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(4′-Phenyl-2,2′:6′,2″-terpyridine-κ^3N,N',N'')bis(thiocyanato-κN)zinc(II) unknown solvate

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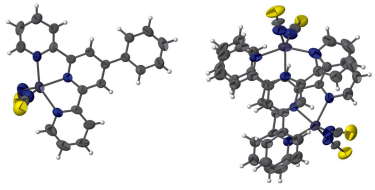
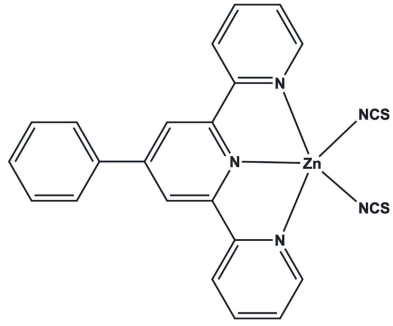
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Zn(NCS)_2(C_{21}H_{15}N_3)]$, crystallizes with three independent complex molecules in the asymmetric unit. In each complex molecule, the Zn^{II} atom is coordinated by three N atoms of a 4′-phenyl-2,2′:6′,2″-terpyridine ligand, and by the N atoms of two NCS^- anions. The Zn^{II} atoms are therefore five-coordinate, ZnN_5, with distorted square-pyramidal geometries. In the crystal, the three independent molecules are linked by a series of offset π–π interactions [intercentroid distances vary between 3.680 (5) and 3.791 (5) Å], forming columns along the *a*-axis direction. The columns are linked *via* C—H···S interactions, forming a fence-like arrangement parallel to the *ab* plane. A small region of disordered electron density was corrected for using the SQUEEZE routine in *PLATON* [Spek (2015). *Acta Cryst.* C**71**, 9–18], but the formula mass and unit-cell characteristics were not taken into account during the refinement.

3D view



Chemical scheme



Structure description

In recent decades, the design of metal–organic compounds has been an important goal for synthetic chemistry as it provides the opportunity to control the properties of materials at the molecular level (Li *et al.*, 2008). Polydentate ligands containing N-donor heterocyclic rings are versatile building blocks in the construction of coordination compounds because of their ability to form stable complexes with transition metals and their various coordination modes (Hancock, 2013; Li *et al.*, 2011; Bhaumik *et al.*, 2011). One such ligand is 4′-phenyl-2,2′:6′,2″-terpyridine (pypyt), first synthesized by Constable *et al.* (1990) and used by them for the formation of nickel complexes. The same ligand has been used by many groups to form metal complexes, both mononuclear, binuclear and polymeric (Crystal Structure Database; Groom *et al.*, 2016). We have studied the reaction of

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···S6^{i}	0.93	2.87	3.748 (8)	159
C41—H41···S6^{ii}	0.93	2.82	3.612 (9)	144

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

this ligand with $Zn(NCS)_2$, and report herein on the crystal structure of the resulting mononuclear complex.

The asymmetric unit of the title compound contains three complex molecules. For simplicity, as the three complexes are very similar, only the structure of one complex, involving atom Zn1, is illustrated in Fig. 1. In each complex molecule, the zinc(II) atom is coordinated by three N atoms of a 4′-phenyl-2,2′:6′,2″-terpyridine ligand in a tridentate manner, and by the N atoms of two NCS^- anions. The zinc atoms are therefore five-coordinate with τ values indicating fivefold coordination (Addison *et al.*, 1984) being 0.33 for the Zn1 complex, 0.30 for Zn2 and 0.13 for Zn3; hence, all have highly distorted square-pyramidal geometries.

In the crystal, the three molecules are linked by offset π–π interactions [intercentroid distances vary between 3.680 (5) and 3.791 (5) Å], forming columns along the *a*-axis direction. The columns are linked *via* C—H···S interactions, forming a fence-like arrangement parallel to the *ab* plane (Table 1 and Fig. 2).

Synthesis and crystallization

The 4′-phenyl-2,2′:6′,2″-terpyridine ligand was synthesized according to a literature method (Mutai *et al.*, 2011). For the preparation of the title complex, a methanol solution of $Zn(NCS)_2$ (0.181 g, 1 mmol) and 4′-phenyl-2,2′:6′,2″-terpyridine (0.64 g, 2 mmol) was refluxed for 2 h. The precipitate that formed was filtered off and recrystallized from methanol solution, giving colourless block-like crystals of the title compound.

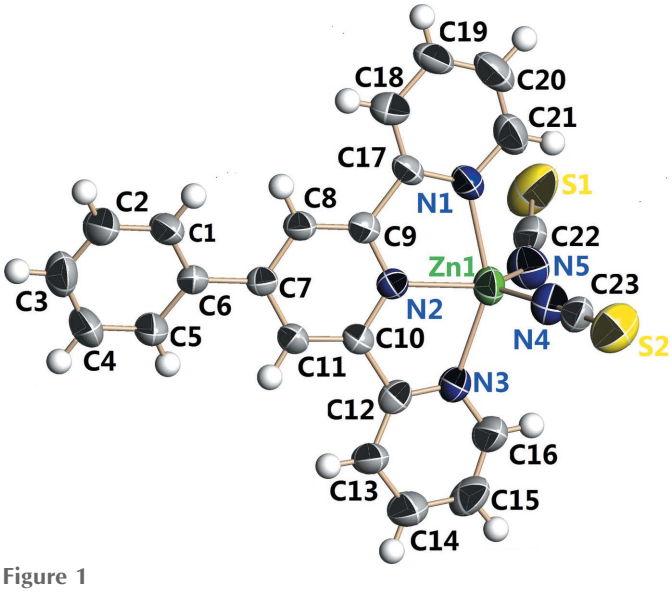


Figure 1
The molecular structure of one of the three title complex molecules, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(NCS)_2(C_{21}H_{15}N_3)]$
M_r	490.89
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, b, c (Å)	11.518 (5), 25.095 (5), 23.137 (5)
β (°)	98.217 (5)
V (Å^3)	6619 (3)
Z	12
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.32
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.692, 0.778
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	47455, 11948, 5625
R_{int}	0.127
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.080, 0.213, 0.98
No. of reflections	11948
No. of parameters	838
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.78, −0.53

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2006) and *PLATON* (Spek, 2009).

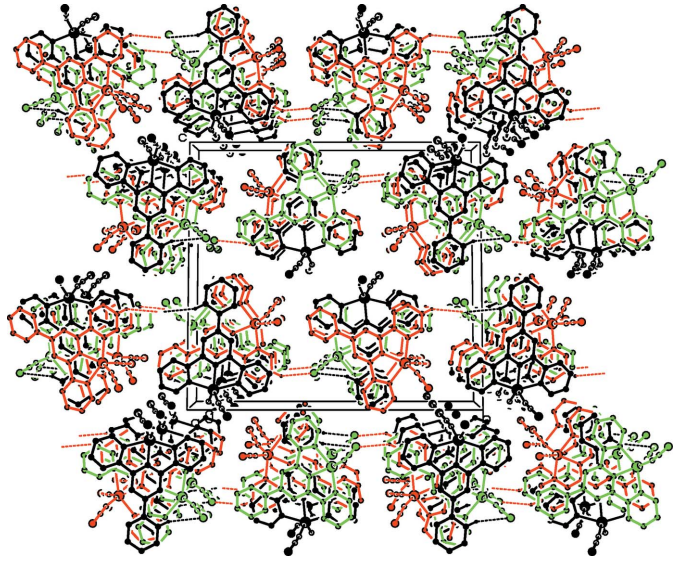


Figure 2
A view along the *a* axis of the crystal packing of the title compound [colour code for the three independent complexes: black (Zn1), red (Zn2), and green (Zn3)]. Hydrogen bonds are shown as dashed lines (see Table 1) and H atoms not involved in these interactions have been omitted for clarity.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Reflections (011), (012), and (020) affected by the beam-stop, were omitted for the final refinement. A small region of disordered electron density was corrected for using the SQUEEZE routine in *PLATON* (Spek, 2015), volume *ca* 60 Å^3 for 12 electrons count; the formula mass and unit-cell characteristics were not taken into account during refinement.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161758 [https://doi.org/10.1107/S2414314616017582]

