

catena-Poly[[tetraqua- μ -aqua-bis(μ_4 -pyrimidine-2-carboxylato)tetralithium] dichloride]

Wojciech Starosta and Janusz Leciejewicz*

Institute of Nuclear Chemistry and Technology, ul.Dorodna 16, 03-195 Warszawa, Poland

Correspondence e-mail: j.leciejewicz@ichtj.waw.pl

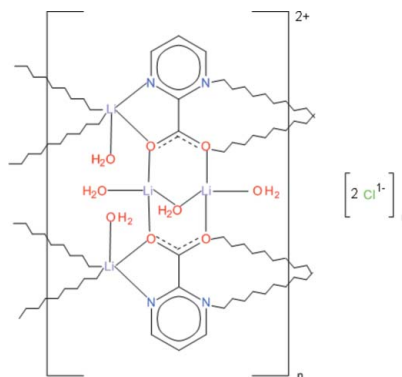
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.044; wR factor = 0.147; data-to-parameter ratio = 18.5.

The asymmetric unit of the title compound, $[Li_4(C_5H_3N_2O_2)_2(H_2O)_5]Cl_2$, contains two Li^I cations, one with a distorted trigonal-bipyramidal and the other with a distorted tetrahedral coordination geometry. Two symmetry-related asymmetric units constitute a building block of the structure, in which both ligand carboxylate O atoms are bidentate and bridge the metal ions, forming a divalent cation. Charge balance is maintained by two chloride anions. The building blocks, bridged by Li^I cations, form cationic ribbons with chloride anions in the space between them. The ribbons propagate in [010] and are held together by a network of weak O—H...O hydrogen bonds which operate in the space between adjacent ribbons.

Related literature

For the structure of a Li complex with pyrimidine-2-carboxylate and nitrate ligands, see: Starosta & Leciejewicz (2011). The structure of a Li^I complex with pyrimidine-4-carboxylate and water ligands was reported recently by Starosta & Leciejewicz (2012).



Experimental

Crystal data

$[Li_4(C_5H_3N_2O_2)_2(H_2O)_5]Cl_2$
 $M_r = 434.93$
 Monoclinic, $C2/c$
 $a = 22.084$ (4) Å
 $b = 8.0773$ (16) Å
 $c = 10.814$ (2) Å
 $\beta = 94.08$ (3)°

$V = 1924.1$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.39$ mm⁻¹
 $T = 293$ K
 $0.37 \times 0.24 \times 0.18$ mm

Data collection

Kuma KM4 four-circle diffractometer
 Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2008)
 $T_{min} = 0.917$, $T_{max} = 0.935$
 2964 measured reflections

2819 independent reflections
 1781 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.029$
 3 standard reflections every 200 reflections
 intensity decay: 2.3%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.147$
 $S = 1.02$
 2819 reflections
 152 parameters
 4 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.51$ e Å⁻³
 $\Delta\rho_{min} = -0.36$ e Å⁻³

Table 1

Selected bond lengths (Å).

Li1—O1	2.069 (3)	Li2—O21	2.140 (6)
Li1—N1	2.175 (4)	Li2—O22	1.915 (4)
Li1—O3	1.987 (4)	Li2—O2 ⁱⁱ	1.968 (4)
Li1—O2 ⁱ	2.029 (4)	Li2—O1	1.993 (4)
Li1—N3 ⁱ	2.221 (4)		

 Symmetry codes: (i) $x, -y + 2, z + \frac{1}{2}$; (ii) $-x, y, -z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O22—H222...O3	0.89 (2)	2.16 (3)	2.841 (3)	133 (3)
O22—H221...Cl1 ⁱⁱⁱ	0.87 (2)	2.36 (2)	3.212 (2)	167 (3)
O3—H31...Cl1	0.83 (4)	2.35 (4)	3.1381 (19)	158 (3)
O3—H32...Cl1 ^{iv}	0.86 (4)	2.29 (4)	3.1429 (19)	168 (4)
O21—H211...Cl1 ^v	0.84 (3)	2.45 (3)	3.288 (2)	175 (3)

 Symmetry codes: (iii) $-x, y, -z + \frac{3}{2}$; (iv) $x, -y + 1, z - \frac{1}{2}$; (v) $-x, -y + 1, -z + 1$.

