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# Dichlorido[2-(pyridin-2-yl-$\kappa N$)-1,5-naphthyridine-$\kappa N^1$]zinc(II)

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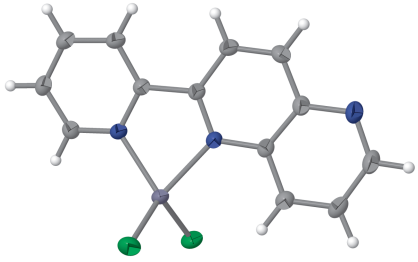
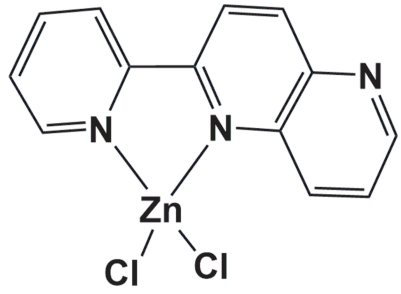
**Structural data:** full structural data are available from iucrdata.iucr.org

The title zinc(II) complex, $[ZnCl_2(C_{13}H_9N_3)]$, crystallizes in the triclinic space group $P\overline{1}$. The coordination environment around the zinc(II) ion in the title complex can be described as a distorted tetrahedron formed by the two N atoms of the NAD$^+$/NADH model ligand pn [pn = 2-(pyridin-2-yl)[1,5]naphthyridine] and two $Cl^-$ ions. There are $\pi$–$\pi$ stacking interactions in the crystal packing of the title compound.

3D view



Chemical scheme




## Structure description

Photo-driven carbon dioxide ($CO_2$) reduction has been one of the most attractive approaches to address global energy and environmental problems because of its capacity to transform $CO_2$ into value-added chemical compounds, such as formic acid and carbon monoxide, under mild conditions by utilizing solar energy (Wang *et al.*, 2022). Transition-metal molecular catalysts are an important tool and play a central role in the roadmap to achieve efficient and novel $CO_2$ photoreduction into valuable chemicals (Kumagai *et al.*, 2022). Our motivation for investigating transition-metal complexes with a coenzyme NAD$^+$/NADH model ligand is based on their potential as candidates for photocatalytic $CO_2$ reduction. The synthesis and use of the NAD$^+$/NADH model ligand pbn [pbn = 2-(pyridin-2-yl)benzo[*b*][1,5]naphthyridine] was first reported by Koizumi & Tanaka (2005), and we have previously developed a novel photocatalytic $CO_2$ reduction process to produce formic acid using a Ru-based pbn complex (Ohtsu & Tanaka, 2012; Ohtsu *et al.*, 2015, 2019).

In order to further develop transition-metal NAD$^+$/NADH model complexes, substituent tuning of NAD$^+$/NADH model ligands offers a potentially powerful means not only to control catalytic activity of the complexes but also to confer new reactivity on the complexes. However, the synthetic pathway to introduce substituents into the benzonaphthyridine skeleton of the pbn ligand is considerably difficult.

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—N3 | 2.0560 (14) | Zn1—Cl1 | 2.2137 (6) |
| Zn1—N2 | 2.0909 (14) | Zn1—Cl2 | 2.2161 (6) |
| N3—Zn1—N2 | 79.59 (6) | N3—Zn1—Cl2 | 120.94 (4) |
| N3—Zn1—Cl1 | 113.63 (4) | N2—Zn1—Cl2 | 108.77 (4) |
| N2—Zn1—Cl1 | 113.74 (4) | Cl1—Zn1—Cl2 | 114.81 (2) |

As part of our ongoing investigation of transition-metal complexes bearing various substituted $NAD^+$/NADH model ligands, we have focused on the non-substituted $NAD^+$/NADH model ligand pn [pn = 2-(pyridin-2-yl)[1,5]naphthyridine] synthesized by Singh & Thummel (2009), which can possess the potential to facilitate the introduction of substituents through a straightforward synthetic process. A new zinc(II) complex with a pn ligand has been structurally characterized and is reported in this paper.

