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# *catena*-Poly[[(ethanol-$\kappa O$)[3-(1-phenyl-1*H*-pyrazol-3-yl)benzoic acid-$\kappa O$]-lithium]-$\mu$-3-(1-phenyl-1*H*-pyrazol-3-yl)benzoato-$\kappa^2 O:O'$]

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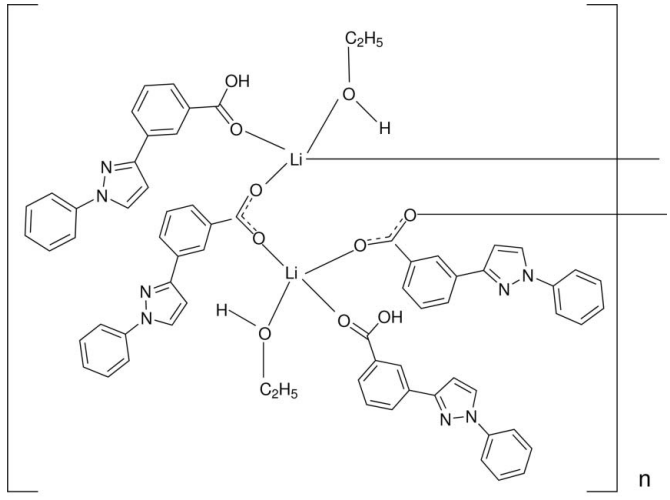
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.066; $wR$ factor = 0.168; data-to-parameter ratio = 21.2.

The asymmetric unit of the title polymeric compound, $[Li_2(C_{16}H_{11}N_2O_2)_2(C_{16}H_{12}N_2O_2)_2(CH_3CH_2OH)_2]_n$, contains two $Li^I$ ions, two 3-(1-phenyl-1*H*-pyrazol-3-yl)benzoate ions, two 3-(1-phenyl-1*H*-pyrazol-3-yl)benzoic acid molecules and two ethanol molecules. In the crystal structure, each of the two $Li^I$ ions has a distorted tetrahedral geometry, coordinated by two carboxylate O atoms, one carboxyl O atom and one ethanol O atom. The carboxylate group bridges the $Li^I$ ions, forming a one-dimensional polymeric chain along [100]. The crystal structure is further stabilized by O—H···O and C—H···N hydrogen bonding, and $\pi$–$\pi$ interactions with centroid–centroid distances in the range 3.6534 (13)–3.8374 (13) Å.

## Related literature

For pyrazole derivatives, see: Isloor *et al.* (2009); Skoutakis *et al.* (1988); Di Marzo *et al.* (2004); Kalluraya *et al.* (2004); Hanamoto *et al.* (2008). For a similar coordination geometry, see: Fischer (2005). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$[Li_2(C_{16}H_{11}N_2O_2)_2(C_{16}H_{12}N_2O_2)_2(C_2H_6O)_2]$
$M_r$ = 1161.10
Triclinic, $P\overline{1}$
$a$ = 7.9607 (1) Å
$b$ = 14.9527 (2) Å
$c$ = 26.5320 (4) Å
$\alpha$ = 103.471 (1)°
$\beta$ = 90.348 (1)°
$\gamma$ = 105.429 (1)°
$V$ = 2952.82 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100 K
0.47 × 0.18 × 0.15 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.960, $T_{max}$ = 0.987
66644 measured reflections
17230 independent reflections
11897 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.168
$S$ = 1.04
17230 reflections
811 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Li1—O1*A* | 1.912 (4) | Li2—O2*C* | 1.912 (4) |
| Li1—O2*D* | 1.931 (4) | Li2—O1*B* | 1.931 (4) |
| Li1—O4 | 1.953 (4) | Li2—O1*D* | 1.940 (4) |
| Li1—O1*C*$^{i}$ | 1.954 (4) | Li2—O3 | 1.960 (4) |

Symmetry code: (i) $x+1, y, z$.

‡ Thomson Reuters ResearcherID: A-3561-2009.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2$A$—H1$OA$···O2$C^{i}$ | 0.91 (3) | 1.70 (3) | 2.594 (2) | 167 (3) |
| O2$B$—H1$OB$···O2$D$ | 0.92 (3) | 1.68 (3) | 2.584 (2) | 165 (3) |
| O3—H1$O3$···O1$C^{i}$ | 0.85 (3) | 1.92 (3) | 2.761 (2) | 171 (3) |
| O4—H1$O4$···O1$D^{i}$ | 0.85 (3) | 1.94 (3) | 2.780 (2) | 170 (2) |
| C7$A$—H7$AA$···N2$D$ | 0.93 | 2.58 | 3.306 (3) | 136 |
| C5$C$—H5$CA$···N2$B^{ii}$ | 0.93 | 2.60 | 3.501 (3) | 163 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2436).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, m917-m918 [ **doi:10.1107/S1600536809026385** ]

# *catena*-Poly[[(ethanol-*κO*)[3-(1-phenyl-1*H*-pyrazol-3-yl)benzoic acid-*κO*]lithium]-$\mu$-3-(1-phenyl-1*H*-pyrazol-3-yl)benzoato-$\kappa^2O$:*O*']

**H.-K. Fun, K. Balasubramani, S. Rai, P. Shetty and A. M. Isloor**

## Comment

Natural antibiotic compounds have become indispensable to the current health care system, assisting and complementing the natural immune system against microbial pathogens. However, because conventional antibiotics are often overused to treat microbial infections, some microorganisms have developed resistance to many of these antibiotics. Pyrazole chemistry has been a focus of medical research for more than five decades due to the versatile biological and pharmacological activities of pyrazole derivatives, including effects as antimicrobial (Isloor *et al.*, 2009), antiviral (Skoutakis *et al.*, 1988), antitumor (Di Marzo *et al.*, 2004), anti-inflammatory (Kalluraya *et al.*, 2004), antihistaminic, antifungal, anti-rheumatoid-arthritic, anticonvulsant and antipyretic (Hanamoto *et al.*, 2008) agents. We report here a lithium salt of the pyrazole derivative.

The asymmetric unit of (I) (Fig. 1), contains two Li ions, two 3-(1-phenyl-1*H*-pyrazol-3-yl)benzoate ions, two 3-(1-phenyl-1*H*-pyrazol-3-yl)benzoic acid and two ethanol molecules. The bond lengths (Allen *et al.*, 1987) and angles are normal. The torsion angles of C6A—N1A—C7A—C8A, C4A—C5A—C6A—N1A, C2A—C1A—C6A—N1A, C10A—C11A—C12A—C16A, C16A—C12A—C13A—C14A, C13A—C12A—C16A—O1A, C11A—C12A—C16A—O2A, C6B—N1B—C7B—C8B, C4B—C5B—C6B—N1B, C2B—C1B—C6B—N1B, C10B—C11B—C12B—C16B, C16B—C12B—C13B—C14B, C13B—C12B—C16B—O1B, C11B—C12B—C16B—O2B, C6C—N1C—C7C—C8C, C4C—C5C—C6C—N1C, C2C—C1C—C6C—N1C, C10C—C11C—C12C—C16C, C16C—C12C—C13C—C14C, C13C—C12C—C16C—O1C, C11C—C12C—C16C—O2C, C6D—N1D—C7D—C8D, C4D—C5D—C6D—N1D, C2D—C1D—C6D—N1D, C10D—C11D—C12D—C16D, C16D—C12D—C13D—C14D, C13D—C12D—C16D—O1D and C11D—C12D—C16D—O2D are -178.7 (2), 178.8 (2), -178.3 (2), 177.4 (2), -177.9 (2), -176.8 (2), -174.7 (2), -179.1 (2), -179.4 (2), -179.9 (2), 177.1 (2), -176.6 (2), 171.3 (2), 176.2 (2), 178.7 (2), 178.3 (2), -179.5 (2), 178.2 (2), -178.3 (2), 172.0 (2), 173.8 (2), -180.0 (2), 177.9 (2), -178.8 (2), 177.7 (2), -177.7 (2), 172.0 (2) and 174.2 (2)°, respectively. The environments of both Li ions adopt a distorted tetrahedral geometry, with each Li atom coordinated by two carboxylate oxygen atoms, one carboxyl oxygen atom and an ethanol oxygen atom (Table 1). This coordination is similar to that observed in the crystal structure of lithium hydrogen (*RS*)-phenylsuccinate (Fischer, 2005). In the crystal packing (Fig. 2), the molecules form one-dimensional polymeric chains along the [100] direction. In each chain, the ethanol hydrogen atom is hydrogen-bonded to the carboxylate oxygen atoms through O—H···O hydrogen bonding. The carboxyl hydrogen atom is also hydrogen-bonded to the carboxylate oxygen atoms *via* O—H···O hydrogen bonding. The crystal structure is further stabilized by C—H···N hydrogen-bonding (Table 2) and π–π interactions. The π–π interaction between the five-membered rings, N1A—N2A/C9A—C7A and N1B—N2B/C9B—C7B, has centroid-to-centroid distance of 3.6534 (13) Å. The π–π interactions between the six-membered rings, C1A—C6A/C10A—C15A and C1B—C6B/C10B—C15B, have centroid-to-centroid distances of between 3.7099 (14) and 3.7589 (14) Å. The π–π interaction between the five-membered and six-membered rings, N1C—N2C/C9C—C7C and C10B—C15B, has centroid-to-centroid distance of 3.8374 (13) Å.

### Experimental

The title compound is obtained by adding 3-bromo-1-phenyl pyrazole (500 mg, 2.2 mmol) into a stirred solution of benzene boronic acid (369 mg, 2.2 mmol) in toluene (10 ml) and water (10 ml). Sodium carbonate (370 mg, 4.4 mmol), and tetrakis(triphenylphosphine)palladium(0) (258 mg, 0.2 mmol) were then added. The reaction mixture was heated to 100°C for 12 hr when TLC showed completion of reaction. Reaction mixture was diluted with water, acidified to pH 3, and extracted with ethyl acetate. The combined organic layer was dried over sodium sulfate, concentrated and the residue purified by column chromatography using 5% methanol in chloroform to get pure product as colorless crystals, Yield: 510 mg (84%), Melting point: 435–438 K. The lithium is an impurity with silica gel. The NMR data is consistent with the structure of the title compound (I).

