—Li1^{ix}	134.7 (6)
O16^{ii}—Gd2—B2	96.20 (14)	O12—B5—Li1^{ix}	93.5 (5)
O16—Gd2—B2	96.20 (14)	O11—B5—Gd5	163.4 (5)
O2—Gd2—B2	101.48 (12)	O13—B5—Gd5	55.1 (4)
O2^{ii}—Gd2—B2	101.48 (12)	O12—B5—Gd5	59.6 (4)
O4^{iv}—Gd2—O14^{ii}	102.64 (13)	Li1^{ix}—B5—Gd5	123.0 (4)
O5—Gd2—O14^{ii}	90.81 (16)	O11—B5—Cs1	67.8 (4)
O5^{ii}—Gd2—O14^{ii}	66.72 (16)	O13—B5—Cs1	67.9 (4)
O16^{ii}—Gd2—O14^{ii}	51.50 (16)	O12—B5—Cs1	139.4 (5)
O16—Gd2—O14^{ii}	132.05 (16)	Li1^{ix}—B5—Cs1	68.3 (3)
O2—Gd2—O14^{ii}	124.22 (15)	Gd5—B5—Cs1	99.2 (2)
O2^{ii}—Gd2—O14^{ii}	61.62 (15)	O14—B6—O16	119.6 (6)
B2—Gd2—O14^{ii}	77.36 (13)	O14—B6—O15	116.2 (6)
O4^{iv}—Gd2—O14	102.64 (13)	O16—B6—O15	124.1 (7)
O5—Gd2—O14	66.72 (16)	O14—B6—Gd3	58.6 (3)
O5^{ii}—Gd2—O14	90.81 (16)	O16—B6—Gd3	165.9 (6)
O16^{ii}—Gd2—O14	132.05 (16)	O15—B6—Gd3	59.0 (3)
O16—Gd2—O14	51.50 (16)	O14—B6—Gd2	72.0 (4)
O2—Gd2—O14	61.62 (15)	O16—B6—Gd2	48.9 (3)
O2^{ii}—Gd2—O14	124.22 (15)	O15—B6—Gd2	164.3 (6)
B2—Gd2—O14	77.36 (13)	Gd3—B6—Gd2	123.9 (3)
O14^{ii}—Gd2—O14	154.7 (3)	O14—B6—Cs1	75.0 (4)
O4^{iv}—Gd2—B6^{ii}	90.41 (16)	O16—B6—Cs1	96.7 (5)
O5—Gd2—B6^{ii}	90.52 (19)	O15—B6—Cs1	99.9 (5)
O5^{ii}—Gd2—B6^{ii}	88.76 (19)	Gd3—B6—Cs1	96.1 (2)
O16^{ii}—Gd2—B6^{ii}	25.60 (19)	Gd2—B6—Cs1	95.2 (2)
O16—Gd2—B6^{ii}	154.60 (19)	O14—B6—Cs1^{iv}	128.9 (5)
O2—Gd2—B6^{ii}	99.31 (18)	O16—B6—Cs1^{iv}	73.6 (4)
O2^{ii}—Gd2—B6^{ii}	80.86 (18)	O15—B6—Cs1^{iv}	70.0 (4)
B2—Gd2—B6^{ii}	89.59 (16)	Gd3—B6—Cs1^{iv}	96.7 (2)
O14^{ii}—Gd2—B6^{ii}	26.27 (17)	Gd2—B6—Cs1^{iv}	94.4 (2)
O14—Gd2—B6^{ii}	153.33 (18)	Cs1—B6—Cs1^{iv}	156.1 (3)

O4^{iv}—Gd2—B6	90.41 (16)	O11^{x}—Li1—O1	115.3 (7)
O5—Gd2—B6	88.76 (19)	O11^{x}—Li1—O6^{iv}	138.4 (7)
O5^{ii}—Gd2—B6	90.52 (19)	O1—Li1—O6^{iv}	106.2 (6)
O16^{ii}—Gd2—B6	154.60 (19)	O11^{x}—Li1—O7^{x}	103.6 (7)
O16—Gd2—B6	25.60 (19)	O1—Li1—O7^{x}	93.9 (6)
O2—Gd2—B6	80.86 (18)	O6^{iv}—Li1—O7^{x}	71.9 (5)
O2^{ii}—Gd2—B6	99.31 (18)	O11^{x}—Li1—O3	95.3 (6)
B2—Gd2—B6	89.59 (16)	O1—Li1—O3	71.5 (5)
O14^{ii}—Gd2—B6	153.33 (18)	O6^{iv}—Li1—O3	98.4 (7)
O14—Gd2—B6	26.27 (17)	O7^{x}—Li1—O3	159.9 (7)
B6^{ii}—Gd2—B6	179.2 (3)	O11^{x}—Li1—B3^{iv}	127.1 (7)
O6^{iv}—Gd3—O7	150.44 (11)	O1—Li1—B3^{iv}	102.6 (6)
