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$[Li_6(C_2N_2H_8)_{11.5}][Fe_4Se_8]$: the first lithium-containing chalcogenidotetraferrate synthesized in solution

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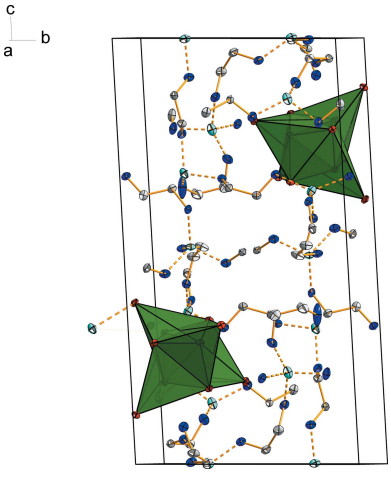
The octaselenidotetraferrate(II/III) with six Li atoms as counter-ions chelated by ethylenediamine (en, $C_2H_8N_2$), $\{[Li_6(en)_{11.5}][Fe_4Se_8]\}_n$, was synthesized from Li, FeSe and Se in an ethylenediamine solution at room temperature. Its crystal structure was determined at 100 K and has triclinic ($P\overline{1}$) symmetry. The $[Fe_4Se_8]^{6-}$ anions show a connectivity comparable to a distorted tetrahedral cluster structure. Contact distances are given, and central structure features compared to literature known selenidoferrates with the same anion motif.

1. Chemical context

Alkali metal chalcogenido ferrates $A_x[Fe_yCh_z]$ (A = Li···Cs; Ch = O···Te) show $[FeCh_4]$ tetrahedra to be the most prominent coordination motif of the anionic moiety. These can be isolated, connected into chains, layers, or three-dimensional networks. A special motive is the connection of four such $[FeCh_4]$ (Ch = S, Se, Te) units *via* three shared edges each to form a tetramer. This secondary structure can be described as a distorted heterocubane $[Fe_4Ch_4]^{x-}$ core, with one additional chalcogenido ligand on every iron corner of the heterocubane (Schwarz & Röhr, 2015). Another approach to describe those tetramers can be as a distorted tetrahedral star (*stella quadrangula;* Stüble *et al.*, 2016).

The first reported ferrate of this type was $Cs_7[Fe_4Te_8]$ published by Bronger *et al.* in 1983. $A_7[Fe_4Ch_8]$ (A = K, Rb, Cs; Ch = S, Se, Te) is the most common sum formula for those ferrates. The respective sulfido and selenido ferrates are only known with Cs as alkali metal [$Cs_7[Fe_4S_8]$ (Schwarz & Röhr, 2015), $Cs_7[Fe_4Se_8]$ (Stüble & Röhr, 2017)], while the tellurido ferrates are known with K, Rb and Cs as alkali metals [$K_7[Fe_4Te_8]$, $Rb_7[Fe_4Te_8]$ (Stüble *et al.*, 2016), $Cs_7[Fe_4Te_8]$ (Bronger *et al.*, 1983)]. The reported tetrachalcogenido ferrates are synthesized in solid-state reactions at temperatures in the range 500–1050 K. With the exception of the potassium tellurido tetraferrates, all these alkali metal chalcogenido tetraferrates crystallize in the space-group type $C2/c$ (Schwarz & Röhr, 2015; Stüble & Röhr, 2017; Stüble *et al.*, 2016, 2018; Bronger *et al.*, 1983). For $K_7[Fe_4Te_8]$, a room-temperature ($P4_2/nmc$) and a low-temperature (100 K, $Pbcn$) polymorph are known. $K_6[Fe_4Se_8]$ ($Pbcn$) is almost isostructural to the low-temperature modification of $K_7[Fe_4Se_8]$ with a missing K site (Stüble *et al.*, 2016).

For the compound presented herein, an initial attempt was to use the solubility of Li and Se in ethylenediamine to form *in situ* Li_2Se, which would then react with iron(II) selenide to a



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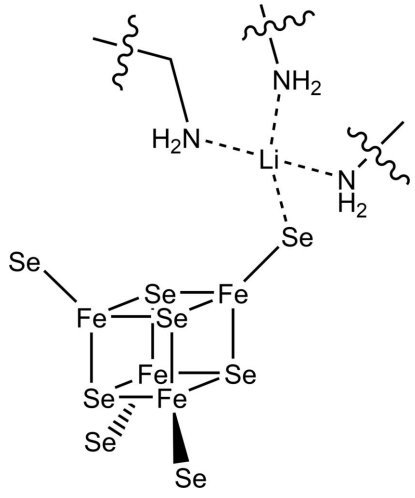
lithium selenidoferrate(II). Instead, the solution approach yielded the mixed-valent tetraferrate $[Li_6(en_{11.5})][Fe_4Se_8]$.



2. Structural commentary

The title compound (Fig. 1) crystallizes in the triclinic space group $P\overline{1}$. The asymmetric unit consists of the cationic $[Li_6(en)_{11.5}]^{6+}$ moiety forming networks and the anionic $[Fe_4Se_8]^{6-}$ unit, where each Fe atom is coordinated by four Se atoms, forming a distorted tetrahedron. The distortion is towards a trigonal–pyramidal geometry. The distorted $[FeSe_4]$ tetrahedra are connected *via* three edges with neighbouring tetrahedra, forming a distorted tetrahedral star $[Fe_4Se_8]^{6-}$ (*stella quadrangula*; Stüble *et al.*, 2016) as a secondary structure (Fig. 2). The terminal Fe—Se distances are 2.3251 (8)–2.3502 (7) Å. The terminal Se3 directly coordinates Li3, at a distance of 2.634 (7) Å, positioned between two anions along the crystallographic *b*-axis (see Fig. 4). The Fe—Se bond lengths within the heterocubane core are in the range 2.3899 (8)—2.4752 (8) Å. Parallel to the *b*-axis the Fe—Se bonds are slightly shorter [2.3899 (8)—2.4157 (8) Å] than the rest of the bonds in the heterocubane [2.4414 (7)—2.4752 (8) Å] (see Figs. 3 and 4), this might be due to partial electron-density polarization towards the Li atom directly coordinated by one terminal Se ligand.

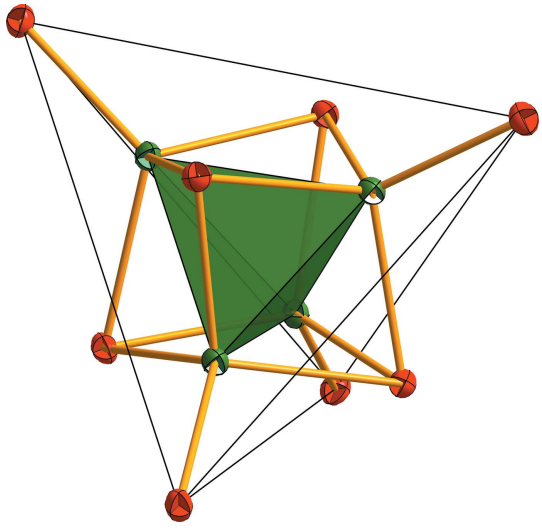


Figure 2
Representation of the anionic tetramer $[Fe_4Se_8]^{6-}$ with tetrahedral shape highlighted. Green: Fe, red: Se, ellipsoids are drawn with 70% probability.

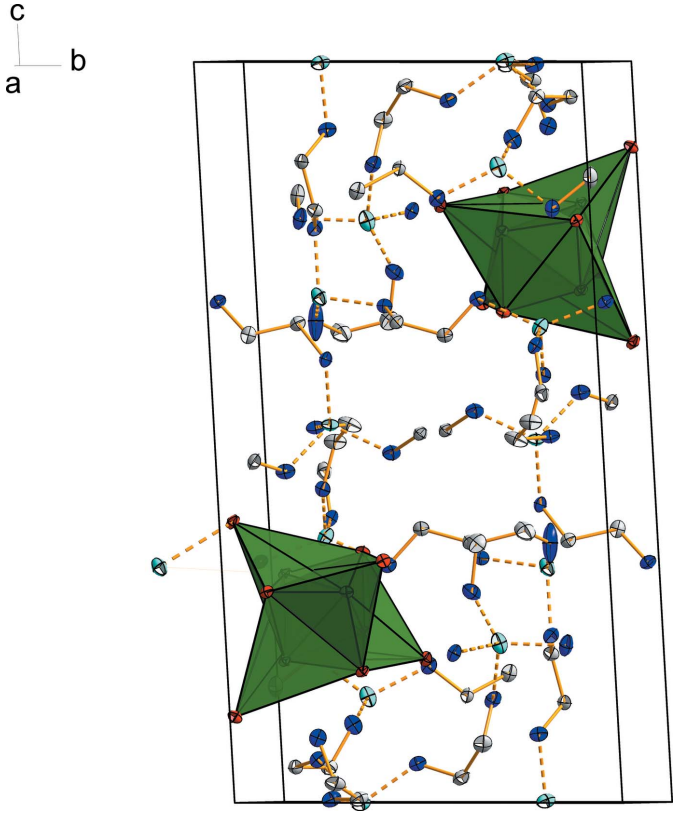


Figure 1
Excerpt from the crystal structure of $[Li_6(en_{11.5})][Fe_4Se_8]$. Green: Fe, red: Se, grey: C, blue: N, light blue: Li. Ellipsoids are drawn with 70% probability. Protons are omitted for clarity.

The Se—Fe—Se angles for the bridging Se atoms are in the range of 101.23 (2)—108.66 (3)° and therefore smaller than the ideal tetrahedron angle. As a result of the contraction of

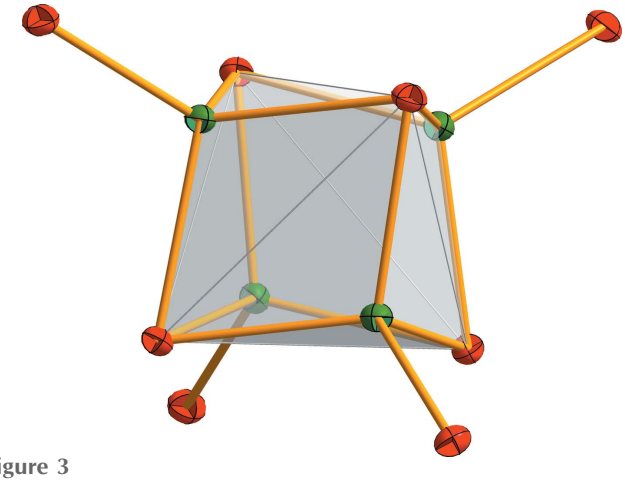


Figure 3
Anionic moiety in $[Li_6(en_{11.5})][Fe_4Se_8]$ with the distorted heterocubane core highlighted. Ellipsoids are drawn with 70% probability.

