Supporting Information

Hydrothermal Synthesis, Crystal Structures and Properties of Zinc(II) Di-nuclear Complex and Copper(I) Coordination Polymer Based on Building Block 2-Phenyl-4,6-di(pyridin-2-yl)pyrimidine

Pusu Zhao,[†,‡,*] Wang Jing,[†] Long Jing,[†] Fangfang Jian,[†] and Yufeng Li[†]

[†]New Materials & Function Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao, Shandong 266042, P.R. China. [*]E-mail: zhaopusu@163.com
[‡]Jiangsu Key Laboratory for Chemistry of Low-Dimensional Materials, Huaiyin Teachers College, Huaian, Jiangsu 223300, P.R. China
Received June 5, 2013, Accepted September 24, 2013

Abstract

Computing details

For both compounds, data collection: CAD-4 Software (Enraf-Nonius, 1989); cell refinement: CAD-4 Software; data reduction: NRCVAX (Gabe *et al.*, 1989); program(s) used to solve structure: SHELXS-97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL-97 (Sheldrick, 1997); molecular graphics: SHELXTL-PC (Sheldrick, 1990); software used to prepare material for publication: WinGX (Farrugia, 1999).

References

NOT FOUND

(qj07190)

Crystal data

$C_{10}H_7CuIN_2$	$F(000) = 1304$
$M_r = 345.63$	$D_x = 2.266$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 25 reflections
$a = 11.760$ (2) Å	$\theta = 4–14°$
$b = 14.750$ (3) Å	$\mu = 5.16$ mm^{-1}
$c = 11.690$ (2) Å	$T = 293$ K
$\beta = 92.29$ (3)°	Bolck, blue
$V = 2026.1$ (6) Å^3	0.35 × 0.25 × 0.25 mm
$Z = 8$	

Data collection

Enraf-Nonius CAD-4 diffractometer	1322 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.065$
graphite	$\theta_{max} = 28.3°$, $\theta_{min} = 2.2°$
ω/2θ scans	$h = -15 \rightarrow 13$
Absorption correction: ψ scan North et al., 1968	$k = -10 \rightarrow 19$
$T_{min} = 0.232$, $T_{max} = 0.275$	$l = -14 \rightarrow 14$
6565 measured reflections	3 standard reflections every 100 reflections
2438 independent reflections	intensity decay: none

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.107$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2438 reflections	$(\Delta/\sigma)_{max} < 0.001$
129 parameters	$\Delta\rangle_{max} = 0.71$ e Å^{-3}
0 restraints	$\Delta\rangle_{min} = -0.77$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$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}
I1	0.13419 (5)	0.23277 (4)	0.14692 (5)	0.0600 (2)
Cu1	0.31791 (8)	0.18978 (6)	0.04508 (7)	0.0448 (3)
N1	0.4389 (5)	0.1347 (3)	0.1673 (4)	0.0318 (13)
N2	0.3148 (5)	0.0537 (4)	0.0028 (5)	0.0413 (16)
C1	0.2543 (7)	0.0177 (6)	-0.0860 (6)	0.055 (2)
H1A	0.2148	0.0568	-0.1358	0.066*
C2	0.2482 (7)	-0.0718 (6)	-0.1065 (7)	0.055 (2)
H2A	0.2055	-0.0942	-0.1690	0.066*
C3	0.3059 (7)	-0.1292 (5)	-0.0337 (7)	0.056 (2)
H3A	0.3024	-0.1915	-0.0452	0.067*
C4	0.3694 (6)	-0.0941 (4)	0.0569 (6)	0.046 (2)
H4A	0.4100	-0.1322	0.1070	0.055*
C5	0.3720 (6)	-0.0029 (4)	0.0723 (5)	0.0331 (16)
C6	0.4400 (6)	0.0430 (4)	0.1667 (5)	0.0313 (16)
C7	0.5000	-0.0045 (6)	0.2500	0.037 (2)
H7A	0.5000	-0.0676	0.2500	0.045*
C8	0.5000	0.1762 (6)	0.2500	0.037 (2)
C9	0.5000	0.2766 (6)	0.2500	0.039 (2)
C10	0.5215 (7)	0.3245 (5)	0.1519 (7)	0.053 (2)
H10A	0.5339	0.2935	0.0842	0.063*
C11	0.5248 (7)	0.4190 (5)	0.1534 (8)	0.068 (3)
H11A	0.5439	0.4509	0.0883	0.082*
C12	0.5000	0.4641 (8)	0.2500	0.074 (5)
H12A	0.5000	0.5271	0.2500	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0605 (4)	0.0709 (4)	0.0494 (3)	0.0258 (3)	0.0124 (3)	0.0214 (3)
Cu1	0.0499 (7)	0.0418 (5)	0.0421 (5)	0.0127 (4)	-0.0062 (5)	0.0039 (4)
N1	0.037 (4)	0.029 (3)	0.030 (3)	0.002 (2)	-0.003 (3)	-0.002 (2)
N2	0.043 (4)	0.039 (3)	0.041 (4)	0.009 (3)	-0.010 (3)	-0.007 (3)
C1	0.049 (6)	0.066 (6)	0.049 (5)	0.007 (4)	-0.022 (5)	-0.013 (4)
C2	0.045 (5)	0.062 (6)	0.057 (5)	0.000 (4)	-0.021 (5)	-0.024 (4)
C3	0.054 (6)	0.050 (5)	0.063 (6)	-0.010 (4)	0.001 (5)	-0.021 (4)
C4	0.047 (5)	0.033 (4)	0.057 (5)	0.003 (3)	-0.009 (4)	-0.015 (4)
C5	0.031 (4)	0.036 (4)	0.032 (4)	0.005 (3)	-0.007 (3)	-0.002 (3)

