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(Isoquinoline-2κN)bis[μ-1-(2-oxidobenzylidene)-4-phenylthiosemicarbazonato]-1:2$\kappa^4 S,N,O:O$;1:2$\kappa^4 O:O,N,S$-(quinoline-1κN)dizinc(II) hemiquinoline hemiisoquinoline solvate

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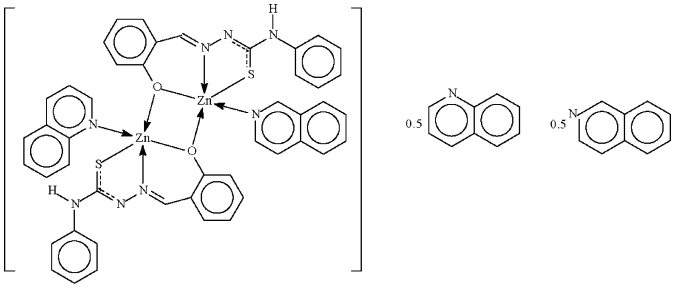
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.059; wR factor = 0.205; data-to-parameter ratio = 20.3.

The deprotonated salicylaldimine-4-phenylthiosemicarbazide dianion chelates in an N,O,S-tridentate manner to zinc in the dinuclear title compound, $[Zn_2(C_{14}H_{11}N_3OS)_2(C_9H_7N)_2]\cdot 0.5C_9H_7N\cdot 0.5C_9H_7N$, which crystallizes with one molecule each of quinoline and isoquinoline in the asymmetric unit; the O atom also bridges the mononuclear units. One Zn atom is coordinated by a quinoline heterocycle in a trigonal–bipyramidal geometry; the other is coordinated by an isoquinoline heterocycle in a square-pyramidal geometry. The two independent dinuclear molecules in the asymmetric unit display similar bond dimensions.

Related literature

For other metal derivatives of *N*-salicyldimine-4-phenylthiosemicarbazide, see: Milanesio *et al.* (2000) for vanadium; Prabhakaran *et al.* (2005) and Soriano-García *et al.* (1985) for nickel; Naik *et al.* (2003) and Thomas *et al.* (2004) for copper.



Experimental

Crystal data

$[Zn_2(C_{14}H_{11}N_3OS)_2(C_9H_7N)_2]\cdot 0.5C_9H_7N\cdot 0.5C_9H_7N$
M_r = 1056.84
Triclinic, $P\overline{1}$
a = 11.1001 (2) Å
b = 21.2080 (5) Å
c = 21.6944 (5) Å
α = 103.5680 (8)°
β = 90.1886 (7)°
γ = 91.6505 (8)°
V = 4962.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 293 (2) K
0.35 × 0.29 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.402, T_{max} = 0.801
49299 measured reflections
22670 independent reflections
15723 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.205
S = 1.05
22670 reflections
1119 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2316).

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supplementary materials

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(Isoquinoline-2κN)bis[μ-1-(2-oxidobenzylidene)-4-phenylthiosemicarbazonato]-1:2$\kappa^4 S,N,O:O$;1:2$\kappa^4 O:O,N,S$-(quinoline-1κN)dizinc(II) hemiquinoline hemiisoquinoline solvate

Z.-P. Deng, S. Gao and S. W. Ng

Comment

The *N*-salicyldimine-4-phenylthiosemicarbazide dianion chelates in a terdentate manner to a number of transition metal ions, but these compounds are mononuclear ones, *e.g.*, the vanadium (Milanesio *et al.*, 2000), nickel (Prabhakaran *et al.*, 2005; Soriano-Garcia *et al.*, 1985), copper (Naik *et al.*, 2003; Thomas *et al.*, 2003). The zinc derivative exists as a dinuclear compound in (I); one zinc site is coordinated by a quinoline in a trigonal bipyramidal geometry whereas the other is coordinated by an isoquinoline in a square pyramidal geometry.

Experimental

N-Salicyldimine-4-phenylthiosemicarbazone was synthesized by condensing salicylaldehyde with 4-phenythiosemicarbazide. Zinc acetate tetrahydrate (1 mmol) and quinoline (1 ml) were added to a methanol solution (15 ml) of the compound (1 mmol). The mixture was heated for 1 h. Yellow crystals were isolated from the solution after a week. C, H & N elemental analysis. Calculated for $C_{55}H_{43}N_9O_2S_2Zn_2$: C 62.50, H 4.10, N 11.93%; found: C 62.48, H 4.14, N 11.90%.

Refinement

Although the synthesis had used quinoline, the crystal structure unambiguously showed the coordination of quinoline as well as isoquinoline to two metal sites. Presumably, the technical-grade quinoline consisted of a large proportion of the other isomer, but this could not be independently verified.

The crystal structure also showed two solvent molecules. These were presumed to be one quinoline and one isoquinoline molecules. They are both each disordered over two sites, and are presumed to be disordered with respect to each other. Each of the six membered rings was refined as rigid hexagons of 1.39 Å sides. The temperature factors of all atoms in each fused-ring were restrained to be the same; the atoms were refined isotropically. Attempts to refine the occupancy factors led to instability and a consideration of the temperature factors resulted in the occupancies being fixed in a 1:2 ratio.

Furthermore, the Zn1 atom is disordered with respect to the Zn1' atom. This occupancy refined to a 0.87 (1):0.13 ratio. The Zn1 atom is coordinated to five atoms in a square-pyramidal enviroment, with the isoquinoline ligand in the apical position. However Zn1' does not bind to the isoquinoline ligand and is coordinated to only four atoms in a square-planar environment.

The carbon- and nitrogen bound H atoms were generated geometrically (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C,*N*).

The final difference Fourier map had a large peak at 2.7 Å from H28.

Figures

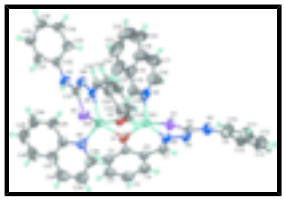


Fig. 1. Thermal ellipsoid plot of one of the two independent dinuclear molecules; displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. The quinoline and isoquinoline solvent molecules and the minor disorder component of the Zn1 atom are not shown.

(Isoquinoline-2κ*N*)bis[μ-1-(2-oxidobenzylidene)-4- phenylthiosemicarbazonato]-1:2κ^4*S*,*N*,*O*:*O*;1:2κ^4*O*:*O*,*N*,*S*-(quinoline- 1κ*N*)dizinc(II) hemiquinoline hemiisoquinoline solvate

Crystal data

$[Zn_2(C_{14}H_{11}N_3OS)_2(C_9H_7N)_2]\cdot 0.5C_9H_7N\cdot 0.5C_9H_7N$	$Z = 4$
$M_r = 1056.84$	$F_{000} = 2176$
Triclinic, $P\overline{1}$	$D_x = 1.415$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.1001$ (2) Å	Cell parameters from 33410 reflections
$b = 21.2080$ (5) Å	$\theta = 3.1$–27.5º
$c = 21.6944$ (5) Å	$\mu = 1.10$ mm^{-1}
$\alpha = 103.5680$ (8)º	$T = 293$ (2) K
$\beta = 90.1886$ (7)º	Block, yellow
$\gamma = 91.6505$ (8)º	0.35 × 0.29 × 0.21 mm
$V = 4962.3$ (2) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	22670 independent reflections
Radiation source: fine-focus sealed tube	15723 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.037$
$T = 295$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -12\rightarrow14$
$T_{min} = 0.402$, $T_{max} = 0.801$	$k = -27\rightarrow27$
49299 measured reflections	$l = -27\rightarrow28$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H-atom parameters constrained
$wR(F^2) = 0.205$	$w = 1/[\sigma^2(F_o^2) + (0.1145P)^2 + 3.0297P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.01$
22670 reflections	$\Delta\rho_{max} = 1.12$ e Å^{-3}
1119 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.72115 (4)	0.23664 (3)	0.53320 (2)	0.04449 (18)	0.8663 (16)
Zn1'	0.7512 (3)	0.29374 (19)	0.52767 (15)	0.0465 (11)	0.1337 (16)
Zn2	0.48642 (4)	0.30194 (2)	0.59473 (2)	0.04593 (13)	
Zn3	0.22034 (4)	0.22651 (2)	1.073283 (19)	0.04117 (12)	
Zn4	−0.01428 (4)	0.29112 (2)	1.041345 (19)	0.03918 (12)	
S1	0.93090 (10)	0.24021 (7)	0.54579 (5)	0.0620 (3)	
S2	0.29298 (9)	0.25700 (7)	0.56429 (5)	0.0594 (3)	
S3	0.42883 (9)	0.22224 (6)	1.05767 (5)	0.0548 (3)	
S4	−0.21091 (9)	0.24885 (6)	1.04974 (5)	0.0518 (3)	
O1	0.5687 (2)	0.27777 (16)	0.50633 (12)	0.0528 (7)	
O2	0.6681 (2)	0.30108 (15)	0.61480 (12)	0.0499 (7)	
O3	0.0671 (2)	0.26625 (14)	1.11791 (11)	0.0436 (6)	
O4	0.1671 (2)	0.28986 (13)	1.02086 (12)	0.0425 (6)	
N1	0.7637 (3)	0.2105 (2)	0.43816 (15)	0.0536 (9)	
N2	0.8760 (3)	0.1830 (2)	0.42137 (16)	0.0562 (9)	
N3	1.0677 (3)	0.1745 (2)	0.45663 (17)	0.0625 (10)	
H3N	1.1166	0.1833	0.4886	0.075*	
N5	0.4615 (3)	0.25449 (17)	0.66868 (15)	0.0469 (8)	
N4	0.6500 (4)	0.1512 (2)	0.55406 (18)	0.0647 (10)	
N6	0.3508 (3)	0.22533 (18)	0.67673 (16)	0.0513 (8)	
N7	0.1597 (3)	0.1985 (2)	0.63502 (17)	0.0598 (10)	
H7N	0.1102	0.2005	0.6050	0.072*	
N8	0.4728 (3)	0.40236 (19)	0.61764 (17)	0.0565 (9)	
N9	0.2654 (3)	0.20194 (16)	1.15674 (14)	0.0431 (7)	
N10	0.3779 (3)	0.17460 (19)	1.16189 (17)	0.0529 (9)	
N11	0.5689 (3)	0.1621 (2)	1.12103 (18)	0.0579 (9)	
H11N	0.6164	0.1681	1.0915	0.069*	
N12	0.1435 (3)	0.14377 (17)	1.01286 (16)	0.0517 (8)	
N13	−0.0243 (3)	0.39203 (16)	1.06756 (15)	0.0436 (7)	
N14	−0.0394 (3)	0.24657 (16)	0.94543 (14)	0.0416 (7)	
N15	−0.1508 (3)	0.21782 (17)	0.92362 (15)	0.0464 (7)	
N16	−0.3409 (3)	0.18983 (19)	0.95085 (16)	0.0531 (9)	
H16N	−0.3902	0.1900	0.9814	0.064*	
C1	0.5260 (3)	0.2778 (2)	0.44866 (17)	0.0449 (9)	
C2	0.4221 (4)	0.3123 (2)	0.4421 (2)	0.0558 (10)	
H2	0.3838	0.3350	0.4782	0.067*	
C3	0.3759 (4)	0.3130 (3)	0.3834 (2)	0.0622 (12)	

H3	0.3068	0.3359	0.3805	0.075*
C4	0.4302 (5)	0.2806 (3)	0.3296 (2)	0.0670 (13)
H4	0.3978	0.2810	0.2901	0.080*
C5	0.5327 (4)	0.2473 (3)	0.3337 (2)	0.0613 (12)
H5	0.5696	0.2256	0.2967	0.074*
C6	0.5836 (4)	0.2452 (2)	0.39314 (18)	0.0493 (9)
C7	0.6972 (4)	0.2135 (2)	0.39089 (18)	0.0518 (10)
H7	0.7247	0.1931	0.3510	0.062*
C8	0.9536 (4)	0.1963 (2)	0.46842 (18)	0.0507 (10)
C9	1.1162 (4)	0.1395 (2)	0.39938 (19)	0.0523 (10)
C10	1.0516 (5)	0.0925 (3)	0.3563 (2)	0.0717 (13)
H10	0.9712	0.0830	0.3632	0.086*
C11	1.1108 (6)	0.0595 (3)	0.3015 (3)	0.0856 (17)
H11	1.0678	0.0279	0.2720	0.103*
C12	1.2274 (6)	0.0718 (3)	0.2901 (3)	0.0801 (16)
H12	1.2641	0.0491	0.2534	0.096*
C13	1.2899 (5)	0.1176 (3)	0.3328 (3)	0.0738 (14)
H13	1.3704	0.1264	0.3252	0.089*
C14	1.2367 (4)	0.1518 (2)	0.3874 (2)	0.0608 (11)
H14	1.2815	0.1832	0.4163	0.073*
C15	0.5349 (5)	0.1344 (3)	0.5432 (2)	0.0681 (13)
H15	0.4884	0.1591	0.5226	0.082*
C16	0.7168 (6)	0.1156 (3)	0.5836 (3)	0.0887 (18)
H16	0.7974	0.1278	0.5922	0.106*
C17	0.6731 (9)	0.0628 (4)	0.6016 (3)	0.110 (2)
H17	0.7237	0.0393	0.6215	0.132*
C18	0.5474 (8)	0.0425 (3)	0.5902 (3)	0.093 (2)
C19	0.4784 (6)	0.0805 (3)	0.5613 (3)	0.0795 (16)
C20	0.3559 (7)	0.0647 (4)	0.5491 (4)	0.116 (3)
H20	0.3079	0.0896	0.5295	0.139*
C21	0.3089 (10)	0.0112 (4)	0.5670 (5)	0.143 (4)
H21	0.2274	0.0007	0.5599	0.171*
C22	0.3751 (13)	−0.0263 (5)	0.5942 (4)	0.138 (4)
H22	0.3404	−0.0629	0.6044	0.165*
C23	0.4937 (12)	−0.0107 (4)	0.6070 (4)	0.139 (4)
H23	0.5393	−0.0361	0.6272	0.167*
C24	0.7187 (3)	0.3057 (2)	0.67205 (17)	0.0455 (9)
C25	0.8342 (4)	0.3335 (2)	0.6844 (2)	0.0535 (10)
H25	0.8749	0.3487	0.6531	0.064*
C26	0.8890 (4)	0.3386 (3)	0.7431 (2)	0.0610 (12)
H26	0.9664	0.3569	0.7507	0.073*
C27	0.8299 (4)	0.3169 (3)	0.7902 (2)	0.0637 (12)
H27	0.8662	0.3214	0.8298	0.076*
C28	0.7175 (4)	0.2888 (2)	0.7783 (2)	0.0565 (11)
H28	0.6791	0.2730	0.8099	0.068*
C29	0.6577 (3)	0.2829 (2)	0.72006 (17)	0.0457 (9)
C30	0.5372 (4)	0.2549 (2)	0.71380 (18)	0.0495 (9)
H30	0.5115	0.2352	0.7457	0.059*
C31	0.2726 (3)	0.2254 (2)	0.63123 (18)	0.0487 (9)