Data collection: *KM-4 Software* (Kuma, 1996); cell refinement: *KM-4 Software*; data reduction: *DATAPROC* (Kuma, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2084).

References

- Kuma (1996). *KM-4 Software*. Kuma Diffraction Ltd. Wrocław, Poland.
Kuma (2001). *DATAPROC*. Kuma Diffraction Ltd. Wrocław, Poland.
Oxford Diffraction (2008). *CrysAlis RED*. Oxford Diffraction Ltd., Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Starosta, W. & Leciejewicz, J. (2011). *Acta Cryst.* **E67**, m818.
Starosta, W. & Leciejewicz, J. (2012). *Acta Cryst.* **E68**, m1065–m1066.

supporting information

Acta Cryst. (2012). E68, m1369–m1370 [doi:10.1107/S1600536812041955]

catena-Poly[[tetraqua- μ -aqua-bis(μ_4 -pyrimidine-2-carboxylato)tetalithium] dichloride]**Wojciech Starosta and Janusz Leciejewicz****S1. Comment**

The asymmetric cell of the title compound contains two symmetry independent Li^{i} ions, one deprotonated pyrimidine-2-carboxylato ligand molecule, three symmetry independent water molecules which are coordinated to metal ions and one chloride anion. The latter maintains charge balance in the cell. Two symmetry related cells form a molecular moiety which can be visualized as a building unit of the structure (Fig. 1). The ligand bridges Li ions in a μ_4 mode using both its carboxylate O atoms which act as bidentate. Ligand bonding groups N1,O1 and N3,O2 chelate Li^{i} and Li^{iii} ions; the O1 and O2 atoms are also bonded to Li^{ii} and Li^{ii} ions, respectively. Since the Li^{i} and Li^{iii} ions are also coordinated by bonding groups from adjacent symmetry related ligands, a $-\text{Li}^{\text{ii}}-\text{O}2-\text{O}1-\text{Li}^{\text{i}}-\text{O}2^{\text{iii}}-\text{O}1^{\text{iii}}-\text{Li}^{\text{iii}}-$ bridging pathway is formed. Apart from two N,O bonding groups, Li^{i} coordination is completed by an aqua O3 atom. On the other hand, pairs of adjacent symmetry related Li^{ii} and Li^{ii} ions are bridged by an aqua O21 atom while the other coordinated to them aqua O22 and $\text{O}22^{\text{i}}$ atoms are not bridging. Symmetry code: ⁱ $-x, y, -z + 1/2$; ⁱⁱ $x, -y + 2, z - 1/2$; ⁱⁱⁱ $x, -y + 2, z + 1/2$. Adjacent moieties linked along the Li^{i} bridging pathway form a cationic ribbon propagating in the unit cell *b* direction (Fig. 2). Chloride anions are located in the space between adjacent ribbons. Fig. 1 shows, that a ribbon can be visualized as built of centro-symmetric molecular clusters in which Li ions form a tetrameric entities additionally connected by $\text{Li}^{\text{ii}}-\text{O}21-\text{Li}^{\text{ii}}$ bridges. The Li^{i} ion exhibits a distorted trigonal bipyramidal coordination environment in which O1, O3 and $\text{N}3^{\text{iii}}$ atoms form an equatorial plane with a Li^{i} ion 0.0619 (2) Å out of it; N1 and $\text{O}2^{\text{iii}}$ atoms are at apical positions. The coordination of the Li^{ii} ion is strongly distorted tetrahedral. The Li—O and Li—N bond distances (Table 1) are close to those reported in the structures of a Li complex with the title and nitrate ligands (Starosta & Leciejewicz, 2011) and pyrimidine-4-carboxylate and water ligands (Starosta & Leciejewicz, 2012). The pyrimidine ring is planar with r.m.s. of 0.0071 (1) Å; the C7/O1/O2 makes with it a dihedral angle of 5.8 (1)°. Weak hydrogen bonds in which water O atoms are as donors and chloride anions act as acceptors operate between adjacent ribbons (Table 2).