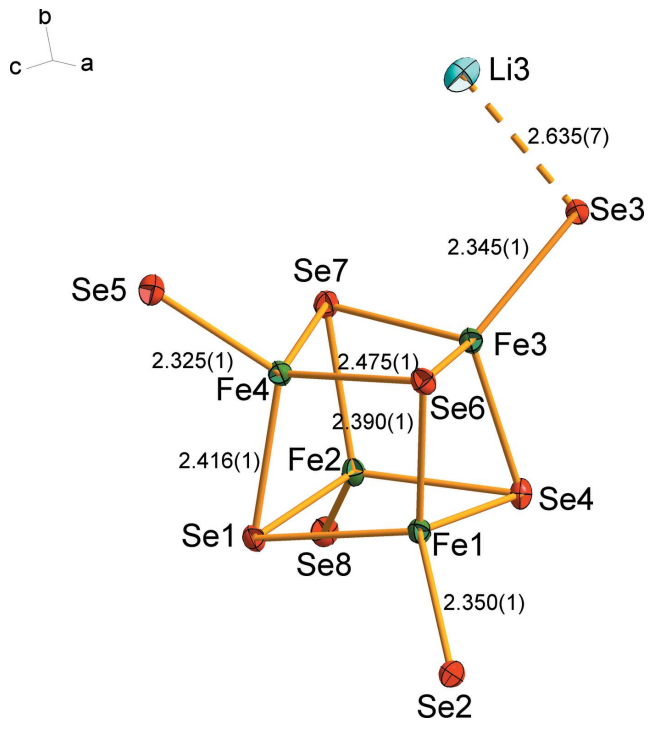


Figure 4
Atom labelling of the anionic moiety in $[Li_6(en_{11.5})][Fe_4Se_8]$ with selected distances. Green: Fe, red: Se, ellipsoids are drawn with 70% probability.

the heterocubane along the crystallographic *b*-axis, the Se—Fe—Se angles are the smallest in this direction, 101.23 (2)–101.90 (2)°. The Se—Fe—Se angles of the terminal Se atoms are in the range of 108.31 (2)—119.59 (3)°.

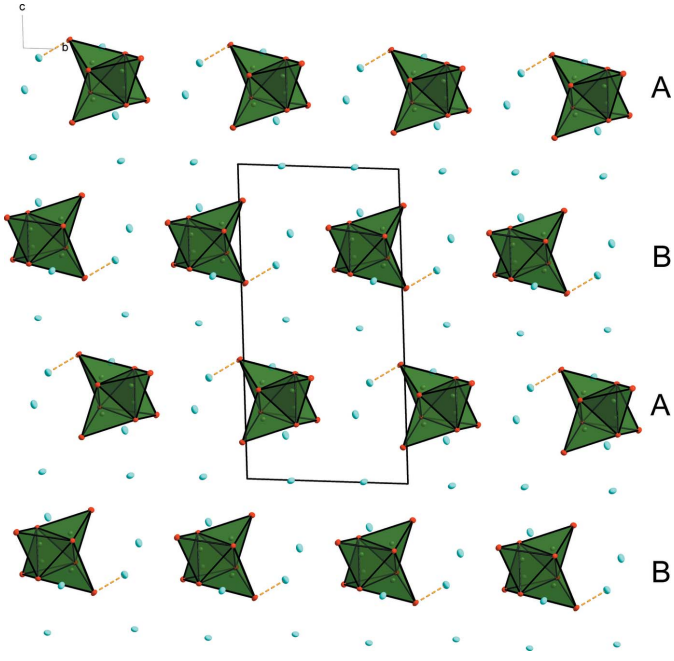


Figure 5
$[Fe_4Se_8]^{6-}$ anion packing in layers with Se—Li coordination sites pointing in different directions along the crystallographic *b*-axis. Green: Fe, red: Se, light blue: Li. For ease of viewing, atoms are drawn as small spheres and ethylenediamine ligands are omitted.

Five of the six crystallographically independent Li cations are tetrahedrally coordinated by one amine group of four ethylenediamine molecules. The ethylenediamine molecules bridge adjacent lithium cations to form an infinite three-dimensionally connected network of $^{3}_{\infty}[Li_6(en)_{11.5}]^{6+}$. The last Li cation is coordinated by three amine groups of three independent ethylenediamine molecules with the fourth coordination site occupied by one of the terminal selenido ligands (Se3) as depicted in Fig. 4. The coordination of Se to the Li cation results in the non-integer number of ethylenediamine ligands in the sum formula. As a result of the individual coordination environments of lithium ions, a complicated 6-nodal net with point symbol $\{3.6.7^3.8\}_2\{3.7^3.8^2\}\{4^2.6.8^2.9\}\{4^2.6^3.8\}\{6.8.9\}$ is obtained (*ToposPro* V 5.4.1.0; Blatov *et al.*, 2014).

3. Supramolecular features

The anion packing can be described as layers stacked in an *AB* type. The Li coordinated to the terminal Se ligand pointing in one direction defines the *A* layer, while the ligand pointing in the opposite direction defines the *B* layer. The layers are shifted with respect to each other such that the anions of one layer are placed between the anions of the other layer. The formation of those layers correlates with the inversion centre in the unit cell containing two asymmetric units. The Li–ethylenediamine network is located both in between and within those layers surrounding the anions (see Fig. 5). It is stabilized by classical N—H···Se and non-classical C—H···Se hydrogen bonds (Table 1).

The hydrogen bonds between the ethylenediamine molecules of the cationic network and the selenium atoms of the anion can be described by graph-set theory (*e.g.* Etter *et al.*, 1990). In graph-set theory, a hydrogen-bond network can be described by a pattern designator (G), the pattern's degree (r) and the number of donors (d) and acceptors (a): $G^a_d(r)$. G can be S (intramolecular), C (chains), R (rings) or D (non-cyclic) and r is the number of atoms before repetition. To be able to determine the graph sets, the Li—N coordination was also counted as a 'bond' in the network, so rings or chains can contain Li atoms. The anionic moiety was not counted as taking part in the network; every acceptor Se atom was looked at individually. Only the smallest/simplest pattern for each set is given. For Se1 the graph set is three times $R^1_2(8)$, for the donor pairs N7, N14; N14, N16; N7, N16. Se2 can be described by two sets of $R^1_2(4)$ for N10, N18; N22, N23 and two $R^1_2(5)$ for N7, N13 and N21, N23. Se3 is bound in two sets of $R^1_2(4)$ to N2, N8; N15, N17 and in $R^1_2(5)$ to N2, N15 and $R^1_2(9)$ to N2, N24. Se4 has two sets, $R^1_2(8)$ N2, N8 and $R^1_2(12)$ N2, N6/N6*A* (the split positions of N6 are counted in a single set). Se5 has five sets of classical hydrogen bonds: three sets of $R^1_2(4)$ for N1, N19; N3, N19 and N12, N13; two sets of $R^1_2(5)$ for N2, N22 and N16, N19 and one set of non-classical hydrogen bonds D for C6. Se6 has one set of classical hydrogen bonds, $R^1_2(5)$ to N1, N18 and one set of non-classical D to C20. Se7 has one set of $R^1_2(5)$ for N4, N17 and one $R^1_2(7)$ for N12, N24*A* and one $R^1_2(9)$ N12, N20. Se8 has three classical sets of hydrogen bonds: one

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Se5^{i}	0.91 (1)	2.94 (1)	3.837 (3)	169 (4)
N1—H1B···Se6^{i}	0.91 (1)	2.98 (3)	3.594 (3)	127 (3)
N2—H2A···Se3^{i}	0.91 (1)	2.60 (2)	3.483 (3)	163 (3)
N2—H2B···Se4^{i}	0.91 (1)	2.81 (2)	3.646 (3)	155 (3)
N3—H3B···Se5	0.91 (1)	2.86 (2)	3.665 (4)	148 (3)
N4—H4A···Se7^{i}	0.91 (1)	2.94 (3)	3.600 (3)	131 (3)
N4—H4B···Se8^{i}	0.91 (1)	2.60 (1)	3.493 (3)	170 (4)
N5—H5B···Se4^{i}	0.91 (1)	3.15 (4)	3.696 (3)	121 (3)
N5—H5B···Se8^{i}	0.91 (1)	2.90 (2)	3.751 (3)	156 (4)
N7—H7A···Se2^{i}	0.91 (1)	2.81 (2)	3.647 (3)	154 (3)
N7—H7B···Se1^{i}	0.91 (1)	2.73 (2)	3.573 (3)	155 (3)
N8—H8A···Se3^{ii}	0.91 (1)	2.68 (2)	3.514 (3)	152 (3)
N9—H9B···Se8^{iii}	0.91 (1)	2.92 (2)	3.786 (3)	161 (3)
N10—H10A···Se2^{iv}	0.91 (1)	2.88 (2)	3.725 (3)	156 (3)
N10—H10B···Se8^{i}	0.91 (1)	2.86 (1)	3.749 (3)	165 (3)
N12—H12A···Se5	0.91 (1)	2.71 (1)	3.611 (4)	173 (4)
N12—H12B···Se7	0.91 (1)	2.91 (4)	3.532 (3)	127 (3)
N13—H13A···Se5	0.91 (1)	3.14 (2)	3.973 (4)	153 (3)
N13—H13B···Se2^{i}	0.91 (1)	2.74 (2)	3.628 (3)	166 (4)
N14—H14A···Se8^{i}	0.91 (1)	2.59 (1)	3.479 (3)	166 (4)
N14—H14B···Se1^{i}	0.90 (1)	2.77 (3)	3.539 (3)	144 (3)
N15—H15A···Se3^{i}	0.91 (1)	2.94 (2)	3.785 (4)	154 (3)
N15—H15B···Se3^{ii}	0.91 (1)	2.68 (2)	3.560 (3)	163 (4)
N16—H16A···Se5^{i}	0.91 (1)	2.82 (2)	3.679 (3)	159 (4)
N16—H16B···Se1^{i}	0.91 (1)	2.67 (2)	3.537 (3)	160 (4)
N17—H17A···Se3^{i}	0.91 (1)	3.01 (2)	3.897 (4)	166 (4)
N17—H17B···Se7^{i}	0.91 (1)	3.07 (4)	3.649 (3)	124 (3)
N18—H18A···Se6^{i}	0.91 (1)	2.96 (2)	3.837 (3)	162 (3)
N18—H18B···Se2^{i}	0.91 (1)	2.80 (3)	3.491 (3)	134 (3)
N19—H19A···Se5^{i}	0.91 (1)	2.98 (2)	3.801 (3)	151 (4)
N20—H20A···Se7	0.89 (5)	2.98 (5)	3.841 (4)	163 (4)
N21—H21A···Se8^{v}	0.91 (1)	2.98 (3)	3.729 (3)	141 (3)
N21—H21B···Se2^{i}	0.91 (1)	2.91 (2)	3.763 (3)	157 (3)
N22—H22A···Se5	0.91 (1)	2.97 (2)	3.785 (3)	150 (4)
N22—H22B···Se2^{i}	0.91 (1)	3.10 (3)	3.818 (4)	138 (3)
N23—H23B···Se2^{i}	0.91 (1)	2.60 (1)	3.505 (3)	173 (4)
C1—H1C···Se8^{v}	0.99	3.14	3.702 (4)	118
C6—H6A···Se5^{vi}	0.99	2.90	3.734 (4)	143
C12—H12C···Se6	0.99	3.05	3.838 (4)	137
C13—H13D···Se8^{iii}	0.99	3.07	3.929 (4)	146
N6—H6D···Se4^{i}	0.90 (1)	3.01 (4)	3.659 (5)	130 (4)
C10—H10D···Se8^{i}	0.99	2.99	3.816 (5)	142
N24—H24B···Se3	0.91 (1)	2.77 (5)	3.327 (4)	121 (4)
N24—H24B···Se7	0.91 (1)	2.88 (4)	3.507 (5)	128 (4)
N6A—H6AA···Se4^{i}	0.91	2.99	3.79 (7)	147
C10A—H10F···Se8^{i}	0.99	2.95	3.74 (5)	137
N24A—H24D···Se7	0.91	3.17	3.94 (6)	145