O6^{iv}—Gd3—O7^{iii}	150.44 (11)	O6^{iv}—Li1—B3^{iv}	36.1 (4)
O7—Gd3—O7^{iii}	59.1 (2)	O7^{x}—Li1—B3^{iv}	35.8 (4)
O6^{iv}—Gd3—O14	103.85 (15)	O3—Li1—B3^{iv}	132.3 (7)
O7—Gd3—O14	85.64 (17)	O11^{x}—Li1—B1	108.6 (6)
O7^{iii}—Gd3—O14	70.10 (17)	O1—Li1—B1	35.4 (4)
O6^{iv}—Gd3—O14^{iii}	103.85 (15)	O6^{iv}—Li1—B1	105.3 (6)
O7—Gd3—O14^{iii}	70.10 (17)	O7^{x}—Li1—B1	128.1 (6)
O7^{iii}—Gd3—O14^{iii}	85.64 (17)	O3—Li1—B1	36.0 (3)
O14—Gd3—O14^{iii}	152.3 (3)	B3^{iv}—Li1—B1	123.3 (6)
O6^{iv}—Gd3—O15^{iii}	81.35 (13)	O11^{x}—Li1—B5^{x}	29.5 (4)
O7—Gd3—O15^{iii}	114.08 (16)	O1—Li1—B5^{x}	106.0 (6)
O7^{iii}—Gd3—O15^{iii}	81.59 (17)	O6^{iv}—Li1—B5^{x}	135.8 (7)
O14—Gd3—O15^{iii}	130.14 (16)	O7^{x}—Li1—B5^{x}	76.6 (5)
O14^{iii}—Gd3—O15^{iii}	55.07 (16)	O3—Li1—B5^{x}	120.1 (6)
O6^{iv}—Gd3—O15	81.34 (13)	B3^{iv}—Li1—B5^{x}	107.2 (6)
O7—Gd3—O15	81.59 (17)	B1—Li1—B5^{x}	118.4 (6)
O7^{iii}—Gd3—O15	114.08 (17)	O11^{x}—Li1—Gd1^{iv}	99.0 (6)
O14—Gd3—O15	55.07 (16)	O1—Li1—Gd1^{iv}	48.7 (4)
O14^{iii}—Gd3—O15	130.14 (16)	O6^{iv}—Li1—Gd1^{iv}	108.1 (5)
O15^{iii}—Gd3—O15	162.7 (3)	O7^{x}—Li1—Gd1^{iv}	51.8 (3)
O6^{iv}—Gd3—O3^{iii}	78.17 (11)	O3—Li1—Gd1^{iv}	118.9 (5)
O7—Gd3—O3^{iii}	73.11 (16)	B3^{iv}—Li1—Gd1^{iv}	79.0 (4)
O7^{iii}—Gd3—O3^{iii}	130.34 (16)	B1—Li1—Gd1^{iv}	83.4 (4)
O14—Gd3—O3^{iii}	121.44 (16)	B5^{x}—Li1—Gd1^{iv}	73.3 (4)
O14^{iii}—Gd3—O3^{iii}	64.95 (16)	O11^{x}—Li1—Gd5^{iii}	48.1 (4)
O15^{iii}—Gd3—O3^{iii}	108.25 (16)	O1—Li1—Gd5^{iii}	109.0 (5)
O15—Gd3—O3^{iii}	67.98 (16)	O6^{iv}—Li1—Gd5^{iii}	118.6 (6)
O6^{iv}—Gd3—O3	78.17 (11)	O7^{x}—Li1—Gd5^{iii}	149.1 (6)
O7—Gd3—O3	130.34 (16)	O3—Li1—Gd5^{iii}	51.0 (3)

O7^{iii}—Gd3—O3	73.11 (16)	B3^{iv}—Li1—Gd5^{iii}	145.5 (5)
O14—Gd3—O3	64.95 (16)	B1—Li1—Gd5^{iii}	79.4 (4)
O14^{iii}—Gd3—O3	121.44 (16)	B5^{x}—Li1—Gd5^{iii}	77.3 (4)
O15^{iii}—Gd3—O3	67.98 (16)	Gd1^{iv}—Li1—Gd5^{iii}	133.0 (4)
O15—Gd3—O3	108.25 (16)	O11^{x}—Li1—Gd3	121.3 (6)
O3^{iii}—Gd3—O3	156.3 (2)	O1—Li1—Gd3	101.7 (6)
O6^{iv}—Gd3—B3	180.000 (3)	O6^{iv}—Li1—Gd3	46.0 (4)
O7—Gd3—B3	29.56 (11)	O7^{x}—Li1—Gd3	117.9 (5)
O7^{iii}—Gd3—B3	29.56 (11)	O3—Li1—Gd3	54.7 (4)