S2. Experimental

1 mmol of methyl pyrimidine-2-carboxylate and ca 2 mmol s of lithium hydroxide dissolved in 50 ml of hot, doubly distilled water were boiled under reflux with stirring for twenty hours. After evaporation to dryness at room temperature the polycrystalline material was dissolved in 50 ml of water. The solution was titrated with 1 N HCl until the pH reached 6.0 and then stirred for 3 h at ca 320 K. Left to crystallize at room temperature, colourless single-crystal blocks deposited after a week. They were washed with cold methanol and dried in the air.

S3. Refinement

Hydrogen atoms belonging to water molecules were located in a difference map and refined isotropically, while three H atoms attached to pyrimidine C atoms were located at calculated positions and treated as riding on the parent atoms with

C—H=0.93 Å and $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$.

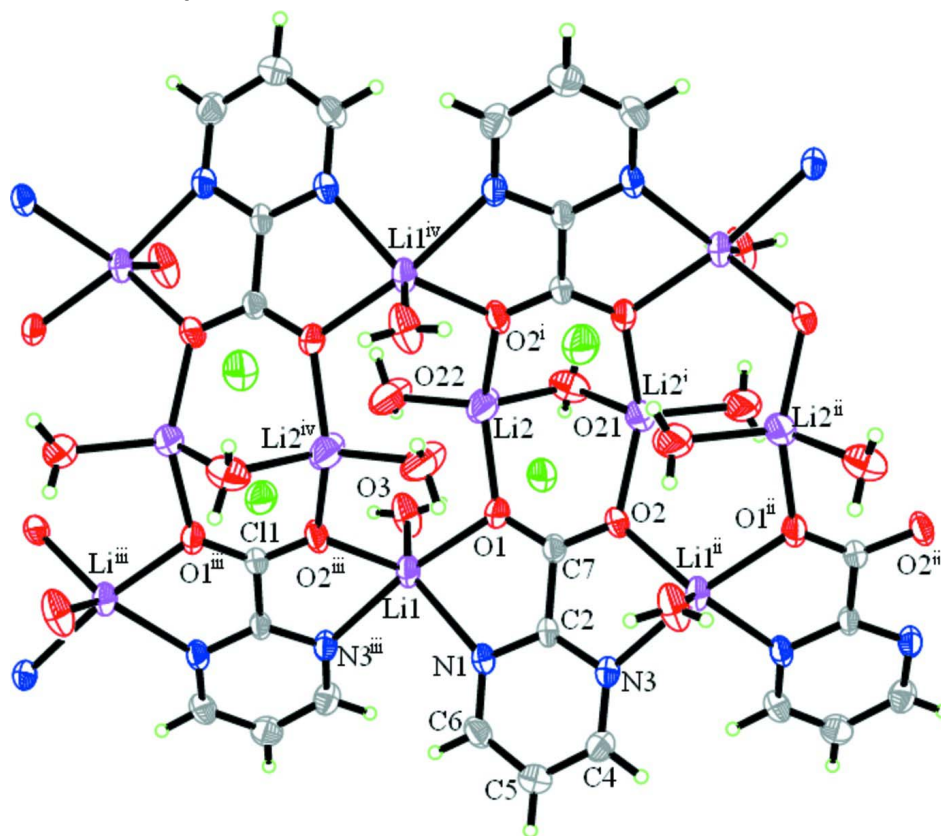
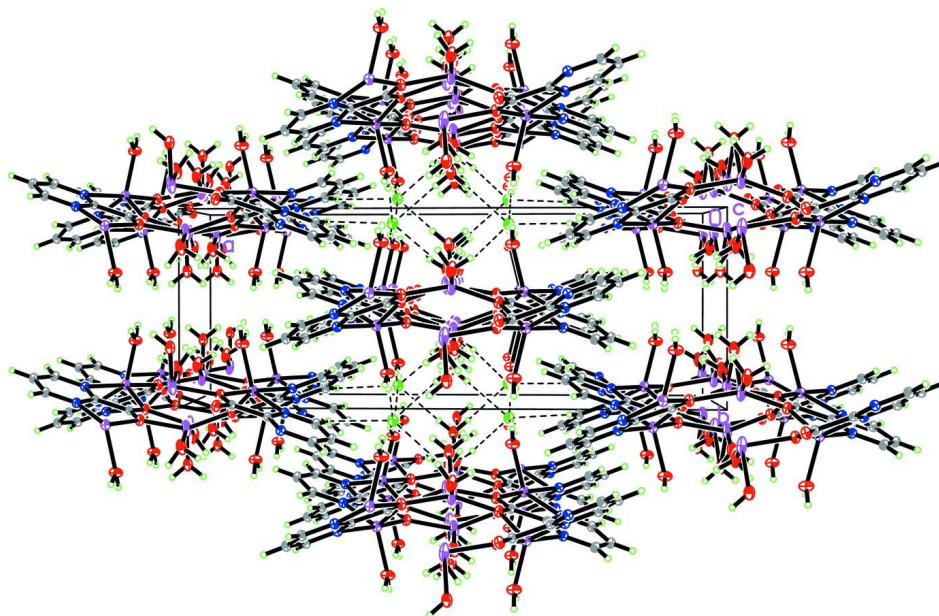


