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[1-(3-Aminopropyl)-4,7-dithia-1-azacyclononane-κ^4N,N',S,S']bis(dimethylformamide-κO)nickel(II) bis(tetraphenylborate) acetonitrile disolvate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.069
wR factor = 0.205
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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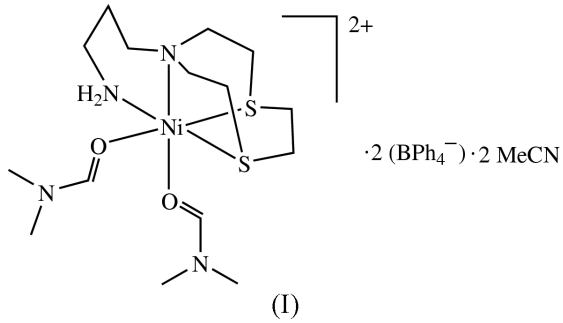
In the title complex, $[Ni(C_3H_7NO)_2(C_9H_{20}N_2S_2)](C_{24}H_{20}B)_2\cdot 2CH_3CN$, the metal centre has a distorted octahedral environment, with four coordination sites occupied by two N- and two S-donor atoms from a 3-aminopropyl pendant arm derivative of the nine-membered macrocycle 1-aza-4,7-dithiacyclononane, and the remaining two positions by two mutually *cis* dimethylformamide ligands.

Comment

The coordination chemistry of mixed thia–aza nine-membered macrocycles is of particular interest since the loss of threefold symmetry with respect to 1,4,7-triazacyclononane ([9]aneN$_3$) and the presence of both hard N- and soft S-donors can have interesting stereochemical consequences and thereby offer specific coordination selectivity (Danks *et al.*, 1998). Recently, we have reported on the coordination chemistry of nitrile and amino pendant arm derivatives of 1,4-diaza-7-thiacyclononane ([9]aneN$_2$S) and 1-aza-4,7-dithiacyclononane ([9]aneNS$_2$) with Pd^{II} and Cu^{II} (Arca *et al.*, 2003). A distorted square-pyramidal coordination is generally observed at these metal centres with 3-aminopropyl pendant arm derivatives of [9]-aneN$_2$S and [9]aneNS$_2$ which show strong basal coordination of the N-donors of the macrocycle and of the primary amine group(s).



(I)

We report here the X-ray crystal structure of the title Ni^{II} complex, (I), obtained by reacting the 3-aminopropyl pendant arm derivative of [9]aneNS$_2$ with NiCl$_2$ in MeOH/H$_2$O followed by addition of excess sodium tetraphenylborate. Crystals were obtained by diffusion of Et$_2$O vapour first into a solution of acetonitrile and subsequently into a solution of the resulting solid in dimethylformamide. The metal centre is in a distorted octahedral geometry (Fig. 1) with two positions occupied by mutually *cis* dimethylformamide ligands and the remaining four by the two N- and two S-donor atoms of the pendant-arm macrocyclic ligand. The Ni—O and Ni—NH$_2$ bond lengths (Table 1) are both slightly shorter than the Ni—N4 distance which involves the tertiary macrocyclic N-donor.

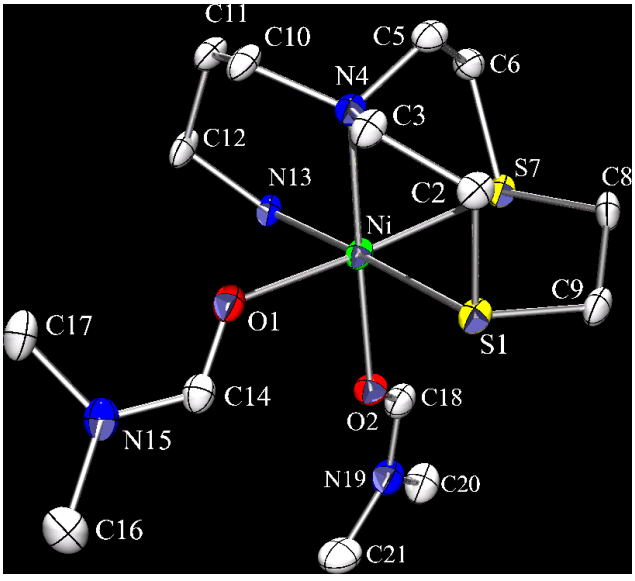


Figure 1
A view of the title cation, with displacement ellipsoids drawn at the 30% probability level. The two counter-anions and two solvent molecules are not shown, and H atoms have been omitted for clarity.

This leads to a trigonal elongation of the octahedron towards the triangular face formed by three of the macrocyclic donors. The S-donor *trans* to the NH_2 group lies slightly further from the metal than the one *trans* to the dimethylformamide donor O1.

Experimental

A solution of the ligand (30 mg, 0.136 mmol) and $NiCl_2$ (17.63 mg, 0.136 mmol) in MeOH/H_2O (10 ml, 1:1 *v*/*v*) was refluxed for 1 h. Excess sodium tetraphenylborate was added and a purple solid formed. Purple crystals were obtained as follows: first, Et_2O vapour was diffused into a solution of this solid in acetonitrile and a solid product isolated; second, this solid was dissolved in dimethylformamide and Et_2O vapour diffused into the solution (yield 51.7 mg, 33%). Found (calculated for $C_{67}H_{80}B_2N_6NiO_2S_2$): C 70.33 (70.23), H 6.98 (7.04), N 7.15% (7.33%).

Crystal data

$[Ni(C_3H_7NO)_2(C_9H_{20}N_2S_2)]$-$(C_{24}H_{20}B)_2{\cdot}2C_2H_3N$
M_r = 1145.82
Monoclinic, $P2_1/n$
a = 20.907 (4) Å
b = 11.951 (4) Å
c = 26.516 (5) Å
β = 111.06 (3)°
V = 6183 (3) Å^3
Z = 4
D_x = 1.231 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 33 reflections
θ = 26–34°
μ = 0.43 mm^{-1}
T = 150 (2) K
Irregular block, purple
0.39 × 0.39 × 0.31 mm

Data collection

Stoe Stadi-4 diffractometer
ω–θ scans
Absorption correction: ψ scan (*X-RED*32; Stoe & Cie, 1996)
T_{min} = 0.741, T_{max} = 0.876
12472 measured reflections
10898 independent reflections
8397 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.0°
$h = -24 \rightarrow 24$
$k = 0 \rightarrow 14$
$l = -31 \rightarrow 31$
3 standard reflections
every 60 reflections
intensity decay: random variation ±5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.205
S = 1.05
10898 reflections
731 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.122P)^2 + 7.311P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni—S1	2.4119 (12)	S1—C2	1.830 (4)
Ni—S7	2.3917 (14)	S1—C9	1.805 (4)
Ni—O1	2.057 (3)	S7—C6	1.812 (4)
Ni—O2	2.086 (3)	S7—C8	1.827 (4)
Ni—N4	2.141 (4)	O1—C14	1.231 (5)
Ni—N13	2.073 (3)	O2—C18	1.232 (5)
S1—Ni—S7	87.66 (5)	O2—Ni—N13	88.61 (12)
S1—Ni—O1	91.47 (8)	N4—Ni—N13	94.77 (12)
S1—Ni—O2	89.78 (8)	Ni—S1—C2	96.27 (12)
S1—Ni—N4	86.83 (8)	Ni—S1—C9	100.88 (13)
S1—Ni—N13	178.23 (11)	C2—S1—C9	102.67 (19)
S7—Ni—O1	176.09 (9)	Ni—S7—C6	93.35 (14)
S7—Ni—O2	93.46 (8)	Ni—S7—C8	103.56 (13)
S7—Ni—N4	87.46 (9)	C6—S7—C8	103.13 (19)
S7—Ni—N13	93.17 (9)	Ni—O1—C14	129.2 (2)
O1—Ni—O2	90.35 (11)	Ni—O2—C18	127.2 (3)
O1—Ni—N4	88.68 (12)	Ni—N4—C3	106.5 (2)
O1—Ni—N13	87.81 (11)	Ni—N4—C5	112.5 (2)
O2—Ni—N4	176.45 (10)	Ni—N13—C12	117.4 (2)