C6	0.033 (4)	0.030 (4)	0.031 (4)	0.001 (3)	-0.008 (3)	0.000 (3)
C7	0.037 (6)	0.020 (5)	0.054 (6)	0.000	-0.001 (5)	0.000
C8	0.037 (6)	0.036 (6)	0.037 (6)	0.000	0.001 (5)	0.000
C9	0.041 (7)	0.030 (5)	0.045 (6)	0.000	-0.009 (5)	0.000
C10	0.049 (6)	0.042 (5)	0.065 (6)	0.001 (4)	-0.013 (5)	0.010 (4)
C11	0.058 (7)	0.052 (6)	0.094 (8)	0.001 (5)	-0.010 (6)	0.024 (5)
C12	0.067 (10)	0.027 (7)	0.124 (13)	0.000	-0.034 (10)	0.000

Geometric parameters (Å, º)

I1—Cu1	2.5871 (13)	C4—C5	1.357 (8)
I1—Cu1^{i}	2.6003 (11)	C4—H4A	0.9300
Cu1—N2	2.068 (5)	C5—C6	1.499 (8)
Cu1—N1	2.136 (5)	C6—C7	1.372 (7)
Cu1—Cu1^{i}	2.5853 (17)	C7—C6^{ii}	1.372 (7)
Cu1—I1^{i}	2.6003 (11)	C7—H7A	0.9300
N1—C8	1.331 (6)	C8—N1^{ii}	1.331 (6)
N1—C6	1.352 (7)	C8—C9	1.481 (12)
N2—C5	1.329 (7)	C9—C10^{ii}	1.379 (8)
N2—C1	1.343 (8)	C9—C10	1.379 (9)
C1—C2	1.344 (9)	C10—C11	1.394 (9)
C1—H1A	0.9300	C10—H10A	0.9300
C2—C3	1.361 (10)	C11—C12	1.352 (10)
C2—H2A	0.9300	C11—H11A	0.9300
C3—C4	1.372 (9)	C12—C11^{ii}	1.352 (10)
C3—H3A	0.9300	C12—H12A	0.9300
Cu1—I1—Cu1^{i}	59.79 (4)	C5—C4—H4A	120.5
N2—Cu1—N1	78.2 (2)	C3—C4—H4A	120.5
N2—Cu1—Cu1^{i}	124.39 (16)	N2—C5—C4	122.2 (6)
N1—Cu1—Cu1^{i}	156.67 (14)	N2—C5—C6	114.1 (5)
N2—Cu1—I1	109.92 (18)	C4—C5—C6	123.6 (6)
N1—Cu1—I1	109.39 (16)	N1—C6—C7	120.8 (6)
Cu1^{i}—Cu1—I1	60.36 (4)	N1—C6—C5	116.8 (5)
N2—Cu1—I1^{i}	102.87 (17)	C7—C6—C5	122.4 (6)
N1—Cu1—I1^{i}	125.64 (16)	C6^{ii}—C7—C6	118.5 (8)
Cu1^{i}—Cu1—I1^{i}	59.86 (4)	C6^{ii}—C7—H7A	120.7
I1—Cu1—I1^{i}	120.22 (4)	C6—C7—H7A	120.7
C8—N1—C6	117.3 (5)	N1^{ii}—C8—N1	125.2 (8)