O14—Gd3—B3	76.15 (15)	B3^{iv}—Li1—Gd3	82.1 (5)
O14^{iii}—Gd3—B3	76.15 (15)	B1—Li1—Gd3	77.0 (5)
O15^{iii}—Gd3—B3	98.65 (13)	B5^{x}—Li1—Gd3	147.7 (5)
O15—Gd3—B3	98.66 (13)	Gd1^{iv}—Li1—Gd3	138.9 (4)
O3^{iii}—Gd3—B3	101.83 (11)	Gd5^{iii}—Li1—Gd3	78.3 (3)
O3—Gd3—B3	101.83 (11)	O11^{x}—Li1—Cs1^{x}	64.3 (4)
O6^{iv}—Gd3—B6	89.68 (16)	O1—Li1—Cs1^{x}	165.0 (7)
O7—Gd3—B6	86.45 (19)	O6^{iv}—Li1—Cs1^{x}	75.4 (3)
O7^{iii}—Gd3—B6	94.11 (19)	O7^{x}—Li1—Cs1^{x}	72.2 (4)
O14—Gd3—B6	27.51 (18)	O3—Li1—Cs1^{x}	123.4 (5)
O14^{iii}—Gd3—B6	152.8 (2)	B3^{iv}—Li1—Cs1^{x}	69.6 (3)
O15^{iii}—Gd3—B6	151.79 (18)	B1—Li1—Cs1^{x}	159.3 (6)
O15—Gd3—B6	28.00 (18)	B5^{x}—Li1—Cs1^{x}	65.9 (3)
O3^{iii}—Gd3—B6	95.82 (18)	Gd1^{iv}—Li1—Cs1^{x}	116.3 (4)
O3—Gd3—B6	84.05 (19)	Gd5^{iii}—Li1—Cs1^{x}	82.2 (3)
B3—Gd3—B6	90.32 (17)	Gd3—Li1—Cs1^{x}	90.1 (3)
O6^{iv}—Gd3—B6^{iii}	89.68 (17)	O8^{xi}—Li2—O1	116.4 (7)
O7—Gd3—B6^{iii}	94.11 (19)	O8^{xi}—Li2—O4^{iv}	130.8 (6)
O7^{iii}—Gd3—B6^{iii}	86.45 (19)	O1—Li2—O4^{iv}	112.7 (6)
O14—Gd3—B6^{iii}	152.8 (2)	O8^{xi}—Li2—O5^{iv}	105.4 (6)
O14^{iii}—Gd3—B6^{iii}	27.51 (18)	O1—Li2—O5^{iv}	95.0 (6)
O15^{iii}—Gd3—B6^{iii}	28.00 (18)	O4^{iv}—Li2—O5^{iv}	73.1 (5)
O15—Gd3—B6^{iii}	151.79 (19)	O8^{xi}—Li2—O2	94.9 (6)
O3^{iii}—Gd3—B6^{iii}	84.05 (19)	O1—Li2—O2	72.1 (5)
O3—Gd3—B6^{iii}	95.82 (18)	O4^{iv}—Li2—O2	96.6 (6)
B3—Gd3—B6^{iii}	90.32 (16)	O5^{iv}—Li2—O2	159.4 (7)
B6—Gd3—B6^{iii}	179.4 (3)	O8^{xi}—Li2—B2^{iv}	123.2 (6)
O9^{v}—Gd4—O13^{v}	92.37 (18)	O1—Li2—B2^{iv}	109.0 (6)
O9^{v}—Gd4—O8^{iv}	89.57 (18)	O4^{iv}—Li2—B2^{iv}	36.4 (4)
O13^{v}—Gd4—O8^{iv}	88.01 (18)	O5^{iv}—Li2—B2^{iv}	36.7 (4)
O9^{v}—Gd4—O16	99.64 (19)	O2—Li2—B2^{iv}	131.5 (6)
O13^{v}—Gd4—O16	166.45 (18)	O8^{xi}—Li2—B1	107.5 (6)

O8^{iv}—Gd4—O16	85.83 (19)	O1—Li2—B1	35.9 (4)
O9^{v}—Gd4—O9	73.0 (2)	O4^{iv}—Li2—B1	109.8 (6)
O13^{v}—Gd4—O9	103.30 (18)	O5^{iv}—Li2—B1	129.7 (6)
O8^{iv}—Gd4—O9	159.41 (17)	O2—Li2—B1	36.3 (3)
O16—Gd4—O9	86.33 (19)	B2^{iv}—Li2—B1	129.2 (6)
O9^{v}—Gd4—O2^{ii}	166.9 (2)	O8^{xi}—Li2—B4^{xi}	30.2 (3)
O13^{v}—Gd4—O2^{ii}	90.96 (17)	O1—Li2—B4^{xi}	106.8 (6)
O8^{iv}—Gd4—O2^{ii}	77.92 (17)	O4^{iv}—Li2—B4^{xi}	132.4 (6)