### Refinement

H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$(methyl C). A rotating–group model was used for the methyl groups. The oxygen H atoms were located from the difference Fourier map [O–H = 0.85 (3)–0.91 (3) Å] and allowed to refine freely.

### Figures

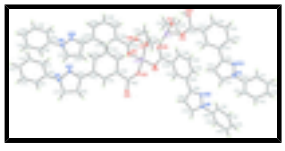

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom numbering scheme.

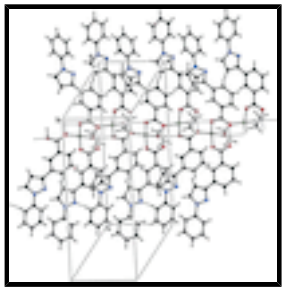

Fig. 2. The polymeric network of (I) along the [100] direction. Dashed lines indicate the hydrogen bonding.

### *catena*-Poly[[(ethanol-κ*O*)[3-(1-phenyl-1*H*-pyrazol- 3-yl)benzoic acid-κ*O*]lithium(I)]-μ-3-(1-phenyl-1*H*-pyrazol-3-yl)benzoato- $\kappa^2O$:$O'$]

*Crystal data*

| | |
|---|---|
| $[Li_2(C_{16}H_{11}N_2O_2)_2(C_{16}H_{12}N_2O_2)_2(C_2H_6O)_2]$ | $Z = 2$ |
| $M_r = 1161.10$ | $F_{000} = 1216$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.306$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| $a = 7.9607$ (1) Å | Cell parameters from 9941 reflections |
| $b = 14.9527$ (2) Å | θ = 2.4–30.1° |
| $c = 26.5320$ (4) Å | μ = 0.09 mm$^{-1}$ |

| | |
|---|---|
| α = 103.471 (1)º | $T$ = 100 K |
| β = 90.348 (1)º | Block, colorless |
| γ = 105.429 (1)º | 0.47 × 0.18 × 0.15 mm |
| $V$ = 2952.82 (7) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 17230 independent reflections |
| Radiation source: fine-focus sealed tube | 11897 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.046 |
| $T$ = 100 K | $\theta_{max}$ = 30.2º |
| φ and ω scans | $\theta_{min}$ = 0.8º |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $h$ = −11→11 |
| $T_{min}$ = 0.960, $T_{max}$ = 0.987 | $k$ = −20→21 |
| 66644 measured reflections | $l$ = −35→37 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.066 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.168 | $w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 3.024P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.04 | $(\Delta/\sigma)_{max} < 0.001$ |
| 17230 reflections | $\Delta\rho_{max}$ = 0.41 e Å$^{-3}$ |
| 811 parameters | $\Delta\rho_{min}$ = −0.31 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Li1 | 1.4484 (4) | 0.4845 (2) | 0.21870 (13) | 0.0220 (7) |
| Li2 | 0.9517 (4) | 0.5029 (3) | 0.27808 (13) | 0.0224 (7) |
| O1A | 1.4132 (2) | 0.35616 (11) | 0.17852 (6) | 0.0327 (4) |
| O2A | 1.6215 (2) | 0.30183 (12) | 0.20755 (6) | 0.0293 (3) |
| N1A | 1.0252 (2) | 0.06256 (12) | −0.06878 (7) | 0.0243 (4) |
| N2A | 1.1522 (2) | 0.05002 (12) | −0.03866 (6) | 0.0230 (4) |
| C1A | 1.0440 (3) | −0.07475 (16) | −0.13585 (8) | 0.0289 (5) |
| H1AA | 1.1124 | −0.0906 | −0.1126 | 0.035* |
| C2A | 1.0046 (3) | −0.13031 (18) | −0.18655 (9) | 0.0347 (5) |
| H2AA | 1.0475 | −0.1833 | −0.1972 | 0.042* |
| C3A | 0.9028 (3) | −0.10783 (19) | −0.22109 (9) | 0.0399 (6) |
| H3AA | 0.8780 | −0.1449 | −0.2551 | 0.048* |
| C4A | 0.8374 (4) | −0.0297 (2) | −0.20491 (10) | 0.0426 (6) |
| H4AA | 0.7666 | −0.0151 | −0.2280 | 0.051* |
| C5A | 0.8762 (3) | 0.02741 (18) | −0.15462 (9) | 0.0359 (5) |
| H5AA | 0.8329 | 0.0803 | −0.1441 | 0.043* |
| C6A | 0.9805 (3) | 0.00437 (15) | −0.12024 (8) | 0.0258 (4) |
| C7A | 0.9607 (3) | 0.13500 (15) | −0.04342 (9) | 0.0309 (5) |
| H7AA | 0.8740 | 0.1563 | −0.0565 | 0.037* |
| C8A | 1.0462 (3) | 0.17068 (15) | 0.00468 (9) | 0.0298 (5) |
| H8AA | 1.0301 | 0.2204 | 0.0309 | 0.036* |
| C9A | 1.1647 (3) | 0.11558 (14) | 0.00604 (8) | 0.0226 (4) |
| C10A | 1.2922 (3) | 0.12322 (15) | 0.04811 (8) | 0.0235 (4) |
| C11A | 1.3292 (3) | 0.20125 (14) | 0.09116 (8) | 0.0225 (4) |
| H11A | 1.2711 | 0.2483 | 0.0937 | 0.027* |
| C12A | 1.4534 (3) | 0.20890 (15) | 0.13040 (8) | 0.0240 (4) |
| C13A | 1.5398 (3) | 0.13848 (17) | 0.12752 (9) | 0.0303 (5) |
| H13A | 1.6220 | 0.1438 | 0.1539 | 0.036* |
| C14A | 1.5021 (3) | 0.06018 (17) | 0.08493 (9) | 0.0331 (5) |
| H14A | 1.5593 | 0.0128 | 0.0827 | 0.040* |
| C15A | 1.3794 (3) | 0.05260 (16) | 0.04567 (8) | 0.0283 (5) |
| H15A | 1.3547 | −0.0001 | 0.0173 | 0.034* |
| C16A | 1.4931 (3) | 0.29600 (15) | 0.17435 (8) | 0.0236 (4) |
| O1B | 1.0385 (2) | 0.63497 (11) | 0.31587 (6) | 0.0289 (3) |
| O2B | 1.3177 (2) | 0.67241 (11) | 0.29641 (6) | 0.0277 (3) |
| N1B | 0.9371 (2) | 0.93770 (12) | 0.56028 (7) | 0.0229 (4) |
| N2B | 1.0854 (2) | 0.93899 (12) | 0.53531 (6) | 0.0216 (3) |
| C1B | 1.1010 (3) | 1.06570 (16) | 0.63134 (8) | 0.0267 (4) |
| H1BA | 1.2014 | 1.0670 | 0.6135 | 0.032* |
| C2B | 1.1088 (3) | 1.12830 (17) | 0.67979 (8) | 0.0308 (5) |
| H2BA | 1.2148 | 1.1709 | 0.6945 | 0.037* |
| C3B | 0.9589 (3) | 1.12698 (18) | 0.70596 (9) | 0.0362 (6) |
| H3BA | 0.9640 | 1.1687 | 0.7383 | 0.043* |
| C4B | 0.8006 (3) | 1.06335 (18) | 0.68384 (9) | 0.0361 (5) |
| H4BA | 0.6997 | 1.0633 | 0.7013 | 0.043* |

| | | | | |
|---|---|---|---|---|
| C5B | 0.7918 (3) | 0.99997 (16) | 0.63590 (9) | 0.0311 (5) |
| H5BA | 0.6858 | 0.9570 | 0.6214 | 0.037* |
| C6B | 0.9428 (3) | 1.00136 (15) | 0.60980 (8) | 0.0243 (4) |
| C7B | 0.7971 (3) | 0.87027 (16) | 0.53268 (9) | 0.0339 (5) |
| H7BA | 0.6828 | 0.8567 | 0.5424 | 0.041* |
| C8B | 0.8557 (3) | 0.82614 (16) | 0.48798 (9) | 0.0317 (5) |
| H8BA | 0.7903 | 0.7769 | 0.4612 | 0.038* |
| C9B | 1.0358 (3) | 0.87105 (14) | 0.49110 (8) | 0.0207 (4) |
| C10B | 1.1659 (3) | 0.84961 (14) | 0.45499 (8) | 0.0227 (4) |
| C11B | 1.1187 (3) | 0.78132 (14) | 0.40765 (7) | 0.0210 (4) |
| H11B | 1.0014 | 0.7500 | 0.3980 | 0.025* |
| C12B | 1.2456 (3) | 0.75986 (14) | 0.37487 (8) | 0.0234 (4) |
| C13B | 1.4212 (3) | 0.80507 (17) | 0.38890 (9) | 0.0318 (5) |
| H13B | 1.5058 | 0.7904 | 0.3670 | 0.038* |
| C14B | 1.4695 (3) | 0.87257 (18) | 0.43609 (9) | 0.0374 (6) |
| H14B | 1.5869 | 0.9033 | 0.4458 | 0.045* |
| C15B | 1.3434 (3) | 0.89403 (16) | 0.46862 (9) | 0.0322 (5) |
| H15B | 1.3773 | 0.9389 | 0.5002 | 0.039* |
| C16B | 1.1898 (3) | 0.68338 (14) | 0.32605 (7) | 0.0215 (4) |
| O1C | 0.45630 (18) | 0.48572 (11) | 0.29247 (5) | 0.0240 (3) |
| O2C | 0.70998 (17) | 0.44937 (10) | 0.28620 (5) | 0.0206 (3) |
| N1C | 0.3491 (2) | 0.71485 (12) | 0.55515 (6) | 0.0203 (3) |
| N2C | 0.4858 (2) | 0.68099 (12) | 0.53726 (6) | 0.0206 (3) |
| C1C | 0.4597 (3) | 0.75143 (15) | 0.64512 (8) | 0.0239 (4) |
| H1CA | 0.5194 | 0.7050 | 0.6362 | 0.029* |
| C2C | 0.4694 (3) | 0.80360 (16) | 0.69617 (8) | 0.0290 (5) |
| H2CA | 0.5379 | 0.7929 | 0.7215 | 0.035* |
| C3C | 0.3778 (3) | 0.87166 (16) | 0.70978 (8) | 0.0321 (5) |
| H3CA | 0.3828 | 0.9054 | 0.7442 | 0.039* |
| C4C | 0.2791 (3) | 0.88917 (17) | 0.67205 (9) | 0.0337 (5) |
| H4CA | 0.2180 | 0.9349 | 0.6812 | 0.040* |
| C5C | 0.2709 (3) | 0.83868 (16) | 0.62051 (8) | 0.0282 (5) |
| H5CA | 0.2063 | 0.8514 | 0.5950 | 0.034* |
| C6C | 0.3598 (3) | 0.76925 (14) | 0.60752 (7) | 0.0214 (4) |
| C7C | 0.2168 (3) | 0.69150 (15) | 0.51775 (8) | 0.0236 (4) |
| H7CA | 0.1113 | 0.7072 | 0.5214 | 0.028* |
| C8C | 0.2681 (3) | 0.64053 (15) | 0.47366 (8) | 0.0229 (4) |
| H8CA | 0.2055 | 0.6145 | 0.4415 | 0.027* |
| C9C | 0.4369 (3) | 0.63602 (14) | 0.48750 (7) | 0.0192 (4) |
| C10C | 0.5541 (2) | 0.58987 (14) | 0.45517 (7) | 0.0185 (4) |
| C11C | 0.5233 (3) | 0.56048 (14) | 0.40109 (7) | 0.0187 (4) |
| H11C | 0.4279 | 0.5709 | 0.3853 | 0.022* |
| C12C | 0.6337 (2) | 0.51578 (13) | 0.37057 (7) | 0.0178 (4) |
| C13C | 0.7780 (3) | 0.50106 (14) | 0.39425 (7) | 0.0197 (4) |
| H13C | 0.8530 | 0.4719 | 0.3742 | 0.024* |
| C14C | 0.8087 (3) | 0.53019 (14) | 0.44790 (8) | 0.0217 (4) |
| H14C | 0.9046 | 0.5202 | 0.4637 | 0.026* |
| C15C | 0.6984 (3) | 0.57396 (14) | 0.47825 (7) | 0.0206 (4) |
| H15C | 0.7203 | 0.5929 | 0.5142 | 0.025* |