The molecular structure of the title complex, $[ZnCl_2(pn)]$, is shown in Fig. 1 and selected geometrical data are listed in Table 1. The zinc(II) ion in $[ZnCl_2(pn)]$ has a tetracoordinate structure formed by the two N atoms of pn ligand [Zn1—N2 = 2.0909 (14) Å, Zn1—N3 = 2.0560 (14) Å] and two $Cl^-$ ions [Zn1—Cl1 = 2.2137 (6) Å, Zn1—Cl2 = 2.2161 (6) Å]. The quantitative difference in four-coordinate geometry is indicated by an index of $\tau_4$. The value can range from $\tau_4 = 1$ for a perfect tetrahedral geometry to $\tau_4 = 0$ for a perfect square planar geometry (Yang *et al.*, 2007). The $\tau_4$ value for the zinc(II) ion of the title complex is obtained as $\tau_4 = 0.88$ by using the equation $\tau_4 = [360–(\alpha+\beta)]/141$ (Yang *et al.*, 2007), where $\alpha$ = N3—Zn1—Cl2 [120.94 (4)°], $\beta$ = Cl1—Zn1—Cl2 [114.81 (2)°]. Thus, the coordination environment of the zinc(II) ion in $[ZnCl_2(pn)]$ is a slightly distorted tetrahedron. The pyridine ring and the naphthyridine ring system in the pn ligand are twisted to give a dihedral angle of 10.57 (5)° between the two least-squares planes.

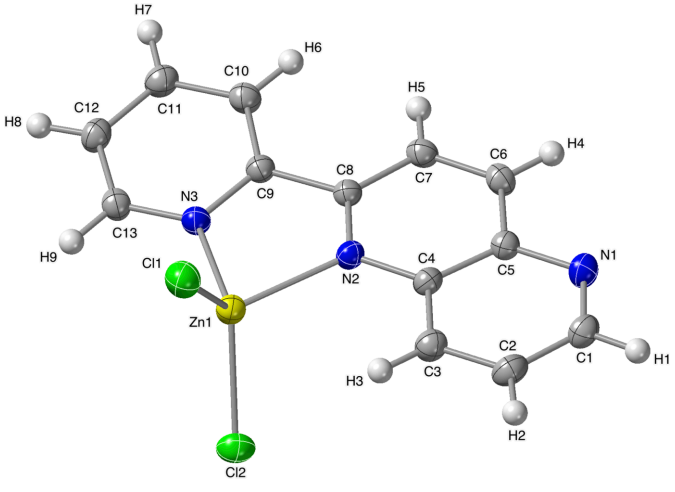



**Figure 1**
The molecular structure of the title compound with displacement ellipsoids for non-hydrogen atoms at the 50% probability level.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[ZnCl_2(C_{13}H_9N_3)]$ |
| $M_r$ | 343.52 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 173 |
| $a, b, c$ (Å) | 8.0634 (15), 8.6146 (17), 10.2087 (19) |
| $\alpha, \beta, \gamma$ (°) | 86.492 (6), 78.622 (6), 70.336 (5) |
| $V$ (Å$^3$) | 654.6 (2) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 2.27 |
| Crystal size (mm) | 0.23 × 0.11 × 0.07 |
| Data collection | |
| Diffractometer | Rigaku R-AXIS RAPID |
| Absorption correction | Multi-scan (*ABSCOR*; Rigaku, 1995) |
| $T_{min}$, $T_{max}$ | 0.630, 0.853 |
| No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections | 6486, 2992, 2693 |
| $R_{int}$ | 0.034 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.649 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.026, 0.069, 1.03 |
| No. of reflections | 2992 |
| No. of parameters | 172 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.43, −0.28 |

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*), *CrystalStructure* (Rigaku, 2019), *CrystalMaker* (Palmer, 2014) and *publCIF* (Westrip, 2010).

The crystal packing of the title complex is shown in Fig. 2. There are noteworthy $\pi$–$\pi$ stacking interactions between neighboring naphthyridine ring systems of the pn ligand, with a centroid–centroid distance of 3.625 (1) Å. No other significant or interesting intermolecular interactions are observed.