C32	0.1143 (4)	0.1682 (2)	0.68145 (18)	0.0492 (9)
C33	0.1826 (4)	0.1293 (2)	0.7102 (2)	0.0613 (11)
H33	0.2636	0.1232	0.7005	0.074*
C34	0.1281 (5)	0.0996 (3)	0.7538 (2)	0.0676 (13)
H34	0.1736	0.0735	0.7732	0.081*
C35	0.0087 (5)	0.1077 (2)	0.7690 (2)	0.0651 (12)
H35	−0.0263	0.0876	0.7986	0.078*
C36	−0.0573 (5)	0.1454 (3)	0.7402 (2)	0.0660 (12)
H36	−0.1384	0.1510	0.7500	0.079*
C37	−0.0062 (4)	0.1754 (2)	0.6969 (2)	0.0578 (11)
H37	−0.0531	0.2010	0.6775	0.069*
C38	0.5365 (5)	0.4339 (3)	0.5827 (3)	0.0762 (15)
H38	0.5832	0.4095	0.5508	0.091*
C39	0.5390 (6)	0.5003 (3)	0.5898 (3)	0.0932 (19)
H39	0.5846	0.5197	0.5630	0.112*
C40	0.4719 (6)	0.5374 (3)	0.6379 (4)	0.0932 (19)
H40	0.4721	0.5823	0.6440	0.112*
C41	0.4035 (5)	0.5068 (3)	0.6777 (3)	0.0739 (14)
C42	0.4040 (4)	0.4380 (2)	0.6655 (2)	0.0577 (11)
C43	0.3345 (5)	0.4069 (3)	0.7038 (2)	0.0711 (13)
H43	0.3330	0.3619	0.6965	0.085*
C44	0.2689 (6)	0.4425 (3)	0.7519 (3)	0.095 (2)
H44	0.2225	0.4213	0.7768	0.114*
C45	0.2697 (6)	0.5091 (4)	0.7642 (4)	0.101 (2)
H45	0.2248	0.5322	0.7977	0.122*
C46	0.3349 (6)	0.5414 (3)	0.7283 (3)	0.0898 (18)
H46	0.3345	0.5865	0.7370	0.108*
C47	0.0261 (3)	0.26839 (19)	1.17620 (17)	0.0409 (8)
C48	−0.0789 (4)	0.3013 (2)	1.1972 (2)	0.0534 (10)
H48	−0.1194	0.3218	1.1701	0.064*
C49	−0.1241 (4)	0.3042 (3)	1.2565 (2)	0.0678 (13)
H49	−0.1947	0.3261	1.2688	0.081*
C50	−0.0650 (5)	0.2747 (3)	1.2982 (2)	0.0744 (15)
H50	−0.0950	0.2768	1.3386	0.089*
C51	0.0379 (4)	0.2425 (3)	1.2788 (2)	0.0632 (12)
H51	0.0772	0.2223	1.3065	0.076*
C52	0.0865 (4)	0.2388 (2)	1.21861 (17)	0.0463 (9)
C53	0.2011 (3)	0.2076 (2)	1.20699 (18)	0.0471 (9)
H53	0.2313	0.1898	1.2390	0.057*
C54	0.4534 (3)	0.1835 (2)	1.11901 (19)	0.0475 (9)
C55	0.6183 (4)	0.1316 (2)	1.1662 (2)	0.0519 (10)
C56	0.5547 (5)	0.0874 (3)	1.1924 (3)	0.0714 (14)
H56	0.4741	0.0774	1.1815	0.086*
C57	0.6116 (5)	0.0580 (3)	1.2354 (3)	0.0780 (15)
H57	0.5686	0.0288	1.2536	0.094*
C58	0.7320 (6)	0.0722 (3)	1.2510 (3)	0.0790 (16)
H58	0.7698	0.0526	1.2796	0.095*
C59	0.7945 (5)	0.1146 (3)	1.2246 (3)	0.0719 (14)
H59	0.8755	0.1238	1.2348	0.086*

C60	0.7388 (4)	0.1444 (2)	1.1825 (2)	0.0613 (11)
H60	0.7830	0.1735	1.1648	0.074*
C61	0.1569 (7)	0.0599 (3)	0.9186 (3)	0.092 (2)
H61	0.2033	0.0375	0.8854	0.111*
C62	0.2059 (5)	0.1106 (2)	0.9619 (2)	0.0700 (13)
H62	0.2854	0.1234	0.9569	0.084*
C63	0.0296 (4)	0.1255 (2)	1.0181 (2)	0.0558 (10)
H63	−0.0131	0.1479	1.0529	0.067*
C64	−0.0310 (5)	0.0750 (2)	0.9752 (2)	0.0647 (13)
C65	0.0355 (7)	0.0408 (3)	0.9237 (2)	0.0802 (17)
C66	−0.0270 (10)	−0.0115 (3)	0.8801 (3)	0.119 (3)
H66	0.0135	−0.0351	0.8451	0.142*
C67	−0.1420 (11)	−0.0269 (4)	0.8889 (4)	0.130 (4)
H67	−0.1803	−0.0613	0.8604	0.156*
C68	−0.2035 (8)	0.0074 (4)	0.9392 (5)	0.119 (3)
H68	−0.2841	−0.0035	0.9442	0.143*
C69	−0.1507 (5)	0.0569 (3)	0.9821 (3)	0.0881 (18)
H69	−0.1945	0.0791	1.0166	0.106*
C70	0.2170 (3)	0.29656 (18)	0.96682 (17)	0.0389 (8)
C71	0.3339 (3)	0.3238 (2)	0.9673 (2)	0.0478 (9)
H71	0.3763	0.3362	1.0055	0.057*
C72	0.3870 (4)	0.3325 (2)	0.9126 (2)	0.0587 (11)
H72	0.4644	0.3509	0.9145	0.070*
C73	0.3270 (4)	0.3144 (2)	0.8548 (2)	0.0610 (12)
H73	0.3625	0.3213	0.8180	0.073*
C74	0.2132 (4)	0.2858 (2)	0.8529 (2)	0.0548 (10)
H74	0.1739	0.2717	0.8140	0.066*
C75	0.1548 (3)	0.27739 (19)	0.90815 (18)	0.0427 (8)
C76	0.0352 (3)	0.2493 (2)	0.90053 (17)	0.0446 (8)
H76	0.0087	0.2312	0.8593	0.054*
C77	−0.2291 (3)	0.2171 (2)	0.96821 (18)	0.0433 (8)
C78	−0.3858 (3)	0.1616 (2)	0.88974 (18)	0.0459 (9)
C79	−0.3175 (4)	0.1241 (2)	0.8422 (2)	0.0587 (11)
H79	−0.2369	0.1173	0.8496	0.070*
C80	−0.3704 (5)	0.0969 (3)	0.7835 (2)	0.0657 (12)
H80	−0.3247	0.0720	0.7514	0.079*
C81	−0.4908 (5)	0.1065 (3)	0.7722 (2)	0.0692 (13)
H81	−0.5255	0.0882	0.7328	0.083*
C82	−0.5587 (4)	0.1432 (3)	0.8195 (2)	0.0662 (12)
H82	−0.6395	0.1494	0.8120	0.079*
C83	−0.5077 (4)	0.1708 (2)	0.8781 (2)	0.0551 (10)
H83	−0.5543	0.1955	0.9098	0.066*
C84	0.0405 (4)	0.4214 (2)	1.1180 (2)	0.0545 (10)
H84	0.0898	0.3964	1.1368	0.065*
C85	0.0387 (5)	0.4881 (3)	1.1445 (2)	0.0670 (12)
H85	0.0847	0.5067	1.1804	0.080*
C86	−0.0330 (4)	0.5256 (2)	1.1162 (2)	0.0623 (11)
H86	−0.0356	0.5701	1.1330	0.075*
C87	−0.1012 (4)	0.4969 (2)	1.0626 (2)	0.0518 (10)

C88	−0.0962 (4)	0.4288 (2)	1.03892 (18)	0.0457 (9)	
C89	−0.1641 (4)	0.3991 (2)	0.9843 (2)	0.0530 (10)	
H89	−0.1632	0.3544	0.9687	0.064*	
C90	−0.2311 (5)	0.4360 (3)	0.9542 (2)	0.0651 (12)	
H90	−0.2737	0.4163	0.9174	0.078*	
C91	−0.2363 (5)	0.5034 (3)	0.9783 (3)	0.0721 (14)	
H91	−0.2834	0.5278	0.9577	0.086*	
C92	−0.1733 (4)	0.5330 (2)	1.0312 (2)	0.0628 (12)	
H92	−0.1779	0.5776	1.0468	0.075*	
N17	0.6850 (11)	0.4931 (5)	0.7626 (5)	0.097 (2)*	0.33
C93	0.7442 (11)	0.5391 (7)	0.7363 (6)	0.097 (2)*	0.33
H93A	0.8004	0.5261	0.7045	0.117*	0.33
C94	0.7195 (12)	0.6044 (6)	0.7577 (7)	0.097 (2)*	0.33
H94A	0.7592	0.6352	0.7401	0.117*	0.33
C95	0.6356 (13)	0.6239 (4)	0.8052 (7)	0.097 (2)*	0.33
H95A	0.6190	0.6676	0.8195	0.117*	0.33
C96	0.5763 (10)	0.5779 (4)	0.8315 (5)	0.097 (2)*	0.33
C97	0.6010 (9)	0.5126 (4)	0.8102 (4)	0.097 (2)*	0.33
C98	0.5417 (13)	0.4666 (4)	0.8364 (6)	0.097 (2)*	0.33
H98A	0.5583	0.4229	0.8221	0.117*	0.33
C99	0.4578 (13)	0.4860 (6)	0.8840 (7)	0.097 (2)*	0.33
H99A	0.4181	0.4553	0.9015	0.117*	0.33
C100	0.4331 (13)	0.5514 (7)	0.9053 (7)	0.097 (2)*	0.33
H10B	0.3769	0.5644	0.9371	0.117*	0.33
C101	0.4923 (13)	0.5973 (5)	0.8790 (7)	0.097 (2)*	0.33
H10C	0.4758	0.6411	0.8933	0.117*	0.33
C102	0.152 (2)	0.4079 (9)	0.5063 (11)	0.193 (5)*	0.33
H10A	0.1786	0.3940	0.5415	0.232*	0.33
N18	0.098 (2)	0.3637 (8)	0.4554 (13)	0.193 (5)*	0.33
C103	0.0588 (19)	0.3845 (10)	0.4028 (11)	0.193 (5)*	0.33
H10D	0.0227	0.3550	0.3687	0.232*	0.33
C104	0.0733 (19)	0.4494 (11)	0.4011 (8)	0.193 (5)*	0.33
H10E	0.0469	0.4632	0.3658	0.232*	0.33
C105	0.1273 (15)	0.4935 (9)	0.4519 (8)	0.193 (5)*	0.33
C106	0.1667 (14)	0.4728 (9)	0.5046 (8)	0.193 (5)*	0.33
C107	0.2207 (18)	0.5169 (11)	0.5555 (9)	0.193 (5)*	0.33
H10F	0.2471	0.5030	0.5907	0.232*	0.33
C108	0.235 (2)	0.5818 (10)	0.5537 (11)	0.193 (5)*	0.33
H10G	0.2713	0.6113	0.5878	0.232*	0.33
C109	0.196 (2)	0.6025 (8)	0.5011 (13)	0.193 (5)*	0.33
H10H	0.2054	0.6459	0.4999	0.232*	0.33
C110	0.142 (2)	0.5584 (9)	0.4502 (11)	0.193 (5)*	0.33
H11A	0.1153	0.5723	0.4150	0.232*	0.33
N1'	0.6659 (6)	0.4720 (2)	0.7697 (3)	0.0924 (11)*	0.67
C1'	0.7315 (6)	0.5063 (3)	0.7331 (3)	0.0924 (11)*	0.67
H1'A	0.7810	0.4844	0.7012	0.111*	0.67
C2'	0.7231 (6)	0.5732 (3)	0.7444 (3)	0.0924 (11)*	0.67
H2'A	0.7669	0.5962	0.7199	0.111*	0.67
C3'	0.6491 (6)	0.6059 (2)	0.7922 (3)	0.0924 (11)*	0.67

