

# Bis[(1-methylimidazol-2-ylmethyl)[2-(2-pyridyl)ethyl]amine- $\kappa^3 N, N', N''$ ]zinc(II) bis(hexafluoridophosphate)

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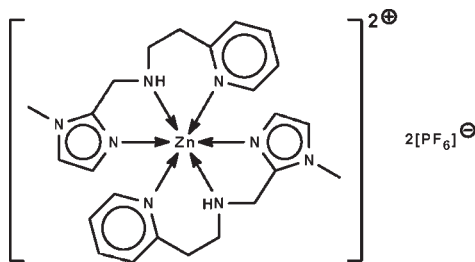
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.147; data-to-parameter ratio = 16.7.

Two tridentate  $N$ -heterocyclic ligands chelate the  $\text{Zn}^{\text{II}}$  atom in the title compound,  $[\text{Zn}(\text{C}_{12}\text{H}_{16}\text{N}_4)_2](\text{PF}_6)_2$ , conferring a *fac*-octahedral geometry. The  $\text{Zn}^{\text{II}}$  atom lies on a center of inversion. The cation is linked to the anion by an  $\text{N}-\text{H}\cdots\text{F}$  hydrogen bond.

## Related literature

No crystal structure studies of metal complexes with the  $N$ -heterocyclic ligand have been reported. For the synthesis of the ligand, see: Greatti *et al.* (2008).



## Experimental

### Crystal data

$[\text{Zn}(\text{C}_{12}\text{H}_{16}\text{N}_4)_2](\text{PF}_6)_2$   
 $M_r = 787.89$   
Orthorhombic,  $Pbca$   
 $a = 13.3147$  (5) Å

$b = 11.8147$  (4) Å  
 $c = 20.3359$  (6) Å  
 $V = 3199.0$  (2) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.97$  mm<sup>-1</sup>

$T = 100$  K  
 $0.40 \times 0.38 \times 0.35$  mm

### Data collection

Bruker APEXII diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996)  
 $T_{\text{min}} = 0.698$ ,  $T_{\text{max}} = 0.728$

18287 measured reflections  
3655 independent reflections  
2740 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.048$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.147$   
 $S = 1.04$   
3655 reflections  
219 parameters  
1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 1.49$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.71$  e Å<sup>-3</sup>

**Table 1**  
Selected bond lengths (Å).

|        |           |        |           |
|--------|-----------|--------|-----------|
| Zn1—N1 | 2.188 (3) | Zn1—N4 | 2.298 (3) |
| Zn1—N2 | 2.095 (3) |        |           |

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

| $D-H\cdots A$     | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------|----------|-------------|-------------|---------------|
| N1—H1 $\cdots$ F1 | 0.88 (1) | 2.21 (1)    | 3.083 (4)   | 179 (3)       |

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2009).

We thank Guangzhou University of Chinese Medicine and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2647).

## References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.  
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Greatti, A., Scarpellini, M., Peralta, R. A., Bortoluzi, A. J., Xavier, F. R., Szoganicz, B., Tomkowicz, Z., Rams, M., Haase, W. & Neves, A. (2008). *Inorg. Chem.* **47**, 1107–1119.  
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Westrip, S. P. (2009). *pubCIF*. In preparation.

**supplementary materials**

*Acta Cryst.* (2009). E65, m1479 [ doi:10.1107/S1600536809044419 ]

**Bis{(1-methylimidazol-2-ylmethyl)[2-(2-pyridyl)ethyl]amine- $\kappa^3N,N',N''$ }zinc(II) bis(hexafluoridophosphate)**

**A.-Z. Wu and S. W. Ng**

**Experimental**

(1-Methylimidazol-2-ylmethyl)(pyridin-2-ylethyl)amine was synthesized according to a literature method (Greatti *et al.*, 2008).