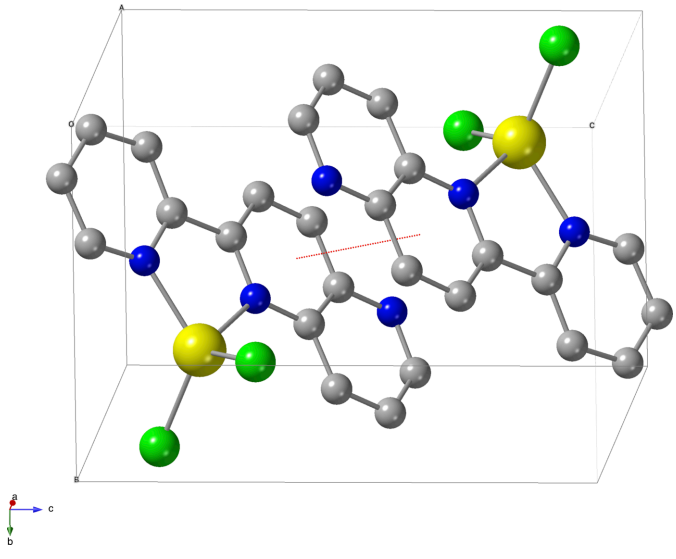


**Figure 2**
Part of the crystal structure showing a $\pi$–$\pi$ interaction (red dotted line). Zn atoms are represented in yellow, Cl in green, N in blue, and C in gray. Hydrogen atoms are omitted for clarity.

## Synthesis and crystallization

The $NAD^+$/NADH model ligand, 2-(pyridin-2-yl)[1,5]naphthyridine abbreviated as pn, was prepared according to the literature procedure (Singh & Thummel, 2009).

To a dichloromethane solution (4.0 ml) of pn (36.44 mg, 17.6 mmol) was added dropwise $ZnCl_2$ (23.95 mg, 17.6 mmol) in acetonitrile (4.0 ml), and the resulting solution was left to stand for a few days at room temperature. Light-yellow crystals of the title compound [$ZnCl_2$(pn)] were obtained (yield; 44.48 mg, 73.7%). Elemental analysis, found: C 45.32, H 2.69, N 12.18%; calculated for $C_{13}H_9Cl_2N_3Zn$: C 45.45, H 2.64, N 12.23%.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Funding information

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# full crystallographic data

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### Dichlorido[2-(pyridin-2-yl-$\kappa N$)-1,5-naphthyridine-$\kappa N^1$]zinc(II)

*Crystal data*

$[ZnCl_2(C_{13}H_9N_3)]$
$M_r$ = 343.52
Triclinic, $P\overline{1}$
$a$ = 8.0634 (15) Å
$b$ = 8.6146 (17) Å
$c$ = 10.2087 (19) Å
$\alpha$ = 86.492 (6)°
$\beta$ = 78.622 (6)°
$\gamma$ = 70.336 (5)°
$V$ = 654.6 (2) Å$^3$
$Z$ = 2
$F(000)$ = 344.00
$D_x$ = 1.743 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71075 Å
Cell parameters from 4464 reflections
$\theta$ = 2.0–27.5°
$\mu$ = 2.27 mm$^{-1}$
$T$ = 173 K
Block, colorless
0.23 × 0.11 × 0.07 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
$T_{min}$ = 0.630, $T_{max}$ = 0.853
6486 measured reflections
2992 independent reflections
2693 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int}$ = 0.034
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.5°
$h$ = −10→10
$k$ = −11→11
$l$ = −13→12