O16—Gd4—O2^{ii}	75.95 (18)	O5^{iv}—Li2—B4^{xi}	78.1 (5)
O9—Gd4—O2^{ii}	118.38 (17)	O2—Li2—B4^{xi}	120.6 (6)
O9^{v}—Gd4—O10	119.01 (18)	B2^{iv}—Li2—B4^{xi}	105.8 (6)
O13^{v}—Gd4—O10	72.09 (17)	B1—Li2—B4^{xi}	117.8 (6)
O8^{iv}—Gd4—O10	144.98 (16)	O8^{xi}—Li2—Gd1^{iv}	101.7 (5)
O16—Gd4—O10	106.88 (18)	O1—Li2—Gd1^{iv}	49.5 (3)
O9—Gd4—O10	55.60 (16)	O4^{iv}—Li2—Gd1^{iv}	112.6 (5)
O2^{ii}—Gd4—O10	74.02 (17)	O5^{iv}—Li2—Gd1^{iv}	51.9 (3)
O9^{v}—Gd4—B4	99.1 (2)	O2—Li2—Gd1^{iv}	120.7 (5)
O13^{v}—Gd4—B4	92.5 (2)	B2^{iv}—Li2—Gd1^{iv}	82.8 (4)
O8^{iv}—Gd4—B4	171.27 (19)	B1—Li2—Gd1^{iv}	84.7 (4)
O16—Gd4—B4	91.8 (2)	B4^{xi}—Li2—Gd1^{iv}	74.8 (4)
O9—Gd4—B4	27.96 (18)	O8^{xi}—Li2—Gd4^{ii}	46.7 (3)
O2^{ii}—Gd4—B4	93.36 (19)	O1—Li2—Gd4^{ii}	107.9 (6)
O10—Gd4—B4	28.77 (18)	O4^{iv}—Li2—Gd4^{ii}	113.9 (5)
O9^{v}—Gd4—Li2^{ii}	123.9 (3)	O5^{iv}—Li2—Gd4^{ii}	149.6 (5)
O13^{v}—Gd4—Li2^{ii}	98.6 (2)	O2—Li2—Gd4^{ii}	50.8 (3)
O8^{iv}—Gd4—Li2^{ii}	36.7 (3)	B2^{iv}—Li2—Gd4^{ii}	140.5 (5)
O16—Gd4—Li2^{ii}	69.5 (3)	B1—Li2—Gd4^{ii}	77.5 (4)
O9—Gd4—Li2^{ii}	151.8 (3)	B4^{xi}—Li2—Gd4^{ii}	76.4 (4)
O2^{ii}—Gd4—Li2^{ii}	43.1 (3)	Gd1^{iv}—Li2—Gd4^{ii}	133.5 (4)
O10—Gd4—Li2^{ii}	116.8 (3)	O8^{xi}—Li2—Gd2	115.0 (5)
B4—Gd4—Li2^{ii}	134.8 (3)	O1—Li2—Gd2	104.2 (5)
O9^{v}—Gd4—Gd4^{v}	38.01 (14)	O4^{iv}—Li2—Gd2	46.6 (4)
O13^{v}—Gd4—Gd4^{v}	99.95 (13)	O5^{iv}—Li2—Gd2	119.6 (5)
O8^{iv}—Gd4—Gd4^{v}	126.73 (12)	O2—Li2—Gd2	51.8 (3)
O16—Gd4—Gd4^{v}	93.40 (13)	B2^{iv}—Li2—Gd2	83.1 (4)
O9—Gd4—Gd4^{v}	35.04 (12)	B1—Li2—Gd2	78.0 (4)
O2^{ii}—Gd4—Gd4^{v}	152.96 (13)	B4^{xi}—Li2—Gd2	142.5 (5)
O10—Gd4—Gd4^{v}	85.84 (11)	Gd1^{iv}—Li2—Gd2	142.6 (4)
B4—Gd4—Gd4^{v}	61.74 (15)	Gd4^{ii}—Li2—Gd2	74.5 (3)
Li2^{ii}—Gd4—Gd4^{v}	154.4 (2)	O8^{xi}—Li2—Cs1^{xi}	59.8 (3)
O9^{v}—Gd4—Gd5^{v}	101.76 (14)	O1—Li2—Cs1^{xi}	167.2 (6)

$O13^{v}$—Gd4—$Gd5^{v}$	36.24 (13)	$O4^{iv}$—Li2—$Cs1^{xi}$	73.0 (3)
$O8^{iv}$—Gd4—$Gd5^{v}$	122.64 (13)	$O5^{iv}$—Li2—$Cs1^{xi}$	75.3 (4)
O16—Gd4—$Gd5^{v}$	144.10 (14)	O2—Li2—$Cs1^{xi}$	119.5 (5)
O9—Gd4—$Gd5^{v}$	72.93 (12)	$B2^{iv}$—Li2—$Cs1^{xi}$	68.2 (3)
$O2^{ii}$—Gd4—$Gd5^{v}$	88.34 (12)	B1—Li2—$Cs1^{xi}$	154.9 (6)
O10—Gd4—$Gd5^{v}$	37.24 (11)	$B4^{xi}$—Li2—$Cs1^{xi}$	63.4 (3)
