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Bis{*N*-[(1*Z*,3*Z*)-1,3-bis(4-fluorophenyl)-3-(phenylimino)prop-1-enyl]aniline(1–)}-zinc(II)

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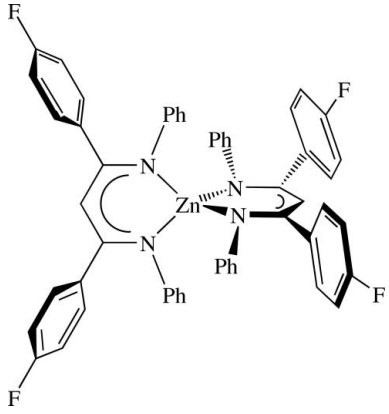
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 15.0.

In the title complex, $[Zn(C_{27}H_{19}F_2N_2)_2]$, a twofold rotation axis passes through the Zn atom, which is tetrahedrally coordinated by four N atoms from two diketiminate ligands. There are no intermolecular interactions of note in the crystal structure.

Related literature

For related literature, see: Chamberlain *et al.* (1999, 2001); Chen *et al.* (2005); Chisholm *et al.* (2003); Duda *et al.* (1990); Endo *et al.* (1987); Ko & Lin (2001); Rieth *et al.* (2002); Sawhney *et al.* (1993); Shueh *et al.* (2004); Simic *et al.* (1997); Stevels *et al.* (1996); Wu *et al.* (2006); Ni & Yu (1998).



Experimental

Crystal data

$[Zn(C_{27}H_{19}F_2N_2)_2]$
M_r = 884.26
Monoclinic, $C2/c$
a = 21.967 (2) Å
b = 10.6232 (10) Å
c = 19.2852 (19) Å
β = 106.102 (2)°
V = 4323.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 298 (2) K
0.50 × 0.25 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*, Sheldrick, 1996)
T_{min} = 0.524, T_{max} = 1.000
(expected range = 0.480–0.916)
12028 measured reflections
4272 independent reflections
3043 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
S = 0.95
4272 reflections
285 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); 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: GG2033).

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supplementary materials

Acta Cryst. (2007). E**63**, m2388 [**doi:10.1107/S1600536807040123**]

Bis{*N*-[(1*Z*,3*Z*)-1,3-bis(4-fluorophenyl)-3-(phenylimino)prop-1-enyl]aniline(1-)}zinc(II)

Y.-L. Peng, M.-L. Hsueh and C.-C. Lin

Comment

Biodegradable polymers have been attracting considerable attention recently due to their potential applications in the environmental protection as well as in the medical field. Among biodegradable polymers, the aliphatic polyesters, such as poly(ε-caprolactone) (PCL), (Endo *et al.*, 1987) poly(lactide) (PLA) (Chamberlain *et al.*, 1999), and their copolymers are especially interested for their applications in the medical field as biodegradable surgical sutures or as a delivery medium for controlled release of drugs (Ni & Yu, 1997). Therefore, there has been increasing interest in the development of efficient catalytic systems for the preparation of PLA and PCL (Wu *et al.*, 2006). The major polymerization method used to synthesize these polymers has been the ring-opening polymerization (ROP) of lactones/lactides and functionally related compounds. For examples, aluminium alkoxides (Duda *et al.*, 1990), stannous (Sawhney *et al.*, 1993), yttrium (Stevels *et al.*, 1996) as well as trivalent lanthanide derivatives (Simic *et al.*, 1997), lithium (Ko & Lin, 2001), magnesium (Shueh *et al.*, 2004; Chamberlain *et al.*, 2001), calcium (Chisholm *et al.*, 2003) and zinc (Chamberlain *et al.*, 2001; Rieth *et al.*, 2002) have been reported to be effective initiators that initiate ROP of lactones/lactides, yielding polymers with both high molecular weights and high yields. Among them, zinc diketiminato-based catalytic systems are especially attracted and well suited as initiators for the ROP of lactones and lactides due to their high Lewis acidity. Recently, we have reported that Zn complexes of diketiminato-based ligands are very active catalysts for ROP of lactide (Chen *et al.*, 2005). Herein, we report the crystal structure of a potentially useful Zn complex with bulky diketiminato ligands.