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
$S$ = 1.03
2992 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.1345P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 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 was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on $F^2$. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma($F^2$) is used only for calculating R-factor (gt).
H atoms were located in a difference map and refined as riding on their parent atoms with C–H = 0.95 Å and with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.52702 (3) | 0.80210 (2) | 0.18747 (2) | 0.02563 (8) |
| Cl1 | 0.70577 (6) | 0.89381 (6) | 0.27656 (5) | 0.03363 (12) |
| Cl2 | 0.29182 (6) | 0.99685 (6) | 0.13125 (5) | 0.03711 (12) |
| N1 | 0.1233 (2) | 0.5604 (2) | 0.59856 (15) | 0.0327 (3) |
| N2 | 0.43844 (18) | 0.62744 (18) | 0.30470 (13) | 0.0220 (3) |
| N3 | 0.66057 (19) | 0.59482 (18) | 0.07077 (14) | 0.0235 (3) |
| C1 | 0.0609 (2) | 0.7111 (3) | 0.64747 (18) | 0.0326 (4) |
| H1 | −0.029364 | 0.732608 | 0.725885 | 0.039* |
| C2 | 0.1173 (2) | 0.8429 (2) | 0.59282 (18) | 0.0305 (4) |
| H2 | 0.068503 | 0.948033 | 0.635055 | 0.037* |
| C3 | 0.2437 (2) | 0.8172 (2) | 0.47777 (18) | 0.0284 (4) |
| H3 | 0.284141 | 0.903886 | 0.438031 | 0.034* |
| C4 | 0.3122 (2) | 0.6578 (2) | 0.41992 (16) | 0.0227 (3) |
| C5 | 0.2495 (2) | 0.5333 (2) | 0.48381 (16) | 0.0250 (3) |
| C6 | 0.3234 (2) | 0.3738 (2) | 0.42718 (18) | 0.0287 (4) |
| H6 | 0.284985 | 0.286671 | 0.468330 | 0.034* |
| C7 | 0.4511 (2) | 0.3448 (2) | 0.31252 (17) | 0.0259 (3) |
| H7 | 0.501827 | 0.237854 | 0.273490 | 0.031* |
| C8 | 0.5059 (2) | 0.4762 (2) | 0.25336 (15) | 0.0215 (3) |
| C9 | 0.6415 (2) | 0.4540 (2) | 0.12667 (15) | 0.0218 (3) |
| C10 | 0.7425 (2) | 0.3016 (2) | 0.06984 (18) | 0.0280 (4) |
| H10 | 0.728308 | 0.203757 | 0.111003 | 0.034* |
| C11 | 0.8650 (2) | 0.2936 (2) | −0.04844 (18) | 0.0303 (4) |
| H11 | 0.937152 | 0.189843 | −0.088050 | 0.036* |
| C12 | 0.8812 (2) | 0.4371 (2) | −0.10788 (17) | 0.0291 (4) |
| H12 | 0.961660 | 0.434432 | −0.190011 | 0.035* |
| C13 | 0.7767 (2) | 0.5854 (2) | −0.04455 (17) | 0.0280 (4) |
| H13 | 0.788006 | 0.684666 | −0.084677 | 0.034* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.02615 (12) | 0.01684 (12) | 0.03053 (12) | −0.00643 (9) | 0.00227 (9) | −0.00346 (8) |
| Cl1 | 0.0383 (2) | 0.0267 (2) | 0.0385 (2) | −0.01520 (19) | −0.0046 (2) | −0.00282 (18) |
| Cl2 | 0.0341 (2) | 0.0217 (2) | 0.0473 (3) | −0.00115 (18) | −0.0029 (2) | −0.00052 (19) |
| N1 | 0.0306 (8) | 0.0319 (9) | 0.0285 (7) | −0.0073 (7) | 0.0053 (7) | 0.0006 (6) |
| N2 | 0.0207 (6) | 0.0200 (7) | 0.0236 (6) | −0.0062 (5) | −0.0003 (6) | −0.0030 (5) |
| N3 | 0.0251 (7) | 0.0181 (7) | 0.0247 (6) | −0.0057 (6) | −0.0007 (6) | −0.0010 (5) |