H3'A	0.6434	0.6508	0.7997	0.111*	0.67
C4'	0.5835 (5)	0.57165 (18)	0.8287 (2)	0.0924 (11)*	0.67
C5'	0.5919 (4)	0.50466 (18)	0.8175 (2)	0.0924 (11)*	0.67
C6'	0.5263 (6)	0.4704 (2)	0.8541 (3)	0.0924 (11)*	0.67
H6'A	0.5320	0.4255	0.8465	0.111*	0.67
C7'	0.4523 (6)	0.5031 (3)	0.9019 (3)	0.0924 (11)*	0.67
H7'A	0.4084	0.4801	0.9263	0.111*	0.67
C8'	0.4439 (7)	0.5701 (3)	0.9131 (3)	0.0924 (11)*	0.67
H8'A	0.3944	0.5919	0.9451	0.111*	0.67
C9'	0.5095 (7)	0.6043 (2)	0.8765 (3)	0.0924 (11)*	0.67
H9'A	0.5038	0.6492	0.8840	0.111*	0.67
C10'	0.1398 (9)	0.4546 (6)	0.5855 (5)	0.202 (3)*	0.67
H10I	0.1438	0.4676	0.6295	0.242*	0.67
N2'	0.1191 (9)	0.3896 (6)	0.5560 (7)	0.202 (3)*	0.67
C11'	0.1131 (10)	0.3702 (5)	0.4902 (7)	0.202 (3)*	0.67
H11B	0.0993	0.3266	0.4704	0.242*	0.67
C12'	0.1276 (11)	0.4158 (5)	0.4539 (5)	0.202 (3)*	0.67
H12A	0.1236	0.4028	0.4099	0.242*	0.67
C13'	0.1483 (7)	0.4809 (5)	0.4834 (4)	0.202 (3)*	0.67
C14'	0.1543 (6)	0.5003 (5)	0.5492 (4)	0.202 (3)*	0.67
C15'	0.1749 (10)	0.5653 (5)	0.5787 (5)	0.202 (3)*	0.67
H15A	0.1790	0.5783	0.6227	0.242*	0.67
C16'	0.1895 (11)	0.6110 (4)	0.5424 (7)	0.202 (3)*	0.67
H16A	0.2033	0.6545	0.5622	0.242*	0.67
C17'	0.1835 (12)	0.5916 (5)	0.4767 (7)	0.202 (3)*	0.67
H17A	0.1932	0.6221	0.4524	0.242*	0.67
C18'	0.1628 (11)	0.5265 (6)	0.4472 (5)	0.202 (3)*	0.67
H18B	0.1588	0.5136	0.4031	0.242*	0.67

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0370 (3)	0.0620 (4)	0.0349 (3)	−0.0005 (2)	−0.0035 (2)	0.0126 (2)
Zn1'	0.0370 (17)	0.064 (2)	0.0393 (17)	−0.0038 (15)	−0.0007 (13)	0.0135 (15)
Zn2	0.0371 (2)	0.0613 (3)	0.0401 (2)	−0.0017 (2)	−0.00168 (18)	0.0138 (2)
Zn3	0.0357 (2)	0.0526 (3)	0.0376 (2)	0.00395 (18)	−0.00196 (17)	0.01519 (19)
Zn4	0.0345 (2)	0.0483 (3)	0.0361 (2)	0.00287 (17)	−0.00326 (16)	0.01260 (18)
S1	0.0411 (5)	0.0968 (9)	0.0415 (5)	0.0043 (6)	−0.0064 (4)	0.0031 (5)
S2	0.0421 (5)	0.0946 (9)	0.0470 (5)	−0.0147 (5)	−0.0099 (4)	0.0300 (6)
S3	0.0375 (5)	0.0799 (8)	0.0579 (6)	0.0093 (5)	0.0053 (4)	0.0372 (6)
S4	0.0398 (5)	0.0763 (7)	0.0391 (5)	−0.0091 (5)	−0.0013 (4)	0.0142 (5)
O1	0.0398 (14)	0.086 (2)	0.0336 (13)	0.0004 (14)	−0.0045 (11)	0.0165 (13)
O2	0.0371 (13)	0.077 (2)	0.0330 (12)	0.0008 (13)	−0.0029 (11)	0.0081 (13)
O3	0.0404 (13)	0.0599 (17)	0.0328 (12)	0.0069 (12)	0.0013 (10)	0.0146 (11)
O4	0.0362 (13)	0.0550 (16)	0.0414 (13)	0.0038 (11)	−0.0015 (11)	0.0214 (12)
N1	0.0377 (17)	0.087 (3)	0.0367 (16)	0.0025 (17)	−0.0054 (13)	0.0150 (17)
N2	0.0451 (18)	0.082 (3)	0.0396 (17)	0.0095 (18)	−0.0022 (15)	0.0098 (17)
N3	0.0439 (19)	0.089 (3)	0.0479 (19)	0.0076 (19)	−0.0066 (16)	0.0024 (19)

N5	0.0375 (16)	0.064 (2)	0.0399 (16)	−0.0040 (15)	−0.0054 (13)	0.0147 (15)
N4	0.072 (3)	0.071 (3)	0.050 (2)	−0.002 (2)	−0.0027 (19)	0.0132 (19)
N6	0.0390 (17)	0.072 (2)	0.0457 (18)	−0.0096 (16)	−0.0036 (14)	0.0196 (17)
N7	0.0376 (17)	0.096 (3)	0.054 (2)	−0.0122 (18)	−0.0088 (15)	0.034 (2)
N8	0.0477 (19)	0.067 (2)	0.056 (2)	−0.0025 (17)	0.0006 (16)	0.0167 (18)
N9	0.0350 (15)	0.058 (2)	0.0409 (16)	0.0058 (14)	−0.0017 (13)	0.0207 (15)
N10	0.0400 (17)	0.072 (2)	0.0552 (19)	0.0109 (16)	0.0001 (15)	0.0308 (18)
N11	0.0379 (17)	0.082 (3)	0.066 (2)	0.0148 (17)	0.0073 (16)	0.039 (2)
N12	0.059 (2)	0.052 (2)	0.0450 (17)	−0.0022 (16)	−0.0031 (16)	0.0150 (15)
N13	0.0380 (16)	0.0482 (18)	0.0460 (17)	0.0029 (13)	−0.0046 (13)	0.0141 (14)
N14	0.0344 (15)	0.0487 (18)	0.0426 (16)	0.0020 (13)	−0.0010 (13)	0.0126 (14)
N15	0.0360 (16)	0.062 (2)	0.0397 (16)	−0.0053 (14)	−0.0037 (13)	0.0094 (15)
N16	0.0351 (16)	0.080 (3)	0.0414 (17)	−0.0078 (16)	−0.0004 (14)	0.0106 (17)
C1	0.0389 (19)	0.061 (2)	0.0387 (18)	−0.0073 (17)	−0.0058 (15)	0.0201 (17)
C2	0.050 (2)	0.067 (3)	0.055 (2)	−0.001 (2)	−0.0053 (19)	0.024 (2)
C3	0.055 (3)	0.076 (3)	0.062 (3)	−0.001 (2)	−0.016 (2)	0.031 (2)
C4	0.068 (3)	0.089 (4)	0.050 (2)	−0.003 (3)	−0.022 (2)	0.032 (2)
C5	0.061 (3)	0.083 (3)	0.039 (2)	−0.002 (2)	−0.0107 (19)	0.016 (2)
C6	0.048 (2)	0.066 (3)	0.0361 (18)	−0.0069 (19)	−0.0087 (16)	0.0162 (18)
C7	0.050 (2)	0.067 (3)	0.0353 (18)	0.000 (2)	−0.0037 (17)	0.0083 (18)
C8	0.041 (2)	0.072 (3)	0.0392 (19)	0.0006 (19)	0.0010 (16)	0.0124 (19)
C9	0.054 (2)	0.058 (3)	0.044 (2)	0.0085 (19)	−0.0031 (18)	0.0107 (19)
C10	0.065 (3)	0.076 (3)	0.065 (3)	−0.003 (3)	−0.008 (2)	0.000 (3)
C11	0.104 (5)	0.074 (4)	0.067 (3)	0.010 (3)	−0.018 (3)	−0.008 (3)
C12	0.099 (4)	0.078 (4)	0.062 (3)	0.032 (3)	0.012 (3)	0.010 (3)
C13	0.072 (3)	0.080 (4)	0.073 (3)	0.020 (3)	0.022 (3)	0.023 (3)
C14	0.056 (3)	0.064 (3)	0.062 (3)	0.005 (2)	0.004 (2)	0.014 (2)
C15	0.074 (3)	0.063 (3)	0.065 (3)	0.001 (2)	0.002 (2)	0.011 (2)
C16	0.107 (5)	0.083 (4)	0.080 (4)	−0.006 (3)	−0.033 (3)	0.029 (3)
C17	0.165 (8)	0.091 (5)	0.082 (4)	0.021 (5)	−0.019 (5)	0.036 (4)
C18	0.158 (7)	0.070 (4)	0.047 (3)	−0.012 (4)	0.003 (3)	0.009 (3)
C19	0.098 (4)	0.065 (3)	0.069 (3)	−0.005 (3)	0.026 (3)	0.003 (3)
C20	0.105 (5)	0.110 (6)	0.117 (6)	−0.034 (4)	0.037 (5)	0.000 (4)
C21	0.168 (9)	0.097 (6)	0.136 (8)	−0.055 (6)	0.076 (7)	−0.022 (5)
C22	0.231 (13)	0.087 (6)	0.087 (5)	−0.054 (7)	0.046 (7)	0.011 (4)
C23	0.263 (13)	0.079 (5)	0.075 (4)	−0.021 (7)	0.035 (7)	0.017 (4)
C24	0.0371 (18)	0.058 (2)	0.0372 (18)	0.0030 (17)	−0.0051 (15)	0.0022 (17)
C25	0.040 (2)	0.066 (3)	0.048 (2)	−0.0026 (19)	−0.0059 (17)	0.0018 (19)
C26	0.042 (2)	0.079 (3)	0.053 (2)	−0.002 (2)	−0.0169 (19)	−0.002 (2)
C27	0.058 (3)	0.079 (3)	0.048 (2)	−0.002 (2)	−0.027 (2)	0.004 (2)
C28	0.054 (2)	0.073 (3)	0.043 (2)	0.003 (2)	−0.0105 (18)	0.016 (2)
C29	0.042 (2)	0.055 (2)	0.0387 (18)	0.0018 (17)	−0.0098 (16)	0.0090 (17)
C30	0.050 (2)	0.060 (3)	0.0386 (19)	−0.0013 (19)	−0.0058 (17)	0.0112 (18)
C31	0.0399 (19)	0.064 (3)	0.043 (2)	−0.0064 (18)	−0.0036 (16)	0.0154 (18)
C32	0.043 (2)	0.061 (3)	0.042 (2)	−0.0090 (18)	−0.0063 (17)	0.0111 (18)
C33	0.046 (2)	0.073 (3)	0.067 (3)	−0.004 (2)	−0.002 (2)	0.024 (2)
C34	0.076 (3)	0.065 (3)	0.067 (3)	−0.003 (2)	−0.013 (3)	0.027 (2)
C35	0.075 (3)	0.065 (3)	0.058 (3)	−0.015 (2)	0.003 (2)	0.022 (2)
C36	0.058 (3)	0.080 (3)	0.062 (3)	−0.008 (2)	0.009 (2)	0.022 (3)

