Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

Crystal structure of dimethyl-1κ^2C-bis(μ-4-methylphenolato-1:2κ^2O:O)(N,N,N',N'-tetramethylethylenediamine-2κ^2N,N')-indium(III)lithium(I)

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Received 20 November 2015; accepted 6 December 2015

Edited by A. J. Lough, University of Toronto, Canada

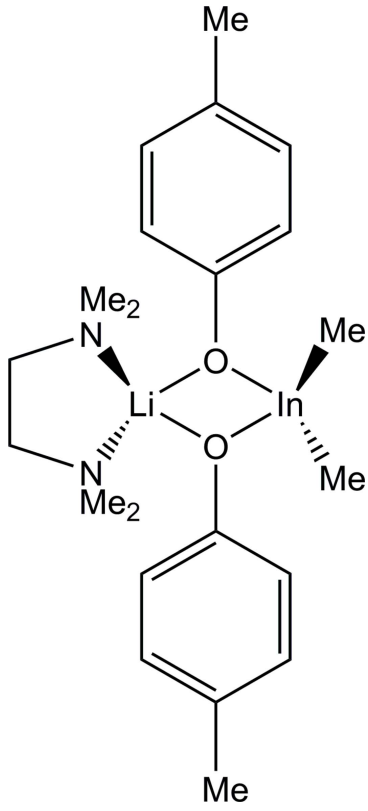
The mixed bimetallic title compound, $[InLi(CH_3)_2(C_7H_7O)_2(C_6H_{16}N_2)]$ or [(tmeda)Li-μ-(4-$MeC_6H_4O)_2InMe_2$] (tmeda is N,N,N',N'-tetramethylethylenediamine), exhibits a four-membered LiO_2In ring core *via* bridging 4-methylphenolate groups. The Li and In atoms are in distorted tetrahedral N_2O_2 and C_2O_2 bonding environments, respectively. The Li atom is further chelated by a tmeda group, yielding a spirocyclic structure.

Keywords: crystal structure; bimetallic; indium; lithium; phenolate; spirocyclic.

CCDC reference: 1440726

1. Related literature

For other bimetallic alkali–triel chalcogenolates, see: Niemeyer & Power (1997); Clegg *et al.* (1999); Muñoz *et al.* (2011, 2014); Uhl *et al.* (1994); Adonin *et al.* (2005); Soki *et al.* (2008); Normand *et al.* (2012). For metal-containing ligands, see Simmonds & Wright (2012). For organometallic precusors for indium tin oxide (ITO), see: Aksu & Driess (2009); Veith & Kunze (1991). For dimeric dimethylindium phenolates $[Me_2InOR]_2$, see: Briand *et al.* (2013, 2010); Beachley *et al.* (2003); Häusslein *et al.* (1999); Blake *et al.* (2011); Bradley *et al.* (1988); Trentler *et al.* (1997).



2. Experimental

2.1. Crystal data

$[InLi(CH_3)_2(C_7H_7O)_2(C_6H_{16}N_2)]$
M_r = 482.29
Monoclinic, $P2_1/c$
a = 9.0991 (8) Å
b = 16.4481 (15) Å
c = 16.4256 (15) Å
β = 91.956 (1)°
V = 2456.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 188 K
0.65 × 0.60 × 0.60 mm

2.2. Data collection

Bruker SMART1000/P4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.569, T_{max} = 0.591
16648 measured reflections
5459 independent reflections
4921 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.067
S = 1.05
5459 reflections
261 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008*b*).

Acknowledgements

This work was supported by the Natural Sciences and Engineering Research Council of Canada, the New Brunswick Innovation Foundation, the Canadian Foundation for Innovation and Mount Allison University.

Supporting information for this paper is available from the IUCr electronic archives (Reference: LH5799).