Figure 1

A fragment of a cationic ribbon of the title compound with atom labelling scheme and 50% probability displacement ellipsoids. Symmetry code: ⁱ $-x, y, -z + 1/2$; ⁱⁱ $x, -y + 2, z - 1/2$; ⁱⁱⁱ $x, -y + 2, z + 1/2$; ^{iv} $-x, -y + 2, z + 1$.

**Figure 2**

The alignment of cationic ribbons and chloride anions in the structure of the title compound viewed along the unit cell *b* direction.

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Crystal data

[Li₄(C₅H₃N₂O₂)₂(H₂O)₅]Cl₂

M_r = 434.93

Monoclinic, *C2/c*

Hall symbol: -C 2yc

a = 22.084 (4) Å

b = 8.0773 (16) Å

c = 10.814 (2) Å

β = 94.08 (3)°

V = 1924.1 (7) Å³

Z = 4

F(000) = 888

D_x = 1.501 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 6–15°

μ = 0.39 mm⁻¹

T = 293 K

Block, colourless

0.37 × 0.24 × 0.18 mm

Data collection

Kuma KM4 four-circle
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

profile data from $\omega/2\theta$ scans

Absorption correction: analytical

(*CrysAlis RED*; Oxford Diffraction, 2008)

T_{min} = 0.917, *T_{max}* = 0.935

2964 measured reflections

2819 independent reflections

1781 reflections with *I* > 2 σ (*I*)

R_{int} = 0.029

θ_{\max} = 30.1°, θ_{\min} = 1.9°

h = -31→31

k = -11→0

l = 0→15

3 standard reflections every 200 reflections

intensity decay: 2.3%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.147$
 $S = 1.02$
 2819 reflections
 152 parameters
 4 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0879P)^2 + 1.2478P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.51 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$