| | | | | |
|---|---|---|---|---|
| C16C | 0.5968 (2) | 0.48180 (14) | 0.31252 (7) | 0.0184 (4) |
| O1D | 0.96510 (18) | 0.49718 (11) | 0.20445 (5) | 0.0230 (3) |
| O2D | 1.25582 (18) | 0.53777 (10) | 0.21192 (5) | 0.0205 (3) |
| N1D | 0.6220 (2) | 0.27979 (12) | −0.05822 (6) | 0.0206 (3) |
| N2D | 0.7938 (2) | 0.31606 (12) | −0.04095 (6) | 0.0200 (3) |
| C1D | 0.6886 (3) | 0.25619 (15) | −0.14861 (8) | 0.0242 (4) |
| H1DA | 0.7943 | 0.3030 | −0.1389 | 0.029* |
| C2D | 0.6411 (3) | 0.20990 (16) | −0.20067 (8) | 0.0276 (5) |
| H2DA | 0.7164 | 0.2257 | −0.2259 | 0.033* |
| C3D | 0.4833 (3) | 0.14069 (16) | −0.21533 (8) | 0.0292 (5) |
| H3DA | 0.4521 | 0.1107 | −0.2502 | 0.035* |
| C4D | 0.3723 (3) | 0.11638 (16) | −0.17781 (9) | 0.0309 (5) |
| H4DA | 0.2660 | 0.0700 | −0.1876 | 0.037* |
| C5D | 0.4182 (3) | 0.16084 (15) | −0.12542 (8) | 0.0267 (4) |
| H5DA | 0.3446 | 0.1436 | −0.1002 | 0.032* |
| C6D | 0.5760 (3) | 0.23139 (14) | −0.11147 (7) | 0.0206 (4) |
| C7D | 0.5147 (3) | 0.29660 (16) | −0.01962 (8) | 0.0246 (4) |
| H7DA | 0.3932 | 0.2783 | −0.0227 | 0.030* |
| C8D | 0.6191 (3) | 0.34543 (15) | 0.02464 (8) | 0.0245 (4) |
| H8DA | 0.5838 | 0.3673 | 0.0575 | 0.029* |
| C9D | 0.7913 (3) | 0.35560 (14) | 0.00984 (7) | 0.0194 (4) |
| C10D | 0.9570 (3) | 0.40278 (13) | 0.04207 (7) | 0.0189 (4) |
| C11D | 0.9577 (3) | 0.42900 (14) | 0.09619 (7) | 0.0195 (4) |
| H11D | 0.8527 | 0.4164 | 0.1119 | 0.023* |
| C12D | 1.1138 (3) | 0.47380 (13) | 0.12698 (7) | 0.0180 (4) |
| C13D | 1.2705 (3) | 0.49167 (14) | 0.10350 (7) | 0.0196 (4) |
| H13D | 1.3750 | 0.5209 | 0.1238 | 0.024* |
| C14D | 1.2716 (3) | 0.46595 (14) | 0.04972 (8) | 0.0221 (4) |
| H14D | 1.3769 | 0.4779 | 0.0341 | 0.027* |
| C15D | 1.1159 (3) | 0.42249 (14) | 0.01917 (7) | 0.0204 (4) |
| H15D | 1.1175 | 0.4064 | −0.0168 | 0.025* |
| C16D | 1.1096 (3) | 0.50458 (14) | 0.18509 (7) | 0.0189 (4) |
| O3 | 1.1049 (2) | 0.44372 (11) | 0.30900 (6) | 0.0254 (3) |
| C17 | 1.0641 (3) | 0.34913 (16) | 0.31647 (10) | 0.0338 (5) |
| H17A | 1.1206 | 0.3108 | 0.2912 | 0.041* |
| H17B | 0.9389 | 0.3204 | 0.3106 | 0.041* |
| C18 | 1.1228 (3) | 0.34828 (19) | 0.37057 (11) | 0.0384 (6) |
| H18A | 1.0993 | 0.2834 | 0.3735 | 0.058* |
| H18B | 1.0606 | 0.3821 | 0.3955 | 0.058* |
| H18C | 1.2460 | 0.3788 | 0.3770 | 0.058* |
| O4 | 1.6609 (2) | 0.54954 (11) | 0.19115 (6) | 0.0267 (3) |
| C19 | 1.7212 (3) | 0.64612 (18) | 0.18609 (11) | 0.0407 (6) |
| H19A | 1.8151 | 0.6818 | 0.2125 | 0.049* |
| H19B | 1.6266 | 0.6761 | 0.1918 | 0.049* |
| C20 | 1.7857 (4) | 0.6501 (2) | 0.13303 (13) | 0.0532 (8) |
| H20A | 1.8269 | 0.7156 | 0.1311 | 0.080* |
| H20B | 1.6919 | 0.6168 | 0.1069 | 0.080* |
| H20C | 1.8795 | 0.6205 | 0.1273 | 0.080* |
| H1OA | 1.642 (4) | 0.357 (2) | 0.2328 (11) | 0.044 (8)* |