| C1 | 0.0269 (9) | 0.0360 (11) | 0.0263 (8) | −0.0041 (8) | 0.0039 (7) | −0.0017 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0252 (8) | 0.0295 (10) | 0.0309 (9) | −0.0023 (7) | −0.0014 (7) | −0.0085 (7) |
| C3 | 0.0275 (8) | 0.0243 (9) | 0.0308 (9) | −0.0075 (7) | −0.0003 (8) | −0.0046 (7) |
| C4 | 0.0188 (7) | 0.0239 (9) | 0.0234 (8) | −0.0049 (6) | −0.0030 (7) | −0.0015 (6) |
| C5 | 0.0230 (8) | 0.0258 (9) | 0.0232 (7) | −0.0058 (7) | −0.0023 (7) | 0.0019 (6) |
| C6 | 0.0322 (9) | 0.0226 (9) | 0.0301 (8) | −0.0106 (7) | −0.0015 (8) | 0.0038 (7) |
| C7 | 0.0292 (8) | 0.0187 (8) | 0.0268 (8) | −0.0052 (7) | −0.0032 (7) | −0.0004 (6) |
| C8 | 0.0211 (7) | 0.0198 (8) | 0.0221 (7) | −0.0053 (6) | −0.0035 (7) | −0.0001 (6) |
| C9 | 0.0220 (7) | 0.0205 (8) | 0.0219 (7) | −0.0060 (6) | −0.0031 (7) | −0.0011 (6) |
| C10 | 0.0322 (9) | 0.0195 (9) | 0.0295 (8) | −0.0071 (7) | −0.0010 (8) | −0.0019 (7) |
| C11 | 0.0299 (9) | 0.0236 (9) | 0.0318 (9) | −0.0049 (7) | 0.0023 (8) | −0.0073 (7) |
| C12 | 0.0272 (8) | 0.0311 (10) | 0.0250 (8) | −0.0081 (7) | 0.0024 (7) | −0.0034 (7) |
| C13 | 0.0298 (9) | 0.0247 (9) | 0.0271 (8) | −0.0094 (7) | 0.0005 (7) | 0.0013 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—N3 | 2.0560 (14) | C4—C5 | 1.408 (2) |
| Zn1—N2 | 2.0909 (14) | C5—C6 | 1.410 (3) |
| Zn1—Cl1 | 2.2137 (6) | C6—C7 | 1.371 (2) |
| Zn1—Cl2 | 2.2161 (6) | C6—H6 | 0.9500 |
| N1—C1 | 1.314 (3) | C7—C8 | 1.410 (2) |
| N1—C5 | 1.366 (2) | C7—H7 | 0.9500 |
| N2—C8 | 1.328 (2) | C8—C9 | 1.496 (2) |
| N2—C4 | 1.369 (2) | C9—C10 | 1.382 (2) |
| N3—C13 | 1.340 (2) | C10—C11 | 1.390 (2) |
| N3—C9 | 1.352 (2) | C10—H10 | 0.9500 |
| C1—C2 | 1.406 (3) | C11—C12 | 1.378 (3) |
| C1—H1 | 0.9500 | C11—H11 | 0.9500 |
| C2—C3 | 1.369 (3) | C12—C13 | 1.386 (3) |
| C2—H2 | 0.9500 | C12—H12 | 0.9500 |
| C3—C4 | 1.414 (2) | C13—H13 | 0.9500 |
| C3—H3 | 0.9500 | | |
| | | | |
| N3—Zn1—N2 | 79.59 (6) | N1—C5—C6 | 119.26 (16) |
| N3—Zn1—Cl1 | 113.63 (4) | C4—C5—C6 | 117.99 (15) |
| N2—Zn1—Cl1 | 113.74 (4) | C7—C6—C5 | 119.77 (16) |
| N3—Zn1—Cl2 | 120.94 (4) | C7—C6—H6 | 120.1 |
| N2—Zn1—Cl2 | 108.77 (4) | C5—C6—H6 | 120.1 |
| Cl1—Zn1—Cl2 | 114.81 (2) | C6—C7—C8 | 119.04 (16) |
| C1—N1—C5 | 116.46 (16) | C6—C7—H7 | 120.5 |
| C8—N2—C4 | 119.22 (14) | C8—C7—H7 | 120.5 |
| C8—N2—Zn1 | 114.20 (11) | N2—C8—C7 | 122.39 (15) |
| C4—N2—Zn1 | 126.40 (11) | N2—C8—C9 | 115.80 (14) |
| C13—N3—C9 | 118.69 (15) | C7—C8—C9 | 121.80 (15) |
| C13—N3—Zn1 | 126.24 (12) | N3—C9—C10 | 121.59 (15) |
| C9—N3—Zn1 | 114.60 (11) | N3—C9—C8 | 115.16 (14) |
| N1—C1—C2 | 125.12 (17) | C10—C9—C8 | 123.25 (15) |
| N1—C1—H1 | 117.4 | C9—C10—C11 | 119.02 (16) |
| C2—C1—H1 | 117.4 | C9—C10—H10 | 120.5 |

