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# Crystal and molecular structures of two silver(I) amidinates, including an unexpected co-crystal with a lithium amidinate

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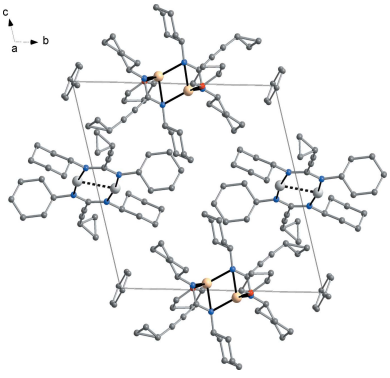
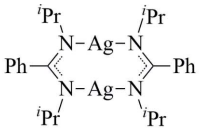
The silver(I) amidinates bis[$\mu$-$N^1$,$N^2$-bis(propan-2-yl)benzamidinato-$\kappa^2N^1$:$N^2$]-disilver(I), $[Ag_2(C_{13}H_{19}N_2)_2]$ or $[Ag\{PhC(N^iPr)_2\}]_2$ (**1**), and bis($\mu$-$N^1$,$N^2$-dicyclohexyl-3-cyclopropylpropynamidinato-$\kappa^2N^1$:$N^2$)disilver(I), $[Ag_2(C_{18}H_{27}N_2)_2]$ or $[Ag\{cyclo\text{-}C_3H_5\text{–}C{\equiv}C\text{–}C(NCy)_2\}]_2$ (**2a**), exist as centrosymmetric dimers with a planar $Ag_2N_4C_2$ ring and a common linear coordination of the metal atoms in the crystalline state. Moiety **2a** forms a co-crystal with the related lithium amidinate, namely bis($\mu$-$N^1$,$N^2$-dicyclohexyl-3-cyclopropylpropynamidinato-$\kappa^2N^1$:$N^2$)disilver(I) bis($\mu$-$N^1$,$N^2$-dicyclohexyl-3-cyclopropylpropynamidinato-$\kappa^3N^1$,$N^2$:$N^1$)bis(tetrahydrofuran-$\kappa O$)lithium(I) toluene monosolvate, $[Ag_2(C_{18}H_{27}N_2)_2][Li_2(C_{18}H_{27}N_2)_2(C_4H_8O)_2]\cdot C_7H_8$ or $[Ag\{cyclo\text{-}C_3H_5\text{–}C{\equiv}C\text{–}C(NCy)_2\}]_2[Li\{cyclo\text{-}C_3H_5\text{–}C{\equiv}C\text{–}C(NCy)_2\}(THF)]_2\cdot C_7H_8$, composed as **2a** × **2b** × toluene. The lithium moiety **2b** features a typical ladder-type dimeric structure with a distorted tetrahedral coordination of the metal atoms. In the silver(I) derivatives **1** and **2a**, the amidinate ligand adopts a $\mu$-$\kappa N$:$\kappa N'$ coordination, while it is a $\mu$-$\kappa N$:$\kappa N$:$\kappa N'$-coordination in the case of lithium derivative **2b**.

## 1. Chemical context

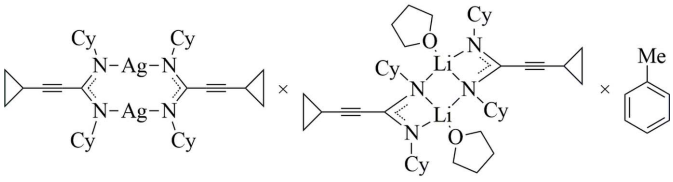
Anionic *N*-chelating donor ligands such as amidinates, $[RC(NR)_2]^-$, and guanidinates, $[R_2NC(NR)_2]^-$, have gained tremendous importance in various fields of organometallic and coordination chemistry over the past two decades. Formally, amidinate anions are the nitrogen analogues of the carboxylate anions, while guanidinates are similarly related to the carbamates. However, in contrast to the carboxylates and carbamates, the steric properties of amidinates and guanidinates can be widely tuned through the use of different substituents, both at the outer nitrogen atoms as well as at the central carbon atom of the NCN unit. Both types of *N*-chelating ligands are often regarded as 'steric cyclopentadienyl equivalents' (Bailey & Pace, 2001; Collins, 2011; Edelmann, 2008, 2013). Meanwhile, amidinato and guanidinato complexes are known for virtually every metallic element in the Periodic Table ranging from lithium to uranium (Edelmann, 2008, 2009, 2012, 2013; Trifonov, 2010). Alkyl-substituted amidinate and guanidinate complexes of various metals have also been established as ALD and MOCVD precursors for the deposition of thin layers of metals, metal oxides, metal nitrides *etc.* (Devi, 2013). The most important starting materials in this field are lithium amidinates and guanidinates. Lithium amidinates are normally prepared in a straightforward manner by addition of lithium alkyls to *N*,*N*′-diorganocarbodiimides in a 1:1 molar ratio, while lithium guanidinates



are formed when lithium-*N*,*N*-dialkylamides are added to *N*,*N*′-diorganocarbodiimides (Stalke *et al.*, 1992; Aharonovich *et al.*, 2008; Chlupatý *et al.*, 2011; Nevoralová *et al.*, 2013; Hong *et al.*, 2013). On the other hand, silver(I) amidinates and guanidinates (Archibald *et al.*, 2000; Lim *et al.*, 2003; Whitehorne *et al.*, 2011; Lane *et al.*, 2014) are of significant importance as potential precursors for vapor deposition processes (Lim *et al.*, 2003; Whitehorne *et al.*, 2011), as precursors for silver nanoparticles (Cure *et al.*, 2015), or as intermediates in silver-catalyzed amidination and guanylation reactions (Pereshivko *et al.*, 2011; Okano *et al.*, 2012; Li *et al.*, 2015).



**1**



**2**

We report here the structural characterization of two silver(I) amidinates, namely $[Ag\{PhC(N^iPr)_2\}]_2$ (**1**), and the unexpected co-crystal (**2**), composed as $[Ag\{cyclo\text{-}C_3H_5{-}C{\equiv}C{-}C(NCy)_2\}]_2$ (**2a**) × $[Li\{cyclo\text{-}C_3H_5{-}C{\equiv}C{-}C(NCy)_2\}(THF)]_2$ (**2b**) × toluene (Cy = cyclohexyl).

## 2. Structural commentary

Silver(I) compound **1** (Fig. 1) and silver moiety **2a** (Fig. 2): Both silver(I) complexes exist as centrosymmetric dimers in the crystalline state. Compound **1** crystallizes without any solvent, and the molecular structure of moiety **2a** was determined from the co-crystal **2** (**2a** × **2b** × toluene). In both **1** and **2a**, each of the two N atoms of the amidinate ligand coordinates to one Ag atom (coordination mode $\mu$-$\kappa N$:$\kappa N'$), and the Ag atoms adopt an almost linear coordination [**1**: N—Ag—N 170.58 (7)°; **2a**: N—Ag—N 170.66 (5)°] by two N atoms of two symmetry-related amidinate ligands, leading to centrosymmetric dimers in each case. The Ag—N separations are very similar in both structures [**1**: 2.0959 (16) and 2.0965 (16) Å, **2a**: 2.0908 (15) and 2.0916 (14) Å]. An $sp^2$ hybridization can be assigned to the N atoms since the coordination environment is almost trigonal–planar. The C—N separations within the amidinate NCN fragment are virtually equal [**1**: twice 1.322 (3) Å, **2a**: 1.329 (2) and 1.331 (2) Å], indicating a typical delocalization of the negative charge. Through the mentioned connectivity pattern, a strictly planar $C_2N_4Ag_2$ eight-membered ring with a short Ag···Ag contact is built [**1**: 2.6604 (3) Å, **2a**: 2.6838 (3) Å]. This constitution might be supported by some attractive $d^{10}$–$d^{10}$ interaction between the Ag atoms that have been frequently discussed in the literature (for a review, *e.g.* see: Jansen, 1987). The molecular structures of the here discussed compounds are closely related to those of the most previously described copper(I) and silver(I) amidinates, namely $[Cu_2\{RC(NR')_2\}_2]$ ($R$, $R'$ = Me, $^n$Bu; Li *et al.*, 2005) and $[M_2\{MeC(N^iPr)_2\}_2]$ ($M$ = Cu, Ag). However, in the case of $Ag\{MeC(N^iPr)_2\}$, also a trimeric structure $[Ag_3\{MeC(N^iPr)_2\}_3]$ was observed (Lim *et al.*, 2003). The bond lengths and angles involving the Ag atoms, *viz*. Ag—N and Ag—Ag distances and N—Ag—N angles, in the compounds discussed herein resemble those observed in the previously reported dimeric silver(I) amidinates. A dimerization or oligomerization under formation of linear N—*M*—N units is also typical for a broad ensemble of copper(I) and silver(I) complexes with other anionic nitrogen ligands, *e.g.* $[Cu_4(NR_2)_4]$ (*e.g.* $R$ = Me, Gambarotta *et al.*, 1987; $R$ = Et, Hope & Power, 1984; $R$ = $SiMe_3$, James *et al.*, 1998), $[Ag_4(N(SiMe_3)_2\}_4]$ and $[Ag_3(N,N,N',N'$-tetramethylpiperidyl$)_3]$ (Hitchcock *et al.*, 1996), $[Cu_2Tl_2(ThioSila)_2]$ and $[Ag_4(ThioSila)_2(THT)_2]$ (ThioSila = $\{Me_2Si(N\text{-}C_6H_4\text{-}2\text{-}SPh)_2\}^{2-}$, THT = tetrahydrothiophene; Liebing & Merzweiler,

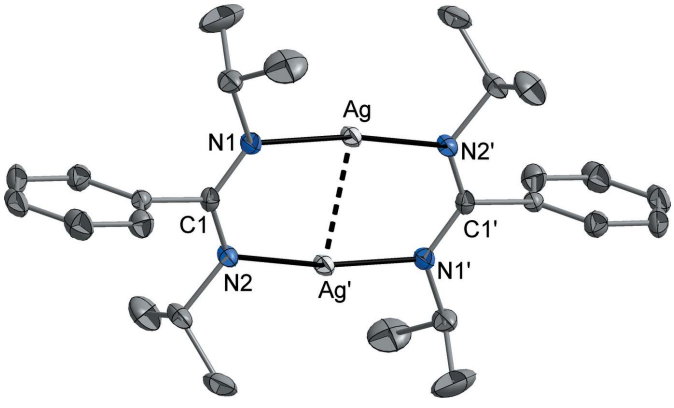



**Figure 1**
The molecular structure of compound **1**. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. [Symmetry code: (′) 2 − *x*, 2 − *y*, 1 − *z*.]