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

set of $R_2^1(4)$ to N4, N21, $C_2^2(4)$ for N5, N9 and $R_2^1(5)$ to N10, N14 and two non-classical sets, $C_2^2(8)$ to C1, C10/C10A (the split positions of C10 are counted in a single set) and $C_2^2(10)$ C1, C13.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.43; Groom *et al.*, 2016) for compounds showing the motif of a heterocubane core containing iron and chalcogens yielded 548 results. Most of those are structures containing sulfidoferrate heterocubane cores, which are investigated with regard to iron–sulfur proteins. For a more direct comparison, only compounds comprising one terminal ligand on each iron atom and solely Se as the chalcogen were chosen, as the bond lengths inside the cubane core differ significantly depending on whether S or Se is part of the heterocubane. First, selenido ferrates, which only differ in the anionic moiety, are compared. In the second step, we analyse compounds that contain organic ligands on the terminal Se atoms.

Regarding the elemental ratios of alkali metal to Fe and Se, $[Li_6(en_{11.5})][Fe_4Se_8]$ is identical to $K_6[Fe_4Se_8]$ (ICSD: 430631; Stüble *et al.*, 2016). In the following, the bond lengths of the anion are compared to the ones in $K_6[Fe_4Se_8]$, despite the differences in the cationic moiety. The Fe—Se bonds to the terminal Se atoms in the potassium selenido tetraferrate are in the range of 2.320 (2)–2.307 (2) Å and therefore shorter than the respective bonds in the title compound, lithium selenido tetraferrate [2.3251 (8)–2.3502 (7) Å]. The Fe—Se distances of the bridging Se atoms are in the range of 2.397 (2)–2.468 (2) Å in the potassium ferrate and 2.3899 (8)–2.4752 (8) Å in the lithium selenido tetraferrate. In known literature for the $A_7[Fe_4Ch_8]$ species, the anion is surrounded by 26 cations, which form a cube with one cation on each corner, edge, and face of the cube: $Cs_7[Fe_4S_8]$ (ICSD: 428508; Schwarz & Röhr, 2015), $Cs_7[Fe_4Se_8]$ (ICSD: 433140; Stüble & Röhr, 2017), ($K_7[Fe_4Te_8]$ (ICSD: 430632), $Rb_7[Fe_4Te_8]$ (ICSD: 430634; Stüble *et al.*, 2016), $Cs_7[Fe_4Te_8]$ (ICSD: 37065; Bronger *et al.*, 1983). In $K_6[Fe_4Se_8]$, 24 cations form a distorted cube around the anions. In the title compound, no such regular shape can be observed for the surrounding cations, probably due to the more complex cation motif with the ethylenediamine ligands interlinking the alkali metal ions.

Comparing the bond angles and distances of the anionic moiety to homologues with aliphatic or arylic ligands at the terminal Se atoms, the bond lengths inside the heterocubane core are in a similar range: Fe—Se distances are found to be 2.3573 (12)–2.4391 (12) Å in $[Yb(THF)_6][Fe_4Se_4(SePh_4)_4]$ (THF = tetrahydrofuran; CCDC 228675; Kornienko *et al.*, 2003) and 2.391–2.434 Å in $(NBu_4)_2[Fe_4Se_4(SeCH_3)_4]$ (CCDC 201198; Kern *et al.*, 2004). In contrast, terminal Fe—Se distances are significantly elongated upon organic substitution: 2.3843 (12)–2.4055 (12) Å for $[Yb(THF)_6][Fe_4Se_4(SePh_4)_4]$ and 2.375 Å in $(NBu_4)_2[Fe_4Se_4(SeCH_3)_4]$.

5. Synthesis and crystallization

500 mg (3.71 mmol, 1 eq.) of iron(II) selenide, 293 mg (3.71 mmol, 1 eq.) of Se and 52 mg (7.49 mmol, 2 eq.) of Li were stirred in 50 mL of dry ethylenediamine under an argon atmosphere. The reaction mixture was stirred for 24 h, during which time several colour changes from brown to green to brown occur; these are most likely associated with the various intermediate polyselenide anions. After 24 h, a final colour change to brown was observed and the solution was filtered and allowed to stand for 16 weeks to afford crystallization. A crystal suitable for X-ray diffraction analysis was chosen in Paratone oil under a light microscope. The obtained crystals were comparably large and visible without a microscope. Breaking the crystal typically yielded very small crystallites that immediately decomposed because of their air and

moisture sensitivity. Therefore, a crystal larger than the X-ray beam was used for analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

The crystal was found to comprise two pieces, mis-aligned by ∼1.6°. For the purpose of integration, and processing, facilities for handling twinning by non-merohedry (namely the HKLF 5 data format in *SHELXL*) were attempted. In combination with the experimentation with different integration box sizes with common-volume overlap of 4% did not result in an improved dataset.

One of the en ligands is disordered, the disorder was treated with RIGU and DELU restraints. H atoms were treated by a mixture of independent and constrained refinement.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Li_6(C_2H_8N_2)_{11.5}][Fe_4Se_8]$
M_r	1587.91
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	11.495 (2), 11.665 (3), 22.233 (5)
α, β, γ (°)	92.885 (8), 92.383 (7), 103.510 (7)
V (Å^3)	2890.9 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	6.06
Crystal size (mm)	0.8 × 0.6 × 0.4
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.323, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	178309, 10708, 9144
R_{int}	0.081
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.059, 1.10
No. of reflections	10708
No. of parameters	752
No. of restraints	193
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.64

Computer programs: *APEX4* (Bruker, 2021), *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

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$[Li_6(C_2N_2H_8)_{11.5}][Fe_4Se_8]$: the first lithium-containing chalcogenidotetraferrate synthesized in solution

Friederike Fuss and Günther Thiele

Computing details

Data collection: *APEX4* (Bruker, 2021); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: Olex2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 (Dolomanov *et al.*, 2009).

Poly[[tricosa(*μ*-ethylenediamine)dodecalithium] bis[octaselenidotetraferrate(II/III)]]

Crystal data

$[Li_6(C_2H_8N_2)_{11.5}][Fe_4Se_8]$
M_r = 1587.91
Triclinic, $P\overline{1}$
a = 11.495 (2) Å
b = 11.665 (3) Å
c = 22.233 (5) Å
α = 92.885 (8)°
β = 92.383 (7)°
γ = 103.510 (7)°
V = 2890.9 (11) Å^3
Z = 2
$F(000)$ = 1570
D_x = 1.824 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9368 reflections
θ = 2.4–25.4°
μ = 6.06 mm^{-1}
T = 100 K
Block, dark black
0.8 × 0.6 × 0.4 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.323, T_{max} = 0.745
178309 measured reflections
10708 independent reflections
9144 reflections with $I > 2\sigma(I)$
R_{int} = 0.081
θ_{max} = 25.5°, θ_{min} = 2.2°
h = −13→13
k = −14→14
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.059
S = 1.10
10708 reflections
752 parameters
193 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 11.5642P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 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)
Se1	0.23309 (3)	−0.31834 (3)	0.82278 (2)	0.00859 (8)	
Se2	0.51559 (3)	−0.44704 (3)	0.80634 (2)	0.01022 (8)	
Se3	0.47570 (3)	0.02579 (3)	0.62160 (2)	0.01098 (8)	
Se4	0.36270 (3)	−0.31909 (3)	0.66142 (2)	0.00930 (8)	
Se5	0.28008 (3)	0.02291 (3)	0.88460 (2)	0.01085 (8)	
Se6	0.51956 (3)	−0.09741 (3)	0.78576 (2)	0.00885 (8)	
Se7	0.19676 (3)	−0.08788 (3)	0.71572 (2)	0.00948 (8)	
Se8	0.00915 (3)	−0.41635 (3)	0.67346 (2)	0.01008 (8)	
Fe1	0.42062 (4)	−0.30404 (5)	0.77046 (2)	0.00816 (11)	
Fe2	0.18670 (4)	−0.29485 (5)	0.71569 (2)	0.00838 (11)	
Fe3	0.39696 (4)	−0.11194 (5)	0.69146 (2)	0.00849 (11)	
Fe4	0.30805 (4)	−0.11068 (5)	0.80853 (2)	0.00818 (11)	
N1	0.4973 (3)	0.8434 (3)	0.94248 (15)	0.0136 (7)	
H1A	0.448 (3)	0.892 (3)	0.9340 (18)	0.016*	
H1B	0.490 (4)	0.802 (3)	0.9063 (10)	0.016*	
N2	0.6222 (3)	0.8083 (3)	0.57712 (14)	0.0126 (7)	
H2A	0.591 (3)	0.873 (2)	0.5816 (18)	0.015*	
H2B	0.571 (3)	0.757 (3)	0.5986 (16)	0.015*	
N3	0.5391 (3)	0.2755 (3)	0.90791 (14)	0.0138 (7)	
H3A	0.534 (4)	0.3467 (19)	0.8947 (18)	0.017*	
H3B	0.4601 (13)	0.238 (3)	0.9060 (19)	0.017*	
N4	−0.0699 (3)	0.8309 (3)	0.61730 (15)	0.0139 (7)	
H4A	−0.026 (3)	0.891 (2)	0.6417 (15)	0.017*	
H4B	−0.039 (3)	0.772 (3)	0.6314 (18)	0.017*	
N5	0.1591 (3)	0.5663 (3)	0.52773 (15)	0.0157 (7)	
H5A	0.223 (2)	0.534 (3)	0.5327 (19)	0.019*	
H5B	0.146 (4)	0.585 (4)	0.5667 (7)	0.019*	
N7	0.3681 (3)	0.5696 (3)	0.94751 (15)	0.0156 (7)	
H7A	0.425 (3)	0.562 (4)	0.9216 (15)	0.019*	
H7B	0.313 (3)	0.594 (4)	0.9239 (16)	0.019*	
N8	0.2417 (3)	1.0029 (3)	0.32400 (15)	0.0135 (7)	
H8A	0.3213 (12)	1.006 (4)	0.3250 (19)	0.016*	
H8B	0.205 (3)	0.982 (4)	0.2869 (9)	0.016*	
N9	0.1297 (3)	0.7187 (3)	0.40169 (14)	0.0118 (7)	
H9A	0.0574 (19)	0.734 (4)	0.4077 (18)	0.014*	
H9B	0.110 (3)	0.6404 (12)	0.3901 (18)	0.014*	
N10	−0.1535 (3)	0.5881 (3)	0.81593 (15)	0.0135 (7)	
H10A	−0.2307 (14)	0.574 (4)	0.8008 (17)	0.016*	
H10B	−0.101 (3)	0.591 (4)	0.7863 (13)	0.016*	