C8—N1—Cu1	129.5 (5)	N1^{ii}—C8—C9	117.4 (4)
C6—N1—Cu1	112.5 (4)	N1—C8—C9	117.4 (4)
C5—N2—C1	117.7 (6)	C10^{ii}—C9—C10	118.4 (9)
C5—N2—Cu1	117.4 (4)	C10^{ii}—C9—C8	120.8 (5)
C1—N2—Cu1	124.9 (5)	C10—C9—C8	120.8 (5)
N2—C1—C2	123.2 (7)	C9—C10—C11	120.5 (8)
N2—C1—H1A	118.4	C9—C10—H10A	119.8
C2—C1—H1A	118.4	C11—C10—H10A	119.8
C1—C2—C3	118.5 (7)	C12—C11—C10	119.7 (9)
C1—C2—H2A	120.7	C12—C11—H11A	120.2
C3—C2—H2A	120.7	C10—C11—H11A	120.2
C2—C3—C4	119.4 (7)	C11^{ii}—C12—C11	121.1 (12)
C2—C3—H3A	120.3	C11^{ii}—C12—H12A	119.5
C4—C3—H3A	120.3	C11—C12—H12A	119.5
C5—C4—C3	119.0 (7)		

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

(qj07238)

Crystal data

$C_{20}H_{14}I_4N_4Zn_2$	$F(000) = 1736$
$M_r = 948.69$	$D_x = 2.406$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
$a = 14.650$ (3) Å	$\theta = 4$–$14°$
$b = 12.555$ (3) Å	$\mu = 6.56$ mm^{-1}
$c = 17.545$ (7) Å	$T = 293$ K
$\beta = 125.763$ (19)°	Block, yellow
$V = 2618.6$ (13) Å^3	0.30 × 0.20 × 0.20 mm
$Z = 4$	

Data collection

Enraf-Nonius CAD-4 diffractometer	3765 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.054$
graphite	$\theta_{max} = 28.3°$, $\theta_{min} = 1.7°$
$\omega/2\theta$ scans	$h = -17 \rightarrow 19$
Absorption correction: ψ scan North et al., 1968	$k = -16 \rightarrow 16$

T_{min} = 0.226, T_{max} = 0.269	l = -23→11
16612 measured reflections	3 standard reflections every 100 reflections
6327 independent reflections	intensity decay: none

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.055	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.160	H-atom parameters constrained
S = 1.04	$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2 + 0.3901P]$ where $P = (F_o^2 + 2F_c^2)/3$
6327 reflections	$(\Delta/\sigma)_{max} < 0.001$
271 parameters	$\Delta\rangle_{max}$ = 1.83 e Å^{-3}
0 restraints	$\Delta\rangle_{min}$ = -1.49 e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$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}
I1	0.40665 (6)	0.23612 (5)	-0.26028 (6)	0.0755 (3)
I2	0.65334 (5)	0.03956 (5)	-0.24732 (6)	0.0710 (2)
I3	-0.11070 (5)	-0.07618 (6)	-0.69902 (5)	0.0698 (2)
I4	0.16185 (6)	-0.30405 (5)	-0.61187 (5)	0.0626 (2)
Zn1	0.47955 (8)	0.05110 (8)	-0.24824 (7)	0.0496 (3)
Zn2	0.05232 (7)	-0.18605 (7)	-0.57378 (6)	0.0417 (2)