The two MeCN solvent molecules were affected by disorder. In one molecule, the components were each half-occupied while the other clearly had major and minor occupancies of 0.694 (19) and 0.306 (19), respectively. Restraints were applied to the C—C, C≡N and 1,3-C···N distances. Restraints for planarity, local C_{2v} symmetry and similarity were applied to and between the phenyl rings. Methyl H atoms were located from ΔF syntheses while all other H atoms were placed geometrically. Methyl H atoms were refined as part of rigid rotating groups, with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were refined using a riding model, with N—H = 0.92 Å, C—H(sp^2 and aryl) = 0.95 and C—H(methylene) = 0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(N,C). The maximum electron-density peak lies 1.25 Å from atom C18.

Data collection: *Stadi*-4 (Stoe & Cie, 1996); cell refinement: *Stadi*-4; data reduction: *X-RED*32 (Stoe & Cie, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004) and *PLATON*.

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supporting information

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Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.205$
$S = 1.05$
10898 reflections
731 parameters
709 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.122P)^2 + 7.311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni	0.53225 (2)	0.25356 (3)	0.30412 (2)	0.0278 (2)	
S1	0.55303 (5)	0.44737 (7)	0.33025 (4)	0.0329 (3)	
S7	0.43746 (5)	0.31491 (7)	0.22720 (4)	0.0320 (3)	
O1	0.60967 (14)	0.2025 (2)	0.37340 (10)	0.0371 (9)	
O2	0.60158 (14)	0.2651 (2)	0.26413 (10)	0.0350 (8)	
N4	0.46381 (16)	0.2510 (2)	0.34781 (12)	0.0296 (9)	
N13	0.51734 (16)	0.0868 (2)	0.28145 (12)	0.0295 (9)	
N15	0.71696 (18)	0.1625 (3)	0.42720 (13)	0.0407 (10)	
N19	0.6385 (2)	0.2352 (3)	0.19491 (15)	0.0455 (11)	
C2	0.4961 (2)	0.4529 (3)	0.36890 (15)	0.0343 (11)	
C3	0.4886 (2)	0.3382 (3)	0.39048 (15)	0.0350 (11)	
C5	0.3916 (2)	0.2766 (3)	0.31271 (16)	0.0368 (11)	
C6	0.3745 (2)	0.2582 (3)	0.25260 (16)	0.0345 (11)	
C8	0.4336 (2)	0.4652 (3)	0.23837 (15)	0.0360 (11)	
C9	0.5032 (2)	0.5161 (3)	0.26788 (16)	0.0381 (11)	
C10	0.4668 (2)	0.1415 (3)	0.37626 (16)	0.0382 (13)	
C11	0.4527 (2)	0.0378 (3)	0.34077 (16)	0.0371 (11)	
C12	0.5098 (2)	0.0062 (3)	0.32159 (16)	0.0386 (13)	
C14	0.6720 (2)	0.2153 (3)	0.38678 (15)	0.0368 (11)	
C16	0.7905 (3)	0.1795 (5)	0.4423 (2)	0.0664 (17)	
C17	0.6947 (3)	0.0836 (4)	0.45954 (17)	0.0502 (14)	
C18	0.5900 (2)	0.2477 (3)	0.21584 (18)	0.0422 (16)	
C20	0.6218 (3)	0.2159 (4)	0.13769 (19)	0.0548 (16)	
C21	0.7076 (3)	0.2403 (4)	0.2272 (2)	0.0603 (17)	
C1A	0.55838 (19)	0.7110 (3)	0.16228 (14)	0.0358 (11)	
C2A	0.6146 (2)	0.6398 (3)	0.17185 (14)	0.0472 (12)	
C3A	0.6084 (2)	0.5274 (3)	0.15748 (17)	0.0578 (16)	
C4A	0.5433 (2)	0.4824 (3)	0.13232 (17)	0.0510 (14)	
C5A	0.4869 (2)	0.5495 (3)	0.12171 (17)	0.0451 (14)	
C6A	0.4942 (2)	0.6620 (3)	0.13659 (15)	0.0385 (12)	
C7A	0.6082 (2)	0.8962 (3)	0.13865 (17)	0.0453 (16)	
C8A	0.6777 (2)	0.9218 (3)	0.1539 (2)	0.0526 (16)	
C9A	0.7058 (3)	0.9618 (4)	0.1168 (3)	0.073 (2)	
C10A	0.6650 (3)	0.9783 (5)	0.0636 (2)	0.086 (3)	
C11A	0.5969 (3)	0.9524 (4)	0.0468 (2)	0.076 (2)	
C12A	0.5692 (3)	0.9118 (4)	0.08334 (17)	0.0560 (16)	
C13A	0.62032 (18)	0.8568 (3)	0.24322 (15)	0.0361 (12)	
C14A	0.65295 (19)	0.9585 (3)	0.26285 (19)	0.0487 (14)	
C15A	0.6939 (2)	0.9747 (4)	0.3161 (2)	0.0602 (17)	
C16A	0.7050 (2)	0.8896 (5)	0.35297 (19)	0.0617 (19)	
C17A	0.6728 (2)	0.7868 (5)	0.33598 (18)	0.0587 (18)	
C18A	0.6311 (2)	0.7712 (4)	0.28135 (16)	0.0441 (14)	
C19A	0.49955 (19)	0.9082 (3)	0.17275 (14)	0.0354 (11)	
C20A	0.45619 (19)	0.8637 (3)	0.19794 (13)	0.0391 (11)	
C21A	0.3951 (2)	0.9147 (3)	0.19475 (15)	0.0444 (12)	

