

Dilithium 1,2,5-thiadiazolidine-3,4-dione 1,1-dioxide dihydrate

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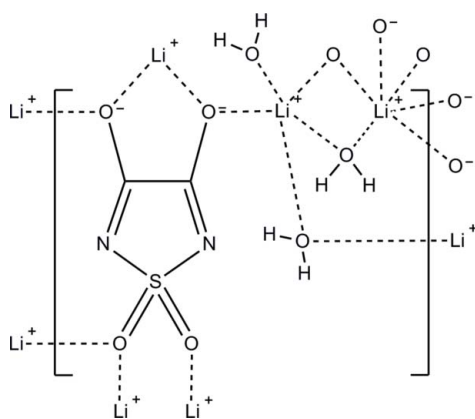
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Key indicators: single-crystal X-ray study; $T = 110$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.022; wR factor = 0.065; data-to-parameter ratio = 29.1.

The title compound, poly[μ -aqua-aqua- μ_6 -(1,1-dioxo-1 λ^6 ,2,5-thiadiazolidine-3,4-diolato)-dilithium], $[\text{Li}_2(\text{C}_2\text{N}_2\text{O}_4\text{S})(\text{H}_2\text{O})_2]_n$ or $(\text{H}_2\text{O})_2\text{Li}_2\text{TDD}$, forms an infinite three-dimensional structure containing five-coordinate (Li/5) and six-coordinate (Li/6) Li^+ cations. Li/5 is coordinated by three water molecules, one carbonyl O atom and one sulfuryl O atom while Li/6 is coordinated by one water molecule, three carbonyl O atoms, and two sulfuryl O atoms. Each water molecule bridges two Li^+ cations, while also hydrogen bonding to either one endocyclic N atom and one sulfuryl O atom or two endocyclic N atoms. While the endocyclic N atoms in the anion do not coordinate the Li^+ cations, the carbonyl and sulfuryl groups each coordinate three Li^+ cations, which gives rise to the infinite three-dimensional structure.

Related literature

For Na salt synthesis, see: Lee & Kohn (1990). For Na salt, K salt, and acid form synthesis, see: Wen *et al.* (1975).



Experimental

Crystal data

$[\text{Li}_2(\text{C}_2\text{N}_2\text{O}_4\text{S})(\text{H}_2\text{O})_2]$
 $M_r = 198.01$
 Monoclinic, $P2_1/c$
 $a = 7.239$ (3) Å
 $b = 11.185$ (3) Å
 $c = 9.786$ (4) Å
 $\beta = 124.27$ (2)°
 $V = 654.8$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.49$ mm⁻¹
 $T = 110$ K
 $0.41 \times 0.24 \times 0.24$ mm

Data collection

Bruker–Nonius Kappa X8 APEXII diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.825$, $T_{\max} = 0.894$
 34710 measured reflections
 3899 independent reflections
 3575 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.065$
 $S = 1.06$
 3899 reflections
 134 parameters
 All H-atom parameters refined
 $\Delta\rho_{\max} = 0.62$ e Å⁻³
 $\Delta\rho_{\min} = -0.40$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1WA}\cdots\text{N2}^{\text{i}}$	0.791 (16)	2.155 (16)	2.9428 (14)	175 (2)
$\text{O1W}-\text{H1WB}\cdots\text{O1}^{\text{ii}}$	0.842 (17)	2.29 (2)	2.9971 (15)	142 (2)
$\text{O2W}-\text{H2WA}\cdots\text{N2}^{\text{iii}}$	0.823 (16)	2.049 (16)	2.8712 (14)	175.7 (16)
$\text{O2W}-\text{H2WB}\cdots\text{N1}^{\text{iv}}$	0.79 (2)	2.01 (2)	2.7947 (14)	168.7 (17)

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2080).