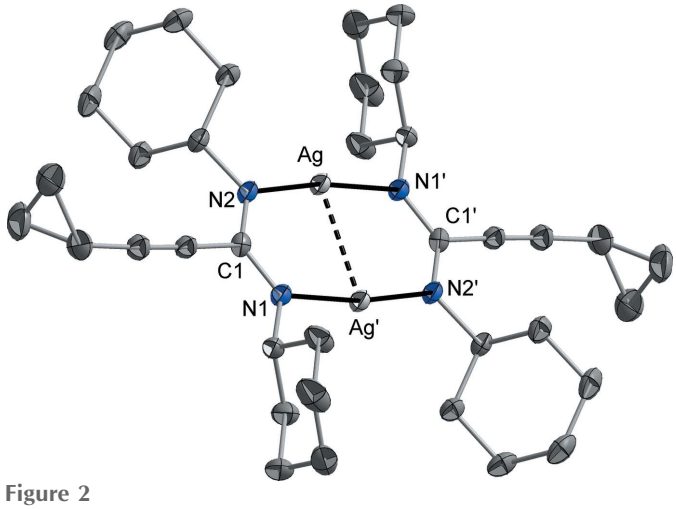



**Figure 2**
The molecular structure of moiety **2a**, determined from the co-crystal **2**. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. [Symmetry code: (′) 2 − *x*, 2 − *y*, 1 − *z*.]

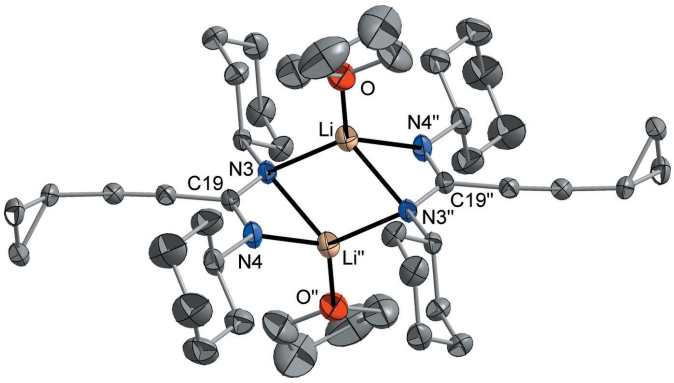



**Figure 3**
The molecular structure of moiety **2a**, determined from the co-crystal **2**. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. [Symmetry code: (″) $2-x, 1-y, -z$.]

2016). The silane diamide complexes $[M_4(\mathrm{ThioSila})_2]$ comprise a planar $Si_2N_4M_2$ ring that is structurally closely related to the $C_2N_4M_2$ ring in the dimeric amidinate complexes.

Lithium moiety **2b** (Fig. 3): The molecular structure of **2b** was determined from the above-mentioned co-crystal **2** (**2a** × **2b** × toluene). Like the silver components **1** and **2a**, the lithium moiety exists as a centrosymmetric dimer in the crystalline state. However, the molecular structure of **2b** is considerably different, featuring a centrosymmetric $Li_2N_2$ four-membered ring formed by $\mu$-bridging coordination of one of the N atoms (N3). The Li—N distances within this ring are 2.033 (4)–2.261 (4) Å and therefore in the expected range. The coordination number of the mentioned N atom N3 is consequently raised to four and an $sp^3$ hybridization fits best to describe the bonding situation. The second N atom of the amidinate ligand (N4) is attached to only one Li atom with a shorter Li—N bond of 2.001 (4) Å, and its coordination environment is trigonal–planar like in the related silver components. Through this $\mu$-$\kappa N$:$\kappa N$:$\kappa N'$-coordination mode of the amidinate ligands, a 'ladder' consisting of three four-membered rings is formed. By coordination of a solvent THF molecule, a typical distorted tetrahedral coordination of the Li atom is completed. Just like in the case of the silver components **1** and **2a**, the C—N bond lengths within the amidinate moiety are very similar with 1.321 (2) and 1.335 (2) Å. The structural motif of ladder-type dimers is typical for this class of compounds and has frequently been observed for most of the previously characterized lithium amidinates and guanidinates (Stalke *et al.*, 1992; Snaith & Wright, 1995; Downard & Chivers, 2001, Brown *et al.*, 2008).

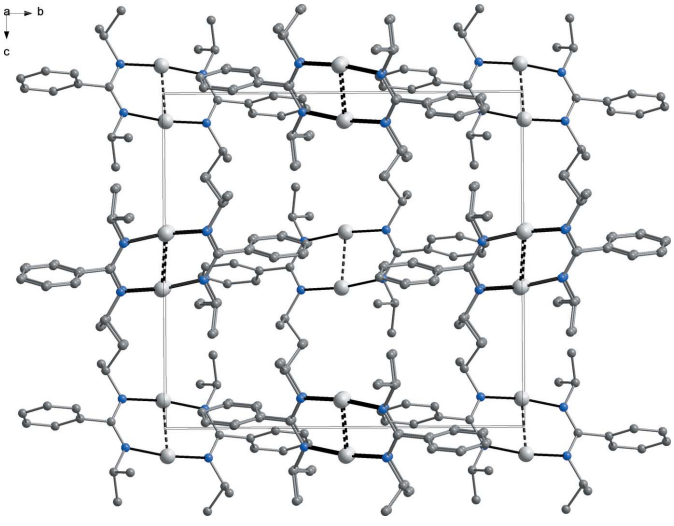



**Figure 4**
Crystal packing of dimeric silver(I) amidinate molecules in compound **1**, viewed in a projection on (100).

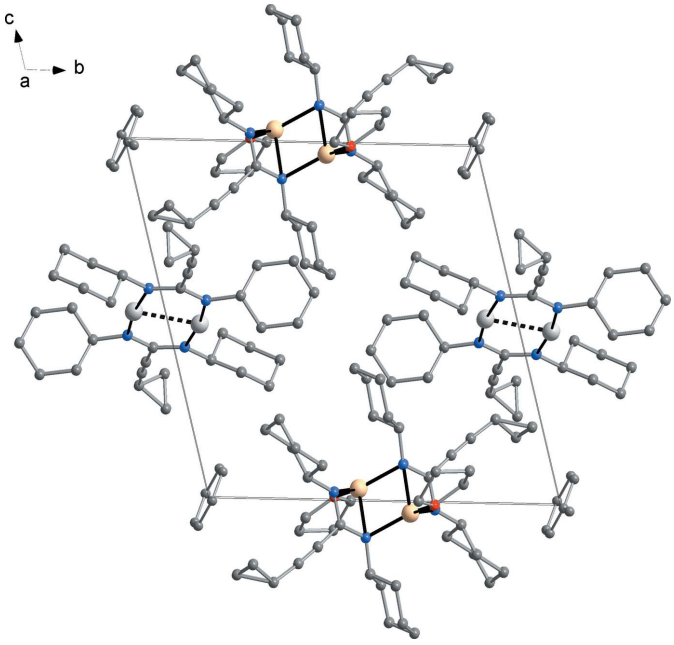



**Figure 5**
Crystal packing of silver(I) amidinate (**2a**), lithium amidinate (**2b**) and disordered toluene molecules in the co-crystal **2**, viewed in a projection on (100).

## 3. Supramolecular features

In both of the presented crystal structures, there are no specific intermolecular interactions. In compound **1** (Fig. 4), the closest intermolecular contacts exist between phenyl groups and isopropyl groups [min. HC···$CH_3$ 3.79 (1) Å]. In the co-crystal **2** (Fig. 5), four silver amidinate molecules (**2a**) are situated on the centres of the four unit-cell edges perpendicular to (001) and four lithium amidinate molecules (**2b**) on the four edges perpendicular to (010). The four remaining unit-cell edges perpendicular to (100) are occupied by four disordered toluene molecules. The closest intermolecular contacts exist between the cyclopropyl moieties of the silver complex and the toluene methyl groups [C6···C44 3.48 (1) Å], followed by cyclopropyl-cyclopropyl contacts between silver amidinate and lithium amidinate molecules [C5···C24 3.57 (1) Å].

**Table 1**
Experimental details.

| | **1** | **2** |
|---|---|---|
| Crystal data | | |
| Chemical formula | $[Ag_2(C_{13}H_{19}N_2)_2]$ | $[Ag_2(C_{18}H_{27}N_2)_2][Li_2(C_{18}H_{27}N_2)_2(C_4H_8O)_2]\cdot C_7H_8$ |
| $M_r$ | 622.34 | 1551.62 |
| Crystal system, space group | Orthorhombic, *Pbca* | Triclinic, $P\overline{1}$ |
| Temperature (K) | 153 | 133 |
| $a, b, c$ (Å) | 11.7112 (6), 15.9238 (6), 14.8703 (6) | 10.5880 (3), 14.5620 (4), 14.9830 (5) |
| $\alpha, \beta, \gamma$ (°) | 90, 90, 90 | 99.871 (2), 102.825 (2), 106.538 (2) |
| $V$ (Å$^3$) | 2773.1 (2) | 2090.17 (11) |
| $Z$ | 4 | 1 |
| Radiation type | Mo $K\alpha$ | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.43 | 0.52 |
| Crystal size (mm) | 0.23 × 0.21 × 0.09 | 0.44 × 0.29 × 0.27 |
| Data collection | | |
| Diffractometer | Stoe IPDS 2T | Stoe IPDS 2T |
| Absorption correction | Numerical (*X-AREA* and *X-RED*; Stoe & Cie, 2002) | – |
| $T_{min}$, $T_{max}$ | 0.713, 0.874 | – |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 9641, 3026, 2360 | 22444, 9099, 8214 |
| $R_{int}$ | 0.030 | 0.043 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.639 | 0.639 |
| Refinement | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.024, 0.047, 0.99 | 0.028, 0.073, 1.03 |
| No. of reflections | 3026 | 9099 |
| No. of parameters | 150 | 461 |
| No. of restraints | 0 | 12 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.34, −0.29 | 0.40, −0.61 |

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXT2013* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999) and *publCIF* (Westrip, 2010).