C37	0.049 (2)	0.071 (3)	0.055 (2)	−0.005 (2)	−0.0036 (19)	0.018 (2)
C38	0.076 (3)	0.080 (4)	0.073 (3)	−0.014 (3)	0.013 (3)	0.021 (3)
C39	0.098 (5)	0.079 (4)	0.106 (5)	−0.013 (3)	0.014 (4)	0.031 (4)
C40	0.095 (4)	0.063 (4)	0.124 (5)	−0.006 (3)	−0.011 (4)	0.030 (4)
C41	0.064 (3)	0.067 (3)	0.089 (4)	0.007 (2)	−0.005 (3)	0.014 (3)
C42	0.048 (2)	0.064 (3)	0.059 (3)	0.004 (2)	−0.007 (2)	0.009 (2)
C43	0.068 (3)	0.076 (3)	0.070 (3)	0.009 (3)	0.011 (3)	0.017 (3)
C44	0.100 (5)	0.094 (5)	0.094 (4)	0.028 (4)	0.037 (4)	0.023 (4)
C45	0.089 (4)	0.101 (5)	0.106 (5)	0.025 (4)	0.017 (4)	0.003 (4)
C46	0.082 (4)	0.070 (4)	0.108 (5)	0.019 (3)	−0.008 (4)	0.001 (3)
C47	0.0385 (18)	0.049 (2)	0.0352 (17)	0.0017 (16)	0.0002 (14)	0.0089 (15)
C48	0.047 (2)	0.065 (3)	0.048 (2)	0.0135 (19)	0.0022 (18)	0.013 (2)
C49	0.055 (3)	0.098 (4)	0.054 (2)	0.026 (3)	0.015 (2)	0.023 (3)
C50	0.069 (3)	0.110 (4)	0.050 (3)	0.017 (3)	0.020 (2)	0.029 (3)
C51	0.063 (3)	0.088 (4)	0.046 (2)	0.014 (2)	0.008 (2)	0.031 (2)
C52	0.046 (2)	0.058 (2)	0.0374 (18)	0.0023 (18)	0.0006 (16)	0.0154 (17)
C53	0.044 (2)	0.057 (2)	0.044 (2)	0.0057 (18)	−0.0027 (17)	0.0206 (18)
C54	0.0399 (19)	0.059 (2)	0.048 (2)	0.0075 (17)	−0.0022 (17)	0.0206 (19)
C55	0.052 (2)	0.057 (3)	0.052 (2)	0.0149 (19)	0.0038 (19)	0.021 (2)
C56	0.058 (3)	0.074 (3)	0.092 (4)	0.009 (2)	−0.001 (3)	0.041 (3)
C57	0.080 (4)	0.084 (4)	0.084 (4)	0.013 (3)	−0.001 (3)	0.048 (3)
C58	0.095 (4)	0.083 (4)	0.065 (3)	0.034 (3)	−0.008 (3)	0.025 (3)
C59	0.061 (3)	0.079 (4)	0.076 (3)	0.017 (3)	−0.017 (3)	0.018 (3)
C60	0.049 (2)	0.072 (3)	0.067 (3)	0.004 (2)	−0.007 (2)	0.023 (2)
C61	0.141 (6)	0.077 (4)	0.054 (3)	−0.005 (4)	0.018 (3)	0.008 (3)
C62	0.088 (4)	0.061 (3)	0.055 (3)	0.000 (3)	0.014 (3)	0.003 (2)
C63	0.063 (3)	0.049 (2)	0.057 (2)	0.002 (2)	−0.008 (2)	0.015 (2)
C64	0.081 (3)	0.050 (3)	0.068 (3)	−0.004 (2)	−0.029 (3)	0.026 (2)
C65	0.137 (6)	0.054 (3)	0.050 (3)	−0.012 (3)	−0.019 (3)	0.014 (2)
C66	0.217 (10)	0.068 (4)	0.066 (4)	−0.029 (5)	−0.049 (5)	0.011 (3)
C67	0.205 (11)	0.070 (5)	0.113 (6)	−0.049 (6)	−0.091 (7)	0.025 (4)
C68	0.130 (7)	0.084 (5)	0.149 (7)	−0.049 (5)	−0.070 (6)	0.046 (5)
C69	0.075 (4)	0.073 (4)	0.119 (5)	−0.018 (3)	−0.037 (3)	0.032 (4)
C70	0.0358 (18)	0.041 (2)	0.0427 (18)	0.0052 (15)	−0.0001 (15)	0.0158 (16)
C71	0.0356 (18)	0.054 (2)	0.058 (2)	0.0005 (17)	−0.0002 (17)	0.0206 (19)
C72	0.045 (2)	0.064 (3)	0.073 (3)	0.000 (2)	0.009 (2)	0.028 (2)
C73	0.052 (2)	0.078 (3)	0.058 (3)	0.002 (2)	0.018 (2)	0.027 (2)
C74	0.054 (2)	0.069 (3)	0.042 (2)	0.004 (2)	0.0079 (18)	0.015 (2)
C75	0.0383 (19)	0.048 (2)	0.0431 (19)	0.0015 (16)	0.0033 (16)	0.0140 (17)
C76	0.044 (2)	0.055 (2)	0.0355 (17)	0.0047 (17)	0.0011 (16)	0.0112 (16)
C77	0.0358 (18)	0.051 (2)	0.0427 (19)	0.0002 (16)	−0.0050 (15)	0.0105 (17)
C78	0.043 (2)	0.055 (2)	0.0400 (19)	−0.0065 (17)	−0.0021 (16)	0.0131 (17)
C79	0.049 (2)	0.066 (3)	0.058 (2)	−0.002 (2)	−0.002 (2)	0.008 (2)
C80	0.068 (3)	0.067 (3)	0.054 (3)	−0.009 (2)	0.006 (2)	0.000 (2)
C81	0.077 (3)	0.070 (3)	0.056 (3)	−0.010 (3)	−0.014 (2)	0.006 (2)
C82	0.055 (3)	0.080 (3)	0.063 (3)	0.001 (2)	−0.018 (2)	0.015 (2)
C83	0.046 (2)	0.066 (3)	0.051 (2)	−0.002 (2)	−0.0067 (18)	0.009 (2)
C84	0.053 (2)	0.058 (3)	0.054 (2)	−0.003 (2)	−0.0111 (19)	0.016 (2)
C85	0.068 (3)	0.066 (3)	0.060 (3)	−0.007 (2)	−0.016 (2)	0.004 (2)

C86	0.068 (3)	0.048 (3)	0.066 (3)	0.002 (2)	0.005 (2)	0.004 (2)
C87	0.051 (2)	0.051 (2)	0.054 (2)	0.0044 (18)	0.0091 (19)	0.0122 (19)
C88	0.048 (2)	0.048 (2)	0.0426 (19)	0.0077 (17)	0.0048 (17)	0.0136 (17)
C89	0.053 (2)	0.051 (2)	0.055 (2)	0.0101 (19)	−0.0048 (19)	0.0123 (19)
C90	0.069 (3)	0.070 (3)	0.059 (3)	0.015 (2)	−0.015 (2)	0.019 (2)
C91	0.072 (3)	0.071 (3)	0.081 (3)	0.023 (3)	−0.005 (3)	0.032 (3)
C92	0.062 (3)	0.052 (3)	0.079 (3)	0.019 (2)	0.006 (2)	0.021 (2)

Geometric parameters (Å, °)

Zn1—Zn1'	1.279 (4)	C49—H49	0.9300
Zn1—O2	2.065 (3)	C50—C51	1.364 (7)
Zn1—N1	2.066 (3)	C50—H50	0.9300
Zn1—O1	2.069 (3)	C51—C52	1.400 (5)
Zn1—N4	2.102 (4)	C51—H51	0.9300
Zn1—S1	2.3403 (12)	C52—C53	1.445 (6)
Zn1—Zn2	3.1388 (7)	C53—H53	0.9300
Zn2—O2	2.064 (3)	C55—C60	1.386 (6)
Zn2—N8	2.080 (4)	C55—C56	1.384 (6)
Zn2—O1	2.086 (3)	C56—C57	1.396 (7)
Zn2—N5	2.099 (3)	C56—H56	0.9300
Zn2—S2	2.3522 (11)	C57—C58	1.385 (8)
Zn3—O4	2.051 (2)	C57—H57	0.9300
Zn3—O3	2.062 (2)	C58—C59	1.352 (8)
Zn3—N9	2.062 (3)	C58—H58	0.9300
Zn3—N12	2.086 (4)	C59—C60	1.378 (6)
Zn3—S3	2.3413 (11)	C59—H59	0.9300
Zn3—Zn4	3.1272 (6)	C60—H60	0.9300
Zn4—O4	2.063 (2)	C61—C62	1.351 (8)
Zn4—O3	2.069 (2)	C61—C65	1.407 (9)
Zn4—N14	2.088 (3)	C61—H61	0.9300
Zn4—N13	2.088 (3)	C62—H62	0.9300
Zn4—S4	2.3595 (10)	C63—C64	1.398 (7)
S1—C8	1.741 (4)	C63—H63	0.9300
S2—C31	1.749 (4)	C64—C69	1.392 (8)
S3—C54	1.745 (4)	C64—C65	1.405 (8)
S4—C77	1.747 (4)	C65—C66	1.439 (9)
O1—C1	1.337 (4)	C66—C67	1.333 (13)
O2—C24	1.343 (4)	C66—H66	0.9300
O3—C47	1.337 (4)	C67—C68	1.361 (13)
O4—C70	1.334 (4)	C67—H67	0.9300
N1—C7	1.276 (5)	C68—C69	1.347 (9)
N1—N2	1.403 (5)	C68—H68	0.9300
N2—C8	1.307 (5)	C69—H69	0.9300
N3—C8	1.366 (5)	C70—C71	1.404 (5)
N3—C9	1.406 (5)	C70—C75	1.413 (5)
N3—H3N	0.8600	C71—C72	1.375 (6)
N5—C30	1.286 (5)	C71—H71	0.9300
N5—N6	1.390 (4)	C72—C73	1.386 (7)

N4—C15	1.322 (7)	C72—H72	0.9300
N4—C16	1.337 (7)	C73—C74	1.381 (6)
N6—C31	1.313 (5)	C73—H73	0.9300
N7—C31	1.373 (5)	C74—C75	1.410 (5)
N7—C32	1.404 (5)	C74—H74	0.9300
N7—H7N	0.8600	C75—C76	1.433 (5)
N8—C38	1.318 (6)	C76—H76	0.9300
N8—C42	1.379 (6)	C78—C79	1.387 (6)
N9—C53	1.289 (5)	C78—C83	1.404 (6)
N9—N10	1.407 (4)	C79—C80	1.391 (6)
N10—C54	1.297 (5)	C79—H79	0.9300
N11—C54	1.376 (5)	C80—C81	1.387 (7)
N11—C55	1.412 (5)	C80—H80	0.9300
N11—H11N	0.8600	C81—C82	1.376 (7)
N12—C63	1.325 (6)	C81—H81	0.9300
N12—C62	1.366 (6)	C82—C83	1.379 (6)
N13—C84	1.324 (5)	C82—H82	0.9300
N13—C88	1.376 (5)	C83—H83	0.9300
N14—C76	1.291 (5)	C84—C85	1.396 (7)
N14—N15	1.393 (4)	C84—H84	0.9300
N15—C77	1.305 (5)	C85—C86	1.382 (7)
N16—C77	1.367 (5)	C85—H85	0.9300
N16—C78	1.404 (5)	C86—C87	1.390 (7)
N16—H16N	0.8600	C86—H86	0.9300
C1—C2	1.408 (6)	C87—C92	1.401 (6)
C1—C6	1.406 (6)	C87—C88	1.418 (6)
C2—C3	1.373 (6)	C88—C89	1.410 (6)
C2—H2	0.9300	C89—C90	1.363 (6)
C3—C4	1.361 (7)	C89—H89	0.9300
C3—H3	0.9300	C90—C91	1.404 (7)
C4—C5	1.369 (7)	C90—H90	0.9300
C4—H4	0.9300	C91—C92	1.353 (7)
C5—C6	1.417 (5)	C91—H91	0.9300
C5—H5	0.9300	C92—H92	0.9300
C6—C7	1.441 (6)	N17—C93	1.3900
C7—H7	0.9300	N17—C97	1.3900
C9—C10	1.378 (7)	C93—C94	1.3900
C9—C14	1.393 (6)	C93—H93A	0.9300
C10—C11	1.405 (8)	C94—C95	1.3900
C10—H10	0.9300	C94—H94A	0.9300
C11—C12	1.349 (9)	C95—C96	1.3900
C11—H11	0.9300	C95—H95A	0.9300
C12—C13	1.348 (8)	C96—C97	1.3900
C12—H12	0.9300	C96—C101	1.3900
C13—C14	1.381 (7)	C97—C98	1.3900
C13—H13	0.9300	C98—C99	1.3900
C14—H14	0.9300	C98—H98A	0.9300
C15—C19	1.424 (7)	C99—C100	1.3900
C15—H15	0.9300	C99—H99A	0.9300