N12	0.0773 (3)	0.1331 (3)	0.78714 (17)	0.0180 (8)
H12A	0.134 (3)	0.111 (4)	0.8107 (16)	0.022*
H12B	0.063 (4)	0.084 (3)	0.7533 (12)	0.022*
N13	0.2564 (3)	0.3522 (3)	0.86096 (15)	0.0153 (7)
H13A	0.290 (3)	0.290 (3)	0.8659 (19)	0.018*
H13B	0.317 (3)	0.413 (3)	0.8513 (19)	0.018*
N14	0.0117 (3)	0.4141 (3)	0.79762 (15)	0.0134 (7)
H14A	0.000 (4)	0.448 (3)	0.7626 (11)	0.016*
H14B	0.064 (3)	0.468 (3)	0.8216 (15)	0.016*
N15	0.4007 (3)	0.7894 (3)	0.49376 (15)	0.0146 (7)
H15A	0.409 (4)	0.824 (3)	0.5317 (8)	0.018*
H15B	0.425 (4)	0.849 (3)	0.4688 (16)	0.018*
N16	0.0241 (3)	0.7795 (3)	0.91254 (15)	0.0146 (7)
H16A	0.077 (3)	0.8511 (19)	0.9124 (19)	0.018*
H16B	0.064 (3)	0.736 (3)	0.8897 (16)	0.018*
N17	0.1663 (3)	0.8433 (3)	0.55308 (15)	0.0163 (7)
H17A	0.234 (2)	0.898 (3)	0.5658 (18)	0.020*
H17B	0.150 (4)	0.802 (3)	0.5863 (12)	0.020*
N18	0.7145 (3)	0.7742 (3)	0.89574 (16)	0.0162 (7)
H18A	0.685 (4)	0.810 (4)	0.8649 (13)	0.019*
H18B	0.659 (3)	0.705 (2)	0.8959 (19)	0.019*
N19	0.2420 (3)	0.7809 (3)	0.99544 (16)	0.0174 (7)
H19A	0.248 (4)	0.814 (4)	0.9592 (10)	0.021*
H19B	0.240 (4)	0.842 (3)	1.0221 (15)	0.021*
N20	−0.0885 (4)	−0.1079 (3)	0.80260 (17)	0.0193 (8)
H20A	−0.019 (4)	−0.115 (4)	0.789 (2)	0.023*
H20B	−0.142 (4)	−0.108 (4)	0.775 (2)	0.023*
N21	0.7131 (3)	0.6615 (3)	0.68026 (14)	0.0129 (7)
H21A	0.784 (2)	0.657 (4)	0.6988 (17)	0.015*
H21B	0.650 (2)	0.646 (4)	0.7040 (15)	0.015*
N22	0.4619 (3)	0.2194 (3)	0.77482 (15)	0.0156 (7)
H22A	0.416 (3)	0.152 (2)	0.7881 (18)	0.019*
H22B	0.433 (4)	0.280 (3)	0.7899 (18)	0.019*
N23	0.5410 (3)	0.3981 (3)	0.67015 (15)	0.0141 (7)
H23A	0.489 (3)	0.425 (4)	0.6460 (16)	0.017*
H23B	0.542 (4)	0.438 (3)	0.7062 (10)	0.017*
C1	0.6909 (3)	0.5686 (3)	0.63090 (17)	0.0123 (8)
H1C	0.762564	0.580950	0.606620	0.015*
H1D	0.623310	0.579231	0.604416	0.015*
C2	0.6124 (3)	0.7679 (4)	0.51350 (17)	0.0177 (9)
H2C	0.661928	0.709742	0.507613	0.021*
H2D	0.645166	0.835994	0.489397	0.021*
C3	0.2137 (3)	0.3794 (4)	0.92042 (18)	0.0173 (9)
H3C	0.176491	0.303972	0.937863	0.021*
H3D	0.150301	0.422983	0.914353	0.021*
C4	0.5863 (3)	0.2379 (4)	0.79921 (17)	0.0136 (8)
H4C	0.628153	0.320933	0.794129	0.016*
H4D	0.626567	0.186916	0.774797	0.016*

C5	0.1255 (3)	0.6950 (4)	0.99522 (18)	0.0180 (9)
H5C	0.113172	0.668570	1.036583	0.022*
H5D	0.128743	0.625057	0.968781	0.022*
C6	0.6203 (3)	0.9169 (3)	0.95251 (17)	0.0140 (8)
H6A	0.627267	0.963798	0.991428	0.017*
H6B	0.637259	0.972722	0.920102	0.017*
C7	0.0182 (3)	0.7406 (4)	0.97419 (18)	0.0175 (9)
H7C	−0.055347	0.677252	0.976673	0.021*
H7D	0.011857	0.807642	1.001954	0.021*
C8	−0.0500 (3)	0.8437 (4)	0.55319 (18)	0.0155 (8)
H8C	−0.108237	0.885511	0.536073	0.019*
H8D	−0.066662	0.764026	0.532432	0.019*
C9	−0.0345 (4)	0.1159 (4)	0.8184 (2)	0.0183 (9)
H9C	−0.098390	0.127796	0.789821	0.022*
H9D	−0.024173	0.177812	0.851663	0.022*
C11	0.1833 (4)	0.7927 (3)	0.35333 (17)	0.0151 (8)
H11A	0.136081	0.765971	0.314823	0.018*
H11B	0.265987	0.783963	0.348170	0.018*
C12	0.6014 (3)	0.2127 (3)	0.86527 (16)	0.0121 (8)
H12C	0.572022	0.126766	0.869137	0.015*
H12D	0.687953	0.233809	0.877319	0.015*
C13	0.0556 (3)	0.4759 (3)	0.50163 (17)	0.0119 (8)
H13C	0.041653	0.406652	0.526690	0.014*
H13D	0.072700	0.449422	0.460623	0.014*
C14	−0.1363 (4)	0.4963 (3)	0.85624 (17)	0.0143 (8)
H14C	−0.211055	0.469010	0.877347	0.017*
H14D	−0.072224	0.532640	0.887239	0.017*
C15	−0.1040 (3)	0.3892 (3)	0.82603 (18)	0.0143 (8)
H15C	−0.102545	0.330553	0.856564	0.017*
H15D	−0.167734	0.352795	0.794877	0.017*
C16	0.0761 (3)	0.9104 (3)	0.53955 (18)	0.0153 (8)
H16C	0.077291	0.927622	0.496395	0.018*
H16D	0.096934	0.986740	0.563707	0.018*
C17	0.4843 (4)	0.7115 (4)	0.48997 (19)	0.0207 (9)
H17C	0.485777	0.683582	0.447283	0.025*
H17D	0.453212	0.641405	0.513020	0.025*
C18	0.6626 (3)	0.4420 (3)	0.64901 (17)	0.0132 (8)
H18C	0.673124	0.390264	0.613966	0.016*
H18D	0.721579	0.434751	0.681476	0.016*
C19	−0.0765 (4)	−0.0038 (4)	0.8445 (2)	0.0218 (9)
H19C	−0.019529	−0.009323	0.878198	0.026*
H19D	−0.155264	−0.007029	0.861602	0.026*
C20	0.7115 (3)	0.8423 (3)	0.95328 (17)	0.0142 (8)
H20C	0.791911	0.894470	0.963200	0.017*
H20D	0.693641	0.786626	0.985673	0.017*
C22	0.3085 (4)	0.4515 (4)	0.96621 (18)	0.0179 (9)
H22C	0.270339	0.461047	1.004661	0.021*
H22D	0.370199	0.406516	0.973909	0.021*

C23	0.1855 (3)	0.9217 (3)	0.36872 (18)	0.0134 (8)	
H23C	0.102221	0.929384	0.372773	0.016*	
H23D	0.229333	0.945997	0.408313	0.016*	
Li1	0.7577 (5)	0.8246 (6)	0.6421 (3)	0.0141 (14)	
Li2	0.4064 (6)	0.7262 (6)	1.0017 (3)	0.0162 (14)	
Li5	0.2141 (5)	0.7278 (6)	0.4896 (3)	0.0129 (13)	
Li6	−0.1309 (5)	0.7527 (6)	0.8581 (3)	0.0154 (14)	
Li4	0.1373 (6)	0.3128 (6)	0.7847 (3)	0.0170 (14)	
N6	0.2336 (6)	0.3899 (6)	0.71564 (18)	0.0195 (9)	0.935 (8)
H6C	0.3101 (18)	0.383 (4)	0.721 (2)	0.023*	0.935 (8)
H6D	0.239 (4)	0.4674 (15)	0.725 (2)	0.023*	0.935 (8)
C10	0.2073 (5)	0.3661 (4)	0.64990 (19)	0.0177 (10)	0.935 (8)
H10C	0.277723	0.405388	0.628182	0.021*	0.935 (8)
H10D	0.138889	0.399250	0.637314	0.021*	0.935 (8)
C21	0.1775 (4)	0.2355 (4)	0.6335 (2)	0.0198 (11)	0.935 (8)
H21C	0.106329	0.196734	0.654849	0.024*	0.935 (8)
H21D	0.157330	0.221581	0.589634	0.024*	0.935 (8)
N24	0.2752 (4)	0.1837 (4)	0.6490 (3)	0.0335 (13)	0.935 (8)
H24A	0.276 (5)	0.186 (5)	0.6897 (6)	0.040*	0.935 (8)
H24B	0.271 (5)	0.1061 (15)	0.640 (2)	0.040*	0.935 (8)
Li3	0.4551 (6)	0.2192 (6)	0.6823 (3)	0.0170 (14)	
N6A	0.221 (8)	0.375 (8)	0.7090 (15)	0.020 (4)	0.065 (8)
H6AA	0.235880	0.454990	0.711734	0.024*	0.065 (8)
H6AB	0.293028	0.354976	0.708873	0.024*	0.065 (8)
C10A	0.155 (6)	0.332 (7)	0.6506 (16)	0.021 (3)	0.065 (8)
H10E	0.082052	0.271092	0.658274	0.025*	0.065 (8)
H10F	0.129397	0.398155	0.632669	0.025*	0.065 (8)
C21A	0.224 (4)	0.280 (5)	0.6064 (18)	0.022 (3)	0.065 (8)
H21E	0.166901	0.235314	0.574121	0.026*	0.065 (8)
H21F	0.278237	0.345660	0.587620	0.026*	0.065 (8)
N24A	0.294 (4)	0.203 (5)	0.629 (3)	0.025 (3)	0.065 (8)
H24C	0.306951	0.161916	0.595230	0.030*	0.065 (8)
H24D	0.240096	0.150678	0.649050	0.030*	0.065 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.00745 (17)	0.01009 (19)	0.00859 (18)	0.00206 (14)	0.00235 (13)	0.00248 (14)
Se2	0.00890 (18)	0.01060 (19)	0.01223 (19)	0.00395 (15)	0.00204 (14)	0.00199 (15)
Se3	0.01273 (18)	0.01107 (19)	0.01146 (18)	0.00579 (15)	0.00575 (14)	0.00452 (15)
Se4	0.00803 (17)	0.01185 (19)	0.00829 (18)	0.00278 (14)	0.00216 (13)	−0.00026 (14)
Se5	0.01063 (18)	0.0120 (2)	0.00995 (18)	0.00294 (15)	0.00167 (14)	−0.00080 (15)
Se6	0.00723 (17)	0.00982 (19)	0.00919 (18)	0.00113 (14)	0.00079 (13)	0.00152 (14)
Se7	0.00895 (17)	0.01200 (19)	0.00890 (18)	0.00486 (15)	0.00133 (14)	0.00209 (15)
Se8	0.00716 (17)	0.0118 (2)	0.01137 (18)	0.00250 (15)	−0.00047 (14)	0.00072 (15)
Fe1	0.0070 (2)	0.0093 (3)	0.0088 (3)	0.0025 (2)	0.0019 (2)	0.0016 (2)
Fe2	0.0068 (2)	0.0102 (3)	0.0083 (3)	0.0021 (2)	0.0010 (2)	0.0007 (2)
Fe3	0.0081 (2)	0.0097 (3)	0.0083 (3)	0.0029 (2)	0.0020 (2)	0.0020 (2)