## 4. Synthesis and crystallization

$[Ag_2\{PhC(N^iPr)_2\}_2]$ (**1**) was obtained following a published procedure (Lim *et al.*, 2003). Therefore, an *in situ* prepared solution of the lithium derivative $Li\{PhC(N^iPr)_2\}$ (Sroor *et al.*, 2013) in THF was treated with a stoichiometric amount of silver(I) chloride at room temperature (Fig. 6). Afterwards the solvent was removed *in vacuo*, the residue was extracted with toluene and the insoluble matter filtered off. After addition of an excess of *n*-pentane to the filtrate, large colorless crystals formed within few days at room temperature. $^1$H NMR (400.1 MHz, THF-$d_8$, 298 K): $\delta$ (p.p.m.) 7.45–7.04 (3×*m*, 10H, C*H* Ph), 3.21 (*sept*, 4H, C*H* $^i$Pr), 1.05 (*d*, 24H, C$H_3$ $^i$Pr). $^{13}$C NMR (100.6 MHz, THF-$d_8$, 298 K): $\delta$ (p.p.m.) 170.4 (N*C*N), 141.1 (*ipso-C* Ph), 128.6 (*C*H Ph), 127.3 (*C*H Ph), 126.7 (*para-C*H Ph), 49.3 (*C*H $^i$Pr), 28.1 (*C*H$_3$ $^i$Pr).

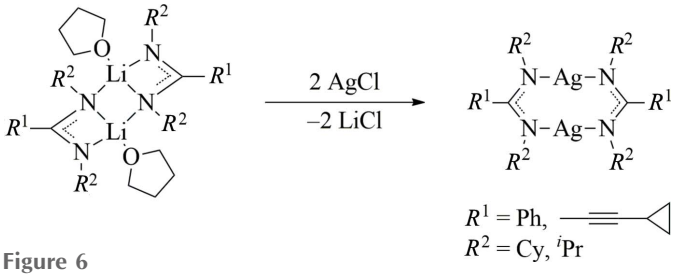



**Figure 6**
Synthesis of silver(I) amidinates from the related lithium derivatives.

Single crystals of the co-crystal (**2**) with composition $[Ag\{c\text{-}C_3H_5{-}C{\equiv}C{-}C(NCy)_2\}]_2$ (**2a**) × $[Li\{c\text{-}C_3H_5{-}C{\equiv}C{-}C(NCy)_2\}(THF)]_2$ (**2b**) × toluene were serendipitously obtained in an attempt to prepare the pure silver(I) derivative **2a**. The reaction of the *in situ* prepared lithium compound **2b** (Sroor *et al.*, 2013) with silver(I) chloride in THF analogous to the procedure described for compound **1** afforded a small quantity of colorless co-crystals of (**2**). Mp. = 393 K. $^1$H NMR (400.1 MHz, THF-$d_8$, 298 K): $\delta$ (p.p.m.): 3.31–3.40 (*m*, 4H, C*H* Cy), 1.55–1.72 (*m*, 20H, C$H_2$ Cy), 1.34–1.40 (*m*, 2H, C*H* *c*-$C_3H_5$), 1.09–1.23 (m, 20H, C$H_2$ Cy), 0.79–0.83 (*m*, 4H, C$H_2$ *c*-$C_3H_5$), 0.64–0.68 (*m*, 4H, C$H_2$ *c*-$C_3H_5$). $^{13}$C NMR (100.6 MHz, THF-$d_8$, 298 K): $\delta$ (p.p.m.) 156.5 (N*C*N), 96.6 (CH−*C*≡C), 69.2 (C≡*C*–-C), 58.8 (*C*H Cy), 38.8 (*C*H$_2$, Cy), 26.3 (*C*H$_2$ Cy), 8.83 (*C*H$_2$ *c*-$C_3H_5$), 0.37 (*C*H *c*-$C_3H_5$).

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were fixed geometrically and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C). C—H distances in $CH_3$ groups were constrained to 0.98 Å, those in $CH_2$ groups to 0.99 Å and those in CH groups to 1.00 Å. All $CH_3$ groups were refined as freely rotating around the C–C vector.

For compound **2**, the reflection (100) was partly obstructed by the beam stop and was therefore omitted from the refinement. The $U_{ij}$ components of the C atoms of the THF molecule (C41–C44) were restrained to be similar for atoms closer than 1.7 Å (SIMU restraint in *SHELXL*; the s.u. applied was 0.01 Å$^2$). The toluene molecule (C41–C44) is located on an inversion center. Consequently, the methyl group (C44) and the *para*-H atom (H64) are disordered over two positions and were refined with a constrained site occupancy factor of 0.5. The *ipso*-C and *para*-C atom (C42*A* and C42*B*) were refined to be equal (EXYZ and EADP restraints in *SHELXL*).

## Acknowledgements

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# supporting information

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## Crystal and molecular structures of two silver(I) amidinates, including an unexpected co-crystal with a lithium amidinate

**Sida Wang, Nicole Harmgarth, Phil Liebing and Frank T. Edelmann**

### Computing details

For both compounds, data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-AREA* and *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: SHELXT2013 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### (compound_1) Bis[$\mu$-$N^1$,$N^2$-bis(propan-2-yl)benzamidinato-$\kappa^2N^1$:$N^2$]disilver(I)

*Crystal data*

$[Ag_2(C_{13}H_{19}N_2)_2]$
$M_r$ = 622.34
Orthorhombic, *Pbca*
$a$ = 11.7112 (6) Å
$b$ = 15.9238 (6) Å
$c$ = 14.8703 (6) Å
$V$ = 2773.1 (2) Å$^3$
$Z$ = 4
$F$(000) = 1264
$D_x$ = 1.491 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 11797 reflections
$\theta$ = 2.6–29.1°
$\mu$ = 1.43 mm$^{-1}$
$T$ = 153 K
Plate, colorless
0.23 × 0.21 × 0.09 mm

*Data collection*

Stoe IPDS 2T diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.67 pixels mm$^{-1}$
area detector scans
Absorption correction: numerical (*X-AREA* and *X-RED*; Stoe & Cie, 2002)
$T_{min}$ = 0.713, $T_{max}$ = 0.874
9641 measured reflections
3026 independent reflections
2360 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.6°
$h$ = −12→14
$k$ = −17→20
$l$ = −18→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.047
$S$ = 0.99
3026 reflections
150 parameters
0 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

Extinction correction: SHELXL2016 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00133 (9)

*Special details*

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.89250 (17) | 0.84957 (11) | 0.52126 (14) | 0.0180 (4) |
| C2 | 0.84003 (17) | 0.76359 (12) | 0.53144 (14) | 0.0192 (4) |
| C3 | 0.72930 (18) | 0.75332 (14) | 0.56240 (15) | 0.0269 (5) |
| H1 | 0.684814 | 0.801041 | 0.577986 | 0.032* |
| C4 | 0.6834 (2) | 0.67346 (15) | 0.57063 (17) | 0.0339 (6) |
| H2 | 0.607343 | 0.666906 | 0.591646 | 0.041* |
| C5 | 0.7464 (2) | 0.60378 (15) | 0.54883 (17) | 0.0347 (6) |
| H3 | 0.714312 | 0.549257 | 0.554655 | 0.042* |
| C6 | 0.8568 (2) | 0.61370 (14) | 0.51837 (17) | 0.0347 (6) |
| H4 | 0.901066 | 0.565694 | 0.503496 | 0.042* |
| C7 | 0.9036 (2) | 0.69336 (13) | 0.50927 (16) | 0.0279 (5) |
| H5 | 0.979524 | 0.699645 | 0.487771 | 0.034* |
| C8 | 0.9646 (2) | 0.83508 (14) | 0.67386 (15) | 0.0307 (5) |
| H6 | 0.926464 | 0.779127 | 0.668444 | 0.037* |
| C9 | 1.0893 (3) | 0.82211 (19) | 0.6933 (2) | 0.0519 (8) |
| H7 | 1.097759 | 0.790334 | 0.749337 | 0.062* |
| H9 | 1.126925 | 0.876767 | 0.699461 | 0.062* |
| H8 | 1.124389 | 0.790784 | 0.643782 | 0.062* |
| C10 | 0.9090 (3) | 0.8841 (2) | 0.7489 (2) | 0.0657 (10) |
| H12 | 0.915326 | 0.852442 | 0.805200 | 0.079* |
| H10 | 0.828196 | 0.893125 | 0.734664 | 0.079* |
| H11 | 0.947262 | 0.938437 | 0.755509 | 0.079* |
| C11 | 0.8084 (2) | 0.85689 (12) | 0.37151 (15) | 0.0255 (5) |
| H13 | 0.793586 | 0.795930 | 0.382647 | 0.031* |
| C12 | 0.6952 (2) | 0.90348 (17) | 0.3702 (2) | 0.0431 (7) |
| H15 | 0.648800 | 0.883280 | 0.319816 | 0.052* |
| H16 | 0.709247 | 0.963797 | 0.363193 | 0.052* |
| H14 | 0.654535 | 0.893414 | 0.426792 | 0.052* |
| C13 | 0.8693 (3) | 0.86641 (16) | 0.28221 (16) | 0.0398 (6) |
| H19 | 0.821450 | 0.843287 | 0.234130 | 0.048* |
| H18 | 0.942018 | 0.836057 | 0.284187 | 0.048* |
| H17 | 0.883690 | 0.926043 | 0.270543 | 0.048* |
| N1 | 0.95209 (16) | 0.88054 (10) | 0.58907 (12) | 0.0225 (4) |
| N2 | 0.88089 (15) | 0.88965 (10) | 0.44393 (12) | 0.0194 (4) |
| AG | 1.04222 (2) | 0.99411 (2) | 0.58280 (2) | 0.01974 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0154 (10) | 0.0156 (8) | 0.0229 (10) | −0.0005 (7) | 0.0023 (8) | −0.0010 (7) |
| C2 | 0.0205 (11) | 0.0201 (9) | 0.0172 (10) | −0.0048 (8) | −0.0028 (8) | 0.0025 (8) |
| C3 | 0.0226 (13) | 0.0312 (10) | 0.0269 (11) | −0.0027 (9) | −0.0015 (9) | 0.0032 (9) |
| C4 | 0.0260 (12) | 0.0422 (12) | 0.0334 (14) | −0.0165 (10) | −0.0069 (10) | 0.0108 (11) |
| C5 | 0.0462 (15) | 0.0267 (10) | 0.0312 (13) | −0.0194 (10) | −0.0126 (12) | 0.0066 (9) |
| C6 | 0.0454 (15) | 0.0207 (10) | 0.0381 (14) | −0.0038 (10) | −0.0069 (12) | −0.0004 (10) |
| C7 | 0.0317 (13) | 0.0213 (9) | 0.0308 (13) | −0.0027 (9) | 0.0007 (10) | 0.0003 (9) |
| C8 | 0.0435 (15) | 0.0276 (10) | 0.0209 (11) | −0.0129 (11) | −0.0057 (11) | 0.0074 (9) |
| C9 | 0.057 (2) | 0.0559 (17) | 0.0424 (17) | 0.0170 (14) | −0.0130 (15) | 0.0194 (14) |
| C10 | 0.068 (2) | 0.101 (3) | 0.0281 (15) | 0.0053 (19) | 0.0150 (17) | 0.0124 (19) |
| C11 | 0.0309 (12) | 0.0185 (9) | 0.0270 (12) | −0.0041 (9) | −0.0118 (10) | −0.0007 (8) |
| C12 | 0.0332 (14) | 0.0476 (14) | 0.0484 (17) | 0.0024 (12) | −0.0179 (13) | −0.0024 (13) |
| C13 | 0.0567 (18) | 0.0383 (12) | 0.0243 (12) | −0.0063 (13) | −0.0097 (12) | −0.0104 (10) |
| N1 | 0.0273 (9) | 0.0213 (7) | 0.0190 (9) | −0.0074 (7) | −0.0039 (8) | 0.0036 (7) |
| N2 | 0.0213 (9) | 0.0169 (7) | 0.0200 (9) | −0.0028 (7) | −0.0058 (7) | 0.0006 (6) |
| AG | 0.02505 (8) | 0.01632 (8) | 0.01784 (8) | −0.00466 (6) | −0.00495 (6) | 0.00110 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.322 (3) | C9—H9 | 0.9800 |
| C1—N2 | 1.322 (3) | C9—H8 | 0.9800 |
| C1—C2 | 1.508 (3) | C10—H12 | 0.9800 |
| C2—C7 | 1.383 (3) | C10—H10 | 0.9800 |
| C2—C3 | 1.386 (3) | C10—H11 | 0.9800 |
| C3—C4 | 1.386 (3) | C11—N2 | 1.467 (3) |
| C3—H1 | 0.9500 | C11—C13 | 1.514 (4) |
| C4—C5 | 1.371 (4) | C11—C12 | 1.520 (3) |
| C4—H2 | 0.9500 | C11—H13 | 1.0000 |
| C5—C6 | 1.379 (4) | C12—H15 | 0.9800 |
| C5—H3 | 0.9500 | C12—H16 | 0.9800 |
| C6—C7 | 1.389 (3) | C12—H14 | 0.9800 |
| C6—H4 | 0.9500 | C13—H19 | 0.9800 |
| C7—H5 | 0.9500 | C13—H18 | 0.9800 |
| C8—N1 | 1.461 (3) | C13—H17 | 0.9800 |
| C8—C9 | 1.502 (4) | N1—AG | 2.0959 (16) |
| C8—C10 | 1.509 (4) | N2—AG$^{i}$ | 2.0965 (16) |
| C8—H6 | 1.0000 | AG—N2$^{i}$ | 2.0965 (16) |
| C9—H7 | 0.9800 | AG—AG$^{i}$ | 2.6604 (3) |
| | | | |
| N1—C1—N2 | 122.53 (17) | C8—C10—H12 | 109.5 |
| N1—C1—C2 | 118.50 (18) | C8—C10—H10 | 109.5 |
| N2—C1—C2 | 118.92 (18) | H12—C10—H10 | 109.5 |
| C7—C2—C3 | 119.2 (2) | C8—C10—H11 | 109.5 |
| C7—C2—C1 | 119.38 (19) | H12—C10—H11 | 109.5 |
| C3—C2—C1 | 121.45 (19) | H10—C10—H11 | 109.5 |