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.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.08301 (6)	0.92604 (19)	0.37614 (11)	0.0321 (3)
O2	0.08768 (6)	0.96441 (19)	0.17202 (11)	0.0319 (3)
N3	0.20103 (7)	1.0854 (2)	0.20733 (13)	0.0277 (3)
N1	0.19897 (7)	1.0170 (2)	0.42115 (13)	0.0277 (3)
C6	0.25599 (9)	1.0720 (3)	0.43984 (17)	0.0326 (4)
H6	0.2752	1.0657	0.5191	0.039*
C2	0.17410 (7)	1.0274 (2)	0.30494 (14)	0.0232 (3)
C4	0.25768 (9)	1.1411 (3)	0.22901 (18)	0.0332 (4)
H4	0.2778	1.1836	0.1634	0.040*
C5	0.28729 (9)	1.1378 (3)	0.3457 (2)	0.0353 (4)
H5	0.3266	1.1781	0.3601	0.042*
Li1	0.13426 (15)	0.9162 (5)	0.5437 (3)	0.0323 (7)
O3	0.11355 (9)	0.6795 (2)	0.56747 (16)	0.0469 (4)
C7	0.10916 (8)	0.9673 (2)	0.28238 (14)	0.0239 (3)
O21	0.0000	0.6868 (4)	0.2500	0.0527 (6)
Li2	-0.00573 (17)	0.8841 (8)	0.3807 (4)	0.0590 (13)
Cl1	0.10829 (3)	0.57231 (8)	0.84542 (5)	0.04391 (17)
H211	-0.0286 (13)	0.622 (4)	0.230 (3)	0.064 (10)*
H32	0.1130 (18)	0.599 (5)	0.515 (4)	0.086 (12)*
H31	0.1170 (14)	0.627 (4)	0.634 (3)	0.065 (9)*
O22	-0.00669 (8)	0.8066 (3)	0.54795 (18)	0.0618 (6)
H221	-0.0386 (10)	0.754 (4)	0.570 (3)	0.075 (10)*
H222	0.0166 (14)	0.717 (4)	0.555 (3)	0.120 (17)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0302 (6)	0.0478 (8)	0.0185 (6)	-0.0032 (6)	0.0031 (5)	0.0039 (5)
O2	0.0313 (6)	0.0472 (8)	0.0164 (5)	-0.0051 (6)	-0.0040 (4)	0.0036 (5)
N3	0.0316 (7)	0.0335 (8)	0.0181 (6)	-0.0022 (6)	0.0028 (5)	0.0009 (6)
N1	0.0312 (7)	0.0352 (8)	0.0165 (6)	-0.0006 (6)	-0.0012 (5)	0.0012 (6)
C6	0.0330 (8)	0.0390 (10)	0.0245 (8)	-0.0006 (8)	-0.0062 (6)	-0.0016 (7)
C2	0.0291 (8)	0.0258 (8)	0.0148 (6)	0.0024 (6)	0.0012 (5)	0.0000 (6)
C4	0.0354 (9)	0.0361 (10)	0.0289 (9)	-0.0051 (8)	0.0075 (7)	0.0008 (7)
C5	0.0289 (9)	0.0392 (10)	0.0373 (10)	-0.0036 (8)	-0.0006 (7)	-0.0014 (8)
Li1	0.0376 (16)	0.0420 (18)	0.0173 (13)	0.0004 (14)	0.0020 (11)	-0.0006 (12)
O3	0.0754 (12)	0.0358 (8)	0.0277 (7)	0.0017 (8)	-0.0090 (7)	0.0005 (7)
C7	0.0258 (7)	0.0285 (8)	0.0171 (7)	0.0017 (6)	0.0006 (5)	0.0009 (6)
O21	0.0337 (11)	0.0675 (17)	0.0551 (15)	0.000	-0.0086 (10)	0.000
Li2	0.0301 (17)	0.116 (4)	0.0305 (18)	0.009 (2)	0.0030 (14)	0.018 (2)
Cl1	0.0420 (3)	0.0553 (3)	0.0345 (3)	-0.0001 (2)	0.00346 (19)	0.0087 (2)
O22	0.0349 (8)	0.0967 (16)	0.0550 (11)	0.0101 (10)	0.0123 (7)	0.0338 (11)

