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## 4,6-Dimethyl-2-(naphthalen-1-yl)-pyrimidine

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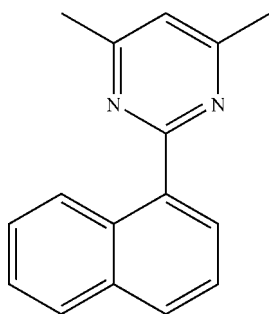
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  
 $R$  factor = 0.044;  $wR$  factor = 0.129; data-to-parameter ratio = 14.4.

The asymmetric unit of the title compound,  $\text{C}_{16}\text{H}_{14}\text{N}_2$ , contains two independent molecules in which the dihedral angles between the pyrimidine and naphthalene rings are  $38.20(5)$  and  $39.35(5)^\circ$ . Intermolecular  $\text{C}-\text{H}\cdots\pi$  contacts and  $\pi-\pi$  stacking interactions [centroid-centroid distances =  $3.766(1)$  and  $3.792(1)$  Å] are present in the crystal structure.

## Related literature

For cyclometalated Ir(III) complexes, see: Chen *et al.* (2010); Talarico *et al.* (2010); Xu *et al.* (2011); Yang *et al.* (2006). For the synthesis, see: Wang *et al.* (2011).



## Experimental

## Crystal data

$\text{C}_{16}\text{H}_{14}\text{N}_2$   
 $M_r = 234.29$   
Monoclinic,  $P2_1/c$   
 $a = 14.9022(18)$  Å  
 $b = 11.4756(14)$  Å

$c = 15.9499(19)$  Å  
 $\beta = 111.028(1)^\circ$   
 $V = 2546.0(5)$  Å<sup>3</sup>  
 $Z = 8$   
Mo  $K\alpha$  radiation

$\mu = 0.07$  mm<sup>-1</sup>  
 $T = 296$  K

 $0.50 \times 0.37 \times 0.29$  mm

## Data collection

Bruker SMART APEX CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.965$ ,  $T_{\max} = 0.979$

18638 measured reflections  
4733 independent reflections  
3442 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.023$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.129$   
 $S = 1.06$   
4733 reflections

329 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.18$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$\text{Cg}1$ ,  $\text{Cg}2$ ,  $\text{Cg}5$  and  $\text{Cg}6$  are the centroids of the  $\text{N}1/\text{N}2/\text{C}11-\text{C}14$ ,  $\text{C}1/\text{C}2/\text{C}7-\text{C}10$ ,  $\text{N}3/\text{N}4/\text{C}27-\text{C}30$  and  $\text{C}17-\text{C}21/\text{C}26$  rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}22-\text{H}22\cdots\text{Cg}1^{\text{i}}$	0.93	2.74	3.651 (4)	167
$\text{C}13-\text{H}13\cdots\text{Cg}2^{\text{ii}}$	0.93	2.76	3.597 (4)	150
$\text{C}6-\text{H}6\cdots\text{Cg}5$	0.93	2.75	3.665 (2)	168
$\text{C}29-\text{H}29\cdots\text{Cg}6^{\text{iii}}$	0.93	2.72	3.546 (3)	149

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2364).

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**supplementary materials**

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## 4,6-Dimethyl-2-(naphthalen-1-yl)pyrimidine

X.-X. Zhang, D.-Y. Zhu, X.-Q. Hao, X.-M. Dong and M.-P. Song

### Comment

In recent years, various types of cyclometalated Ir(III) complexes have been developed, such as homoleptic complexes, heteroleptic neutral complexes and cationic complexes (Chen *et al.*, 2010; Talarico *et al.*, 2010). In contrast to the most phenylpyridine ligands, few examples of naphthalenylpyrimidine iridium complexes have been reported (Xu *et al.*, 2011; Yang *et al.*, 2006). The title compound was obtained from the Suzuki coupling reaction with 1-naphthaleneboronic acid and 2-iodo-4,6-dimethylpyrimidine.