| | | | |
|---|---|---|---|
| C2—C3—C4 | 120.0 (2) | N2—C11—C13 | 109.64 (19) |
| C2—C3—H1 | 120.0 | N2—C11—C12 | 109.90 (19) |
| C4—C3—H1 | 120.0 | C13—C11—C12 | 110.5 (2) |
| C5—C4—C3 | 120.9 (2) | N2—C11—H13 | 108.9 |
| C5—C4—H2 | 119.6 | C13—C11—H13 | 108.9 |
| C3—C4—H2 | 119.6 | C12—C11—H13 | 108.9 |
| C4—C5—C6 | 119.3 (2) | C11—C12—H15 | 109.5 |
| C4—C5—H3 | 120.4 | C11—C12—H16 | 109.5 |
| C6—C5—H3 | 120.4 | H15—C12—H16 | 109.5 |
| C5—C6—C7 | 120.5 (2) | C11—C12—H14 | 109.5 |
| C5—C6—H4 | 119.8 | H15—C12—H14 | 109.5 |
| C7—C6—H4 | 119.8 | H16—C12—H14 | 109.5 |
| C2—C7—C6 | 120.2 (2) | C11—C13—H19 | 109.5 |
| C2—C7—H5 | 119.9 | C11—C13—H18 | 109.5 |
| C6—C7—H5 | 119.9 | H19—C13—H18 | 109.5 |
| N1—C8—C9 | 109.4 (2) | C11—C13—H17 | 109.5 |
| N1—C8—C10 | 109.8 (2) | H19—C13—H17 | 109.5 |
| C9—C8—C10 | 110.4 (2) | H18—C13—H17 | 109.5 |
| N1—C8—H6 | 109.1 | C1—N1—C8 | 121.76 (16) |
| C9—C8—H6 | 109.1 | C1—N1—AG | 123.63 (13) |
| C10—C8—H6 | 109.1 | C8—N1—AG | 114.54 (13) |
| C8—C9—H7 | 109.5 | C1—N2—C11 | 121.76 (17) |
| C8—C9—H9 | 109.5 | C1—N2—AG$^{i}$ | 123.15 (13) |
| H7—C9—H9 | 109.5 | C11—N2—AG$^{i}$ | 115.04 (12) |
| C8—C9—H8 | 109.5 | N1—AG—N2$^{i}$ | 170.58 (7) |
| H7—C9—H8 | 109.5 | N1—AG—AG$^{i}$ | 85.12 (5) |
| H9—C9—H8 | 109.5 | N2$^{i}$—AG—AG$^{i}$ | 85.52 (5) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C7 | −87.4 (3) | N2—C1—N1—AG | −2.7 (3) |
| N2—C1—C2—C7 | 90.1 (3) | C2—C1—N1—AG | 174.65 (14) |
| N1—C1—C2—C3 | 92.7 (3) | C9—C8—N1—C1 | 122.8 (2) |
| N2—C1—C2—C3 | −89.8 (3) | C10—C8—N1—C1 | −116.0 (3) |
| C7—C2—C3—C4 | −0.2 (3) | C9—C8—N1—AG | −54.4 (2) |
| C1—C2—C3—C4 | 179.7 (2) | C10—C8—N1—AG | 66.9 (3) |
| C2—C3—C4—C5 | 0.3 (4) | N1—C1—N2—C11 | −176.00 (19) |
| C3—C4—C5—C6 | 0.0 (4) | C2—C1—N2—C11 | 6.6 (3) |
| C4—C5—C6—C7 | −0.4 (4) | N1—C1—N2—AG$^{i}$ | 1.4 (3) |
| C3—C2—C7—C6 | −0.2 (3) | C2—C1—N2—AG$^{i}$ | −175.99 (14) |
| C1—C2—C7—C6 | 179.9 (2) | C13—C11—N2—C1 | −137.0 (2) |
| C5—C6—C7—C2 | 0.5 (4) | C12—C11—N2—C1 | 101.3 (2) |
| N2—C1—N1—C8 | −179.6 (2) | C13—C11—N2—AG$^{i}$ | 45.4 (2) |
| C2—C1—N1—C8 | −2.2 (3) | C12—C11—N2—AG$^{i}$ | −76.2 (2) |

Symmetry code: (i) −*x*+2, −*y*+2, −*z*+1.

**(compound_2) Bis(μ-*N*¹,*N*²-dicyclohexyl-3-cyclopropylpropynamidinato-κ²*N*¹:*N*²)disilver(I) bis(μ-*N*¹,*N*²-dicyclohexyl-3-cyclopropylpropynamidinato-κ³*N*¹,*N*²:*N*¹)bis(tetrahydrofuran- κ*O*)lithium(I) toluene monosolvate**

*Crystal data*

$[Ag_2(C_{18}H_{27}N_2)_2][Li_2(C_{18}H_{27}N_2)_2(C_4H_8O)_2]\cdot C_7H_8$
$M_r$ = 1551.62
Triclinic, $P\overline{1}$
$a$ = 10.5880 (3) Å
$b$ = 14.5620 (4) Å
$c$ = 14.9830 (5) Å
$\alpha$ = 99.871 (2)°
$\beta$ = 102.825 (2)°
$\gamma$ = 106.538 (2)°
$V$ = 2090.17 (11) Å³
$Z$ = 1
$F(000)$ = 826
$D_x$ = 1.233 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 27393 reflections
$\theta$ = 2.1–29.2°
$\mu$ = 0.52 mm$^{-1}$
$T$ = 133 K
Rod, colorless
0.44 × 0.29 × 0.27 mm

*Data collection*

Stoe IPDS 2T diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.67 pixels mm$^{-1}$
area detector scans
22444 measured reflections
9099 independent reflections
8214 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.1°
$h$ = −12→13
$k$ = −18→18
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
$S$ = 1.03
9099 reflections
461 parameters
12 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.4823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.61 e Å$^{-3}$