| | | | | |
|---|---|---|---|---|
| H1OB | 1.276 (4) | 0.623 (2) | 0.2673 (12) | 0.052 (9)* |
| H1O3 | 1.215 (4) | 0.460 (2) | 0.3076 (11) | 0.043 (8)* |
| H1O4 | 1.750 (4) | 0.5287 (19) | 0.1914 (10) | 0.036 (7)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Li1 | 0.0187 (17) | 0.0279 (17) | 0.0179 (15) | 0.0079 (14) | −0.0006 (13) | 0.0011 (13) |
| Li2 | 0.0185 (17) | 0.0281 (17) | 0.0166 (15) | 0.0050 (14) | −0.0007 (13) | −0.0006 (13) |
| O1A | 0.0382 (9) | 0.0259 (8) | 0.0301 (8) | 0.0127 (7) | −0.0098 (7) | −0.0050 (6) |
| O2A | 0.0300 (8) | 0.0321 (8) | 0.0224 (7) | 0.0123 (7) | −0.0044 (6) | −0.0044 (6) |
| N1A | 0.0245 (9) | 0.0213 (8) | 0.0246 (9) | 0.0058 (7) | −0.0021 (7) | 0.0017 (7) |
| N2A | 0.0220 (9) | 0.0242 (8) | 0.0211 (8) | 0.0056 (7) | −0.0005 (7) | 0.0030 (7) |
| C1A | 0.0267 (11) | 0.0301 (11) | 0.0251 (10) | 0.0061 (9) | −0.0023 (9) | −0.0007 (8) |
| C2A | 0.0316 (13) | 0.0357 (12) | 0.0303 (12) | 0.0098 (10) | −0.0009 (10) | −0.0051 (10) |
| C3A | 0.0395 (14) | 0.0464 (15) | 0.0256 (11) | 0.0085 (12) | −0.0054 (10) | −0.0034 (10) |
| C4A | 0.0431 (15) | 0.0504 (16) | 0.0320 (13) | 0.0112 (12) | −0.0103 (11) | 0.0076 (11) |
| C5A | 0.0381 (14) | 0.0358 (12) | 0.0332 (12) | 0.0129 (11) | −0.0050 (10) | 0.0045 (10) |
| C6A | 0.0246 (11) | 0.0262 (10) | 0.0229 (10) | 0.0038 (8) | −0.0013 (8) | 0.0026 (8) |
| C7A | 0.0307 (12) | 0.0232 (10) | 0.0357 (12) | 0.0102 (9) | −0.0069 (9) | −0.0018 (9) |
| C8A | 0.0321 (12) | 0.0216 (10) | 0.0326 (11) | 0.0101 (9) | −0.0036 (9) | −0.0022 (8) |
| C9A | 0.0234 (10) | 0.0187 (9) | 0.0233 (10) | 0.0035 (8) | 0.0016 (8) | 0.0030 (7) |
| C10A | 0.0225 (10) | 0.0231 (9) | 0.0213 (9) | 0.0037 (8) | 0.0021 (8) | 0.0016 (8) |
| C11A | 0.0230 (10) | 0.0204 (9) | 0.0228 (10) | 0.0053 (8) | 0.0028 (8) | 0.0035 (7) |
| C12A | 0.0261 (11) | 0.0242 (10) | 0.0195 (9) | 0.0066 (8) | 0.0034 (8) | 0.0012 (8) |
| C13A | 0.0321 (12) | 0.0346 (12) | 0.0241 (10) | 0.0140 (10) | −0.0011 (9) | 0.0014 (9) |
| C14A | 0.0380 (13) | 0.0318 (11) | 0.0304 (11) | 0.0181 (10) | −0.0006 (10) | −0.0002 (9) |
| C15A | 0.0320 (12) | 0.0280 (11) | 0.0221 (10) | 0.0104 (9) | 0.0017 (9) | −0.0019 (8) |
| C16A | 0.0233 (10) | 0.0242 (10) | 0.0196 (9) | 0.0041 (8) | 0.0014 (8) | 0.0010 (8) |
| O1B | 0.0251 (8) | 0.0263 (7) | 0.0276 (8) | 0.0035 (6) | 0.0030 (6) | −0.0043 (6) |
| O2B | 0.0231 (8) | 0.0327 (8) | 0.0204 (7) | 0.0054 (6) | 0.0029 (6) | −0.0048 (6) |
| N1B | 0.0251 (9) | 0.0195 (8) | 0.0227 (8) | 0.0053 (7) | 0.0074 (7) | 0.0029 (6) |
| N2B | 0.0222 (9) | 0.0241 (8) | 0.0192 (8) | 0.0095 (7) | 0.0041 (6) | 0.0032 (6) |
| C1B | 0.0275 (11) | 0.0304 (11) | 0.0211 (10) | 0.0098 (9) | 0.0046 (8) | 0.0016 (8) |
| C2B | 0.0313 (12) | 0.0313 (11) | 0.0255 (11) | 0.0081 (9) | 0.0004 (9) | −0.0009 (9) |
| C3B | 0.0437 (15) | 0.0368 (13) | 0.0235 (11) | 0.0119 (11) | 0.0053 (10) | −0.0024 (9) |
| C4B | 0.0372 (14) | 0.0394 (13) | 0.0286 (12) | 0.0092 (11) | 0.0128 (10) | 0.0034 (10) |
| C5B | 0.0303 (12) | 0.0289 (11) | 0.0296 (11) | 0.0041 (9) | 0.0070 (9) | 0.0031 (9) |
| C6B | 0.0311 (11) | 0.0231 (10) | 0.0194 (9) | 0.0102 (8) | 0.0064 (8) | 0.0034 (8) |
| C7B | 0.0254 (12) | 0.0266 (11) | 0.0382 (13) | −0.0021 (9) | 0.0107 (10) | −0.0038 (9) |
| C8B | 0.0275 (12) | 0.0229 (10) | 0.0341 (12) | −0.0007 (9) | 0.0057 (9) | −0.0047 (9) |
| C9B | 0.0226 (10) | 0.0184 (9) | 0.0210 (9) | 0.0071 (8) | 0.0019 (8) | 0.0030 (7) |
| C10B | 0.0243 (10) | 0.0228 (9) | 0.0194 (9) | 0.0069 (8) | 0.0019 (8) | 0.0014 (7) |
| C11B | 0.0214 (10) | 0.0199 (9) | 0.0197 (9) | 0.0047 (7) | −0.0008 (7) | 0.0024 (7) |
| C12B | 0.0239 (10) | 0.0223 (9) | 0.0207 (9) | 0.0061 (8) | 0.0001 (8) | −0.0008 (7) |
| C13B | 0.0254 (11) | 0.0345 (12) | 0.0290 (11) | 0.0076 (9) | 0.0045 (9) | −0.0039 (9) |
| C14B | 0.0215 (11) | 0.0407 (13) | 0.0360 (13) | 0.0020 (10) | −0.0008 (9) | −0.0102 (10) |
| C15B | 0.0282 (12) | 0.0311 (11) | 0.0266 (11) | 0.0041 (9) | −0.0008 (9) | −0.0093 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16B | 0.0241 (10) | 0.0214 (9) | 0.0185 (9) | 0.0084 (8) | 0.0001 (8) | 0.0014 (7) |
| O1C | 0.0165 (7) | 0.0393 (8) | 0.0175 (7) | 0.0114 (6) | 0.0007 (5) | 0.0052 (6) |
| O2C | 0.0157 (7) | 0.0264 (7) | 0.0176 (6) | 0.0064 (6) | 0.0009 (5) | 0.0007 (5) |
| N1C | 0.0202 (8) | 0.0228 (8) | 0.0174 (8) | 0.0067 (7) | 0.0020 (6) | 0.0031 (6) |
| N2C | 0.0193 (8) | 0.0210 (8) | 0.0199 (8) | 0.0051 (6) | 0.0015 (6) | 0.0024 (6) |
| C1C | 0.0256 (11) | 0.0228 (9) | 0.0217 (10) | 0.0061 (8) | 0.0021 (8) | 0.0027 (8) |
| C2C | 0.0322 (12) | 0.0306 (11) | 0.0204 (10) | 0.0044 (9) | −0.0014 (9) | 0.0039 (8) |
| C3C | 0.0423 (14) | 0.0295 (11) | 0.0196 (10) | 0.0091 (10) | 0.0031 (9) | −0.0029 (8) |
| C4C | 0.0437 (14) | 0.0286 (11) | 0.0289 (11) | 0.0163 (10) | 0.0039 (10) | −0.0002 (9) |
| C5C | 0.0353 (12) | 0.0278 (11) | 0.0228 (10) | 0.0126 (9) | 0.0016 (9) | 0.0038 (8) |
| C6C | 0.0227 (10) | 0.0210 (9) | 0.0169 (9) | 0.0032 (8) | 0.0029 (7) | 0.0011 (7) |
| C7C | 0.0232 (10) | 0.0280 (10) | 0.0217 (9) | 0.0104 (8) | 0.0012 (8) | 0.0063 (8) |
| C8C | 0.0230 (10) | 0.0276 (10) | 0.0183 (9) | 0.0090 (8) | 0.0004 (8) | 0.0037 (8) |
| C9C | 0.0204 (10) | 0.0195 (9) | 0.0167 (8) | 0.0039 (7) | 0.0012 (7) | 0.0040 (7) |
| C10C | 0.0163 (9) | 0.0211 (9) | 0.0168 (8) | 0.0031 (7) | 0.0013 (7) | 0.0045 (7) |
| C11C | 0.0159 (9) | 0.0220 (9) | 0.0176 (9) | 0.0047 (7) | −0.0006 (7) | 0.0042 (7) |
| C12C | 0.0167 (9) | 0.0194 (8) | 0.0158 (8) | 0.0034 (7) | −0.0003 (7) | 0.0036 (7) |
| C13C | 0.0175 (9) | 0.0227 (9) | 0.0183 (9) | 0.0055 (7) | 0.0017 (7) | 0.0039 (7) |
| C14C | 0.0181 (10) | 0.0259 (10) | 0.0217 (9) | 0.0061 (8) | −0.0029 (7) | 0.0068 (8) |
| C15C | 0.0199 (10) | 0.0239 (9) | 0.0159 (8) | 0.0033 (8) | −0.0012 (7) | 0.0041 (7) |
| C16C | 0.0152 (9) | 0.0217 (9) | 0.0173 (9) | 0.0037 (7) | 0.0009 (7) | 0.0045 (7) |
| O1D | 0.0169 (7) | 0.0365 (8) | 0.0163 (6) | 0.0113 (6) | 0.0010 (5) | 0.0033 (6) |
| O2D | 0.0168 (7) | 0.0282 (7) | 0.0159 (6) | 0.0095 (6) | −0.0008 (5) | 0.0003 (5) |
| N1D | 0.0192 (8) | 0.0234 (8) | 0.0171 (8) | 0.0048 (7) | −0.0004 (6) | 0.0021 (6) |
| N2D | 0.0189 (8) | 0.0212 (8) | 0.0185 (8) | 0.0065 (6) | −0.0015 (6) | 0.0014 (6) |
| C1D | 0.0240 (10) | 0.0238 (10) | 0.0221 (10) | 0.0058 (8) | 0.0006 (8) | 0.0008 (8) |
| C2D | 0.0335 (12) | 0.0306 (11) | 0.0188 (9) | 0.0116 (9) | 0.0049 (8) | 0.0026 (8) |
| C3D | 0.0334 (12) | 0.0318 (11) | 0.0185 (9) | 0.0116 (9) | −0.0038 (8) | −0.0044 (8) |
| C4D | 0.0288 (12) | 0.0283 (11) | 0.0270 (11) | 0.0015 (9) | −0.0039 (9) | −0.0023 (9) |
| C5D | 0.0267 (11) | 0.0262 (10) | 0.0232 (10) | 0.0033 (9) | 0.0003 (8) | 0.0029 (8) |
| C6D | 0.0229 (10) | 0.0220 (9) | 0.0164 (9) | 0.0076 (8) | −0.0018 (7) | 0.0019 (7) |
| C7D | 0.0191 (10) | 0.0329 (11) | 0.0202 (9) | 0.0063 (8) | 0.0022 (8) | 0.0041 (8) |
| C8D | 0.0228 (10) | 0.0299 (10) | 0.0189 (9) | 0.0067 (8) | 0.0019 (8) | 0.0032 (8) |
| C9D | 0.0225 (10) | 0.0202 (9) | 0.0158 (8) | 0.0076 (7) | 0.0003 (7) | 0.0028 (7) |
| C10D | 0.0205 (10) | 0.0196 (9) | 0.0160 (8) | 0.0074 (7) | −0.0009 (7) | 0.0012 (7) |
| C11D | 0.0181 (9) | 0.0227 (9) | 0.0176 (9) | 0.0071 (7) | 0.0010 (7) | 0.0030 (7) |
| C12D | 0.0193 (9) | 0.0196 (9) | 0.0155 (8) | 0.0081 (7) | −0.0004 (7) | 0.0020 (7) |
| C13D | 0.0174 (9) | 0.0227 (9) | 0.0178 (9) | 0.0062 (7) | 0.0007 (7) | 0.0023 (7) |
| C14D | 0.0194 (10) | 0.0263 (10) | 0.0206 (9) | 0.0075 (8) | 0.0052 (7) | 0.0043 (8) |
| C15D | 0.0233 (10) | 0.0235 (9) | 0.0151 (8) | 0.0092 (8) | 0.0026 (7) | 0.0026 (7) |
| C16D | 0.0189 (9) | 0.0223 (9) | 0.0165 (8) | 0.0090 (7) | 0.0007 (7) | 0.0028 (7) |
| O3 | 0.0161 (7) | 0.0327 (8) | 0.0292 (8) | 0.0069 (6) | 0.0020 (6) | 0.0104 (6) |
| C17 | 0.0301 (12) | 0.0253 (11) | 0.0423 (13) | 0.0059 (9) | −0.0002 (10) | 0.0032 (10) |
| C18 | 0.0286 (12) | 0.0413 (14) | 0.0541 (16) | 0.0120 (10) | 0.0023 (11) | 0.0261 (12) |
| O4 | 0.0189 (8) | 0.0343 (8) | 0.0309 (8) | 0.0116 (6) | 0.0037 (6) | 0.0104 (6) |
| C19 | 0.0317 (13) | 0.0292 (12) | 0.0580 (17) | 0.0092 (10) | 0.0030 (12) | 0.0033 (11) |
| C20 | 0.0403 (16) | 0.0542 (17) | 0.085 (2) | 0.0220 (14) | 0.0269 (15) | 0.0441 (17) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Li1—O1A | 1.912 (4) | N1C—N2C | 1.361 (2) |
| Li1—O2D | 1.931 (4) | N1C—C6C | 1.427 (2) |
| Li1—O4 | 1.953 (4) | N2C—C9C | 1.337 (2) |
| Li1—O1C$^{i}$ | 1.954 (4) | C1C—C2C | 1.387 (3) |
| Li2—O2C | 1.912 (4) | C1C—C6C | 1.388 (3) |
| Li2—O1B | 1.931 (4) | C1C—H1CA | 0.9300 |
| Li2—O1D | 1.940 (4) | C2C—C3C | 1.387 (3) |
| Li2—O3 | 1.960 (4) | C2C—H2CA | 0.9300 |
| O1A—C16A | 1.218 (3) | C3C—C4C | 1.382 (3) |
| O2A—C16A | 1.317 (3) | C3C—H3CA | 0.9300 |
| O2A—H1OA | 0.91 (3) | C4C—C5C | 1.391 (3) |
| N1A—C7A | 1.360 (3) | C4C—H4CA | 0.9300 |
| N1A—N2A | 1.363 (2) | C5C—C6C | 1.387 (3) |
| N1A—C6A | 1.423 (3) | C5C—H5CA | 0.9300 |
| N2A—C9A | 1.335 (2) | C7C—C8C | 1.368 (3) |
| C1A—C6A | 1.385 (3) | C7C—H7CA | 0.9300 |
| C1A—C2A | 1.390 (3) | C8C—C9C | 1.414 (3) |
| C1A—H1AA | 0.9300 | C8C—H8CA | 0.9300 |
| C2A—C3A | 1.375 (4) | C9C—C10C | 1.469 (3) |
| C2A—H2AA | 0.9300 | C10C—C15C | 1.398 (3) |
| C3A—C4A | 1.383 (4) | C10C—C11C | 1.399 (3) |
| C3A—H3AA | 0.9300 | C11C—C12C | 1.394 (3) |
| C4A—C5A | 1.389 (3) | C11C—H11C | 0.9300 |
| C4A—H4AA | 0.9300 | C12C—C13C | 1.398 (3) |
| C5A—C6A | 1.389 (3) | C12C—C16C | 1.506 (3) |
| C5A—H5AA | 0.9300 | C13C—C14C | 1.388 (3) |
| C7A—C8A | 1.362 (3) | C13C—H13C | 0.9300 |
| C7A—H7AA | 0.9300 | C14C—C15C | 1.385 (3) |
| C8A—C9A | 1.413 (3) | C14C—H14C | 0.9300 |
| C8A—H8AA | 0.9300 | C15C—H15C | 0.9300 |
| C9A—C10A | 1.468 (3) | O1D—C16D | 1.251 (2) |
| C10A—C11A | 1.395 (3) | O2D—C16D | 1.275 (2) |
| C10A—C15A | 1.400 (3) | N1D—C7D | 1.359 (3) |
| C11A—C12A | 1.395 (3) | N1D—N2D | 1.363 (2) |
| C11A—H11A | 0.9300 | N1D—C6D | 1.425 (2) |
| C12A—C13A | 1.391 (3) | N2D—C9D | 1.342 (2) |
| C12A—C16A | 1.492 (3) | C1D—C6D | 1.384 (3) |
| C13A—C14A | 1.389 (3) | C1D—C2D | 1.392 (3) |
| C13A—H13A | 0.9300 | C1D—H1DA | 0.9300 |
| C14A—C15A | 1.388 (3) | C2D—C3D | 1.384 (3) |
| C14A—H14A | 0.9300 | C2D—H2DA | 0.9300 |
| C15A—H15A | 0.9300 | C3D—C4D | 1.383 (3) |
| O1B—C16B | 1.220 (3) | C3D—H3DA | 0.9300 |
| O2B—C16B | 1.312 (2) | C4D—C5D | 1.394 (3) |
| O2B—H1OB | 0.92 (3) | C4D—H4DA | 0.9300 |
| N1B—N2B | 1.356 (2) | C5D—C6D | 1.391 (3) |