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

O1—C7	1.247 (2)	Li1—N3 ⁱⁱⁱ	2.221 (4)
Li1—O1	2.069 (3)	Li1—Li2 ^{iv}	3.414 (6)
O2—C7	1.2528 (19)	O3—H32	0.86 (4)
O2—Li2 ⁱ	1.968 (4)	O3—H31	0.83 (4)
O2—Li1 ⁱⁱ	2.029 (4)	Li2—O21	2.140 (6)
N3—C2	1.333 (2)	O21—Li2 ⁱ	2.140 (6)
N3—C4	1.335 (2)	O21—H211	0.84 (3)
N3—Li1 ⁱⁱ	2.221 (4)	Li2—O22	1.915 (4)
N1—C6	1.337 (2)	Li2—O2 ⁱ	1.968 (4)
N1—C2	1.338 (2)	Li2—O1	1.993 (4)
Li1—N1	2.175 (4)	Li2—O22 ^{iv}	2.623 (7)
C6—C5	1.377 (3)	Li2—Li2 ⁱ	2.856 (8)
C6—H6	0.9300	Li2—Li2 ^{iv}	3.183 (11)
C2—C7	1.517 (2)	Li2—Li1 ^{iv}	3.414 (6)
C4—C5	1.379 (3)	Li2—H222	2.343 (18)
C4—H4	0.9300	O22—Li2 ^{iv}	2.623 (7)
C5—H5	0.9300	O22—H221	0.868 (18)
Li1—O3	1.987 (4)	O22—H222	0.891 (18)
Li1—O2 ⁱⁱⁱ	2.029 (4)		
C7—O1—Li2	125.36 (16)	Li2—O21—Li2 ⁱ	83.7 (3)
C7—O1—Li1	117.79 (15)	Li2—O21—H211	124 (2)
Li2—O1—Li1	116.70 (16)	Li2 ⁱ —O21—H211	112 (2)
C7—O2—Li2 ⁱ	124.07 (17)	O22—Li2—O2 ⁱ	108.02 (19)
C7—O2—Li1 ⁱⁱ	117.82 (15)	O22—Li2—O1	98.98 (19)
Li2 ⁱ —O2—Li1 ⁱⁱ	117.32 (18)	O2 ⁱ —Li2—O1	145.3 (3)
C2—N3—C4	116.42 (15)	O22—Li2—O21	112.7 (3)