*Special details*

**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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.72575 (17) | 0.93982 (12) | 0.41483 (12) | 0.0218 (3) | |
| C2 | 0.57831 (19) | 0.90959 (12) | 0.37327 (13) | 0.0246 (3) | |
| C3 | 0.45722 (19) | 0.89050 (13) | 0.34225 (14) | 0.0288 (4) | |
| C4 | 0.3132 (2) | 0.87385 (16) | 0.30639 (16) | 0.0372 (4) | |
| H1 | 0.250264 | 0.804282 | 0.293635 | 0.045* | |
| C5 | 0.2590 (3) | 0.9540 (2) | 0.33985 (19) | 0.0530 (6) | |
| H3 | 0.166275 | 0.933659 | 0.349156 | 0.064* | |

| | | | | |
|---|---|---|---|---|
| H2 | 0.325410 | 1.015476 | 0.385331 | 0.064* |
| C6 | 0.2683 (3) | 0.9347 (2) | 0.24215 (18) | 0.0517 (6) |
| H4 | 0.340640 | 0.984016 | 0.226610 | 0.062* |
| H5 | 0.181473 | 0.902183 | 0.190427 | 0.062* |
| C7 | 0.68836 (18) | 0.77293 (12) | 0.43251 (13) | 0.0250 (3) |
| H6 | 0.591076 | 0.771776 | 0.420229 | 0.030* |
| C8 | 0.6996 (2) | 0.70587 (14) | 0.34709 (15) | 0.0364 (5) |
| H8 | 0.796825 | 0.710104 | 0.356146 | 0.044* |
| H7 | 0.670205 | 0.728808 | 0.289972 | 0.044* |
| C9 | 0.6106 (3) | 0.59800 (16) | 0.3322 (2) | 0.0523 (7) |
| H9 | 0.512424 | 0.592466 | 0.315540 | 0.063* |
| H10 | 0.625175 | 0.555915 | 0.278802 | 0.063* |
| C10 | 0.6448 (3) | 0.56124 (16) | 0.4195 (2) | 0.0543 (7) |
| H12 | 0.739052 | 0.558114 | 0.431136 | 0.065* |
| H11 | 0.580377 | 0.493464 | 0.409075 | 0.065* |
| C11 | 0.6355 (2) | 0.62794 (16) | 0.50555 (18) | 0.0436 (5) |
| H13 | 0.665684 | 0.604587 | 0.562243 | 0.052* |
| H14 | 0.538532 | 0.624002 | 0.497493 | 0.052* |
| C12 | 0.7243 (2) | 0.73533 (15) | 0.52052 (16) | 0.0361 (4) |
| H16 | 0.710784 | 0.777303 | 0.574501 | 0.043* |
| H15 | 0.822439 | 0.740615 | 0.536326 | 0.043* |
| C13 | 0.73199 (18) | 1.09818 (12) | 0.38343 (12) | 0.0228 (3) |
| H17 | 0.651330 | 1.058023 | 0.327716 | 0.027* |
| C14 | 0.6799 (2) | 1.14824 (14) | 0.45820 (14) | 0.0304 (4) |
| H18 | 0.758111 | 1.186566 | 0.514822 | 0.037* |
| H19 | 0.614428 | 1.097199 | 0.477180 | 0.037* |
| C15 | 0.6084 (2) | 1.21748 (16) | 0.42102 (17) | 0.0398 (5) |
| H21 | 0.525174 | 1.178218 | 0.368054 | 0.048* |
| H20 | 0.579014 | 1.251029 | 0.471881 | 0.048* |
| C16 | 0.7029 (2) | 1.29438 (15) | 0.38732 (16) | 0.0400 (5) |
| H22 | 0.780227 | 1.339007 | 0.441950 | 0.048* |
| H23 | 0.651693 | 1.334757 | 0.359347 | 0.048* |
| C17 | 0.7593 (2) | 1.24632 (14) | 0.31411 (15) | 0.0350 (4) |
| H25 | 0.826715 | 1.298382 | 0.297605 | 0.042* |
| H24 | 0.683240 | 1.209012 | 0.255944 | 0.042* |
| C18 | 0.8288 (2) | 1.17612 (13) | 0.35133 (14) | 0.0293 (4) |
| H27 | 0.859313 | 1.143032 | 0.300877 | 0.035* |
| H26 | 0.911196 | 1.214723 | 0.405123 | 0.035* |
| C19 | 0.94671 (19) | 0.64290 (12) | 0.06927 (13) | 0.0254 (4) |
| C20 | 0.92323 (19) | 0.72135 (13) | 0.13212 (13) | 0.0261 (4) |
| C21 | 0.90549 (19) | 0.78792 (13) | 0.17990 (13) | 0.0255 (4) |
| C22 | 0.88536 (19) | 0.87128 (13) | 0.23412 (13) | 0.0259 (4) |
| H28 | 0.887959 | 0.871143 | 0.301222 | 0.031* |
| C23 | 0.7900 (2) | 0.91816 (15) | 0.18509 (15) | 0.0342 (4) |
| H30 | 0.744110 | 0.889465 | 0.116586 | 0.041* |
| H29 | 0.734145 | 0.944081 | 0.220953 | 0.041* |
| C24 | 0.9408 (2) | 0.97115 (14) | 0.21517 (16) | 0.0355 (4) |
| H31 | 0.978425 | 1.029887 | 0.269721 | 0.043* |

| | | | | |
|---|---|---|---|---|
| H32 | 0.988391 | 0.975263 | 0.165338 | 0.043* |
| C25 | 1.03702 (19) | 0.59030 (12) | 0.20584 (12) | 0.0248 (3) |
| H33 | 1.054854 | 0.660915 | 0.237426 | 0.030* |
| C26 | 0.9230 (2) | 0.52439 (15) | 0.23685 (15) | 0.0338 (4) |
| H34 | 0.840624 | 0.544594 | 0.221742 | 0.041* |
| H35 | 0.897781 | 0.454947 | 0.200854 | 0.041* |
| C27 | 0.9664 (2) | 0.53054 (16) | 0.34234 (15) | 0.0401 (5) |
| H36 | 0.983959 | 0.598669 | 0.378675 | 0.048* |
| H37 | 0.890966 | 0.485109 | 0.358858 | 0.048* |
| C28 | 1.0950 (3) | 0.50317 (16) | 0.36923 (15) | 0.0405 (5) |
| H39 | 1.075296 | 0.433155 | 0.337186 | 0.049* |
| H38 | 1.123447 | 0.510441 | 0.438347 | 0.049* |
| C29 | 1.2107 (2) | 0.56912 (18) | 0.34099 (15) | 0.0417 (5) |
| H41 | 1.291641 | 0.547196 | 0.355210 | 0.050* |
| H40 | 1.237522 | 0.637984 | 0.378925 | 0.050* |
| C30 | 1.1689 (2) | 0.56665 (15) | 0.23579 (14) | 0.0324 (4) |
| H42 | 1.244177 | 0.615136 | 0.221918 | 0.039* |
| H43 | 1.156115 | 0.500118 | 0.198041 | 0.039* |
| C31 | 0.8585 (2) | 0.70279 (15) | −0.06282 (14) | 0.0359 (4) |
| H44 | 0.882137 | 0.765597 | −0.013568 | 0.043* |
| C32 | 0.7040 (3) | 0.6540 (2) | −0.0967 (2) | 0.0536 (6) |
| H45 | 0.669609 | 0.640626 | −0.042284 | 0.064* |
| H46 | 0.680299 | 0.589873 | −0.142688 | 0.064* |
| C33 | 0.6331 (4) | 0.7193 (3) | −0.1434 (3) | 0.0720 (9) |
| H48 | 0.532751 | 0.683588 | −0.167797 | 0.086* |
| H47 | 0.648538 | 0.780594 | −0.095703 | 0.086* |
| C34 | 0.6882 (4) | 0.7455 (3) | −0.2231 (2) | 0.0704 (9) |
| H50 | 0.661290 | 0.684754 | −0.274381 | 0.084* |
| H49 | 0.646067 | 0.791608 | −0.248707 | 0.084* |
| C35 | 0.8414 (3) | 0.7924 (2) | −0.1931 (2) | 0.0610 (7) |
| H51 | 0.867929 | 0.857776 | −0.148375 | 0.073* |
| H52 | 0.873055 | 0.803077 | −0.249146 | 0.073* |
| C36 | 0.9122 (3) | 0.72721 (18) | −0.14558 (17) | 0.0465 (5) |
| H54 | 0.895094 | 0.665048 | −0.192628 | 0.056* |
| H53 | 1.012784 | 0.762288 | −0.122444 | 0.056* |
| C37 | 0.6472 (3) | 0.4020 (2) | −0.0033 (3) | 0.0705 (8) |
| H55 | 0.680375 | 0.468615 | −0.014340 | 0.085* |
| H56 | 0.613828 | 0.407387 | 0.053486 | 0.085* |
| C38 | 0.5371 (4) | 0.3329 (4) | −0.0867 (3) | 0.0974 (13) |
| H58 | 0.445435 | 0.330165 | −0.079680 | 0.117* |
| H57 | 0.546322 | 0.354115 | −0.145022 | 0.117* |
| C39 | 0.5549 (4) | 0.2359 (3) | −0.0907 (3) | 0.1037 (14) |
| H60 | 0.505404 | 0.199991 | −0.051531 | 0.124* |
| H59 | 0.522228 | 0.194648 | −0.156541 | 0.124* |
| C40 | 0.7025 (4) | 0.2623 (2) | −0.0526 (3) | 0.0784 (10) |
| H62 | 0.723819 | 0.214845 | −0.016809 | 0.094* |
| H61 | 0.746114 | 0.260588 | −0.104635 | 0.094* |
| C41 | 0.5148 (4) | 0.9502 (2) | −0.08088 (19) | 0.0607 (8) |