The ligand (1 mmol, 0.26 g) dissolved in methanol (5 ml) was reacted with zinc hexafluorophosphat (1 mmol, 0.36 g) dissolved in water (5 ml). The mixture was filtered and the solution set aside for the growth of colorless block-shaped crystals that formed after several days in 60% yield. CH&N elemental analysis. Found: C 36.24, H 4.07, N 13.36%; calculated: C 36.55, H 4.06, N 14.22%.

**Refinement**

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with  $U(H)$  set to 1.2 to 1.5 $U(C)$ .

The imino H-atom was located in a difference Fourier map, and was refined with a distance restraint of N—H 0.88±0.01 Å; its temperature factor was freely refined.

The final difference Fourier map had a peak in the vicinity of Zn1 but was otherwise featureless.

**Figures**

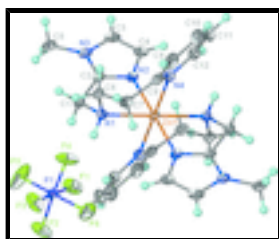


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of  $[Zn(C_{12}H_{16}N_4)_2] 2[PF_6]$  at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

**Bis{(1-methylimidazol-2-ylmethyl)[2-(2-pyridyl)ethyl]amine- $\kappa^3N,N',N''$ }zinc(II) bis(hexafluoridophosphate)**

*Crystal data*

$[Zn(C_{12}H_{16}N_4)_2](PF_6)_2$

$M_r = 787.89$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$F_{000} = 1600$

$D_x = 1.636 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4790 reflections

# supplementary materials

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$a = 13.3147 (5) \text{ \AA}$   
 $b = 11.8147 (4) \text{ \AA}$   
 $c = 20.3359 (6) \text{ \AA}$   
 $V = 3199.0 (2) \text{ \AA}^3$   
 $Z = 4$

$\theta = 2.5\text{--}28.2^\circ$   
 $\mu = 0.97 \text{ mm}^{-1}$   
 $T = 100 \text{ K}$   
Block, colorless  
 $0.40 \times 0.38 \times 0.35 \text{ mm}$

## Data collection

Bruker APEXII diffractometer  
Radiation source: fine-focus sealed tube  
Monochromator: graphite  
 $T = 100 \text{ K}$   
 $\omega$  scans  
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.698$ ,  $T_{\max} = 0.728$   
18287 measured reflections

3655 independent reflections  
2740 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.048$   
 $\theta_{\max} = 27.5^\circ$   
 $\theta_{\min} = 2.0^\circ$   
 $h = -10 \rightarrow 17$   
 $k = -13 \rightarrow 15$   
 $l = -22 \rightarrow 26$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.147$   
 $S = 1.04$   
3655 reflections  
219 parameters  
1 restraint  
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map  
Hydrogen site location: inferred from neighbouring sites  
H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 5.7073P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.49 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.71 \text{ e \AA}^{-3}$   
Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

|     | <i>x</i>     | <i>y</i>    | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|--------------|----------------------------------|
| Zn1 | 0.5000       | 0.5000      | 0.5000       | 0.02098 (16)                     |
| P1  | 0.38657 (6)  | 0.83958 (7) | 0.68434 (4)  | 0.0251 (2)                       |
| F1  | 0.47058 (17) | 0.7507 (2)  | 0.66130 (14) | 0.0524 (7)                       |
| F2  | 0.47025 (19) | 0.9039 (2)  | 0.72513 (13) | 0.0563 (7)                       |
| F3  | 0.30477 (18) | 0.9306 (2)  | 0.70513 (12) | 0.0540 (7)                       |
| F4  | 0.30581 (18) | 0.7775 (2)  | 0.63902 (15) | 0.0586 (7)                       |
| F5  | 0.3608 (2)   | 0.7641 (3)  | 0.74431 (16) | 0.0840 (11)                      |
| F6  | 0.4135 (2)   | 0.9157 (2)  | 0.62167 (13) | 0.0588 (7)                       |
| N1  | 0.40722 (19) | 0.5353 (2)  | 0.58640 (13) | 0.0231 (6)                       |
| H1  | 0.424 (3)    | 0.5969 (18) | 0.6075 (15)  | 0.027 (9)*                       |