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Crystal data

$[Zn(NCS)_2(C_{21}H_{15}N_3)]$
M_r = 490.89
Monoclinic, $P2_1/n$
a = 11.518 (5) Å
b = 25.095 (5) Å
c = 23.137 (5) Å
β = 98.217 (5)°
V = 6619 (3) Å^3
Z = 12
$F(000)$ = 3000
D_x = 1.478 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 2976 reflections
θ = 2.3–17.9°
μ = 1.32 mm^{-1}
T = 298 K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.692, T_{max} = 0.778
47455 measured reflections
11948 independent reflections
5625 reflections with $I > 2\sigma(I)$
R_{int} = 0.127
θ_{max} = 25.3°, θ_{min} = 1.8°
h = −13→13
k = −30→27
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.213
S = 0.98
11948 reflections
838 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.093P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.40821 (8)	0.09997 (4)	0.08583 (3)	0.0588 (3)
S1	0.0197 (3)	0.09060 (15)	0.01774 (13)	0.1266 (13)
S2	0.7367 (2)	0.15375 (12)	0.00189 (12)	0.1003 (9)
N1	0.3470 (6)	0.1807 (2)	0.1066 (3)	0.0576 (17)
N2	0.4488 (5)	0.1072 (2)	0.1756 (2)	0.0443 (14)
N3	0.4745 (6)	0.0217 (2)	0.1153 (2)	0.0563 (17)
N10	0.2607 (7)	0.0800 (3)	0.0387 (3)	0.079 (2)
N11	0.5373 (7)	0.1201 (3)	0.0425 (3)	0.071 (2)
C1	0.5630 (8)	0.1283 (4)	0.4818 (4)	0.078 (3)
H1	0.5720	0.1308	0.5223	0.094*
C2	0.5519 (8)	0.1729 (4)	0.4485 (3)	0.078 (3)
H2	0.5568	0.2062	0.4663	0.094*
C3	0.5332 (7)	0.1694 (3)	0.3882 (3)	0.062 (2)
H3	0.5259	0.2004	0.3660	0.075*
C4	0.5254 (6)	0.1205 (3)	0.3605 (3)	0.0479 (18)
C5	0.5406 (7)	0.0750 (3)	0.3955 (3)	0.065 (2)
H5	0.5370	0.0416	0.3781	0.078*
C6	0.5609 (9)	0.0792 (4)	0.4552 (4)	0.084 (3)
H6	0.5732	0.0486	0.4779	0.101*
C7	0.5002 (6)	0.1160 (3)	0.2963 (3)	0.0422 (17)
C8	0.4496 (6)	0.1578 (3)	0.2620 (3)	0.0464 (18)
H8	0.4319	0.1894	0.2798	0.056*
C9	0.4256 (6)	0.1530 (3)	0.2026 (3)	0.0439 (17)
C10	0.4990 (6)	0.0661 (3)	0.2068 (3)	0.0417 (17)
C11	0.5248 (6)	0.0697 (3)	0.2672 (3)	0.0476 (18)
H11	0.5589	0.0409	0.2884	0.057*
C12	0.3702 (6)	0.1956 (3)	0.1630 (3)	0.0487 (19)
C13	0.3427 (8)	0.2456 (3)	0.1806 (4)	0.070 (2)
H13	0.3585	0.2549	0.2199	0.084*
C14	0.2918 (8)	0.2821 (3)	0.1406 (4)	0.073 (3)
H14	0.2731	0.3162	0.1522	0.088*
C15	0.2694 (8)	0.2672 (4)	0.0836 (4)	0.083 (3)
H15	0.2348	0.2911	0.0556	0.100*
C16	0.2983 (8)	0.2162 (4)	0.0672 (4)	0.077 (3)
H16	0.2835	0.2066	0.0281	0.092*
C17	0.5169 (6)	0.0180 (3)	0.1716 (3)	0.0491 (19)
C18	0.5750 (7)	−0.0266 (3)	0.1945 (3)	0.060 (2)
H18	0.6055	−0.0280	0.2339	0.072*
C19	0.5875 (8)	−0.0690 (3)	0.1588 (4)	0.074 (2)
H19	0.6261	−0.0997	0.1735	0.089*

C20	0.5416 (8)	−0.0652 (4)	0.1007 (4)	0.076 (3)
H20	0.5482	−0.0933	0.0752	0.091*
C21	0.4867 (8)	−0.0196 (4)	0.0815 (3)	0.075 (3)
H21	0.4559	−0.0172	0.0422	0.090*
C69	0.1643 (10)	0.0857 (4)	0.0302 (3)	0.076 (3)
C70	0.6193 (7)	0.1331 (3)	0.0252 (3)	0.056 (2)
Zn2	0.62013 (8)	0.26836 (4)	0.81912 (4)	0.0645 (3)
S3	0.3027 (2)	0.19842 (10)	0.90059 (10)	0.0783 (7)
S4	0.9905 (2)	0.18933 (11)	0.83004 (16)	0.1121 (10)
N4	0.5505 (6)	0.2600 (2)	0.7256 (3)	0.0597 (17)
N5	0.6317 (5)	0.3445 (2)	0.7843 (3)	0.0493 (15)
N6	0.6784 (6)	0.3198 (3)	0.8944 (3)	0.0694 (19)
N12	0.4919 (6)	0.2319 (3)	0.8506 (3)	0.075 (2)
N13	0.7654 (7)	0.2278 (3)	0.8221 (3)	0.074 (2)
C22	0.7660 (9)	0.5882 (3)	0.6572 (5)	0.083 (3)
H22	0.7842	0.6202	0.6405	0.099*
C23	0.7027 (9)	0.5510 (4)	0.6247 (4)	0.082 (3)
H23	0.6764	0.5573	0.5854	0.098*
C24	0.6767 (8)	0.5028 (3)	0.6504 (4)	0.072 (3)
H24	0.6345	0.4770	0.6274	0.087*
C25	0.7115 (6)	0.4924 (3)	0.7086 (3)	0.0504 (19)
C26	0.7760 (8)	0.5309 (3)	0.7400 (4)	0.075 (3)
H26	0.8025	0.5251	0.7793	0.089*
C27	0.8031 (10)	0.5786 (4)	0.7144 (5)	0.094 (3)
H27	0.8471	0.6042	0.7369	0.112*
C28	0.6848 (6)	0.4406 (3)	0.7344 (3)	0.0452 (18)
C29	0.6335 (7)	0.3986 (3)	0.7014 (3)	0.055 (2)
H29	0.6158	0.4023	0.6611	0.066*
C30	0.6085 (6)	0.3518 (3)	0.7268 (3)	0.0481 (18)
C31	0.7037 (6)	0.4328 (3)	0.7951 (3)	0.054 (2)
H31	0.7318	0.4606	0.8198	0.065*
C32	0.6803 (6)	0.3834 (3)	0.8181 (3)	0.0485 (18)
C33	0.7007 (7)	0.3705 (3)	0.8812 (3)	0.054 (2)
C34	0.7416 (7)	0.4059 (4)	0.9239 (4)	0.072 (2)
H34	0.7564	0.4409	0.9140	0.087*
C35	0.7615 (9)	0.3903 (5)	0.9823 (4)	0.096 (3)
H35	0.7908	0.4140	1.0117	0.115*
C36	0.7362 (9)	0.3395 (6)	0.9942 (4)	0.101 (4)
H36	0.7445	0.3280	1.0327	0.122*
C37	0.6981 (8)	0.3044 (4)	0.9498 (4)	0.084 (3)
H37	0.6858	0.2689	0.9588	0.101*
C38	0.5532 (7)	0.3049 (3)	0.6939 (4)	0.058 (2)
C39	0.5141 (7)	0.3051 (3)	0.6352 (4)	0.063 (2)
H39	0.5200	0.3361	0.6137	0.075*
C40	0.4666 (8)	0.2605 (4)	0.6077 (4)	0.079 (3)
H40	0.4373	0.2609	0.5681	0.095*
C41	0.4633 (8)	0.2149 (4)	0.6404 (4)	0.078 (3)
H41	0.4344	0.1833	0.6228	0.093*