C2—N3—Li1 ⁱⁱ	108.69 (14)	O2 ⁱ —Li2—O21	98.6 (2)
C4—N3—Li1 ⁱⁱ	134.65 (15)	O1—Li2—O21	90.32 (18)
C6—N1—C2	116.14 (15)	O22—Li2—O22 ^{iv}	92.4 (2)
C6—N1—Li1	133.22 (14)	O2 ⁱ —Li2—O22 ^{iv}	81.1 (2)
C2—N1—Li1	110.62 (14)	O1—Li2—O22 ^{iv}	76.29 (19)
N1—C6—C5	122.22 (17)	O21—Li2—O22 ^{iv}	153.3 (2)
N1—C6—H6	118.9	O22—Li2—Li2 ⁱ	160.4 (2)
C5—C6—H6	118.9	O2 ⁱ —Li2—Li2 ⁱ	81.81 (19)
N3—C2—N1	126.11 (16)	O1—Li2—Li2 ⁱ	79.56 (18)
N3—C2—C7	117.06 (14)	O21—Li2—Li2 ⁱ	48.13 (14)
N1—C2—C7	116.82 (15)	O22 ^{iv} —Li2—Li2 ⁱ	106.04 (10)
N3—C4—C5	122.10 (17)	O22—Li2—Li2 ^{iv}	55.42 (15)
N3—C4—H4	119.0	O2 ⁱ —Li2—Li2 ^{iv}	93.4 (2)
C5—C4—H4	119.0	O1—Li2—Li2 ^{iv}	84.2 (2)
C6—C5—C4	116.98 (18)	O21—Li2—Li2 ^{iv}	165.6 (3)
C6—C5—H5	121.5	O22 ^{iv} —Li2—Li2 ^{iv}	36.95 (15)
C4—C5—H5	121.5	Li2 ⁱ —Li2—Li2 ^{iv}	142.6 (2)
O3—Li1—O2 ⁱⁱⁱ	103.68 (16)	O22—Li2—Li1 ^{iv}	82.13 (16)
O3—Li1—O1	91.92 (15)	O2 ⁱ —Li2—Li1 ^{iv}	31.87 (10)
O2 ⁱⁱⁱ —Li1—O1	107.96 (16)	O1—Li2—Li1 ^{iv}	139.6 (3)
O3—Li1—N1	127.32 (18)	O21—Li2—Li1 ^{iv}	126.81 (17)
O2 ⁱⁱⁱ —Li1—N1	128.74 (19)	O22 ^{iv} —Li2—Li1 ^{iv}	63.32 (13)
O1—Li1—N1	78.11 (12)	Li2 ⁱ —Li2—Li1 ^{iv}	111.75 (17)
O3—Li1—N3 ⁱⁱⁱ	92.14 (15)	Li2 ^{iv} —Li2—Li1 ^{iv}	63.10 (15)
O2 ⁱⁱⁱ —Li1—N3 ⁱⁱⁱ	78.36 (12)	O22—Li2—H222	21.2 (6)
O1—Li1—N3 ⁱⁱⁱ	171.42 (18)	O2 ⁱ —Li2—H222	124.0 (7)
N1—Li1—N3 ⁱⁱⁱ	93.42 (14)	O1—Li2—H222	88.1 (8)
O3—Li1—Li2 ^{iv}	102.75 (17)	O21—Li2—H222	94.7 (9)
O2 ⁱⁱⁱ —Li1—Li2 ^{iv}	30.81 (10)	O22 ^{iv} —Li2—H222	107.6 (10)
O1—Li1—Li2 ^{iv}	77.24 (13)	Li2 ⁱ —Li2—H222	140.1 (7)
N1—Li1—Li2 ^{iv}	124.23 (17)	Li2 ^{iv} —Li2—H222	71.8 (9)
N3 ⁱⁱⁱ —Li1—Li2 ^{iv}	109.16 (14)	Li1 ^{iv} —Li2—H222	102.2 (6)
Li1—O3—H32	129 (3)	Li2—O22—Li2 ^{iv}	87.6 (2)
Li1—O3—H31	126 (2)	Li2—O22—H221	119 (2)
H32—O3—H31	101 (3)	Li2 ^{iv} —O22—H221	117 (2)
O1—C7—O2	127.12 (16)	Li2—O22—H222	107.6 (17)
O1—C7—C2	116.22 (14)	Li2 ^{iv} —O22—H222	135 (3)
O2—C7—C2	116.65 (15)	H221—O22—H222	93 (2)

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $x, -y+2, z-1/2$; (iii) $x, -y+2, z+1/2$; (iv) $-x, -y+2, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O22—H222 \cdots O3	0.89 (2)	2.16 (3)	2.841 (3)	133 (3)
O22—H221 \cdots C11 ^v	0.87 (2)	2.36 (2)	3.212 (2)	167 (3)
O3—H31 \cdots C11	0.83 (4)	2.35 (4)	3.1381 (19)	158 (3)

O3—H32...C11 ^{vi}	0.86 (4)	2.29 (4)	3.1429 (19)	168 (4)
O21—H211...C11 ^{vii}	0.84 (3)	2.45 (3)	3.288 (2)	175 (3)

Symmetry codes: (v) $-x, y, -z+3/2$; (vi) $x, -y+1, z-1/2$; (vii) $-x, -y+1, -z+1$.