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Bis(5-aminoisoquinoline)diazidozinc(II)

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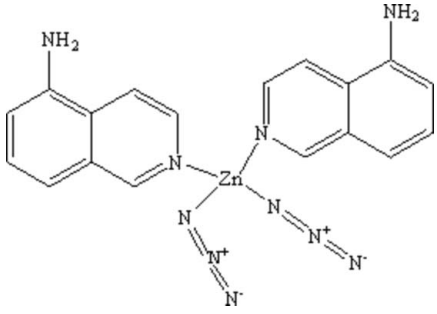
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.076; data-to-parameter ratio = 12.7.

The solution reaction of Zn^{2+} with 5-aminoisoquinoline and NaN_3 afforded the mononuclear title complex, $[Zn(N_3)_2(C_9H_8N_2)_2]$. The azide anions and the 5-aminoisoquinoline molecules act as monodentate ligands, resulting in a slightly distorted ZnN_4 tetrahedron. A network of weak N—H···N hydrogen bonds helps to consolidate the crystal packing.

Related literature

For related structures, see: Liu *et al.* (2004); Gao *et al.* (2006); Li *et al.* (2006); Miao *et al.* (2006). For related literature, see: Robin & Fromm (2006); Yaghi *et al.* (2003).



Experimental

Crystal data

$[Zn(N_3)_2(C_9H_8N_2)_2]$
M_r = 437.78
Orthorhombic, *Pbca*
a = 14.4330 (4) Å
b = 16.0837 (4) Å
c = 16.4677 (5) Å
V = 3822.75 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.31 mm^{-1}
T = 273 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.779, T_{max} = 0.880
22267 measured reflections
3338 independent reflections
2560 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.077
S = 1.02
3338 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	1.963 (2)	Zn1—N9	2.0118 (19)
Zn1—N4	1.981 (2)	Zn1—N7	2.018 (2)
N2—N1—Zn1	123.62 (19)	N5—N4—Zn1	120.44 (19)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N10—H10B···N1^{i}	0.86	2.46	3.225 (3)	148
N10—H10A···N4^{ii}	0.86	2.36	3.182 (3)	160
N8—H8B···N10^{iii}	0.86	2.50	3.294 (3)	154
N8—H8A···N3^{iv}	0.86	2.40	3.155 (4)	147

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); 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: HB2440).

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supplementary materials

Acta Cryst. (2007). E**63**, m1808 [**doi:10.1107/S1600536807026700**]

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Comment

Intense attention has been received to azide complexes due to their diverse structural topologies from discrete molecules to three-dimensional networks and their potential applications in functional materials (Robin & Fromm, 2006; Yaghi *et al.*, 2003). The azido group can act as a monodentate ligand as well as bridging ligand which adopting end-on or end-to-end bridging modes to generate many complexes with interesting structures (Liu *et al.*, 2004; Gao *et al.*, 2006). Here we report a new azide complex using 5-aminoisoquinoline as co-ligand, $Zn(C_9H_8N_2)_2(N_3)_2$ (I). To our knowledge, no other structurally characterized example of a 5-aminoisoquinoline complex has been documented.

As shown in Figure 1, the Zn(II) atom of (I) is coordinated tetrahedrally by four nitrogen atoms, of which two N-donor atoms are from azide groups and the others are from 5-aminoisoquinoline ligands (Table 1). The Zn—N—N bond angles in (I) compare well to equivalent values in related structures (Li *et al.*, 2006; Miao *et al.*, 2006). The 5-aminoisoquinoline aromatic planes are nearly perpendicular to one another with a dihedral angle of 82.106(*x*)°. A network of weak N—H···N hydrogen bonds (Table 2) completes the structure (Fig. 2).

Experimental

Complex (I) was synthesized in a solution reaction. NaN_3 (0.2 mmol) dissolved in 2 ml water was added to 5 ml aqueous solution of $Zn(CH_3COO)_2 2H_2O$ (0.1 mmol) with stirring. Then an ethanol solution (5 ml) of 5-aminoisoquinoline (0.2 mmol) was added into the solution and stirred for 5 h. The mixture was filtered and the clear solution was kept at room temperature to evaporate slowly·After one week, light-yellow single crystals suitable for X-ray diffraction were obtained.