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supporting information

Acta Cryst. (2015). E**71**, m257–m258 [https://doi.org/10.1107/S2056989015023476]

Crystal structure of dimethyl-1κ^2C-bis(μ-4-methylphenolato-1:2κ^2O:O)(N,N,N',N'-tetramethylethylenediamine-2κ^2N,N')indium(III)lithium(I)

Glen G. Briand, Andreas Decken and Marshall R. Hoey

S1. Comment

Ligands containing metal bridgeheads are useful for the generation of mixed metal species with novel physical properties and reactivity (Simmonds *et al.*, 2012). In our efforts to generate organometallic In/Sn precusors for indium tin oxide (ITO) semiconductor species (Aksu *et al.*, 2009; Veith *et al.*, 1991), we have isolated the Li^+ salt of the anionic ligand [(4-$MeC_6H_4O)_2InMe_2]^-$. The structure of [(tmeda)Li-μ-(4-$MeC_6H_4O)_2InMe_2$] (tmeda = *N*,*N*,*N*′,*N*′-tetramethylethylenediamine) (**I**) (Fig. 1) exhibits a four-membered LiO_2In ring core in which Li1 and In1 centre are bridged via the oxygen atoms of two 4-MeC_6H_4O ligands. The In—O bond distances [In1—O1 = 2.125 (1), In1—O2 = 2.141 (1) Å] are larger than the Li—O bond distances [Li1—O1 = 1.889 (4), Li1—O2 = 1.926 (3) Å] as a result of the larger covalent radius of In versus Li. However, the LiO_2In ring is nearly planar [In1—O1—Li1—O2 = -4.5 (1)°]. In addition to the In—O bonds, In1 is also bonded to the carbon atoms of two methyl groups, resulting in a distorted tetrahedral C_2O_2 bonding environment for indium [O1—In1—O2 = 78.32 (5), C1—In1—C2 = 133.8 (1)°]. Li1 is also bonded to two nitrogen atoms of a chelating tmeda ligand, resulting in a distorted tetrahedral N_2O_2 bonding environment for lithium [O1—Li1—O2 = 89.9 (2), N1—In1—N2 = 86.8 (2)°]. The overall result is a bimetallic spirocyclic arrangement. The 4-MeC_6H_5 rings are displaced slightly toward the Me_2In group [C3—O1—In1 = 121.0 (1), C10—O2—In1 = 125.0 (1), C3—O1—Li1 = 142.4 (2), C10—O2—Li1 = 137.9 (2)°] and are nearly orthogonal [88.63 (6)°]. The geometries at the bridging O atoms are distorted trigonal planar [Σ X—O1—X = 360.0, Σ X—O2—X = 357.9°]. The structure resembles those of dimethylindium phenolates [$Me_2InOR]_2$, which form bimetallic species in the solid state *via* intermolecular In—O coordinate bonding interactions (Briand *et al.*, 2013; Briand *et al.*, 2010; Beachley *et al.*, 2003; Häußlein *et al.*, 1999; Blake *et al.*, 2011; Bradley *et al.*, 1988; Trentler *et al.*, 1997). These structures feature distorted tetrahedral geometries at In, distorted trigonal planar or slightly pyramidal geometries at O, and near planar In_2O_2 ring cores. For other bimetallic alkali-triel chalcogenolates, see: Niemeyer *et al.* (1997); Clegg *et al.* (1999); Muñoz *et al.* (2011); Uhl *et al.* (1994); Adonin *et al.* (2005); Soki *et al.* (2008); Muñoz *et al.* (2014); Normand *et al.* (2012).

S2. Synthesis and Crystallization

Synthesis of [(tmeda)Li-μ-(4-$MeC_6H_4O)_2InMe_2$]. [4-MeC_6H_4O]Li (0.143 g, 1.25 mmol) was added to a stirrred solution of $InMe_3$ (0.200 g, 1.25 mmol) in diethyl ether (10 mL). After1 h, 4-MeC_6H_4OH (0.064 g, 0.60 mmol) in diethyl ether (3 mL) was added. After 2 h, tmeda (0.145 g, 1.25 mmol) was added. After 1 h, the reaction mixture was filtered, and the filtrate concentrated to 5 mL and allowed to sit at 277 K. After 1 d, the solution was filtered to yield colourless crystals of **I** (0.188 g, 0.490 mmol, 82 %). Anal. Calc. for $C_{22}H_{36}InLiN_2O_2$: C, 54.78; H, 7.52; N, 5.81. Found: C, 54.56; H, 8.01; N, 5.67. Mp 426-428 K. FT-Raman (cm^{-1}): 127 s, 170 m, 297 w, 342 w, 502 *vs* [ν_{sym} (Me—In—Me)], 519 w [ν_{asym} (Me—In—Me)], 646 w, 766 m, 791 m, 857 m, 1155 m, 1212 w, 1288 w, 1383 w, 1438 w, 1607 w, 2841 w, 2921 m, 2959 m, 3045 w. ^{1}H NMR (thf-d_8, ppm): 0.00 (s, 6H, Me_2In), 2.31 (s, 6H, MeC_6H_4), 2.33 (s, 12H, Me_2N), 2.48 (s, 4H, NCH_2), 6.60 (d,