The crystal structure analysis of the title compound revealed that the asymmetric unit consists of two independent molecules (Fig. 1). The pyrimidine ring and naphthalene ring are not coplanar with the dihedral angles of 38.20 (5)° and 39.35 (5)°. All the bond distances and angles are within normal ranges. In the crystal of title compound there exist intermolecular C—H $\cdots$  $\pi$  interactions (Table 1) and  $\pi$ — $\pi$  stacking interactions [centroid-centroid distances Cg1 (N1,C11,N2,C12,C13,C14) $\cdots$ Cg7<sup>ii</sup> (C21–C26) and Cg3 (C2–C7) $\cdots$ Cg5<sup>iii</sup> (N3,C27,N4,C28,C29,C30) are 3.7659 (12) and 3.7915 (12) Å, the perpendicular distances Cg1 on Cg7<sup>ii</sup> and Cg3 on Cg5<sup>iii</sup> are 3.4761 (7) and 3.5318 (8) Å, respectively; [symmetry codes: ii = 1 - x, 1/2 + y, 1/2 - z; iii = -x, 1/2 + y, 1/2 - z] (see also Table 1). Cg2 and Cg6 are the centroids of the six-membered rings of the independent naphthyl units (C1,C2,C7,C8,C9,C10) and (C17 - C21,C26), respectively.

### Experimental

The title compound was obtained from the coupling reaction of 1-naphthaleneboronic acid and 2-iodo-4,6-dimethylpyrimidine as described in literature (Wang *et al.*, 2011) and recrystallized from dichloromethane- petroleum ether solution at room temperature to give the desired crystals suitable for single-crystal X-ray diffraction.

### Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with  $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$ ,  $1.5U_{\text{eq}}(\text{methyl H})$ .

### Figures

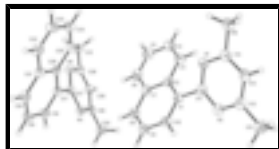


Fig. 1. The molecular structure of the title compound with displacement ellipsoids at the 30% probability level.

## 4,6-Dimethyl-2-(naphthalen-1-yl)pyrimidine

### Crystal data

$C_{16}H_{14}N_2$	$F(000) = 992$
$M_r = 234.29$	$D_x = 1.222 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 14.9022 (18) \text{ \AA}$	Cell parameters from 5588 reflections
$b = 11.4756 (14) \text{ \AA}$	$\theta = 2.4\text{--}27.4^\circ$
$c = 15.9499 (19) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$\beta = 111.028 (1)^\circ$	$T = 296 \text{ K}$
$V = 2546.0 (5) \text{ \AA}^3$	Block, colourless
$Z = 8$	$0.50 \times 0.37 \times 0.29 \text{ mm}$

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	4733 independent reflections
Radiation source: fine-focus sealed tube graphite	3442 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.023$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 25.5^\circ$ , $\theta_{\text{min}} = 2.4^\circ$
$T_{\text{min}} = 0.965$ , $T_{\text{max}} = 0.979$	$h = -18 \rightarrow 18$
18638 measured reflections	$k = -13 \rightarrow 13$
	$l = -19 \rightarrow 19$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.129$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.8594P]$
4733 reflections	where $P = (F_o^2 + 2F_c^2)/3$
329 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