Refinement

The H atoms were geometrically placed (C—H = 0.93 Å, N—H = 0.86 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

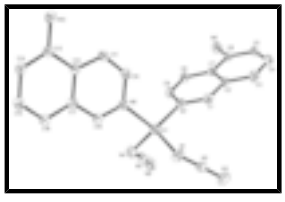

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are omitted for clarity

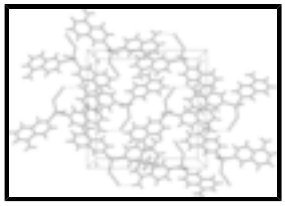

Fig. 2. A packing diagram for (I).

Bis(5-aminoisoquinoline)diazidozinc(II)

Crystal data

$[Zn(N_3)_2(C_9H_8N_2)_2]$	F_{000} = 1792
M_r = 437.78	D_x = 1.521 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5531 reflections
a = 14.4330 (4) Å	θ = 2.8–23.6º
b = 16.0837 (4) Å	μ = 1.31 mm^{-1}
c = 16.4677 (5) Å	*T* = 273 (2) K
V = 3822.75 (18) Å^3	Block, light-yellow
Z = 8	0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer	3338 independent reflections
Radiation source: fine-focus sealed tube	2560 reflections with *I* > \2s(*I*)
Monochromator: graphite	R_{int} = 0.036
T = 273(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −17→17
T_{min} = 0.779, T_{max} = 0.880	*k* = −19→18
22267 measured reflections	*l* = −19→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H-atom parameters constrained
$wR(F^2)$ = 0.077	$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 1.8397P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3338 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
262 parameters	$\Delta\rho_{min}$ = −0.28 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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
Zn1	0.94645 (2)	0.032733 (17)	0.680773 (16)	0.04710 (11)
C1	0.89609 (17)	0.02149 (15)	0.85389 (15)	0.0470 (6)
H1	0.8616	−0.0239	0.8364	0.056*
C2	0.89393 (16)	0.04197 (14)	0.93744 (14)	0.0435 (6)
C3	0.83983 (19)	−0.00398 (18)	0.99208 (17)	0.0609 (7)
H3	0.8046	−0.0488	0.9742	0.073*
C4	0.8399 (2)	0.01836 (18)	1.07239 (17)	0.0651 (8)
H4	0.8037	−0.0112	1.1092	0.078*
C5	0.89341 (19)	0.08466 (17)	1.09951 (16)	0.0574 (7)
H5	0.8923	0.0981	1.1544	0.069*
C6	0.94764 (17)	0.13088 (15)	1.04849 (15)	0.0490 (6)
C7	0.94798 (16)	0.11029 (14)	0.96325 (14)	0.0415 (5)
C8	0.99863 (18)	0.15350 (15)	0.90421 (15)	0.0507 (6)
H8	1.0346	0.1990	0.9192	0.061*
C9	0.99554 (19)	0.12939 (15)	0.82568 (15)	0.0517 (6)
H9	1.0298	0.1591	0.7877	0.062*
C10	0.80985 (18)	0.16731 (15)	0.64571 (14)	0.0496 (6)
H10	0.7998	0.1662	0.7015	0.060*
C11	0.76044 (17)	0.22168 (14)	0.60011 (14)	0.0457 (6)
H11	0.7184	0.2573	0.6250	0.055*
C12	0.77234 (16)	0.22461 (13)	0.51551 (13)	0.0393 (5)
C13	0.72056 (17)	0.27742 (14)	0.46242 (14)	0.0435 (6)
C14	0.73427 (19)	0.26955 (16)	0.38043 (15)	0.0558 (7)
H14	0.6997	0.3025	0.3453	0.067*
C15	0.7983 (2)	0.21394 (17)	0.34800 (16)	0.0631 (8)
H15	0.8048	0.2102	0.2919	0.076*
C16	0.85134 (19)	0.16508 (16)	0.39660 (15)	0.0557 (7)
H16	0.8955	0.1296	0.3745	0.067*
C17	0.83801 (16)	0.16920 (14)	0.48121 (13)	0.0412 (5)
C18	0.88677 (17)	0.11636 (14)	0.53447 (15)	0.0474 (6)
H18	0.9309	0.0808	0.5124	0.057*