$^3J_{H—H}$ = 11 Hz, 4H, C_6H_4), 6.96 (d, $^3J_{H—H}$ = 11 Hz, 4H, C_6H_4). $^{13}C\{^1H\}$ NMR (thf-d_8, ppm): -1.8 (Me_2In), 19.8 (MeC_6H_4), 45.4 (Me_2N), 58.2 (NCH_2), 118.0 (C_6H_4), 129.5 (C_6H_4).

S3. Refinement

H atoms were included in calculated positions and refined using a riding model.

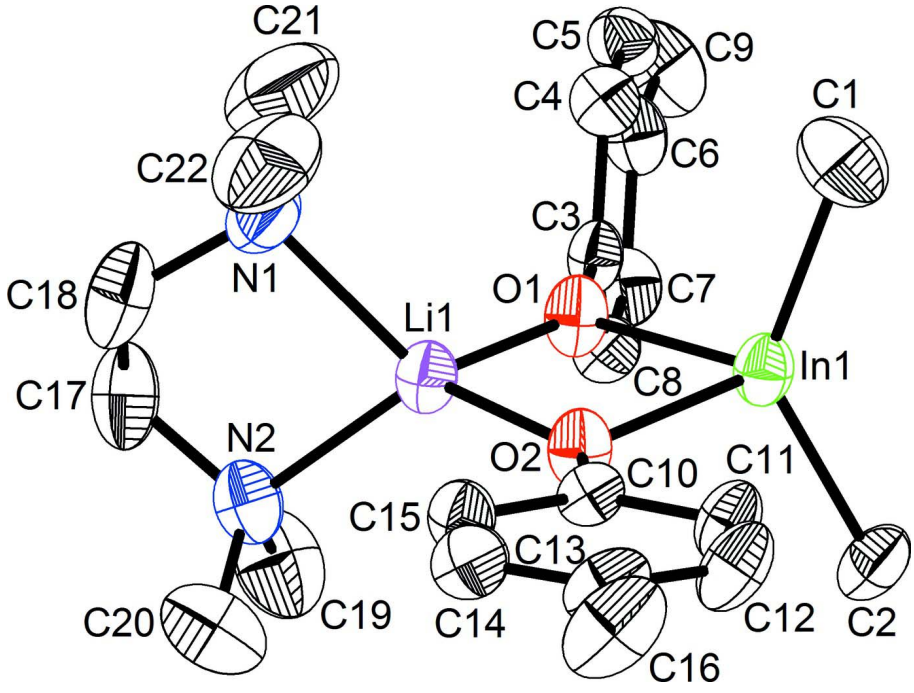

Figure 1

The molecular structure of (**I**), with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

Dimethyl-1κ^2C-bis(μ-4-methylphenolato-1:2κ^2O:O)(N,N,N',N'-tetramethylethylenediamine-2κ^2N,N')indium(III)lithium(I)

Crystal data

$[InLi(CH_3)_2(C_7H_7O)_2(C_6H_{16}N_2)]$
M_r = 482.29
Monoclinic, $P2_1/c$
a = 9.0991 (8) Å
b = 16.4481 (15) Å
c = 16.4256 (15) Å
β = 91.956 (1)°
V = 2456.9 (4) Å^3
Z = 4
$F(000)$ = 1000
D_x = 1.304 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5977 reflections
θ = 2.5–28.4°
μ = 0.98 mm^{-1}
T = 188 K
Irregular, colourless
0.65 × 0.60 × 0.60 mm