Fe4	0.0081 (2)	0.0090 (3)	0.0078 (3)	0.0023 (2)	0.0014 (2)	0.0015 (2)
N1	0.0103 (16)	0.0163 (19)	0.0150 (17)	0.0044 (14)	0.0014 (13)	0.0031 (14)
N2	0.0105 (16)	0.0159 (18)	0.0134 (17)	0.0074 (14)	0.0009 (13)	0.0005 (14)
N3	0.0100 (16)	0.0203 (19)	0.0124 (17)	0.0060 (14)	0.0001 (13)	0.0021 (14)
N4	0.0136 (17)	0.0142 (18)	0.0149 (17)	0.0045 (14)	0.0004 (13)	0.0041 (14)
N5	0.0135 (17)	0.0185 (19)	0.0142 (17)	0.0022 (14)	−0.0012 (14)	0.0010 (15)
N7	0.0177 (18)	0.0172 (19)	0.0129 (17)	0.0050 (15)	0.0022 (14)	0.0036 (14)
N8	0.0129 (16)	0.0155 (18)	0.0126 (17)	0.0041 (14)	0.0004 (13)	0.0034 (14)
N9	0.0103 (16)	0.0101 (17)	0.0144 (17)	0.0009 (14)	0.0015 (13)	0.0028 (14)
N10	0.0093 (16)	0.0172 (18)	0.0171 (18)	0.0081 (14)	0.0031 (13)	0.0045 (14)
N12	0.0160 (18)	0.0123 (18)	0.028 (2)	0.0057 (15)	0.0062 (15)	0.0043 (15)
N13	0.0128 (17)	0.0168 (19)	0.0176 (18)	0.0045 (14)	0.0067 (14)	0.0053 (15)
N14	0.0099 (16)	0.0141 (18)	0.0169 (18)	0.0031 (14)	0.0019 (13)	0.0055 (14)
N15	0.0120 (16)	0.0206 (19)	0.0119 (17)	0.0044 (14)	0.0017 (13)	0.0032 (14)
N16	0.0079 (16)	0.0178 (19)	0.0180 (18)	0.0027 (14)	0.0013 (13)	0.0015 (15)
N17	0.0138 (17)	0.023 (2)	0.0137 (17)	0.0068 (15)	0.0013 (14)	0.0022 (15)
N18	0.0081 (16)	0.0187 (19)	0.0211 (19)	0.0029 (14)	−0.0002 (14)	−0.0029 (15)
N19	0.0148 (17)	0.021 (2)	0.0158 (18)	0.0020 (15)	0.0009 (14)	0.0042 (15)
N20	0.025 (2)	0.0123 (18)	0.021 (2)	0.0047 (16)	−0.0019 (16)	0.0015 (15)
N21	0.0092 (16)	0.0157 (18)	0.0143 (17)	0.0036 (14)	0.0017 (13)	0.0028 (14)
N22	0.0154 (17)	0.0153 (19)	0.0153 (18)	0.0018 (14)	−0.0009 (14)	0.0044 (14)
N23	0.0164 (17)	0.0138 (18)	0.0118 (17)	0.0029 (14)	0.0005 (14)	0.0003 (14)
C1	0.0104 (18)	0.014 (2)	0.0123 (19)	0.0033 (16)	0.0016 (15)	0.0011 (16)
C2	0.0113 (19)	0.029 (2)	0.014 (2)	0.0075 (18)	−0.0002 (16)	−0.0001 (18)
C3	0.014 (2)	0.020 (2)	0.019 (2)	0.0035 (17)	0.0080 (16)	0.0029 (17)
C4	0.0127 (19)	0.015 (2)	0.014 (2)	0.0040 (16)	0.0027 (15)	0.0009 (16)
C5	0.018 (2)	0.020 (2)	0.015 (2)	0.0017 (18)	0.0015 (16)	0.0050 (17)
C6	0.016 (2)	0.013 (2)	0.0120 (19)	0.0021 (16)	−0.0002 (15)	0.0010 (16)
C7	0.014 (2)	0.024 (2)	0.014 (2)	0.0031 (17)	0.0062 (16)	0.0004 (17)
C8	0.015 (2)	0.014 (2)	0.019 (2)	0.0056 (17)	−0.0013 (16)	0.0001 (17)
C9	0.016 (2)	0.011 (2)	0.028 (2)	0.0025 (17)	0.0021 (17)	0.0045 (18)
C11	0.019 (2)	0.014 (2)	0.012 (2)	0.0027 (17)	0.0023 (16)	0.0026 (16)
C12	0.0121 (19)	0.014 (2)	0.0126 (19)	0.0078 (16)	0.0002 (15)	0.0007 (16)
C13	0.0121 (19)	0.012 (2)	0.0115 (19)	0.0013 (16)	0.0025 (15)	0.0016 (15)
C14	0.019 (2)	0.011 (2)	0.015 (2)	0.0054 (16)	0.0036 (16)	0.0024 (16)
C15	0.0102 (18)	0.014 (2)	0.019 (2)	0.0027 (16)	0.0039 (15)	0.0031 (17)
C16	0.017 (2)	0.013 (2)	0.017 (2)	0.0044 (17)	0.0036 (16)	0.0052 (17)
C17	0.016 (2)	0.032 (3)	0.015 (2)	0.0097 (19)	−0.0016 (16)	−0.0083 (18)
C18	0.0135 (19)	0.013 (2)	0.0132 (19)	0.0050 (16)	−0.0014 (15)	−0.0001 (16)
C19	0.025 (2)	0.013 (2)	0.029 (2)	0.0053 (18)	0.0082 (19)	0.0025 (18)
C20	0.0130 (19)	0.015 (2)	0.015 (2)	0.0037 (16)	−0.0010 (15)	0.0009 (16)
C22	0.021 (2)	0.018 (2)	0.014 (2)	0.0029 (18)	0.0031 (16)	0.0046 (17)
C23	0.0102 (18)	0.013 (2)	0.017 (2)	0.0028 (16)	0.0012 (15)	0.0023 (16)
Li1	0.009 (3)	0.017 (4)	0.018 (3)	0.006 (3)	−0.001 (3)	0.004 (3)
Li2	0.015 (3)	0.020 (4)	0.013 (3)	0.002 (3)	0.001 (3)	0.003 (3)
Li5	0.011 (3)	0.016 (3)	0.010 (3)	0.001 (3)	−0.001 (2)	0.000 (3)
Li6	0.007 (3)	0.015 (4)	0.023 (4)	0.002 (3)	0.000 (3)	−0.003 (3)
Li4	0.011 (3)	0.014 (4)	0.025 (3)	0.001 (3)	0.001 (3)	−0.002 (3)

N6	0.020 (2)	0.019 (3)	0.0166 (19)	−0.0016 (17)	0.0021 (17)	−0.0056 (17)
C10	0.013 (2)	0.020 (2)	0.021 (2)	0.0058 (18)	−0.0039 (17)	0.0005 (18)
C21	0.019 (2)	0.020 (2)	0.021 (2)	0.0077 (18)	−0.0066 (18)	−0.0024 (18)
N24	0.015 (2)	0.015 (2)	0.072 (3)	0.0062 (17)	−0.001 (2)	0.007 (2)
Li3	0.017 (3)	0.016 (4)	0.020 (4)	0.008 (3)	0.001 (3)	−0.002 (3)
N6A	0.017 (6)	0.019 (6)	0.022 (5)	0.002 (6)	−0.002 (5)	−0.002 (5)
C10A	0.017 (5)	0.019 (5)	0.025 (4)	0.004 (5)	−0.005 (4)	−0.003 (5)
C21A	0.016 (5)	0.017 (5)	0.034 (5)	0.007 (4)	−0.004 (5)	0.001 (5)
N24A	0.018 (6)	0.017 (6)	0.041 (6)	0.006 (5)	−0.004 (6)	0.005 (6)

Geometric parameters (Å, º)