C16—C17	1.348 (9)	C100—C101	1.3900
C16—H16	0.9300	C100—H10B	0.9300
C17—C18	1.451 (11)	C101—H10C	0.9300
C17—H17	0.9300	C102—N18	1.3900
C18—C19	1.378 (9)	C102—C106	1.3900
C18—C23	1.383 (10)	C102—H10A	0.9300
C19—C20	1.400 (9)	N18—C103	1.3900
C20—C21	1.372 (11)	C103—C104	1.3900
C20—H20	0.9300	C103—H10D	0.9300
C21—C22	1.330 (15)	C104—C105	1.3900
C21—H21	0.9300	C104—H10E	0.9300
C22—C23	1.360 (15)	C105—C106	1.3900
C22—H22	0.9300	C105—C110	1.3900
C23—H23	0.9300	C106—C107	1.3900
C24—C25	1.394 (5)	C107—C108	1.3900
C24—C29	1.414 (6)	C107—H10F	0.9300
C25—C26	1.390 (6)	C108—C109	1.3900
C25—H25	0.9300	C108—H10G	0.9300
C26—C27	1.376 (7)	C109—C110	1.3900
C26—H26	0.9300	C109—H10H	0.9300
C27—C28	1.366 (6)	C110—H11A	0.9300
C27—H27	0.9300	N1'—C1'	1.3900
C28—C29	1.402 (5)	N1'—C5'	1.3900
C28—H28	0.9300	C1'—C2'	1.3900
C29—C30	1.441 (6)	C1'—H1'A	0.9300
C30—H30	0.9300	C2'—C3'	1.3900
C32—C37	1.384 (6)	C2'—H2'A	0.9300
C32—C33	1.386 (6)	C3'—C4'	1.3900
C33—C34	1.383 (6)	C3'—H3'A	0.9300
C33—H33	0.9300	C4'—C5'	1.3900
C34—C35	1.373 (7)	C4'—C9'	1.3900
C34—H34	0.9300	C5'—C6'	1.3900
C35—C36	1.353 (7)	C6'—C7'	1.3900
C35—H35	0.9300	C6'—H6'A	0.9300
C36—C37	1.370 (6)	C7'—C8'	1.3900
C36—H36	0.9300	C7'—H7'A	0.9300
C37—H37	0.9300	C8'—C9'	1.3900
C38—C39	1.381 (8)	C8'—H8'A	0.9300
C38—H38	0.9300	C9'—H9'A	0.9300
C39—C40	1.384 (9)	C10'—N2'	1.3900
C39—H39	0.9300	C10'—C14'	1.3900
C40—C41	1.406 (8)	C10'—H10I	0.9300
C40—H40	0.9300	N2'—C11'	1.3900
C41—C46	1.409 (8)	C11'—C12'	1.3900
C41—C42	1.422 (7)	C11'—H11B	0.9300
C42—C43	1.397 (7)	C12'—C13'	1.3900
C43—C44	1.361 (7)	C12'—H12A	0.9300
C43—H43	0.9300	C13'—C14'	1.3900
C44—C45	1.374 (9)	C13'—C18'	1.3900

C44—H44	0.9300	C14'—C15'	1.3900
C45—C46	1.351 (9)	C15'—C16'	1.3900
C45—H45	0.9300	C15'—H15A	0.9300
C46—H46	0.9300	C16'—C17'	1.3900
C47—C48	1.398 (5)	C16'—H16A	0.9300
C47—C52	1.408 (5)	C17'—C18'	1.3900
C48—C49	1.370 (6)	C17'—H17A	0.9300
C48—H48	0.9300	C18'—H18B	0.9300
C49—C50	1.389 (7)		
Zn1'—Zn1—O2	72.67 (17)	C46—C45—H45	119.6
Zn1'—Zn1—N1	83.57 (19)	C44—C45—H45	119.6
O2—Zn1—N1	153.81 (14)	C45—C46—C41	120.0 (6)
Zn1'—Zn1—O1	72.35 (17)	C45—C46—H46	120.0
O2—Zn1—O1	75.49 (11)	C41—C46—H46	120.0
N1—Zn1—O1	87.10 (12)	O3—C47—C48	120.3 (3)
Zn1'—Zn1—N4	169.91 (19)	O3—C47—C52	121.9 (3)
O2—Zn1—N4	97.92 (14)	C48—C47—C52	117.7 (3)
N1—Zn1—N4	104.88 (16)	C49—C48—C47	122.0 (4)
O1—Zn1—N4	102.17 (15)	C49—C48—H48	119.0
Zn1'—Zn1—S1	76.90 (16)	C47—C48—H48	119.0
O2—Zn1—S1	102.00 (8)	C48—C49—C50	120.4 (4)
N1—Zn1—S1	82.65 (9)	C48—C49—H49	119.8
O1—Zn1—S1	148.46 (9)	C50—C49—H49	119.8
N4—Zn1—S1	109.27 (13)	C51—C50—C49	118.6 (4)
Zn1'—Zn1—Zn2	84.53 (15)	C51—C50—H50	120.7
O2—Zn1—Zn2	40.50 (7)	C49—C50—H50	120.7
N1—Zn1—Zn2	127.95 (9)	C50—C51—C52	122.4 (4)
O1—Zn1—Zn2	41.15 (7)	C50—C51—H51	118.8
N4—Zn1—Zn2	85.88 (12)	C52—C51—H51	118.8
S1—Zn1—Zn2	142.20 (4)	C51—C52—C47	118.8 (4)
O2—Zn2—N8	96.29 (13)	C51—C52—C53	115.8 (4)
O2—Zn2—O1	75.16 (10)	C47—C52—C53	125.3 (3)
N8—Zn2—O1	106.41 (13)	N9—C53—C52	126.5 (3)
O2—Zn2—N5	85.80 (11)	N9—C53—H53	116.7
N8—Zn2—N5	116.88 (14)	C52—C53—H53	116.7
O1—Zn2—N5	134.27 (13)	N10—C54—N11	118.7 (3)
O2—Zn2—S2	156.31 (10)	N10—C54—S3	127.8 (3)
N8—Zn2—S2	107.37 (11)	N11—C54—S3	113.5 (3)
O1—Zn2—S2	98.58 (8)	C60—C55—C56	118.5 (4)
N5—Zn2—S2	82.59 (9)	C60—C55—N11	117.8 (4)
O2—Zn2—Zn1	40.54 (7)	C56—C55—N11	123.6 (4)
N8—Zn2—Zn1	120.87 (10)	C55—C56—C57	119.9 (5)
O1—Zn2—Zn1	40.73 (8)	C55—C56—H56	120.1
N5—Zn2—Zn1	100.60 (9)	C57—C56—H56	120.1
S2—Zn2—Zn1	122.10 (4)	C56—C57—C58	120.1 (5)
O4—Zn3—O3	75.88 (10)	C56—C57—H57	120.0
O4—Zn3—N9	153.59 (13)	C58—C57—H57	120.0
O3—Zn3—N9	87.39 (11)	C59—C58—C57	119.9 (5)
O4—Zn3—N12	95.64 (12)	C59—C58—H58	120.0

O3—Zn3—N12	99.50 (13)	C57—C58—H58	120.0
N9—Zn3—N12	107.32 (13)	C58—C59—C60	120.4 (5)
O4—Zn3—S3	103.30 (7)	C58—C59—H59	119.8
O3—Zn3—S3	153.57 (9)	C60—C59—H59	119.8
N9—Zn3—S3	82.72 (9)	C59—C60—C55	121.1 (5)
N12—Zn3—S3	106.83 (11)	C59—C60—H60	119.4
O4—Zn3—Zn4	40.67 (7)	C55—C60—H60	119.4
O3—Zn3—Zn4	40.89 (7)	C62—C61—C65	120.0 (6)
N9—Zn3—Zn4	128.12 (9)	C62—C61—H61	120.0
N12—Zn3—Zn4	83.40 (10)	C65—C61—H61	120.0
S3—Zn3—Zn4	143.93 (3)	C61—C62—N12	122.6 (5)
O4—Zn4—O3	75.45 (9)	C61—C62—H62	118.7
O4—Zn4—N14	85.41 (11)	N12—C62—H62	118.7
O3—Zn4—N14	135.30 (11)	N12—C63—C64	124.6 (5)
O4—Zn4—N13	95.79 (12)	N12—C63—H63	117.7
O3—Zn4—N13	104.84 (12)	C64—C63—H63	117.7
N14—Zn4—N13	117.17 (12)	C69—C64—C63	123.2 (6)
O4—Zn4—S4	157.53 (9)	C69—C64—C65	119.8 (5)
O3—Zn4—S4	99.71 (8)	C63—C64—C65	117.0 (5)
N14—Zn4—S4	83.02 (9)	C64—C65—C61	118.3 (5)
N13—Zn4—S4	106.63 (9)	C64—C65—C66	116.6 (7)
O4—Zn4—Zn3	40.37 (7)	C61—C65—C66	125.1 (7)
O3—Zn4—Zn3	40.71 (7)	C67—C66—C65	121.2 (8)
N14—Zn4—Zn3	101.58 (8)	C67—C66—H66	119.4
N13—Zn4—Zn3	118.96 (9)	C65—C66—H66	119.4
S4—Zn4—Zn3	124.14 (3)	C66—C67—C68	120.4 (7)
C8—S1—Zn1	93.11 (14)	C66—C67—H67	119.8
C31—S2—Zn2	94.85 (14)	C68—C67—H67	119.8
C54—S3—Zn3	93.71 (13)	C69—C68—C67	121.6 (8)
C77—S4—Zn4	94.44 (13)	C69—C68—H68	119.2
C1—O1—Zn1	130.4 (3)	C67—C68—H68	119.2
C1—O1—Zn2	130.5 (2)	C68—C69—C64	120.3 (8)
Zn1—O1—Zn2	98.12 (10)	C68—C69—H69	119.9
C24—O2—Zn2	126.6 (2)	C64—C69—H69	119.9
C24—O2—Zn1	123.8 (2)	O4—C70—C71	120.0 (3)
Zn2—O2—Zn1	98.96 (11)	O4—C70—C75	121.7 (3)
C47—O3—Zn3	130.8 (2)	C71—C70—C75	118.2 (3)
C47—O3—Zn4	130.4 (2)	C72—C71—C70	121.5 (4)
Zn3—O3—Zn4	98.40 (10)	C72—C71—H71	119.3
C70—O4—Zn3	125.4 (2)	C70—C71—H71	119.3
C70—O4—Zn4	126.6 (2)	C71—C72—C73	121.1 (4)
Zn3—O4—Zn4	98.96 (10)	C71—C72—H72	119.5
C7—N1—N2	114.0 (3)	C73—C72—H72	119.5
C7—N1—Zn1	127.7 (3)	C74—C73—C72	118.4 (4)
N2—N1—Zn1	118.2 (2)	C74—C73—H73	120.8
C8—N2—N1	112.5 (3)	C72—C73—H73	120.8
C8—N3—C9	128.8 (4)	C73—C74—C75	122.1 (4)
C8—N3—H3N	115.6	C73—C74—H74	119.0
C9—N3—H3N	115.6	C75—C74—H74	119.0

C30—N5—N6	113.3 (3)	C70—C75—C74	118.7 (4)
C30—N5—Zn2	125.8 (3)	C70—C75—C76	124.3 (3)
N6—N5—Zn2	120.5 (2)	C74—C75—C76	117.0 (4)
C15—N4—C16	118.2 (5)	N14—C76—C75	126.3 (4)
C15—N4—Zn1	120.5 (4)	N14—C76—H76	116.9
C16—N4—Zn1	121.0 (4)	C75—C76—H76	116.9
C31—N6—N5	113.6 (3)	N15—C77—N16	118.1 (3)
C31—N7—C32	128.6 (3)	N15—C77—S4	127.9 (3)
C31—N7—H7N	115.7	N16—C77—S4	114.0 (3)
C32—N7—H7N	115.7	C79—C78—N16	123.5 (4)
C38—N8—C42	118.1 (4)	C79—C78—C83	119.5 (4)
C38—N8—Zn2	115.9 (4)	N16—C78—C83	116.9 (4)
C42—N8—Zn2	126.0 (3)	C78—C79—C80	119.5 (4)
C53—N9—N10	113.2 (3)	C78—C79—H79	120.2
C53—N9—Zn3	127.7 (3)	C80—C79—H79	120.2
N10—N9—Zn3	119.1 (2)	C81—C80—C79	120.6 (5)
C54—N10—N9	113.0 (3)	C81—C80—H80	119.7
C54—N11—C55	127.3 (3)	C79—C80—H80	119.7
C54—N11—H11N	116.4	C82—C81—C80	119.8 (5)
C55—N11—H11N	116.4	C82—C81—H81	120.1
C63—N12—C62	117.5 (4)	C80—C81—H81	120.1
C63—N12—Zn3	121.8 (3)	C83—C82—C81	120.5 (5)
C62—N12—Zn3	120.3 (3)	C83—C82—H82	119.8
C84—N13—C88	118.7 (4)	C81—C82—H82	119.8
C84—N13—Zn4	115.8 (3)	C82—C83—C78	120.1 (4)
C88—N13—Zn4	125.4 (3)	C82—C83—H83	120.0
C76—N14—N15	113.5 (3)	C78—C83—H83	120.0
C76—N14—Zn4	125.9 (3)	N13—C84—C85	123.5 (4)
N15—N14—Zn4	120.0 (2)	N13—C84—H84	118.2
C77—N15—N14	114.3 (3)	C85—C84—H84	118.2
C77—N16—C78	128.5 (3)	C86—C85—C84	118.4 (4)
C77—N16—H16N	115.7	C86—C85—H85	120.8
C78—N16—H16N	115.7	C84—C85—H85	120.8
O1—C1—C2	120.2 (4)	C87—C86—C85	120.1 (4)
O1—C1—C6	121.8 (4)	C87—C86—H86	120.0
C2—C1—C6	117.9 (3)	C85—C86—H86	120.0
C3—C2—C1	121.5 (4)	C86—C87—C92	122.4 (4)
C3—C2—H2	119.3	C86—C87—C88	118.3 (4)
C1—C2—H2	119.3	C92—C87—C88	119.3 (4)
C4—C3—C2	120.7 (5)	N13—C88—C89	120.0 (4)
C4—C3—H3	119.6	N13—C88—C87	121.0 (4)
C2—C3—H3	119.6	C89—C88—C87	118.9 (4)
C3—C4—C5	119.8 (4)	C90—C89—C88	120.0 (4)
C3—C4—H4	120.1	C90—C89—H89	120.0
C5—C4—H4	120.1	C88—C89—H89	120.0
C4—C5—C6	121.4 (4)	C89—C90—C91	120.6 (5)
C4—C5—H5	119.3	C89—C90—H90	119.7
C6—C5—H5	119.3	C91—C90—H90	119.7
C1—C6—C5	118.6 (4)	C92—C91—C90	120.6 (4)