B4—Gd4—$Gd5^{v}$	56.64 (16)	$Gd1^{iv}$—Li2—$Cs1^{xi}$	118.0 (4)
$Li2^{ii}$—Gd4—$Gd5^{v}$	119.0 (2)	$Gd4^{ii}$—Li2—$Cs1^{xi}$	78.7 (3)
$Gd4^{v}$—Gd4—$Gd5^{v}$	86.18 (2)	Gd2—Li2—$Cs1^{xi}$	88.0 (3)
$O9^{v}$—Gd4—Gd2	136.44 (13)	B1—O1—Li2	88.1 (6)
$O13^{v}$—Gd4—Gd2	130.73 (13)	B1—O1—Li1	88.2 (6)
$O8^{iv}$—Gd4—Gd2	86.43 (12)	Li2—O1—Li1	173.9 (7)
O16—Gd4—Gd2	36.82 (13)	B1—O1—$Gd1^{iv}$	166.2 (5)
O9—Gd4—Gd2	98.50 (13)	Li2—O1—$Gd1^{iv}$	91.0 (5)
$O2^{ii}$—Gd4—Gd2	40.10 (12)	Li1—O1—$Gd1^{iv}$	91.5 (5)
O10—Gd4—Gd2	85.46 (11)	B1—O2—Li2	78.0 (5)
B4—Gd4—Gd2	86.62 (15)	B1—O2—$Gd4^{ii}$	127.6 (4)
$Li2^{ii}$—Gd4—Gd2	53.4 (2)	Li2—O2—$Gd4^{ii}$	86.1 (4)
$Gd4^{v}$—Gd4—Gd2	122.01 (2)	B1—O2—Gd1	90.8 (5)
$Gd5^{v}$—Gd4—Gd2	116.732 (17)	Li2—O2—Gd1	167.6 (4)
$O11^{iv}$—Gd5—O15	84.81 (19)	$Gd4^{ii}$—O2—Gd1	105.3 (2)
$O11^{iv}$—Gd5—$O10^{v}$	90.68 (19)	B1—O2—Gd2	126.5 (4)
O15—Gd5—$O10^{v}$	110.01 (17)	Li2—O2—Gd2	86.0 (4)
$O11^{iv}$—Gd5—$O12^{vi}$	89.85 (18)	$Gd4^{ii}$—O2—Gd2	101.29 (17)
O15—Gd5—$O12^{vi}$	173.27 (18)	Gd1—O2—Gd2	96.45 (18)
$O10^{v}$—Gd5—$O12^{vi}$	74.05 (18)	B1—O3—Li1	79.8 (6)
$O11^{iv}$—Gd5—O13	157.13 (17)	B1—O3—$Gd5^{iii}$	132.9 (4)
O15—Gd5—O13	84.69 (18)	Li1—O3—$Gd5^{iii}$	85.3 (4)
$O10^{v}$—Gd5—O13	74.01 (19)	B1—O3—Gd1	92.3 (5)
$O12^{vi}$—Gd5—O13	101.74 (17)	Li1—O3—Gd1	167.3 (4)
$O11^{iv}$—Gd5—$O3^{iii}$	79.26 (19)	$Gd5^{iii}$—O3—Gd1	107.36 (19)
O15—Gd5—$O3^{iii}$	75.92 (18)	B1—O3—Gd3	118.3 (4)
$O10^{v}$—Gd5—$O3^{iii}$	167.96 (19)	Li1—O3—Gd3	83.9 (4)
$O12^{vi}$—Gd5—$O3^{iii}$	99.10 (17)	$Gd5^{iii}$—O3—Gd3	103.96 (17)
O13—Gd5—$O3^{iii}$	117.54 (17)	Gd1—O3—Gd3	91.14 (16)
$O11^{iv}$—Gd5—O12	145.68 (17)	B2—O4—$Li2^{viii}$	84.3 (5)
O15—Gd5—O12	107.87 (18)	B2—O4—$Li2^{i}$	84.3 (5)
$O10^{v}$—Gd5—O12	113.12 (17)	$Li2^{viii}$—O4—$Li2^{i}$	168.6 (9)
$O12^{vi}$—Gd5—O12	74.52 (19)	B2—O4—$Gd2^{i}$	180.000 (2)
O13—Gd5—O12	57.18 (16)	$Li2^{viii}$—O4—$Gd2^{i}$	95.7 (5)
$O3^{iii}$—Gd5—O12	73.51 (17)	$Li2^{i}$—O4—$Gd2^{i}$	95.7 (5)

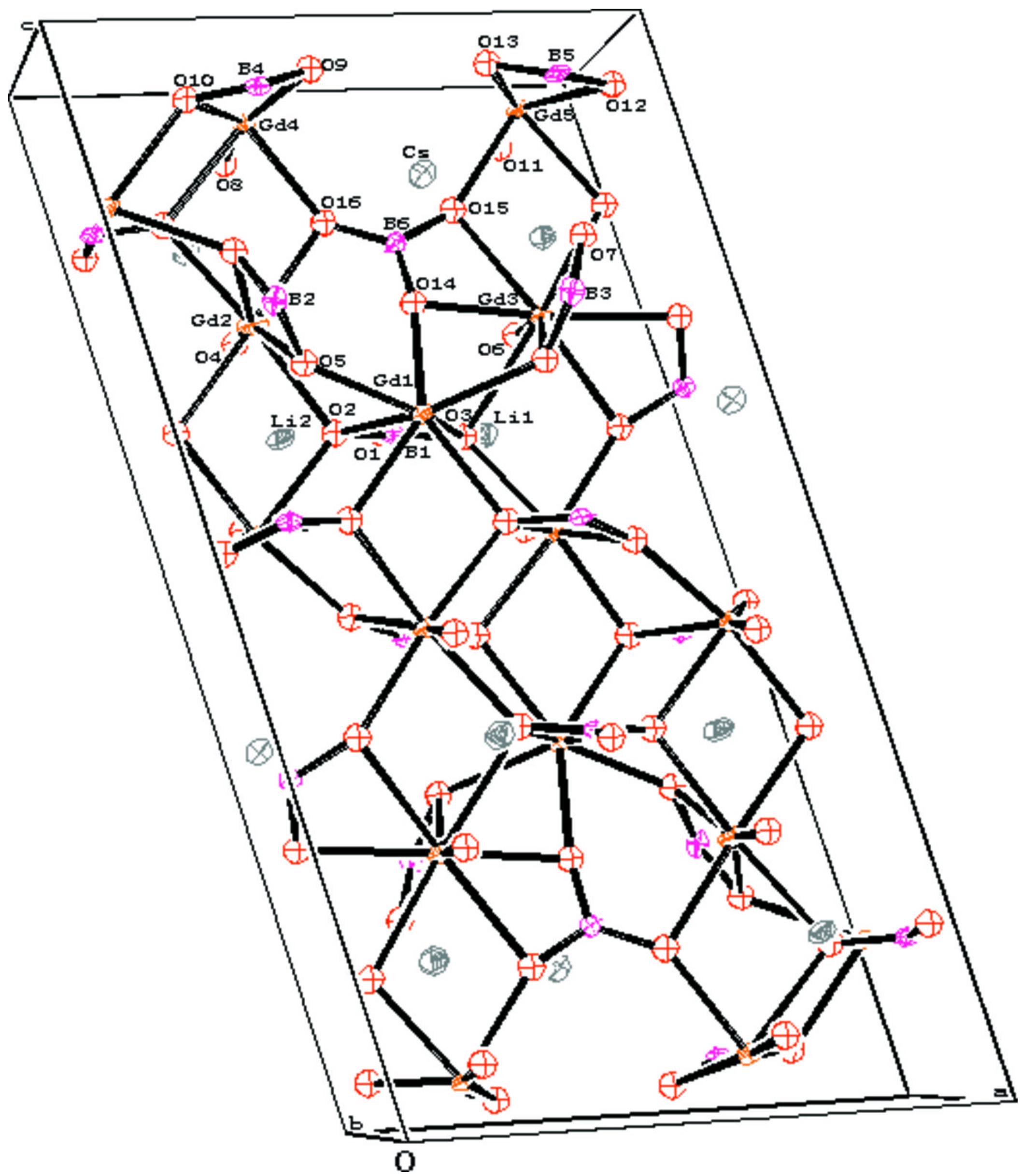
$O11^{iv}$—Gd5—B5	172.2 (2)	B2—O4—Cs1	75.18 (13)
O15—Gd5—B5	92.5 (2)	$Li2^{viii}$—O4—Cs1	74.8 (4)