| | | | | | |
|---|---|---|---|---|---|
| H65 | 0.523425 | 0.914834 | −0.137403 | 0.073* | |
| C42A | 0.6311 (4) | 1.0072 (2) | −0.00946 (18) | 0.0573 (7) | 0.5 |
| C42B | 0.6311 (4) | 1.0072 (2) | −0.00946 (18) | 0.0573 (7) | 0.5 |
| H64 | 0.719917 | 1.012313 | −0.016020 | 0.069* | 0.5 |
| C43 | 0.6154 (4) | 1.0569 (2) | 0.07242 (19) | 0.0604 (7) | |
| H63 | 0.694287 | 1.096225 | 0.123303 | 0.072* | |
| C44 | 0.7893 (6) | 1.0222 (4) | −0.0176 (4) | 0.0552 (13) | 0.5 |
| H67 | 0.851023 | 1.031026 | 0.044882 | 0.066* | 0.5 |
| H68 | 0.821343 | 1.080825 | −0.041261 | 0.066* | 0.5 |
| H66 | 0.788893 | 0.963722 | −0.061378 | 0.066* | 0.5 |
| N1 | 0.77781 (15) | 0.87526 (10) | 0.44791 (10) | 0.0232 (3) | |
| N2 | 0.80123 (15) | 1.03151 (10) | 0.41855 (10) | 0.0228 (3) | |
| N3 | 0.99709 (17) | 0.57779 (11) | 0.10369 (10) | 0.0262 (3) | |
| N4 | 0.9242 (2) | 0.63837 (12) | −0.02199 (11) | 0.0335 (4) | |
| AG | 0.98689 (2) | 0.91010 (2) | 0.51539 (2) | 0.02283 (5) | |
| LI | 0.9428 (4) | 0.4339 (2) | 0.0324 (3) | 0.0376 (8) | |
| O | 0.75344 (18) | 0.35921 (12) | 0.00793 (13) | 0.0502 (4) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0194 (8) | 0.0237 (8) | 0.0225 (8) | 0.0091 (6) | 0.0054 (6) | 0.0037 (6) |
| C2 | 0.0249 (9) | 0.0215 (8) | 0.0282 (8) | 0.0090 (7) | 0.0071 (7) | 0.0068 (7) |
| C3 | 0.0243 (9) | 0.0273 (8) | 0.0339 (9) | 0.0084 (7) | 0.0072 (7) | 0.0078 (7) |
| C4 | 0.0201 (9) | 0.0420 (11) | 0.0444 (12) | 0.0061 (8) | 0.0043 (8) | 0.0117 (9) |
| C5 | 0.0333 (12) | 0.0762 (17) | 0.0590 (15) | 0.0316 (12) | 0.0130 (11) | 0.0194 (13) |
| C6 | 0.0328 (12) | 0.0764 (17) | 0.0522 (14) | 0.0245 (12) | 0.0060 (10) | 0.0296 (13) |
| C7 | 0.0216 (8) | 0.0224 (8) | 0.0331 (9) | 0.0071 (7) | 0.0096 (7) | 0.0103 (7) |
| C8 | 0.0399 (11) | 0.0230 (9) | 0.0437 (11) | 0.0020 (8) | 0.0210 (9) | 0.0042 (8) |
| C9 | 0.0569 (15) | 0.0252 (10) | 0.0702 (17) | −0.0004 (10) | 0.0374 (13) | −0.0006 (10) |
| C10 | 0.0546 (15) | 0.0255 (10) | 0.104 (2) | 0.0185 (10) | 0.0504 (15) | 0.0257 (12) |
| C11 | 0.0429 (13) | 0.0381 (11) | 0.0662 (15) | 0.0175 (10) | 0.0275 (11) | 0.0327 (11) |
| C12 | 0.0337 (11) | 0.0366 (10) | 0.0427 (11) | 0.0111 (9) | 0.0129 (9) | 0.0206 (9) |
| C13 | 0.0212 (8) | 0.0217 (8) | 0.0249 (8) | 0.0100 (7) | 0.0025 (6) | 0.0045 (6) |
| C14 | 0.0336 (10) | 0.0322 (9) | 0.0304 (9) | 0.0182 (8) | 0.0102 (8) | 0.0066 (7) |
| C15 | 0.0431 (12) | 0.0388 (11) | 0.0472 (12) | 0.0278 (10) | 0.0158 (10) | 0.0080 (9) |
| C16 | 0.0504 (13) | 0.0281 (9) | 0.0447 (12) | 0.0238 (9) | 0.0084 (10) | 0.0066 (8) |
| C17 | 0.0446 (12) | 0.0247 (9) | 0.0381 (10) | 0.0161 (8) | 0.0089 (9) | 0.0104 (8) |
| C18 | 0.0317 (10) | 0.0237 (8) | 0.0372 (10) | 0.0131 (7) | 0.0115 (8) | 0.0106 (7) |
| C19 | 0.0282 (9) | 0.0203 (8) | 0.0275 (9) | 0.0087 (7) | 0.0095 (7) | 0.0024 (7) |
| C20 | 0.0314 (10) | 0.0227 (8) | 0.0265 (8) | 0.0105 (7) | 0.0099 (7) | 0.0074 (7) |
| C21 | 0.0274 (9) | 0.0234 (8) | 0.0273 (9) | 0.0090 (7) | 0.0096 (7) | 0.0072 (7) |
| C22 | 0.0310 (9) | 0.0234 (8) | 0.0253 (8) | 0.0112 (7) | 0.0117 (7) | 0.0031 (7) |
| C23 | 0.0333 (10) | 0.0332 (10) | 0.0404 (11) | 0.0183 (8) | 0.0125 (9) | 0.0050 (8) |
| C24 | 0.0366 (11) | 0.0224 (8) | 0.0512 (12) | 0.0110 (8) | 0.0192 (9) | 0.0080 (8) |
| C25 | 0.0300 (9) | 0.0204 (8) | 0.0236 (8) | 0.0091 (7) | 0.0085 (7) | 0.0022 (6) |
| C26 | 0.0302 (10) | 0.0368 (10) | 0.0374 (10) | 0.0110 (8) | 0.0146 (8) | 0.0107 (8) |
| C27 | 0.0507 (13) | 0.0404 (11) | 0.0387 (11) | 0.0178 (10) | 0.0248 (10) | 0.0140 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C28 | 0.0592 (14) | 0.0392 (11) | 0.0284 (10) | 0.0218 (10) | 0.0138 (10) | 0.0110 (8) |
| C29 | 0.0391 (12) | 0.0524 (13) | 0.0327 (10) | 0.0189 (10) | 0.0044 (9) | 0.0098 (9) |
| C30 | 0.0301 (10) | 0.0401 (10) | 0.0289 (9) | 0.0143 (8) | 0.0096 (8) | 0.0078 (8) |
| C31 | 0.0546 (13) | 0.0294 (9) | 0.0297 (9) | 0.0227 (9) | 0.0119 (9) | 0.0084 (8) |
| C32 | 0.0553 (16) | 0.0652 (16) | 0.0641 (16) | 0.0338 (13) | 0.0295 (13) | 0.0382 (14) |
| C33 | 0.068 (2) | 0.096 (2) | 0.085 (2) | 0.0532 (19) | 0.0291 (17) | 0.0537 (19) |
| C34 | 0.077 (2) | 0.088 (2) | 0.0618 (17) | 0.0413 (19) | 0.0155 (16) | 0.0424 (17) |
| C35 | 0.084 (2) | 0.0543 (15) | 0.0544 (15) | 0.0230 (15) | 0.0245 (15) | 0.0324 (13) |
| C36 | 0.0538 (15) | 0.0424 (12) | 0.0468 (13) | 0.0146 (11) | 0.0181 (11) | 0.0183 (10) |
| C37 | 0.0471 (16) | 0.0643 (18) | 0.095 (2) | 0.0133 (14) | 0.0204 (16) | 0.0159 (17) |
| C38 | 0.0507 (19) | 0.154 (4) | 0.078 (2) | 0.026 (2) | 0.0113 (17) | 0.028 (2) |
| C39 | 0.059 (2) | 0.096 (3) | 0.104 (3) | −0.016 (2) | 0.014 (2) | −0.021 (2) |
| C40 | 0.070 (2) | 0.0409 (14) | 0.098 (2) | −0.0083 (14) | 0.0217 (18) | −0.0008 (15) |
| C41 | 0.100 (2) | 0.0539 (15) | 0.0398 (13) | 0.0408 (16) | 0.0238 (15) | 0.0118 (11) |
| C42A | 0.092 (2) | 0.0514 (14) | 0.0405 (13) | 0.0388 (15) | 0.0191 (14) | 0.0177 (11) |
| C42B | 0.092 (2) | 0.0514 (14) | 0.0405 (13) | 0.0388 (15) | 0.0191 (14) | 0.0177 (11) |
| C43 | 0.090 (2) | 0.0562 (15) | 0.0389 (13) | 0.0335 (15) | 0.0151 (14) | 0.0113 (11) |
| C44 | 0.059 (3) | 0.068 (3) | 0.045 (3) | 0.026 (3) | 0.017 (2) | 0.021 (2) |
| N1 | 0.0202 (7) | 0.0207 (7) | 0.0289 (7) | 0.0077 (6) | 0.0051 (6) | 0.0073 (6) |
| N2 | 0.0196 (7) | 0.0214 (7) | 0.0281 (7) | 0.0098 (6) | 0.0036 (6) | 0.0070 (6) |
| N3 | 0.0341 (8) | 0.0220 (7) | 0.0235 (7) | 0.0120 (6) | 0.0087 (6) | 0.0031 (6) |
| N4 | 0.0515 (11) | 0.0293 (8) | 0.0265 (8) | 0.0233 (8) | 0.0118 (7) | 0.0069 (6) |
| AG | 0.01875 (7) | 0.02032 (7) | 0.02912 (8) | 0.00771 (5) | 0.00391 (5) | 0.00737 (5) |
| LI | 0.042 (2) | 0.0290 (16) | 0.0412 (19) | 0.0127 (15) | 0.0145 (16) | 0.0037 (14) |
| O | 0.0445 (10) | 0.0380 (8) | 0.0559 (10) | 0.0024 (7) | 0.0143 (8) | 0.0005 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.329 (2) | C26—H35 | 0.9900 |
| C1—N2 | 1.331 (2) | C27—C28 | 1.515 (3) |
| C1—C2 | 1.450 (2) | C27—H36 | 0.9900 |
| C2—C3 | 1.194 (3) | C27—H37 | 0.9900 |
| C3—C4 | 1.433 (3) | C28—C29 | 1.517 (3) |
| C4—C5 | 1.501 (3) | C28—H39 | 0.9900 |
| C4—C6 | 1.505 (3) | C28—H38 | 0.9900 |
| C4—H1 | 1.0000 | C29—C30 | 1.531 (3) |
| C5—C6 | 1.473 (4) | C29—H41 | 0.9900 |
| C5—H3 | 0.9900 | C29—H40 | 0.9900 |
| C5—H2 | 0.9900 | C30—H42 | 0.9900 |
| C6—H4 | 0.9900 | C30—H43 | 0.9900 |
| C6—H5 | 0.9900 | C31—N4 | 1.455 (2) |
| C7—N1 | 1.467 (2) | C31—C32 | 1.512 (4) |
| C7—C8 | 1.520 (3) | C31—C36 | 1.529 (3) |
| C7—C12 | 1.526 (3) | C31—H44 | 1.0000 |
| C7—H6 | 1.0000 | C32—C33 | 1.536 (3) |
| C8—C9 | 1.533 (3) | C32—H45 | 0.9900 |
| C8—H8 | 0.9900 | C32—H46 | 0.9900 |
| C8—H7 | 0.9900 | C33—C34 | 1.501 (4) |