N1	0.89962 (19)	−0.08021 (14)	0.66187 (14)	0.0667 (7)
N2	0.91573 (16)	−0.13681 (14)	0.70470 (13)	0.0548 (6)
N3	0.9294 (2)	−0.19444 (16)	0.74305 (16)	0.0981 (11)
N4	1.07524 (17)	0.04730 (15)	0.64174 (15)	0.0639 (6)
N5	1.13908 (18)	0.03513 (14)	0.68614 (14)	0.0574 (6)
N6	1.2017 (2)	0.0247 (2)	0.72680 (17)	0.0886 (9)
N7	0.94411 (13)	0.06303 (12)	0.79965 (12)	0.0447 (5)
N8	0.99928 (17)	0.19602 (15)	1.07584 (13)	0.0684 (7)
H8A	0.9983	0.2091	1.1265	0.082*
H8B	1.0328	0.2241	1.0425	0.082*
N9	0.87372 (14)	0.11419 (11)	0.61346 (11)	0.0447 (5)
N10	0.65323 (15)	0.32964 (13)	0.49322 (13)	0.0568 (6)
H10A	0.6189	0.3580	0.4608	0.068*
H10B	0.6456	0.3338	0.5449	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0574 (2)	0.04234 (17)	0.04158 (18)	0.00293 (13)	−0.00621 (13)	0.00430 (12)
C1	0.0435 (14)	0.0449 (14)	0.0526 (16)	−0.0007 (11)	−0.0049 (12)	0.0029 (11)
C2	0.0377 (13)	0.0431 (13)	0.0495 (15)	0.0018 (11)	0.0000 (11)	0.0102 (11)
C3	0.0577 (17)	0.0577 (16)	0.0674 (19)	−0.0124 (14)	0.0064 (14)	0.0087 (14)
C4	0.0646 (19)	0.0693 (19)	0.0614 (19)	−0.0035 (15)	0.0146 (15)	0.0156 (15)
C5	0.0613 (17)	0.0665 (18)	0.0443 (15)	0.0104 (15)	0.0089 (13)	0.0099 (13)
C6	0.0482 (14)	0.0503 (15)	0.0484 (15)	0.0069 (12)	−0.0036 (12)	0.0027 (12)
C7	0.0375 (12)	0.0429 (13)	0.0442 (14)	0.0045 (11)	−0.0029 (10)	0.0052 (10)
C8	0.0554 (16)	0.0467 (14)	0.0502 (16)	−0.0116 (12)	−0.0006 (12)	0.0022 (12)
C9	0.0615 (17)	0.0483 (15)	0.0454 (15)	−0.0086 (13)	0.0026 (12)	0.0048 (12)
C10	0.0606 (16)	0.0529 (15)	0.0353 (13)	0.0029 (13)	0.0003 (12)	0.0017 (11)
C11	0.0507 (15)	0.0467 (14)	0.0397 (13)	0.0051 (11)	0.0006 (11)	−0.0031 (11)
C12	0.0409 (13)	0.0364 (12)	0.0405 (13)	−0.0052 (10)	−0.0026 (10)	0.0010 (10)
C13	0.0470 (14)	0.0418 (13)	0.0418 (14)	−0.0032 (11)	−0.0027 (11)	0.0012 (11)
C14	0.0693 (18)	0.0540 (16)	0.0440 (15)	0.0074 (14)	−0.0073 (13)	0.0095 (12)
C15	0.089 (2)	0.0653 (18)	0.0347 (14)	0.0120 (16)	0.0043 (14)	0.0037 (13)
C16	0.0677 (18)	0.0547 (16)	0.0448 (15)	0.0113 (13)	0.0079 (13)	0.0024 (12)
C17	0.0467 (14)	0.0388 (13)	0.0382 (13)	−0.0028 (11)	−0.0007 (11)	0.0024 (10)
C18	0.0510 (15)	0.0436 (14)	0.0477 (15)	0.0036 (11)	0.0006 (11)	0.0014 (11)
N1	0.0943 (19)	0.0471 (14)	0.0588 (14)	−0.0042 (13)	−0.0196 (13)	0.0005 (12)
N2	0.0735 (15)	0.0459 (13)	0.0449 (13)	−0.0026 (11)	0.0015 (11)	−0.0107 (11)
N3	0.184 (3)	0.0486 (15)	0.0620 (16)	0.0097 (18)	−0.0026 (19)	0.0045 (14)
N4	0.0618 (15)	0.0745 (16)	0.0554 (15)	0.0016 (13)	0.0062 (12)	0.0147 (12)
N5	0.0574 (15)	0.0640 (15)	0.0506 (14)	−0.0022 (12)	0.0126 (13)	0.0046 (12)
N6	0.0590 (17)	0.138 (3)	0.0689 (18)	0.0028 (17)	0.0005 (14)	0.0083 (17)
N7	0.0482 (12)	0.0424 (11)	0.0435 (11)	0.0007 (9)	−0.0049 (9)	0.0042 (9)
N8	0.0839 (18)	0.0761 (16)	0.0451 (13)	−0.0167 (14)	−0.0014 (12)	−0.0071 (12)
N9	0.0529 (12)	0.0421 (11)	0.0391 (12)	0.0009 (9)	−0.0047 (9)	0.0039 (9)
N10	0.0636 (14)	0.0598 (13)	0.0471 (12)	0.0182 (11)	−0.0054 (11)	0.0047 (10)