$O10^{v}$—Gd5—B5	97.1 (2)	$Li2^{i}$—O4—Cs1	102.2 (4)
$O12^{vi}$—Gd5—B5	92.3 (2)	$Gd2^{i}$—O4—Cs1	104.82 (13)
O13—Gd5—B5	28.69 (19)	B2—O4—$Cs1^{ii}$	75.19 (13)
$O3^{iii}$—Gd5—B5	93.0 (2)	$Li2^{viii}$—O4—$Cs1^{ii}$	102.2 (4)
O12—Gd5—B5	29.22 (19)	$Li2^{i}$—O4—$Cs1^{ii}$	74.8 (3)
$O11^{iv}$—Gd5—$Li1^{iii}$	38.4 (3)	$Gd2^{i}$—O4—$Cs1^{ii}$	104.81 (13)
O15—Gd5—$Li1^{iii}$	66.2 (3)	Cs1—O4—$Cs1^{ii}$	150.4 (3)
$O10^{v}$—Gd5—$Li1^{iii}$	128.0 (3)	B2—O5—$Li2^{i}$	80.8 (6)
$O12^{vi}$—Gd5—$Li1^{iii}$	107.1 (3)	B2—O5—Gd1	139.4 (3)
O13—Gd5—$Li1^{iii}$	147.6 (3)	$Li2^{i}$—O5—Gd1	85.5 (4)
$O3^{iii}$—Gd5—$Li1^{iii}$	43.7 (3)	B2—O5—Gd2	92.0 (5)
O12—Gd5—$Li1^{iii}$	117.1 (3)	$Li2^{i}$—O5—Gd2	171.2 (4)
B5—Gd5—$Li1^{iii}$	134.0 (3)	Gd1—O5—Gd2	103.29 (19)
$O11^{iv}$—Gd5—$Gd4^{v}$	125.57 (13)	B2—O5—$Cs1^{ii}$	71.2 (2)
O15—Gd5—$Gd4^{v}$	90.44 (13)	$Li2^{i}$—O5—$Cs1^{ii}$	71.7 (4)
$O10^{v}$—Gd5—$Gd4^{v}$	41.03 (13)	Gd1—O5—$Cs1^{ii}$	138.87 (17)
$O12^{vi}$—Gd5—$Gd4^{v}$	95.99 (12)	Gd2—O5—$Cs1^{ii}$	101.16 (14)
O13—Gd5—$Gd4^{v}$	34.40 (12)	B3—O6—$Li1^{ix}$	84.6 (5)
$O3^{iii}$—Gd5—$Gd4^{v}$	150.98 (12)	B3—O6—$Li1^{i}$	84.6 (5)
O12—Gd5—$Gd4^{v}$	86.96 (12)	$Li1^{ix}$—O6—$Li1^{i}$	169.1 (10)
B5—Gd5—$Gd4^{v}$	61.61 (16)	B3—O6—$Gd3^{i}$	180.000 (2)
$Li1^{iii}$—Gd5—$Gd4^{v}$	150.0 (2)	$Li1^{ix}$—O6—$Gd3^{i}$	95.4 (5)
$O11^{iv}$—Gd5—$Gd1^{vii}$	96.38 (14)	$Li1^{i}$—O6—$Gd3^{i}$	95.4 (5)
O15—Gd5—$Gd1^{vii}$	146.63 (13)	B3—O6—Cs1	74.35 (13)
$O10^{v}$—Gd5—$Gd1^{vii}$	36.80 (12)	$Li1^{ix}$—O6—Cs1	71.0 (4)
$O12^{vi}$—Gd5—$Gd1^{vii}$	38.09 (12)	$Li1^{i}$—O6—Cs1	105.9 (4)
O13—Gd5—$Gd1^{vii}$	81.61 (13)	$Gd3^{i}$—O6—Cs1	105.65 (13)
$O3^{iii}$—Gd5—$Gd1^{vii}$	137.19 (12)	B3—O6—$Cs1^{iii}$	74.35 (13)
O12—Gd5—$Gd1^{vii}$	89.83 (12)	$Li1^{ix}$—O6—$Cs1^{iii}$	105.9 (4)
B5—Gd5—$Gd1^{vii}$	89.87 (15)	$Li1^{i}$—O6—$Cs1^{iii}$	71.0 (4)
$Li1^{iii}$—Gd5—$Gd1^{vii}$	130.7 (3)	$Gd3^{i}$—O6—$Cs1^{iii}$	105.65 (13)
$Gd4^{v}$—Gd5—$Gd1^{vii}$	61.771 (15)	Cs1—O6—$Cs1^{iii}$	148.7 (3)
$O11^{iv}$—Gd5—$Gd5^{vi}$	121.94 (13)	B3—O7—$Li1^{ix}$	83.6 (7)
O15—Gd5—$Gd5^{vi}$	143.78 (13)	B3—O7—$Gd1^{iii}$	131.6 (3)
$O10^{v}$—Gd5—$Gd5^{vi}$	94.80 (12)	$Li1^{ix}$—O7—$Gd1^{iii}$	86.1 (4)