|     |              |            |              |             |
|-----|--------------|------------|--------------|-------------|
| N2  | 0.48361 (19) | 0.3368 (2) | 0.53888 (14) | 0.0248 (6)  |
| N3  | 0.4460 (2)   | 0.2326 (2) | 0.62505 (14) | 0.0282 (6)  |
| N4  | 0.3548 (2)   | 0.4794 (2) | 0.44007 (14) | 0.0267 (6)  |
| C1  | 0.4281 (3)   | 0.4463 (3) | 0.63589 (16) | 0.0274 (7)  |
| H1A | 0.3690       | 0.4358     | 0.6648       | 0.033*      |
| H1B | 0.4861       | 0.4685     | 0.6635       | 0.033*      |
| C2  | 0.4510 (2)   | 0.3384 (3) | 0.60004 (16) | 0.0243 (7)  |
| C3  | 0.4784 (3)   | 0.1600 (3) | 0.57608 (19) | 0.0326 (8)  |
| H3  | 0.4838       | 0.0800     | 0.5790       | 0.039*      |
| C4  | 0.5009 (2)   | 0.2245 (3) | 0.5236 (2)   | 0.0294 (7)  |
| H4  | 0.5248       | 0.1972     | 0.4825       | 0.035*      |
| C5  | 0.4136 (3)   | 0.1995 (3) | 0.69075 (18) | 0.0372 (9)  |
| H5A | 0.3915       | 0.2667     | 0.7150       | 0.056*      |
| H5B | 0.4697       | 0.1638     | 0.7141       | 0.056*      |
| H5C | 0.3578       | 0.1457     | 0.6874       | 0.056*      |
| C6  | 0.2980 (2)   | 0.5415 (3) | 0.57167 (17) | 0.0254 (7)  |
| H6A | 0.2621       | 0.5715     | 0.6106       | 0.031*      |
| H6B | 0.2724       | 0.4643     | 0.5629       | 0.031*      |
| C7  | 0.2758 (2)   | 0.6170 (3) | 0.51236 (17) | 0.0292 (7)  |
| H7A | 0.2092       | 0.6529     | 0.5181       | 0.035*      |
| H7B | 0.3267       | 0.6778     | 0.5099       | 0.035*      |
| C8  | 0.2766 (2)   | 0.5506 (3) | 0.44925 (17) | 0.0277 (7)  |
| C9  | 0.1977 (3)   | 0.5560 (4) | 0.40485 (19) | 0.0391 (9)  |
| H9  | 0.1448       | 0.6087     | 0.4116       | 0.047*      |
| C10 | 0.1957 (3)   | 0.4854 (4) | 0.3511 (2)   | 0.0498 (11) |
| H10 | 0.1425       | 0.4895     | 0.3201       | 0.060*      |
| C11 | 0.2727 (3)   | 0.4086 (4) | 0.34328 (19) | 0.0449 (10) |
| H11 | 0.2724       | 0.3564     | 0.3078       | 0.054*      |
| C12 | 0.3505 (3)   | 0.4095 (3) | 0.38849 (17) | 0.0330 (8)  |
| H12 | 0.4040       | 0.3573     | 0.3825       | 0.040*      |

Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$      | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|---------------|--------------|--------------|
| Zn1 | 0.0169 (3)  | 0.0213 (3)  | 0.0247 (3)  | -0.00221 (18) | 0.00329 (19) | 0.00056 (19) |
| P1  | 0.0221 (4)  | 0.0233 (4)  | 0.0299 (5)  | 0.0017 (3)    | -0.0017 (3)  | -0.0007 (3)  |
| F1  | 0.0394 (12) | 0.0431 (13) | 0.0747 (18) | 0.0150 (11)   | -0.0061 (12) | -0.0213 (12) |
| F2  | 0.0428 (13) | 0.0550 (15) | 0.0710 (18) | 0.0110 (12)   | -0.0256 (12) | -0.0275 (13) |
| F3  | 0.0449 (13) | 0.0636 (16) | 0.0534 (15) | 0.0283 (12)   | -0.0118 (11) | -0.0196 (12) |
| F4  | 0.0410 (13) | 0.0396 (13) | 0.095 (2)   | -0.0040 (10)  | -0.0220 (13) | -0.0184 (13) |
| F5  | 0.0588 (18) | 0.106 (3)   | 0.087 (2)   | 0.0105 (17)   | 0.0142 (15)  | 0.069 (2)    |
| F6  | 0.0594 (16) | 0.0596 (16) | 0.0573 (17) | -0.0066 (13)  | -0.0012 (13) | 0.0243 (13)  |
| N1  | 0.0209 (12) | 0.0230 (12) | 0.0253 (15) | -0.0035 (10)  | 0.0010 (10)  | -0.0006 (11) |
| N2  | 0.0218 (13) | 0.0216 (12) | 0.0309 (16) | -0.0020 (10)  | 0.0017 (11)  | 0.0006 (11)  |
| N3  | 0.0248 (13) | 0.0270 (14) | 0.0328 (16) | -0.0074 (11)  | -0.0075 (11) | 0.0064 (12)  |
| N4  | 0.0197 (13) | 0.0328 (14) | 0.0277 (15) | -0.0047 (11)  | 0.0012 (11)  | 0.0005 (11)  |
| C1  | 0.0271 (15) | 0.0277 (16) | 0.0273 (18) | -0.0017 (13)  | 0.0014 (13)  | 0.0013 (13)  |
| C2  | 0.0196 (14) | 0.0218 (15) | 0.0317 (18) | -0.0034 (12)  | -0.0024 (12) | 0.0040 (13)  |

## supplementary materials

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|     |             |             |             |              |              |              |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C3  | 0.0272 (16) | 0.0223 (15) | 0.048 (2)   | -0.0028 (13) | -0.0097 (15) | 0.0008 (15)  |
| C4  | 0.0221 (15) | 0.0250 (16) | 0.041 (2)   | -0.0027 (12) | -0.0029 (14) | -0.0050 (14) |
| C5  | 0.043 (2)   | 0.0341 (18) | 0.035 (2)   | -0.0167 (16) | -0.0106 (16) | 0.0121 (15)  |
| C6  | 0.0171 (14) | 0.0282 (15) | 0.0310 (18) | -0.0024 (12) | 0.0061 (12)  | -0.0010 (13) |
| C7  | 0.0164 (14) | 0.0285 (16) | 0.043 (2)   | 0.0007 (12)  | 0.0027 (13)  | 0.0011 (14)  |
| C8  | 0.0176 (14) | 0.0335 (17) | 0.0321 (19) | -0.0035 (12) | 0.0036 (13)  | 0.0048 (14)  |
| C9  | 0.0227 (17) | 0.057 (2)   | 0.037 (2)   | 0.0016 (16)  | -0.0007 (15) | 0.0107 (18)  |
| C10 | 0.0278 (19) | 0.087 (3)   | 0.034 (2)   | -0.006 (2)   | -0.0050 (16) | 0.003 (2)    |
| C11 | 0.0316 (19) | 0.076 (3)   | 0.027 (2)   | -0.012 (2)   | 0.0021 (15)  | -0.0128 (19) |
| C12 | 0.0235 (16) | 0.044 (2)   | 0.031 (2)   | -0.0061 (15) | 0.0052 (13)  | -0.0049 (15) |