### 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.33022 (12)	0.56804 (15)	0.19201 (11)	0.0391 (4)
C2	0.28518 (12)	0.54003 (15)	0.25537 (11)	0.0382 (4)
C3	0.31319 (13)	0.58798 (17)	0.34283 (12)	0.0466 (5)
H3	0.3632	0.6417	0.3614	0.056*
C4	0.26816 (14)	0.55681 (19)	0.40020 (13)	0.0545 (5)
H4	0.2882	0.5891	0.4575	0.065*
C5	0.19230 (15)	0.47692 (19)	0.37416 (14)	0.0574 (5)
H5	0.1631	0.4549	0.4144	0.069*
C6	0.16151 (14)	0.43166 (18)	0.29020 (14)	0.0535 (5)
H6	0.1102	0.3797	0.2729	0.064*
C7	0.20588 (12)	0.46173 (16)	0.22806 (12)	0.0429 (4)
C8	0.17279 (13)	0.41556 (17)	0.14022 (13)	0.0493 (5)
H8	0.1219	0.3630	0.1230	0.059*
C9	0.21425 (13)	0.44683 (17)	0.08061 (13)	0.0507 (5)
H9	0.1905	0.4175	0.0224	0.061*
C10	0.29303 (12)	0.52348 (16)	0.10659 (12)	0.0453 (4)
H10	0.3206	0.5445	0.0649	0.054*
C11	0.41918 (12)	0.63937 (15)	0.21483 (12)	0.0399 (4)
C12	0.50852 (13)	0.76663 (16)	0.16641 (13)	0.0466 (4)
C13	0.58104 (13)	0.75808 (17)	0.24906 (13)	0.0481 (5)
H13	0.6379	0.7995	0.2612	0.058*
C14	0.56827 (13)	0.68750 (16)	0.31349 (12)	0.0450 (4)
C15	0.51631 (16)	0.8421 (2)	0.09295 (15)	0.0643 (6)
H15A	0.4803	0.8079	0.0358	0.097*
H15B	0.5826	0.8489	0.0991	0.097*
H15C	0.4910	0.9180	0.0968	0.097*
C16	0.64365 (14)	0.67278 (19)	0.40496 (13)	0.0588 (5)
H16A	0.6343	0.7300	0.4450	0.088*
H16B	0.7061	0.6828	0.4014	0.088*
H16C	0.6388	0.5962	0.4271	0.088*
C17	0.12658 (11)	0.06318 (15)	0.19754 (11)	0.0357 (4)
C18	0.09762 (13)	0.01305 (17)	0.11404 (11)	0.0435 (4)
H18	0.0368	0.0304	0.0729	0.052*
C19	0.15642 (13)	-0.06341 (16)	0.08848 (12)	0.0454 (4)
H19	0.1345	-0.0962	0.0313	0.054*

