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(4-Hydroxycinnamato)[tris(*N*-methylbenzimidazol-2-ylmethyl)amine]zinc(II)] perchlorate–dimethylformamide–ethanol–methanol (2/2/2/1)

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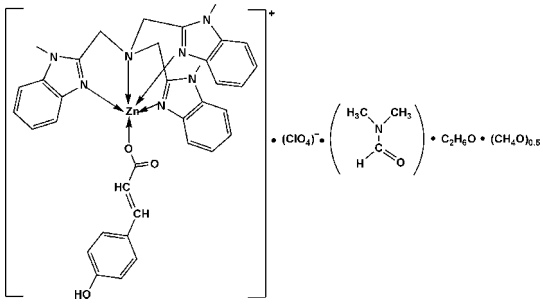
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.046; wR factor = 0.155; data-to-parameter ratio = 14.4.

In the title complex, $[Zn(C_9H_7O_3)(C_{27}H_{27}N_7)]ClO_4\cdot C_3H_7NO\cdot C_2H_6O\cdot 0.5CH_4O$, the Zn^{II} ion is five-coordinated by four N atoms from a tris(*N*-methylbenzimidazol-2-ylmethyl)amine ligand and one O atom from a 4-hydroxycinnamate ligand in a distorted trigonal–bipyramidal geometry. The atoms of the ethanol and methanol solvent molecules are disordered over two sites with equal occupancy.

Related literature

For related literature, see: Allen *et al.* (1987); Youngme *et al.* (2007).



Experimental

Crystal data

$[Zn(C_9H_7O_3)(C_{27}H_{27}N_7)]ClO_4\cdot C_3H_7NO\cdot C_2H_6O\cdot 0.5CH_4O$
M_r = 912.71
Monoclinic, $C2/c$
a = 32.0342 (8) Å
b = 15.5594 (5) Å
c = 22.1536 (5) Å
β = 125.338 (10)°
V = 9007.6 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 153 (2) K
0.58 × 0.53 × 0.38 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Absorption correction: multi-scan (Higashi; 1995)
T_{min} = 0.698, T_{max} = 0.786
36372 measured reflections
8367 independent reflections
7232 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.155
S = 1.04
8367 reflections
582 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2554).

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supplementary materials

Acta Cryst. (2007). E**63**, m3022 [**doi:10.1107/S1600536807058023**]

(4-Hydroxycinnamato)[tris(*N*-methylbenzimidazol-2-ylmethyl)amine]zinc(II)] perchlorate-dimethylformamide-ethanol-methanol (2/2/2/1)

H. Wu, R. Yun, J. Ding and J. Yuan

Comment

The asymmetric unit of the title compound (Fig. 1) consists of a [Zn(Mentb)(4-hydroxycinnamate)] cation, a perchlorate anion, one molecule of DMF and ethanol, and a hemimethanol molecule. The zinc ion is five-coordinate with a N_4O ligand set. The Mentb ligand acts as a tetradentate N-donor, and an O atom of carboxylate groups of the 4-hydroxycinnamate completes the coordination. The coordination geometry of the Zn^{II} may be best described as distorted trigonal bipyramid (τ = 0.86). The parameter τ is defined as (β - α)/60 [where β = O1—Zn—N7, α = O1—Zn—N1] and its value varies from 0 (in regular square-based pyramidal) to 1 (in regular trigonal bipyramidal) (Youngme *et al.*, 2007). The equatorial plane is occupied by three N atoms of three benzimidazolyl groups, while the Zn^{II} atom protrudes towards O1 and is 0.561Å from the plane of atoms N1, N3 and N5. The axial positions are occupyied by N7 and O1, with Zn—N7 2.453 (2) Å, Zn—O1 1.974 (2)Å and O1—Zn—N7 167.13 (8)°. The three benzimidazole ring arms of the Mentb ligand form a cone-shaped cavity. The angles N3—Zn—N1, N5—Zn—N1 and N5—Zn—N3 are 110.28 (9), 114.28 (8) and 113.99 (9)°, respectively. The N7—Zn—N1 74.74 (9), N7—Zn—N3 74.15 (8) and N7—Zn—N5, 73.65 (8)° angles, which are all less than 90°. The distance between Zn^{II} and O2 is 3.063 (2) Å, so O2 is not coordinated. The angles and distance in the Mentb and 4-hydroxycinnamate are normal (Allen *et al.*, 1987). The rystal packing is stabilized by O—H···O hydrogen-bonding interactions (Fig. 2).

Experimental

To a stirred solution of tris(*N*-methylbenzimidazol-2-ylmethyl)amine (0.0899 g, 0.2 mmol) in hot MeOH (10 ml) was added $Zn(ClO_4)_2(H_2O)_6$ (0.0745 g, 0.2 mmol), followed by a solution of Na(4-hydroxycinnamate) (0.0372 g, 0.2 mmol) in MeOH (5 ml). A colorless crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH,EtOH and absolute Et_2O, and dried *in vacuo*. The dried precipitate was dissolved in DMF to a colorless solution that was allowed to evaporate at room temperature. colorless crystals suitable for X-ray diffraction studies were obtained after two weeks. Yield, 0.135 g (74%). (found: C, 54.37; H, 5.22; N,12.36. Calcd. for $C_{41.50}H_{49}ClN_8O_{9.50}Zn$: C, 54.61; H, 5.41; N, 12.28)

Refinement

The atoms of the ethanol and methanol solvate are disordered of two sites with equal occupancy. All H atoms were geometrically positioned and refined using a riding-model with C—H distances ranging from 0.95 to 0.99 Å and O—H = 0.84Å and U_{iso}(H) = 1.2 U_{eq}(C) or U_{iso}(H) = 1.5 U_{eq}(C_{methyl},*O*).

Figures

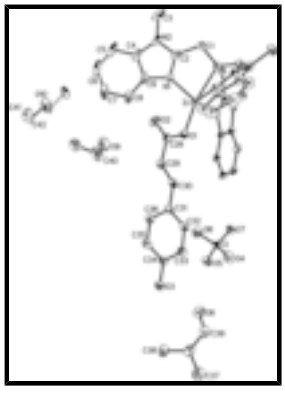


Fig. 1. Crystal structure and atom numbering of the title compound.

Fig. 2. The Packing diagram of the title compound. H bonds shown as dashed lines.