In the title mononuclear Zn^{II} compound, the Zn atom is tetracoordinated with four N atoms from two diketiminato ligands (Fig. 1). The Zn atom lies on a C_2 rotation symmetry. By comparison with the Zn complexes reported in the literature, we notice that the Zn—N coordinated bond distances (1.989 (2) and 1.994 (2) Å)(Table 1) of the title compound are consistent with that reported for [(BDI-**2**)Zn(μ–O*i*Pr)]$_2$ (1.990 (8) and 2.021 (7) Å) (Chamberlain *et al.*, 2001).

Experimental

The title compound was prepared by the reaction of *N*-((1*Z*,3*Z*)-1,3-bis(4-fluorophenyl)-3-(phenylimino)prop-1-enyl)benzenamine (0.82 g, 2.0 mmol) with $ZnEt_2$ (1.1 ml, 1.0 *M* in hexane, 1.1 mmol) in hexane (20 ml). The mixture was stirred at 25°C for 6 h and was then evaporated to dryness under vacuum. The residue was extracted with hot hexane (30 ml), and the resulting hexane solution was then concentrated to *ca* 15 ml. Yellow crystals were obtained at room temperature after 16 h. Yield: 0.61 g (69%).

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

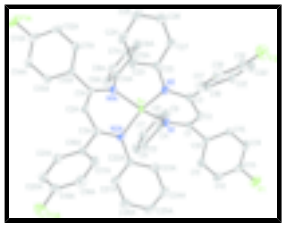


Fig. 1. A view of the molecular structure of (I) with displacement ellipsoids shown at the 20% probability level. All the H atoms are omitted for clarity.

Bis{*N*-[(1*Z*,3*Z*)-1,3-bis(4-fluorophenyl)-3- (phenylimino)prop-1-enyl]aniline(1-)}zinc(II)

Crystal data

$[Zn(C_{27}H_{19}F_2N_2)_2]$	F_{000} = 1824
M_r = 884.26	D_x = 1.358 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3748 reflections
a = 21.967 (2) Å	θ = 2.5–25.5º
b = 10.6232 (10) Å	μ = 0.63 mm^{-1}
c = 19.2852 (19) Å	*T* = 298 (2) K
β = 106.102 (2)º	Parallelpiped, yellow
V = 4323.8 (7) Å^3	0.50 × 0.25 × 0.14 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	4272 independent reflections
Radiation source: fine-focus sealed tube	3043 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.048
T = 298(2) K	θ_{max} = 26.1º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS, Sheldrick, 1996)	*h* = −27→24
T_{min} = 0.524, T_{max} = 1.000	*k* = −13→11
12028 measured reflections	*l* = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.95	$(\Delta/\sigma)_{max}$ = 0.001

4272 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
285 parameters	$\Delta\rho_{min} = -0.30$ 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.5000	0.15528 (4)	1.2500	0.03975 (14)
F1	0.72953 (9)	0.0113 (2)	0.97921 (11)	0.0977 (7)
F2	0.33272 (10)	0.65322 (18)	0.92235 (10)	0.0936 (6)
N1	0.54684 (9)	0.06780 (18)	1.18950 (9)	0.0403 (5)
N2	0.44306 (9)	0.25386 (19)	1.16987 (9)	0.0424 (5)
C1	0.55117 (11)	0.1220 (2)	1.12847 (11)	0.0391 (5)
C2	0.51558 (11)	0.2276 (2)	1.09706 (11)	0.0428 (6)
H2A	0.5292	0.2669	1.0609	0.051*
C3	0.46282 (11)	0.2823 (2)	1.11195 (11)	0.0412 (5)
C4	0.57425 (12)	−0.0522 (2)	1.21246 (12)	0.0429 (6)
C5	0.62314 (13)	−0.0624 (3)	1.27565 (13)	0.0550 (7)
H5A	0.6406	0.0097	1.3008	0.066*
C6	0.64604 (16)	−0.1804 (3)	1.30144 (15)	0.0682 (9)
H6A	0.6791	−0.1869	1.3436	0.082*
C7	0.62031 (17)	−0.2870 (3)	1.26521 (18)	0.0714 (9)
H7A	0.6355	−0.3658	1.2828	0.086*
C8	0.57228 (17)	−0.2772 (3)	1.20321 (18)	0.0709 (9)
H8A	0.5551	−0.3497	1.1784	0.085*
C9	0.54883 (15)	−0.1610 (3)	1.17676 (15)	0.0587 (7)
H9A	0.5157	−0.1559	1.1346	0.070*
C10	0.59870 (11)	0.0783 (2)	1.09063 (12)	0.0401 (5)
C11	0.66212 (12)	0.0696 (2)	1.12655 (13)	0.0495 (6)
H11A	0.6753	0.0790	1.1764	0.059*
C12	0.70666 (13)	0.0471 (3)	1.08923 (16)	0.0581 (7)
H12A	0.7495	0.0419	1.1135	0.070*
C13	0.68610 (14)	0.0326 (3)	1.01600 (16)	0.0596 (7)
C14	0.62417 (15)	0.0373 (3)	0.97884 (14)	0.0583 (7)
H14A	0.6115	0.0241	0.9292	0.070*