Geometric parameters (Å, °)

Zn1—N1	1.963 (2)	C10—H10	0.9300
Zn1—N4	1.981 (2)	C11—C12	1.404 (3)
Zn1—N9	2.0118 (19)	C11—H11	0.9300
Zn1—N7	2.018 (2)	C12—C17	1.418 (3)
C1—N7	1.313 (3)	C12—C13	1.430 (3)
C1—C2	1.415 (3)	C13—C14	1.370 (3)
C1—H1	0.9300	C13—N10	1.381 (3)
C2—C3	1.402 (3)	C14—C15	1.392 (4)
C2—C7	1.413 (3)	C14—H14	0.9300
C3—C4	1.370 (4)	C15—C16	1.358 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.391 (4)	C16—C17	1.408 (3)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.368 (3)	C17—C18	1.409 (3)
C5—H5	0.9300	C18—N9	1.315 (3)
C6—N8	1.362 (3)	C18—H18	0.9300
C6—C7	1.442 (3)	N1—N2	1.175 (3)
C7—C8	1.401 (3)	N2—N3	1.139 (3)
C8—C9	1.351 (3)	N4—N5	1.193 (3)
C8—H8	0.9300	N5—N6	1.137 (3)
C9—N7	1.369 (3)	N8—H8A	0.8600
C9—H9	0.9300	N8—H8B	0.8600
C10—C11	1.356 (3)	N10—H10A	0.8600
C10—N9	1.364 (3)	N10—H10B	0.8600
N1—Zn1—N4	112.41 (11)	C12—C11—H11	119.8
N1—Zn1—N9	109.61 (9)	C11—C12—C17	117.1 (2)
N4—Zn1—N9	103.52 (9)	C11—C12—C13	124.2 (2)
N1—Zn1—N7	111.81 (9)	C17—C12—C13	118.6 (2)
N4—Zn1—N7	107.58 (9)	C14—C13—N10	121.3 (2)
N9—Zn1—N7	111.63 (8)	C14—C13—C12	118.2 (2)
N7—C1—C2	123.7 (2)	N10—C13—C12	120.3 (2)
N7—C1—H1	118.2	C13—C14—C15	122.2 (2)
C2—C1—H1	118.2	C13—C14—H14	118.9
C3—C2—C7	121.6 (2)	C15—C14—H14	118.9
C3—C2—C1	120.9 (2)	C16—C15—C14	121.3 (2)
C7—C2—C1	117.5 (2)	C16—C15—H15	119.3
C4—C3—C2	118.8 (3)	C14—C15—H15	119.3
C4—C3—H3	120.6	C15—C16—C17	118.6 (2)
C2—C3—H3	120.6	C15—C16—H16	120.7
C3—C4—C5	120.7 (3)	C17—C16—H16	120.7
C3—C4—H4	119.6	C16—C17—C18	121.3 (2)
C5—C4—H4	119.6	C16—C17—C12	121.0 (2)
C6—C5—C4	122.5 (3)	C18—C17—C12	117.7 (2)
C6—C5—H5	118.7	N9—C18—C17	124.1 (2)
C4—C5—H5	118.7	N9—C18—H18	118.0
N8—C6—C5	121.9 (2)	C17—C18—H18	118.0