C22A	0.3743 (2)	1.0134 (3)	0.16582 (17)	0.0483 (14)	
C23A	0.4157 (2)	1.0600 (3)	0.14108 (17)	0.0453 (14)	
C24A	0.4768 (2)	1.0078 (3)	0.14469 (16)	0.0416 (12)	
B1A	0.5719 (2)	0.8437 (3)	0.17923 (17)	0.0352 (12)	
C1B	0.19466 (18)	0.3343 (3)	0.09965 (12)	0.0292 (10)	
C2B	0.17187 (19)	0.4455 (3)	0.08957 (11)	0.0321 (11)	
C3B	0.2150 (2)	0.5335 (3)	0.08894 (13)	0.0379 (13)	
C4B	0.2835 (2)	0.5145 (3)	0.09805 (15)	0.0408 (12)	
C5B	0.3085 (2)	0.4055 (3)	0.10865 (15)	0.0397 (11)	
C6B	0.26450 (18)	0.3192 (3)	0.11012 (14)	0.0347 (11)	
C7B	0.17758 (16)	0.1646 (3)	0.15799 (13)	0.0297 (10)	
C8B	0.18290 (17)	0.2239 (3)	0.20539 (14)	0.0351 (11)	
C9B	0.21021 (18)	0.1760 (3)	0.25666 (15)	0.0396 (11)	
C10B	0.23367 (19)	0.0675 (3)	0.26295 (15)	0.0385 (11)	
C11B	0.23000 (18)	0.0067 (3)	0.21773 (15)	0.0359 (11)	
C12B	0.20176 (18)	0.0542 (3)	0.16615 (14)	0.0314 (11)	
C13B	0.06573 (18)	0.2622 (2)	0.08526 (13)	0.0287 (10)	
C14B	0.02787 (19)	0.2398 (2)	0.11819 (15)	0.0327 (11)	
C15B	−0.0405 (2)	0.2696 (3)	0.10455 (17)	0.0403 (14)	
C16B	−0.0741 (2)	0.3250 (3)	0.05718 (17)	0.0442 (14)	
C17B	−0.03912 (19)	0.3501 (3)	0.02307 (16)	0.0424 (12)	
C18B	0.02869 (19)	0.3181 (3)	0.03666 (14)	0.0367 (11)	
C19B	0.14494 (17)	0.1365 (3)	0.05077 (13)	0.0291 (10)	
C20B	0.18528 (17)	0.1423 (3)	0.01914 (13)	0.0347 (11)	
C21B	0.18392 (19)	0.0618 (3)	−0.01901 (15)	0.0417 (12)	
C22B	0.1425 (2)	−0.0308 (3)	−0.02642 (15)	0.0412 (14)	
C23B	0.0998 (2)	−0.0393 (3)	0.00324 (14)	0.0369 (11)	
C24B	0.10131 (19)	0.0433 (3)	0.04044 (14)	0.0340 (11)	
B2B	0.1457 (2)	0.2260 (3)	0.09876 (15)	0.0283 (11)	
N2S	0.3399 (7)	0.6785 (9)	−0.0131 (4)	0.119 (4)*	0.694 (19)
C3S	0.3273 (7)	0.7415 (8)	0.0151 (4)	0.078 (3)*	0.694 (19)
C4S	0.3161 (5)	0.8261 (7)	0.0515 (4)	0.073 (3)*	0.694 (19)
N2S′	0.2963 (19)	0.704 (2)	−0.0134 (10)	0.127 (10)*	0.306 (19)
C3S′	0.2953 (12)	0.7660 (15)	0.0191 (7)	0.065 (6)*	0.306 (19)
C4S′	0.2856 (15)	0.829 (2)	0.0635 (9)	0.097 (9)*	0.306 (19)
N1S	0.5597 (3)	0.7363 (5)	−0.0595 (2)	0.095 (3)	
C1S	0.5347 (10)	0.6416 (11)	0.0177 (5)	0.073 (5)*	0.50 (4)
C2S	0.5436 (4)	0.7006 (6)	−0.0271 (2)	0.081 (2)	
C1S′	0.499 (2)	0.669 (2)	0.0046 (12)	0.136 (9)*	0.50 (4)
H2A	0.51490	0.50580	0.39940	0.0410*	
H2B	0.45050	0.48070	0.34540	0.0410*	
H3A	0.53350	0.31470	0.41690	0.0420*	
H3B	0.45610	0.34340	0.40990	0.0420*	
H5A	0.38190	0.35570	0.31850	0.0440*	
H5B	0.36060	0.22960	0.32450	0.0440*	
H6A	0.32950	0.29290	0.23260	0.0410*	
H6B	0.37020	0.17680	0.24520	0.0410*	
H8A	0.41240	0.50300	0.20300	0.0430*	

H8B	0.40380	0.47870	0.25960	0.0430*
H9A	0.49690	0.59540	0.27580	0.0460*
H9B	0.52970	0.51500	0.24350	0.0460*
H10A	0.43330	0.14390	0.39470	0.0460*
H10B	0.51300	0.13390	0.40450	0.0460*
H11A	0.44380	−0.02580	0.36120	0.0440*
H11B	0.41050	0.05050	0.30880	0.0440*
H12A	0.55340	0.00280	0.35300	0.0460*
H12B	0.50070	−0.06930	0.30510	0.0460*
H13A	0.47870	0.08210	0.25080	0.0350*
H13B	0.55380	0.06400	0.27230	0.0350*
H14	0.68820	0.26630	0.36660	0.0440*
H16A	0.81250	0.10800	0.44050	0.0990*
H16B	0.80950	0.20890	0.47920	0.0990*
H16C	0.79890	0.23300	0.41740	0.0990*
H17A	0.73050	0.02720	0.47500	0.0750*
H17B	0.65240	0.04670	0.43660	0.0750*
H17C	0.68640	0.12380	0.48880	0.0750*
H18	0.54360	0.24300	0.19220	0.0510*
H20A	0.64310	0.14580	0.13250	0.0820*
H20B	0.63920	0.27800	0.12220	0.0820*
H20C	0.57200	0.21070	0.11970	0.0820*
H21A	0.72840	0.30640	0.21750	0.0910*
H21B	0.73090	0.17280	0.22160	0.0910*
H21C	0.71230	0.24520	0.26530	0.0910*
H2C	0.65930	0.66980	0.18900	0.0560*
H3C	0.64800	0.48200	0.16470	0.0690*
H4A	0.53800	0.40550	0.12260	0.0610*
H5C	0.44240	0.51910	0.10410	0.0540*
H6C	0.45430	0.70670	0.12900	0.0460*
H8C	0.70680	0.91170	0.19050	0.0630*
H9C	0.75340	0.97770	0.12840	0.0880*
H10C	0.68400	1.00750	0.03870	0.1030*
H11C	0.56860	0.96240	0.01000	0.0910*
H12C	0.52190	0.89350	0.07060	0.0680*
H14A	0.64660	1.01910	0.23830	0.0590*
H15A	0.71470	1.04560	0.32740	0.0720*
H16D	0.73410	0.90040	0.38950	0.0750*
H17D	0.67910	0.72750	0.36120	0.0700*
H18A	0.60970	0.70070	0.27010	0.0530*
H20D	0.46920	0.79620	0.21790	0.0470*
H21D	0.36740	0.88190	0.21240	0.0530*
H22A	0.33230	1.04810	0.16310	0.0580*
H23A	0.40250	1.12800	0.12150	0.0540*
H24A	0.50430	1.04180	0.12720	0.0500*
H2D	0.12500	0.46120	0.08290	0.0380*
H3D	0.19720	0.60750	0.08220	0.0450*
H4D	0.31290	0.57440	0.09710	0.0490*