(4-Hydroxycinnamato)[tris(*N*-methylbenzimidazol-2-ylmethyl)amine]zinc(II)] perchlorate–dimethylformamide–ethanol–methanol (2/2/2/1)

Crystal data

$[Zn(C_9H_7O_3)(C_{27}H_{27}N_7)]ClO_4·C_3H_7NO·C_2H_6O·0.5CH_4O$	F_{000} = 3816
M_r = 912.71	D_x = 1.346 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 32.0342 (8) Å	Cell parameters from 32283 reflections
b = 15.5594 (5) Å	θ = 3.0–27.5º
c = 22.1536 (5) Å	μ = 0.67 mm^{-1}
β = 125.338 (10)º	*T* = 153 (2) K
V = 9007.6 (4) Å^3	Block, colorless
Z = 8	0.58 × 0.53 × 0.38 mm

Data collection

Rigaku R-axis Spider diffractometer	8367 independent reflections
Radiation source: Rotating Anode	7232 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 153(2) K	θ_{max} = 25.5º
ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (Higashi; 1995)	*h* = −38→38
T_{min} = 0.698, T_{max} = 0.786	*k* = −18→18
36372 measured reflections	*l* = −26→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.155$	$w = 1/[\sigma^2(F_o^2) + (0.1005P)^2 + 14.7697P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
8367 reflections	$\Delta\rho_{max} = 1.20$ e Å^{-3}
582 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn	0.078081 (11)	0.750336 (17)	0.059720 (15)	0.02571 (12)	
Cl	0.09422 (3)	0.26335 (5)	0.27601 (4)	0.03521 (18)	
O1	0.08765 (8)	0.71180 (13)	0.15189 (11)	0.0406 (5)	
O2	0.08059 (11)	0.84273 (15)	0.18386 (13)	0.0596 (7)	
O3	0.17586 (9)	0.50549 (16)	0.56220 (11)	0.0470 (5)	
H3	0.1929	0.4605	0.5706	0.056*	
O4	0.14662 (10)	0.2631 (2)	0.33752 (16)	0.0781 (10)	
O5	0.06623 (10)	0.20352 (16)	0.28876 (13)	0.0544 (6)	
O6	0.07260 (12)	0.34759 (16)	0.26806 (15)	0.0659 (7)	
O7	0.08874 (10)	0.24106 (15)	0.20881 (13)	0.0499 (6)	
O8	0.22487 (11)	0.35802 (17)	0.58986 (15)	0.0632 (7)	
O9	0.0375 (3)	0.8967 (4)	0.2674 (4)	0.0854 (19)	0.50
H9	0.0419	0.8963	0.2336	0.128*	0.50
O10	−0.19155 (11)	0.9252 (2)	0.03371 (18)	0.0792 (9)	
H10	−0.1636	0.9060	0.0443	0.095*	
N1	0.01650 (8)	0.82827 (15)	−0.00654 (12)	0.0326 (5)	
N2	−0.02600 (10)	0.92314 (16)	−0.09803 (14)	0.0463 (7)	
N3	0.14463 (8)	0.81120 (14)	0.08906 (11)	0.0284 (5)	

N4	0.20541 (9)	0.83904 (16)	0.07238 (14)	0.0367 (5)
N5	0.07008 (8)	0.62744 (14)	0.01897 (11)	0.0268 (4)
N6	0.04009 (8)	0.53490 (14)	−0.07408 (12)	0.0297 (5)
N7	0.07240 (9)	0.76521 (14)	−0.05503 (12)	0.0298 (5)
N8	0.25900 (11)	0.34541 (19)	0.71284 (16)	0.0521 (7)
C1	0.04634 (11)	0.84674 (18)	−0.08750 (15)	0.0369 (6)
H1A	0.0260	0.8434	−0.1421	0.044*
H1B	0.0718	0.8934	−0.0708	0.044*
C2	0.01215 (10)	0.86516 (17)	−0.06387 (14)	0.0350 (6)
C3	−0.04099 (17)	0.9714 (2)	−0.16462 (19)	0.0703 (13)
H3A	−0.0104	0.9946	−0.1586	0.084*
H3B	−0.0637	1.0187	−0.1721	0.084*
H3C	−0.0589	0.9331	−0.2076	0.084*
C4	−0.04866 (11)	0.9244 (2)	−0.06052 (18)	0.0477 (8)
C5	−0.08978 (14)	0.9717 (2)	−0.0720 (2)	0.0691 (13)
H5	−0.1070	1.0132	−0.1104	0.083*
C6	−0.10405 (13)	0.9561 (3)	−0.0264 (3)	0.0762 (15)
H6	−0.1319	0.9872	−0.0330	0.091*
C7	−0.07855 (14)	0.8949 (3)	0.0305 (3)	0.0685 (13)
H7	−0.0899	0.8852	0.0612	0.082*
C8	−0.03720 (12)	0.8481 (2)	0.0431 (2)	0.0489 (8)
H8	−0.0199	0.8071	0.0819	0.059*
C9	−0.02249 (10)	0.86409 (19)	−0.00359 (17)	0.0397 (7)
C10	0.12566 (11)	0.76483 (19)	−0.03122 (16)	0.0346 (6)
H10A	0.1286	0.7967	−0.0673	0.042*
H10B	0.1372	0.7050	−0.0284	0.042*
C11	0.15818 (10)	0.80646 (17)	0.04318 (14)	0.0309 (5)
C12	0.23281 (13)	0.8447 (2)	0.0380 (2)	0.0516 (8)
H12A	0.2134	0.8145	−0.0096	0.062*
H12B	0.2666	0.8181	0.0705	0.062*
H12C	0.2368	0.9052	0.0299	0.062*
C13	0.22484 (11)	0.86450 (18)	0.14409 (16)	0.0378 (6)
C14	0.27295 (12)	0.8962 (2)	0.2012 (2)	0.0519 (8)
H14	0.2993	0.9058	0.1945	0.062*
C15	0.27985 (13)	0.9126 (2)	0.26715 (19)	0.0562 (9)
H15	0.3121	0.9333	0.3075	0.067*
C16	0.24137 (13)	0.9001 (2)	0.27703 (18)	0.0531 (8)
H16	0.2476	0.9139	0.3234	0.064*
C17	0.19373 (12)	0.8677 (2)	0.22069 (16)	0.0411 (7)
H17	0.1674	0.8592	0.2275	0.049*
C18	0.18653 (10)	0.84843 (17)	0.15427 (15)	0.0326 (6)
C19	0.04282 (10)	0.69104 (17)	−0.10112 (14)	0.0317 (6)
H19A	0.0537	0.6753	−0.1334	0.038*
H19B	0.0059	0.7055	−0.1329	0.038*
C20	0.05185 (9)	0.61738 (16)	−0.05163 (14)	0.0275 (5)
C21	0.01773 (11)	0.50181 (19)	−0.14887 (15)	0.0386 (6)
H21A	0.0070	0.5500	−0.1833	0.046*
H21B	−0.0121	0.4660	−0.1642	0.046*
H21C	0.0432	0.4673	−0.1490	0.046*