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| N1B—C7B | 1.357 (3) | C5D—H5DA | 0.9300 |
| N1B—C6B | 1.424 (2) | C7D—C8D | 1.367 (3) |
| N2B—C9B | 1.338 (2) | C7D—H7DA | 0.9300 |
| C1B—C6B | 1.388 (3) | C8D—C9D | 1.408 (3) |
| C1B—C2B | 1.393 (3) | C8D—H8DA | 0.9300 |
| C1B—H1BA | 0.9300 | C9D—C10D | 1.475 (3) |
| C2B—C3B | 1.382 (3) | C10D—C15D | 1.397 (3) |
| C2B—H2BA | 0.9300 | C10D—C11D | 1.397 (3) |
| C3B—C4B | 1.390 (4) | C11D—C12D | 1.397 (3) |
| C3B—H3BA | 0.9300 | C11D—H11D | 0.9300 |
| C4B—C5B | 1.387 (3) | C12D—C13D | 1.388 (3) |
| C4B—H4BA | 0.9300 | C12D—C16D | 1.506 (3) |
| C5B—C6B | 1.389 (3) | C13D—C14D | 1.389 (3) |
| C5B—H5BA | 0.9300 | C13D—H13D | 0.9300 |
| C7B—C8B | 1.366 (3) | C14D—C15D | 1.389 (3) |
| C7B—H7BA | 0.9300 | C14D—H14D | 0.9300 |
| C8B—C9B | 1.405 (3) | C15D—H15D | 0.9300 |
| C8B—H8BA | 0.9300 | O3—C17 | 1.426 (3) |
| C9B—C10B | 1.463 (3) | O3—H1O3 | 0.85 (3) |
| C10B—C15B | 1.396 (3) | C17—C18 | 1.511 (3) |
| C10B—C11B | 1.398 (3) | C17—H17A | 0.9700 |
| C11B—C12B | 1.390 (3) | C17—H17B | 0.9700 |
| C11B—H11B | 0.9300 | C18—H18A | 0.9600 |
| C12B—C13B | 1.387 (3) | C18—H18B | 0.9600 |
| C12B—C16B | 1.488 (3) | C18—H18C | 0.9600 |
| C13B—C14B | 1.390 (3) | O4—C19 | 1.434 (3) |
| C13B—H13B | 0.9300 | O4—H1O4 | 0.85 (3) |
| C14B—C15B | 1.381 (3) | C19—C20 | 1.510 (4) |
| C14B—H14B | 0.9300 | C19—H19A | 0.9700 |
| C15B—H15B | 0.9300 | C19—H19B | 0.9700 |
| O1C—C16C | 1.257 (2) | C20—H20A | 0.9600 |
| O1C—Li1$^{ii}$ | 1.954 (4) | C20—H20B | 0.9600 |
| O2C—C16C | 1.272 (2) | C20—H20C | 0.9600 |
| N1C—C7C | 1.359 (3) | | |
| O1A—Li1—O2D | 114.37 (17) | C1C—C2C—C3C | 120.5 (2) |
| O1A—Li1—O4 | 100.80 (17) | C1C—C2C—H2CA | 119.8 |
| O2D—Li1—O4 | 113.07 (19) | C3C—C2C—H2CA | 119.8 |
| O1A—Li1—O1C$^{i}$ | 109.10 (19) | C4C—C3C—C2C | 119.8 (2) |
| O2D—Li1—O1C$^{i}$ | 102.01 (16) | C4C—C3C—H3CA | 120.1 |
| O4—Li1—O1C$^{i}$ | 118.00 (17) | C2C—C3C—H3CA | 120.1 |
| O2C—Li2—O1B | 112.91 (18) | C3C—C4C—C5C | 120.3 (2) |
| O2C—Li2—O1D | 105.03 (16) | C3C—C4C—H4CA | 119.8 |
| O1B—Li2—O1D | 108.16 (19) | C5C—C4C—H4CA | 119.8 |
| O2C—Li2—O3 | 112.76 (19) | C6C—C5C—C4C | 119.4 (2) |
| O1B—Li2—O3 | 101.30 (16) | C6C—C5C—H5CA | 120.3 |
| O1D—Li2—O3 | 116.84 (18) | C4C—C5C—H5CA | 120.3 |
| C16A—O2A—H1OA | 110.3 (18) | C5C—C6C—C1C | 120.70 (18) |
| C7A—N1A—N2A | 111.37 (17) | C5C—C6C—N1C | 120.26 (18) |