References

- Bruker (2009). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Lee, C.-H. & Kohn, H. (1990). *J. Am. Chem. Soc.* **55**, 6098–6104.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Wen, R., Komin, A., Street, R. & Carmack, M. (1975). *J. Org. Chem.* **40**, 2743–2748.

supporting information

Acta Cryst. (2012). E68, m1228 [doi:10.1107/S1600536812036379]

Dilithium 1,2,5-thiadiazolidine-3,4-dione 1,1-dioxide dihydrate

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S1. Comment

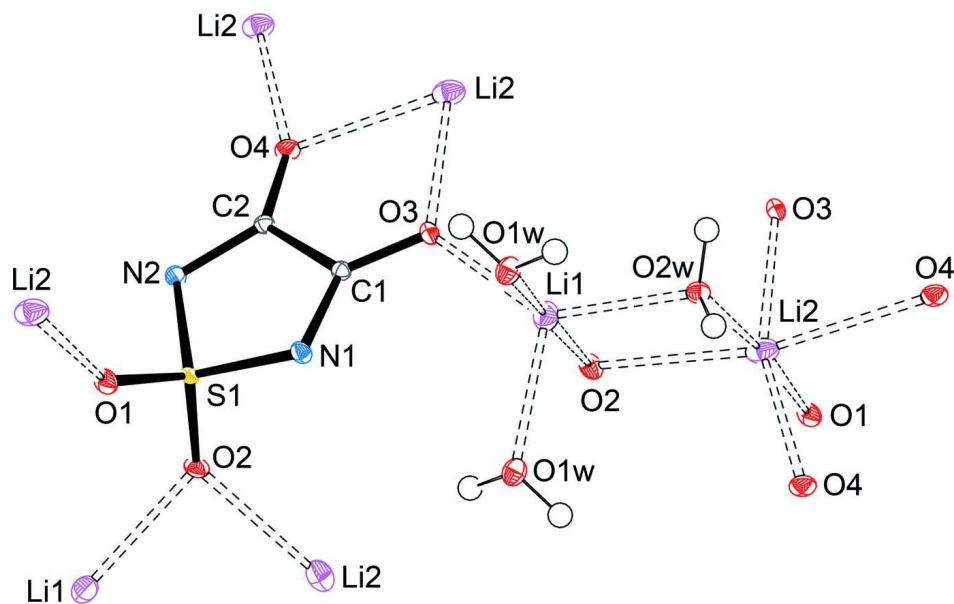
Dilithium 1,2,5-thiadiazolidine-3,4-dione 1,1-dioxide (Li₂TDD) was synthesized following methods reported in the literature for the anion (Lee *et al.*, Wen *et al.*). The salt forms a dihydrate in which the carbonyl and sulfonyl oxygen atoms each coordinate multiple Li⁺ cations forming a highly aggregated structure. In addition, each water molecule bridges two Li⁺ cations. The endocyclic nitrogen atoms, however, are not coordinated to the Li⁺ cations, indicating that the O atoms exhibit the greatest Lewis basicity.

S2. Experimental

Sulfamide (1.00 eq.) was dissolved in methanol and slowly added to a solution of LiMeO (2.10 eq.) at room temperature, resulting in a cloudy white solution. After addition of diethyl oxalate (1.05 eq.), the solution became clear. After gently refluxing for 20 h, the solvent was removed under vacuum and a clear viscous solution was obtained. Upon addition of deionized water, crystals suitable for characterization formed.

S3. Refinement

The structure was solved by direct methods using the XS program. All non-hydrogen atoms were obtained from the initial solution. The hydrogen atoms were introduced at idealized positions and were allowed to refine isotropically. The structural model was fit to the data using full matrix least-squares based on F². The calculated structure factors included corrections for anomalous dispersion from the usual tabulation. The structure was refined using the XL program from *SHELXTL*, graphic plots were produced using the *ORTEP-3* crystallographic program suite.

**Figure 1**

Asymmetric unit of the Li_2TDD dihydrate crystal structure. Thermal ellipsoids are at 50% probability (Li-purple, O-red, S-yellow, N-blue).