C43	0.5028 (8)	0.2164 (3)	0.6988 (4)	0.073 (3)
H43	0.4963	0.1858	0.7208	0.088*
C65	0.8564 (9)	0.2108 (3)	0.8268 (4)	0.065 (2)
C66	0.4157 (7)	0.2176 (3)	0.8730 (3)	0.055 (2)
Zn3	0.39549 (8)	0.48965 (3)	0.81136 (4)	0.0524 (3)
S5	0.7473 (2)	0.56688 (12)	0.89780 (12)	0.0956 (9)
S6	0.0596 (2)	0.57143 (10)	0.86627 (12)	0.0856 (8)
N7	0.3859 (5)	0.5012 (2)	0.7189 (3)	0.0544 (16)
N8	0.3436 (4)	0.4158 (2)	0.7753 (2)	0.0397 (13)
N9	0.4070 (6)	0.4335 (2)	0.8843 (2)	0.0596 (17)
N14	0.5383 (6)	0.5294 (3)	0.8402 (3)	0.071 (2)
N15	0.2609 (6)	0.5312 (3)	0.8320 (3)	0.0655 (19)
C44	0.1194 (9)	0.1752 (3)	0.6482 (4)	0.083 (3)
H44	0.0901	0.1435	0.6312	0.099*
C45	0.1755 (10)	0.1755 (4)	0.7046 (4)	0.096 (3)
H45	0.1864	0.1439	0.7256	0.116*
C46	0.2160 (8)	0.2231 (3)	0.7302 (3)	0.074 (3)
H46	0.2521	0.2231	0.7688	0.089*
C47	0.2041 (6)	0.2703 (3)	0.6997 (3)	0.0487 (18)
C48	0.1500 (7)	0.2686 (3)	0.6430 (3)	0.055 (2)
H48	0.1422	0.2998	0.6212	0.066*
C49	0.1067 (8)	0.2214 (3)	0.6174 (4)	0.069 (2)
H49	0.0689	0.2214	0.5791	0.082*
C50	0.2509 (6)	0.3211 (3)	0.7260 (3)	0.0415 (17)
C51	0.2798 (6)	0.3269 (3)	0.7869 (3)	0.0464 (18)
H51	0.2671	0.2989	0.8115	0.056*
C52	0.3269 (6)	0.3739 (3)	0.8098 (3)	0.0464 (18)
C53	0.2717 (6)	0.3646 (3)	0.6920 (3)	0.0442 (18)
H53	0.2550	0.3621	0.6516	0.053*
C54	0.3166 (6)	0.4117 (3)	0.7169 (3)	0.0444 (17)
C55	0.3415 (6)	0.4608 (3)	0.6844 (3)	0.0460 (18)
C56	0.3223 (7)	0.4638 (3)	0.6243 (3)	0.066 (2)
H56	0.2926	0.4347	0.6020	0.079*
C57	0.3476 (9)	0.5101 (4)	0.5983 (4)	0.086 (3)
H57	0.3346	0.5132	0.5578	0.104*
C58	0.3927 (9)	0.5528 (4)	0.6324 (4)	0.080 (3)
H58	0.4110	0.5846	0.6152	0.095*
C59	0.4099 (7)	0.5470 (3)	0.6918 (4)	0.062 (2)
H59	0.4393	0.5758	0.7146	0.074*
C60	0.3616 (6)	0.3851 (3)	0.8729 (3)	0.0449 (18)
C61	0.3562 (7)	0.3476 (3)	0.9159 (3)	0.059 (2)
H61	0.3262	0.3137	0.9066	0.071*
C62	0.3959 (8)	0.3611 (4)	0.9726 (3)	0.074 (3)
H62	0.3913	0.3364	1.0022	0.088*
C63	0.4422 (9)	0.4104 (4)	0.9863 (4)	0.086 (3)
H63	0.4708	0.4200	1.0245	0.103*
C64	0.4443 (8)	0.4451 (4)	0.9403 (4)	0.081 (3)
H64	0.4738	0.4791	0.9488	0.098*

C67	0.1803 (8)	0.5478 (3)	0.8479 (3)	0.052 (2)
C68	0.6241 (8)	0.5454 (3)	0.8634 (3)	0.058 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0606 (6)	0.0714 (7)	0.0429 (5)	0.0004 (5)	0.0021 (4)	−0.0018 (4)
S1	0.082 (2)	0.190 (4)	0.099 (2)	0.036 (2)	−0.0135 (16)	−0.056 (2)
S2	0.086 (2)	0.109 (2)	0.113 (2)	−0.0146 (17)	0.0391 (16)	−0.0114 (16)
N1	0.068 (5)	0.055 (4)	0.047 (4)	0.007 (4)	0.000 (3)	0.009 (3)
N2	0.040 (4)	0.050 (4)	0.043 (3)	0.004 (3)	0.008 (3)	0.002 (3)
N3	0.069 (5)	0.055 (4)	0.044 (4)	0.004 (3)	0.005 (3)	−0.009 (3)
N10	0.059 (5)	0.098 (6)	0.073 (5)	0.002 (5)	−0.015 (4)	−0.002 (4)
N11	0.070 (5)	0.081 (5)	0.064 (5)	−0.001 (4)	0.010 (4)	−0.005 (4)
C1	0.079 (7)	0.109 (8)	0.043 (5)	0.006 (6)	0.000 (4)	0.001 (5)
C2	0.104 (8)	0.075 (6)	0.050 (5)	0.016 (6)	−0.010 (5)	−0.009 (5)
C3	0.076 (6)	0.054 (5)	0.053 (5)	0.017 (5)	−0.006 (4)	−0.001 (4)
C4	0.053 (5)	0.047 (5)	0.044 (4)	0.011 (4)	0.006 (3)	0.001 (4)
C5	0.092 (7)	0.053 (5)	0.050 (5)	0.014 (5)	0.008 (4)	0.000 (4)
C6	0.114 (8)	0.084 (7)	0.049 (5)	0.026 (6)	−0.007 (5)	0.014 (5)
C7	0.041 (4)	0.040 (4)	0.046 (4)	0.002 (4)	0.006 (3)	−0.002 (3)
C8	0.048 (5)	0.042 (4)	0.048 (4)	0.008 (4)	0.001 (3)	−0.001 (3)
C9	0.038 (4)	0.047 (5)	0.049 (4)	−0.002 (4)	0.013 (3)	0.005 (3)
C10	0.037 (4)	0.042 (4)	0.046 (4)	−0.002 (4)	0.005 (3)	0.004 (3)
C11	0.043 (5)	0.055 (5)	0.043 (4)	0.012 (4)	0.001 (3)	0.002 (3)
C12	0.040 (4)	0.055 (5)	0.053 (5)	0.012 (4)	0.015 (3)	0.020 (4)
C13	0.091 (7)	0.049 (5)	0.072 (6)	0.014 (5)	0.015 (5)	0.008 (4)
C14	0.078 (7)	0.057 (6)	0.086 (7)	0.025 (5)	0.016 (5)	0.022 (5)
C15	0.079 (7)	0.093 (8)	0.076 (7)	0.021 (6)	0.008 (5)	0.039 (6)
C16	0.073 (6)	0.101 (8)	0.054 (5)	0.027 (6)	0.000 (4)	0.017 (5)
C17	0.049 (5)	0.050 (5)	0.049 (5)	−0.005 (4)	0.010 (4)	−0.012 (4)
C18	0.069 (6)	0.053 (5)	0.057 (5)	0.014 (4)	−0.001 (4)	−0.008 (4)
C19	0.092 (7)	0.056 (6)	0.072 (6)	0.011 (5)	0.008 (5)	−0.010 (5)
C20	0.079 (7)	0.083 (7)	0.064 (6)	0.003 (6)	0.004 (5)	−0.035 (5)
C21	0.098 (7)	0.072 (7)	0.052 (5)	0.025 (6)	−0.003 (5)	−0.014 (5)
C69	0.103 (8)	0.082 (7)	0.040 (5)	0.025 (7)	0.000 (5)	−0.010 (4)
C70	0.054 (6)	0.065 (6)	0.048 (5)	0.007 (5)	0.008 (4)	−0.008 (4)
Zn2	0.0525 (6)	0.0569 (6)	0.0868 (7)	0.0081 (5)	0.0192 (5)	0.0252 (5)
S3	0.0770 (17)	0.0734 (16)	0.0919 (17)	−0.0114 (13)	0.0371 (13)	0.0076 (12)
S4	0.0651 (18)	0.0662 (18)	0.204 (3)	0.0199 (15)	0.0143 (19)	0.0062 (18)
N4	0.059 (4)	0.038 (4)	0.086 (5)	−0.005 (3)	0.021 (4)	0.009 (3)
N5	0.044 (4)	0.043 (4)	0.061 (4)	0.009 (3)	0.010 (3)	0.005 (3)
N6	0.060 (5)	0.081 (5)	0.070 (5)	0.007 (4)	0.016 (4)	0.025 (4)
N12	0.052 (5)	0.075 (5)	0.100 (6)	0.000 (4)	0.020 (4)	0.027 (4)
N13	0.065 (5)	0.064 (5)	0.097 (5)	0.022 (4)	0.023 (4)	0.021 (4)
C22	0.108 (8)	0.040 (6)	0.107 (8)	0.009 (6)	0.035 (7)	0.008 (5)
C23	0.110 (8)	0.059 (6)	0.074 (6)	0.013 (6)	0.006 (5)	0.011 (5)
C24	0.100 (7)	0.044 (6)	0.070 (6)	−0.007 (5)	0.002 (5)	0.006 (4)