C22	0.05093 (9)	0.48669 (17)	−0.01402 (14)	0.0299 (5)	
C23	0.04592 (10)	0.39947 (18)	−0.00567 (17)	0.0378 (6)	
H23	0.0324	0.3605	−0.0459	0.045*	
C24	0.06148 (11)	0.37225 (19)	0.06356 (17)	0.0388 (6)	
H24	0.0593	0.3129	0.0715	0.047*	
C25	0.08045 (10)	0.42973 (19)	0.12242 (16)	0.0371 (6)	
H25	0.0904	0.4086	0.1692	0.044*	
C26	0.08518 (10)	0.51715 (18)	0.11426 (15)	0.0325 (6)	
H26	0.0982	0.5560	0.1545	0.039*	
C27	0.07000 (9)	0.54537 (17)	0.04436 (14)	0.0281 (5)	
C28	0.08855 (12)	0.76500 (19)	0.19611 (17)	0.0377 (6)	
C29	0.10197 (13)	0.7321 (2)	0.26800 (18)	0.0443 (7)	
H29	0.1019	0.7716	0.3006	0.053*	
C30	0.11405 (12)	0.6513 (2)	0.28966 (16)	0.0410 (7)	
H30	0.1130	0.6129	0.2555	0.049*	
C31	0.12889 (11)	0.6139 (2)	0.36029 (16)	0.0392 (6)	
C32	0.14191 (12)	0.5278 (2)	0.37396 (17)	0.0418 (7)	
H32	0.1396	0.4938	0.3366	0.050*	
C33	0.15824 (11)	0.4897 (2)	0.44118 (16)	0.0405 (7)	
H33	0.1677	0.4307	0.4497	0.049*	
C34	0.16062 (11)	0.5385 (2)	0.49557 (15)	0.0380 (6)	
C35	0.14651 (12)	0.6246 (2)	0.48222 (16)	0.0422 (7)	
H35	0.1477	0.6580	0.5190	0.051*	
C36	0.13084 (12)	0.6615 (2)	0.41574 (17)	0.0424 (7)	
H36	0.1212	0.7204	0.4072	0.051*	
C37	0.30445 (16)	0.3253 (3)	0.7867 (2)	0.0781 (13)	
H37A	0.3333	0.3134	0.7837	0.094*	
H37B	0.2977	0.2747	0.8061	0.094*	
H37C	0.3128	0.3744	0.8196	0.094*	
C38	0.21247 (14)	0.3648 (2)	0.7068 (2)	0.0561 (9)	
H38A	0.1843	0.3730	0.6546	0.067*	
H38B	0.2173	0.4174	0.7344	0.067*	
H38C	0.2043	0.3170	0.7272	0.067*	
C39	0.26060 (14)	0.3424 (2)	0.6547 (2)	0.0560 (9)	
H39	0.2923	0.3266	0.6634	0.067*	
C40	0.0000	0.8452 (6)	0.2500	0.097 (2)	
H40A	−0.0110	0.8569	0.2823	0.150*	0.50
H40B	0.0117	0.7856	0.2566	0.150*	0.50
H40C	−0.0287	0.8546	0.1983	0.150*	0.50
C41	−0.1478 (3)	1.0074 (5)	0.1414 (4)	0.063 (2)	0.50
H41A	−0.1141	0.9799	0.1684	0.076*	0.50
H41B	−0.1532	1.0333	0.1767	0.076*	0.50
H41C	−0.1495	1.0522	0.1089	0.076*	0.50
C42	−0.18727 (19)	0.9434 (4)	0.0970 (3)	0.0335 (12)	0.50
H42A	−0.1789	0.8901	0.1264	0.040*	0.50
H42B	−0.2205	0.9651	0.0844	0.040*	0.50
C41'	−0.2317 (3)	0.8500 (5)	−0.0807 (4)	0.0530 (18)	0.50
H41D	−0.2421	0.9042	−0.1082	0.064*	0.50
H41E	−0.2574	0.8057	−0.1107	0.064*	0.50