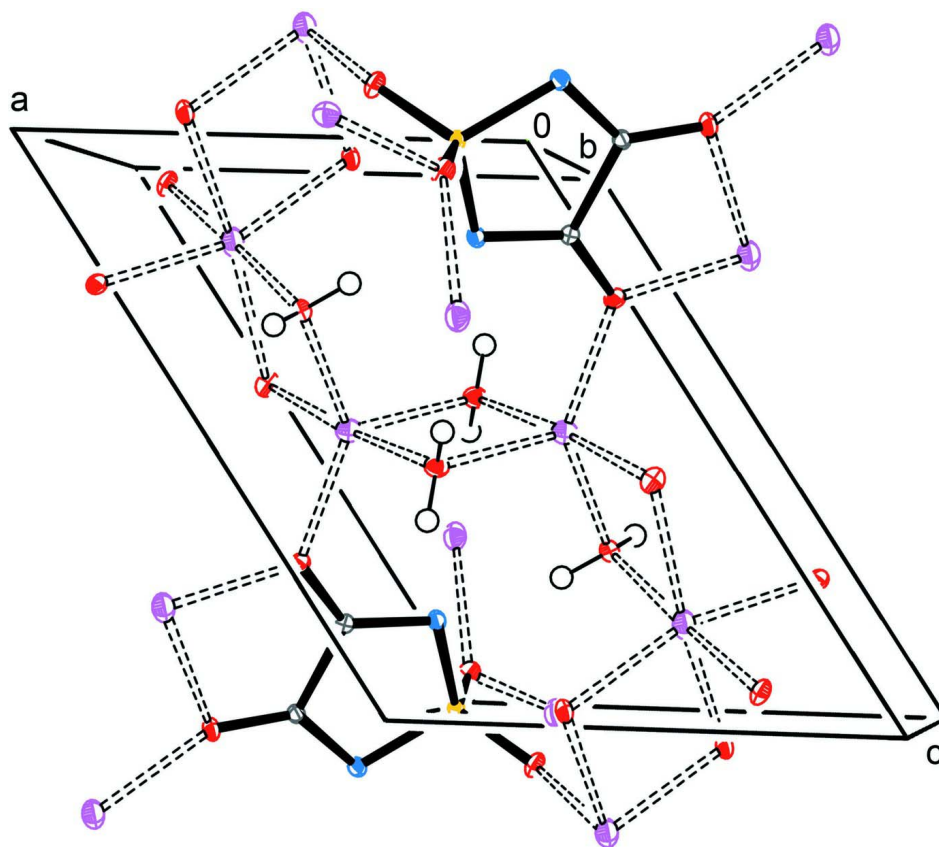


Figure 2

Packing diagram for the Li₂TDD dihydrate crystal structure (Li-purple, O-red, S-yellow, N-blue).

Poly[μ -aqua-aqua- μ_6 -(1,1-dioxo-1 λ^6 ,2,5-thiadiazolidine-3,4-diolato)- dilithium]

Crystal data

[Li₂(C₂N₂O₄S)(H₂O₂)]

$M_r = 198.01$

Monoclinic, $P2_1/c$

$a = 7.239$ (3) Å

$b = 11.185$ (3) Å

$c = 9.786$ (4) Å

$\beta = 124.27$ (2)°

$V = 654.8$ (4) Å³

$Z = 4$

$F(000) = 400$

$D_x = 2.008$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9851 reflections

$\theta = 3.1$ – 42.4 °

$\mu = 0.49$ mm⁻¹

$T = 110$ K

Prism, colourless

$0.41 \times 0.24 \times 0.24$ mm

Data collection

Bruker–Nonius Kappa X8 APEXII
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and ϕ scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.825$, $T_{\max} = 0.894$

34710 measured reflections

3899 independent reflections

3575 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 42.7$ °, $\theta_{\min} = 3.1$ °