### *Geometric parameters (Å, °)*

|                                      |             |            |           |
|--------------------------------------|-------------|------------|-----------|
| Zn1—N1                               | 2.188 (3)   | C1—H1A     | 0.9900    |
| Zn1—N1 <sup>i</sup>                  | 2.188 (3)   | C1—H1B     | 0.9900    |
| Zn1—N2 <sup>i</sup>                  | 2.095 (3)   | C3—C4      | 1.345 (5) |
| Zn1—N2                               | 2.095 (3)   | C3—H3      | 0.9500    |
| Zn1—N4                               | 2.298 (3)   | C4—H4      | 0.9500    |
| Zn1—N4 <sup>i</sup>                  | 2.298 (3)   | C5—H5A     | 0.9800    |
| P1—F5                                | 1.549 (3)   | C5—H5B     | 0.9800    |
| P1—F2                                | 1.583 (2)   | C5—H5C     | 0.9800    |
| P1—F3                                | 1.588 (2)   | C6—C7      | 1.529 (5) |
| P1—F4                                | 1.595 (2)   | C6—H6A     | 0.9900    |
| P1—F6                                | 1.601 (3)   | C6—H6B     | 0.9900    |
| P1—F1                                | 1.605 (2)   | C7—C8      | 1.504 (5) |
| N1—C1                                | 1.482 (4)   | C7—H7A     | 0.9900    |
| N1—C6                                | 1.486 (4)   | C7—H7B     | 0.9900    |
| N1—H1                                | 0.875 (10)  | C8—C9      | 1.386 (5) |
| N2—C2                                | 1.317 (4)   | C9—C10     | 1.375 (6) |
| N2—C4                                | 1.382 (4)   | C9—H9      | 0.9500    |
| N3—C2                                | 1.351 (4)   | C10—C11    | 1.378 (6) |
| N3—C3                                | 1.383 (5)   | C10—H10    | 0.9500    |
| N3—C5                                | 1.457 (4)   | C11—C12    | 1.385 (5) |
| N4—C12                               | 1.336 (4)   | C11—H11    | 0.9500    |
| N4—C8                                | 1.352 (4)   | C12—H12    | 0.9500    |
| C1—C2                                | 1.500 (4)   |            |           |
| N2 <sup>i</sup> —Zn1—N2              | 180.00 (6)  | C2—C1—H1A  | 110.1     |
| N2 <sup>i</sup> —Zn1—N1              | 100.73 (10) | N1—C1—H1B  | 110.1     |
| N2—Zn1—N1                            | 79.27 (10)  | C2—C1—H1B  | 110.1     |
| N2 <sup>i</sup> —Zn1—N1 <sup>i</sup> | 79.27 (10)  | H1A—C1—H1B | 108.4     |
| N2—Zn1—N1 <sup>i</sup>               | 100.73 (10) | N2—C2—N3   | 111.0 (3) |
| N1—Zn1—N1 <sup>i</sup>               | 180.0       | N2—C2—C1   | 122.5 (3) |
| N2 <sup>i</sup> —Zn1—N4              | 89.13 (10)  | N3—C2—C1   | 126.4 (3) |
| N2—Zn1—N4                            | 90.87 (10)  | C4—C3—N3   | 106.8 (3) |
| N1—Zn1—N4                            | 88.35 (10)  | C4—C3—H3   | 126.6     |
| N1 <sup>i</sup> —Zn1—N4              | 91.65 (9)   | N3—C3—H3   | 126.6     |
| N2 <sup>i</sup> —Zn1—N4 <sup>i</sup> | 90.87 (10)  | C3—C4—N2   | 109.2 (3) |