## supplementary materials

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C20	0.24584 (13)	-0.08964 (16)	0.14757 (12)	0.0440 (4)
H20	0.2842	-0.1420	0.1311	0.053*
C21	0.28081 (12)	-0.03786 (15)	0.23378 (11)	0.0381 (4)
C22	0.37491 (13)	-0.06205 (18)	0.29471 (13)	0.0501 (5)
H22	0.4136	-0.1140	0.2783	0.060*
C23	0.40930 (13)	-0.0107 (2)	0.37641 (13)	0.0561 (5)
H23	0.4709	-0.0283	0.4159	0.067*
C24	0.35244 (13)	0.06895 (18)	0.40169 (12)	0.0500 (5)
H24	0.3771	0.1048	0.4576	0.060*
C25	0.26154 (12)	0.09449 (16)	0.34545 (11)	0.0413 (4)
H25	0.2250	0.1479	0.3634	0.050*
C26	0.22168 (11)	0.04068 (14)	0.25978 (10)	0.0345 (4)
C27	0.05443 (11)	0.13401 (15)	0.21966 (11)	0.0360 (4)
C28	-0.01736 (12)	0.18418 (16)	0.31890 (12)	0.0425 (4)
C29	-0.08211 (12)	0.25082 (16)	0.25319 (12)	0.0432 (4)
H29	-0.1305	0.2911	0.2649	0.052*
C30	-0.07448 (12)	0.25720 (15)	0.16983 (12)	0.0407 (4)
C31	-0.02058 (15)	0.1730 (2)	0.41097 (13)	0.0608 (6)
H31A	0.0023	0.0973	0.4347	0.091*
H31B	-0.0855	0.1828	0.4082	0.091*
H31C	0.0195	0.2317	0.4493	0.091*
C32	-0.14053 (14)	0.33086 (18)	0.09602 (13)	0.0548 (5)
H32A	-0.1143	0.4079	0.0998	0.082*
H32B	-0.2023	0.3348	0.1019	0.082*
H32C	-0.1473	0.2971	0.0390	0.082*
N1	0.48627 (10)	0.62722 (13)	0.29660 (10)	0.0437 (4)
N2	0.42607 (10)	0.70672 (13)	0.14848 (10)	0.0443 (4)
N3	-0.00560 (10)	0.19787 (12)	0.15203 (9)	0.0395 (3)
N4	0.05243 (10)	0.12487 (13)	0.30227 (9)	0.0406 (4)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0340 (9)	0.0402 (10)	0.0421 (10)	0.0027 (7)	0.0125 (7)	0.0004 (8)
C2	0.0324 (8)	0.0386 (10)	0.0423 (10)	0.0043 (7)	0.0119 (7)	0.0018 (7)
C3	0.0382 (9)	0.0543 (12)	0.0478 (11)	-0.0007 (8)	0.0160 (8)	-0.0062 (9)
C4	0.0525 (12)	0.0654 (13)	0.0480 (11)	0.0035 (10)	0.0212 (9)	-0.0036 (10)
C5	0.0562 (12)	0.0655 (14)	0.0593 (13)	-0.0010 (10)	0.0315 (10)	0.0055 (11)
C6	0.0465 (11)	0.0546 (12)	0.0631 (13)	-0.0071 (9)	0.0240 (10)	0.0014 (10)
C7	0.0358 (9)	0.0429 (10)	0.0493 (11)	0.0013 (8)	0.0145 (8)	0.0025 (8)
C8	0.0402 (10)	0.0505 (12)	0.0530 (11)	-0.0065 (8)	0.0118 (9)	-0.0033 (9)
C9	0.0485 (11)	0.0533 (12)	0.0447 (11)	-0.0035 (9)	0.0100 (9)	-0.0068 (9)
C10	0.0433 (10)	0.0496 (11)	0.0437 (10)	0.0003 (8)	0.0165 (8)	0.0014 (8)
C11	0.0382 (9)	0.0386 (10)	0.0453 (10)	0.0041 (7)	0.0178 (8)	-0.0016 (8)
C12	0.0456 (10)	0.0429 (11)	0.0573 (12)	0.0013 (8)	0.0257 (9)	-0.0002 (9)
C13	0.0406 (10)	0.0461 (11)	0.0606 (12)	-0.0068 (8)	0.0220 (9)	-0.0064 (9)
C14	0.0396 (9)	0.0449 (11)	0.0516 (11)	0.0005 (8)	0.0179 (8)	-0.0064 (9)
C15	0.0676 (14)	0.0621 (14)	0.0678 (14)	-0.0064 (11)	0.0298 (11)	0.0121 (11)

C16	0.0483 (11)	0.0662 (14)	0.0560 (12)	-0.0050 (10)	0.0115 (9)	-0.0046 (10)
C17	0.0349 (9)	0.0390 (9)	0.0348 (9)	0.0030 (7)	0.0143 (7)	0.0021 (7)
C18	0.0406 (9)	0.0518 (11)	0.0356 (9)	0.0068 (8)	0.0108 (8)	-0.0008 (8)
C19	0.0510 (11)	0.0490 (11)	0.0377 (10)	0.0040 (9)	0.0179 (8)	-0.0056 (8)
C20	0.0470 (10)	0.0450 (11)	0.0468 (10)	0.0067 (8)	0.0251 (8)	-0.0020 (8)
C21	0.0360 (9)	0.0390 (10)	0.0433 (10)	0.0033 (7)	0.0190 (8)	0.0053 (7)
C22	0.0404 (10)	0.0549 (12)	0.0557 (12)	0.0135 (9)	0.0182 (9)	0.0046 (9)
C23	0.0373 (10)	0.0699 (14)	0.0528 (12)	0.0095 (10)	0.0061 (9)	0.0055 (10)
C24	0.0425 (10)	0.0611 (13)	0.0412 (10)	-0.0032 (9)	0.0086 (8)	-0.0025 (9)
C25	0.0380 (9)	0.0453 (10)	0.0418 (10)	0.0000 (8)	0.0159 (8)	-0.0017 (8)
C26	0.0340 (8)	0.0365 (9)	0.0366 (9)	0.0012 (7)	0.0169 (7)	0.0035 (7)
C27	0.0333 (8)	0.0366 (9)	0.0375 (9)	0.0001 (7)	0.0121 (7)	-0.0011 (7)
C28	0.0379 (9)	0.0501 (11)	0.0412 (10)	0.0036 (8)	0.0163 (8)	-0.0003 (8)
C29	0.0380 (9)	0.0469 (11)	0.0458 (10)	0.0099 (8)	0.0165 (8)	-0.0017 (8)
C30	0.0381 (9)	0.0391 (10)	0.0435 (10)	0.0044 (8)	0.0129 (8)	-0.0002 (8)
C31	0.0629 (13)	0.0800 (16)	0.0458 (11)	0.0202 (11)	0.0271 (10)	0.0076 (10)
C32	0.0602 (12)	0.0546 (12)	0.0471 (11)	0.0209 (10)	0.0162 (9)	0.0075 (9)
N1	0.0383 (8)	0.0447 (9)	0.0482 (9)	-0.0011 (7)	0.0158 (7)	-0.0022 (7)
N2	0.0426 (8)	0.0431 (9)	0.0499 (9)	0.0018 (7)	0.0200 (7)	0.0003 (7)
N3	0.0381 (8)	0.0402 (8)	0.0399 (8)	0.0045 (6)	0.0136 (6)	0.0015 (6)
N4	0.0377 (8)	0.0465 (9)	0.0392 (8)	0.0066 (7)	0.0159 (6)	0.0019 (7)