N1	0.5154 (5)	-0.0335 (5)	-0.1325 (5)	0.0428 (16)
N2	0.3470 (5)	-0.0629 (5)	-0.3118 (4)	0.0348 (14)
N3	0.1725 (4)	-0.1379 (5)	-0.4337 (4)	0.0339 (14)
N4	0.0050 (5)	-0.2772 (5)	-0.5040 (4)	0.0422 (16)
C1	0.6055 (7)	-0.0175 (8)	-0.0449 (6)	0.059 (3)
H1A	0.6544	0.0377	-0.0334	0.071*
C2	0.6291 (7)	-0.0797 (9)	0.0294 (7)	0.074 (3)
H2A	0.6930	-0.0669	0.0897	0.089*
C3	0.5571 (8)	-0.1608 (9)	0.0131 (6)	0.068 (3)
H3A	0.5707	-0.2030	0.0623	0.082*
C4	0.4628 (7)	-0.1789 (7)	-0.0788 (6)	0.055 (2)
H4A	0.4134	-0.2342	-0.0918	0.066*
C5	0.4441 (6)	-0.1131 (6)	-0.1501 (6)	0.0411 (19)
C6	0.3484 (6)	-0.1241 (6)	-0.2480 (5)	0.0357 (17)
C7	0.2575 (6)	-0.1929 (6)	-0.2756 (5)	0.0375 (17)
H7A	0.2558	-0.2333	-0.2320	0.045*
C8	0.1693 (6)	-0.1973 (6)	-0.3724 (6)	0.0369 (17)
C9	0.0737 (6)	-0.2743 (6)	-0.4099 (6)	0.0384 (17)
C10	0.0566 (7)	-0.3344 (7)	-0.3557 (7)	0.053 (2)
H10A	0.1053	-0.3281	-0.2907	0.064*
C11	-0.0321 (8)	-0.4052 (8)	-0.3950 (8)	0.067 (3)
H11A	-0.0444	-0.4481	-0.3586	0.080*
C12	-0.1027 (7)	-0.4079 (8)	-0.4937 (8)	0.069 (3)
H12A	-0.1640	-0.4539	-0.5245	0.083*
C13	-0.0824 (7)	-0.3448 (8)	-0.5439 (7)	0.060 (2)
H13A	-0.1309	-0.3480	-0.6090	0.072*
C14	0.2590 (6)	-0.0701 (6)	-0.4031 (5)	0.0373 (17)
C15	0.2576 (6)	-0.0020 (6)	-0.4725 (5)	0.0398 (18)
C16	0.1664 (8)	0.0611 (8)	-0.5325 (7)	0.066 (3)
H16A	0.1069	0.0646	-0.5272	0.080*
C17	0.1629 (10)	0.1206 (9)	-0.6020 (8)	0.079 (3)
H17A	0.1001	0.1615	-0.6446	0.094*
C18	0.2507 (10)	0.1175 (10)	-0.6059 (8)	0.087 (4)
H18A	0.2494	0.1581	-0.6508	0.104*
C19	0.3433 (9)	0.0559 (11)	-0.5453 (9)	0.090 (4)
H19A	0.4040	0.0560	-0.5490	0.108*
C20	0.3466 (8)	-0.0051 (9)	-0.4800 (7)	0.066 (3)
H20A	0.4082	-0.0487	-0.4404	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0839 (5)	0.0492 (4)	0.1124 (7)	0.0034 (3)	0.0681 (5)	0.0067 (4)
I2	0.0571 (4)	0.0644 (4)	0.0953 (6)	-0.0031 (3)	0.0467 (4)	0.0034 (4)