H5D	0.35530	0.39030	0.11480	0.0480*	
H6D	0.28300	0.24600	0.11870	0.0420*	
H8D	0.16730	0.29920	0.20220	0.0420*	
H9D	0.21260	0.21870	0.28750	0.0470*	
H10D	0.25210	0.03480	0.29790	0.0470*	
H11D	0.24670	−0.06790	0.22160	0.0430*	
H12D	0.19890	0.01000	0.13560	0.0380*	
H14B	0.05000	0.20230	0.15150	0.0390*	
H15B	−0.06400	0.25150	0.12820	0.0480*	
H16E	−0.12070	0.34600	0.04780	0.0530*	
H17E	−0.06170	0.38920	−0.00970	0.0510*	
H18B	0.05120	0.33450	0.01220	0.0440*	
H20E	0.21530	0.20440	0.02380	0.0420*	
H21E	0.21190	0.07070	−0.04020	0.0500*	
H22B	0.14300	−0.08770	−0.05130	0.0500*	
H23B	0.06970	−0.10130	−0.00190	0.0440*	
H24B	0.07130	0.03630	0.05990	0.0410*	
H4S1	0.29970	0.78920	0.07760	0.1090*	0.694 (19)
H4S2	0.28180	0.88030	0.03030	0.1090*	0.694 (19)
H4S3	0.35920	0.86480	0.07090	0.1090*	0.694 (19)
H4S4	0.24710	0.79650	0.07140	0.1460*	0.306 (19)
H4S5	0.27590	0.90710	0.05290	0.1460*	0.306 (19)
H4S6	0.32740	0.82380	0.09570	0.1460*	0.306 (19)
H1S2	0.49240	0.59740	0.00450	0.1100*	0.50 (4)
H1S3	0.57390	0.59170	0.03440	0.1100*	0.50 (4)
H1S1	0.53180	0.69580	0.04450	0.1100*	0.50 (4)
H1S4	0.49450	0.58780	0.00500	0.2040*	0.50 (4)
H1S5	0.52000	0.69700	0.04170	0.2040*	0.50 (4)
H1S6	0.45360	0.70310	−0.01240	0.2040*	0.50 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0370 (3)	0.0243 (2)	0.0272 (3)	0.0033 (2)	0.0177 (2)	0.0024 (2)
S1	0.0416 (5)	0.0278 (4)	0.0330 (5)	−0.0005 (4)	0.0179 (4)	−0.0001 (4)
S7	0.0399 (5)	0.0275 (4)	0.0317 (5)	0.0035 (4)	0.0166 (4)	0.0032 (3)
O1	0.0466 (17)	0.0333 (13)	0.0354 (14)	0.0051 (11)	0.0196 (13)	0.0052 (11)
O2	0.0399 (15)	0.0387 (14)	0.0326 (14)	0.0006 (11)	0.0205 (12)	0.0012 (11)
N4	0.0374 (17)	0.0272 (15)	0.0303 (15)	0.0029 (12)	0.0197 (14)	0.0005 (12)
N13	0.0413 (17)	0.0244 (14)	0.0272 (14)	0.0083 (12)	0.0178 (13)	0.0051 (12)
N15	0.048 (2)	0.0344 (17)	0.0383 (17)	0.0040 (14)	0.0137 (15)	0.0000 (14)
N19	0.052 (2)	0.0415 (19)	0.046 (2)	0.0023 (15)	0.0212 (18)	0.0054 (15)
C2	0.044 (2)	0.0300 (18)	0.0342 (19)	−0.0011 (15)	0.0204 (17)	−0.0052 (15)
C3	0.052 (2)	0.0293 (18)	0.0318 (18)	0.0005 (16)	0.0250 (18)	−0.0019 (15)
C5	0.044 (2)	0.0337 (19)	0.042 (2)	−0.0007 (16)	0.0269 (18)	−0.0027 (16)
C6	0.035 (2)	0.0321 (19)	0.039 (2)	0.0017 (15)	0.0165 (17)	−0.0006 (15)
C8	0.045 (2)	0.0257 (17)	0.037 (2)	0.0121 (15)	0.0145 (17)	0.0088 (15)
C9	0.054 (2)	0.0221 (17)	0.045 (2)	0.0031 (16)	0.026 (2)	0.0065 (16)

C10	0.060 (3)	0.0290 (18)	0.039 (2)	0.0022 (17)	0.034 (2)	0.0053 (16)
C11	0.052 (2)	0.0271 (18)	0.041 (2)	−0.0032 (16)	0.0273 (19)	0.0029 (15)
C12	0.066 (3)	0.0191 (16)	0.042 (2)	0.0049 (16)	0.033 (2)	0.0059 (15)
C14	0.047 (2)	0.0335 (19)	0.0330 (19)	0.0045 (17)	0.0181 (18)	0.0023 (16)
C16	0.052 (3)	0.073 (3)	0.070 (3)	0.006 (2)	0.017 (3)	0.009 (3)
C17	0.069 (3)	0.043 (2)	0.037 (2)	0.008 (2)	0.017 (2)	0.0094 (18)
C18	0.053 (3)	0.031 (2)	0.051 (3)	0.0030 (17)	0.029 (2)	0.0048 (17)
C20	0.074 (3)	0.047 (2)	0.054 (3)	0.008 (2)	0.036 (3)	0.002 (2)
C21	0.061 (3)	0.063 (3)	0.074 (3)	−0.002 (2)	0.045 (3)	0.001 (2)
C1A	0.045 (2)	0.0333 (19)	0.0324 (19)	0.0005 (16)	0.0178 (17)	0.0017 (15)
C2A	0.045 (2)	0.040 (2)	0.050 (2)	0.0032 (18)	0.009 (2)	−0.0057 (19)
C3A	0.063 (3)	0.038 (2)	0.065 (3)	0.012 (2)	0.014 (2)	−0.003 (2)
C4A	0.073 (3)	0.030 (2)	0.050 (2)	0.000 (2)	0.022 (2)	−0.0031 (18)
C5A	0.053 (3)	0.039 (2)	0.046 (2)	−0.0070 (18)	0.021 (2)	−0.0056 (18)
C6A	0.045 (2)	0.036 (2)	0.036 (2)	0.0018 (16)	0.0163 (18)	0.0021 (16)
C7A	0.061 (3)	0.032 (2)	0.056 (3)	0.0100 (18)	0.037 (2)	0.0030 (18)
C8A	0.062 (3)	0.038 (2)	0.076 (3)	0.010 (2)	0.047 (3)	0.010 (2)
C9A	0.079 (4)	0.058 (3)	0.116 (5)	0.015 (3)	0.075 (4)	0.017 (3)
C10A	0.117 (5)	0.077 (4)	0.106 (5)	0.044 (4)	0.092 (5)	0.049 (4)
C11A	0.112 (5)	0.070 (3)	0.072 (3)	0.037 (3)	0.066 (4)	0.027 (3)
C12A	0.079 (3)	0.059 (3)	0.041 (2)	0.016 (2)	0.035 (2)	0.010 (2)
C13A	0.039 (2)	0.039 (2)	0.039 (2)	−0.0023 (16)	0.0246 (17)	−0.0086 (16)
C14A	0.047 (2)	0.041 (2)	0.066 (3)	0.0011 (18)	0.030 (2)	−0.018 (2)
C15A	0.052 (3)	0.060 (3)	0.068 (3)	0.005 (2)	0.021 (2)	−0.029 (3)
C16A	0.047 (3)	0.096 (4)	0.045 (3)	0.008 (3)	0.020 (2)	−0.030 (3)
C17A	0.047 (3)	0.098 (4)	0.041 (2)	0.013 (3)	0.028 (2)	0.011 (3)
C18A	0.042 (2)	0.058 (3)	0.038 (2)	−0.0072 (19)	0.0214 (19)	0.0005 (19)
C19A	0.044 (2)	0.0321 (19)	0.035 (2)	−0.0023 (16)	0.0200 (17)	−0.0048 (15)
C20A	0.048 (2)	0.0338 (19)	0.042 (2)	−0.0001 (17)	0.0240 (19)	0.0012 (17)
C21A	0.050 (2)	0.040 (2)	0.049 (2)	−0.0025 (18)	0.025 (2)	−0.0047 (18)
C22A	0.047 (2)	0.046 (2)	0.057 (3)	0.0014 (19)	0.025 (2)	−0.009 (2)
C23A	0.058 (3)	0.032 (2)	0.046 (2)	0.0091 (18)	0.019 (2)	0.0013 (17)
C24A	0.052 (2)	0.037 (2)	0.041 (2)	−0.0047 (18)	0.0230 (19)	−0.0020 (17)
B1A	0.045 (2)	0.027 (2)	0.040 (2)	0.0018 (17)	0.023 (2)	0.0008 (17)
C1B	0.041 (2)	0.0269 (17)	0.0229 (16)	−0.0035 (14)	0.0155 (15)	−0.0001 (13)
C2B	0.043 (2)	0.0299 (18)	0.0260 (17)	0.0031 (15)	0.0156 (16)	0.0009 (14)
C3B	0.057 (3)	0.0242 (17)	0.036 (2)	−0.0022 (16)	0.0208 (18)	0.0017 (15)
C4B	0.053 (2)	0.038 (2)	0.034 (2)	−0.0143 (18)	0.0189 (19)	0.0026 (16)
C5B	0.042 (2)	0.042 (2)	0.0342 (19)	−0.0054 (17)	0.0128 (17)	0.0063 (17)
C6B	0.038 (2)	0.0302 (18)	0.0347 (19)	−0.0004 (15)	0.0115 (16)	0.0066 (15)
C7B	0.0307 (18)	0.0310 (18)	0.0307 (18)	−0.0023 (14)	0.0151 (15)	0.0029 (14)
C8B	0.048 (2)	0.0279 (18)	0.0324 (19)	−0.0030 (16)	0.0181 (17)	−0.0035 (15)
C9B	0.048 (2)	0.044 (2)	0.0304 (19)	−0.0054 (18)	0.0183 (18)	−0.0031 (16)
C10B	0.043 (2)	0.046 (2)	0.0278 (18)	−0.0057 (17)	0.0142 (17)	0.0067 (16)
C11B	0.036 (2)	0.0325 (19)	0.039 (2)	0.0019 (15)	0.0133 (17)	0.0078 (16)
C12B	0.0359 (19)	0.0307 (18)	0.0304 (18)	0.0000 (14)	0.0154 (16)	0.0000 (14)
C13B	0.037 (2)	0.0217 (16)	0.0284 (17)	−0.0021 (13)	0.0129 (15)	−0.0065 (13)
C14B	0.042 (2)	0.0226 (17)	0.038 (2)	−0.0065 (14)	0.0200 (17)	−0.0075 (14)