*Geometric parameters (Å, °)*

C1—C10	1.372 (2)	C17—C18	1.371 (2)
C1—C2	1.436 (2)	C17—C26	1.432 (2)
C1—C11	1.488 (2)	C17—C27	1.488 (2)
C2—C3	1.416 (2)	C18—C19	1.400 (2)
C2—C7	1.423 (2)	C18—H18	0.9300
C3—C4	1.362 (3)	C19—C20	1.361 (2)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.398 (3)	C20—C21	1.415 (2)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.354 (3)	C21—C22	1.418 (2)
C5—H5	0.9300	C21—C26	1.422 (2)
C6—C7	1.417 (3)	C22—C23	1.353 (3)
C6—H6	0.9300	C22—H22	0.9300
C7—C8	1.411 (3)	C23—C24	1.400 (3)
C8—C9	1.355 (3)	C23—H23	0.9300
C8—H8	0.9300	C24—C25	1.361 (2)
C9—C10	1.405 (3)	C24—H24	0.9300
C9—H9	0.9300	C25—C26	1.421 (2)
C10—H10	0.9300	C25—H25	0.9300
C11—N1	1.336 (2)	C27—N4	1.333 (2)
C11—N2	1.344 (2)	C27—N3	1.345 (2)
C12—N2	1.346 (2)	C28—N4	1.347 (2)
C12—C13	1.376 (3)	C28—C29	1.374 (2)
C12—C15	1.495 (3)	C28—C31	1.492 (2)
C13—C14	1.374 (3)	C29—C30	1.376 (2)