Data collection

Bruker SMART1000/P4 diffractometer
Radiation source: fine-focus sealed tube, K760
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.569, T_{max} = 0.591
16648 measured reflections
5459 independent reflections
4921 reflections with $I > 2\sigma(I)$

R_{int} = 0.025
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −11→11
k = −21→21
l = −21→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.067
S = 1.05
5459 reflections
261 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 1.1193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Experimental. Crystal decay was monitored by repeating the initial 50 frames at the end of the data collection and analyzing duplicate reflections

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
In1	0.26596 (2)	0.05874 (2)	0.78772 (2)	0.03548 (6)
O1	0.37283 (15)	0.14787 (8)	0.71713 (8)	0.0396 (3)
O2	0.12094 (14)	0.16051 (8)	0.79780 (8)	0.0390 (3)
Li1	0.2425 (4)	0.2341 (2)	0.7385 (2)	0.0375 (7)
N1	0.3343 (2)	0.34149 (12)	0.79061 (12)	0.0511 (5)
N2	0.1764 (2)	0.30590 (12)	0.63874 (11)	0.0489 (4)
C1	0.3935 (4)	0.04698 (19)	0.89888 (16)	0.0686 (8)
H1A	0.4979	0.0543	0.8879	0.103*
H1B	0.3783	−0.0072	0.9220	0.103*
H1C	0.3628	0.0884	0.9376	0.103*
C2	0.1651 (2)	−0.02775 (13)	0.70346 (14)	0.0475 (5)
H2A	0.0581	−0.0208	0.7024	0.071*
H2B	0.1899	−0.0831	0.7211	0.071*
H2C	0.2016	−0.0185	0.6488	0.071*
C3	0.4953 (2)	0.12953 (11)	0.67653 (11)	0.0333 (4)
C4	0.6347 (2)	0.13756 (12)	0.71342 (11)	0.0382 (4)
H4	0.6443	0.1558	0.7682	0.046*
C5	0.7597 (2)	0.11910 (13)	0.67083 (12)	0.0408 (4)
H5	0.8537	0.1252	0.6971	0.049*
C6	0.7502 (2)	0.09210 (13)	0.59107 (12)	0.0415 (4)
C7	0.6121 (2)	0.08379 (13)	0.55467 (12)	0.0426 (5)
H7	0.6032	0.0653	0.4999	0.051*
C8	0.4854 (2)	0.10193 (12)	0.59630 (12)	0.0384 (4)