C25	0.045 (5)	0.039 (4)	0.066 (5)	−0.002 (4)	0.006 (4)	−0.001 (4)
C26	0.094 (7)	0.058 (6)	0.072 (6)	−0.019 (5)	0.014 (5)	0.002 (5)
C27	0.130 (10)	0.059 (6)	0.095 (8)	−0.029 (6)	0.027 (7)	−0.021 (6)
C28	0.035 (4)	0.046 (5)	0.057 (5)	0.010 (4)	0.014 (3)	0.010 (4)
C29	0.058 (5)	0.052 (5)	0.055 (5)	−0.008 (4)	0.005 (4)	0.004 (4)
C30	0.048 (5)	0.040 (5)	0.058 (5)	0.006 (4)	0.013 (4)	0.002 (4)
C31	0.051 (5)	0.047 (5)	0.065 (5)	0.002 (4)	0.013 (4)	−0.011 (4)
C32	0.047 (5)	0.050 (5)	0.050 (4)	0.009 (4)	0.011 (4)	0.002 (4)
C33	0.048 (5)	0.062 (6)	0.054 (5)	0.002 (4)	0.014 (4)	0.000 (4)
C34	0.060 (6)	0.086 (7)	0.070 (6)	0.013 (5)	0.006 (5)	0.009 (5)
C35	0.079 (7)	0.143 (11)	0.063 (6)	−0.004 (8)	0.004 (5)	0.000 (6)
C36	0.085 (8)	0.154 (12)	0.063 (7)	0.005 (8)	−0.001 (5)	0.037 (8)
C37	0.085 (7)	0.086 (7)	0.081 (7)	−0.005 (6)	0.014 (6)	0.031 (6)
C38	0.059 (5)	0.046 (5)	0.072 (6)	0.000 (4)	0.020 (4)	0.003 (4)
C39	0.072 (6)	0.051 (5)	0.066 (6)	−0.008 (5)	0.012 (4)	0.001 (4)
C40	0.082 (7)	0.070 (7)	0.084 (6)	−0.008 (6)	0.009 (5)	−0.006 (5)
C41	0.077 (7)	0.058 (6)	0.095 (7)	−0.008 (5)	−0.002 (6)	−0.009 (5)
C43	0.072 (6)	0.037 (5)	0.112 (8)	−0.007 (5)	0.019 (6)	0.015 (5)
C65	0.071 (7)	0.027 (4)	0.096 (6)	0.005 (5)	0.006 (5)	0.010 (4)
C66	0.054 (5)	0.053 (5)	0.057 (5)	0.002 (4)	0.002 (4)	0.012 (4)
Zn3	0.0495 (6)	0.0417 (5)	0.0650 (6)	−0.0042 (4)	0.0047 (4)	−0.0081 (4)
S5	0.0707 (17)	0.109 (2)	0.1016 (19)	−0.0259 (16)	−0.0078 (14)	−0.0296 (16)
S6	0.0731 (17)	0.0666 (16)	0.121 (2)	0.0156 (13)	0.0259 (15)	−0.0121 (14)
N7	0.053 (4)	0.040 (4)	0.073 (4)	−0.013 (3)	0.017 (3)	−0.001 (3)
N8	0.035 (3)	0.039 (3)	0.046 (3)	0.001 (3)	0.007 (3)	−0.003 (3)
N9	0.078 (5)	0.053 (4)	0.045 (4)	0.001 (4)	−0.002 (3)	−0.006 (3)
N14	0.054 (5)	0.059 (5)	0.099 (6)	−0.013 (4)	0.007 (4)	−0.016 (4)
N15	0.068 (5)	0.045 (4)	0.080 (5)	−0.003 (4)	0.000 (4)	−0.014 (3)
C44	0.108 (8)	0.043 (6)	0.103 (8)	−0.024 (5)	0.033 (6)	−0.026 (5)
C45	0.159 (11)	0.046 (6)	0.082 (7)	−0.018 (6)	0.009 (7)	0.001 (5)
C46	0.103 (7)	0.058 (6)	0.058 (5)	−0.022 (5)	0.002 (5)	−0.002 (4)
C47	0.058 (5)	0.040 (5)	0.048 (4)	−0.002 (4)	0.006 (4)	−0.002 (3)
C48	0.066 (5)	0.037 (5)	0.061 (5)	0.003 (4)	0.010 (4)	−0.008 (4)
C49	0.082 (7)	0.051 (6)	0.071 (5)	−0.007 (5)	0.004 (5)	−0.015 (4)
C50	0.037 (4)	0.037 (4)	0.048 (4)	0.006 (3)	−0.002 (3)	−0.005 (3)
C51	0.047 (5)	0.038 (4)	0.053 (4)	0.005 (4)	0.005 (3)	0.005 (3)
C52	0.053 (5)	0.036 (4)	0.050 (4)	0.000 (4)	0.005 (3)	0.004 (3)
C53	0.056 (5)	0.034 (4)	0.041 (4)	0.003 (4)	0.005 (3)	0.001 (3)
C54	0.049 (5)	0.041 (4)	0.042 (4)	−0.001 (4)	0.003 (3)	0.003 (3)
C55	0.050 (5)	0.024 (4)	0.066 (5)	−0.012 (3)	0.014 (4)	−0.003 (3)
C56	0.090 (7)	0.050 (5)	0.057 (5)	−0.020 (5)	0.006 (4)	0.003 (4)
C57	0.131 (9)	0.072 (7)	0.056 (5)	−0.021 (6)	0.012 (5)	0.003 (5)
C58	0.114 (8)	0.059 (6)	0.068 (6)	−0.008 (6)	0.020 (5)	0.018 (5)
C59	0.059 (6)	0.038 (5)	0.088 (6)	−0.004 (4)	0.012 (4)	−0.012 (4)
C60	0.046 (5)	0.038 (5)	0.050 (4)	0.011 (4)	0.006 (3)	−0.001 (3)
C61	0.076 (6)	0.051 (5)	0.049 (5)	0.005 (4)	0.006 (4)	−0.001 (4)
C62	0.086 (7)	0.081 (7)	0.054 (5)	−0.004 (6)	0.011 (5)	0.008 (5)
C63	0.130 (9)	0.079 (7)	0.046 (5)	−0.009 (7)	0.001 (5)	−0.008 (5)