H41F	−0.1985	0.8321	−0.0693	0.064*	0.50
C42'	−0.22735 (18)	0.8618 (3)	−0.0117 (3)	0.0302 (11)	0.50
H42C	−0.2612	0.8779	−0.0236	0.036*	0.50
H42D	−0.2171	0.8066	0.0155	0.036*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.02397 (19)	0.02513 (19)	0.02573 (19)	−0.00064 (10)	0.01306 (15)	−0.00058 (10)
Cl	0.0322 (4)	0.0421 (4)	0.0278 (3)	−0.0025 (3)	0.0153 (3)	−0.0015 (3)
O1	0.0539 (12)	0.0346 (11)	0.0384 (11)	0.0028 (9)	0.0296 (10)	0.0020 (9)
O2	0.0795 (17)	0.0370 (13)	0.0493 (13)	0.0159 (12)	0.0297 (13)	0.0025 (10)
O3	0.0449 (12)	0.0595 (15)	0.0357 (11)	−0.0006 (10)	0.0227 (10)	0.0042 (10)
O4	0.0324 (13)	0.143 (3)	0.0455 (15)	−0.0061 (14)	0.0147 (12)	−0.0068 (15)
O5	0.0643 (15)	0.0533 (15)	0.0580 (14)	−0.0133 (12)	0.0425 (12)	−0.0063 (11)
O6	0.097 (2)	0.0418 (14)	0.0601 (16)	0.0092 (13)	0.0463 (15)	−0.0019 (11)
O7	0.0620 (15)	0.0550 (15)	0.0397 (13)	0.0018 (11)	0.0334 (12)	−0.0026 (9)
O8	0.0632 (16)	0.0553 (16)	0.0582 (16)	0.0020 (13)	0.0276 (14)	−0.0032 (12)
O9	0.117 (5)	0.066 (4)	0.118 (5)	−0.008 (4)	0.094 (5)	−0.009 (4)
O10	0.0611 (17)	0.089 (2)	0.096 (2)	−0.0030 (16)	0.0507 (17)	−0.0127 (17)
N1	0.0275 (11)	0.0283 (12)	0.0342 (12)	0.0002 (9)	0.0133 (9)	−0.0037 (9)
N2	0.0421 (14)	0.0289 (13)	0.0353 (13)	0.0103 (11)	0.0036 (11)	−0.0054 (10)
N3	0.0260 (10)	0.0274 (11)	0.0258 (11)	−0.0033 (9)	0.0115 (9)	−0.0019 (8)
N4	0.0298 (12)	0.0365 (13)	0.0456 (14)	−0.0049 (10)	0.0227 (11)	−0.0034 (10)
N5	0.0242 (10)	0.0266 (11)	0.0277 (11)	−0.0011 (8)	0.0138 (9)	−0.0001 (8)
N6	0.0265 (11)	0.0279 (11)	0.0314 (11)	−0.0013 (9)	0.0149 (9)	−0.0043 (9)
N7	0.0281 (11)	0.0292 (11)	0.0265 (11)	−0.0023 (9)	0.0126 (9)	−0.0009 (8)
N8	0.0413 (15)	0.0469 (16)	0.0565 (17)	−0.0029 (12)	0.0217 (13)	−0.0056 (13)
C1	0.0424 (16)	0.0288 (14)	0.0314 (14)	−0.0004 (12)	0.0168 (12)	0.0032 (11)
C2	0.0318 (14)	0.0232 (13)	0.0304 (14)	0.0003 (11)	0.0066 (11)	−0.0038 (10)
C3	0.085 (3)	0.0337 (18)	0.0385 (18)	0.0203 (18)	0.0048 (18)	0.0020 (14)
C4	0.0305 (14)	0.0344 (16)	0.0473 (18)	0.0033 (12)	0.0047 (13)	−0.0187 (13)
C5	0.0387 (18)	0.047 (2)	0.073 (3)	0.0137 (16)	0.0042 (18)	−0.0307 (18)
C6	0.0307 (17)	0.065 (3)	0.097 (3)	0.0073 (17)	0.017 (2)	−0.049 (2)
C7	0.045 (2)	0.062 (2)	0.106 (3)	−0.0182 (19)	0.048 (2)	−0.050 (2)
C8	0.0380 (16)	0.0386 (17)	0.072 (2)	−0.0078 (13)	0.0332 (16)	−0.0209 (15)
C9	0.0237 (13)	0.0309 (15)	0.0496 (17)	−0.0008 (11)	0.0125 (12)	−0.0175 (12)
C10	0.0344 (15)	0.0385 (15)	0.0344 (15)	−0.0066 (12)	0.0219 (13)	−0.0046 (11)
C11	0.0264 (12)	0.0287 (13)	0.0343 (14)	−0.0010 (10)	0.0157 (11)	−0.0003 (10)
C12	0.0405 (17)	0.062 (2)	0.064 (2)	−0.0087 (15)	0.0372 (16)	−0.0047 (16)
C13	0.0294 (14)	0.0309 (14)	0.0418 (16)	−0.0038 (11)	0.0141 (12)	−0.0035 (12)
C14	0.0300 (15)	0.049 (2)	0.062 (2)	−0.0117 (14)	0.0186 (15)	−0.0070 (16)
C15	0.0369 (17)	0.054 (2)	0.0478 (19)	−0.0147 (15)	0.0070 (14)	−0.0144 (15)
C16	0.0488 (19)	0.051 (2)	0.0386 (17)	−0.0127 (15)	0.0131 (14)	−0.0116 (14)
C17	0.0398 (16)	0.0385 (16)	0.0345 (15)	−0.0076 (13)	0.0155 (13)	−0.0071 (12)
C18	0.0266 (13)	0.0260 (13)	0.0340 (14)	−0.0036 (10)	0.0110 (11)	−0.0023 (10)
C19	0.0322 (13)	0.0309 (14)	0.0273 (13)	−0.0048 (11)	0.0145 (11)	−0.0028 (10)
C20	0.0206 (11)	0.0282 (13)	0.0321 (13)	−0.0014 (10)	0.0144 (10)	−0.0027 (10)

C21	0.0391 (15)	0.0366 (16)	0.0340 (15)	−0.0045 (12)	0.0177 (12)	−0.0112 (12)
C22	0.0213 (12)	0.0307 (14)	0.0357 (14)	−0.0012 (10)	0.0154 (10)	−0.0014 (10)
C23	0.0300 (14)	0.0287 (14)	0.0503 (17)	−0.0034 (11)	0.0208 (13)	−0.0046 (12)
C24	0.0331 (14)	0.0276 (14)	0.0550 (18)	−0.0002 (11)	0.0251 (13)	0.0057 (12)
C25	0.0324 (14)	0.0346 (15)	0.0441 (16)	0.0035 (12)	0.0220 (12)	0.0095 (12)
C26	0.0272 (13)	0.0322 (14)	0.0371 (14)	0.0016 (11)	0.0180 (11)	0.0025 (11)
C27	0.0204 (11)	0.0268 (13)	0.0343 (13)	0.0000 (10)	0.0142 (10)	0.0017 (10)
C28	0.0375 (16)	0.0370 (16)	0.0394 (16)	0.0037 (12)	0.0227 (13)	−0.0004 (12)
C29	0.0499 (18)	0.0475 (18)	0.0404 (17)	0.0026 (14)	0.0290 (15)	−0.0028 (13)
C30	0.0473 (17)	0.0427 (17)	0.0394 (16)	−0.0042 (13)	0.0288 (14)	−0.0061 (12)
C31	0.0408 (15)	0.0434 (17)	0.0385 (15)	−0.0075 (13)	0.0258 (13)	−0.0043 (12)
C32	0.0463 (17)	0.0444 (17)	0.0403 (16)	−0.0071 (13)	0.0283 (14)	−0.0057 (13)
C33	0.0405 (15)	0.0425 (17)	0.0427 (16)	−0.0062 (13)	0.0265 (13)	−0.0002 (13)
C34	0.0311 (14)	0.0500 (18)	0.0331 (15)	−0.0073 (12)	0.0187 (12)	−0.0005 (12)
C35	0.0434 (16)	0.0506 (18)	0.0377 (16)	−0.0070 (14)	0.0265 (13)	−0.0069 (13)
C36	0.0441 (16)	0.0423 (17)	0.0445 (17)	−0.0028 (13)	0.0278 (14)	−0.0037 (13)
C37	0.055 (2)	0.100 (4)	0.061 (2)	0.003 (2)	0.023 (2)	−0.006 (2)
C38	0.054 (2)	0.0449 (19)	0.068 (2)	−0.0019 (16)	0.0347 (18)	−0.0066 (16)
C39	0.050 (2)	0.050 (2)	0.066 (2)	−0.0037 (16)	0.0325 (19)	−0.0086 (17)
C40	0.094 (5)	0.111 (6)	0.125 (6)	0.000	0.086 (5)	0.000
C41	0.042 (4)	0.078 (5)	0.033 (3)	0.011 (3)	0.000 (3)	−0.023 (3)
C42	0.025 (2)	0.046 (3)	0.018 (2)	0.016 (2)	0.006 (2)	0.008 (2)
C41'	0.040 (3)	0.076 (5)	0.051 (4)	−0.020 (3)	0.031 (3)	−0.033 (3)
C42'	0.015 (2)	0.032 (3)	0.041 (3)	0.0020 (19)	0.014 (2)	−0.007 (2)