C1—C6—C7	125.4 (3)	C92—C91—H91	119.7
C5—C6—C7	115.8 (4)	C90—C91—H91	119.7
N1—C7—C6	126.6 (4)	C91—C92—C87	120.5 (5)
N1—C7—H7	116.7	C91—C92—H92	119.7
C6—C7—H7	116.7	C87—C92—H92	119.7
N2—C8—N3	117.6 (4)	C93—N17—C97	120.0
N2—C8—S1	127.9 (3)	N17—C93—C94	120.0
N3—C8—S1	114.5 (3)	N17—C93—H93A	120.0
C10—C9—C14	119.1 (4)	C94—C93—H93A	120.0
C10—C9—N3	123.2 (4)	C95—C94—C93	120.0
C14—C9—N3	117.7 (4)	C95—C94—H94A	120.0
C9—C10—C11	118.0 (5)	C93—C94—H94A	120.0
C9—C10—H10	121.0	C94—C95—C96	120.0
C11—C10—H10	121.0	C94—C95—H95A	120.0
C12—C11—C10	122.6 (6)	C96—C95—H95A	120.0
C12—C11—H11	118.7	C97—C96—C95	120.0
C10—C11—H11	118.7	C97—C96—C101	120.0
C13—C12—C11	118.9 (5)	C95—C96—C101	120.0
C13—C12—H12	120.6	C98—C97—C96	120.0
C11—C12—H12	120.6	C98—C97—N17	120.0
C12—C13—C14	121.2 (5)	C96—C97—N17	120.0
C12—C13—H13	119.4	C99—C98—C97	120.0
C14—C13—H13	119.4	C99—C98—H98A	120.0
C13—C14—C9	120.2 (5)	C97—C98—H98A	120.0
C13—C14—H14	119.9	C98—C99—C100	120.0
C9—C14—H14	119.9	C98—C99—H99A	120.0
N4—C15—C19	123.5 (5)	C100—C99—H99A	120.0
N4—C15—H15	118.3	C101—C100—C99	120.0
C19—C15—H15	118.3	C101—C100—H10B	120.0
N4—C16—C17	123.2 (7)	C99—C100—H10B	120.0
N4—C16—H16	118.4	C100—C101—C96	120.0
C17—C16—H16	118.4	C100—C101—H10C	120.0
C16—C17—C18	120.3 (6)	C96—C101—H10C	120.0
C16—C17—H17	119.9	N18—C102—C106	120.0
C18—C17—H17	119.9	N18—C102—H10A	120.0
C19—C18—C23	119.1 (9)	C106—C102—H10A	120.0
C19—C18—C17	116.1 (6)	C102—N18—C103	120.0
C23—C18—C17	124.8 (8)	C104—C103—N18	120.0
C18—C19—C20	119.8 (7)	C104—C103—H10D	120.0
C18—C19—C15	118.6 (6)	N18—C103—H10D	120.0
C20—C19—C15	121.5 (7)	C105—C104—C103	120.0
C21—C20—C19	117.9 (10)	C105—C104—H10E	120.0
C21—C20—H20	121.1	C103—C104—H10E	120.0
C19—C20—H20	121.1	C104—C105—C106	120.0
C22—C21—C20	122.9 (10)	C104—C105—C110	120.0
C22—C21—H21	118.6	C106—C105—C110	120.0
C20—C21—H21	118.6	C107—C106—C105	120.0
C21—C22—C23	119.5 (9)	C107—C106—C102	120.0
C21—C22—H22	120.2	C105—C106—C102	120.0

C23—C22—H22	120.2	C106—C107—C108	120.0
C22—C23—C18	120.9 (10)	C106—C107—H10F	120.0
C22—C23—H23	119.6	C108—C107—H10F	120.0
C18—C23—H23	119.6	C109—C108—C107	120.0
O2—C24—C25	119.1 (4)	C109—C108—H10G	120.0
O2—C24—C29	121.6 (3)	C107—C108—H10G	120.0
C25—C24—C29	119.3 (3)	C108—C109—C110	120.0
C26—C25—C24	120.4 (4)	C108—C109—H10H	120.0
C26—C25—H25	119.8	C110—C109—H10H	120.0
C24—C25—H25	119.8	C109—C110—C105	120.0
C27—C26—C25	120.6 (4)	C109—C110—H11A	120.0
C27—C26—H26	119.7	C105—C110—H11A	120.0
C25—C26—H26	119.7	C1'—N1'—C5'	120.0
C28—C27—C26	119.3 (4)	N1'—C1'—C2'	120.0
C28—C27—H27	120.3	N1'—C1'—H1'A	120.0
C26—C27—H27	120.3	C2'—C1'—H1'A	120.0
C27—C28—C29	122.3 (4)	C1'—C2'—C3'	120.0
C27—C28—H28	118.8	C1'—C2'—H2'A	120.0
C29—C28—H28	118.8	C3'—C2'—H2'A	120.0
C28—C29—C24	118.0 (4)	C4'—C3'—C2'	120.0
C28—C29—C30	117.5 (4)	C4'—C3'—H3'A	120.0
C24—C29—C30	124.5 (3)	C2'—C3'—H3'A	120.0
N5—C30—C29	126.7 (4)	C5'—C4'—C3'	120.0
N5—C30—H30	116.7	C5'—C4'—C9'	120.0
C29—C30—H30	116.7	C3'—C4'—C9'	120.0
N6—C31—N7	118.3 (3)	C6'—C5'—C4'	120.0
N6—C31—S2	127.8 (3)	C6'—C5'—N1'	120.0
N7—C31—S2	113.8 (3)	C4'—C5'—N1'	120.0
C37—C32—C33	118.8 (4)	C7'—C6'—C5'	120.0
C37—C32—N7	117.8 (4)	C7'—C6'—H6'A	120.0
C33—C32—N7	123.3 (4)	C5'—C6'—H6'A	120.0
C34—C33—C32	118.8 (4)	C6'—C7'—C8'	120.0
C34—C33—H33	120.6	C6'—C7'—H7'A	120.0
C32—C33—H33	120.6	C8'—C7'—H7'A	120.0
C35—C34—C33	121.9 (5)	C7'—C8'—C9'	120.0
C35—C34—H34	119.1	C7'—C8'—H8'A	120.0
C33—C34—H34	119.1	C9'—C8'—H8'A	120.0
C36—C35—C34	118.8 (4)	C8'—C9'—C4'	120.0
C36—C35—H35	120.6	C8'—C9'—H9'A	120.0
C34—C35—H35	120.6	C4'—C9'—H9'A	120.0
C35—C36—C37	120.9 (5)	N2'—C10'—C14'	120.0
C35—C36—H36	119.6	N2'—C10'—H10I	120.0
C37—C36—H36	119.6	C14'—C10'—H10I	120.0
C36—C37—C32	120.9 (4)	C11'—N2'—C10'	120.0
C36—C37—H37	119.5	N2'—C11'—C12'	120.0
C32—C37—H37	119.5	N2'—C11'—H11B	120.0
N8—C38—C39	124.9 (6)	C12'—C11'—H11B	120.0
N8—C38—H38	117.5	C11'—C12'—C13'	120.0
C39—C38—H38	117.5	C11'—C12'—H12A	120.0

C38—C39—C40	118.2 (6)	C13'—C12'—H12A	120.0
C38—C39—H39	120.9	C14'—C13'—C12'	120.0
C40—C39—H39	120.9	C14'—C13'—C18'	120.0
C39—C40—C41	119.7 (6)	C12'—C13'—C18'	120.0
C39—C40—H40	120.2	C15'—C14'—C13'	120.0
C41—C40—H40	120.2	C15'—C14'—C10'	120.0
C46—C41—C40	122.9 (6)	C13'—C14'—C10'	120.0
C46—C41—C42	119.1 (5)	C14'—C15'—C16'	120.0
C40—C41—C42	118.0 (5)	C14'—C15'—H15A	120.0
N8—C42—C43	120.4 (4)	C16'—C15'—H15A	120.0
N8—C42—C41	121.0 (4)	C17'—C16'—C15'	120.0
C43—C42—C41	118.5 (5)	C17'—C16'—H16A	120.0
C44—C43—C42	120.0 (6)	C15'—C16'—H16A	120.0
C44—C43—H43	120.0	C18'—C17'—C16'	120.0
C42—C43—H43	120.0	C18'—C17'—H17A	120.0
C43—C44—C45	121.5 (6)	C16'—C17'—H17A	120.0
C43—C44—H44	119.3	C17'—C18'—C13'	120.0
C45—C44—H44	119.3	C17'—C18'—H18B	120.0
C46—C45—C44	120.8 (6)	C13'—C18'—H18B	120.0
Zn1'—Zn1—Zn2—O2	−69.6 (2)	C14—C9—C10—C11	−0.6 (8)
N1—Zn1—Zn2—O2	−147.04 (19)	N3—C9—C10—C11	−178.2 (5)
O1—Zn1—Zn2—O2	−138.91 (19)	C9—C10—C11—C12	0.4 (9)
N4—Zn1—Zn2—O2	107.28 (17)	C10—C11—C12—C13	0.0 (9)
S1—Zn1—Zn2—O2	−9.26 (14)	C11—C12—C13—C14	−0.1 (9)
Zn1'—Zn1—Zn2—N8	−9.75 (19)	C12—C13—C14—C9	−0.2 (8)
O2—Zn1—Zn2—N8	59.85 (17)	C10—C9—C14—C13	0.5 (7)
N1—Zn1—Zn2—N8	−87.19 (19)	N3—C9—C14—C13	178.2 (4)
O1—Zn1—Zn2—N8	−79.06 (18)	C16—N4—C15—C19	0.1 (8)
N4—Zn1—Zn2—N8	167.13 (16)	Zn1—N4—C15—C19	−174.2 (4)
S1—Zn1—Zn2—N8	50.58 (14)	C15—N4—C16—C17	1.4 (9)
Zn1'—Zn1—Zn2—O1	69.3 (2)	Zn1—N4—C16—C17	175.6 (5)
O2—Zn1—Zn2—O1	138.91 (19)	N4—C16—C17—C18	−1.0 (11)
N1—Zn1—Zn2—O1	−8.13 (19)	C16—C17—C18—C19	−0.8 (10)
N4—Zn1—Zn2—O1	−113.81 (17)	C16—C17—C18—C23	−179.8 (7)
S1—Zn1—Zn2—O1	129.65 (15)	C23—C18—C19—C20	−0.3 (9)
Zn1'—Zn1—Zn2—N5	−140.12 (18)	C17—C18—C19—C20	−179.4 (6)
O2—Zn1—Zn2—N5	−70.52 (16)	C23—C18—C19—C15	−178.8 (6)
N1—Zn1—Zn2—N5	142.44 (17)	C17—C18—C19—C15	2.1 (8)
O1—Zn1—Zn2—N5	150.56 (16)	N4—C15—C19—C18	−1.9 (8)
N4—Zn1—Zn2—N5	36.76 (14)	N4—C15—C19—C20	179.6 (5)
S1—Zn1—Zn2—N5	−79.79 (11)	C18—C19—C20—C21	0.3 (10)
Zn1'—Zn1—Zn2—S2	132.02 (15)	C15—C19—C20—C21	178.7 (6)
O2—Zn1—Zn2—S2	−158.38 (13)	C19—C20—C21—C22	−1.2 (13)
N1—Zn1—Zn2—S2	54.58 (15)	C20—C21—C22—C23	2.1 (15)
O1—Zn1—Zn2—S2	62.71 (14)	C21—C22—C23—C18	−2.1 (14)
N4—Zn1—Zn2—S2	−51.10 (11)	C19—C18—C23—C22	1.2 (11)
S1—Zn1—Zn2—S2	−167.64 (7)	C17—C18—C23—C22	−179.8 (8)
O3—Zn3—Zn4—O4	140.56 (17)	Zn2—O2—C24—C25	−150.7 (3)
N9—Zn3—Zn4—O4	146.48 (17)	Zn1—O2—C24—C25	72.4 (5)