I3	0.0529 (4)	0.0920 (5)	0.0485 (4)	0.0271 (3)	0.0206 (3)	0.0140 (3)
I4	0.0760 (4)	0.0673 (4)	0.0641 (4)	0.0241 (3)	0.0520 (4)	0.0135 (3)
Zn1	0.0439 (5)	0.0476 (5)	0.0527 (6)	-0.0078 (4)	0.0258 (5)	-0.0046 (5)
Zn2	0.0353 (5)	0.0536 (6)	0.0323 (5)	0.0030 (4)	0.0176 (4)	0.0002 (4)
N1	0.032 (3)	0.044 (4)	0.039 (4)	-0.007 (3)	0.014 (3)	-0.012 (3)
N2	0.027 (3)	0.040 (3)	0.033 (3)	-0.004 (2)	0.015 (3)	-0.005 (3)
N3	0.033 (3)	0.037 (3)	0.034 (3)	-0.001 (3)	0.021 (3)	-0.004 (3)
N4	0.028 (3)	0.062 (4)	0.034 (4)	-0.010 (3)	0.017 (3)	-0.009 (3)
C1	0.035 (4)	0.074 (6)	0.045 (5)	-0.007 (4)	0.010 (4)	-0.019 (5)
C2	0.041 (5)	0.097 (8)	0.044 (6)	0.004 (5)	0.002 (4)	-0.012 (6)
C3	0.066 (6)	0.087 (7)	0.034 (5)	0.024 (6)	0.018 (5)	0.004 (5)
C4	0.057 (5)	0.062 (6)	0.042 (5)	0.008 (4)	0.027 (4)	0.006 (4)
C5	0.034 (4)	0.048 (4)	0.041 (4)	0.005 (3)	0.021 (4)	-0.005 (4)
C6	0.039 (4)	0.043 (4)	0.024 (4)	0.004 (3)	0.018 (3)	-0.004 (3)
C7	0.035 (4)	0.052 (4)	0.028 (4)	-0.005 (3)	0.020 (3)	0.003 (3)
C8	0.032 (4)	0.039 (4)	0.043 (4)	-0.002 (3)	0.023 (3)	-0.010 (3)
C9	0.036 (4)	0.048 (4)	0.037 (4)	-0.005 (3)	0.024 (3)	-0.005 (4)
C10	0.059 (5)	0.060 (5)	0.047 (5)	-0.021 (4)	0.034 (4)	-0.012 (4)
C11	0.070 (6)	0.076 (7)	0.063 (6)	-0.021 (5)	0.044 (6)	-0.001 (5)
C12	0.050 (5)	0.082 (7)	0.070 (7)	-0.036 (5)	0.032 (5)	-0.020 (6)
C13	0.052 (5)	0.083 (7)	0.046 (5)	-0.019 (5)	0.030 (4)	-0.010 (5)
C14	0.035 (4)	0.039 (4)	0.034 (4)	0.002 (3)	0.018 (3)	0.000 (3)
C15	0.041 (4)	0.041 (4)	0.037 (4)	-0.007 (3)	0.023 (4)	-0.001 (4)
C16	0.064 (6)	0.075 (6)	0.062 (6)	0.002 (5)	0.038 (5)	0.017 (5)
C17	0.086 (8)	0.070 (7)	0.070 (7)	0.009 (6)	0.040 (7)	0.020 (6)
C18	0.086 (8)	0.103 (9)	0.060 (7)	-0.010 (7)	0.037 (7)	0.023 (6)
C19	0.059 (6)	0.142 (11)	0.078 (8)	0.000 (7)	0.044 (6)	0.025 (8)
C20	0.059 (6)	0.088 (7)	0.052 (6)	0.003 (5)	0.034 (5)	0.011 (5)