Geometric parameters (Å, °)

Zn—O1	1.9745 (19)	C13—C14	1.401 (4)
Zn—N1	2.041 (2)	C14—C15	1.370 (5)
Zn—N3	2.064 (2)	C14—H14	0.9500
Zn—N5	2.066 (2)	C15—C16	1.385 (5)
Zn—N7	2.452 (2)	C15—H15	0.9500
Cl—O4	1.424 (3)	C16—C17	1.392 (4)
Cl—O5	1.429 (2)	C16—H16	0.9500
Cl—O7	1.437 (2)	C17—C18	1.384 (4)
Cl—O6	1.445 (3)	C17—H17	0.9500
O1—C28	1.270 (4)	C19—C20	1.494 (4)
O2—C28	1.233 (4)	C19—H19A	0.9900
O3—C34	1.359 (3)	C19—H19B	0.9900
O3—H3	0.8400	C21—H21A	0.9800
O8—C39	1.237 (4)	C21—H21B	0.9800
O9—C40	1.302 (8)	C21—H21C	0.9800
O9—H9	0.8400	C22—C23	1.391 (4)
O10—C42	1.358 (6)	C22—C27	1.402 (4)
O10—C42'	1.402 (6)	C23—C24	1.377 (4)
O10—H10	0.8400	C23—H23	0.9500
N1—C2	1.325 (4)	C24—C25	1.397 (4)
N1—C9	1.403 (4)	C24—H24	0.9500
N2—C2	1.345 (4)	C25—C26	1.392 (4)

N2—C4	1.384 (5)	C25—H25	0.9500
N2—C3	1.467 (5)	C26—C27	1.398 (4)
N3—C11	1.318 (3)	C26—H26	0.9500
N3—C18	1.407 (3)	C28—C29	1.480 (4)
N4—C11	1.354 (3)	C29—C30	1.321 (5)
N4—C13	1.387 (4)	C29—H29	0.9500
N4—C12	1.461 (4)	C30—C31	1.467 (4)
N5—C20	1.325 (3)	C30—H30	0.9500
N5—C27	1.396 (3)	C31—C32	1.384 (5)
N6—C20	1.349 (3)	C31—C36	1.404 (4)
N6—C22	1.385 (3)	C32—C33	1.394 (4)
N6—C21	1.466 (3)	C32—H32	0.9500
N7—C1	1.459 (4)	C33—C34	1.389 (4)
N7—C10	1.466 (4)	C33—H33	0.9500
N7—C19	1.467 (3)	C34—C35	1.389 (5)
N8—C39	1.320 (5)	C35—C36	1.378 (4)
N8—C38	1.449 (5)	C35—H35	0.9500
N8—C37	1.462 (5)	C36—H36	0.9500
C1—C2	1.490 (4)	C37—H37A	0.9800
C1—H1A	0.9900	C37—H37B	0.9800
C1—H1B	0.9900	C37—H37C	0.9800
C3—H3A	0.9800	C38—H38A	0.9800
C3—H3B	0.9800	C38—H38B	0.9800
C3—H3C	0.9800	C38—H38C	0.9800
C4—C9	1.397 (5)	C39—H39	0.9500
C4—C5	1.398 (5)	C40—O9^{i}	1.302 (8)
C5—C6	1.350 (7)	C40—H40A	0.9801
C5—H5	0.9500	C40—H40B	0.9801
C6—C7	1.404 (7)	C40—H40C	0.9801
C6—H6	0.9500	C41—C42	1.456 (9)
C7—C8	1.391 (5)	C41—H41A	0.9800
C7—H7	0.9500	C41—H41B	0.9800
C8—C9	1.385 (5)	C41—H41C	0.9800
C8—H8	0.9500	C42—H42A	0.9900
C10—C11	1.495 (4)	C42—H42B	0.9900
C10—H10A	0.9900	C41'—C42'	1.462 (8)
C10—H10B	0.9900	C41'—H41D	0.9800
C12—H12A	0.9800	C41'—H41E	0.9800
C12—H12B	0.9800	C41'—H41F	0.9800
C12—H12C	0.9800	C42'—H42C	0.9900
C13—C18	1.393 (4)	C42'—H42D	0.9900
O1—Zn—N1	115.56 (9)	C13—C14—H14	121.9
O1—Zn—N3	107.42 (9)	C14—C15—C16	122.2 (3)
N1—Zn—N3	110.27 (9)	C14—C15—H15	118.9
O1—Zn—N5	94.39 (8)	C16—C15—H15	118.9
N1—Zn—N5	114.30 (8)	C15—C16—C17	121.6 (3)
N3—Zn—N5	114.00 (8)	C15—C16—H16	119.2
O1—Zn—N7	167.08 (8)	C17—C16—H16	119.2