H8	0.3917	0.0955	0.5699	0.046*
C9	0.8866 (3)	0.06967 (18)	0.54574 (16)	0.0625 (7)
H9A	0.9076	0.0117	0.5534	0.094*
H9B	0.9702	0.1018	0.5669	0.094*
H9C	0.8702	0.0810	0.4876	0.094*
C10	0.0086 (2)	0.16495 (12)	0.84883 (11)	0.0334 (4)
C11	−0.0424 (2)	0.09752 (13)	0.89039 (13)	0.0415 (4)
H11	0.0019	0.0460	0.8824	0.050*
C12	−0.1578 (3)	0.10467 (14)	0.94352 (14)	0.0502 (5)
H12	−0.1910	0.0575	0.9708	0.060*
C13	−0.2252 (2)	0.17834 (15)	0.95769 (13)	0.0471 (5)
C14	−0.1765 (2)	0.24514 (14)	0.91485 (13)	0.0458 (5)
H14	−0.2227	0.2963	0.9220	0.055*
C15	−0.0617 (2)	0.23886 (13)	0.86159 (12)	0.0407 (4)
H15	−0.0305	0.2859	0.8333	0.049*
C16	−0.3460 (3)	0.18714 (19)	1.01892 (18)	0.0705 (8)
H16A	−0.4306	0.2151	0.9931	0.106*
H16B	−0.3090	0.2188	1.0658	0.106*
H16C	−0.3762	0.1331	1.0372	0.106*
C17	0.2618 (4)	0.37967 (17)	0.64916 (18)	0.0716 (8)
H17A	0.2149	0.4236	0.6164	0.086*
H17B	0.3615	0.3706	0.6285	0.086*
C18	0.2747 (4)	0.40580 (16)	0.7358 (2)	0.0719 (8)
H18A	0.3396	0.4540	0.7399	0.086*
H18B	0.1764	0.4221	0.7540	0.086*
C19	0.2068 (4)	0.2688 (2)	0.55914 (15)	0.0742 (8)
H19A	0.1775	0.3065	0.5154	0.111*
H19B	0.1509	0.2181	0.5528	0.111*
H19C	0.3121	0.2571	0.5565	0.111*
C20	0.0174 (3)	0.3218 (2)	0.64082 (18)	0.0748 (8)
H20A	−0.0056	0.3462	0.6933	0.112*
H20B	−0.0365	0.2705	0.6339	0.112*
H20C	−0.0115	0.3592	0.5967	0.112*
C21	0.4918 (3)	0.3336 (2)	0.7846 (3)	0.1069 (14)
H21A	0.5149	0.3171	0.7291	0.160*
H21B	0.5284	0.2924	0.8233	0.160*
H21C	0.5389	0.3859	0.7972	0.160*
C22	0.2953 (4)	0.3605 (2)	0.87428 (18)	0.0885 (10)
H22A	0.3377	0.3194	0.9114	0.133*
H22B	0.1881	0.3606	0.8781	0.133*
H22C	0.3341	0.4142	0.8894	0.133*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.03663 (9)	0.03030 (8)	0.04007 (8)	−0.00028 (5)	0.00951 (6)	0.00208 (5)
O1	0.0382 (7)	0.0336 (7)	0.0480 (7)	0.0027 (6)	0.0178 (6)	0.0033 (6)
O2	0.0386 (7)	0.0350 (7)	0.0443 (7)	0.0027 (6)	0.0159 (6)	0.0039 (6)

Li1	0.0400 (17)	0.0319 (16)	0.0410 (16)	−0.0002 (13)	0.0065 (13)	0.0024 (13)
N1	0.0498 (11)	0.0399 (10)	0.0635 (12)	−0.0054 (8)	0.0004 (9)	−0.0099 (9)
N2	0.0563 (11)	0.0452 (10)	0.0454 (9)	0.0051 (9)	0.0050 (8)	0.0086 (8)
C1	0.0794 (19)	0.079 (2)	0.0467 (13)	0.0079 (15)	−0.0064 (13)	0.0139 (13)
C2	0.0454 (12)	0.0363 (11)	0.0613 (13)	−0.0092 (9)	0.0056 (10)	−0.0113 (10)
C3	0.0357 (9)	0.0257 (9)	0.0390 (9)	0.0004 (7)	0.0109 (7)	0.0026 (7)
C4	0.0403 (10)	0.0406 (10)	0.0338 (9)	0.0028 (8)	0.0047 (8)	−0.0026 (8)
C5	0.0340 (10)	0.0437 (11)	0.0449 (10)	0.0035 (8)	0.0025 (8)	0.0018 (9)
C6	0.0427 (11)	0.0387 (11)	0.0441 (10)	0.0097 (9)	0.0145 (9)	0.0038 (9)
C7	0.0524 (12)	0.0421 (11)	0.0337 (9)	0.0043 (9)	0.0078 (8)	−0.0047 (8)
C8	0.0375 (10)	0.0367 (10)	0.0411 (9)	−0.0021 (8)	0.0027 (8)	−0.0021 (8)
C9	0.0531 (14)	0.0774 (18)	0.0584 (14)	0.0221 (13)	0.0217 (12)	0.0033 (13)
C10	0.0319 (9)	0.0356 (10)	0.0329 (8)	−0.0025 (7)	0.0048 (7)	−0.0049 (7)
C11	0.0453 (11)	0.0326 (10)	0.0475 (10)	−0.0047 (8)	0.0158 (9)	−0.0079 (9)
C12	0.0567 (13)	0.0429 (12)	0.0525 (12)	−0.0154 (10)	0.0244 (10)	−0.0091 (10)
C13	0.0376 (10)	0.0536 (13)	0.0512 (11)	−0.0087 (9)	0.0145 (9)	−0.0189 (10)
C14	0.0381 (10)	0.0452 (12)	0.0546 (12)	0.0059 (9)	0.0073 (9)	−0.0123 (10)
C15	0.0388 (10)	0.0376 (10)	0.0461 (10)	0.0028 (8)	0.0073 (8)	−0.0001 (9)
C16	0.0580 (15)	0.0729 (18)	0.0832 (18)	−0.0151 (13)	0.0398 (14)	−0.0275 (15)
C17	0.093 (2)	0.0459 (14)	0.0762 (18)	−0.0046 (14)	0.0121 (16)	0.0229 (13)
C18	0.092 (2)	0.0334 (12)	0.091 (2)	−0.0066 (13)	0.0130 (17)	−0.0044 (13)
C19	0.100 (2)	0.077 (2)	0.0470 (13)	0.0161 (17)	0.0141 (14)	0.0074 (13)
C20	0.0626 (16)	0.100 (2)	0.0619 (15)	0.0196 (16)	−0.0017 (13)	0.0061 (16)
C21	0.0563 (18)	0.080 (2)	0.184 (4)	−0.0067 (16)	−0.005 (2)	−0.043 (3)
C22	0.117 (3)	0.085 (2)	0.0633 (17)	−0.023 (2)	−0.0025 (17)	−0.0287 (17)