| | | | |
|---|---|---|---|
| C9—C10 | 1.506 (4) | C33—H48 | 0.9900 |
| C9—H9 | 0.9900 | C33—H47 | 0.9900 |
| C9—H10 | 0.9900 | C34—C35 | 1.497 (5) |
| C10—C11 | 1.516 (4) | C34—H50 | 0.9900 |
| C10—H12 | 0.9900 | C34—H49 | 0.9900 |
| C10—H11 | 0.9900 | C35—C36 | 1.540 (4) |
| C11—C12 | 1.526 (3) | C35—H51 | 0.9900 |
| C11—H13 | 0.9900 | C35—H52 | 0.9900 |
| C11—H14 | 0.9900 | C36—H54 | 0.9900 |
| C12—H16 | 0.9900 | C36—H53 | 0.9900 |
| C12—H15 | 0.9900 | C37—O | 1.426 (4) |
| C13—N2 | 1.472 (2) | C37—C38 | 1.479 (5) |
| C13—C18 | 1.521 (3) | C37—H55 | 0.9900 |
| C13—C14 | 1.521 (2) | C37—H56 | 0.9900 |
| C13—H17 | 1.0000 | C38—C39 | 1.470 (6) |
| C14—C15 | 1.530 (3) | C38—H58 | 0.9900 |
| C14—H18 | 0.9900 | C38—H57 | 0.9900 |
| C14—H19 | 0.9900 | C39—C40 | 1.450 (5) |
| C15—C16 | 1.513 (3) | C39—H60 | 0.9900 |
| C15—H21 | 0.9900 | C39—H59 | 0.9900 |
| C15—H20 | 0.9900 | C40—O | 1.419 (3) |
| C16—C17 | 1.522 (3) | C40—H62 | 0.9900 |
| C16—H22 | 0.9900 | C40—H61 | 0.9900 |
| C16—H23 | 0.9900 | C41—C42B | 1.371 (4) |
| C17—C18 | 1.529 (2) | C41—C42A | 1.371 (4) |
| C17—H25 | 0.9900 | C41—C43$^{ii}$ | 1.388 (5) |
| C17—H24 | 0.9900 | C41—H65 | 0.9500 |
| C18—H27 | 0.9900 | C42A—C43 | 1.383 (4) |
| C18—H26 | 0.9900 | C42A—C44 | 1.661 (6) |
| C19—N4 | 1.321 (2) | C42B—C43 | 1.383 (4) |
| C19—N3 | 1.335 (2) | C42B—H64 | 0.9500 |
| C19—C20 | 1.466 (2) | C43—C41$^{ii}$ | 1.388 (5) |
| C19—LI$^{i}$ | 2.428 (4) | C43—H63 | 0.9500 |
| C20—C21 | 1.189 (3) | C44—H67 | 0.9800 |
| C21—C22 | 1.437 (2) | C44—H68 | 0.9800 |
| C22—C23 | 1.503 (3) | C44—H66 | 0.9800 |
| C22—C24 | 1.507 (3) | N1—AG | 2.0908 (15) |
| C22—H28 | 1.0000 | N2—AG$^{iii}$ | 2.0916 (14) |
| C23—C24 | 1.486 (3) | N3—LI | 2.033 (4) |
| C23—H30 | 0.9900 | N3—LI$^{i}$ | 2.261 (4) |
| C23—H29 | 0.9900 | N4—LI$^{i}$ | 2.001 (4) |
| C24—H31 | 0.9900 | AG—N2$^{iii}$ | 2.0917 (15) |
| C24—H32 | 0.9900 | AG—AG$^{iii}$ | 2.6838 (3) |
| C25—N3 | 1.459 (2) | LI—O | 1.906 (4) |
| C25—C30 | 1.523 (3) | LI—N4$^{i}$ | 2.001 (4) |
| C25—C26 | 1.528 (3) | LI—N3$^{i}$ | 2.261 (4) |
| C25—H33 | 1.0000 | LI—C19$^{i}$ | 2.428 (4) |
| C26—C27 | 1.524 (3) | LI—LI$^{i}$ | 2.440 (7) |

| | | | |
|---|---|---|---|
| C26—H34 | 0.9900 | | |
| | | | |
| N1—C1—N2 | 123.71 (15) | C26—C27—H37 | 109.4 |
| N1—C1—C2 | 118.48 (15) | H36—C27—H37 | 108.0 |
| N2—C1—C2 | 117.81 (15) | C27—C28—C29 | 110.48 (17) |
| C3—C2—C1 | 175.75 (19) | C27—C28—H39 | 109.6 |
| C2—C3—C4 | 176.6 (2) | C29—C28—H39 | 109.6 |
| C3—C4—C5 | 118.31 (19) | C27—C28—H38 | 109.6 |
| C3—C4—C6 | 118.78 (19) | C29—C28—H38 | 109.6 |
| C5—C4—C6 | 58.69 (17) | H39—C28—H38 | 108.1 |
| C3—C4—H1 | 116.3 | C28—C29—C30 | 111.95 (18) |
| C5—C4—H1 | 116.3 | C28—C29—H41 | 109.2 |
| C6—C4—H1 | 116.3 | C30—C29—H41 | 109.2 |
| C6—C5—C4 | 60.81 (16) | C28—C29—H40 | 109.2 |
| C6—C5—H3 | 117.7 | C30—C29—H40 | 109.2 |
| C4—C5—H3 | 117.7 | H41—C29—H40 | 107.9 |
| C6—C5—H2 | 117.7 | C25—C30—C29 | 112.68 (16) |
| C4—C5—H2 | 117.7 | C25—C30—H42 | 109.1 |
| H3—C5—H2 | 114.8 | C29—C30—H42 | 109.1 |
| C5—C6—C4 | 60.50 (16) | C25—C30—H43 | 109.1 |
| C5—C6—H4 | 117.7 | C29—C30—H43 | 109.1 |
| C4—C6—H4 | 117.7 | H42—C30—H43 | 107.8 |
| C5—C6—H5 | 117.7 | N4—C31—C32 | 110.88 (18) |
| C4—C6—H5 | 117.7 | N4—C31—C36 | 109.39 (18) |
| H4—C6—H5 | 114.8 | C32—C31—C36 | 109.73 (19) |
| N1—C7—C8 | 110.92 (14) | N4—C31—H44 | 108.9 |
| N1—C7—C12 | 110.30 (15) | C32—C31—H44 | 108.9 |
| C8—C7—C12 | 110.42 (16) | C36—C31—H44 | 108.9 |
| N1—C7—H6 | 108.4 | C31—C32—C33 | 111.7 (2) |
| C8—C7—H6 | 108.4 | C31—C32—H45 | 109.3 |
| C12—C7—H6 | 108.4 | C33—C32—H45 | 109.3 |
| C7—C8—C9 | 111.51 (17) | C31—C32—H46 | 109.3 |
| C7—C8—H8 | 109.3 | C33—C32—H46 | 109.3 |
| C9—C8—H8 | 109.3 | H45—C32—H46 | 107.9 |
| C7—C8—H7 | 109.3 | C34—C33—C32 | 110.7 (2) |
| C9—C8—H7 | 109.3 | C34—C33—H48 | 109.5 |
| H8—C8—H7 | 108.0 | C32—C33—H48 | 109.5 |
| C10—C9—C8 | 111.6 (2) | C34—C33—H47 | 109.5 |
| C10—C9—H9 | 109.3 | C32—C33—H47 | 109.5 |
| C8—C9—H9 | 109.3 | H48—C33—H47 | 108.1 |
| C10—C9—H10 | 109.3 | C35—C34—C33 | 112.6 (3) |
| C8—C9—H10 | 109.3 | C35—C34—H50 | 109.1 |
| H9—C9—H10 | 108.0 | C33—C34—H50 | 109.1 |
| C9—C10—C11 | 111.62 (18) | C35—C34—H49 | 109.1 |
| C9—C10—H12 | 109.3 | C33—C34—H49 | 109.1 |
| C11—C10—H12 | 109.3 | H50—C34—H49 | 107.8 |
| C9—C10—H11 | 109.3 | C34—C35—C36 | 111.3 (2) |
| C11—C10—H11 | 109.3 | C34—C35—H51 | 109.4 |

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| H12—C10—H11 | 108.0 | C36—C35—H51 | 109.4 |
| C10—C11—C12 | 111.61 (18) | C34—C35—H52 | 109.4 |
| C10—C11—H13 | 109.3 | C36—C35—H52 | 109.4 |
| C12—C11—H13 | 109.3 | H51—C35—H52 | 108.0 |
| C10—C11—H14 | 109.3 | C31—C36—C35 | 111.1 (2) |
| C12—C11—H14 | 109.3 | C31—C36—H54 | 109.4 |
| H13—C11—H14 | 108.0 | C35—C36—H54 | 109.4 |
| C7—C12—C11 | 111.45 (18) | C31—C36—H53 | 109.4 |
| C7—C12—H16 | 109.3 | C35—C36—H53 | 109.4 |
| C11—C12—H16 | 109.3 | H54—C36—H53 | 108.0 |
| C7—C12—H15 | 109.3 | O—C37—C38 | 104.5 (3) |
| C11—C12—H15 | 109.3 | O—C37—H55 | 110.8 |
| H16—C12—H15 | 108.0 | C38—C37—H55 | 110.8 |
| N2—C13—C18 | 110.41 (14) | O—C37—H56 | 110.8 |
| N2—C13—C14 | 111.62 (14) | C38—C37—H56 | 110.8 |
| C18—C13—C14 | 109.78 (15) | H55—C37—H56 | 108.9 |
| N2—C13—H17 | 108.3 | C39—C38—C37 | 105.6 (3) |
| C18—C13—H17 | 108.3 | C39—C38—H58 | 110.6 |
| C14—C13—H17 | 108.3 | C37—C38—H58 | 110.6 |
| C13—C14—C15 | 111.17 (16) | C39—C38—H57 | 110.6 |
| C13—C14—H18 | 109.4 | C37—C38—H57 | 110.6 |
| C15—C14—H18 | 109.4 | H58—C38—H57 | 108.8 |
| C13—C14—H19 | 109.4 | C40—C39—C38 | 102.6 (3) |
| C15—C14—H19 | 109.4 | C40—C39—H60 | 111.3 |
| H18—C14—H19 | 108.0 | C38—C39—H60 | 111.3 |
| C16—C15—C14 | 111.29 (18) | C40—C39—H59 | 111.3 |
| C16—C15—H21 | 109.4 | C38—C39—H59 | 111.3 |
| C14—C15—H21 | 109.4 | H60—C39—H59 | 109.2 |
| C16—C15—H20 | 109.4 | O—C40—C39 | 108.0 (3) |
| C14—C15—H20 | 109.4 | O—C40—H62 | 110.1 |
| H21—C15—H20 | 108.0 | C39—C40—H62 | 110.1 |
| C15—C16—C17 | 111.32 (17) | O—C40—H61 | 110.1 |
| C15—C16—H22 | 109.4 | C39—C40—H61 | 110.1 |
| C17—C16—H22 | 109.4 | H62—C40—H61 | 108.4 |
| C15—C16—H23 | 109.4 | C42B—C41—C43$^{ii}$ | 121.4 (3) |
| C17—C16—H23 | 109.4 | C42A—C41—C43$^{ii}$ | 121.4 (3) |
| H22—C16—H23 | 108.0 | C42A—C41—H65 | 119.3 |
| C16—C17—C18 | 111.25 (17) | C43$^{ii}$—C41—H65 | 119.3 |
| C16—C17—H25 | 109.4 | C41—C42A—C43 | 118.0 (3) |
| C18—C17—H25 | 109.4 | C41—C42A—C44 | 123.4 (3) |
| C16—C17—H24 | 109.4 | C43—C42A—C44 | 118.5 (3) |
| C18—C17—H24 | 109.4 | C41—C42B—C43 | 118.0 (3) |
| H25—C17—H24 | 108.0 | C41—C42B—H64 | 121.0 |
| C13—C18—C17 | 111.56 (16) | C43—C42B—H64 | 121.0 |
| C13—C18—H27 | 109.3 | C42B—C43—C41$^{ii}$ | 120.6 (3) |
| C17—C18—H27 | 109.3 | C42A—C43—C41$^{ii}$ | 120.6 (3) |
| C13—C18—H26 | 109.3 | C42A—C43—H63 | 119.7 |
| C17—C18—H26 | 109.3 | C41$^{ii}$—C43—H63 | 119.7 |