N1—Zn—N7	74.75 (9)	C18—C17—C16	117.0 (3)
N3—Zn—N7	74.16 (8)	C18—C17—H17	121.5
N5—Zn—N7	73.64 (8)	C16—C17—H17	121.5
O4—Cl—O5	109.65 (18)	C17—C18—C13	120.8 (3)
O4—Cl—O7	111.16 (17)	C17—C18—N3	130.8 (3)
O5—Cl—O7	109.44 (14)	C13—C18—N3	108.3 (2)
O4—Cl—O6	109.59 (19)	N7—C19—C20	108.6 (2)
O5—Cl—O6	107.67 (16)	N7—C19—H19A	110.0
O7—Cl—O6	109.26 (15)	C20—C19—H19A	110.0
C28—O1—Zn	121.4 (2)	N7—C19—H19B	110.0
C34—O3—H3	109.5	C20—C19—H19B	110.0
C40—O9—H9	109.5	H19A—C19—H19B	108.3
O9—C40—H40A	109.4	N5—C20—N6	112.7 (2)
O9—C40—H40B	109.5	N5—C20—C19	122.8 (2)
H40A—C40—H40B	109.5	N6—C20—C19	124.4 (2)
O9—C40—H40C	109.6	N6—C21—H21A	109.5
H40A—C40—H40C	109.5	N6—C21—H21B	109.5
H40B—C40—H40C	109.5	H21A—C21—H21B	109.5
C42—O10—C42'	116.2 (4)	N6—C21—H21C	109.5
C42—O10—H10	109.5	H21A—C21—H21C	109.5
C42'—O10—H10	104.3	H21B—C21—H21C	109.5
C2—N1—C9	105.6 (2)	N6—C22—C23	132.2 (2)
C2—N1—Zn	117.95 (19)	N6—C22—C27	105.5 (2)
C9—N1—Zn	135.9 (2)	C23—C22—C27	122.3 (3)
C2—N2—C4	107.0 (3)	C24—C23—C22	116.9 (3)
C2—N2—C3	124.8 (3)	C24—C23—H23	121.5
C4—N2—C3	128.1 (3)	C22—C23—H23	121.5
C11—N3—C18	105.7 (2)	C23—C24—C25	121.6 (3)
C11—N3—Zn	118.18 (17)	C23—C24—H24	119.2
C18—N3—Zn	135.24 (18)	C25—C24—H24	119.2
C11—N4—C13	106.9 (2)	C26—C25—C24	121.7 (3)
C11—N4—C12	128.0 (3)	C26—C25—H25	119.1
C13—N4—C12	125.0 (3)	C24—C25—H25	119.1
C20—N5—C27	105.4 (2)	C25—C26—C27	117.2 (3)
C20—N5—Zn	118.93 (17)	C25—C26—H26	121.4
C27—N5—Zn	134.36 (17)	C27—C26—H26	121.4
C20—N6—C22	107.4 (2)	N5—C27—C26	130.8 (2)
C20—N6—C21	126.9 (2)	N5—C27—C22	109.0 (2)
C22—N6—C21	125.6 (2)	C26—C27—C22	120.3 (2)
C1—N7—C10	113.3 (2)	O2—C28—O1	124.0 (3)
C1—N7—C19	112.7 (2)	O2—C28—C29	118.0 (3)
C10—N7—C19	113.3 (2)	O1—C28—C29	117.9 (3)
C1—N7—Zn	105.75 (17)	C30—C29—C28	124.1 (3)
C10—N7—Zn	104.69 (16)	C30—C29—H29	117.9
C19—N7—Zn	106.14 (16)	C28—C29—H29	117.9
C39—N8—C38	122.4 (3)	C29—C30—C31	127.6 (3)
C39—N8—C37	120.6 (3)	C29—C30—H30	116.2
C38—N8—C37	117.0 (3)	C31—C30—H30	116.2
N7—C1—C2	108.7 (2)	C32—C31—C36	117.6 (3)