C15B	0.043 (2)	0.0297 (19)	0.055 (3)	−0.0060 (16)	0.026 (2)	−0.0131 (18)
C16B	0.038 (2)	0.036 (2)	0.059 (3)	0.0041 (17)	0.018 (2)	−0.0184 (19)
C17B	0.039 (2)	0.039 (2)	0.041 (2)	0.0077 (17)	0.0046 (18)	−0.0062 (17)
C18B	0.043 (2)	0.036 (2)	0.0306 (18)	0.0011 (16)	0.0126 (17)	−0.0005 (15)
C19B	0.0355 (19)	0.0273 (17)	0.0264 (17)	0.0016 (14)	0.0133 (15)	0.0015 (14)
C20B	0.045 (2)	0.0286 (18)	0.0370 (19)	0.0001 (15)	0.0226 (17)	−0.0016 (15)
C21B	0.054 (2)	0.041 (2)	0.043 (2)	0.0049 (18)	0.033 (2)	−0.0010 (17)
C22B	0.057 (3)	0.034 (2)	0.036 (2)	0.0046 (18)	0.0209 (19)	−0.0096 (16)
C23B	0.045 (2)	0.0288 (18)	0.036 (2)	−0.0042 (16)	0.0136 (18)	−0.0039 (15)
C24B	0.044 (2)	0.0328 (19)	0.0310 (18)	−0.0042 (16)	0.0207 (17)	−0.0032 (15)
B2B	0.036 (2)	0.0267 (19)	0.0258 (19)	−0.0021 (16)	0.0154 (17)	−0.0031 (15)
N1S	0.089 (4)	0.120 (5)	0.071 (4)	−0.018 (3)	0.022 (3)	0.007 (3)
C2S	0.095 (5)	0.090 (4)	0.055 (3)	−0.027 (4)	0.023 (3)	−0.010 (3)

Geometric parameters (Å, º)

Ni—S1	2.4119 (12)	C20A—C21A	1.390 (6)
Ni—S7	2.3917 (14)	C21A—C22A	1.389 (5)
Ni—O1	2.057 (3)	C22A—C23A	1.378 (6)
Ni—O2	2.086 (3)	C23A—C24A	1.394 (6)
Ni—N4	2.141 (4)	C2A—H2C	0.9500
Ni—N13	2.073 (3)	C3A—H3C	0.9500
S1—C2	1.830 (4)	C4A—H4A	0.9500
S1—C9	1.805 (4)	C5A—H5C	0.9500
S7—C6	1.812 (4)	C6A—H6C	0.9500
S7—C8	1.827 (4)	C8A—H8C	0.9500
O1—C14	1.231 (5)	C9A—H9C	0.9500
O2—C18	1.232 (5)	C10A—H10C	0.9500
N4—C3	1.488 (5)	C11A—H11C	0.9500
N4—C5	1.493 (5)	C12A—H12C	0.9500
N4—C10	1.501 (5)	C14A—H14A	0.9500
N13—C12	1.485 (5)	C15A—H15A	0.9500
N15—C14	1.306 (5)	C16A—H16D	0.9500
N15—C16	1.457 (8)	C17A—H17D	0.9500
N15—C17	1.459 (6)	C18A—H18A	0.9500
N19—C18	1.328 (6)	C20A—H20D	0.9500
N19—C20	1.448 (6)	C21A—H21D	0.9500
N19—C21	1.391 (7)	C22A—H22A	0.9500
N13—H13B	0.9200	C23A—H23A	0.9500
N13—H13A	0.9200	C24A—H24A	0.9500
N2S′—C3S′	1.14 (3)	C1B—C2B	1.405 (5)
N2S—C3S	1.156 (16)	C1B—B2B	1.645 (5)
N1S—C2S	1.114 (9)	C1B—C6B	1.397 (6)
C2—C3	1.515 (5)	C2B—C3B	1.389 (6)
C5—C6	1.519 (6)	C3B—C4B	1.383 (6)
C8—C9	1.510 (6)	C4B—C5B	1.394 (5)
C10—C11	1.520 (5)	C5B—C6B	1.392 (6)
C11—C12	1.504 (6)	C7B—C12B	1.402 (5)

C2—H2B	0.9900	C7B—B2B	1.642 (5)
C2—H2A	0.9900	C7B—C8B	1.412 (5)
C3—H3A	0.9900	C8B—C9B	1.394 (5)
C3—H3B	0.9900	C9B—C10B	1.375 (5)
C5—H5A	0.9900	C10B—C11B	1.380 (5)
C5—H5B	0.9900	C11B—C12B	1.400 (5)
C6—H6B	0.9900	C13B—C18B	1.411 (5)
C6—H6A	0.9900	C13B—B2B	1.637 (6)
C8—H8B	0.9900	C13B—C14B	1.399 (5)
C8—H8A	0.9900	C14B—C15B	1.389 (6)
C9—H9A	0.9900	C15B—C16B	1.369 (6)
C9—H9B	0.9900	C16B—C17B	1.385 (6)
C10—H10A	0.9900	C17B—C18B	1.385 (6)
C10—H10B	0.9900	C19B—C24B	1.403 (5)
C11—H11B	0.9900	C19B—C20B	1.389 (5)
C11—H11A	0.9900	C19B—B2B	1.658 (5)
C12—H12B	0.9900	C20B—C21B	1.389 (5)
C12—H12A	0.9900	C21B—C22B	1.375 (5)
C14—H14	0.9500	C22B—C23B	1.389 (6)
C16—H16B	0.9800	C23B—C24B	1.388 (5)
C16—H16C	0.9800	C2B—H2D	0.9500
C16—H16A	0.9800	C3B—H3D	0.9500
C17—H17B	0.9800	C4B—H4D	0.9500
C17—H17C	0.9800	C5B—H5D	0.9500
C17—H17A	0.9800	C6B—H6D	0.9500
C18—H18	0.9500	C8B—H8D	0.9500
C20—H20C	0.9800	C9B—H9D	0.9500
C20—H20A	0.9800	C10B—H10D	0.9500
C20—H20B	0.9800	C11B—H11D	0.9500
C21—H21B	0.9800	C12B—H12D	0.9500
C21—H21C	0.9800	C14B—H14B	0.9500
C21—H21A	0.9800	C15B—H15B	0.9500
C1A—C2A	1.398 (6)	C16B—H16E	0.9500
C1A—B1A	1.645 (5)	C17B—H17E	0.9500
C1A—C6A	1.397 (6)	C18B—H18B	0.9500
C2A—C3A	1.390 (5)	C20B—H20E	0.9500
C3A—C4A	1.391 (6)	C21B—H21E	0.9500
C4A—C5A	1.369 (6)	C22B—H22B	0.9500
C5A—C6A	1.394 (5)	C23B—H23B	0.9500
C7A—C8A	1.395 (6)	C24B—H24B	0.9500
C7A—C12A	1.411 (6)	C3S′—C4S′	1.47 (3)
C7A—B1A	1.648 (6)	C3S—C4S	1.474 (14)
C8A—C9A	1.399 (8)	C4S′—H4S5	0.9700
C9A—C10A	1.375 (9)	C4S′—H4S6	0.9800
C10A—C11A	1.366 (9)	C4S′—H4S4	0.9800
C11A—C12A	1.383 (8)	C4S—H4S2	0.9800
C13A—B1A	1.641 (6)	C4S—H4S3	0.9800
C13A—C18A	1.399 (6)	C4S—H4S1	0.9800