Se1—Fe1	2.4674 (7)	N21—H21A	0.909 (10)
Se1—Fe2	2.4611 (8)	N21—H21B	0.908 (10)
Se1—Fe4	2.4157 (8)	N21—C1	1.473 (5)
Se2—Fe1	2.3502 (7)	N21—Li1	2.084 (7)
Se3—Fe3	2.3456 (7)	N22—H22A	0.905 (10)
Se3—Li3	2.634 (7)	N22—H22B	0.907 (10)
Se4—Fe1	2.4739 (8)	N22—C4	1.471 (5)
Se4—Fe2	2.4629 (7)	N22—Li3	2.055 (8)
Se4—Fe3	2.4108 (8)	N23—H23A	0.906 (10)
Se5—Fe4	2.3251 (8)	N23—H23B	0.906 (10)
Se6—Fe1	2.4133 (8)	N23—C18	1.477 (5)
Se6—Fe3	2.4531 (8)	N23—Li3	2.126 (8)
Se6—Fe4	2.4752 (8)	C1—H1C	0.9900
Se7—Fe2	2.3899 (8)	C1—H1D	0.9900
Se7—Fe3	2.4608 (8)	C1—C18	1.516 (5)
Se7—Fe4	2.4414 (7)	C2—H2C	0.9900
Se8—Fe2	2.3262 (7)	C2—H2D	0.9900
Fe1—Fe2	2.9327 (9)	C2—C17	1.524 (5)
Fe1—Fe3	2.9702 (9)	C3—H3C	0.9900
Fe1—Fe4	2.9566 (9)	C3—H3D	0.9900
Fe2—Fe3	2.9154 (9)	C3—C22	1.524 (6)
Fe2—Fe4	2.9556 (9)	C4—H4C	0.9900
Fe3—Fe4	2.8362 (9)	C4—H4D	0.9900
N1—H1A	0.907 (10)	C4—C12	1.523 (5)
N1—H1B	0.908 (10)	C5—H5C	0.9900
N1—C6	1.474 (5)	C5—H5D	0.9900
N1—Li2	2.079 (7)	C5—C7	1.519 (5)
N2—H2A	0.907 (10)	C6—H6A	0.9900
N2—H2B	0.907 (10)	C6—H6B	0.9900
N2—C2	1.460 (5)	C6—C20	1.511 (5)
N2—Li1	2.049 (7)	C7—H7C	0.9900
N3—H3A	0.909 (10)	C7—H7D	0.9900
N3—H3B	0.909 (10)	C8—H8C	0.9900
N3—C12	1.476 (5)	C8—H8D	0.9900
N3—Li2^{i}	2.082 (7)	C8—C16	1.527 (5)
N4—H4A	0.906 (10)	C9—H9C	0.9900

N4—H4B	0.907 (10)	C9—H9D	0.9900
N4—C8	1.463 (5)	C9—C19	1.519 (5)
N4—Li1^{ii}	2.065 (7)	C11—H11A	0.9900
N5—H5A	0.908 (10)	C11—H11B	0.9900
N5—H5B	0.908 (10)	C11—C23	1.521 (5)
N5—C13	1.470 (5)	C12—H12C	0.9900
N5—Li5	2.077 (7)	C12—H12D	0.9900
N7—H7A	0.907 (10)	C13—C13^{vi}	1.513 (7)
N7—H7B	0.908 (10)	C13—H13C	0.9900
N7—C22	1.477 (5)	C13—H13D	0.9900
N7—Li2	2.085 (8)	C14—H14C	0.9900
N8—H8A	0.907 (10)	C14—H14D	0.9900
N8—H8B	0.906 (10)	C14—C15	1.518 (5)
N8—C23	1.471 (5)	C15—H15C	0.9900
N8—Li1^{iii}	2.111 (8)	C15—H15D	0.9900
N9—H9A	0.906 (10)	C16—H16C	0.9900
N9—H9B	0.910 (10)	C16—H16D	0.9900
N9—C11	1.476 (5)	C17—H17C	0.9900
N9—Li5	2.133 (7)	C17—H17D	0.9900
N10—H10A	0.909 (7)	C18—H18C	0.9900
N10—H10B	0.910 (7)	C18—H18D	0.9900
N10—C14	1.474 (5)	C19—H19C	0.9900
N10—Li6	2.049 (8)	C19—H19D	0.9900
N12—H12A	0.905 (10)	C20—H20C	0.9900
N12—H12B	0.908 (10)	C20—H20D	0.9900
N12—C9	1.464 (5)	C22—H22C	0.9900
N12—Li4	2.052 (8)	C22—H22D	0.9900
N13—H13A	0.908 (10)	C23—H23C	0.9900
N13—H13B	0.908 (10)	C23—H23D	0.9900
N13—C3	1.474 (5)	Li1—H2B	2.26 (4)
N13—Li4	2.097 (8)	Li2—H7B	2.31 (4)
N14—H14A	0.908 (10)	Li4—H14B	2.30 (4)
N14—H14B	0.902 (10)	Li4—N6	2.051 (8)
N14—C15	1.469 (5)	Li4—N6A	2.05 (2)
N14—Li4	2.088 (7)	N6—H6C	0.907 (10)
N15—H15A	0.909 (10)	N6—H6D	0.903 (10)
N15—H15B	0.909 (10)	N6—C10	1.479 (6)
N15—C17	1.470 (5)	C10—H10C	0.9900
N15—Li5	2.094 (7)	C10—H10D	0.9900
N16—H16A	0.909 (10)	C10—C21	1.504 (6)
N16—H16B	0.908 (10)	C21—H21C	0.9900
N16—C7	1.465 (5)	C21—H21D	0.9900
N16—Li6	2.064 (7)	C21—N24	1.431 (6)
N17—H17A	0.907 (10)	N24—H24A	0.902 (10)
N17—H17B	0.908 (10)	N24—H24B	0.906 (10)
N17—C16	1.468 (5)	N24—Li3	2.107 (8)
N17—Li5	2.080 (7)	Li3—H24A	2.01 (6)
N18—H18A	0.909 (10)	Li3—N24A	2.12 (2)

N18—H18B	0.907 (10)	N6A—H6AA	0.9100
N18—C20	1.477 (5)	N6A—H6AB	0.9100
N18—Li6^{iv}	2.058 (7)	N6A—C10A	1.48 (2)
N19—H19A	0.910 (10)	C10A—H10E	0.9900
N19—H19B	0.907 (10)	C10A—H10F	0.9900
N19—C5	1.472 (5)	C10A—C21A	1.48 (2)
N19—Li2	2.133 (7)	C21A—H21E	0.9900
N20—H20A	0.89 (5)	C21A—H21F	0.9900
N20—H20B	0.85 (5)	C21A—N24A	1.44 (2)
N20—C19	1.469 (6)	N24A—H24C	0.9100
N20—Li6^{v}	2.070 (7)	N24A—H24D	0.9100

Fe2—Se1—Fe1	73.03 (2)	C18—C1—H1D	108.1
Fe4—Se1—Fe1	74.52 (2)	N2—C2—H2C	108.9
Fe4—Se1—Fe2	74.60 (2)	N2—C2—H2D	108.9
Fe3—Se3—Li3	98.63 (15)	N2—C2—C17	113.6 (3)
Fe2—Se4—Fe1	72.89 (2)	H2C—C2—H2D	107.7
Fe3—Se4—Fe1	74.89 (2)	C17—C2—H2C	108.9
Fe3—Se4—Fe2	73.47 (2)	C17—C2—H2D	108.9
Fe1—Se6—Fe3	75.23 (2)	N13—C3—H3C	108.3
Fe1—Se6—Fe4	74.42 (2)	N13—C3—H3D	108.3
Fe3—Se6—Fe4	70.27 (2)	N13—C3—C22	115.9 (3)
Fe2—Se7—Fe3	73.87 (2)	H3C—C3—H3D	107.4
Fe2—Se7—Fe4	75.43 (2)	C22—C3—H3C	108.3
Fe4—Se7—Fe3	70.70 (2)	C22—C3—H3D	108.3
Se1—Fe1—Se4	105.83 (3)	N22—C4—H4C	108.4
Se1—Fe1—Fe2	53.39 (2)	N22—C4—H4D	108.4
Se1—Fe1—Fe3	97.87 (2)	N22—C4—C12	115.7 (3)
Se1—Fe1—Fe4	51.944 (18)	H4C—C4—H4D	107.4
Se2—Fe1—Se1	108.31 (2)	C12—C4—H4C	108.4
Se2—Fe1—Se4	117.08 (3)	C12—C4—H4D	108.4
Se2—Fe1—Se6	119.59 (3)	N19—C5—H5C	108.5
Se2—Fe1—Fe2	138.02 (3)	N19—C5—H5D	108.5
Se2—Fe1—Fe3	153.78 (3)	N19—C5—C7	115.1 (3)
Se2—Fe1—Fe4	143.63 (3)	H5C—C5—H5D	107.5
Se4—Fe1—Fe2	53.381 (17)	C7—C5—H5C	108.5
Se4—Fe1—Fe3	51.589 (19)	C7—C5—H5D	108.5
Se4—Fe1—Fe4	98.75 (2)	N1—C6—H6A	109.3
Se6—Fe1—Se1	103.23 (2)	N1—C6—H6B	109.3
Se6—Fe1—Se4	101.23 (2)	N1—C6—C20	111.5 (3)
Se6—Fe1—Fe2	102.13 (2)	H6A—C6—H6B	108.0
Se6—Fe1—Fe3	53.00 (2)	C20—C6—H6A	109.3
Se6—Fe1—Fe4	53.75 (2)	C20—C6—H6B	109.3
Fe2—Fe1—Fe3	59.189 (18)	N16—C7—C5	113.9 (3)
Fe2—Fe1—Fe4	60.25 (2)	N16—C7—H7C	108.8
Fe4—Fe1—Fe3	57.18 (2)	N16—C7—H7D	108.8
Se1—Fe2—Se4	106.37 (2)	C5—C7—H7C	108.8
Se1—Fe2—Fe1	53.582 (17)	C5—C7—H7D	108.8

Se1—Fe2—Fe3	99.46 (2)	H7C—C7—H7D	107.7
Se1—Fe2—Fe4	52.00 (2)	N4—C8—H8C	108.6
Se4—Fe2—Fe1	53.73 (2)	N4—C8—H8D	108.6
Se4—Fe2—Fe3	52.44 (2)	N4—C8—C16	114.7 (3)
Se4—Fe2—Fe4	99.03 (2)	H8C—C8—H8D	107.6
Se7—Fe2—Se1	101.70 (2)	C16—C8—H8C	108.6
Se7—Fe2—Se4	104.06 (2)	C16—C8—H8D	108.6
Se7—Fe2—Fe1	103.32 (2)	N12—C9—H9C	108.4
Se7—Fe2—Fe3	54.18 (2)	N12—C9—H9D	108.4
Se7—Fe2—Fe4	53.076 (19)	N12—C9—C19	115.6 (3)
Se8—Fe2—Se1	116.00 (2)	H9C—C9—H9D	107.4
Se8—Fe2—Se4	112.40 (3)	C19—C9—H9C	108.4
Se8—Fe2—Se7	115.01 (3)	C19—C9—H9D	108.4
Se8—Fe2—Fe1	141.65 (3)	N9—C11—H11A	109.6
Se8—Fe2—Fe3	144.53 (3)	N9—C11—H11B	109.6
Se8—Fe2—Fe4	148.55 (3)	N9—C11—C23	110.4 (3)
Fe1—Fe2—Fe4	60.28 (2)	H11A—C11—H11B	108.1
Fe3—Fe2—Fe1	61.05 (2)	C23—C11—H11A	109.6
Fe3—Fe2—Fe4	57.77 (2)	C23—C11—H11B	109.6
Se3—Fe3—Se4	118.26 (3)	N3—C12—C4	115.6 (3)
Se3—Fe3—Se6	114.85 (3)	N3—C12—H12C	108.4
Se3—Fe3—Se7	108.75 (2)	N3—C12—H12D	108.4
Se3—Fe3—Fe1	150.72 (3)	C4—C12—H12C	108.4
Se3—Fe3—Fe2	143.27 (3)	C4—C12—H12D	108.4
Se3—Fe3—Fe4	137.92 (3)	H12C—C12—H12D	107.4
Se4—Fe3—Se6	101.90 (2)	N5—C13—C13^{vi}	110.8 (4)
Se4—Fe3—Se7	103.50 (2)	N5—C13—H13C	109.5
Se4—Fe3—Fe1	53.52 (2)	N5—C13—H13D	109.5
Se4—Fe3—Fe2	54.084 (19)	C13^{vi}—C13—H13C	109.5
Se4—Fe3—Fe4	103.67 (2)	C13^{vi}—C13—H13D	109.5
Se6—Fe3—Se7	108.66 (3)	H13C—C13—H13D	108.1
Se6—Fe3—Fe1	51.778 (19)	N10—C14—H14C	108.3
Se6—Fe3—Fe2	101.62 (2)	N10—C14—H14D	108.3
Se6—Fe3—Fe4	55.23 (2)	N10—C14—C15	115.8 (3)
Se7—Fe3—Fe1	100.50 (2)	H14C—C14—H14D	107.4
Se7—Fe3—Fe2	51.95 (2)	C15—C14—H14C	108.3
Se7—Fe3—Fe4	54.331 (17)	C15—C14—H14D	108.3
Fe2—Fe3—Fe1	59.76 (2)	N14—C15—C14	114.8 (3)
Fe4—Fe3—Fe1	61.17 (2)	N14—C15—H15C	108.6
Fe4—Fe3—Fe2	61.83 (2)	N14—C15—H15D	108.6
Se1—Fe4—Se6	102.93 (2)	C14—C15—H15C	108.6
Se1—Fe4—Se7	101.53 (2)	C14—C15—H15D	108.6
Se1—Fe4—Fe1	53.54 (2)	H15C—C15—H15D	107.5
Se1—Fe4—Fe2	53.40 (2)	N17—C16—C8	112.3 (3)
Se1—Fe4—Fe3	102.80 (2)	N17—C16—H16C	109.1
Se5—Fe4—Se1	117.39 (3)	N17—C16—H16D	109.1
Se5—Fe4—Se6	114.88 (3)	C8—C16—H16C	109.1
Se5—Fe4—Se7	110.38 (3)	C8—C16—H16D	109.1