## supplementary materials

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C13—H13	0.9300	C29—H29	0.9300
C14—N1	1.345 (2)	C30—N3	1.344 (2)
C14—C16	1.498 (3)	C30—C32	1.496 (2)
C15—H15A	0.9600	C31—H31A	0.9600
C15—H15B	0.9600	C31—H31B	0.9600
C15—H15C	0.9600	C31—H31C	0.9600
C16—H16A	0.9600	C32—H32A	0.9600
C16—H16B	0.9600	C32—H32B	0.9600
C16—H16C	0.9600	C32—H32C	0.9600
C10—C1—C2	119.41 (16)	C26—C17—C27	123.63 (14)
C10—C1—C11	117.06 (15)	C17—C18—C19	122.29 (16)
C2—C1—C11	123.47 (15)	C17—C18—H18	118.9
C3—C2—C7	117.77 (16)	C19—C18—H18	118.9
C3—C2—C1	124.01 (16)	C20—C19—C18	119.77 (16)
C7—C2—C1	118.20 (16)	C20—C19—H19	120.1
C4—C3—C2	121.16 (18)	C18—C19—H19	120.1
C4—C3—H3	119.4	C19—C20—C21	120.51 (16)
C2—C3—H3	119.4	C19—C20—H20	119.7
C3—C4—C5	120.89 (19)	C21—C20—H20	119.7
C3—C4—H4	119.6	C20—C21—C22	120.85 (16)
C5—C4—H4	119.6	C20—C21—C26	119.93 (15)
C6—C5—C4	119.76 (18)	C22—C21—C26	119.22 (16)
C6—C5—H5	120.1	C23—C22—C21	120.97 (17)
C4—C5—H5	120.1	C23—C22—H22	119.5
C5—C6—C7	121.38 (19)	C21—C22—H22	119.5
C5—C6—H6	119.3	C22—C23—C24	120.18 (17)
C7—C6—H6	119.3	C22—C23—H23	119.9
C8—C7—C6	121.22 (17)	C24—C23—H23	119.9
C8—C7—C2	119.81 (16)	C25—C24—C23	120.84 (18)
C6—C7—C2	118.97 (17)	C25—C24—H24	119.6
C9—C8—C7	120.82 (17)	C23—C24—H24	119.6
C9—C8—H8	119.6	C24—C25—C26	120.92 (17)
C7—C8—H8	119.6	C24—C25—H25	119.5
C8—C9—C10	120.13 (18)	C26—C25—H25	119.5
C8—C9—H9	119.9	C25—C26—C21	117.83 (15)
C10—C9—H9	119.9	C25—C26—C17	123.81 (15)
C1—C10—C9	121.54 (17)	C21—C26—C17	118.34 (15)
C1—C10—H10	119.2	N4—C27—N3	126.26 (15)
C9—C10—H10	119.2	N4—C27—C17	117.76 (14)
N1—C11—N2	125.94 (16)	N3—C27—C17	115.91 (14)
N1—C11—C1	118.07 (15)	N4—C28—C29	120.77 (16)
N2—C11—C1	115.91 (15)	N4—C28—C31	116.77 (16)
N2—C12—C13	120.69 (17)	C29—C28—C31	122.47 (16)
N2—C12—C15	116.82 (17)	C28—C29—C30	119.18 (16)
C13—C12—C15	122.50 (18)	C28—C29—H29	120.4
C14—C13—C12	119.12 (17)	C30—C29—H29	120.4
C14—C13—H13	120.4	N3—C30—C29	120.73 (16)
C12—C13—H13	120.4	N3—C30—C32	117.18 (16)
N1—C14—C13	120.87 (17)	C29—C30—C32	122.09 (16)