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| C7A—N1A—C6A | 128.98 (18) | C1C—C6C—N1C | 119.04 (18) |
| N2A—N1A—C6A | 119.62 (17) | N1C—C7C—C8C | 107.01 (18) |
| C9A—N2A—N1A | 104.87 (16) | N1C—C7C—H7CA | 126.5 |
| C6A—C1A—C2A | 119.4 (2) | C8C—C7C—H7CA | 126.5 |
| C6A—C1A—H1AA | 120.3 | C7C—C8C—C9C | 105.17 (17) |
| C2A—C1A—H1AA | 120.3 | C7C—C8C—H8CA | 127.4 |
| C3A—C2A—C1A | 120.7 (2) | C9C—C8C—H8CA | 127.4 |
| C3A—C2A—H2AA | 119.6 | N2C—C9C—C8C | 111.09 (17) |
| C1A—C2A—H2AA | 119.6 | N2C—C9C—C10C | 120.22 (17) |
| C2A—C3A—C4A | 119.4 (2) | C8C—C9C—C10C | 128.69 (17) |
| C2A—C3A—H3AA | 120.3 | C15C—C10C—C11C | 118.81 (18) |
| C4A—C3A—H3AA | 120.3 | C15C—C10C—C9C | 120.20 (17) |
| C3A—C4A—C5A | 120.9 (2) | C11C—C10C—C9C | 120.99 (17) |
| C3A—C4A—H4AA | 119.5 | C12C—C11C—C10C | 120.83 (18) |
| C5A—C4A—H4AA | 119.5 | C12C—C11C—H11C | 119.6 |
| C4A—C5A—C6A | 119.0 (2) | C10C—C11C—H11C | 119.6 |
| C4A—C5A—H5AA | 120.5 | C11C—C12C—C13C | 119.60 (17) |
| C6A—C5A—H5AA | 120.5 | C11C—C12C—C16C | 120.53 (17) |
| C1A—C6A—C5A | 120.4 (2) | C13C—C12C—C16C | 119.87 (17) |
| C1A—C6A—N1A | 119.27 (19) | C14C—C13C—C12C | 119.65 (18) |
| C5A—C6A—N1A | 120.3 (2) | C14C—C13C—H13C | 120.2 |
| N1A—C7A—C8A | 107.58 (19) | C12C—C13C—H13C | 120.2 |
| N1A—C7A—H7AA | 126.2 | C15C—C14C—C13C | 120.75 (18) |
| C8A—C7A—H7AA | 126.2 | C15C—C14C—H14C | 119.6 |
| C7A—C8A—C9A | 104.95 (19) | C13C—C14C—H14C | 119.6 |
| C7A—C8A—H8AA | 127.5 | C14C—C15C—C10C | 120.37 (18) |
| C9A—C8A—H8AA | 127.5 | C14C—C15C—H15C | 119.8 |
| N2A—C9A—C8A | 111.22 (18) | C10C—C15C—H15C | 119.8 |
| N2A—C9A—C10A | 119.82 (18) | O1C—C16C—O2C | 123.21 (17) |
| C8A—C9A—C10A | 128.95 (18) | O1C—C16C—C12C | 119.02 (17) |
| C11A—C10A—C15A | 118.78 (19) | O2C—C16C—C12C | 117.76 (16) |
| C11A—C10A—C9A | 120.57 (19) | C7D—N1D—N2D | 111.97 (15) |
| C15A—C10A—C9A | 120.65 (18) | C7D—N1D—C6D | 128.50 (17) |
| C10A—C11A—C12A | 120.12 (19) | N2D—N1D—C6D | 119.53 (16) |
| C10A—C11A—H11A | 119.9 | C9D—N2D—N1D | 104.39 (16) |
| C12A—C11A—H11A | 119.9 | C6D—C1D—C2D | 119.0 (2) |
| C13A—C12A—C11A | 120.64 (19) | C6D—C1D—H1DA | 120.5 |
| C13A—C12A—C16A | 121.64 (19) | C2D—C1D—H1DA | 120.5 |
| C11A—C12A—C16A | 117.70 (19) | C3D—C2D—C1D | 120.8 (2) |
| C14A—C13A—C12A | 119.4 (2) | C3D—C2D—H2DA | 119.6 |
| C14A—C13A—H13A | 120.3 | C1D—C2D—H2DA | 119.6 |
| C12A—C13A—H13A | 120.3 | C4D—C3D—C2D | 119.66 (19) |
| C15A—C14A—C13A | 120.1 (2) | C4D—C3D—H3DA | 120.2 |
| C15A—C14A—H14A | 120.0 | C2D—C3D—H3DA | 120.2 |
| C13A—C14A—H14A | 120.0 | C3D—C4D—C5D | 120.5 (2) |
| C14A—C15A—C10A | 120.93 (19) | C3D—C4D—H4DA | 119.7 |
| C14A—C15A—H15A | 119.5 | C5D—C4D—H4DA | 119.7 |
| C10A—C15A—H15A | 119.5 | C6D—C5D—C4D | 119.0 (2) |
| O1A—C16A—O2A | 123.60 (18) | C6D—C5D—H5DA | 120.5 |

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| O1A—C16A—C12A | 122.29 (19) | C4D—C5D—H5DA | 120.5 |
| O2A—C16A—C12A | 114.10 (18) | C1D—C6D—C5D | 121.04 (18) |
| C16B—O2B—H1OB | 109.8 (19) | C1D—C6D—N1D | 119.29 (18) |
| N2B—N1B—C7B | 111.66 (17) | C5D—C6D—N1D | 119.67 (19) |
| N2B—N1B—C6B | 120.00 (17) | N1D—C7D—C8D | 107.07 (18) |
| C7B—N1B—C6B | 128.33 (19) | N1D—C7D—H7DA | 126.5 |
| C9B—N2B—N1B | 104.95 (16) | C8D—C7D—H7DA | 126.5 |
| C6B—C1B—C2B | 119.8 (2) | C7D—C8D—C9D | 105.26 (18) |
| C6B—C1B—H1BA | 120.1 | C7D—C8D—H8DA | 127.4 |
| C2B—C1B—H1BA | 120.1 | C9D—C8D—H8DA | 127.4 |
| C3B—C2B—C1B | 119.9 (2) | N2D—C9D—C8D | 111.31 (17) |
| C3B—C2B—H2BA | 120.0 | N2D—C9D—C10D | 119.98 (18) |
| C1B—C2B—H2BA | 120.0 | C8D—C9D—C10D | 128.71 (17) |
| C2B—C3B—C4B | 120.0 (2) | C15D—C10D—C11D | 118.67 (17) |
| C2B—C3B—H3BA | 120.0 | C15D—C10D—C9D | 120.79 (17) |
| C4B—C3B—H3BA | 120.0 | C11D—C10D—C9D | 120.54 (18) |
| C5B—C4B—C3B | 120.5 (2) | C12D—C11D—C10D | 120.91 (18) |
| C5B—C4B—H4BA | 119.7 | C12D—C11D—H11D | 119.5 |
| C3B—C4B—H4BA | 119.7 | C10D—C11D—H11D | 119.5 |
| C4B—C5B—C6B | 119.3 (2) | C13D—C12D—C11D | 119.53 (17) |
| C4B—C5B—H5BA | 120.3 | C13D—C12D—C16D | 120.82 (17) |
| C6B—C5B—H5BA | 120.3 | C11D—C12D—C16D | 119.63 (17) |
| C1B—C6B—C5B | 120.43 (19) | C12D—C13D—C14D | 120.13 (18) |
| C1B—C6B—N1B | 119.14 (19) | C12D—C13D—H13D | 119.9 |
| C5B—C6B—N1B | 120.42 (19) | C14D—C13D—H13D | 119.9 |
| N1B—C7B—C8B | 107.2 (2) | C15D—C14D—C13D | 120.21 (19) |
| N1B—C7B—H7BA | 126.4 | C15D—C14D—H14D | 119.9 |
| C8B—C7B—H7BA | 126.4 | C13D—C14D—H14D | 119.9 |
| C7B—C8B—C9B | 105.23 (19) | C14D—C15D—C10D | 120.55 (18) |
| C7B—C8B—H8BA | 127.4 | C14D—C15D—H15D | 119.7 |
| C9B—C8B—H8BA | 127.4 | C10D—C15D—H15D | 119.7 |
| N2B—C9B—C8B | 111.01 (18) | O1D—C16D—O2D | 123.56 (17) |
| N2B—C9B—C10B | 119.97 (18) | O1D—C16D—C12D | 119.06 (17) |
| C8B—C9B—C10B | 128.95 (18) | O2D—C16D—C12D | 117.38 (17) |
| C15B—C10B—C11B | 118.17 (19) | C17—O3—H1O3 | 105 (2) |
| C15B—C10B—C9B | 120.05 (18) | Li2—O3—H1O3 | 123 (2) |
| C11B—C10B—C9B | 121.70 (19) | O3—C17—C18 | 111.84 (19) |
| C12B—C11B—C10B | 120.53 (19) | O3—C17—H17A | 109.2 |
| C12B—C11B—H11B | 119.7 | C18—C17—H17A | 109.2 |
| C10B—C11B—H11B | 119.7 | O3—C17—H17B | 109.2 |
| C13B—C12B—C11B | 120.52 (18) | C18—C17—H17B | 109.2 |
| C13B—C12B—C16B | 120.77 (19) | H17A—C17—H17B | 107.9 |
| C11B—C12B—C16B | 118.61 (18) | C17—C18—H18A | 109.5 |
| C12B—C13B—C14B | 119.3 (2) | C17—C18—H18B | 109.5 |
| C12B—C13B—H13B | 120.3 | H18A—C18—H18B | 109.5 |
| C14B—C13B—H13B | 120.3 | C17—C18—H18C | 109.5 |
| C15B—C14B—C13B | 120.1 (2) | H18A—C18—H18C | 109.5 |
| C15B—C14B—H14B | 119.9 | H18B—C18—H18C | 109.5 |
| C13B—C14B—H14B | 119.9 | C19—O4—H1O4 | 106.9 (19) |