C15	0.57990 (12)	0.0620 (3)	1.01597 (12)	0.0486 (6)
H15A	0.5372	0.0678	0.9909	0.058*
C16	0.42858 (11)	0.3809 (2)	1.06036 (12)	0.0411 (6)
C17	0.41609 (13)	0.4975 (2)	1.08620 (14)	0.0534 (7)
H17A	0.4291	0.5132	1.1356	0.064*
C18	0.38494 (15)	0.5900 (3)	1.04009 (16)	0.0625 (8)
H18A	0.3771	0.6682	1.0576	0.075*
C19	0.36572 (14)	0.5641 (3)	0.96792 (16)	0.0629 (8)
C20	0.37753 (14)	0.4522 (3)	0.93986 (14)	0.0633 (8)
H20A	0.3641	0.4377	0.8904	0.076*
C21	0.40987 (13)	0.3606 (3)	0.98648 (13)	0.0540 (7)
H21A	0.4192	0.2844	0.9681	0.065*
C22	0.37975 (12)	0.2775 (2)	1.17125 (12)	0.0434 (6)
C23	0.36800 (14)	0.3224 (3)	1.23379 (14)	0.0563 (7)
H23A	0.4014	0.3478	1.2725	0.068*
C24	0.30590 (17)	0.3294 (3)	1.23820 (17)	0.0731 (10)
H24A	0.2982	0.3601	1.2801	0.088*
C25	0.25627 (16)	0.2920 (3)	1.1824 (2)	0.0775 (10)
H25A	0.2151	0.2958	1.1866	0.093*
C26	0.26751 (14)	0.2485 (3)	1.11993 (17)	0.0688 (8)
H26A	0.2338	0.2239	1.0813	0.083*
C27	0.32846 (12)	0.2416 (2)	1.11452 (14)	0.0513 (6)
H27A	0.3355	0.2123	1.0720	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0429 (2)	0.0499 (3)	0.0307 (2)	0.000	0.01727 (16)	0.000
F1	0.0807 (14)	0.1299 (18)	0.1090 (14)	0.0018 (12)	0.0703 (12)	−0.0228 (13)
F2	0.1059 (16)	0.0791 (13)	0.0928 (13)	0.0291 (11)	0.0227 (12)	0.0447 (11)
N1	0.0457 (12)	0.0467 (11)	0.0319 (9)	0.0068 (9)	0.0167 (8)	0.0036 (9)
N2	0.0427 (12)	0.0517 (12)	0.0372 (10)	0.0062 (9)	0.0182 (9)	0.0043 (9)
C1	0.0383 (13)	0.0491 (14)	0.0323 (11)	0.0012 (10)	0.0138 (10)	0.0006 (10)
C2	0.0458 (15)	0.0536 (15)	0.0345 (11)	0.0054 (11)	0.0202 (10)	0.0083 (11)
C3	0.0437 (14)	0.0472 (14)	0.0349 (11)	0.0016 (11)	0.0144 (10)	0.0003 (11)
C4	0.0498 (15)	0.0502 (15)	0.0354 (11)	0.0061 (12)	0.0231 (11)	0.0050 (11)
C5	0.0649 (19)	0.0583 (17)	0.0425 (13)	0.0105 (14)	0.0163 (13)	0.0038 (12)
C6	0.082 (2)	0.074 (2)	0.0500 (16)	0.0247 (17)	0.0200 (15)	0.0170 (15)
C7	0.097 (3)	0.0561 (19)	0.074 (2)	0.0246 (18)	0.0461 (19)	0.0225 (17)
C8	0.094 (3)	0.0479 (18)	0.081 (2)	−0.0023 (16)	0.041 (2)	−0.0005 (16)
C9	0.0685 (19)	0.0552 (17)	0.0527 (15)	−0.0006 (15)	0.0174 (13)	−0.0014 (14)
C10	0.0419 (14)	0.0427 (13)	0.0406 (12)	0.0028 (10)	0.0196 (11)	0.0040 (10)
C11	0.0504 (17)	0.0556 (16)	0.0461 (13)	0.0068 (12)	0.0195 (12)	0.0024 (12)
C12	0.0415 (16)	0.0621 (18)	0.0756 (18)	0.0077 (13)	0.0247 (14)	0.0039 (15)
C13	0.0573 (19)	0.0666 (19)	0.0701 (18)	0.0022 (14)	0.0431 (15)	−0.0042 (15)
C14	0.071 (2)	0.0680 (18)	0.0461 (14)	−0.0005 (15)	0.0338 (14)	−0.0049 (13)
C15	0.0453 (15)	0.0631 (17)	0.0417 (12)	−0.0008 (12)	0.0190 (11)	−0.0033 (12)
C16	0.0411 (14)	0.0450 (14)	0.0416 (12)	0.0035 (10)	0.0186 (11)	0.0039 (10)