Se5—Fe4—Fe1	148.27 (3)	H16C—C16—H16D	107.9
Se5—Fe4—Fe2	144.99 (3)	N15—C17—C2	115.0 (4)
Se5—Fe4—Fe3	139.68 (3)	N15—C17—H17C	108.5
Se6—Fe4—Fe1	51.836 (18)	N15—C17—H17D	108.5
Se6—Fe4—Fe2	99.98 (2)	C2—C17—H17C	108.5
Se6—Fe4—Fe3	54.502 (17)	C2—C17—H17D	108.5
Se7—Fe4—Se6	108.57 (3)	H17C—C17—H17D	107.5
Se7—Fe4—Fe1	101.35 (2)	N23—C18—C1	115.2 (3)
Se7—Fe4—Fe2	51.50 (2)	N23—C18—H18C	108.5
Se7—Fe4—Fe3	54.97 (2)	N23—C18—H18D	108.5
Fe2—Fe4—Fe1	59.48 (2)	C1—C18—H18C	108.5
Fe3—Fe4—Fe1	61.652 (19)	C1—C18—H18D	108.5
Fe3—Fe4—Fe2	60.40 (2)	H18C—C18—H18D	107.5
H1A—N1—H1B	99 (4)	N20—C19—C9	116.5 (4)
C6—N1—H1A	108 (3)	N20—C19—H19C	108.2
C6—N1—H1B	109 (3)	N20—C19—H19D	108.2
C6—N1—Li2	126.1 (3)	C9—C19—H19C	108.2
Li2—N1—H1A	105 (3)	C9—C19—H19D	108.2
Li2—N1—H1B	106 (3)	H19C—C19—H19D	107.3
H2A—N2—H2B	100 (4)	N18—C20—C6	114.0 (3)
C2—N2—H2A	109 (3)	N18—C20—H20C	108.8
C2—N2—H2B	111 (3)	N18—C20—H20D	108.8
C2—N2—Li1	131.7 (3)	C6—C20—H20C	108.8
Li1—N2—H2A	108 (3)	C6—C20—H20D	108.8
Li1—N2—H2B	92 (3)	H20C—C20—H20D	107.7
H3A—N3—H3B	100 (4)	N7—C22—C3	114.5 (3)
C12—N3—H3A	111 (3)	N7—C22—H22C	108.6
C12—N3—H3B	109 (3)	N7—C22—H22D	108.6
C12—N3—Li2^{i}	114.9 (3)	C3—C22—H22C	108.6
Li2^{i}—N3—H3A	116 (3)	C3—C22—H22D	108.6
Li2^{i}—N3—H3B	104 (3)	H22C—C22—H22D	107.6
H4A—N4—H4B	98 (4)	N8—C23—C11	114.3 (3)
C8—N4—H4A	114 (3)	N8—C23—H23C	108.7
C8—N4—H4B	111 (3)	N8—C23—H23D	108.7
C8—N4—Li1^{ii}	115.7 (3)	C11—C23—H23C	108.7
Li1^{ii}—N4—H4A	102 (3)	C11—C23—H23D	108.7
Li1^{ii}—N4—H4B	114 (3)	H23C—C23—H23D	107.6
H5A—N5—H5B	101 (4)	N2—Li1—H2B	23.6 (5)
C13—N5—H5A	110 (3)	N2—Li1—N4^{iv}	119.8 (3)
C13—N5—H5B	109 (3)	N2—Li1—N8^{iii}	97.3 (3)
C13—N5—Li5	121.3 (3)	N2—Li1—N21	102.0 (3)
Li5—N5—H5A	109 (3)	N4^{iv}—Li1—H2B	136.0 (10)
Li5—N5—H5B	105 (3)	N4^{iv}—Li1—N8^{iii}	105.9 (3)
H7A—N7—H7B	103 (4)	N4^{iv}—Li1—N21	101.7 (3)
C22—N7—H7A	109 (3)	N8^{iii}—Li1—H2B	103.6 (11)
C22—N7—H7B	106 (3)	N21—Li1—H2B	81.1 (7)
C22—N7—Li2	126.1 (3)	N21—Li1—N8^{iii}	132.1 (3)
Li2—N7—H7A	115 (3)	N1—Li2—N3^{i}	123.8 (4)

Li2—N7—H7B	93 (3)	N1—Li2—N7	100.6 (3)
H8A—N8—H8B	113 (4)	N1—Li2—H7B	92.4 (10)
C23—N8—H8A	109 (3)	N1—Li2—N19	96.7 (3)
C23—N8—H8B	111 (3)	N3^{i}—Li2—N7	119.6 (3)
C23—N8—Li1^{iii}	106.9 (3)	N3^{i}—Li2—H7B	138.6 (9)
Li1^{iii}—N8—H8A	101 (3)	N3^{i}—Li2—N19	109.5 (3)
Li1^{iii}—N8—H8B	115 (3)	N7—Li2—H7B	23.1 (5)
H9A—N9—H9B	103 (4)	N7—Li2—N19	102.7 (3)
C11—N9—H9A	107 (3)	N19—Li2—H7B	82.3 (7)
C11—N9—H9B	113 (3)	N5—Li5—N9	109.6 (3)
C11—N9—Li5	122.9 (3)	N5—Li5—N15	112.6 (3)
Li5—N9—H9A	105 (3)	N5—Li5—N17	102.1 (3)
Li5—N9—H9B	105 (3)	N15—Li5—N9	114.8 (3)
H10A—N10—H10B	112 (4)	N17—Li5—N9	115.7 (3)
C14—N10—H10A	112 (3)	N17—Li5—N15	101.2 (3)
C14—N10—H10B	108 (3)	N10—Li6—N16	106.0 (3)
C14—N10—Li6	114.3 (3)	N10—Li6—N18^{ii}	111.6 (3)
Li6—N10—H10A	101 (3)	N10—Li6—N20^{vii}	115.3 (3)
Li6—N10—H10B	109 (3)	N16—Li6—N20^{vii}	101.4 (3)
H12A—N12—H12B	108 (4)	N18^{ii}—Li6—N16	118.9 (4)
C9—N12—H12A	109 (3)	N18^{ii}—Li6—N20^{vii}	103.7 (3)
C9—N12—H12B	107 (3)	N12—Li4—N13	101.3 (3)
C9—N12—Li4	105.0 (3)	N12—Li4—N14	117.0 (3)
Li4—N12—H12A	104 (3)	N12—Li4—H14B	132.6 (10)
Li4—N12—H12B	123 (3)	N12—Li4—N6A	117 (3)
H13A—N13—H13B	105 (4)	N13—Li4—H14B	84.9 (7)
C3—N13—H13A	106 (3)	N14—Li4—N13	105.8 (3)
C3—N13—H13B	110 (3)	N14—Li4—H14B	23.1 (5)
C3—N13—Li4	120.5 (3)	N6—Li4—N12	122.4 (4)
Li4—N13—H13A	109 (3)	N6—Li4—N13	105.0 (3)
Li4—N13—H13B	106 (3)	N6—Li4—N14	103.6 (4)
H14A—N14—H14B	107 (4)	N6—Li4—H14B	100.2 (11)
C15—N14—H14A	107 (3)	N6A—Li4—N13	111 (2)
C15—N14—H14B	108 (3)	N6A—Li4—N14	104 (4)
C15—N14—Li4	131.9 (3)	N6A—Li4—H14B	104 (3)
Li4—N14—H14A	108 (3)	Li4—N6—H6C	108 (3)
Li4—N14—H14B	92 (3)	Li4—N6—H6D	102 (3)
H15A—N15—H15B	106 (4)	H6C—N6—H6D	103 (4)
C17—N15—H15A	108 (3)	C10—N6—Li4	128.5 (4)
C17—N15—H15B	108 (3)	C10—N6—H6C	104 (3)
C17—N15—Li5	123.7 (3)	C10—N6—H6D	109 (3)
Li5—N15—H15A	98 (3)	N6—C10—H10C	109.5
Li5—N15—H15B	112 (3)	N6—C10—H10D	109.5
H16A—N16—H16B	99 (4)	N6—C10—C21	110.7 (4)
C7—N16—H16A	109 (3)	H10C—C10—H10D	108.1
C7—N16—H16B	110 (3)	C21—C10—H10C	109.5
C7—N16—Li6	119.8 (3)	C21—C10—H10D	109.5
Li6—N16—H16A	117 (3)	C10—C21—H21C	109.3