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| C14B—C15B—C10B | 121.29 (19) | Li1—O4—H1O4 | 118.8 (19) |
| C14B—C15B—H15B | 119.4 | O4—C19—C20 | 111.6 (2) |
| C10B—C15B—H15B | 119.4 | O4—C19—H19A | 109.3 |
| O1B—C16B—O2B | 124.17 (18) | C20—C19—H19A | 109.3 |
| O1B—C16B—C12B | 121.93 (19) | O4—C19—H19B | 109.3 |
| O2B—C16B—C12B | 113.89 (18) | C20—C19—H19B | 109.3 |
| C7C—N1C—N2C | 111.96 (16) | H19A—C19—H19B | 108.0 |
| C7C—N1C—C6C | 128.46 (17) | C19—C20—H20A | 109.5 |
| N2C—N1C—C6C | 119.58 (16) | C19—C20—H20B | 109.5 |
| C9C—N2C—N1C | 104.77 (16) | H20A—C20—H20B | 109.5 |
| C2C—C1C—C6C | 119.3 (2) | C19—C20—H20C | 109.5 |
| C2C—C1C—H1CA | 120.4 | H20A—C20—H20C | 109.5 |
| C6C—C1C—H1CA | 120.4 | H20B—C20—H20C | 109.5 |
| O2D—Li1—O1A—C16A | −174.1 (2) | N2C—N1C—C6C—C1C | −29.7 (3) |
| O4—Li1—O1A—C16A | 64.3 (3) | N2C—N1C—C7C—C8C | −0.1 (2) |
| O1C$^{i}$—Li1—O1A—C16A | −60.6 (3) | C6C—N1C—C7C—C8C | 178.71 (19) |
| C16C$^{i}$—Li1—O1A—C16A | −36.5 (3) | N1C—C7C—C8C—C9C | −0.2 (2) |
| C7A—N1A—N2A—C9A | 0.4 (2) | N1C—N2C—C9C—C8C | −0.4 (2) |
| C6A—N1A—N2A—C9A | 178.84 (18) | N1C—N2C—C9C—C10C | 179.91 (17) |
| C6A—C1A—C2A—C3A | −0.4 (4) | C7C—C8C—C9C—N2C | 0.4 (2) |
| C1A—C2A—C3A—C4A | −0.8 (4) | C7C—C8C—C9C—C10C | −180.0 (2) |
| C2A—C3A—C4A—C5A | 1.3 (4) | N2C—C9C—C10C—C15C | 14.1 (3) |
| C3A—C4A—C5A—C6A | −0.7 (4) | C8C—C9C—C10C—C15C | −165.4 (2) |
| C2A—C1A—C6A—C5A | 0.9 (4) | N2C—C9C—C10C—C11C | −166.31 (19) |
| C2A—C1A—C6A—N1A | −178.3 (2) | C8C—C9C—C10C—C11C | 14.1 (3) |
| C4A—C5A—C6A—C1A | −0.4 (4) | C15C—C10C—C11C—C12C | 0.2 (3) |
| C4A—C5A—C6A—N1A | 178.8 (2) | C9C—C10C—C11C—C12C | −179.32 (18) |
| C7A—N1A—C6A—C1A | −170.6 (2) | C10C—C11C—C12C—C13C | −0.7 (3) |
| N2A—N1A—C6A—C1A | 11.3 (3) | C10C—C11C—C12C—C16C | 178.23 (18) |
| C7A—N1A—C6A—C5A | 10.1 (4) | C11C—C12C—C13C—C14C | 0.7 (3) |
| N2A—N1A—C6A—C5A | −168.0 (2) | C16C—C12C—C13C—C14C | −178.26 (18) |
| N2A—N1A—C7A—C8A | −0.4 (3) | C12C—C13C—C14C—C15C | −0.2 (3) |
| C6A—N1A—C7A—C8A | −178.7 (2) | C13C—C14C—C15C—C10C | −0.2 (3) |
| N1A—C7A—C8A—C9A | 0.3 (3) | C11C—C10C—C15C—C14C | 0.2 (3) |
| N1A—N2A—C9A—C8A | −0.2 (2) | C9C—C10C—C15C—C14C | 179.79 (18) |
| N1A—N2A—C9A—C10A | −179.50 (18) | Li1$^{ii}$—O1C—C16C—O2C | −21.6 (3) |
| C7A—C8A—C9A—N2A | 0.0 (3) | Li1$^{ii}$—O1C—C16C—C12C | 159.17 (18) |
| C7A—C8A—C9A—C10A | 179.2 (2) | Li2—O2C—C16C—O1C | 121.9 (2) |
| N2A—C9A—C10A—C11A | 168.5 (2) | Li2—O2C—C16C—C12C | −58.9 (3) |
| C8A—C9A—C10A—C11A | −10.6 (4) | Li2—O2C—C16C—Li1$^{ii}$ | 108.4 (2) |
| N2A—C9A—C10A—C15A | −11.2 (3) | C11C—C12C—C16C—O1C | −6.9 (3) |
| C8A—C9A—C10A—C15A | 169.7 (2) | C13C—C12C—C16C—O1C | 172.00 (19) |
| C15A—C10A—C11A—C12A | 1.1 (3) | C11C—C12C—C16C—O2C | 173.83 (18) |
| C9A—C10A—C11A—C12A | −178.6 (2) | C13C—C12C—C16C—O2C | −7.3 (3) |
| C10A—C11A—C12A—C13A | −0.9 (3) | C11C—C12C—C16C—Li1$^{ii}$ | 22.7 (4) |
| C10A—C11A—C12A—C16A | 177.42 (19) | C13C—C12C—C16C—Li1$^{ii}$ | −158.4 (3) |
| C11A—C12A—C13A—C14A | 0.3 (4) | O2C—Li2—O1D—C16D | −162.18 (17) |

| | | | |
|---|---|---|---|
| C16A—C12A—C13A—C14A | −177.9 (2) | O1B—Li2—O1D—C16D | 77.0 (2) |
| C12A—C13A—C14A—C15A | 0.0 (4) | O3—Li2—O1D—C16D | −36.4 (3) |
| C13A—C14A—C15A—C10A | 0.2 (4) | O1A—Li1—O2D—C16D | −1.3 (3) |
| C11A—C10A—C15A—C14A | −0.8 (3) | O4—Li1—O2D—C16D | 113.3 (2) |
| C9A—C10A—C15A—C14A | 178.9 (2) | O1C$^{i}$—Li1—O2D—C16D | −118.9 (2) |
| Li1—O1A—C16A—O2A | 14.2 (4) | C16C$^{i}$—Li1—O2D—C16D | −128.7 (2) |
| Li1—O1A—C16A—C12A | −165.4 (2) | C7D—N1D—N2D—C9D | 0.4 (2) |
| C13A—C12A—C16A—O1A | −176.8 (2) | C6D—N1D—N2D—C9D | −179.65 (17) |
| C11A—C12A—C16A—O1A | 4.9 (3) | C6D—C1D—C2D—C3D | 0.5 (3) |
| C13A—C12A—C16A—O2A | 3.6 (3) | C1D—C2D—C3D—C4D | −0.8 (3) |
| C11A—C12A—C16A—O2A | −174.68 (19) | C2D—C3D—C4D—C5D | −0.2 (4) |
| O2C—Li2—O1B—C16B | 165.81 (19) | C3D—C4D—C5D—C6D | 1.3 (3) |
| O1D—Li2—O1B—C16B | −78.4 (3) | C2D—C1D—C6D—C5D | 0.6 (3) |
| O3—Li2—O1B—C16B | 45.0 (3) | C2D—C1D—C6D—N1D | −178.75 (19) |
| C16D—Li2—O1B—C16B | −55.5 (2) | C4D—C5D—C6D—C1D | −1.5 (3) |
| C7B—N1B—N2B—C9B | 0.3 (2) | C4D—C5D—C6D—N1D | 177.85 (19) |
| C6B—N1B—N2B—C9B | 179.24 (18) | C7D—N1D—C6D—C1D | 151.3 (2) |
| C6B—C1B—C2B—C3B | −0.8 (4) | N2D—N1D—C6D—C1D | −28.6 (3) |
| C1B—C2B—C3B—C4B | −0.1 (4) | C7D—N1D—C6D—C5D | −28.1 (3) |
| C2B—C3B—C4B—C5B | 0.9 (4) | N2D—N1D—C6D—C5D | 152.06 (19) |
| C3B—C4B—C5B—C6B | −0.7 (4) | N2D—N1D—C7D—C8D | −0.1 (2) |
| C2B—C1B—C6B—C5B | 1.0 (3) | C6D—N1D—C7D—C8D | −179.99 (19) |
| C2B—C1B—C6B—N1B | −179.9 (2) | N1D—C7D—C8D—C9D | −0.3 (2) |
| C4B—C5B—C6B—C1B | −0.2 (4) | N1D—N2D—C9D—C8D | −0.6 (2) |
| C4B—C5B—C6B—N1B | −179.4 (2) | N1D—N2D—C9D—C10D | 180.00 (17) |
| N2B—N1B—C6B—C1B | 1.4 (3) | C7D—C8D—C9D—N2D | 0.6 (2) |
| C7B—N1B—C6B—C1B | −179.8 (2) | C7D—C8D—C9D—C10D | 179.9 (2) |
| N2B—N1B—C6B—C5B | −179.4 (2) | N2D—C9D—C10D—C15D | 11.7 (3) |
| C7B—N1B—C6B—C5B | −0.7 (3) | C8D—C9D—C10D—C15D | −167.5 (2) |
| N2B—N1B—C7B—C8B | −0.3 (3) | N2D—C9D—C10D—C11D | −168.53 (18) |
| C6B—N1B—C7B—C8B | −179.1 (2) | C8D—C9D—C10D—C11D | 12.2 (3) |
| N1B—C7B—C8B—C9B | 0.1 (3) | C15D—C10D—C11D—C12D | −0.2 (3) |
| N1B—N2B—C9B—C8B | −0.2 (2) | C9D—C10D—C11D—C12D | −179.91 (18) |
| N1B—N2B—C9B—C10B | −177.43 (18) | C10D—C11D—C12D—C13D | −0.6 (3) |
| C7B—C8B—C9B—N2B | 0.1 (3) | C10D—C11D—C12D—C16D | 177.67 (18) |
| C7B—C8B—C9B—C10B | 177.0 (2) | C11D—C12D—C13D—C14D | 0.6 (3) |
| N2B—C9B—C10B—C15B | 5.5 (3) | C16D—C12D—C13D—C14D | −177.66 (18) |
| C8B—C9B—C10B—C15B | −171.1 (2) | C12D—C13D—C14D—C15D | 0.2 (3) |
| N2B—C9B—C10B—C11B | −177.91 (19) | C13D—C14D—C15D—C10D | −1.0 (3) |
| C8B—C9B—C10B—C11B | 5.4 (3) | C11D—C10D—C15D—C14D | 1.0 (3) |
| C15B—C10B—C11B—C12B | −1.1 (3) | C9D—C10D—C15D—C14D | −179.27 (18) |
| C9B—C10B—C11B—C12B | −177.69 (19) | Li2—O1D—C16D—O2D | −17.1 (3) |
| C10B—C11B—C12B—C13B | 0.7 (3) | Li2—O1D—C16D—C12D | 163.43 (18) |
| C10B—C11B—C12B—C16B | 177.13 (19) | Li1—O2D—C16D—O1D | 121.8 (2) |
| C11B—C12B—C13B—C14B | −0.3 (4) | Li1—O2D—C16D—C12D | −58.7 (3) |
| C16B—C12B—C13B—C14B | −176.6 (2) | Li1—O2D—C16D—Li2 | 111.5 (2) |
| C12B—C13B—C14B—C15B | 0.1 (4) | C13D—C12D—C16D—O1D | 171.96 (18) |
| C13B—C14B—C15B—C10B | −0.5 (4) | C11D—C12D—C16D—O1D | −6.3 (3) |