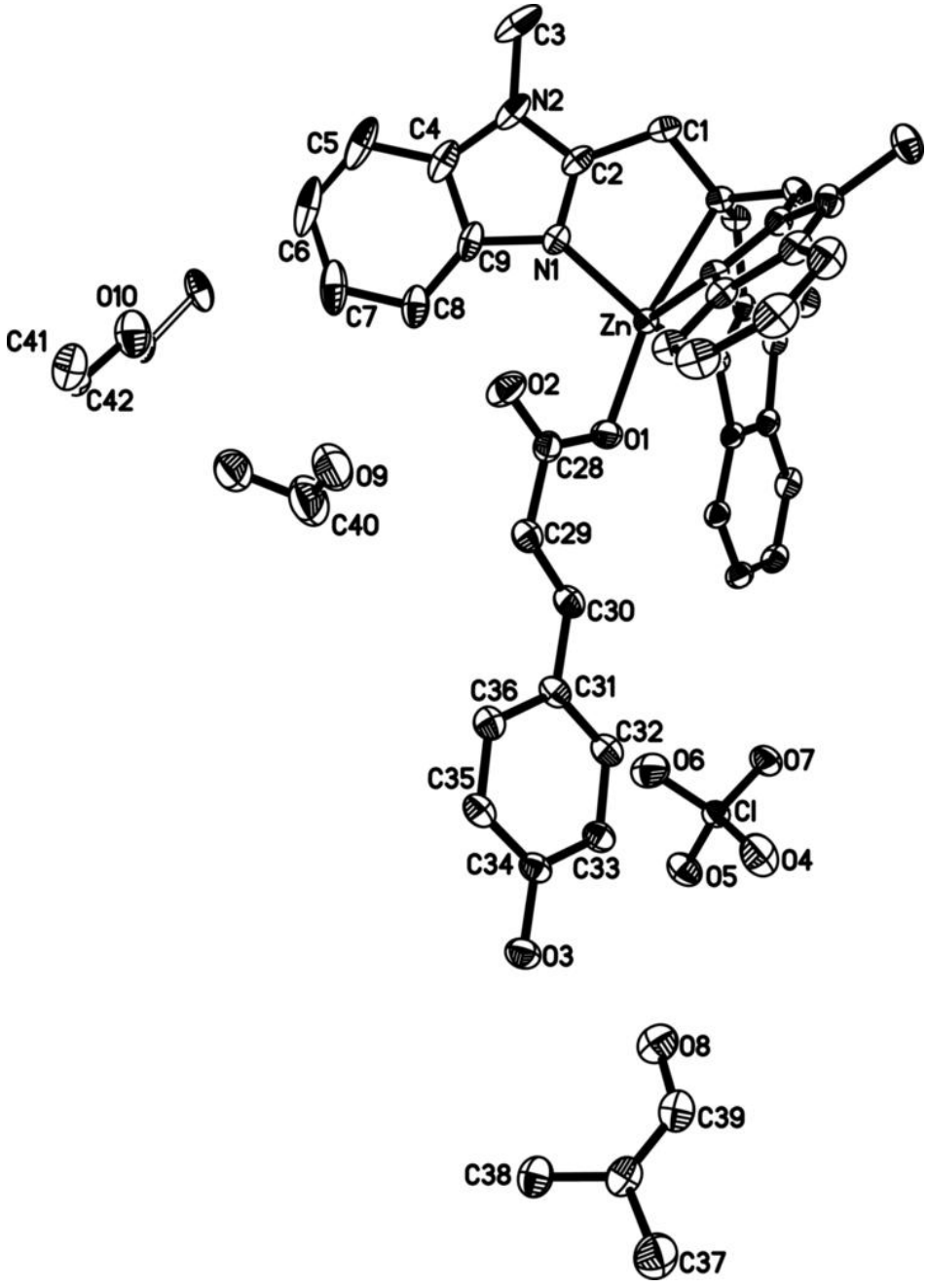
N7—C1—H1A	109.9	C32—C31—C30	119.2 (3)
C2—C1—H1A	109.9	C36—C31—C30	123.1 (3)
N7—C1—H1B	109.9	C31—C32—C33	121.7 (3)
C2—C1—H1B	109.9	C31—C32—H32	119.2
H1A—C1—H1B	108.3	C33—C32—H32	119.2
N1—C2—N2	112.8 (3)	C34—C33—C32	119.5 (3)
N1—C2—C1	124.2 (2)	C34—C33—H33	120.2
N2—C2—C1	123.0 (3)	C32—C33—H33	120.2
N2—C3—H3A	109.5	O3—C34—C33	122.7 (3)
N2—C3—H3B	109.5	O3—C34—C35	117.6 (3)
H3A—C3—H3B	109.5	C33—C34—C35	119.6 (3)
N2—C3—H3C	109.5	C36—C35—C34	120.2 (3)
H3A—C3—H3C	109.5	C36—C35—H35	119.9
H3B—C3—H3C	109.5	C34—C35—H35	119.9
N2—C4—C9	106.5 (3)	C35—C36—C31	121.3 (3)
N2—C4—C5	131.6 (4)	C35—C36—H36	119.4
C9—C4—C5	121.9 (4)	C31—C36—H36	119.4
C6—C5—C4	117.4 (4)	N8—C37—H37A	109.5
C6—C5—H5	121.3	N8—C37—H37B	109.5
C4—C5—H5	121.3	H37A—C37—H37B	109.5
C5—C6—C7	121.4 (3)	N8—C37—H37C	109.5
C5—C6—H6	119.3	H37A—C37—H37C	109.5
C7—C6—H6	119.3	H37B—C37—H37C	109.5
C8—C7—C6	121.9 (4)	N8—C38—H38A	109.5
C8—C7—H7	119.1	N8—C38—H38B	109.5
C6—C7—H7	119.1	H38A—C38—H38B	109.5
C9—C8—C7	116.8 (4)	N8—C38—H38C	109.5
C9—C8—H8	121.6	H38A—C38—H38C	109.5
C7—C8—H8	121.6	H38B—C38—H38C	109.5
C8—C9—C4	120.6 (3)	O8—C39—N8	126.4 (4)
C8—C9—N1	131.3 (3)	O8—C39—H39	116.8
C4—C9—N1	108.1 (3)	N8—C39—H39	116.8
N7—C10—C11	108.6 (2)	O9—C40—O9^{i}	104.1 (9)
N7—C10—H10A	110.0	O10—C42—C41	111.7 (5)
C11—C10—H10A	110.0	O10—C42—H42A	109.3
N7—C10—H10B	110.0	C41—C42—H42A	109.3
C11—C10—H10B	110.0	O10—C42—H42B	109.3
H10A—C10—H10B	108.4	C41—C42—H42B	109.3
N3—C11—N4	112.7 (2)	H42A—C42—H42B	107.9
N3—C11—C10	123.0 (2)	C42'—C41'—H41D	109.5
N4—C11—C10	124.2 (2)	C42'—C41'—H41E	109.5
N4—C12—H12A	109.5	H41D—C41'—H41E	109.5
N4—C12—H12B	109.5	C42'—C41'—H41F	109.5
H12A—C12—H12B	109.5	H41D—C41'—H41F	109.5
N4—C12—H12C	109.5	H41E—C41'—H41F	109.5
H12A—C12—H12C	109.5	O10—C42'—C41'	112.5 (5)
H12B—C12—H12C	109.5	O10—C42'—H42C	109.1
N4—C13—C18	106.3 (2)	C41'—C42'—H42C	109.1
N4—C13—C14	131.7 (3)	O10—C42'—H42D	109.1