$h = -13 \rightarrow 12$

$k = -18 \rightarrow 19$

$l = -16 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.065$

$S = 1.06$

3899 reflections

134 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.1822P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.62$ e Å⁻³

$\Delta\rho_{\min} = -0.40$ e Å⁻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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Li1	0.7137 (2)	0.01566 (12)	0.50356 (15)	0.0135 (2)
Li2	0.7135 (2)	0.05125 (12)	0.18236 (17)	0.0149 (2)

S1	0.89112 (2)	0.223295 (11)	0.983764 (16)	0.00633 (4)
O1	0.79819 (8)	0.19195 (4)	1.07658 (6)	0.01045 (7)
O2	0.84435 (8)	0.34610 (4)	0.92528 (6)	0.01025 (7)
N1	0.79993 (8)	0.13338 (4)	0.82836 (6)	0.00815 (8)
N2	1.16044 (8)	0.19981 (5)	1.09118 (6)	0.00814 (7)
C1	0.97800 (9)	0.08981 (5)	0.83782 (7)	0.00681 (8)
C2	1.19895 (9)	0.12853 (5)	0.99882 (7)	0.00704 (8)
O3	0.97919 (7)	0.02518 (4)	0.73492 (5)	0.00883 (7)
O4	1.38036 (7)	0.09387 (4)	1.02912 (6)	0.01080 (8)
O1W	0.56092 (8)	-0.12147 (4)	0.56167 (6)	0.01060 (7)
H1WA	0.642 (3)	-0.1436 (15)	0.654 (2)	0.038 (4)*
H1WB	0.497 (3)	-0.1828 (15)	0.504 (2)	0.037 (4)*
O2W	0.64205 (7)	-0.06718 (4)	0.30255 (6)	0.00860 (7)
H2WA	0.702 (2)	-0.1334 (14)	0.3304 (18)	0.030 (3)*
H2WB	0.512 (3)	-0.0804 (14)	0.2543 (19)	0.032 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Li1	0.0127 (5)	0.0155 (5)	0.0110 (5)	-0.0009 (4)	0.0059 (4)	-0.0018 (4)
Li2	0.0120 (5)	0.0169 (5)	0.0176 (5)	0.0033 (4)	0.0094 (5)	0.0054 (4)
S1	0.00648 (6)	0.00602 (6)	0.00737 (6)	0.00044 (3)	0.00444 (5)	-0.00002 (3)
O1	0.01270 (18)	0.01092 (17)	0.01269 (18)	0.00098 (14)	0.01016 (16)	0.00139 (13)
O2	0.01357 (18)	0.00648 (15)	0.01303 (18)	0.00244 (13)	0.00890 (16)	0.00195 (13)
N1	0.00613 (17)	0.00947 (17)	0.00851 (17)	-0.00019 (13)	0.00391 (15)	-0.00189 (14)
N2	0.00659 (17)	0.00924 (17)	0.00772 (17)	-0.00007 (14)	0.00350 (15)	-0.00125 (14)
C1	0.00696 (19)	0.00660 (18)	0.00715 (18)	0.00008 (14)	0.00413 (16)	0.00011 (14)
C2	0.00620 (18)	0.00760 (18)	0.00714 (18)	0.00043 (14)	0.00365 (16)	0.00069 (14)
O3	0.00976 (17)	0.00902 (16)	0.00814 (16)	0.00060 (13)	0.00530 (14)	-0.00166 (12)
O4	0.00685 (16)	0.01436 (18)	0.01147 (17)	0.00300 (13)	0.00532 (15)	0.00209 (14)
O1W	0.01054 (17)	0.01104 (17)	0.00911 (17)	-0.00189 (13)	0.00487 (15)	-0.00023 (13)
O2W	0.00740 (16)	0.00840 (15)	0.00953 (16)	0.00014 (12)	0.00449 (14)	0.00025 (12)

Geometric parameters (Å, °)