Geometric parameters (Å, º)

In1—O1	2.1252 (13)	C9—H9B	0.9800
In1—C1	2.138 (3)	C9—H9C	0.9800
In1—O2	2.1414 (13)	C10—C11	1.391 (3)
In1—C2	2.167 (2)	C10—C15	1.393 (3)
O1—C3	1.352 (2)	C11—C12	1.393 (3)
O1—Li1	1.889 (4)	C11—H11	0.9500
O2—C10	1.346 (2)	C12—C13	1.382 (3)
O2—Li1	1.926 (3)	C12—H12	0.9500
Li1—N2	2.092 (4)	C13—C14	1.386 (3)
Li1—N1	2.122 (4)	C13—C16	1.522 (3)
N1—C21	1.446 (4)	C14—C15	1.389 (3)
N1—C22	1.465 (4)	C14—H14	0.9500
N1—C18	1.480 (4)	C15—H15	0.9500
N2—C17	1.448 (3)	C16—H16A	0.9800
N2—C20	1.471 (3)	C16—H16B	0.9800
N2—C19	1.478 (3)	C16—H16C	0.9800
C1—H1A	0.9800	C17—C18	1.487 (4)
C1—H1B	0.9800	C17—H17A	0.9900
C1—H1C	0.9800	C17—H17B	0.9900
C2—H2A	0.9800	C18—H18A	0.9900

C2—H2B	0.9800	C18—H18B	0.9900
C2—H2C	0.9800	C19—H19A	0.9800
C3—C4	1.393 (3)	C19—H19B	0.9800
C3—C8	1.394 (3)	C19—H19C	0.9800
C4—C5	1.389 (3)	C20—H20A	0.9800
C4—H4	0.9500	C20—H20B	0.9800
C5—C6	1.383 (3)	C20—H20C	0.9800
C5—H5	0.9500	C21—H21A	0.9800
C6—C7	1.380 (3)	C21—H21B	0.9800
C6—C9	1.514 (3)	C21—H21C	0.9800
C7—C8	1.392 (3)	C22—H22A	0.9800
C7—H7	0.9500	C22—H22B	0.9800
C8—H8	0.9500	C22—H22C	0.9800
C9—H9A	0.9800		