C64	0.113 (8)	0.067 (6)	0.062 (6)	−0.016 (6)	0.003 (5)	−0.010 (5)
C67	0.066 (6)	0.030 (4)	0.059 (5)	0.006 (4)	0.001 (4)	−0.009 (3)
C68	0.079 (7)	0.040 (5)	0.061 (5)	0.002 (5)	0.025 (5)	−0.009 (4)

Geometric parameters (Å, º)

Zn1—N10	1.949 (7)	C27—H27	0.9300
Zn1—N11	1.975 (8)	C28—C29	1.384 (10)
Zn1—N2	2.071 (5)	C28—C31	1.404 (9)
Zn1—N3	2.181 (6)	C29—C30	1.363 (9)
Zn1—N1	2.219 (6)	C29—H29	0.9300
S1—C69	1.654 (12)	C30—C38	1.492 (10)
S2—C70	1.611 (9)	C31—C32	1.390 (10)
N1—C16	1.339 (9)	C31—H31	0.9300
N1—C12	1.347 (9)	C32—C33	1.481 (10)
N2—C10	1.339 (8)	C33—C34	1.361 (11)
N2—C9	1.353 (8)	C34—C35	1.393 (12)
N3—C21	1.317 (9)	C34—H34	0.9300
N3—C17	1.328 (8)	C35—C36	1.345 (13)
N10—C69	1.108 (10)	C35—H35	0.9300
N11—C70	1.125 (9)	C36—C37	1.377 (13)
C1—C2	1.356 (11)	C36—H36	0.9300
C1—C6	1.375 (12)	C37—H37	0.9300
C1—H1	0.9300	C38—C39	1.370 (10)
C2—C3	1.383 (10)	C39—C40	1.361 (11)
C2—H2	0.9300	C39—H39	0.9300
C3—C4	1.382 (9)	C40—C41	1.376 (12)
C3—H3	0.9300	C40—H40	0.9300
C4—C5	1.394 (10)	C41—C43	1.362 (11)
C4—C7	1.478 (9)	C41—H41	0.9300
C5—C6	1.373 (10)	C43—H43	0.9300
C5—H5	0.9300	Zn3—N14	1.958 (7)
C6—H6	0.9300	Zn3—N15	1.982 (8)
C7—C8	1.391 (9)	Zn3—N8	2.085 (5)
C7—C11	1.391 (9)	Zn3—N7	2.145 (6)
C8—C9	1.368 (9)	Zn3—N9	2.188 (6)
C8—H8	0.9300	S5—C68	1.616 (10)
C9—C12	1.492 (9)	S6—C67	1.624 (9)
C10—C11	1.390 (8)	N7—C55	1.344 (8)
C10—C17	1.488 (9)	N7—C59	1.358 (9)
C11—H11	0.9300	N8—C54	1.348 (8)
C12—C13	1.371 (10)	N8—C52	1.350 (8)
C13—C14	1.373 (10)	N9—C60	1.335 (8)
C13—H13	0.9300	N9—C64	1.336 (9)
C14—C15	1.361 (11)	N14—C68	1.128 (9)
C14—H14	0.9300	N15—C67	1.125 (9)
C15—C16	1.386 (12)	C44—C49	1.358 (11)
C15—H15	0.9300	C44—C45	1.371 (12)

C16—H16	0.9300	C44—H44	0.9300
C17—C18	1.370 (10)	C45—C46	1.383 (11)
C18—C19	1.367 (10)	C45—H45	0.9300
C18—H18	0.9300	C46—C47	1.375 (10)
C19—C20	1.376 (10)	C46—H46	0.9300
C19—H19	0.9300	C47—C48	1.370 (9)
C20—C21	1.351 (11)	C47—C50	1.480 (9)
C20—H20	0.9300	C48—C49	1.384 (10)
C21—H21	0.9300	C48—H48	0.9300
Zn2—N13	1.951 (8)	C49—H49	0.9300
Zn2—N12	1.963 (7)	C50—C53	1.387 (9)
Zn2—N5	2.086 (6)	C50—C51	1.408 (9)
Zn2—N6	2.195 (7)	C51—C52	1.373 (9)
Zn2—N4	2.209 (7)	C51—H51	0.9300
S3—C66	1.603 (9)	C52—C60	1.483 (9)
S4—C65	1.628 (10)	C53—C54	1.381 (9)
N4—C43	1.336 (10)	C53—H53	0.9300
N4—C38	1.348 (9)	C54—C55	1.492 (9)
N5—C32	1.324 (9)	C55—C56	1.379 (9)
N5—C30	1.332 (8)	C56—C57	1.360 (11)
N6—C37	1.325 (10)	C56—H56	0.9300
N6—C33	1.344 (9)	C57—C58	1.386 (11)
N12—C66	1.140 (9)	C57—H57	0.9300
N13—C65	1.122 (9)	C58—C59	1.368 (10)
C22—C23	1.345 (12)	C58—H58	0.9300
C22—C27	1.352 (12)	C59—H59	0.9300
C22—H22	0.9300	C60—C61	1.379 (9)
C23—C24	1.399 (11)	C61—C62	1.369 (10)
C23—H23	0.9300	C61—H61	0.9300
C24—C25	1.372 (10)	C62—C63	1.366 (11)
C24—H24	0.9300	C62—H62	0.9300
C25—C26	1.364 (10)	C63—C64	1.378 (11)
C25—C28	1.482 (10)	C63—H63	0.9300
C26—C27	1.390 (12)	C64—H64	0.9300
C26—H26	0.9300		

N10—Zn1—N11	116.2 (3)	C30—C29—H29	119.4
N10—Zn1—N2	129.6 (3)	C28—C29—H29	119.4
N11—Zn1—N2	114.1 (2)	N5—C30—C29	121.6 (7)
N10—Zn1—N3	100.5 (3)	N5—C30—C38	114.3 (6)
N11—Zn1—N3	97.7 (3)	C29—C30—C38	124.0 (7)
N2—Zn1—N3	75.3 (2)	C32—C31—C28	119.7 (7)
N10—Zn1—N1	94.4 (3)	C32—C31—H31	120.1
N11—Zn1—N1	99.3 (3)	C28—C31—H31	120.1
N2—Zn1—N1	74.7 (2)	N5—C32—C31	121.3 (6)
N3—Zn1—N1	149.5 (2)	N5—C32—C33	114.5 (7)
C16—N1—C12	118.5 (7)	C31—C32—C33	124.1 (7)
C16—N1—Zn1	125.2 (6)	N6—C33—C34	120.7 (7)