$O12^{vi}$—Gd5—$Gd5^{vi}$	38.26 (13)	B3—O7—Gd3	90.3 (5)
O13—Gd5—$Gd5^{vi}$	77.09 (12)	$Li1^{ix}$—O7—Gd3	173.9 (5)
$O3^{iii}$—Gd5—$Gd5^{vi}$	85.11 (12)	$Gd1^{iii}$—O7—Gd3	98.39 (18)
O12—Gd5—$Gd5^{vi}$	36.27 (11)	B3—O7—Cs1	78.3 (2)

B5—Gd5—Gd5^{vi}	57.56 (16)
Li1^{iii}—Gd5—Gd5^{vi}	118.3 (2)
Gd4^{v}—Gd5—Gd5^{vi}	91.72 (2)
Gd1^{vii}—Gd5—Gd5^{vi}	60.984 (16)
O8—Cs1—O9	45.95 (14)
O8—Cs1—O11	117.84 (15)
O9—Cs1—O11	100.84 (14)
O8—Cs1—O13	102.18 (13)
O9—Cs1—O13	63.08 (13)
O11—Cs1—O13	45.78 (14)
O8—Cs1—O15^{i}	98.52 (14)
O9—Cs1—O15^{i}	128.84 (14)
O11—Cs1—O15^{i}	59.50 (14)
O13—Cs1—O15^{i}	103.66 (13)
O8—Cs1—O16^{i}	60.46 (14)
O9—Cs1—O16^{i}	104.80 (14)
O11—Cs1—O16^{i}	99.76 (15)
O13—Cs1—O16^{i}	131.98 (13)
O15^{i}—Cs1—O16^{i}	45.32 (14)
O8—Cs1—O14	119.24 (13)
O9—Cs1—O14	95.46 (14)
O11—Cs1—O14	113.65 (14)
O13—Cs1—O14	91.31 (14)
O15^{i}—Cs1—O14	135.44 (14)
O16^{i}—Cs1—O14	136.69 (14)
O8—Cs1—B6	108.20 (17)
O9—Cs1—B6	73.76 (17)
O11—Cs1—B6	106.59 (17)
O13—Cs1—B6	71.94 (16)
O15^{i}—Cs1—B6	153.27 (16)
O16^{i}—Cs1—B6	153.43 (16)
O14—Cs1—B6	24.31 (16)
O8—Cs1—B6^{i}	84.15 (16)
O9—Cs1—B6^{i}	126.20 (17)
O11—Cs1—B6^{i}	84.04 (17)
O13—Cs1—B6^{i}	126.61 (16)
O15^{i}—Cs1—B6^{i}	24.72 (15)
O16^{i}—Cs1—B6^{i}	24.23 (15)
O14—Cs1—B6^{i}	131.79 (18)
B6—Cs1—B6^{i}	156.1 (3)
O8—Cs1—B4	24.0 (2)
Li1^{ix}—O7—Cs1	73.2 (4)
Gd1^{iii}—O7—Cs1	142.00 (18)
Gd3—O7—Cs1	105.05 (14)
B4—O8—Li2^{viii}	105.4 (6)
B4—O8—Gd4^{i}	154.9 (5)
Li2^{viii}—O8—Gd4^{i}	96.6 (5)
B4—O8—Cs1	88.9 (4)
Li2^{viii}—O8—Cs1	88.2 (4)
Gd4^{i}—O8—Cs1	103.90 (17)
B4—O9—Gd4^{v}	147.7 (5)
B4—O9—Gd4	96.9 (5)
Gd4^{v}—O9—Gd4	107.0 (2)
B4—O9—Cs1	87.3 (5)
Gd4^{v}—O9—Cs1	100.41 (16)
Gd4—O9—Cs1	116.95 (19)
B4—O10—Gd5^{v}	119.8 (4)
B4—O10—Gd1^{ii}	126.6 (5)
Gd5^{v}—O10—Gd1^{ii}	107.16 (18)
B4—O10—Gd4	90.2 (5)
Gd5^{v}—O10—Gd4	101.73 (19)
Gd1^{ii}—O10—Gd4	104.58 (19)
B5—O11—Li1^{ix}	106.8 (7)
B5—O11—Gd5^{i}	157.8 (5)
Li1^{ix}—O11—Gd5^{i}	93.4 (5)
B5—O11—Cs1	88.4 (4)
Li1^{ix}—O11—Cs1	82.1 (4)
Gd5^{i}—O11—Cs1	103.60 (18)
B5—O12—Gd5^{vi}	123.5 (4)
B5—O12—Gd1^{iii}	122.7 (4)
Gd5^{vi}—O12—Gd1^{iii}	104.79 (18)
B5—O12—Gd5	91.1 (5)
Gd5^{vi}—O12—Gd5	105.47 (19)
Gd1^{iii}—O12—Gd5	104.85 (19)