Li6—N16—H16B	98 (3)	C10—C21—H21D	109.3
H17A—N17—H17B	102 (4)	H21C—C21—H21D	107.9
C16—N17—H17A	106 (3)	N24—C21—C10	111.8 (4)
C16—N17—H17B	112 (3)	N24—C21—H21C	109.3
C16—N17—Li5	122.6 (3)	N24—C21—H21D	109.3
Li5—N17—H17A	107 (3)	C21—N24—H24A	103 (4)
Li5—N17—H17B	105 (3)	C21—N24—H24B	121 (4)
H18A—N18—H18B	102 (4)	C21—N24—Li3	144.7 (4)
C20—N18—H18A	110 (3)	H24A—N24—H24B	101 (5)
C20—N18—H18B	108 (3)	Li3—N24—H24A	72 (4)
C20—N18—Li6^{iv}	124.2 (3)	Li3—N24—H24B	94 (4)
Li6^{iv}—N18—H18A	98 (3)	Se3—Li3—H24A	100.9 (15)
Li6^{iv}—N18—H18B	112 (3)	N22—Li3—Se3	117.6 (3)
H19A—N19—H19B	104 (4)	N22—Li3—N23	100.7 (3)
C5—N19—H19A	109 (3)	N22—Li3—N24	109.6 (4)
C5—N19—H19B	108 (3)	N22—Li3—H24A	84.5 (5)
C5—N19—Li2	121.3 (3)	N22—Li3—N24A	123 (2)
Li2—N19—H19A	100 (3)	N23—Li3—Se3	129.2 (3)
Li2—N19—H19B	113 (3)	N23—Li3—H24A	115.6 (17)
H20A—N20—H20B	114 (4)	N24—Li3—Se3	88.4 (3)
C19—N20—H20A	113 (3)	N24—Li3—N23	109.9 (3)
C19—N20—H20B	109 (3)	N24—Li3—H24A	25.2 (4)
C19—N20—Li6^{v}	103.1 (3)	N24A—Li3—Se3	86.1 (15)
Li6^{v}—N20—H20A	103 (3)	N24A—Li3—N23	100.3 (16)
Li6^{v}—N20—H20B	114 (3)	Li4—N6A—H6AA	108.3
H21A—N21—H21B	114 (4)	Li4—N6A—H6AB	108.3
C1—N21—H21A	104 (3)	H6AA—N6A—H6AB	107.4
C1—N21—H21B	107 (3)	C10A—N6A—Li4	116 (3)
C1—N21—Li1	107.9 (3)	C10A—N6A—H6AA	108.3
Li1—N21—H21A	103 (3)	C10A—N6A—H6AB	108.3
Li1—N21—H21B	119 (3)	N6A—C10A—H10E	108.6
H22A—N22—H22B	107 (4)	N6A—C10A—H10F	108.6
C4—N22—H22A	110 (3)	H10E—C10A—H10F	107.5
C4—N22—H22B	107 (3)	C21A—C10A—N6A	115 (3)
C4—N22—Li3	110.9 (3)	C21A—C10A—H10E	108.6
Li3—N22—H22A	112 (3)	C21A—C10A—H10F	108.6
Li3—N22—H22B	109 (3)	C10A—C21A—H21E	108.2
H23A—N23—H23B	104 (4)	C10A—C21A—H21F	108.2
C18—N23—H23A	108 (3)	H21E—C21A—H21F	107.3
C18—N23—H23B	105 (3)	N24A—C21A—C10A	116 (3)
C18—N23—Li3	126.5 (3)	N24A—C21A—H21E	108.2
Li3—N23—H23A	105 (3)	N24A—C21A—H21F	108.2
Li3—N23—H23B	107 (3)	Li3—N24A—H24C	102.7
N21—C1—H1C	108.1	Li3—N24A—H24D	102.7
N21—C1—H1D	108.1	C21A—N24A—Li3	138 (3)
N21—C1—C18	116.6 (3)	C21A—N24A—H24C	102.7
H1C—C1—H1D	107.3	C21A—N24A—H24D	102.7
C18—C1—H1C	108.1	H24C—N24A—H24D	105.0

N1—C6—C20—N18	62.8 (4)	Li5—N9—C11—C23	−67.9 (4)
N2—C2—C17—N15	60.7 (5)	Li5—N15—C17—C2	−161.3 (3)
N4—C8—C16—N17	69.1 (4)	Li5—N17—C16—C8	90.2 (4)
N9—C11—C23—N8	177.8 (3)	Li6—N10—C14—C15	−157.0 (3)
N10—C14—C15—N14	63.8 (5)	Li6—N16—C7—C5	144.6 (4)
N12—C9—C19—N20	−53.8 (5)	Li6^{iv}—N18—C20—C6	139.2 (4)
N13—C3—C22—N7	60.9 (5)	Li6^{v}—N20—C19—C9	174.9 (3)
N19—C5—C7—N16	59.9 (5)	Li4—N12—C9—C19	−160.7 (4)
N21—C1—C18—N23	74.6 (4)	Li4—N13—C3—C22	−157.0 (3)
N22—C4—C12—N3	−54.0 (5)	Li4—N14—C15—C14	148.6 (4)
Li1—N2—C2—C17	150.7 (4)	Li4—N6—C10—C21	−48.1 (9)
Li1^{ii}—N4—C8—C16	149.4 (3)	Li4—N6A—C10A—C21A	−128 (6)
Li1^{iii}—N8—C23—C11	−176.9 (3)	N6—C10—C21—N24	−61.0 (6)
Li1—N21—C1—C18	177.2 (3)	C10—C21—N24—Li3	−5.6 (10)
Li2—N1—C6—C20	67.1 (5)	Li3—N22—C4—C12	−166.9 (3)
Li2^{i}—N3—C12—C4	−165.5 (3)	Li3—N23—C18—C1	166.7 (3)
Li2—N7—C22—C3	136.6 (4)	N6A—C10A—C21A—N24A	43 (9)
Li2—N19—C5—C7	−164.6 (3)	C10A—C21A—N24A—Li3	−74 (8)
Li5—N5—C13—C13^{vi}	−57.2 (5)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Se5^{vii}	0.91 (1)	2.94 (1)	3.837 (3)	169 (4)
N1—H1*B*···Se6^{vii}	0.91 (1)	2.98 (3)	3.594 (3)	127 (3)
N2—H2*A*···Se3^{vii}	0.91 (1)	2.60 (2)	3.483 (3)	163 (3)
N2—H2*B*···Se4^{vii}	0.91 (1)	2.81 (2)	3.646 (3)	155 (3)
N3—H3*B*···Se5	0.91 (1)	2.86 (2)	3.665 (4)	148 (3)
N4—H4*A*···Se7^{vii}	0.91 (1)	2.94 (3)	3.600 (3)	131 (3)
N4—H4*B*···Se8^{vii}	0.91 (1)	2.60 (1)	3.493 (3)	170 (4)
N5—H5*B*···Se4^{vii}	0.91 (1)	3.15 (4)	3.696 (3)	121 (3)
N5—H5*B*···Se8^{vii}	0.91 (1)	2.90 (2)	3.751 (3)	156 (4)
N7—H7*A*···Se2^{vii}	0.91 (1)	2.81 (2)	3.647 (3)	154 (3)
N7—H7*B*···Se1^{vii}	0.91 (1)	2.73 (2)	3.573 (3)	155 (3)
N8—H8*A*···Se3^{viii}	0.91 (1)	2.68 (2)	3.514 (3)	152 (3)
N9—H9*B*···Se8^{ix}	0.91 (1)	2.92 (2)	3.786 (3)	161 (3)
N10—H10*A*···Se2^{x}	0.91 (1)	2.88 (2)	3.725 (3)	156 (3)
N10—H10*B*···Se8^{vii}	0.91 (1)	2.86 (1)	3.749 (3)	165 (3)
N12—H12*A*···Se5	0.91 (1)	2.71 (1)	3.611 (4)	173 (4)
N12—H12*B*···Se7	0.91 (1)	2.91 (4)	3.532 (3)	127 (3)
N13—H13*A*···Se5	0.91 (1)	3.14 (2)	3.973 (4)	153 (3)
N13—H13*B*···Se2^{vii}	0.91 (1)	2.74 (2)	3.628 (3)	166 (4)
N14—H14*A*···Se8^{vii}	0.91 (1)	2.59 (1)	3.479 (3)	166 (4)
N14—H14*B*···Se1^{vii}	0.90 (1)	2.77 (3)	3.539 (3)	144 (3)
N15—H15*A*···Se3^{vii}	0.91 (1)	2.94 (2)	3.785 (4)	154 (3)

N15—H15*B*···Se3^{viii}	0.91 (1)	2.68 (2)	3.560 (3)	163 (4)
N16—H16*A*···Se5^{vii}	0.91 (1)	2.82 (2)	3.679 (3)	159 (4)
N16—H16*B*···Se1^{vii}	0.91 (1)	2.67 (2)	3.537 (3)	160 (4)
N17—H17*A*···Se3^{vii}	0.91 (1)	3.01 (2)	3.897 (4)	166 (4)
N17—H17*B*···Se7^{vii}	0.91 (1)	3.07 (4)	3.649 (3)	124 (3)
N18—H18*A*···Se6^{vii}	0.91 (1)	2.96 (2)	3.837 (3)	162 (3)
N18—H18*B*···Se2^{vii}	0.91 (1)	2.80 (3)	3.491 (3)	134 (3)
N19—H19*A*···Se5^{vii}	0.91 (1)	2.98 (2)	3.801 (3)	151 (4)
N20—H20*A*···Se7	0.89 (5)	2.98 (5)	3.841 (4)	163 (4)
N21—H21*A*···Se8^{xi}	0.91 (1)	2.98 (3)	3.729 (3)	141 (3)
N21—H21*B*···Se2^{vii}	0.91 (1)	2.91 (2)	3.763 (3)	157 (3)
N22—H22*A*···Se5	0.91 (1)	2.97 (2)	3.785 (3)	150 (4)
N22—H22*B*···Se2^{vii}	0.91 (1)	3.10 (3)	3.818 (4)	138 (3)
N23—H23*B*···Se2^{vii}	0.91 (1)	2.60 (1)	3.505 (3)	173 (4)
C1—H1*C*···Se8^{xi}	0.99	3.14	3.702 (4)	118
C6—H6*A*···Se5^{i}	0.99	2.90	3.734 (4)	143
C12—H12*C*···Se6	0.99	3.05	3.838 (4)	137
C13—H13*D*···Se8^{ix}	0.99	3.07	3.929 (4)	146
N6—H6*D*···Se4^{vii}	0.90 (1)	3.01 (4)	3.659 (5)	130 (4)
C10—H10*D*···Se8^{vii}	0.99	2.99	3.816 (5)	142
N24—H24*B*···Se3	0.91 (1)	2.77 (5)	3.327 (4)	121 (4)
N24—H24*B*···Se7	0.91 (1)	2.88 (4)	3.507 (5)	128 (4)
N6*A*—H6*AA*···Se4^{vii}	0.91	2.99	3.79 (7)	147
C10*A*—H10*F*···Se8^{vii}	0.99	2.95	3.74 (5)	137
N24*A*—H24*D*···Se7	0.91	3.17	3.94 (6)	145

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (vii) *x*, *y*+1, *z*; (viii) −*x*+1, −*y*+1, −*z*+1; (ix) −*x*, −*y*, −*z*+1; (x) *x*−1, *y*+1, *z*; (xi) *x*+1, *y*+1, *z*.