C12—N1—Zn1	116.0 (5)	N6—C33—C32	115.0 (7)
C10—N2—C9	120.2 (6)	C34—C33—C32	124.3 (8)
C10—N2—Zn1	119.4 (5)	C33—C34—C35	120.8 (9)
C9—N2—Zn1	120.4 (4)	C33—C34—H34	119.6
C21—N3—C17	118.1 (7)	C35—C34—H34	119.6
C21—N3—Zn1	125.8 (5)	C36—C35—C34	117.0 (10)
C17—N3—Zn1	115.7 (5)	C36—C35—H35	121.5
C69—N10—Zn1	146.8 (8)	C34—C35—H35	121.5
C70—N11—Zn1	170.4 (7)	C35—C36—C37	120.6 (9)
C2—C1—C6	119.4 (8)	C35—C36—H36	119.7
C2—C1—H1	120.3	C37—C36—H36	119.7
C6—C1—H1	120.3	N6—C37—C36	121.8 (9)
C1—C2—C3	120.5 (8)	N6—C37—H37	119.1
C1—C2—H2	119.7	C36—C37—H37	119.1
C3—C2—H2	119.7	N4—C38—C39	120.8 (7)
C4—C3—C2	121.0 (7)	N4—C38—C30	115.1 (7)
C4—C3—H3	119.5	C39—C38—C30	124.0 (7)
C2—C3—H3	119.5	C40—C39—C38	120.9 (8)
C3—C4—C5	117.6 (6)	C40—C39—H39	119.5
C3—C4—C7	121.7 (6)	C38—C39—H39	119.5
C5—C4—C7	120.8 (6)	C39—C40—C41	117.9 (9)
C6—C5—C4	120.7 (7)	C39—C40—H40	121.0
C6—C5—H5	119.6	C41—C40—H40	121.0
C4—C5—H5	119.6	C43—C41—C40	119.4 (8)
C5—C6—C1	120.6 (8)	C43—C41—H41	120.3
C5—C6—H6	119.7	C40—C41—H41	120.3
C1—C6—H6	119.7	N4—C43—C41	122.6 (8)
C8—C7—C11	116.8 (6)	N4—C43—H43	118.7
C8—C7—C4	121.4 (6)	C41—C43—H43	118.7
C11—C7—C4	121.7 (6)	N13—C65—S4	175.7 (8)
C9—C8—C7	120.9 (6)	N12—C66—S3	176.2 (7)
C9—C8—H8	119.5	N14—Zn3—N15	107.3 (3)
C7—C8—H8	119.5	N14—Zn3—N8	140.2 (2)
N2—C9—C8	120.9 (6)	N15—Zn3—N8	112.0 (2)
N2—C9—C12	114.9 (6)	N14—Zn3—N7	101.1 (3)
C8—C9—C12	124.2 (7)	N15—Zn3—N7	103.8 (3)
N2—C10—C11	120.3 (6)	N8—Zn3—N7	75.5 (2)
N2—C10—C17	114.4 (6)	N14—Zn3—N9	96.3 (3)
C11—C10—C17	125.2 (6)	N15—Zn3—N9	96.7 (3)
C10—C11—C7	120.8 (6)	N8—Zn3—N9	73.7 (2)
C10—C11—H11	119.6	N7—Zn3—N9	147.6 (2)
C7—C11—H11	119.6	C55—N7—C59	116.7 (6)
N1—C12—C13	121.5 (6)	C55—N7—Zn3	116.8 (5)
N1—C12—C9	113.8 (6)	C59—N7—Zn3	126.2 (5)
C13—C12—C9	124.7 (7)	C54—N8—C52	120.2 (6)
C12—C13—C14	120.3 (8)	C54—N8—Zn3	118.8 (4)
C12—C13—H13	119.9	C52—N8—Zn3	120.8 (4)
C14—C13—H13	119.9	C60—N9—C64	116.9 (7)

C15—C14—C13	118.2 (8)	C60—N9—Zn3	117.0 (4)
C15—C14—H14	120.9	C64—N9—Zn3	125.7 (6)
C13—C14—H14	120.9	C68—N14—Zn3	168.2 (8)
C14—C15—C16	119.9 (8)	C67—N15—Zn3	169.3 (7)
C14—C15—H15	120.0	C49—C44—C45	119.8 (8)
C16—C15—H15	120.0	C49—C44—H44	120.1
N1—C16—C15	121.5 (8)	C45—C44—H44	120.1
N1—C16—H16	119.2	C44—C45—C46	119.6 (8)
C15—C16—H16	119.2	C44—C45—H45	120.2
N3—C17—C18	121.8 (6)	C46—C45—H45	120.2
N3—C17—C10	114.7 (7)	C47—C46—C45	121.5 (8)
C18—C17—C10	123.4 (6)	C47—C46—H46	119.2
C19—C18—C17	119.4 (7)	C45—C46—H46	119.2
C19—C18—H18	120.3	C48—C47—C46	117.5 (7)
C17—C18—H18	120.3	C48—C47—C50	120.6 (6)
C18—C19—C20	118.5 (8)	C46—C47—C50	121.9 (7)
C18—C19—H19	120.7	C47—C48—C49	121.6 (7)
C20—C19—H19	120.7	C47—C48—H48	119.2
C21—C20—C19	118.4 (8)	C49—C48—H48	119.2
C21—C20—H20	120.8	C44—C49—C48	120.0 (8)
C19—C20—H20	120.8	C44—C49—H49	120.0
N3—C21—C20	123.8 (8)	C48—C49—H49	120.0
N3—C21—H21	118.1	C53—C50—C51	116.8 (6)
C20—C21—H21	118.1	C53—C50—C47	121.9 (6)
N10—C69—S1	176.9 (10)	C51—C50—C47	121.3 (6)
N11—C70—S2	177.8 (8)	C52—C51—C50	120.0 (6)
N13—Zn2—N12	115.6 (3)	C52—C51—H51	120.0
N13—Zn2—N5	112.9 (3)	C50—C51—H51	120.0
N12—Zn2—N5	131.5 (3)	N8—C52—C51	121.4 (6)
N13—Zn2—N6	96.6 (3)	N8—C52—C60	113.2 (6)
N12—Zn2—N6	98.1 (3)	C51—C52—C60	125.4 (6)
N5—Zn2—N6	74.9 (3)	C54—C53—C50	121.5 (6)
N13—Zn2—N4	100.0 (3)	C54—C53—H53	119.3
N12—Zn2—N4	97.6 (3)	C50—C53—H53	119.3
N5—Zn2—N4	75.1 (2)	N8—C54—C53	120.1 (6)
N6—Zn2—N4	149.5 (2)	N8—C54—C55	114.1 (6)
C43—N4—C38	118.2 (7)	C53—C54—C55	125.8 (6)
C43—N4—Zn2	126.9 (6)	N7—C55—C56	123.4 (6)
C38—N4—Zn2	114.8 (5)	N7—C55—C54	114.1 (6)
C32—N5—C30	119.8 (6)	C56—C55—C54	122.5 (6)
C32—N5—Zn2	119.5 (5)	C57—C56—C55	118.7 (7)
C30—N5—Zn2	119.7 (5)	C57—C56—H56	120.7
C37—N6—C33	118.9 (8)	C55—C56—H56	120.7
C37—N6—Zn2	125.9 (7)	C56—C57—C58	119.6 (8)
C33—N6—Zn2	115.1 (5)	C56—C57—H57	120.2
C66—N12—Zn2	170.0 (8)	C58—C57—H57	120.2
C65—N13—Zn2	170.5 (8)	C59—C58—C57	118.6 (8)
C23—C22—C27	119.6 (9)	C59—C58—H58	120.7