C17	0.0628 (18)	0.0510 (17)	0.0505 (14)	0.0008 (13)	0.0226 (13)	0.0026 (12)
C18	0.077 (2)	0.0423 (16)	0.0741 (19)	0.0078 (14)	0.0312 (16)	0.0065 (15)
C19	0.0630 (19)	0.0569 (18)	0.0716 (19)	0.0122 (14)	0.0232 (15)	0.0256 (15)
C20	0.070 (2)	0.075 (2)	0.0444 (14)	0.0102 (16)	0.0153 (13)	0.0124 (14)
C21	0.0635 (18)	0.0565 (16)	0.0446 (13)	0.0094 (13)	0.0191 (12)	0.0041 (12)
C22	0.0463 (15)	0.0452 (14)	0.0443 (13)	0.0088 (11)	0.0219 (11)	0.0082 (11)
C23	0.0637 (18)	0.0658 (19)	0.0468 (14)	0.0173 (14)	0.0274 (13)	0.0049 (13)
C24	0.084 (2)	0.087 (2)	0.0666 (19)	0.0328 (19)	0.0501 (18)	0.0177 (17)
C25	0.059 (2)	0.092 (2)	0.096 (2)	0.0266 (18)	0.047 (2)	0.029 (2)
C26	0.0512 (19)	0.075 (2)	0.081 (2)	0.0045 (15)	0.0209 (16)	0.0123 (17)
C27	0.0484 (16)	0.0565 (16)	0.0531 (15)	0.0051 (13)	0.0207 (13)	0.0034 (13)