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| H27—C18—H26 | 108.0 | C42A—C44—H67 | 109.5 |
| N4—C19—N3 | 118.85 (16) | C42A—C44—H68 | 109.5 |
| N4—C19—C20 | 120.31 (16) | H67—C44—H68 | 109.5 |
| N3—C19—C20 | 120.77 (16) | C42A—C44—H66 | 109.5 |
| N4—C19—LI$^{i}$ | 55.46 (13) | H67—C44—H66 | 109.5 |
| N3—C19—LI$^{i}$ | 66.70 (13) | H68—C44—H66 | 109.5 |
| C20—C19—LI$^{i}$ | 158.53 (15) | C1—N1—C7 | 119.72 (14) |
| C21—C20—C19 | 176.60 (19) | C1—N1—AG | 122.90 (11) |
| C20—C21—C22 | 177.03 (19) | C7—N1—AG | 117.28 (11) |
| C21—C22—C23 | 118.85 (16) | C1—N2—C13 | 119.09 (14) |
| C21—C22—C24 | 118.48 (16) | C1—N2—AG$^{iii}$ | 122.58 (11) |
| C23—C22—C24 | 59.15 (13) | C13—N2—AG$^{iii}$ | 118.05 (11) |
| C21—C22—H28 | 116.1 | C19—N3—C25 | 118.58 (14) |
| C23—C22—H28 | 116.1 | C19—N3—LI | 123.43 (16) |
| C24—C22—H28 | 116.1 | C25—N3—LI | 111.73 (15) |
| C24—C23—C22 | 60.54 (13) | C19—N3—LI$^{i}$ | 80.46 (14) |
| C24—C23—H30 | 117.7 | C25—N3—LI$^{i}$ | 148.51 (16) |
| C22—C23—H30 | 117.7 | LI—N3—LI$^{i}$ | 69.00 (17) |
| C24—C23—H29 | 117.7 | C19—N4—C31 | 119.98 (16) |
| C22—C23—H29 | 117.7 | C19—N4—LI$^{i}$ | 91.58 (16) |
| H30—C23—H29 | 114.8 | C31—N4—LI$^{i}$ | 144.63 (18) |
| C23—C24—C22 | 60.31 (13) | N1—AG—N2$^{iii}$ | 170.66 (5) |
| C23—C24—H31 | 117.7 | N1—AG—AG$^{iii}$ | 85.27 (4) |
| C22—C24—H31 | 117.7 | N2$^{iii}$—AG—AG$^{iii}$ | 85.45 (4) |
| C23—C24—H32 | 117.7 | O—LI—N4$^{i}$ | 118.78 (19) |
| C22—C24—H32 | 117.7 | O—LI—N3 | 114.34 (19) |
| H31—C24—H32 | 114.9 | N4$^{i}$—LI—N3 | 124.4 (2) |
| N3—C25—C30 | 109.55 (15) | O—LI—N3$^{i}$ | 110.21 (18) |
| N3—C25—C26 | 111.24 (15) | N4$^{i}$—LI—N3$^{i}$ | 64.58 (12) |
| C30—C25—C26 | 110.27 (15) | N3—LI—N3$^{i}$ | 111.00 (17) |
| N3—C25—H33 | 108.6 | O—LI—C19$^{i}$ | 112.66 (17) |
| C30—C25—H33 | 108.6 | N4$^{i}$—LI—C19$^{i}$ | 32.96 (8) |
| C26—C25—H33 | 108.6 | N3—LI—C19$^{i}$ | 129.55 (18) |
| C27—C26—C25 | 112.17 (17) | N3$^{i}$—LI—C19$^{i}$ | 32.85 (7) |
| C27—C26—H34 | 109.2 | O—LI—LI$^{i}$ | 131.6 (3) |
| C25—C26—H34 | 109.2 | N4$^{i}$—LI—LI$^{i}$ | 94.2 (2) |
| C27—C26—H35 | 109.2 | N3—LI—LI$^{i}$ | 59.91 (14) |
| C25—C26—H35 | 109.2 | N3$^{i}$—LI—LI$^{i}$ | 51.08 (14) |
| H34—C26—H35 | 107.9 | C19$^{i}$—LI—LI$^{i}$ | 75.64 (17) |
| C28—C27—C26 | 110.99 (17) | C40—O—C37 | 109.2 (2) |
| C28—C27—H36 | 109.4 | C40—O—LI | 118.0 (2) |
| C26—C27—H36 | 109.4 | C37—O—LI | 123.21 (19) |
| C28—C27—H37 | 109.4 | | |

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| C3—C4—C5—C6 | 108.2 (2) | C44—C42A—C43—C41$^{ii}$ | 177.3 (3) |
| C3—C4—C6—C5 | −107.4 (2) | N2—C1—N1—C7 | −174.14 (16) |
| N1—C7—C8—C9 | 177.97 (19) | C2—C1—N1—C7 | 6.6 (2) |
| C12—C7—C8—C9 | 55.4 (2) | N2—C1—N1—AG | 2.2 (2) |

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| C7—C8—C9—C10 | −55.3 (3) | C2—C1—N1—AG | −177.07 (12) |
| C8—C9—C10—C11 | 54.4 (3) | C8—C7—N1—C1 | 96.9 (2) |
| C9—C10—C11—C12 | −54.5 (3) | C12—C7—N1—C1 | −140.43 (17) |
| N1—C7—C12—C11 | −178.41 (16) | C8—C7—N1—AG | −79.60 (17) |
| C8—C7—C12—C11 | −55.5 (2) | C12—C7—N1—AG | 43.06 (18) |
| C10—C11—C12—C7 | 55.2 (3) | N1—C1—N2—C13 | −177.37 (16) |
| N2—C13—C14—C15 | 179.88 (16) | C2—C1—N2—C13 | 1.9 (2) |
| C18—C13—C14—C15 | 57.1 (2) | N1—C1—N2—AG$^{iii}$ | −3.6 (2) |
| C13—C14—C15—C16 | −56.7 (2) | C2—C1—N2—AG$^{iii}$ | 175.62 (12) |
| C14—C15—C16—C17 | 54.8 (2) | C18—C13—N2—C1 | −153.85 (16) |
| C15—C16—C17—C18 | −54.2 (2) | C14—C13—N2—C1 | 83.74 (19) |
| N2—C13—C18—C17 | 179.80 (15) | C18—C13—N2—AG$^{iii}$ | 32.10 (18) |
| C14—C13—C18—C17 | −56.7 (2) | C14—C13—N2—AG$^{iii}$ | −90.30 (16) |
| C16—C17—C18—C13 | 55.6 (2) | N4—C19—N3—C25 | 172.85 (17) |
| C21—C22—C23—C24 | −107.76 (19) | C20—C19—N3—C25 | −4.1 (3) |
| C21—C22—C24—C23 | 108.4 (2) | LI$^{i}$—C19—N3—C25 | 153.26 (19) |
| N3—C25—C26—C27 | 175.81 (16) | N4—C19—N3—LI | −37.3 (3) |
| C30—C25—C26—C27 | 54.1 (2) | C20—C19—N3—LI | 145.79 (19) |
| C25—C26—C27—C28 | −57.2 (2) | LI$^{i}$—C19—N3—LI | −56.9 (2) |
| C26—C27—C28—C29 | 56.8 (2) | N4—C19—N3—LI$^{i}$ | 19.59 (19) |
| C27—C28—C29—C30 | −55.1 (2) | C20—C19—N3—LI$^{i}$ | −157.33 (19) |
| N3—C25—C30—C29 | −174.89 (16) | C30—C25—N3—C19 | −140.43 (17) |
| C26—C25—C30—C29 | −52.1 (2) | C26—C25—N3—C19 | 97.41 (19) |
| C28—C29—C30—C25 | 53.6 (2) | C30—C25—N3—LI | 66.4 (2) |
| N4—C31—C32—C33 | −177.9 (2) | C26—C25—N3—LI | −55.8 (2) |
| C36—C31—C32—C33 | −56.9 (3) | C30—C25—N3—LI$^{i}$ | −18.6 (3) |
| C31—C32—C33—C34 | 56.0 (4) | C26—C25—N3—LI$^{i}$ | −140.7 (2) |
| C32—C33—C34—C35 | −54.5 (4) | N3—C19—N4—C31 | 174.79 (18) |
| C33—C34—C35—C36 | 54.4 (4) | C20—C19—N4—C31 | −8.3 (3) |
| N4—C31—C36—C35 | 178.0 (2) | LI$^{i}$—C19—N4—C31 | −163.3 (2) |
| C32—C31—C36—C35 | 56.1 (3) | N3—C19—N4—LI$^{i}$ | −21.9 (2) |
| C34—C35—C36—C31 | −55.0 (3) | C20—C19—N4—LI$^{i}$ | 154.99 (18) |
| O—C37—C38—C39 | 26.4 (4) | C32—C31—N4—C19 | −90.0 (2) |
| C37—C38—C39—C40 | −32.0 (4) | C36—C31—N4—C19 | 148.8 (2) |
| C38—C39—C40—O | 26.0 (4) | C32—C31—N4—LI$^{i}$ | 119.8 (3) |
| C43$^{ii}$—C41—C42A—C43 | 0.8 (4) | C36—C31—N4—LI$^{i}$ | −1.3 (4) |
| C43$^{ii}$—C41—C42A—C44 | −177.2 (3) | C39—C40—O—C37 | −10.2 (4) |
| C43$^{ii}$—C41—C42B—C43 | 0.8 (4) | C39—C40—O—LI | −157.6 (3) |
| C41—C42B—C43—C41$^{ii}$ | −0.8 (4) | C38—C37—O—C40 | −10.2 (4) |
| C41—C42A—C43—C41$^{ii}$ | −0.8 (4) | C38—C37—O—LI | 135.2 (3) |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+2, −*y*+2, −*z*+1.