C23—C22—H22	120.2	C57—C58—H58	120.7
C27—C22—H22	120.2	N7—C59—C58	123.0 (7)
C22—C23—C24	119.6 (9)	N7—C59—H59	118.5
C22—C23—H23	120.2	C58—C59—H59	118.5
C24—C23—H23	120.2	N9—C60—C61	122.4 (7)
C25—C24—C23	122.0 (8)	N9—C60—C52	114.2 (6)
C25—C24—H24	119.0	C61—C60—C52	123.2 (7)
C23—C24—H24	119.0	C62—C61—C60	118.6 (8)
C26—C25—C24	116.6 (7)	C62—C61—H61	120.7
C26—C25—C28	122.4 (7)	C60—C61—H61	120.7
C24—C25—C28	120.9 (7)	C63—C62—C61	120.8 (8)
C25—C26—C27	121.5 (8)	C63—C62—H62	119.6
C25—C26—H26	119.3	C61—C62—H62	119.6
C27—C26—H26	119.3	C62—C63—C64	116.3 (8)
C22—C27—C26	120.7 (9)	C62—C63—H63	121.9
C22—C27—H27	119.7	C64—C63—H63	121.9
C26—C27—H27	119.7	N9—C64—C63	124.9 (8)
C29—C28—C31	116.1 (6)	N9—C64—H64	117.5
C29—C28—C25	122.9 (7)	C63—C64—H64	117.5
C31—C28—C25	120.9 (7)	N15—C67—S6	176.1 (8)
C30—C29—C28	121.2 (7)	N14—C68—S5	178.5 (9)

N10—Zn1—N1—C16	−52.1 (7)	C32—N5—C30—C29	0.0 (10)
N11—Zn1—N1—C16	65.4 (7)	Zn2—N5—C30—C29	−168.9 (6)
N2—Zn1—N1—C16	178.0 (7)	C32—N5—C30—C38	−179.7 (6)
N3—Zn1—N1—C16	−171.5 (6)	Zn2—N5—C30—C38	11.4 (8)
N10—Zn1—N1—C12	133.5 (5)	C28—C29—C30—N5	0.3 (11)
N11—Zn1—N1—C12	−109.1 (5)	C28—C29—C30—C38	179.9 (7)
N2—Zn1—N1—C12	3.5 (5)	C29—C28—C31—C32	5.3 (10)
N3—Zn1—N1—C12	14.1 (8)	C25—C28—C31—C32	−178.6 (6)
N10—Zn1—N2—C10	95.6 (6)	C30—N5—C32—C31	2.5 (10)
N11—Zn1—N2—C10	−87.9 (5)	Zn2—N5—C32—C31	171.4 (5)
N3—Zn1—N2—C10	4.1 (5)	C30—N5—C32—C33	179.5 (6)
N1—Zn1—N2—C10	178.6 (5)	Zn2—N5—C32—C33	−11.5 (8)
N10—Zn1—N2—C9	−84.9 (6)	C28—C31—C32—N5	−5.3 (11)
N11—Zn1—N2—C9	91.6 (5)	C28—C31—C32—C33	178.0 (6)
N3—Zn1—N2—C9	−176.4 (5)	C37—N6—C33—C34	−0.8 (12)
N1—Zn1—N2—C9	−1.9 (5)	Zn2—N6—C33—C34	−177.6 (6)
N10—Zn1—N3—C21	52.8 (8)	C37—N6—C33—C32	177.8 (7)
N11—Zn1—N3—C21	−65.7 (7)	Zn2—N6—C33—C32	1.0 (8)
N2—Zn1—N3—C21	−178.7 (7)	N5—C32—C33—N6	6.5 (9)
N1—Zn1—N3—C21	170.8 (6)	C31—C32—C33—N6	−176.6 (7)
N10—Zn1—N3—C17	−134.6 (5)	N5—C32—C33—C34	−175.0 (7)
N11—Zn1—N3—C17	106.9 (5)	C31—C32—C33—C34	1.9 (12)
N2—Zn1—N3—C17	−6.1 (5)	N6—C33—C34—C35	0.1 (12)
N1—Zn1—N3—C17	−16.6 (8)	C32—C33—C34—C35	−178.3 (8)
N11—Zn1—N10—C69	−130.0 (15)	C33—C34—C35—C36	−1.3 (14)
N2—Zn1—N10—C69	46.5 (17)	C34—C35—C36—C37	3.1 (16)

N3—Zn1—N10—C69	126.0 (16)	C33—N6—C37—C36	2.7 (13)
N1—Zn1—N10—C69	−27.4 (16)	Zn2—N6—C37—C36	179.1 (7)
N10—Zn1—N11—C70	176 (5)	C35—C36—C37—N6	−4.0 (16)
N2—Zn1—N11—C70	−1 (5)	C43—N4—C38—C39	−3.6 (11)
N3—Zn1—N11—C70	−78 (5)	Zn2—N4—C38—C39	179.2 (6)
N1—Zn1—N11—C70	77 (5)	C43—N4—C38—C30	−179.6 (7)
C6—C1—C2—C3	2.9 (14)	Zn2—N4—C38—C30	3.1 (8)
C1—C2—C3—C4	0.1 (14)	N5—C30—C38—N4	−9.2 (9)
C2—C3—C4—C5	−1.9 (12)	C29—C30—C38—N4	171.1 (7)
C2—C3—C4—C7	177.2 (7)	N5—C30—C38—C39	174.8 (7)
C3—C4—C5—C6	0.9 (12)	C29—C30—C38—C39	−4.8 (12)
C7—C4—C5—C6	−178.2 (8)	N4—C38—C39—C40	2.9 (12)
C4—C5—C6—C1	2.0 (14)	C30—C38—C39—C40	178.7 (8)
C2—C1—C6—C5	−3.9 (15)	C38—C39—C40—C41	−2.4 (13)
C3—C4—C7—C8	−19.4 (11)	C39—C40—C41—C43	2.6 (14)
C5—C4—C7—C8	159.7 (7)	C38—N4—C43—C41	3.9 (13)
C3—C4—C7—C11	161.3 (7)	Zn2—N4—C43—C41	−179.2 (6)
C5—C4—C7—C11	−19.6 (11)	C40—C41—C43—N4	−3.4 (14)
C11—C7—C8—C9	0.0 (10)	Zn2—N13—C65—S4	−62 (15)
C4—C7—C8—C9	−179.3 (6)	Zn2—N12—C66—S3	97 (13)
C10—N2—C9—C8	−1.9 (10)	N14—Zn3—N7—C55	146.3 (5)
Zn1—N2—C9—C8	178.5 (5)	N15—Zn3—N7—C55	−102.5 (5)
C10—N2—C9—C12	179.7 (6)	N8—Zn3—N7—C55	7.1 (5)
Zn1—N2—C9—C12	0.1 (8)	N9—Zn3—N7—C55	25.1 (8)
C7—C8—C9—N2	1.0 (10)	N14—Zn3—N7—C59	−40.3 (6)
C7—C8—C9—C12	179.3 (6)	N15—Zn3—N7—C59	70.9 (6)
C9—N2—C10—C11	1.7 (10)	N8—Zn3—N7—C59	−179.6 (6)
Zn1—N2—C10—C11	−178.7 (5)	N9—Zn3—N7—C59	−161.5 (6)
C9—N2—C10—C17	178.7 (6)	N14—Zn3—N8—C54	−97.6 (6)
Zn1—N2—C10—C17	−1.7 (8)	N15—Zn3—N8—C54	91.7 (5)
N2—C10—C11—C7	−0.7 (10)	N7—Zn3—N8—C54	−7.5 (5)
C17—C10—C11—C7	−177.3 (6)	N9—Zn3—N8—C54	−177.5 (5)
C8—C7—C11—C10	−0.2 (10)	N14—Zn3—N8—C52	88.5 (6)
C4—C7—C11—C10	179.2 (6)	N15—Zn3—N8—C52	−82.2 (5)
C16—N1—C12—C13	1.5 (11)	N7—Zn3—N8—C52	178.5 (5)
Zn1—N1—C12—C13	176.3 (6)	N9—Zn3—N8—C52	8.5 (5)
C16—N1—C12—C9	−179.4 (7)	N14—Zn3—N9—C60	−150.2 (5)
Zn1—N1—C12—C9	−4.5 (8)	N15—Zn3—N9—C60	101.5 (5)
N2—C9—C12—N1	3.0 (9)	N8—Zn3—N9—C60	−9.5 (5)
C8—C9—C12—N1	−175.4 (6)	N7—Zn3—N9—C60	−27.8 (8)
N2—C9—C12—C13	−177.9 (7)	N14—Zn3—N9—C64	37.2 (7)
C8—C9—C12—C13	3.8 (11)	N15—Zn3—N9—C64	−71.1 (7)
N1—C12—C13—C14	−0.9 (12)	N8—Zn3—N9—C64	177.9 (7)
C9—C12—C13—C14	180.0 (7)	N7—Zn3—N9—C64	159.6 (6)
C12—C13—C14—C15	0.3 (13)	N15—Zn3—N14—C68	111 (3)
C13—C14—C15—C16	−0.2 (14)	N8—Zn3—N14—C68	−60 (4)
C12—N1—C16—C15	−1.4 (13)	N7—Zn3—N14—C68	−141 (3)
Zn1—N1—C16—C15	−175.7 (7)	N9—Zn3—N14—C68	12 (3)