C13A—C14A	1.399 (5)	C1S′—C2S	1.51 (4)
C14A—C15A	1.377 (7)	C1S—C2S	1.450 (16)
C15A—C16A	1.372 (7)	C1S′—H1S4	0.9800
C16A—C17A	1.396 (8)	C1S′—H1S5	0.9800
C17A—C18A	1.409 (6)	C1S′—H1S6	0.9800
C19A—C24A	1.394 (5)	C1S—H1S1	0.9800
C19A—B1A	1.651 (6)	C1S—H1S2	0.9800
C19A—C20A	1.409 (6)	C1S—H1S3	0.9800
S1—Ni—S7	87.66 (5)	C22A—C23A—C24A	120.2 (4)
S1—Ni—O1	91.47 (8)	C19A—C24A—C23A	123.2 (4)
S1—Ni—O2	89.78 (8)	C3A—C2A—H2C	118.00
S1—Ni—N4	86.83 (8)	C1A—C2A—H2C	118.00
S1—Ni—N13	178.23 (11)	C2A—C3A—H3C	121.00
S7—Ni—O1	176.09 (9)	C4A—C3A—H3C	121.00
S7—Ni—O2	93.46 (8)	C5A—C4A—H4A	120.00
S7—Ni—N4	87.46 (9)	C3A—C4A—H4A	120.00
S7—Ni—N13	93.17 (9)	C4A—C5A—H5C	120.00
O1—Ni—O2	90.35 (11)	C6A—C5A—H5C	120.00
O1—Ni—N4	88.68 (12)	C1A—C6A—H6C	119.00
O1—Ni—N13	87.81 (11)	C5A—C6A—H6C	119.00
O2—Ni—N4	176.45 (10)	C9A—C8A—H8C	119.00
O2—Ni—N13	88.61 (12)	C7A—C8A—H8C	119.00
N4—Ni—N13	94.77 (12)	C8A—C9A—H9C	120.00
Ni—S1—C2	96.27 (12)	C10A—C9A—H9C	120.00
Ni—S1—C9	100.88 (13)	C9A—C10A—H10C	120.00
C2—S1—C9	102.67 (19)	C11A—C10A—H10C	120.00
Ni—S7—C6	93.35 (14)	C12A—C11A—H11C	120.00
Ni—S7—C8	103.56 (13)	C10A—C11A—H11C	120.00
C6—S7—C8	103.13 (19)	C7A—C12A—H12C	119.00
Ni—O1—C14	129.2 (2)	C11A—C12A—H12C	118.00
Ni—O2—C18	127.2 (3)	C13A—C14A—H14A	119.00
Ni—N4—C3	106.5 (2)	C15A—C14A—H14A	119.00
Ni—N4—C5	112.5 (2)	C16A—C15A—H15A	120.00
Ni—N4—C10	111.7 (2)	C14A—C15A—H15A	120.00
C3—N4—C5	109.2 (3)	C15A—C16A—H16D	121.00
C3—N4—C10	106.8 (3)	C17A—C16A—H16D	120.00
C5—N4—C10	110.0 (3)	C18A—C17A—H17D	120.00
Ni—N13—C12	117.4 (2)	C16A—C17A—H17D	120.00
C14—N15—C16	122.4 (4)	C13A—C18A—H18A	119.00
C14—N15—C17	120.5 (4)	C17A—C18A—H18A	119.00
C16—N15—C17	117.2 (4)	C19A—C20A—H20D	119.00
C18—N19—C20	121.5 (4)	C21A—C20A—H20D	119.00
C18—N19—C21	121.2 (4)	C22A—C21A—H21D	120.00
C20—N19—C21	117.3 (5)	C20A—C21A—H21D	120.00
H13A—N13—H13B	107.00	C21A—C22A—H22A	121.00
Ni—N13—H13A	108.00	C23A—C22A—H22A	121.00
Ni—N13—H13B	108.00	C22A—C23A—H23A	120.00

C12—N13—H13A	108.00	C24A—C23A—H23A	120.00
C12—N13—H13B	108.00	C23A—C24A—H24A	118.00
S1—C2—C3	110.8 (3)	C19A—C24A—H24A	118.00
N4—C3—C2	113.7 (3)	C2B—C1B—B2B	125.1 (3)
N4—C5—C6	115.4 (3)	C6B—C1B—B2B	120.1 (3)
S7—C6—C5	114.0 (3)	C2B—C1B—C6B	114.8 (3)
S7—C8—C9	112.9 (3)	C1B—C2B—C3B	122.8 (4)
S1—C9—C8	115.0 (3)	C2B—C3B—C4B	120.6 (3)
N4—C10—C11	115.9 (3)	C3B—C4B—C5B	118.6 (4)
C10—C11—C12	114.4 (3)	C4B—C5B—C6B	119.6 (4)
N13—C12—C11	112.4 (3)	C1B—C6B—C5B	123.6 (3)
O1—C14—N15	123.5 (4)	C8B—C7B—C12B	115.2 (3)
O2—C18—N19	124.0 (4)	C8B—C7B—B2B	120.1 (3)
S1—C2—H2A	109.00	C12B—C7B—B2B	124.6 (3)
S1—C2—H2B	109.00	C7B—C8B—C9B	122.4 (3)
C3—C2—H2A	110.00	C8B—C9B—C10B	120.6 (3)
C3—C2—H2B	110.00	C9B—C10B—C11B	119.0 (3)
H2A—C2—H2B	108.00	C10B—C11B—C12B	120.5 (3)
N4—C3—H3A	109.00	C7B—C12B—C11B	122.3 (3)
N4—C3—H3B	109.00	C14B—C13B—C18B	114.4 (3)
C2—C3—H3A	109.00	C18B—C13B—B2B	120.5 (3)
C2—C3—H3B	109.00	C14B—C13B—B2B	125.1 (3)
H3A—C3—H3B	108.00	C13B—C14B—C15B	123.3 (3)
N4—C5—H5A	108.00	C14B—C15B—C16B	120.2 (4)
N4—C5—H5B	108.00	C15B—C16B—C17B	119.1 (4)
C6—C5—H5A	108.00	C16B—C17B—C18B	120.1 (4)
C6—C5—H5B	108.00	C13B—C18B—C17B	122.9 (4)
H5A—C5—H5B	107.00	C20B—C19B—B2B	126.2 (3)
S7—C6—H6A	109.00	C24B—C19B—B2B	119.2 (3)
S7—C6—H6B	109.00	C20B—C19B—C24B	114.5 (3)
C5—C6—H6A	109.00	C19B—C20B—C21B	123.2 (3)
C5—C6—H6B	109.00	C20B—C21B—C22B	120.6 (4)
H6A—C6—H6B	108.00	C21B—C22B—C23B	118.5 (3)
S7—C8—H8A	109.00	C22B—C23B—C24B	119.7 (4)
S7—C8—H8B	109.00	C19B—C24B—C23B	123.4 (4)
C9—C8—H8A	109.00	C3B—C2B—H2D	119.00
C9—C8—H8B	109.00	C1B—C2B—H2D	119.00
H8A—C8—H8B	108.00	C2B—C3B—H3D	120.00
S1—C9—H9A	109.00	C4B—C3B—H3D	120.00
S1—C9—H9B	109.00	C5B—C4B—H4D	121.00
C8—C9—H9A	109.00	C3B—C4B—H4D	121.00
C8—C9—H9B	108.00	C6B—C5B—H5D	120.00
H9A—C9—H9B	107.00	C4B—C5B—H5D	120.00
N4—C10—H10A	108.00	C5B—C6B—H6D	118.00
N4—C10—H10B	108.00	C1B—C6B—H6D	118.00
C11—C10—H10A	108.00	C9B—C8B—H8D	119.00
C11—C10—H10B	108.00	C7B—C8B—H8D	119.00
H10A—C10—H10B	107.00	C8B—C9B—H9D	120.00