Li1—O2W	1.9615 (15)	S1—N2	1.6331 (9)
Li1—O3	1.9825 (16)	O1—Li2 ^{vii}	2.1539 (14)
Li1—O1W ⁱ	2.0814 (16)	O2—Li1 ^{viii}	2.1650 (14)
Li1—O1W	2.1468 (15)	O2—Li2 ^{viii}	2.3088 (17)
Li1—O2 ⁱⁱ	2.1650 (14)	N1—C1	1.3317 (9)
Li1—Li1 ⁱ	3.076 (3)	N2—C2	1.3469 (8)
Li1—Li2	3.167 (2)	C1—O3	1.2435 (7)
Li1—H2WB	2.286 (16)	C1—C2	1.5460 (10)
Li2—O2W	2.0226 (14)	C2—O4	1.2346 (8)
Li2—O4 ⁱⁱⁱ	2.0539 (17)	O3—Li2 ^{iv}	2.0755 (16)
Li2—O3 ^{iv}	2.0755 (16)	O4—Li2 ^{ix}	2.0539 (17)
Li2—O1 ^v	2.1539 (14)	O4—Li2 ^{iv}	2.4075 (17)
Li2—O2 ⁱⁱ	2.3088 (17)	O1W—Li1 ⁱ	2.0814 (16)