|                                      |              |              |            |
|--------------------------------------|--------------|--------------|------------|
| N2—Zn1—N4 <sup>i</sup>               | 89.13 (10)   | C3—C4—H4     | 125.4      |
| N1—Zn1—N4 <sup>i</sup>               | 91.65 (9)    | N2—C4—H4     | 125.4      |
| N1 <sup>i</sup> —Zn1—N4 <sup>i</sup> | 88.35 (10)   | N3—C5—H5A    | 109.5      |
| N4—Zn1—N4 <sup>i</sup>               | 180.0        | N3—C5—H5B    | 109.5      |
| F5—P1—F2                             | 91.12 (18)   | H5A—C5—H5B   | 109.5      |
| F5—P1—F3                             | 91.64 (17)   | N3—C5—H5C    | 109.5      |
| F2—P1—F3                             | 91.04 (13)   | H5A—C5—H5C   | 109.5      |
| F5—P1—F4                             | 92.36 (18)   | H5B—C5—H5C   | 109.5      |
| F2—P1—F4                             | 176.28 (17)  | N1—C6—C7     | 112.2 (2)  |
| F3—P1—F4                             | 90.16 (13)   | N1—C6—H6A    | 109.2      |
| F5—P1—F6                             | 179.05 (19)  | C7—C6—H6A    | 109.2      |
| F2—P1—F6                             | 89.42 (16)   | N1—C6—H6B    | 109.2      |
| F3—P1—F6                             | 89.12 (15)   | C7—C6—H6B    | 109.2      |
| F4—P1—F6                             | 87.08 (15)   | H6A—C6—H6B   | 107.9      |
| F5—P1—F1                             | 90.41 (17)   | C8—C7—C6     | 111.6 (3)  |
| F2—P1—F1                             | 88.66 (13)   | C8—C7—H7A    | 109.3      |
| F3—P1—F1                             | 177.93 (16)  | C6—C7—H7A    | 109.3      |
| F4—P1—F1                             | 90.02 (13)   | C8—C7—H7B    | 109.3      |
| F6—P1—F1                             | 88.83 (15)   | C6—C7—H7B    | 109.3      |
| C1—N1—C6                             | 110.8 (2)    | H7A—C7—H7B   | 108.0      |
| C1—N1—Zn1                            | 107.68 (19)  | N4—C8—C9     | 121.5 (3)  |
| C6—N1—Zn1                            | 113.6 (2)    | N4—C8—C7     | 116.6 (3)  |
| C1—N1—H1                             | 102 (2)      | C9—C8—C7     | 121.8 (3)  |
| C6—N1—H1                             | 108 (2)      | C10—C9—C8    | 120.3 (4)  |
| Zn1—N1—H1                            | 114 (2)      | C10—C9—H9    | 119.8      |
| C2—N2—C4                             | 106.3 (3)    | C8—C9—H9     | 119.8      |
| C2—N2—Zn1                            | 112.2 (2)    | C9—C10—C11   | 118.5 (4)  |
| C4—N2—Zn1                            | 141.4 (2)    | C9—C10—H10   | 120.8      |
| C2—N3—C3                             | 106.7 (3)    | C11—C10—H10  | 120.8      |
| C2—N3—C5                             | 127.4 (3)    | C10—C11—C12  | 118.3 (4)  |
| C3—N3—C5                             | 125.9 (3)    | C10—C11—H11  | 120.8      |
| C12—N4—C8                            | 117.4 (3)    | C12—C11—H11  | 120.8      |
| C12—N4—Zn1                           | 121.2 (2)    | N4—C12—C11   | 123.9 (4)  |
| C8—N4—Zn1                            | 120.6 (2)    | N4—C12—H12   | 118.0      |
| N1—C1—C2                             | 108.1 (3)    | C11—C12—H12  | 118.0      |
| N1—C1—H1A                            | 110.1        |              |            |
| N2 <sup>i</sup> —Zn1—N1—C1           | -152.89 (19) | Zn1—N2—C2—C1 | 0.5 (4)    |
| N2—Zn1—N1—C1                         | 27.11 (19)   | C3—N3—C2—N2  | 0.4 (4)    |
| N4—Zn1—N1—C1                         | 118.3 (2)    | C5—N3—C2—N2  | -180.0 (3) |
| N4 <sup>i</sup> —Zn1—N1—C1           | -61.7 (2)    | C3—N3—C2—C1  | -176.9 (3) |
| N2 <sup>i</sup> —Zn1—N1—C6           | 84.0 (2)     | C5—N3—C2—C1  | 2.7 (5)    |
| N2—Zn1—N1—C6                         | -96.0 (2)    | N1—C1—C2—N2  | 23.2 (4)   |
| N4—Zn1—N1—C6                         | -4.8 (2)     | N1—C1—C2—N3  | -159.8 (3) |
| N4 <sup>i</sup> —Zn1—N1—C6           | 175.2 (2)    | C2—N3—C3—C4  | -0.4 (4)   |
| N1—Zn1—N2—C2                         | -15.5 (2)    | C5—N3—C3—C4  | 179.9 (3)  |
| N1 <sup>i</sup> —Zn1—N2—C2           | 164.5 (2)    | N3—C3—C4—N2  | 0.3 (4)    |
| N4—Zn1—N2—C2                         | -103.7 (2)   | C2—N2—C4—C3  | -0.1 (4)   |