N1—C14—C16	116.57 (17)	C28—C31—H31A	109.5
C13—C14—C16	122.56 (17)	C28—C31—H31B	109.5
C12—C15—H15A	109.5	H31A—C31—H31B	109.5
C12—C15—H15B	109.5	C28—C31—H31C	109.5
H15A—C15—H15B	109.5	H31A—C31—H31C	109.5
C12—C15—H15C	109.5	H31B—C31—H31C	109.5
H15A—C15—H15C	109.5	C30—C32—H32A	109.5
H15B—C15—H15C	109.5	C30—C32—H32B	109.5
C14—C16—H16A	109.5	H32A—C32—H32B	109.5
C14—C16—H16B	109.5	C30—C32—H32C	109.5
H16A—C16—H16B	109.5	H32A—C32—H32C	109.5
C14—C16—H16C	109.5	H32B—C32—H32C	109.5
H16A—C16—H16C	109.5	C11—N1—C14	116.74 (15)
H16B—C16—H16C	109.5	C11—N2—C12	116.63 (15)
C18—C17—C26	119.09 (15)	C30—N3—C27	116.44 (14)
C18—C17—C27	117.21 (14)	C27—N4—C28	116.61 (14)
C10—C1—C2—C3	-175.15 (17)	C21—C22—C23—C24	-0.8 (3)
C11—C1—C2—C3	7.8 (3)	C22—C23—C24—C25	1.1 (3)
C10—C1—C2—C7	3.1 (2)	C23—C24—C25—C26	0.3 (3)
C11—C1—C2—C7	-173.91 (16)	C24—C25—C26—C21	-1.9 (3)
C7—C2—C3—C4	2.5 (3)	C24—C25—C26—C17	179.75 (17)
C1—C2—C3—C4	-179.26 (18)	C20—C21—C26—C25	-177.21 (15)
C2—C3—C4—C5	-0.4 (3)	C22—C21—C26—C25	2.0 (2)
C3—C4—C5—C6	-1.5 (3)	C20—C21—C26—C17	1.3 (2)
C4—C5—C6—C7	1.3 (3)	C22—C21—C26—C17	-179.48 (15)
C5—C6—C7—C8	-179.16 (19)	C18—C17—C26—C25	175.28 (16)
C5—C6—C7—C2	0.8 (3)	C27—C17—C26—C25	-7.9 (3)
C3—C2—C7—C8	177.34 (16)	C18—C17—C26—C21	-3.1 (2)
C1—C2—C7—C8	-1.0 (3)	C27—C17—C26—C21	173.76 (15)
C3—C2—C7—C6	-2.6 (3)	C18—C17—C27—N4	140.10 (17)
C1—C2—C7—C6	179.01 (16)	C26—C17—C27—N4	-36.8 (2)
C6—C7—C8—C9	178.50 (19)	C18—C17—C27—N3	-37.2 (2)
C2—C7—C8—C9	-1.5 (3)	C26—C17—C27—N3	145.92 (16)
C7—C8—C9—C10	1.9 (3)	N4—C28—C29—C30	-0.5 (3)
C2—C1—C10—C9	-2.8 (3)	C31—C28—C29—C30	179.84 (19)
C11—C1—C10—C9	174.40 (16)	C28—C29—C30—N3	1.0 (3)
C8—C9—C10—C1	0.3 (3)	C28—C29—C30—C32	-178.10 (17)
C10—C1—C11—N1	-140.99 (17)	N2—C11—N1—C14	-0.5 (3)
C2—C1—C11—N1	36.1 (2)	C1—C11—N1—C14	176.14 (15)
C10—C1—C11—N2	35.9 (2)	C13—C14—N1—C11	0.2 (2)
C2—C1—C11—N2	-146.97 (16)	C16—C14—N1—C11	-179.46 (16)
N2—C12—C13—C14	-0.1 (3)	N1—C11—N2—C12	0.4 (3)
C15—C12—C13—C14	179.50 (18)	C1—C11—N2—C12	-176.27 (15)
C12—C13—C14—N1	0.0 (3)	C13—C12—N2—C11	-0.1 (2)
C12—C13—C14—C16	179.70 (18)	C15—C12—N2—C11	-179.72 (17)
C26—C17—C18—C19	2.7 (3)	C29—C30—N3—C27	-0.5 (2)
C27—C17—C18—C19	-174.41 (17)	C32—C30—N3—C27	178.65 (16)
C17—C18—C19—C20	-0.2 (3)	N4—C27—N3—C30	-0.6 (3)
C18—C19—C20—C21	-1.7 (3)	C17—C27—N3—C30	176.45 (15)

## supplementary materials

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C19—C20—C21—C22	-178.11 (18)	N3—C27—N4—C28	1.0 (3)
C19—C20—C21—C26	1.1 (3)	C17—C27—N4—C28	-175.97 (15)
C20—C21—C22—C23	178.51 (18)	C29—C28—N4—C27	-0.4 (3)
C26—C21—C22—C23	-0.7 (3)	C31—C28—N4—C27	179.27 (17)

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

Cg1, Cg2, Cg5 and Cg6 are the centroids of the N1/N2/C11–C14, C1/C2/C7–C10, N3/N4,C27–C30 and C17–C21/C26 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C22—H22 $\cdots$ Cg1 <sup>i</sup>	0.93	2.74	3.651 (4)	167
C13—H13 $\cdots$ Cg2 <sup>ii</sup>	0.93	2.76	3.597 (4)	150
C6—H6 $\cdots$ Cg5	0.93	2.75	3.665 (2)	168
C29—H29 $\cdots$ Cg6 <sup>iii</sup>	0.93	2.72	3.546 (3)	149

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

Fig. 1