Li2—O4 ^{iv}	2.4075 (17)	O1W—H1WA	0.792 (17)
Li2—Li2 ^{vi}	3.344 (3)	O1W—H1WB	0.840 (17)
S1—O1	1.4453 (6)	O2W—H2WA	0.824 (16)
S1—O2	1.4529 (6)	O2W—H2WB	0.794 (16)
S1—N1	1.6216 (7)		
O2W—Li1—O3	135.20 (8)	O1 ^v —Li2—Li1	136.68 (7)
O2W—Li1—O1W ⁱ	107.07 (7)	O2 ⁱⁱ —Li2—Li1	43.12 (4)
O3—Li1—O1W ⁱ	117.64 (7)	O4 ^{iv} —Li2—Li1	127.63 (6)
O2W—Li1—O1W	92.49 (6)	O2W—Li2—Li2 ^{vi}	90.62 (7)
O3—Li1—O1W	92.78 (6)	O4 ⁱⁱⁱ —Li2—Li2 ^{vi}	45.64 (4)
O1W ⁱ —Li1—O1W	86.66 (6)	O3 ^{iv} —Li2—Li2 ^{vi}	114.74 (8)
O2W—Li1—O2 ⁱⁱ	84.50 (6)	O1 ^v —Li2—Li2 ^{vi}	94.57 (7)
O3—Li1—O2 ⁱⁱ	91.73 (6)	O2 ⁱⁱ —Li2—Li2 ^{vi}	150.02 (7)
O1W ⁱ —Li1—O2 ⁱⁱ	91.01 (6)	O4 ^{iv} —Li2—Li2 ^{vi}	37.58 (4)
O1W—Li1—O2 ⁱⁱ	175.48 (7)	Li1—Li2—Li2 ^{vi}	119.99 (7)
O2W—Li1—Li1 ⁱ	103.23 (7)	O1—S1—O2	112.91 (3)
O3—Li1—Li1 ⁱ	110.35 (8)	O1—S1—N1	110.57 (4)
O1W ⁱ —Li1—Li1 ⁱ	44.16 (4)	O2—S1—N1	109.60 (4)
O1W—Li1—Li1 ⁱ	42.49 (4)	O1—S1—N2	111.47 (4)
O2 ⁱⁱ —Li1—Li1 ⁱ	135.04 (8)	O2—S1—N2	109.54 (3)
O2W—Li1—Li2	38.02 (4)	N1—S1—N2	102.23 (3)
O3—Li1—Li2	125.81 (7)	S1—O1—Li2 ^{vii}	146.99 (5)
O1W ⁱ —Li1—Li2	99.07 (6)	S1—O2—Li1 ^{viii}	125.95 (5)
O1W—Li1—Li2	129.81 (6)	S1—O2—Li2 ^{viii}	138.18 (4)
O2 ⁱⁱ —Li1—Li2	46.80 (4)	Li1 ^{viii} —O2—Li2 ^{viii}	90.08 (5)
Li1 ⁱ —Li1—Li2	123.61 (7)	C1—N1—S1	107.15 (5)
O2W—Li1—H2WB	19.7 (4)	C2—N2—S1	106.65 (5)
O3—Li1—H2WB	150.4 (4)	O3—C1—N1	127.18 (6)
O1W ⁱ —Li1—H2WB	90.8 (4)	O3—C1—C2	120.88 (5)
O1W—Li1—H2WB	80.3 (4)	N1—C1—C2	111.95 (5)
O2 ⁱⁱ —Li1—H2WB	95.9 (4)	O4—C2—N2	128.23 (6)
Li1 ⁱ —Li1—H2WB	83.8 (4)	O4—C2—C1	120.46 (6)
Li2—Li1—H2WB	50.0 (4)	N2—C2—C1	111.31 (5)
O2W—Li2—O4 ⁱⁱⁱ	89.83 (6)	C1—O3—Li1	120.78 (6)
O2W—Li2—O3 ^{iv}	94.15 (6)	C1—O3—Li2 ^{iv}	114.73 (6)
O4 ⁱⁱⁱ —Li2—O3 ^{iv}	160.11 (8)	Li1—O3—Li2 ^{iv}	124.06 (6)
O2W—Li2—O1 ^v	173.35 (8)	C2—O4—Li2 ^{ix}	154.29 (6)
O4 ⁱⁱⁱ —Li2—O1 ^v	90.83 (6)	C2—O4—Li2 ^{iv}	104.96 (5)
O3 ^{iv} —Li2—O1 ^v	87.46 (5)	Li2 ^{ix} —O4—Li2 ^{iv}	96.78 (6)
O2W—Li2—O2 ⁱⁱ	79.51 (6)	Li1 ⁱ —O1W—Li1	93.34 (6)
O4 ⁱⁱⁱ —Li2—O2 ⁱⁱ	105.58 (6)	Li1 ⁱ —O1W—H1WA	119.4 (12)
O3 ^{iv} —Li2—O2 ⁱⁱ	94.31 (6)	Li1—O1W—H1WA	111.6 (12)
O1 ^v —Li2—O2 ⁱⁱ	93.94 (6)	Li1 ⁱ —O1W—H1WB	100.8 (11)
O2W—Li2—O4 ^{iv}	91.01 (6)	Li1—O1W—H1WB	125.3 (11)
O4 ⁱⁱⁱ —Li2—O4 ^{iv}	83.22 (6)	H1WA—O1W—H1WB	106.4 (16)
O3 ^{iv} —Li2—O4 ^{iv}	77.24 (5)	Li1—O2W—Li2	105.30 (7)
O1 ^v —Li2—O4 ^{iv}	95.64 (6)	Li1—O2W—H2WA	107.5 (10)