## supplementary materials

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|                             |            |                |            |
|-----------------------------|------------|----------------|------------|
| N4 <sup>i</sup> —Zn1—N2—C2  | 76.3 (2)   | Zn1—N2—C4—C3   | 175.0 (3)  |
| N1—Zn1—N2—C4                | 169.6 (4)  | C1—N1—C6—C7    | -169.8 (3) |
| N1 <sup>i</sup> —Zn1—N2—C4  | -10.4 (4)  | Zn1—N1—C6—C7   | -48.4 (3)  |
| N4—Zn1—N2—C4                | 81.4 (4)   | N1—C6—C7—C8    | 90.1 (3)   |
| N4 <sup>i</sup> —Zn1—N2—C4  | -98.6 (4)  | C12—N4—C8—C9   | -3.8 (5)   |
| N2 <sup>i</sup> —Zn1—N4—C12 | 109.5 (3)  | Zn1—N4—C8—C9   | 165.9 (3)  |
| N2—Zn1—N4—C12               | -70.5 (3)  | C12—N4—C8—C7   | 171.8 (3)  |
| N1—Zn1—N4—C12               | -149.8 (3) | Zn1—N4—C8—C7   | -18.5 (4)  |
| N1 <sup>i</sup> —Zn1—N4—C12 | 30.2 (3)   | C6—C7—C8—N4    | -47.0 (4)  |
| N2 <sup>i</sup> —Zn1—N4—C8  | -59.9 (2)  | C6—C7—C8—C9    | 128.7 (3)  |
| N2—Zn1—N4—C8                | 120.1 (2)  | N4—C8—C9—C10   | 2.3 (6)    |
| N1—Zn1—N4—C8                | 40.9 (2)   | C7—C8—C9—C10   | -173.1 (3) |
| N1 <sup>i</sup> —Zn1—N4—C8  | -139.1 (2) | C8—C9—C10—C11  | 1.0 (6)    |
| C6—N1—C1—C2                 | 92.0 (3)   | C9—C10—C11—C12 | -2.6 (6)   |
| Zn1—N1—C1—C2                | -32.7 (3)  | C8—N4—C12—C11  | 2.2 (5)    |
| C4—N2—C2—N3                 | -0.2 (3)   | Zn1—N4—C12—C11 | -167.5 (3) |
| Zn1—N2—C2—N3                | -176.9 (2) | C10—C11—C12—N4 | 1.1 (6)    |
| C4—N2—C2—C1                 | 177.2 (3)  |                |            |

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

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

| $D-H\cdots A$     | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------|----------|-------------|-------------|---------------|
| N1—H1 $\cdots$ F1 | 0.88 (1) | 2.21 (1)    | 3.083 (4)   | 179 (3)       |

Fig. 1