| | | | |
|---|---|---|---|
| C3—C2—C1 | 118.96 (17) | C11—C10—H10 | 120.5 |
| C3—C2—H2 | 120.5 | C12—C11—C10 | 119.61 (17) |
| C1—C2—H2 | 120.5 | C12—C11—H11 | 120.2 |
| C2—C3—C4 | 117.95 (17) | C10—C11—H11 | 120.2 |
| C2—C3—H3 | 121.0 | C11—C12—C13 | 118.17 (16) |
| C4—C3—H3 | 121.0 | C11—C12—H12 | 120.9 |
| N2—C4—C5 | 121.59 (15) | C13—C12—H12 | 120.9 |
| N2—C4—C3 | 119.67 (16) | N3—C13—C12 | 122.88 (17) |
| C5—C4—C3 | 118.74 (15) | N3—C13—H13 | 118.6 |
| N1—C5—C4 | 122.75 (16) | C12—C13—H13 | 118.6 |

| | | | |
|---|---|---|---|
| C5—N1—C1—C2 | −1.7 (3) | C4—N2—C8—C9 | 179.39 (14) |
| N1—C1—C2—C3 | 1.8 (3) | Zn1—N2—C8—C9 | 3.94 (17) |
| C1—C2—C3—C4 | −0.4 (3) | C6—C7—C8—N2 | 0.0 (3) |
| C8—N2—C4—C5 | −1.3 (2) | C6—C7—C8—C9 | −178.65 (15) |
| Zn1—N2—C4—C5 | 173.50 (12) | C13—N3—C9—C10 | 2.0 (2) |
| C8—N2—C4—C3 | 177.99 (15) | Zn1—N3—C9—C10 | −170.68 (13) |
| Zn1—N2—C4—C3 | −7.2 (2) | C13—N3—C9—C8 | −178.52 (15) |
| C2—C3—C4—N2 | 179.83 (15) | Zn1—N3—C9—C8 | 8.83 (18) |
| C2—C3—C4—C5 | −0.8 (2) | N2—C8—C9—N3 | −8.6 (2) |
| C1—N1—C5—C4 | 0.3 (3) | C7—C8—C9—N3 | 170.21 (15) |
| C1—N1—C5—C6 | 179.19 (17) | N2—C8—C9—C10 | 170.93 (15) |
| N2—C4—C5—N1 | −179.78 (16) | C7—C8—C9—C10 | −10.3 (2) |
| C3—C4—C5—N1 | 0.9 (2) | N3—C9—C10—C11 | −0.7 (3) |
| N2—C4—C5—C6 | 1.4 (2) | C8—C9—C10—C11 | 179.82 (16) |
| C3—C4—C5—C6 | −177.98 (16) | C9—C10—C11—C12 | −1.2 (3) |
| N1—C5—C6—C7 | −179.57 (16) | C10—C11—C12—C13 | 1.8 (3) |
| C4—C5—C6—C7 | −0.7 (3) | C9—N3—C13—C12 | −1.4 (3) |
| C5—C6—C7—C8 | 0.0 (3) | Zn1—N3—C13—C12 | 170.35 (13) |
| C4—N2—C8—C7 | 0.6 (2) | C11—C12—C13—N3 | −0.5 (3) |
| Zn1—N2—C8—C7 | −174.83 (13) | | |