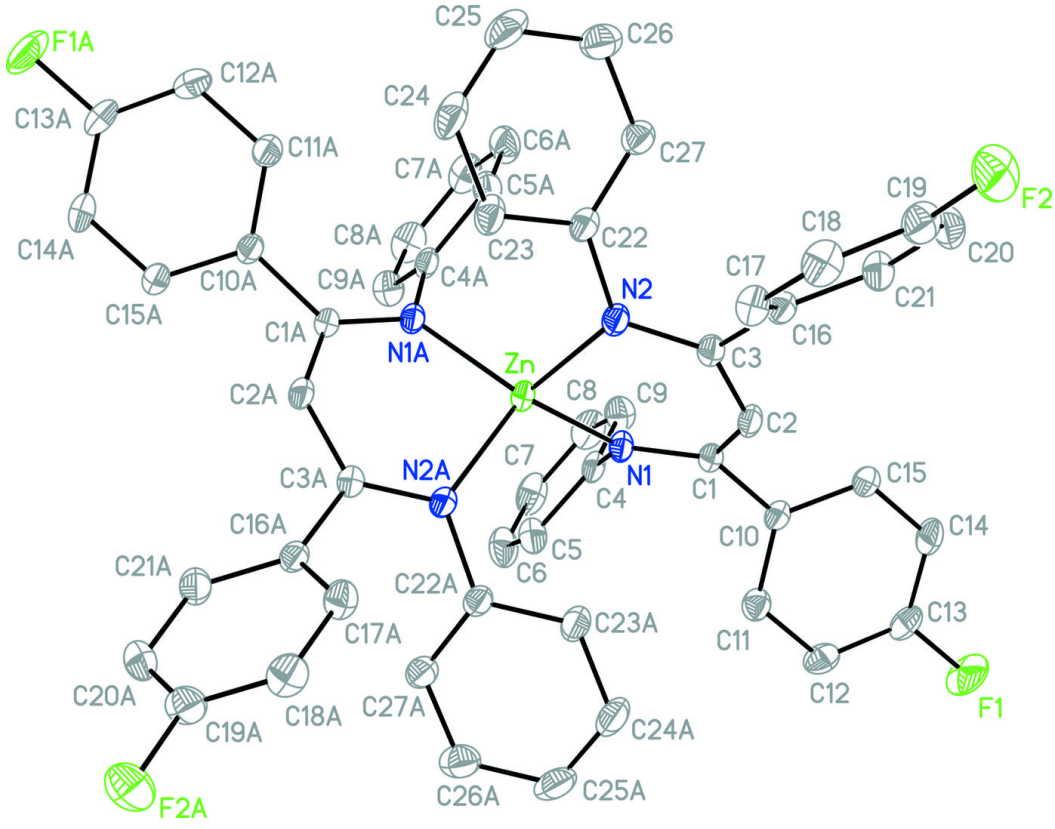
Geometric parameters (Å, °)

Zn—N1^{i}	1.9875 (18)	C11—H11A	0.9300
Zn—N1	1.9875 (18)	C12—C13	1.367 (4)
Zn—N2^{i}	1.9942 (19)	C12—H12A	0.9300
Zn—N2	1.9942 (19)	C13—C14	1.351 (4)
F1—C13	1.356 (3)	C14—C15	1.383 (3)
F2—C19	1.356 (3)	C14—H14A	0.9300
N1—C1	1.337 (3)	C15—H15A	0.9300
N1—C4	1.427 (3)	C16—C21	1.386 (3)
N2—C3	1.340 (3)	C16—C17	1.391 (3)
N2—C22	1.421 (3)	C17—C18	1.374 (4)
C1—C2	1.405 (3)	C17—H17A	0.9300
C1—C10	1.503 (3)	C18—C19	1.366 (4)
C2—C3	1.396 (3)	C18—H18A	0.9300
C2—H2A	0.9300	C19—C20	1.361 (4)
C3—C16	1.496 (3)	C20—C21	1.380 (4)
C4—C9	1.382 (4)	C20—H20A	0.9300
C4—C5	1.387 (3)	C21—H21A	0.9300
C5—C6	1.390 (4)	C22—C27	1.389 (4)
C5—H5A	0.9300	C22—C23	1.386 (3)
C6—C7	1.368 (4)	C23—C24	1.392 (4)
C6—H6A	0.9300	C23—H23A	0.9300
C7—C8	1.362 (4)	C24—C25	1.361 (5)
C7—H7A	0.9300	C24—H24A	0.9300
C8—C9	1.379 (4)	C25—C26	1.376 (4)
C8—H8A	0.9300	C25—H25A	0.9300
C9—H9A	0.9300	C26—C27	1.374 (4)
C10—C11	1.376 (3)	C26—H26A	0.9300
C10—C15	1.394 (3)	C27—H27A	0.9300
C11—C12	1.387 (3)		
N1^{i}—Zn—N1	124.24 (11)	C11—C12—H12A	120.7
N1^{i}—Zn—N2^{i}	96.10 (7)	C14—C13—F1	118.6 (3)
N1—Zn—N2^{i}	112.64 (8)	C14—C13—C12	122.6 (2)
N1^{i}—Zn—N2	112.64 (8)	F1—C13—C12	118.7 (3)
N1—Zn—N2	96.10 (7)	C13—C14—C15	118.8 (2)