N12—Zn3—Zn4—O4	−106.65 (15)	Zn2—O2—C24—C29	29.3 (5)
S3—Zn3—Zn4—O4	3.00 (13)	Zn1—O2—C24—C29	−107.5 (4)
O4—Zn3—Zn4—O3	−140.56 (17)	O2—C24—C25—C26	−179.8 (4)
N9—Zn3—Zn4—O3	5.91 (17)	C29—C24—C25—C26	0.2 (6)
N12—Zn3—Zn4—O3	112.78 (15)	C24—C25—C26—C27	−0.6 (7)
S3—Zn3—Zn4—O3	−137.57 (14)	C25—C26—C27—C28	1.5 (8)
O4—Zn3—Zn4—N14	68.47 (15)	C26—C27—C28—C29	−2.0 (8)
O3—Zn3—Zn4—N14	−150.96 (15)	C27—C28—C29—C24	1.6 (7)
N9—Zn3—Zn4—N14	−145.05 (15)	C27—C28—C29—C30	−177.3 (4)
N12—Zn3—Zn4—N14	−38.18 (13)	O2—C24—C29—C28	179.3 (4)
S3—Zn3—Zn4—N14	71.47 (11)	C25—C24—C29—C28	−0.7 (6)
O4—Zn3—Zn4—N13	−61.78 (15)	O2—C24—C29—C30	−1.9 (6)
O3—Zn3—Zn4—N13	78.79 (15)	C25—C24—C29—C30	178.2 (4)
N9—Zn3—Zn4—N13	84.70 (16)	N6—N5—C30—C29	−178.3 (4)
N12—Zn3—Zn4—N13	−168.43 (13)	Zn2—N5—C30—C29	−5.8 (6)
S3—Zn3—Zn4—N13	−58.78 (12)	C28—C29—C30—N5	168.5 (4)
O4—Zn3—Zn4—S4	157.84 (12)	C24—C29—C30—N5	−10.4 (7)
O3—Zn3—Zn4—S4	−61.60 (12)	N5—N6—C31—N7	−179.2 (4)
N9—Zn3—Zn4—S4	−55.68 (13)	N5—N6—C31—S2	0.2 (6)
N12—Zn3—Zn4—S4	51.19 (10)	C32—N7—C31—N6	−1.8 (7)
S3—Zn3—Zn4—S4	160.84 (7)	C32—N7—C31—S2	178.7 (4)
Zn1'—Zn1—S1—C8	−101.1 (2)	Zn2—S2—C31—N6	−5.1 (4)
O2—Zn1—S1—C8	−169.88 (18)	Zn2—S2—C31—N7	174.3 (3)
N1—Zn1—S1—C8	−16.04 (19)	C31—N7—C32—C37	146.0 (5)
O1—Zn1—S1—C8	−88.1 (2)	C31—N7—C32—C33	−36.9 (7)
N4—Zn1—S1—C8	87.21 (19)	C37—C32—C33—C34	−0.6 (7)
Zn2—Zn1—S1—C8	−163.74 (15)	N7—C32—C33—C34	−177.6 (4)
O2—Zn2—S2—C31	66.7 (2)	C32—C33—C34—C35	0.0 (8)
N8—Zn2—S2—C31	−110.52 (19)	C33—C34—C35—C36	0.4 (8)
O1—Zn2—S2—C31	139.20 (18)	C34—C35—C36—C37	−0.4 (8)
N5—Zn2—S2—C31	5.39 (18)	C35—C36—C37—C32	−0.2 (8)
Zn1—Zn2—S2—C31	103.29 (16)	C33—C32—C37—C36	0.7 (7)
O4—Zn3—S3—C54	166.95 (17)	N7—C32—C37—C36	177.9 (4)
O3—Zn3—S3—C54	82.0 (2)	C42—N8—C38—C39	−0.6 (9)
N9—Zn3—S3—C54	13.11 (18)	Zn2—N8—C38—C39	179.4 (5)
N12—Zn3—S3—C54	−92.85 (18)	N8—C38—C39—C40	1.3 (11)
Zn4—Zn3—S3—C54	164.95 (15)	C38—C39—C40—C41	−0.2 (10)
O4—Zn4—S4—C77	−63.0 (2)	C39—C40—C41—C46	178.8 (6)
O3—Zn4—S4—C77	−138.32 (16)	C39—C40—C41—C42	−1.5 (9)
N14—Zn4—S4—C77	−3.44 (16)	C38—N8—C42—C43	179.7 (5)
N13—Zn4—S4—C77	112.89 (16)	Zn2—N8—C42—C43	−0.3 (6)
Zn3—Zn4—S4—C77	−102.72 (14)	C38—N8—C42—C41	−1.2 (7)
Zn1'—Zn1—O1—C1	88.6 (4)	Zn2—N8—C42—C41	178.8 (4)
O2—Zn1—O1—C1	164.7 (4)	C46—C41—C42—N8	−178.0 (5)
N1—Zn1—O1—C1	4.4 (4)	C40—C41—C42—N8	2.2 (8)
N4—Zn1—O1—C1	−100.2 (3)	C46—C41—C42—C43	1.1 (8)
S1—Zn1—O1—C1	75.3 (4)	C40—C41—C42—C43	−178.7 (5)
Zn2—Zn1—O1—C1	−169.2 (4)	N8—C42—C43—C44	178.6 (5)
Zn1'—Zn1—O1—Zn2	−102.24 (19)	C41—C42—C43—C44	−0.5 (8)

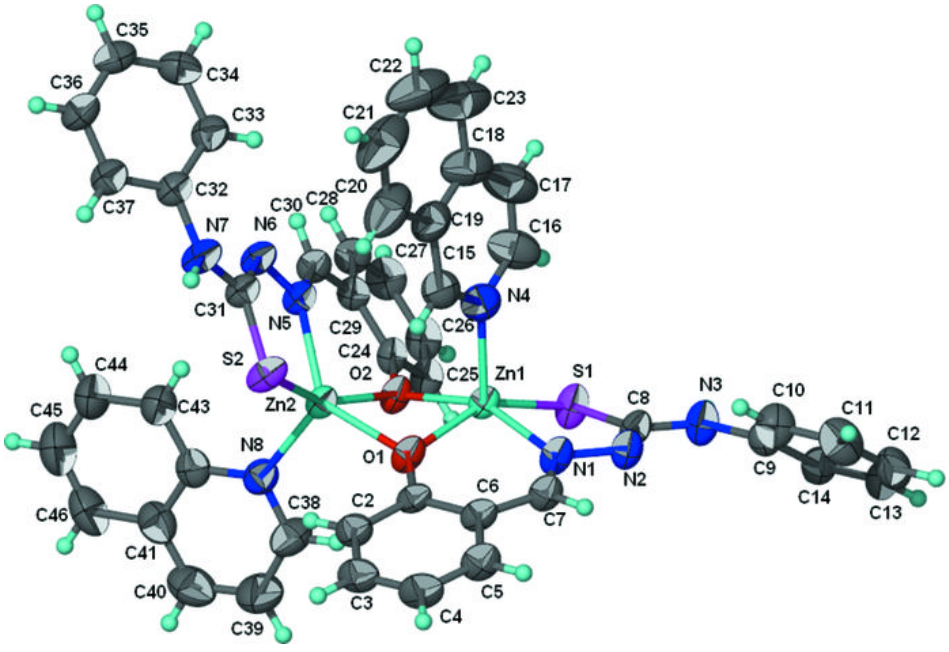
O2—Zn1—O1—Zn2	−26.16 (12)	C42—C43—C44—C45	−0.4 (10)
N1—Zn1—O1—Zn2	173.59 (15)	C43—C44—C45—C46	0.9 (12)
N4—Zn1—O1—Zn2	68.99 (16)	C44—C45—C46—C41	−0.3 (11)
S1—Zn1—O1—Zn2	−115.54 (13)	C40—C41—C46—C45	179.1 (6)
O2—Zn2—O1—C1	−164.6 (4)	C42—C41—C46—C45	−0.7 (9)
N8—Zn2—O1—C1	−72.3 (4)	Zn3—O3—C47—C48	176.9 (3)
N5—Zn2—O1—C1	126.7 (3)	Zn4—O3—C47—C48	−12.1 (6)
S2—Zn2—O1—C1	38.7 (4)	Zn3—O3—C47—C52	−2.4 (6)
Zn1—Zn2—O1—C1	169.2 (4)	Zn4—O3—C47—C52	168.6 (3)
O2—Zn2—O1—Zn1	26.23 (12)	O3—C47—C48—C49	179.6 (4)
N8—Zn2—O1—Zn1	118.53 (14)	C52—C47—C48—C49	−1.1 (7)
N5—Zn2—O1—Zn1	−42.4 (2)	C47—C48—C49—C50	0.7 (8)
S2—Zn2—O1—Zn1	−130.42 (10)	C48—C49—C50—C51	−0.4 (9)
N8—Zn2—O2—C24	83.4 (3)	C49—C50—C51—C52	0.6 (9)
O1—Zn2—O2—C24	−171.2 (4)	C50—C51—C52—C47	−1.0 (8)
N5—Zn2—O2—C24	−33.2 (3)	C50—C51—C52—C53	175.1 (5)
S2—Zn2—O2—C24	−93.9 (4)	O3—C47—C52—C51	−179.5 (4)
Zn1—Zn2—O2—C24	−144.9 (4)	C48—C47—C52—C51	1.2 (6)
N8—Zn2—O2—Zn1	−131.69 (14)	O3—C47—C52—C53	4.7 (7)
O1—Zn2—O2—Zn1	−26.34 (12)	C48—C47—C52—C53	−174.6 (4)
N5—Zn2—O2—Zn1	111.69 (14)	N10—N9—C53—C52	174.2 (4)
S2—Zn2—O2—Zn1	51.0 (2)	Zn3—N9—C53—C52	−6.8 (7)
Zn1'—Zn1—O2—C24	−111.5 (3)	C51—C52—C53—N9	−175.8 (4)
N1—Zn1—O2—C24	−137.3 (3)	C47—C52—C53—N9	0.0 (7)
O1—Zn1—O2—C24	172.8 (3)	N9—N10—C54—N11	176.5 (4)
N4—Zn1—O2—C24	72.2 (3)	N9—N10—C54—S3	−1.7 (6)
S1—Zn1—O2—C24	−39.5 (3)	C55—N11—C54—N10	−1.2 (7)
Zn2—Zn1—O2—C24	146.3 (4)	C55—N11—C54—S3	177.2 (4)
Zn1'—Zn1—O2—Zn2	102.21 (19)	Zn3—S3—C54—N10	−10.9 (4)
N1—Zn1—O2—Zn2	76.4 (3)	Zn3—S3—C54—N11	170.8 (3)
O1—Zn1—O2—Zn2	26.53 (12)	C54—N11—C55—C60	−145.8 (5)
N4—Zn1—O2—Zn2	−74.06 (15)	C54—N11—C55—C56	37.4 (8)
S1—Zn1—O2—Zn2	174.21 (9)	C60—C55—C56—C57	1.4 (8)
O4—Zn3—O3—C47	−161.7 (3)	N11—C55—C56—C57	178.1 (5)
N9—Zn3—O3—C47	−2.3 (3)	C55—C56—C57—C58	−1.0 (9)
N12—Zn3—O3—C47	104.9 (3)	C56—C57—C58—C59	0.0 (9)
S3—Zn3—O3—C47	−70.1 (4)	C57—C58—C59—C60	0.6 (9)
Zn4—Zn3—O3—C47	173.1 (4)	C58—C59—C60—C55	−0.2 (8)
O4—Zn3—O3—Zn4	25.27 (11)	C56—C55—C60—C59	−0.8 (8)
N9—Zn3—O3—Zn4	−175.35 (13)	N11—C55—C60—C59	−177.7 (5)
N12—Zn3—O3—Zn4	−68.22 (13)	C65—C61—C62—N12	2.3 (9)
S3—Zn3—O3—Zn4	116.80 (14)	C63—N12—C62—C61	−1.6 (7)
O4—Zn4—O3—C47	161.7 (3)	Zn3—N12—C62—C61	−174.6 (4)
N14—Zn4—O3—C47	−130.6 (3)	C62—N12—C63—C64	−0.3 (6)
N13—Zn4—O3—C47	69.5 (3)	Zn3—N12—C63—C64	172.6 (3)
S4—Zn4—O3—C47	−40.7 (3)	N12—C63—C64—C69	179.9 (4)
Zn3—Zn4—O3—C47	−173.1 (4)	N12—C63—C64—C65	1.3 (7)
O4—Zn4—O3—Zn3	−25.16 (11)	C69—C64—C65—C61	−179.1 (5)
N14—Zn4—O3—Zn3	42.53 (19)	C63—C64—C65—C61	−0.5 (7)