O2 ⁱⁱ —Li2—O4 ^{iv}	166.89 (6)	Li2—O2W—H2WA	121.4 (10)
O2W—Li2—Li1	36.68 (4)	Li1—O2W—H2WB	103.9 (11)
O4 ⁱⁱⁱ —Li2—Li1	95.63 (6)	Li2—O2W—H2WB	112.5 (11)
O3 ^{iv} —Li2—Li1	99.19 (6)	H2WA—O2W—H2WB	104.9 (15)
O3—Li1—Li2—O2W	119.85 (9)	O2—S1—N1—C1	107.86 (4)
O1W ⁱ —Li1—Li2—O2W	-106.16 (7)	N2—S1—N1—C1	-8.27 (4)
O1W—Li1—Li2—O2W	-12.94 (6)	O1—S1—N2—C2	125.58 (5)
O2 ⁱⁱ —Li1—Li2—O2W	171.05 (8)	O2—S1—N2—C2	-108.72 (5)
Li1 ⁱ —Li1—Li2—O2W	-66.17 (8)	N1—S1—N2—C2	7.45 (4)
O2W—Li1—Li2—O4 ⁱⁱⁱ	82.11 (7)	S1—N1—C1—O3	-173.88 (5)
O3—Li1—Li2—O4 ⁱⁱⁱ	-158.04 (7)	S1—N1—C1—C2	6.29 (5)
O1W ⁱ —Li1—Li2—O4 ⁱⁱⁱ	-24.05 (6)	S1—N2—C2—O4	175.91 (5)
O1W—Li1—Li2—O4 ⁱⁱⁱ	69.17 (9)	S1—N2—C2—C1	-4.32 (5)
O2 ⁱⁱ —Li1—Li2—O4 ⁱⁱⁱ	-106.84 (7)	O3—C1—C2—O4	-1.36 (8)
Li1 ⁱ —Li1—Li2—O4 ⁱⁱⁱ	15.94 (10)	N1—C1—C2—O4	178.47 (5)
O2W—Li1—Li2—O3 ^{iv}	-84.58 (7)	O3—C1—C2—N2	178.85 (5)
O3—Li1—Li2—O3 ^{iv}	35.28 (9)	N1—C1—C2—N2	-1.32 (6)
O1W ⁱ —Li1—Li2—O3 ^{iv}	169.26 (6)	N1—C1—O3—Li1	19.12 (9)
O1W—Li1—Li2—O3 ^{iv}	-97.52 (9)	C2—C1—O3—Li1	-161.08 (6)
O2 ⁱⁱ —Li1—Li2—O3 ^{iv}	86.47 (6)	N1—C1—O3—Li2 ^{iv}	-168.10 (6)
Li1 ⁱ —Li1—Li2—O3 ^{iv}	-150.75 (8)	C2—C1—O3—Li2 ^{iv}	11.71 (7)
O2W—Li1—Li2—O1 ^v	179.33 (11)	O2W—Li1—O3—C1	177.90 (8)
O3—Li1—Li2—O1 ^v	-60.82 (12)	O1W ⁱ —Li1—O3—C1	1.93 (10)
O1W ⁱ —Li1—Li2—O1 ^v	73.17 (10)	O1W—Li1—O3—C1	-85.75 (7)
O1W—Li1—Li2—O1 ^v	166.39 (7)	O2 ⁱⁱ —Li1—O3—C1	93.97 (6)
O2 ⁱⁱ —Li1—Li2—O1 ^v	-9.62 (8)	Li1 ⁱ —Li1—O3—C1	-46.05 (10)
Li1 ⁱ —Li1—Li2—O1 ^v	113.16 (10)	Li2—Li1—O3—C1	128.60 (7)
O2W—Li1—Li2—O2 ⁱⁱ	-171.05 (8)	O2W—Li1—O3—Li2 ^{iv}	5.82 (13)
O3—Li1—Li2—O2 ⁱⁱ	-51.20 (7)	O1W ⁱ —Li1—O3—Li2 ^{iv}	-170.16 (6)
O1W ⁱ —Li1—Li2—O2 ⁱⁱ	82.79 (6)	O1W—Li1—O3—Li2 ^{iv}	102.16 (7)
O1W—Li1—Li2—O2 ⁱⁱ	176.01 (9)	O2 ⁱⁱ —Li1—O3—Li2 ^{iv}	-78.11 (7)
Li1 ⁱ —Li1—Li2—O2 ⁱⁱ	122.78 (10)	Li1 ⁱ —Li1—O3—Li2 ^{iv}	141.87 (7)
O2W—Li1—Li2—O4 ^{iv}	-3.65 (6)	Li2—Li1—O3—Li2 ^{iv}	-43.48 (11)
O3—Li1—Li2—O4 ^{iv}	116.20 (8)	N2—C2—O4—Li2 ^{ix}	25.13 (16)
O1W ⁱ —Li1—Li2—O4 ^{iv}	-109.82 (7)	C1—C2—O4—Li2 ^{ix}	-154.62 (11)
O1W—Li1—Li2—O4 ^{iv}	-16.60 (11)	N2—C2—O4—Li2 ^{iv}	171.92 (6)
O2 ⁱⁱ —Li1—Li2—O4 ^{iv}	167.39 (8)	C1—C2—O4—Li2 ^{iv}	-7.83 (7)
Li1 ⁱ —Li1—Li2—O4 ^{iv}	-69.83 (10)	O2W—Li1—O1W—Li1 ⁱ	-106.96 (7)
O2W—Li1—Li2—Li2 ^{vi}	41.08 (7)	O3—Li1—O1W—Li1 ⁱ	117.54 (7)
O3—Li1—Li2—Li2 ^{vi}	160.93 (7)	O1W ⁱ —Li1—O1W—Li1 ⁱ	0.0
O1W ⁱ —Li1—Li2—Li2 ^{vi}	-65.09 (9)	O2 ⁱⁱ —Li1—O1W—Li1 ⁱ	-58.9 (9)
O1W—Li1—Li2—Li2 ^{vi}	28.13 (11)	Li2—Li1—O1W—Li1 ⁱ	-99.03 (8)
O2 ⁱⁱ —Li1—Li2—Li2 ^{vi}	-147.88 (9)	O3—Li1—O2W—Li2	-93.45 (11)
Li1 ⁱ —Li1—Li2—Li2 ^{vi}	-25.09 (12)	O1W ⁱ —Li1—O2W—Li2	82.82 (7)
O2—S1—O1—Li2 ^{vii}	166.26 (8)	O1W—Li1—O2W—Li2	170.08 (5)
N1—S1—O1—Li2 ^{vii}	43.06 (9)	O2 ⁱⁱ —Li1—O2W—Li2	-6.54 (6)
N2—S1—O1—Li2 ^{vii}	-69.93 (9)	Li1 ⁱ —Li1—O2W—Li2	128.50 (7)