Geometric parameters (Å, º)

I1—Zn1	2.5134 (13)	C6—C7	1.414 (10)
I2—Zn1	2.5408 (13)	C7—C8	1.411 (10)
I3—Zn2	2.5101 (12)	C7—H7A	0.9300
I4—Zn2	2.5438 (12)	C8—C9	1.501 (10)

Zn1—N1	2.069 (7)	C9—C10	1.347 (12)
Zn1—N2	2.129 (6)	C10—C11	1.380 (12)
Zn2—N4	2.070 (7)	C10—H10A	0.9300
Zn2—N3	2.109 (6)	C11—C12	1.406 (14)
N1—C1	1.332 (10)	C11—H11A	0.9300
N1—C5	1.344 (10)	C12—C13	1.340 (14)
N2—C6	1.349 (10)	C12—H12A	0.9300
N2—C14	1.350 (9)	C13—H13A	0.9300
N3—C8	1.332 (10)	C14—C15	1.479 (11)
N3—C14	1.350 (9)	C15—C16	1.370 (12)
N4—C9	1.341 (10)	C15—C20	1.384 (13)
N4—C13	1.342 (10)	C16—C17	1.406 (15)
C1—C2	1.379 (15)	C16—H16A	0.9300
C1—H1A	0.9300	C17—C18	1.328 (16)
C2—C3	1.370 (15)	C17—H17A	0.9300
C2—H2A	0.9300	C18—C19	1.372 (15)
C3—C4	1.398 (12)	C18—H18A	0.9300
C3—H3A	0.9300	C19—C20	1.355 (15)
C4—C5	1.387 (12)	C19—H19A	0.9300
C4—H4A	0.9300	C20—H20A	0.9300
C5—C6	1.455 (10)		
N1—Zn1—N2	78.4 (2)	C8—C7—C6	116.9 (7)
N1—Zn1—I1	114.13 (18)	C8—C7—H7A	121.5
N2—Zn1—I1	111.37 (16)	C6—C7—H7A	121.5
N1—Zn1—I2	106.60 (18)	N3—C8—C7	120.7 (6)
N2—Zn1—I2	124.69 (17)	N3—C8—C9	118.1 (7)
I1—Zn1—I2	115.35 (4)	C7—C8—C9	121.1 (7)
N4—Zn2—N3	79.0 (2)	N4—C9—C10	122.5 (7)
N4—Zn2—I3	110.21 (17)	N4—C9—C8	113.2 (7)
N3—Zn2—I3	125.57 (16)	C10—C9—C8	124.2 (7)
N4—Zn2—I4	108.32 (19)	C9—C10—C11	121.1 (9)
N3—Zn2—I4	104.37 (16)	C9—C10—H10A	119.4
I3—Zn2—I4	120.90 (5)	C11—C10—H10A	119.4
C1—N1—C5	119.4 (8)	C10—C11—C12	115.6 (9)
C1—N1—Zn1	124.5 (6)	C10—C11—H11A	122.2
C5—N1—Zn1	116.0 (5)	C12—C11—H11A	122.2
C6—N2—C14	119.2 (6)	C13—C12—C11	120.6 (8)
C6—N2—Zn1	112.4 (5)	C13—C12—H12A	119.7

C14—N2—Zn1	127.8 (5)	C11—C12—H12A	119.7
C8—N3—C14	119.9 (6)	C12—C13—N4	122.8 (9)
C8—N3—Zn2	112.4 (4)	C12—C13—H13A	118.6
C14—N3—Zn2	126.5 (5)	N4—C13—H13A	118.6
C9—N4—C13	117.4 (7)	N3—C14—N2	122.6 (7)
C9—N4—Zn2	116.3 (5)	N3—C14—C15	118.6 (6)
C13—N4—Zn2	126.0 (6)	N2—C14—C15	118.8 (6)
N1—C1—C2	122.5 (9)	C16—C15—C20	119.5 (9)
N1—C1—H1A	118.8	C16—C15—C14	120.3 (8)
C2—C1—H1A	118.8	C20—C15—C14	120.1 (7)
C3—C2—C1	119.2 (8)	C15—C16—C17	119.9 (10)
C3—C2—H2A	120.4	C15—C16—H16A	120.0
C1—C2—H2A	120.4	C17—C16—H16A	120.0
C2—C3—C4	118.8 (10)	C18—C17—C16	118.9 (11)
C2—C3—H3A	120.6	C18—C17—H17A	120.6
C4—C3—H3A	120.6	C16—C17—H17A	120.6
C5—C4—C3	119.0 (9)	C17—C18—C19	121.7 (11)
C5—C4—H4A	120.5	C17—C18—H18A	119.1
C3—C4—H4A	120.5	C19—C18—H18A	119.1
N1—C5—C4	121.2 (7)	C20—C19—C18	120.3 (11)
N1—C5—C6	115.2 (7)	C20—C19—H19A	119.8
C4—C5—C6	123.6 (7)	C18—C19—H19A	119.8
N2—C6—C7	120.6 (6)	C19—C20—C15	119.6 (10)
N2—C6—C5	117.5 (7)	C19—C20—H20A	120.2
C7—C6—C5	121.9 (7)	C15—C20—H20A	120.2