C10—C11—H11A	109.00	C10B—C9B—H9D	120.00
C10—C11—H11B	109.00	C9B—C10B—H10D	121.00
C12—C11—H11A	109.00	C11B—C10B—H10D	120.00
C12—C11—H11B	109.00	C12B—C11B—H11D	120.00
H11A—C11—H11B	108.00	C10B—C11B—H11D	120.00
N13—C12—H12A	109.00	C7B—C12B—H12D	119.00
N13—C12—H12B	109.00	C11B—C12B—H12D	119.00
C11—C12—H12A	109.00	C13B—C14B—H14B	118.00
C11—C12—H12B	109.00	C15B—C14B—H14B	118.00
H12A—C12—H12B	108.00	C16B—C15B—H15B	120.00
O1—C14—H14	118.00	C14B—C15B—H15B	120.00
N15—C14—H14	118.00	C15B—C16B—H16E	121.00
N15—C16—H16A	109.00	C17B—C16B—H16E	120.00
N15—C16—H16B	109.00	C18B—C17B—H17E	120.00
N15—C16—H16C	109.00	C16B—C17B—H17E	120.00
H16A—C16—H16B	109.00	C17B—C18B—H18B	119.00
H16A—C16—H16C	110.00	C13B—C18B—H18B	119.00
H16B—C16—H16C	109.00	C19B—C20B—H20E	118.00
N15—C17—H17A	109.00	C21B—C20B—H20E	118.00
N15—C17—H17B	109.00	C22B—C21B—H21E	120.00
N15—C17—H17C	109.00	C20B—C21B—H21E	120.00
H17A—C17—H17B	109.00	C21B—C22B—H22B	121.00
H17A—C17—H17C	109.00	C23B—C22B—H22B	121.00
H17B—C17—H17C	110.00	C22B—C23B—H23B	120.00
O2—C18—H18	118.00	C24B—C23B—H23B	120.00
N19—C18—H18	118.00	C23B—C24B—H24B	118.00
N19—C20—H20A	109.00	C19B—C24B—H24B	118.00
N19—C20—H20B	109.00	N2S′—C3S′—C4S′	169 (3)
N19—C20—H20C	110.00	N2S—C3S—C4S	175.7 (15)
H20A—C20—H20B	109.00	C3S′—C4S′—H4S6	109.00
H20A—C20—H20C	110.00	C3S′—C4S′—H4S5	109.00
H20B—C20—H20C	110.00	C3S′—C4S′—H4S4	109.00
N19—C21—H21A	110.00	H4S5—C4S′—H4S6	110.00
N19—C21—H21B	109.00	H4S4—C4S′—H4S5	110.00
N19—C21—H21C	110.00	H4S4—C4S′—H4S6	109.00
H21A—C21—H21B	109.00	H4S1—C4S—H4S2	109.00
H21A—C21—H21C	109.00	C3S—C4S—H4S1	109.00
H21B—C21—H21C	109.00	H4S2—C4S—H4S3	110.00
C2A—C1A—C6A	115.5 (3)	H4S1—C4S—H4S3	109.00
C2A—C1A—B1A	119.1 (3)	C3S—C4S—H4S3	110.00
C6A—C1A—B1A	125.3 (3)	C3S—C4S—H4S2	109.00
C1A—C2A—C3A	123.3 (4)	N1S—C2S—C1S	168.9 (11)
C2A—C3A—C4A	119.0 (4)	N1S—C2S—C1S′	160.5 (15)
C3A—C4A—C5A	119.6 (3)	C2S—C1S′—H1S5	109.00
C4A—C5A—C6A	120.5 (4)	H1S4—C1S′—H1S5	110.00
C1A—C6A—C5A	122.1 (4)	C2S—C1S′—H1S6	109.00
C8A—C7A—C12A	115.2 (4)	C2S—C1S′—H1S4	110.00
C8A—C7A—B1A	124.8 (4)	H1S4—C1S′—H1S6	110.00

C12A—C7A—B1A	120.0 (4)	H1S5—C1S′—H1S6	109.00
C7A—C8A—C9A	121.9 (5)	H1S1—C1S—H1S3	110.00
C8A—C9A—C10A	120.5 (6)	C2S—C1S—H1S3	109.00
C9A—C10A—C11A	119.5 (5)	H1S1—C1S—H1S2	109.00
C10A—C11A—C12A	120.1 (5)	H1S2—C1S—H1S3	109.00
C7A—C12A—C11A	122.9 (5)	C2S—C1S—H1S2	110.00
C14A—C13A—C18A	115.9 (4)	C2S—C1S—H1S1	109.00
C14A—C13A—B1A	120.3 (3)	C7A—B1A—C19A	112.0 (3)
C18A—C13A—B1A	123.8 (3)	C1A—B1A—C7A	105.3 (3)
C13A—C14A—C15A	123.0 (4)	C1A—B1A—C13A	110.9 (3)
C14A—C15A—C16A	120.7 (4)	C1A—B1A—C19A	111.1 (3)
C15A—C16A—C17A	119.0 (4)	C7A—B1A—C13A	112.4 (3)
C16A—C17A—C18A	119.8 (5)	C13A—B1A—C19A	105.4 (3)
C13A—C18A—C17A	121.7 (4)	C7B—B2B—C19B	109.5 (3)
C20A—C19A—C24A	114.9 (4)	C13B—B2B—C19B	106.0 (3)
C20A—C19A—B1A	119.7 (3)	C1B—B2B—C7B	107.5 (3)
C24A—C19A—B1A	125.4 (4)	C1B—B2B—C13B	112.1 (3)
C19A—C20A—C21A	122.6 (3)	C1B—B2B—C19B	110.7 (3)
C20A—C21A—C22A	120.3 (4)	C7B—B2B—C13B	111.0 (3)
C21A—C22A—C23A	118.7 (4)		