C14—C15—C16—N1	0.8 (14)	N14—Zn3—N15—C67	−124 (4)
C21—N3—C17—C18	1.8 (11)	N8—Zn3—N15—C67	50 (4)
Zn1—N3—C17—C18	−171.4 (6)	N7—Zn3—N15—C67	129 (4)
C21—N3—C17—C10	−179.7 (7)	N9—Zn3—N15—C67	−25 (4)
Zn1—N3—C17—C10	7.1 (8)	C49—C44—C45—C46	1.7 (15)
N2—C10—C17—N3	−3.7 (9)	C44—C45—C46—C47	−1.8 (16)
C11—C10—C17—N3	173.1 (6)	C45—C46—C47—C48	0.3 (13)
N2—C10—C17—C18	174.8 (7)	C45—C46—C47—C50	−177.8 (8)
C11—C10—C17—C18	−8.4 (11)	C46—C47—C48—C49	1.3 (12)
N3—C17—C18—C19	−1.5 (12)	C50—C47—C48—C49	179.3 (7)
C10—C17—C18—C19	−179.9 (7)	C45—C44—C49—C48	−0.3 (14)
C17—C18—C19—C20	0.4 (13)	C47—C48—C49—C44	−1.3 (13)
C18—C19—C20—C21	0.3 (14)	C48—C47—C50—C53	−18.0 (11)
C17—N3—C21—C20	−1.0 (14)	C46—C47—C50—C53	160.0 (8)
Zn1—N3—C21—C20	171.4 (7)	C48—C47—C50—C51	164.0 (7)
C19—C20—C21—N3	0.0 (15)	C46—C47—C50—C51	−18.1 (11)
Zn1—N10—C69—S1	−127 (15)	C53—C50—C51—C52	−0.4 (10)
Zn1—N11—C70—S2	−51 (27)	C47—C50—C51—C52	177.8 (6)
N13—Zn2—N4—C43	73.7 (7)	C54—N8—C52—C51	−1.5 (10)
N12—Zn2—N4—C43	−44.1 (7)	Zn3—N8—C52—C51	172.4 (5)
N5—Zn2—N4—C43	−175.1 (7)	C54—N8—C52—C60	179.7 (6)
N6—Zn2—N4—C43	−164.3 (6)	Zn3—N8—C52—C60	−6.4 (8)
N13—Zn2—N4—C38	−109.3 (6)	C50—C51—C52—N8	1.7 (11)
N12—Zn2—N4—C38	132.9 (6)	C50—C51—C52—C60	−179.7 (6)
N5—Zn2—N4—C38	1.9 (5)	C51—C50—C53—C54	−1.1 (10)
N6—Zn2—N4—C38	12.7 (8)	C47—C50—C53—C54	−179.3 (6)
N13—Zn2—N5—C32	−81.7 (6)	C52—N8—C54—C53	0.0 (10)
N12—Zn2—N5—C32	96.6 (6)	Zn3—N8—C54—C53	−174.0 (5)
N6—Zn2—N5—C32	9.2 (5)	C52—N8—C54—C55	−179.1 (6)
N4—Zn2—N5—C32	−176.5 (6)	Zn3—N8—C54—C55	6.9 (8)
N13—Zn2—N5—C30	87.3 (6)	C50—C53—C54—N8	1.4 (11)
N12—Zn2—N5—C30	−94.5 (6)	C50—C53—C54—C55	−179.7 (7)
N6—Zn2—N5—C30	178.1 (6)	C59—N7—C55—C56	1.3 (11)
N4—Zn2—N5—C30	−7.5 (5)	Zn3—N7—C55—C56	175.3 (6)
N13—Zn2—N6—C37	−69.5 (7)	C59—N7—C55—C54	−179.8 (6)
N12—Zn2—N6—C37	47.5 (7)	Zn3—N7—C55—C54	−5.7 (8)
N5—Zn2—N6—C37	178.4 (7)	N8—C54—C55—N7	−0.5 (9)
N4—Zn2—N6—C37	167.6 (6)	C53—C54—C55—N7	−179.6 (7)
N13—Zn2—N6—C33	106.9 (6)	N8—C54—C55—C56	178.4 (7)
N12—Zn2—N6—C33	−136.0 (6)	C53—C54—C55—C56	−0.6 (12)
N5—Zn2—N6—C33	−5.1 (5)	N7—C55—C56—C57	−1.0 (13)
N4—Zn2—N6—C33	−15.9 (8)	C54—C55—C56—C57	−179.9 (8)
N13—Zn2—N12—C66	133 (4)	C55—C56—C57—C58	0.6 (14)
N5—Zn2—N12—C66	−45 (4)	C56—C57—C58—C59	−0.4 (15)
N6—Zn2—N12—C66	32 (4)	C55—N7—C59—C58	−1.1 (11)
N4—Zn2—N12—C66	−122 (4)	Zn3—N7—C59—C58	−174.5 (6)
N12—Zn2—N13—C65	−133 (4)	C57—C58—C59—N7	0.7 (14)
N5—Zn2—N13—C65	45 (5)	C64—N9—C60—C61	−2.1 (11)

N6—Zn2—N13—C65	−31 (5)	Zn3—N9—C60—C61	−175.4 (6)
N4—Zn2—N13—C65	123 (4)	C64—N9—C60—C52	−177.4 (7)
C27—C22—C23—C24	−0.4 (15)	Zn3—N9—C60—C52	9.3 (8)
C22—C23—C24—C25	1.5 (14)	N8—C52—C60—N9	−2.3 (9)
C23—C24—C25—C26	−1.8 (13)	C51—C52—C60—N9	179.0 (7)
C23—C24—C25—C28	−178.8 (8)	N8—C52—C60—C61	−177.5 (7)
C24—C25—C26—C27	1.1 (13)	C51—C52—C60—C61	3.8 (11)
C28—C25—C26—C27	178.0 (8)	N9—C60—C61—C62	1.9 (12)
C23—C22—C27—C26	−0.3 (16)	C52—C60—C61—C62	176.8 (7)
C25—C26—C27—C22	−0.1 (15)	C60—C61—C62—C63	−1.4 (13)
C26—C25—C28—C29	−170.9 (8)	C61—C62—C63—C64	1.1 (14)
C24—C25—C28—C29	5.9 (11)	C60—N9—C64—C63	2.0 (13)
C26—C25—C28—C31	13.3 (11)	Zn3—N9—C64—C63	174.6 (8)
C24—C25—C28—C31	−169.9 (7)	C62—C63—C64—N9	−1.5 (15)
C31—C28—C29—C30	−2.9 (10)	Zn3—N15—C67—S6	−106 (11)
C25—C28—C29—C30	−178.9 (7)	Zn3—N14—C68—S5	0 (36)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···S6^{i}	0.93	2.87	3.748 (8)	159
C41—H41···S6^{ii}	0.93	2.82	3.612 (9)	144

Symmetry codes: (i) $x+1/2, -y+1/2, z-1/2$; (ii) $-x+1/2, y-1/2, -z+3/2$.