N13—Zn4—O3—Zn3	−117.39 (12)	C69—C64—C65—C66	0.7 (7)
S4—Zn4—O3—Zn3	132.39 (9)	C63—C64—C65—C66	179.3 (5)
O3—Zn3—O4—C70	−173.9 (3)	C62—C61—C65—C64	−1.2 (9)
N9—Zn3—O4—C70	133.8 (3)	C62—C61—C65—C66	179.0 (6)
N12—Zn3—O4—C70	−75.5 (3)	C64—C65—C66—C67	−0.7 (9)
S3—Zn3—O4—C70	33.3 (3)	C61—C65—C66—C67	179.2 (7)
Zn4—Zn3—O4—C70	−148.5 (3)	C65—C66—C67—C68	0.9 (12)
O3—Zn3—O4—Zn4	−25.39 (11)	C66—C67—C68—C69	−1.1 (12)
N9—Zn3—O4—Zn4	−77.6 (3)	C67—C68—C69—C64	1.2 (11)
N12—Zn3—O4—Zn4	73.01 (14)	C63—C64—C69—C68	−179.5 (5)
S3—Zn3—O4—Zn4	−178.19 (8)	C65—C64—C69—C68	−1.0 (8)
O3—Zn4—O4—C70	173.3 (3)	Zn3—O4—C70—C71	−69.2 (4)
N14—Zn4—O4—C70	34.1 (3)	Zn4—O4—C70—C71	150.8 (3)
N13—Zn4—O4—C70	−82.8 (3)	Zn3—O4—C70—C75	111.4 (3)
S4—Zn4—O4—C70	93.2 (3)	Zn4—O4—C70—C75	−28.6 (5)
Zn3—Zn4—O4—C70	148.0 (4)	O4—C70—C71—C72	−178.7 (4)
O3—Zn4—O4—Zn3	25.34 (11)	C75—C70—C71—C72	0.7 (6)
N14—Zn4—O4—Zn3	−113.90 (13)	C70—C71—C72—C73	−0.3 (7)
N13—Zn4—O4—Zn3	129.21 (12)	C71—C72—C73—C74	−1.5 (7)
S4—Zn4—O4—Zn3	−54.8 (2)	C72—C73—C74—C75	2.9 (7)
Zn1'—Zn1—N1—C7	−82.8 (4)	O4—C70—C75—C74	−179.9 (4)
O2—Zn1—N1—C7	−58.1 (5)	C71—C70—C75—C74	0.7 (6)
O1—Zn1—N1—C7	−10.3 (4)	O4—C70—C75—C76	−0.3 (6)
N4—Zn1—N1—C7	91.5 (4)	C71—C70—C75—C76	−179.7 (4)
S1—Zn1—N1—C7	−160.4 (4)	C73—C74—C75—C70	−2.5 (6)
Zn2—Zn1—N1—C7	−4.9 (5)	C73—C74—C75—C76	177.8 (4)
Zn1'—Zn1—N1—N2	100.7 (4)	N15—N14—C76—C75	178.4 (4)
O2—Zn1—N1—N2	125.4 (3)	Zn4—N14—C76—C75	7.0 (6)
O1—Zn1—N1—N2	173.3 (3)	C70—C75—C76—N14	11.5 (6)
N4—Zn1—N1—N2	−84.9 (3)	C74—C75—C76—N14	−168.8 (4)
S1—Zn1—N1—N2	23.1 (3)	N14—N15—C77—N16	179.9 (4)
Zn2—Zn1—N1—N2	178.6 (3)	N14—N15—C77—S4	1.4 (5)
C7—N1—N2—C8	162.6 (4)	C78—N16—C77—N15	−0.3 (7)
Zn1—N1—N2—C8	−20.5 (5)	C78—N16—C77—S4	178.4 (4)
O2—Zn2—N5—C30	21.2 (4)	Zn4—S4—C77—N15	2.4 (4)
N8—Zn2—N5—C30	−73.7 (4)	Zn4—S4—C77—N16	−176.2 (3)
O1—Zn2—N5—C30	85.7 (4)	C77—N16—C78—C79	38.0 (7)
S2—Zn2—N5—C30	−179.5 (4)	C77—N16—C78—C83	−144.2 (4)
Zn1—Zn2—N5—C30	59.1 (4)	N16—C78—C79—C80	178.6 (4)
O2—Zn2—N5—N6	−166.8 (3)	C83—C78—C79—C80	0.8 (7)
N8—Zn2—N5—N6	98.3 (3)	C78—C79—C80—C81	−0.5 (7)
O1—Zn2—N5—N6	−102.3 (3)	C79—C80—C81—C82	−0.1 (8)
S2—Zn2—N5—N6	−7.5 (3)	C80—C81—C82—C83	0.3 (8)
Zn1—Zn2—N5—N6	−128.9 (3)	C81—C82—C83—C78	0.1 (8)
Zn1'—Zn1—N4—C15	61.6 (12)	C79—C78—C83—C82	−0.6 (7)
O2—Zn1—N4—C15	82.3 (4)	N16—C78—C83—C82	−178.5 (4)
N1—Zn1—N4—C15	−84.7 (4)	C88—N13—C84—C85	0.9 (6)
O1—Zn1—N4—C15	5.5 (4)	Zn4—N13—C84—C85	−175.9 (4)
S1—Zn1—N4—C15	−172.0 (3)	N13—C84—C85—C86	−1.0 (7)

Zn2—Zn1—N4—C15	43.5 (4)	C84—C85—C86—C87	0.0 (7)
Zn1'—Zn1—N4—C16	−112.5 (11)	C85—C86—C87—C92	−178.6 (4)
O2—Zn1—N4—C16	−91.8 (4)	C85—C86—C87—C88	0.9 (7)
N1—Zn1—N4—C16	101.2 (4)	C84—N13—C88—C89	178.6 (4)
O1—Zn1—N4—C16	−168.6 (4)	Zn4—N13—C88—C89	−5.0 (5)
S1—Zn1—N4—C16	13.9 (5)	C84—N13—C88—C87	0.1 (5)
Zn2—Zn1—N4—C16	−130.6 (4)	Zn4—N13—C88—C87	176.6 (3)
C30—N5—N6—C31	179.2 (4)	C86—C87—C88—N13	−1.0 (6)
Zn2—N5—N6—C31	6.2 (5)	C92—C87—C88—N13	178.5 (4)
O2—Zn2—N8—C38	62.9 (4)	C86—C87—C88—C89	−179.5 (4)
O1—Zn2—N8—C38	−13.4 (4)	C92—C87—C88—C89	0.0 (6)
N5—Zn2—N8—C38	151.4 (4)	N13—C88—C89—C90	−177.0 (4)
S2—Zn2—N8—C38	−118.2 (4)	C87—C88—C89—C90	1.5 (6)
Zn1—Zn2—N8—C38	28.5 (4)	C88—C89—C90—C91	−2.0 (7)
O2—Zn2—N8—C42	−117.0 (4)	C89—C90—C91—C92	1.1 (8)
O1—Zn2—N8—C42	166.6 (3)	C90—C91—C92—C87	0.4 (8)
N5—Zn2—N8—C42	−28.6 (4)	C86—C87—C92—C91	178.5 (5)
S2—Zn2—N8—C42	61.9 (4)	C88—C87—C92—C91	−0.9 (7)
Zn1—Zn2—N8—C42	−151.5 (3)	C97—N17—C93—C94	0.0
O4—Zn3—N9—C53	56.8 (5)	N17—C93—C94—C95	0.0
O3—Zn3—N9—C53	6.7 (4)	C93—C94—C95—C96	0.0
N12—Zn3—N9—C53	−92.5 (4)	C94—C95—C96—C97	0.0
S3—Zn3—N9—C53	162.1 (4)	C94—C95—C96—C101	180.0
Zn4—Zn3—N9—C53	2.8 (4)	C95—C96—C97—C98	180.0
O4—Zn3—N9—N10	−124.3 (3)	C101—C96—C97—C98	0.0
O3—Zn3—N9—N10	−174.4 (3)	C95—C96—C97—N17	0.0
N12—Zn3—N9—N10	86.4 (3)	C101—C96—C97—N17	180.0
S3—Zn3—N9—N10	−19.0 (3)	C93—N17—C97—C98	180.0
Zn4—Zn3—N9—N10	−178.3 (2)	C93—N17—C97—C96	0.0
C53—N9—N10—C54	−164.0 (4)	C96—C97—C98—C99	0.0
Zn3—N9—N10—C54	17.0 (5)	N17—C97—C98—C99	180.0
O4—Zn3—N12—C63	−86.6 (3)	C97—C98—C99—C100	0.0
O3—Zn3—N12—C63	−10.0 (3)	C98—C99—C100—C101	0.0
N9—Zn3—N12—C63	80.2 (3)	C99—C100—C101—C96	0.0
S3—Zn3—N12—C63	167.7 (3)	C97—C96—C101—C100	0.0
Zn4—Zn3—N12—C63	−47.7 (3)	C95—C96—C101—C100	180.0
O4—Zn3—N12—C62	86.1 (4)	C106—C102—N18—C103	0.0
O3—Zn3—N12—C62	162.7 (3)	C102—N18—C103—C104	0.0
N9—Zn3—N12—C62	−107.1 (3)	N18—C103—C104—C105	0.0
S3—Zn3—N12—C62	−19.6 (4)	C103—C104—C105—C106	0.0
Zn4—Zn3—N12—C62	125.0 (3)	C103—C104—C105—C110	180.0
O4—Zn4—N13—C84	−63.4 (3)	C104—C105—C106—C107	180.0
O3—Zn4—N13—C84	13.0 (3)	C110—C105—C106—C107	0.0
N14—Zn4—N13—C84	−151.2 (3)	C104—C105—C106—C102	0.0
S4—Zn4—N13—C84	118.1 (3)	C110—C105—C106—C102	180.0
Zn3—Zn4—N13—C84	−28.4 (3)	N18—C102—C106—C107	180.0
O4—Zn4—N13—C88	120.1 (3)	N18—C102—C106—C105	0.0
O3—Zn4—N13—C88	−163.5 (3)	C105—C106—C107—C108	0.0
N14—Zn4—N13—C88	32.2 (3)	C102—C106—C107—C108	180.0

S4—Zn4—N13—C88	−58.4 (3)	C106—C107—C108—C109	0.0
Zn3—Zn4—N13—C88	155.1 (3)	C107—C108—C109—C110	0.0
O4—Zn4—N14—C76	−23.0 (3)	C108—C109—C110—C105	0.0
O3—Zn4—N14—C76	−87.0 (4)	C104—C105—C110—C109	180.0
N13—Zn4—N14—C76	71.1 (3)	C106—C105—C110—C109	0.0
S4—Zn4—N14—C76	176.3 (3)	C5'—N1'—C1'—C2'	0.0
Zn3—Zn4—N14—C76	−60.2 (3)	N1'—C1'—C2'—C3'	0.0
O4—Zn4—N14—N15	166.1 (3)	C1'—C2'—C3'—C4'	0.0
O3—Zn4—N14—N15	102.2 (3)	C2'—C3'—C4'—C5'	0.0
N13—Zn4—N14—N15	−99.7 (3)	C2'—C3'—C4'—C9'	180.0
S4—Zn4—N14—N15	5.5 (3)	C3'—C4'—C5'—C6'	180.0
Zn3—Zn4—N14—N15	129.0 (3)	C9'—C4'—C5'—C6'	0.0
C76—N14—N15—C77	−177.3 (3)	C3'—C4'—C5'—N1'	0.0
Zn4—N14—N15—C77	−5.4 (4)	C9'—C4'—C5'—N1'	180.0
Zn1—O1—C1—C2	−176.8 (3)	C1'—N1'—C5'—C6'	180.0
Zn2—O1—C1—C2	17.3 (6)	C1'—N1'—C5'—C4'	0.0
Zn1—O1—C1—C6	1.8 (6)	C4'—C5'—C6'—C7'	0.0
Zn2—O1—C1—C6	−164.1 (3)	N1'—C5'—C6'—C7'	180.0
O1—C1—C2—C3	−179.8 (4)	C5'—C6'—C7'—C8'	0.0
C6—C1—C2—C3	1.6 (6)	C6'—C7'—C8'—C9'	0.0
C1—C2—C3—C4	−0.4 (7)	C7'—C8'—C9'—C4'	0.0
C2—C3—C4—C5	−0.6 (8)	C5'—C4'—C9'—C8'	0.0
C3—C4—C5—C6	0.6 (8)	C3'—C4'—C9'—C8'	180.0
O1—C1—C6—C5	179.8 (4)	C14'—C10'—N2'—C11'	0.0
C2—C1—C6—C5	−1.6 (6)	C10'—N2'—C11'—C12'	0.0
O1—C1—C6—C7	−5.5 (7)	N2'—C11'—C12'—C13'	0.0
C2—C1—C6—C7	173.1 (4)	C11'—C12'—C13'—C14'	0.0
C4—C5—C6—C1	0.6 (7)	C11'—C12'—C13'—C18'	180.0
C4—C5—C6—C7	−174.6 (5)	C12'—C13'—C14'—C15'	180.0
N2—N1—C7—C6	−172.9 (4)	C18'—C13'—C14'—C15'	0.0
Zn1—N1—C7—C6	10.5 (7)	C12'—C13'—C14'—C10'	0.0
C1—C6—C7—N1	−0.9 (8)	C18'—C13'—C14'—C10'	180.0
C5—C6—C7—N1	173.9 (5)	N2'—C10'—C14'—C15'	180.0
N1—N2—C8—N3	−177.1 (4)	N2'—C10'—C14'—C13'	0.0
N1—N2—C8—S1	1.9 (6)	C13'—C14'—C15'—C16'	0.0
C9—N3—C8—N2	1.0 (7)	C10'—C14'—C15'—C16'	180.0
C9—N3—C8—S1	−178.1 (4)	C14'—C15'—C16'—C17'	0.0
Zn1—S1—C8—N2	13.5 (4)	C15'—C16'—C17'—C18'	0.0
Zn1—S1—C8—N3	−167.6 (3)	C16'—C17'—C18'—C13'	0.0
C8—N3—C9—C10	−36.7 (8)	C14'—C13'—C18'—C17'	0.0
C8—N3—C9—C14	145.7 (5)	C12'—C13'—C18'—C17'	180.0

Fig. 1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N6
C30
C28
C20
C22
C23
C21
C18
C17
C19
C16
C27
C15
N4
N5
C29
C26
C24
S2
O2
C25
Zn1
S1
C8
N3
C10
C11
C12
C44
C45
C43
Zn2
N8
O1
N1
N2
C9
C14
C13
C46
C38
C2
C6
C7
C41
C40
C3
C5
C39
C4