| | | | |
|---|---|---|---|
| C11B—C10B—C15B—C14B | 1.0 (4) | C13D—C12D—C16D—O2D | −7.5 (3) |
| C9B—C10B—C15B—C14B | 177.6 (2) | C11D—C12D—C16D—O2D | 174.21 (18) |
| Li2—O1B—C16B—O2B | 31.3 (3) | C13D—C12D—C16D—Li2 | −165.2 (3) |
| Li2—O1B—C16B—C12B | −147.2 (2) | C11D—C12D—C16D—Li2 | 16.6 (4) |
| C13B—C12B—C16B—O1B | 171.3 (2) | O2C—Li2—C16D—O1D | 21.7 (2) |
| C11B—C12B—C16B—O1B | −5.1 (3) | O1B—Li2—C16D—O1D | −109.0 (2) |
| C13B—C12B—C16B—O2B | −7.4 (3) | O3—Li2—C16D—O1D | 147.7 (2) |
| C11B—C12B—C16B—O2B | 176.24 (19) | O2C—Li2—C16D—O2D | −172.6 (2) |
| O1B—Li2—O2C—C16C | −2.6 (3) | O1B—Li2—C16D—O2D | 56.79 (17) |
| O1D—Li2—O2C—C16C | −120.3 (2) | O1D—Li2—C16D—O2D | 165.8 (2) |
| O3—Li2—O2C—C16C | 111.5 (2) | O3—Li2—C16D—O2D | −46.51 (16) |
| C16D—Li2—O2C—C16C | −128.9 (2) | O2C—Li2—C16D—C12D | −12.3 (5) |
| C7C—N1C—N2C—C9C | 0.3 (2) | O1B—Li2—C16D—C12D | −143.0 (3) |
| C6C—N1C—N2C—C9C | −178.58 (17) | O1D—Li2—C16D—C12D | −34.0 (4) |
| C6C—C1C—C2C—C3C | 1.2 (3) | O3—Li2—C16D—C12D | 113.7 (3) |
| C1C—C2C—C3C—C4C | −1.5 (4) | O2C—Li2—O3—C17 | 27.5 (3) |
| C2C—C3C—C4C—C5C | 0.2 (4) | O1B—Li2—O3—C17 | 148.46 (19) |
| C3C—C4C—C5C—C6C | 1.3 (4) | O1D—Li2—O3—C17 | −94.3 (3) |
| C4C—C5C—C6C—C1C | −1.5 (3) | C16D—Li2—O3—C17 | −107.9 (2) |
| C4C—C5C—C6C—N1C | 178.3 (2) | Li2—O3—C17—C18 | −133.1 (2) |
| C2C—C1C—C6C—C5C | 0.3 (3) | O1A—Li1—O4—C19 | 150.1 (2) |
| C2C—C1C—C6C—N1C | −179.53 (19) | O2D—Li1—O4—C19 | 27.6 (3) |
| C7C—N1C—C6C—C5C | −28.2 (3) | O1C$^{i}$—Li1—O4—C19 | −91.3 (3) |
| N2C—N1C—C6C—C5C | 150.5 (2) | C16C$^{i}$—Li1—O4—C19 | −104.9 (2) |
| C7C—N1C—C6C—C1C | 151.6 (2) | Li1—O4—C19—C20 | −133.6 (2) |

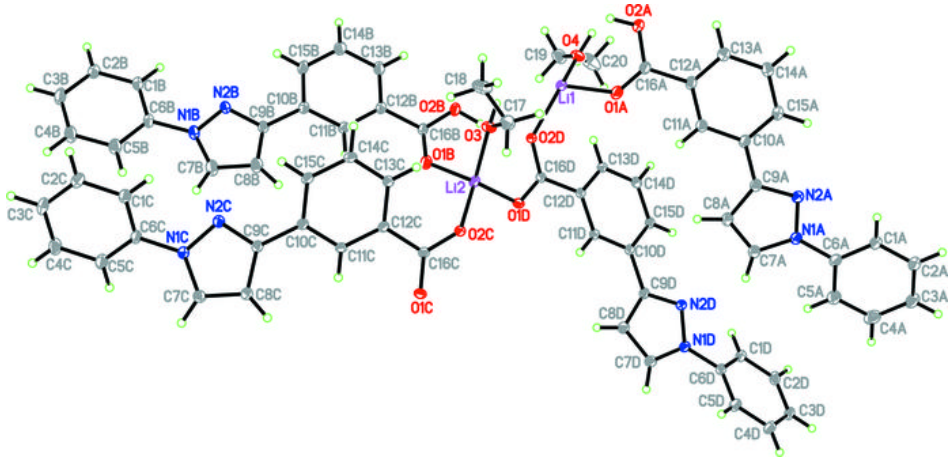
Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*, *z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2A—H1OA···O2C$^{i}$ | 0.91 (3) | 1.70 (3) | 2.594 (2) | 167 (3) |
| O2B—H1OB···O2D | 0.92 (3) | 1.68 (3) | 2.584 (2) | 165 (3) |
| O3—H1O3···O1C$^{i}$ | 0.85 (3) | 1.92 (3) | 2.761 (2) | 171 (3) |
| O4—H1O4···O1D$^{i}$ | 0.85 (3) | 1.94 (3) | 2.780 (2) | 170 (2) |
| C7A—H7AA···N2D | 0.93 | 2.58 | 3.306 (3) | 136 |
| C5C—H5CA···N2B$^{ii}$ | 0.93 | 2.60 | 3.501 (3) | 163 |

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*, *z*.

**Fig. 1**


O2A
O4
C19
C20
C13A
C12A
C14A
C16A
C15A
Li1
O1A
C11A
C10A
C9A
N2A
C8A
N1A
C6A
C1A
C7A
C2A
C5A
C3A
C4A
C14B
C15B
C13B
C18
C17
C2B
C3B
C1B
C6B
N1B
N2B
C9B
C10B
C12B
O2B
C16B
O3
O2D
C4B
C5B
C11B
C14C
O1B
C7B
C8B
C15C
C13C
C16D
C13D
C14D
C2C
C1C
C3C
C6C
N1C
N2C
C9C
C10C
C11C
C12C
Li2
O1D
C12D
C15D
C11D
C10D
C4C
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C7C
C8C
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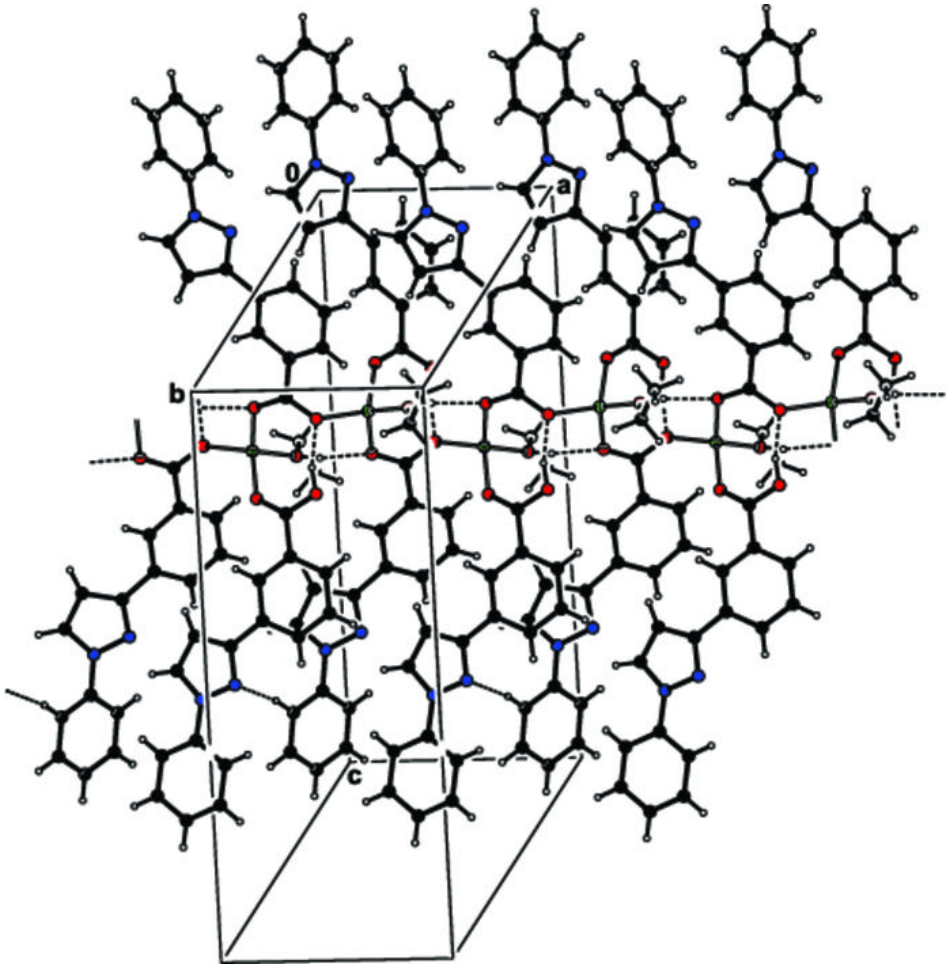
**Fig. 2**