N8—C6—C7	119.8 (2)	N2—N1—Zn1	123.62 (19)
C5—C6—C7	118.4 (2)	N3—N2—N1	176.3 (3)
C8—C7—C2	117.7 (2)	N5—N4—Zn1	120.44 (19)
C8—C7—C6	124.3 (2)	N6—N5—N4	177.9 (3)
C2—C7—C6	118.0 (2)	C1—N7—C9	118.0 (2)
C9—C8—C7	120.3 (2)	C1—N7—Zn1	123.09 (17)
C9—C8—H8	119.8	C9—N7—Zn1	118.89 (16)
C7—C8—H8	119.8	C6—N8—H8A	120.0
C8—C9—N7	122.8 (2)	C6—N8—H8B	120.0
C8—C9—H9	118.6	H8A—N8—H8B	120.0
N7—C9—H9	118.6	C18—N9—C10	117.7 (2)
C11—C10—N9	122.9 (2)	C18—N9—Zn1	119.19 (16)
C11—C10—H10	118.5	C10—N9—Zn1	123.08 (15)
N9—C10—H10	118.5	C13—N10—H10A	120.0
C10—C11—C12	120.5 (2)	C13—N10—H10B	120.0
C10—C11—H11	119.8	H10A—N10—H10B	120.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10B···N1^{i}	0.86	2.46	3.225 (3)	148
N10—H10A···N4^{ii}	0.86	2.36	3.182 (3)	160
N8—H8B···N10^{iii}	0.86	2.50	3.294 (3)	154
N8—H8A···N3^{iv}	0.86	2.40	3.155 (4)	147

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*; (ii) *x*−1/2, −*y*+1/2, −*z*+1; (iii) *x*+1/2, *y*, −*z*+3/2; (iv) −*x*+2, −*y*, −*z*+2.

Fig. 1

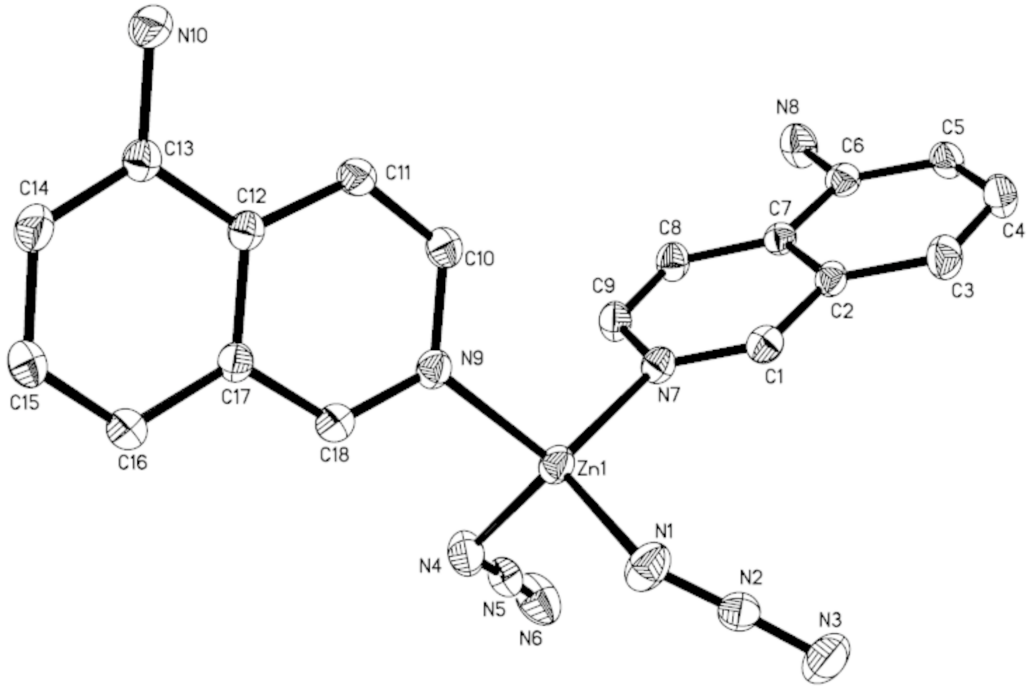
N10
C13
C14
C12
C11
C10
N9
C15
C17
C16
C18
N8
C6
C5
C7
C4
C8
C9
C2
C3
C1
N7
Zn1
N1
N4
N2
N5
N3
N6

Fig. 2