O1—S1—O2—Li1 ^{viii}	12.38 (6)	O4 ⁱⁱⁱ —Li2—O2W—Li1	-99.68 (6)
N1—S1—O2—Li1 ^{viii}	136.11 (6)	O3 ^{iv} —Li2—O2W—Li1	99.83 (7)
N2—S1—O2—Li1 ^{viii}	-112.48 (6)	O1 ^v —Li2—O2W—Li1	-4.0 (6)
O1—S1—O2—Li2 ^{viii}	-132.04 (7)	O2 ⁱⁱ —Li2—O2W—Li1	6.21 (6)
N1—S1—O2—Li2 ^{viii}	-8.31 (7)	O4 ^{iv} —Li2—O2W—Li1	177.11 (5)
N2—S1—O2—Li2 ^{viii}	103.09 (7)	Li2 ^{vi} —Li2—O2W—Li1	-145.31 (6)
O1—S1—N1—C1	-127.04 (4)		

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

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1 <i>W</i> —H1 <i>WA</i> \cdots N2 ^x	0.791 (16)	2.155 (16)	2.9428 (14)	175 (2)
O1 <i>W</i> —H1 <i>WB</i> \cdots O1 ^{xi}	0.842 (17)	2.29 (2)	2.9971 (15)	142 (2)
O2 <i>W</i> —H2 <i>WA</i> \cdots N2 ^{xii}	0.823 (16)	2.049 (16)	2.8712 (14)	175.7 (16)
O2 <i>W</i> —H2 <i>WB</i> \cdots N1 ⁱ	0.79 (2)	2.01 (2)	2.7947 (14)	168.7 (17)

Symmetry codes: (i) $-x+1, -y, -z+1$; (x) $-x+2, -y, -z+2$; (xi) $-x+1, y-1/2, -z+3/2$; (xii) $-x+2, y-1/2, -z+3/2$.