$N2^{i}$—Zn—N2	116.65 (12)	C13—C14—H14A	120.6
C1—N1—C4	122.07 (19)	C15—C14—H14A	120.6
C1—N1—Zn	119.36 (16)	C14—C15—C10	120.6 (2)
C4—N1—Zn	118.57 (13)	C14—C15—H15A	119.7
C3—N2—C22	121.39 (19)	C10—C15—H15A	119.7
C3—N2—Zn	119.06 (16)	C21—C16—C17	118.4 (2)
C22—N2—Zn	119.01 (14)	C21—C16—C3	121.7 (2)
N1—C1—C2	123.8 (2)	C17—C16—C3	119.9 (2)
N1—C1—C10	121.5 (2)	C18—C17—C16	121.2 (2)
C2—C1—C10	114.56 (19)	C18—C17—H17A	119.4
C3—C2—C1	129.7 (2)	C16—C17—H17A	119.4
C3—C2—H2A	115.2	C19—C18—C17	118.3 (3)
C1—C2—H2A	115.2	C19—C18—H18A	120.9
N2—C3—C2	123.8 (2)	C17—C18—H18A	120.9
N2—C3—C16	119.5 (2)	F2—C19—C20	118.6 (3)
C2—C3—C16	116.61 (19)	F2—C19—C18	118.6 (3)
C9—C4—C5	118.7 (2)	C20—C19—C18	122.8 (3)
C9—C4—N1	121.0 (2)	C19—C20—C21	118.5 (3)
C5—C4—N1	120.0 (2)	C19—C20—H20A	120.7
C4—C5—C6	120.0 (3)	C21—C20—H20A	120.7
C4—C5—H5A	120.0	C20—C21—C16	120.8 (3)
C6—C5—H5A	120.0	C20—C21—H21A	119.6
C7—C6—C5	120.4 (3)	C16—C21—H21A	119.6
C7—C6—H6A	119.8	C27—C22—C23	118.3 (2)
C5—C6—H6A	119.8	C27—C22—N2	121.4 (2)
C8—C7—C6	119.6 (3)	C23—C22—N2	119.8 (2)
C8—C7—H7A	120.2	C22—C23—C24	119.6 (3)
C6—C7—H7A	120.2	C22—C23—H23A	120.2
C7—C8—C9	120.8 (3)	C24—C23—H23A	120.2
C7—C8—H8A	119.6	C25—C24—C23	121.4 (3)
C9—C8—H8A	119.6	C25—C24—H24A	119.3
C8—C9—C4	120.4 (3)	C23—C24—H24A	119.3
C8—C9—H9A	119.8	C24—C25—C26	119.4 (3)
C4—C9—H9A	119.8	C24—C25—H25A	120.3
C11—C10—C15	118.7 (2)	C26—C25—H25A	120.3
C11—C10—C1	121.2 (2)	C27—C26—C25	120.0 (3)
C15—C10—C1	119.5 (2)	C27—C26—H26A	120.0
C10—C11—C12	120.8 (2)	C25—C26—H26A	120.0
C10—C11—H11A	119.6	C26—C27—C22	121.4 (3)
C12—C11—H11A	119.6	C26—C27—H27A	119.3
C13—C12—C11	118.5 (3)	C22—C27—H27A	119.3
C13—C12—H12A	120.7		

Symmetry codes: (i) $-x+1, y, -z+5/2$.

Fig. 1


F1A
C12A
C13A
C11A
C14A
C10A
C15A
C25
C26
C24
C27
C6A
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C8A
C23
C22
C9A
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C2
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F1
C19A
C24A
F2A
C26A
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C18
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C17
C21
C16