O1—In1—C1	106.45 (10)	C6—C9—H9C	109.5
O1—In1—O2	78.32 (5)	H9A—C9—H9C	109.5
C1—In1—O2	108.82 (9)	H9B—C9—H9C	109.5
O1—In1—C2	107.23 (7)	O2—C10—C11	122.42 (17)
C1—In1—C2	133.76 (11)	O2—C10—C15	120.24 (17)
O2—In1—C2	108.30 (8)	C11—C10—C15	117.34 (17)
C3—O1—Li1	142.41 (15)	C10—C11—C12	120.8 (2)
C3—O1—In1	121.02 (11)	C10—C11—H11	119.6
Li1—O1—In1	96.57 (11)	C12—C11—H11	119.6
C10—O2—Li1	137.92 (16)	C13—C12—C11	121.9 (2)
C10—O2—In1	125.00 (12)	C13—C12—H12	119.1
Li1—O2—In1	94.94 (11)	C11—C12—H12	119.1
O1—Li1—O2	89.85 (15)	C12—C13—C14	117.28 (18)
O1—Li1—N2	116.35 (17)	C12—C13—C16	122.0 (2)
O2—Li1—N2	126.61 (19)	C14—C13—C16	120.7 (2)
O1—Li1—N1	117.30 (18)	C13—C14—C15	121.4 (2)
O2—Li1—N1	122.97 (18)	C13—C14—H14	119.3
N2—Li1—N1	86.82 (15)	C15—C14—H14	119.3
C21—N1—C22	110.9 (3)	C14—C15—C10	121.3 (2)
C21—N1—C18	111.5 (3)	C14—C15—H15	119.4
C22—N1—C18	108.8 (2)	C10—C15—H15	119.4
C21—N1—Li1	105.9 (2)	C13—C16—H16A	109.5
C22—N1—Li1	116.8 (2)	C13—C16—H16B	109.5
C18—N1—Li1	102.62 (18)	H16A—C16—H16B	109.5
C17—N2—C20	111.9 (2)	C13—C16—H16C	109.5
C17—N2—C19	109.5 (2)	H16A—C16—H16C	109.5
C20—N2—C19	107.9 (2)	H16B—C16—H16C	109.5
C17—N2—Li1	103.99 (18)	N2—C17—C18	112.3 (2)
C20—N2—Li1	109.79 (18)	N2—C17—H17A	109.1
C19—N2—Li1	113.73 (18)	C18—C17—H17A	109.1
In1—C1—H1A	109.5	N2—C17—H17B	109.1
In1—C1—H1B	109.5	C18—C17—H17B	109.1
H1A—C1—H1B	109.5	H17A—C17—H17B	107.9

In1—C1—H1C	109.5	N1—C18—C17	113.0 (2)
H1A—C1—H1C	109.5	N1—C18—H18A	109.0
H1B—C1—H1C	109.5	C17—C18—H18A	109.0
In1—C2—H2A	109.5	N1—C18—H18B	109.0
In1—C2—H2B	109.5	C17—C18—H18B	109.0
H2A—C2—H2B	109.5	H18A—C18—H18B	107.8
In1—C2—H2C	109.5	N2—C19—H19A	109.5
H2A—C2—H2C	109.5	N2—C19—H19B	109.5
H2B—C2—H2C	109.5	H19A—C19—H19B	109.5
O1—C3—C4	121.17 (17)	N2—C19—H19C	109.5
O1—C3—C8	120.74 (17)	H19A—C19—H19C	109.5
C4—C3—C8	118.09 (17)	H19B—C19—H19C	109.5
C5—C4—C3	120.61 (17)	N2—C20—H20A	109.5
C5—C4—H4	119.7	N2—C20—H20B	109.5
C3—C4—H4	119.7	H20A—C20—H20B	109.5
C6—C5—C4	121.43 (19)	N2—C20—H20C	109.5
C6—C5—H5	119.3	H20A—C20—H20C	109.5
C4—C5—H5	119.3	H20B—C20—H20C	109.5
C7—C6—C5	117.92 (18)	N1—C21—H21A	109.5
C7—C6—C9	120.8 (2)	N1—C21—H21B	109.5
C5—C6—C9	121.2 (2)	H21A—C21—H21B	109.5
C6—C7—C8	121.53 (18)	N1—C21—H21C	109.5
C6—C7—H7	119.2	H21A—C21—H21C	109.5
C8—C7—H7	119.2	H21B—C21—H21C	109.5
C7—C8—C3	120.41 (19)	N1—C22—H22A	109.5
C7—C8—H8	119.8	N1—C22—H22B	109.5
C3—C8—H8	119.8	H22A—C22—H22B	109.5
C6—C9—H9A	109.5	N1—C22—H22C	109.5
C6—C9—H9B	109.5	H22A—C22—H22C	109.5
H9A—C9—H9B	109.5	H22B—C22—H22C	109.5