C2—S1—C9—C8	−56.5 (3)	C20A—C19A—B1A—C7A	170.2 (3)
C9—S1—C2—C3	129.2 (3)	C20A—C19A—B1A—C13A	−67.4 (4)
C6—S7—C8—C9	128.9 (3)	C24A—C19A—B1A—C1A	−128.8 (4)
C8—S7—C6—C5	−63.5 (3)	C24A—C19A—B1A—C7A	−11.4 (5)
C10—N4—C3—C2	173.8 (3)	C24A—C19A—B1A—C13A	111.1 (4)
C3—N4—C5—C6	139.1 (3)	C19A—C20A—C21A—C22A	0.2 (6)
C3—N4—C10—C11	−172.1 (4)	C20A—C21A—C22A—C23A	−0.8 (6)
C5—N4—C3—C2	−67.3 (4)	C21A—C22A—C23A—C24A	0.8 (6)
C10—N4—C5—C6	−104.1 (4)	C22A—C23A—C24A—C19A	−0.1 (6)
C5—N4—C10—C11	69.5 (4)	C6B—C1B—C2B—C3B	1.3 (4)
C17—N15—C14—O1	−0.2 (6)	B2B—C1B—C2B—C3B	−177.6 (3)
C16—N15—C14—O1	−179.8 (4)	C2B—C1B—C6B—C5B	−2.6 (5)
C21—N19—C18—O2	0.5 (6)	B2B—C1B—C6B—C5B	176.3 (3)
C20—N19—C18—O2	−179.4 (4)	C2B—C1B—B2B—C7B	−123.0 (3)
S1—C2—C3—N4	−56.3 (4)	C2B—C1B—B2B—C13B	−0.7 (4)
N4—C5—C6—S7	−46.0 (4)	C2B—C1B—B2B—C19B	117.4 (3)
S7—C8—C9—S1	−52.5 (4)	C6B—C1B—B2B—C7B	58.2 (4)
N4—C10—C11—C12	73.2 (5)	C6B—C1B—B2B—C13B	−179.5 (3)
C10—C11—C12—N13	−69.9 (4)	C6B—C1B—B2B—C19B	−61.4 (4)
C6A—C1A—C2A—C3A	−0.4 (5)	C1B—C2B—C3B—C4B	0.5 (5)
B1A—C1A—C2A—C3A	−178.0 (4)	C2B—C3B—C4B—C5B	−0.9 (5)
C2A—C1A—C6A—C5A	0.2 (5)	C3B—C4B—C5B—C6B	−0.4 (6)
B1A—C1A—C6A—C5A	177.6 (4)	C4B—C5B—C6B—C1B	2.3 (6)
C2A—C1A—B1A—C7A	66.8 (4)	C12B—C7B—C8B—C9B	−0.1 (5)
C2A—C1A—B1A—C13A	−55.0 (5)	B2B—C7B—C8B—C9B	−179.3 (4)
C2A—C1A—B1A—C19A	−171.8 (3)	C8B—C7B—C12B—C11B	−0.8 (6)
C6A—C1A—B1A—C7A	−110.6 (4)	B2B—C7B—C12B—C11B	178.4 (4)

C6A—C1A—B1A—C13A	127.7 (4)	C8B—C7B—B2B—C1B	60.3 (4)
C6A—C1A—B1A—C19A	10.9 (5)	C8B—C7B—B2B—C13B	−62.7 (4)
C1A—C2A—C3A—C4A	0.0 (6)	C8B—C7B—B2B—C19B	−179.4 (3)
C2A—C3A—C4A—C5A	0.7 (6)	C12B—C7B—B2B—C1B	−118.9 (4)
C3A—C4A—C5A—C6A	−0.9 (6)	C12B—C7B—B2B—C13B	118.1 (4)
C4A—C5A—C6A—C1A	0.4 (6)	C12B—C7B—B2B—C19B	1.4 (5)
C12A—C7A—C8A—C9A	1.0 (6)	C7B—C8B—C9B—C10B	0.4 (6)
B1A—C7A—C8A—C9A	177.2 (4)	C8B—C9B—C10B—C11B	0.2 (6)
C8A—C7A—C12A—C11A	−1.7 (6)	C9B—C10B—C11B—C12B	−1.1 (6)
B1A—C7A—C12A—C11A	−178.1 (4)	C10B—C11B—C12B—C7B	1.4 (6)
C8A—C7A—B1A—C1A	−104.6 (4)	C18B—C13B—C14B—C15B	0.1 (4)
C8A—C7A—B1A—C13A	16.2 (5)	B2B—C13B—C14B—C15B	−178.3 (3)
C8A—C7A—B1A—C19A	134.6 (4)	C14B—C13B—C18B—C17B	1.2 (5)
C12A—C7A—B1A—C1A	71.4 (4)	B2B—C13B—C18B—C17B	179.7 (3)
C12A—C7A—B1A—C13A	−167.8 (4)	C14B—C13B—B2B—C1B	−123.1 (3)
C12A—C7A—B1A—C19A	−49.5 (5)	C14B—C13B—B2B—C7B	−2.8 (4)
C7A—C8A—C9A—C10A	0.7 (7)	C14B—C13B—B2B—C19B	116.1 (3)
C8A—C9A—C10A—C11A	−1.8 (8)	C18B—C13B—B2B—C1B	58.6 (4)
C9A—C10A—C11A—C12A	1.1 (8)	C18B—C13B—B2B—C7B	178.9 (3)
C10A—C11A—C12A—C7A	0.7 (8)	C18B—C13B—B2B—C19B	−62.2 (4)
C18A—C13A—C14A—C15A	0.7 (6)	C13B—C14B—C15B—C16B	−0.9 (5)
B1A—C13A—C14A—C15A	179.7 (4)	C14B—C15B—C16B—C17B	0.4 (6)
C14A—C13A—C18A—C17A	−0.5 (6)	C15B—C16B—C17B—C18B	0.8 (6)
B1A—C13A—C18A—C17A	−179.5 (4)	C16B—C17B—C18B—C13B	−1.6 (6)
C14A—C13A—B1A—C1A	163.2 (4)	C24B—C19B—C20B—C21B	−1.2 (5)
C14A—C13A—B1A—C7A	45.7 (5)	B2B—C19B—C20B—C21B	177.4 (3)
C14A—C13A—B1A—C19A	−76.5 (4)	C20B—C19B—C24B—C23B	2.3 (5)
C18A—C13A—B1A—C1A	−17.9 (5)	B2B—C19B—C24B—C23B	−176.3 (3)
C18A—C13A—B1A—C7A	−135.3 (4)	C20B—C19B—B2B—C1B	7.1 (5)
C18A—C13A—B1A—C19A	102.5 (4)	C20B—C19B—B2B—C7B	−111.3 (4)
C13A—C14A—C15A—C16A	0.4 (7)	C20B—C19B—B2B—C13B	128.8 (4)
C14A—C15A—C16A—C17A	−1.5 (7)	C24B—C19B—B2B—C1B	−174.5 (3)
C15A—C16A—C17A—C18A	1.6 (7)	C24B—C19B—B2B—C7B	67.2 (4)
C16A—C17A—C18A—C13A	−0.6 (7)	C24B—C19B—B2B—C13B	−52.7 (4)
C24A—C19A—C20A—C21A	0.5 (5)	C19B—C20B—C21B—C22B	−1.5 (6)
B1A—C19A—C20A—C21A	179.0 (3)	C20B—C21B—C22B—C23B	3.0 (6)
C20A—C19A—C24A—C23A	−0.5 (6)	C21B—C22B—C23B—C24B	−1.9 (6)
B1A—C19A—C24A—C23A	−179.0 (4)	C22B—C23B—C24B—C19B	−0.9 (6)
C20A—C19A—B1A—C1A	52.8 (4)		