B5—O13—Gd4^{v}	145.3 (5)
B5—O13—Gd5	96.2 (5)
Gd4^{v}—O13—Gd5	109.4 (2)
B5—O13—Cs1	87.7 (4)
Gd4^{v}—O13—Cs1	98.94 (15)
Gd5—O13—Cs1	119.64 (19)
B6—O14—Gd1	169.7 (4)
B6—O14—Gd3	93.9 (4)

O9—Cs1—B4	24.33 (19)	Gd1—O14—Gd3	95.26 (17)
O11—Cs1—B4	117.98 (16)	B6—O14—Gd2	81.7 (4)
O13—Cs1—B4	86.60 (18)	Gd1—O14—Gd2	88.05 (15)
O15^{i}—Cs1—B4	120.3 (2)	Gd3—O14—Gd2	152.1 (3)
O16^{i}—Cs1—B4	84.4 (2)	B6—O14—Cs1	80.7 (4)
O14—Cs1—B4	102.0 (2)	Gd1—O14—Cs1	100.8 (2)
B6—Cs1—B4	86.1 (2)	Gd3—O14—Cs1	107.41 (18)
B6^{i}—Cs1—B4	108.1 (2)	Gd2—O14—Cs1	99.10 (15)
O8—Cs1—B5	118.94 (16)	B6—O15—Gd5	150.6 (5)
O9—Cs1—B5	86.34 (17)	B6—O15—Gd3	93.0 (4)
O11—Cs1—B5	23.8 (2)	Gd5—O15—Gd3	109.51 (18)
O13—Cs1—B5	24.39 (17)	B6—O15—Cs1^{iv}	85.3 (4)
O15^{i}—Cs1—B5	83.3 (2)	Gd5—O15—Cs1^{iv}	102.85 (18)
O16^{i}—Cs1—B5	122.1 (2)	Gd3—O15—Cs1^{iv}	111.43 (19)
O14—Cs1—B5	96.7 (2)	B6—O15—Cs1	58.9 (4)
B6—Cs1—B5	84.5 (2)	Gd5—O15—Cs1	100.28 (17)
B6^{i}—Cs1—B5	107.9 (2)	Gd3—O15—Cs1	92.58 (15)
B4—Cs1—B5	108.6 (2)	Cs1^{iv}—O15—Cs1	138.22 (15)
O8—Cs1—B3	168.12 (13)	B6—O16—Gd4	144.3 (5)
O9—Cs1—B3	143.5 (2)	B6—O16—Gd2	105.5 (4)
O11—Cs1—B3	71.00 (12)	Gd4—O16—Gd2	107.11 (19)
O13—Cs1—B3	89.69 (14)	B6—O16—Cs1^{iv}	82.2 (4)
O15^{i}—Cs1—B3	78.9 (2)	Gd4—O16—Cs1^{iv}	98.27 (18)
O16^{i}—Cs1—B3	111.7 (2)	Gd2—O16—Cs1^{iv}	112.5 (2)
O14—Cs1—B3	59.2 (2)	B6—O16—Cs1	61.7 (4)
B6—Cs1—B3	74.8 (3)	Gd4—O16—Cs1	99.34 (18)
B6^{i}—Cs1—B3	89.2 (2)	Gd2—O16—Cs1	98.23 (17)
B4—Cs1—B3	160.8 (3)	Cs1^{iv}—O16—Cs1	137.95 (15)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1/2, *y*, −*z*+3/2; (iii) −*x*+3/2, *y*, −*z*+3/2; (iv) *x*, *y*+1, *z*; (v) −*x*+1, −*y*+1, −*z*+2; (vi) −*x*+2, −*y*+1, −*z*+2; (vii) *x*+1/2, −*y*+1, *z*+1/2; (viii) −*x*+1/2, *y*−1, −*z*+3/2; (ix) −*x*+3/2, *y*−1, −*z*+3/2; (x) −*x*+3/2, *y*+1, −*z*+3/2; (xi) −*x*+1/2, *y*+1, −*z*+3/2.

Fig. 1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O10
B4
O9
O13
B5
O12
Gd5
Gd4
Cs
O11
O8
O16
B6
O15
O7
O14
Gd3
B3
B2
Gd2
O4
O6
O5
Gd1
O2
O3
Li1
Li2
O1
B1
b
a
O

Fig. 2

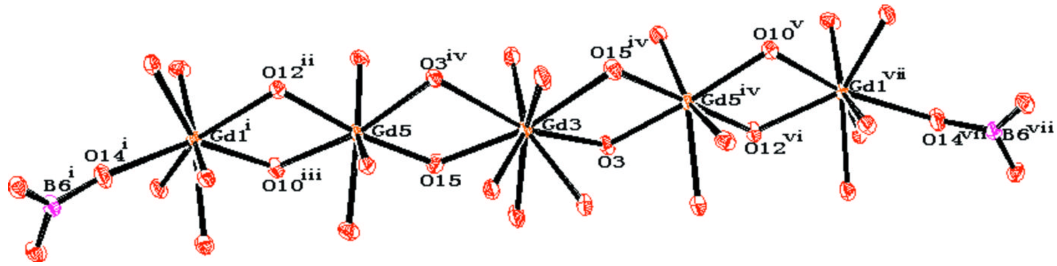
O12ii
O3iv
O15iv
O10v
Gd1vii
O14i
Gd1i
Gd5
Gd3
Gd5iv
B6i
O10iii
O15
O3
O12vi
O14vii
B6vii

Fig. 3