C18—C13—C14	122.0 (3)	C41'—C42'—H42D	109.1
C15—C14—C13	116.3 (3)	H42C—C42'—H42D	107.8
C15—C14—H14	121.9		
N1—Zn—O1—C28	−51.9 (3)	C13—N4—C11—N3	2.1 (3)
N3—Zn—O1—C28	71.7 (2)	C12—N4—C11—N3	−180.0 (3)
N5—Zn—O1—C28	−171.5 (2)	C13—N4—C11—C10	−174.6 (3)
N7—Zn—O1—C28	166.7 (3)	C12—N4—C11—C10	3.4 (5)
O1—Zn—N1—C2	171.17 (18)	N7—C10—C11—N3	23.3 (4)
N3—Zn—N1—C2	49.1 (2)	N7—C10—C11—N4	−160.3 (3)
N5—Zn—N1—C2	−80.8 (2)	C11—N4—C13—C18	−2.1 (3)
N7—Zn—N1—C2	−17.14 (18)	C12—N4—C13—C18	179.8 (3)
O1—Zn—N1—C9	0.7 (3)	C11—N4—C13—C14	174.6 (3)
N3—Zn—N1—C9	−121.3 (3)	C12—N4—C13—C14	−3.4 (5)
N5—Zn—N1—C9	108.7 (3)	N4—C13—C14—C15	−177.9 (3)
N7—Zn—N1—C9	172.4 (3)	C18—C13—C14—C15	−1.6 (5)
O1—Zn—N3—C11	148.31 (19)	C13—C14—C15—C16	−1.0 (5)
N1—Zn—N3—C11	−85.0 (2)	C14—C15—C16—C17	1.8 (6)
N5—Zn—N3—C11	45.2 (2)	C15—C16—C17—C18	0.1 (5)
N7—Zn—N3—C11	−18.31 (19)	C16—C17—C18—C13	−2.6 (4)
O1—Zn—N3—C18	−19.2 (3)	C16—C17—C18—N3	176.2 (3)
N1—Zn—N3—C18	107.5 (2)	N4—C13—C18—C17	−179.4 (3)
N5—Zn—N3—C18	−122.3 (2)	C14—C13—C18—C17	3.5 (5)
N7—Zn—N3—C18	174.2 (3)	N4—C13—C18—N3	1.5 (3)
O1—Zn—N5—C20	165.98 (18)	C14—C13—C18—N3	−175.6 (3)
N1—Zn—N5—C20	45.3 (2)	C11—N3—C18—C17	−179.2 (3)
N3—Zn—N5—C20	−82.75 (19)	Zn—N3—C18—C17	−10.7 (5)
N7—Zn—N5—C20	−18.98 (17)	C11—N3—C18—C13	−0.3 (3)
O1—Zn—N5—C27	1.3 (2)	Zn—N3—C18—C13	168.3 (2)
N1—Zn—N5—C27	−119.3 (2)	C1—N7—C19—C20	−145.2 (2)
N3—Zn—N5—C27	112.6 (2)	C10—N7—C19—C20	84.4 (3)
N7—Zn—N5—C27	176.3 (2)	Zn—N7—C19—C20	−29.9 (2)
O1—Zn—N7—C1	169.7 (3)	C27—N5—C20—N6	−0.3 (3)
N1—Zn—N7—C1	25.38 (17)	Zn—N5—C20—N6	−168.96 (16)
N3—Zn—N7—C1	−91.39 (17)	C27—N5—C20—C19	176.5 (2)
N5—Zn—N7—C1	147.02 (18)	Zn—N5—C20—C19	7.8 (3)
O1—Zn—N7—C10	−70.4 (4)	C22—N6—C20—N5	0.5 (3)
N1—Zn—N7—C10	145.32 (18)	C21—N6—C20—N5	178.0 (2)
N3—Zn—N7—C10	28.54 (16)	C22—N6—C20—C19	−176.2 (2)
N5—Zn—N7—C10	−93.05 (17)	C21—N6—C20—C19	1.3 (4)
O1—Zn—N7—C19	49.8 (4)	N7—C19—C20—N5	18.8 (3)
N1—Zn—N7—C19	−94.54 (17)	N7—C19—C20—N6	−164.8 (2)
N3—Zn—N7—C19	148.68 (18)	C20—N6—C22—C23	179.4 (3)
N5—Zn—N7—C19	27.09 (16)	C21—N6—C22—C23	1.9 (4)
C10—N7—C1—C2	−142.1 (2)	C20—N6—C22—C27	−0.6 (3)
C19—N7—C1—C2	87.5 (3)	C21—N6—C22—C27	−178.0 (2)
Zn—N7—C1—C2	−28.0 (2)	N6—C22—C23—C24	178.9 (3)
C9—N1—C2—N2	0.9 (3)	C27—C22—C23—C24	−1.1 (4)
Zn—N1—C2—N2	−172.19 (18)	C22—C23—C24—C25	1.3 (4)
C9—N1—C2—C1	179.5 (2)	C23—C24—C25—C26	−0.8 (4)

Zn—N1—C2—C1	6.4 (3)	C24—C25—C26—C27	0.1 (4)
C4—N2—C2—N1	−0.2 (3)	C20—N5—C27—C26	179.8 (3)
C3—N2—C2—N1	−177.5 (3)	Zn—N5—C27—C26	−14.0 (4)
C4—N2—C2—C1	−178.8 (2)	C20—N5—C27—C22	−0.1 (3)
C3—N2—C2—C1	3.9 (4)	Zn—N5—C27—C22	166.01 (18)
N7—C1—C2—N1	18.5 (4)	C25—C26—C27—N5	−179.9 (3)
N7—C1—C2—N2	−163.1 (2)	C25—C26—C27—C22	0.0 (4)
C2—N2—C4—C9	−0.6 (3)	N6—C22—C27—N5	0.4 (3)
C3—N2—C4—C9	176.6 (3)	C23—C22—C27—N5	−179.6 (2)
C2—N2—C4—C5	−179.6 (3)	N6—C22—C27—C26	−179.5 (2)
C3—N2—C4—C5	−2.4 (5)	C23—C22—C27—C26	0.5 (4)
N2—C4—C5—C6	177.9 (3)	Zn—O1—C28—O2	4.6 (4)
C9—C4—C5—C6	−1.0 (5)	Zn—O1—C28—C29	−172.9 (2)
C4—C5—C6—C7	0.2 (5)	O2—C28—C29—C30	−176.3 (3)
C5—C6—C7—C8	0.6 (5)	O1—C28—C29—C30	1.4 (5)
C6—C7—C8—C9	−0.5 (5)	C28—C29—C30—C31	178.5 (3)
C7—C8—C9—C4	−0.3 (4)	C29—C30—C31—C32	−177.9 (3)
C7—C8—C9—N1	−179.3 (3)	C29—C30—C31—C36	1.9 (5)
N2—C4—C9—C8	−178.0 (3)	C36—C31—C32—C33	−2.3 (4)
C5—C4—C9—C8	1.1 (4)	C30—C31—C32—C33	177.4 (3)
N2—C4—C9—N1	1.2 (3)	C31—C32—C33—C34	1.4 (5)
C5—C4—C9—N1	−179.7 (3)	C32—C33—C34—O3	179.6 (3)
C2—N1—C9—C8	177.8 (3)	C32—C33—C34—C35	0.3 (4)
Zn—N1—C9—C8	−11.0 (5)	O3—C34—C35—C36	179.8 (3)
C2—N1—C9—C4	−1.3 (3)	C33—C34—C35—C36	−0.8 (4)
Zn—N1—C9—C4	170.0 (2)	C34—C35—C36—C31	−0.2 (5)
C1—N7—C10—C11	81.8 (3)	C32—C31—C36—C35	1.8 (4)
C19—N7—C10—C11	−148.2 (2)	C30—C31—C36—C35	−178.0 (3)
Zn—N7—C10—C11	−32.9 (2)	C38—N8—C39—O8	2.8 (6)
C18—N3—C11—N4	−1.1 (3)	C37—N8—C39—O8	−179.9 (4)
Zn—N3—C11—N4	−172.02 (18)	C42'—O10—C42—C41	177.7 (5)
C18—N3—C11—C10	175.6 (2)	C42—O10—C42'—C41'	176.5 (5)
Zn—N3—C11—C10	4.7 (3)		

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

Fig. 1


C3
N2
C4
C5
C1
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C6
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N1
C7
C8
Zn
O10
C41
C42
O2
O1
C28
O9
C40
C29
C30
C36
C31
C32
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C34
C33
O5
O4
O3
O8
C39
C38
C37

Fig. 2