

Acta Crystallographica Section E

## Structure Reports

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**(*E,E*)-3,3'-Dimethyl-1,1'-diphenyl-4,4'-  
 {[3-azapentane-1,5-diylbis(azanediyl)]-  
 bis(phenylmethylidene)}di-1*H*-pyrazol-  
 5(4*H*)-one**

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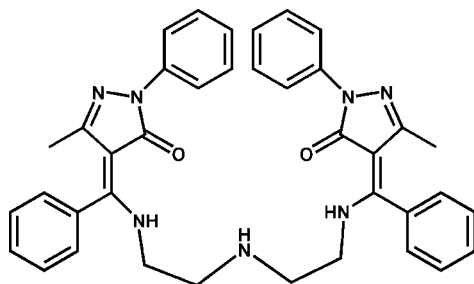
Received 21 November 2010; accepted 23 November 2010

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.054;  $wR$  factor = 0.179; data-to-parameter ratio = 17.6.

The asymmetric unit of the title compound,  $\text{C}_{38}\text{H}_{37}\text{N}_7\text{O}_2$ , contains one half-molecule, situated on a twofold rotational axis, in which one amino group is involved in intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond and the two phenyl rings are twisted from the plane of pyrazolone ring by 26.69 (10) and 79.64 (8)°. The crystal packing exhibits no classical intermolecular contacts.

## Related literature

For the synthesis of the title compound and the DNA binding properties of its transition metal complexes, see: Yang *et al.* (2000); Wang & Yang (2005). For the similar structure of (*E,E*)-3,3'-dimethyl-1,1'-diphenyl-4,4'-{(ethane-1,2-diyl-di-imino)bis[(2-furyl)-methylidene]}di-1*H*-pyrazol-5(4*H*)-one, see: Wang (2010).



## Experimental

## Crystal data

$\text{C}_{38}\text{H}_{37}\text{N}_7\text{O}_2$   
 $M_r = 623.75$   
 Monoclinic,  $C2/c$   
 $a = 20.3219$  (8) Å  
 $b = 8.1990$  (2) Å  
 $c = 20.5468$  (6) Å  
 $\beta = 106.748$  (2)°

$V = 3278.27$  (18) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.23 \times 0.21 \times 0.15$  mm

## Data collection

Bruker SMART APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2007)  
 $T_{\min} = 0.982$ ,  $T_{\max} = 0.988$

8269 measured reflections  
 3765 independent reflections  
 1886 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.021$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.179$   
 $S = 1.01$   
 3765 reflections

214 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.29$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N3}-\text{H3A}\cdots\text{O1}$	0.86	2.00	2.722 (2)	140

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); 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: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5005).

## References

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## supporting information

*Acta Cryst.* (2010). E66, o3326 [https://doi.org/10.1107/S1600536810048981]

**(*E,E*)-3,3'-Dimethyl-1,1'-diphenyl-4,4'-{[3-azapentane-1,5-diylbis(azanediy)]bis(phenylmethyldiylne)}di-1*H*-pyrazol-5(4*H*)-one**

**Zhao-Po Zhang, Yuan Wang, Xiao-Xia Li and Yan-Wei Li**

### S1. Comment

The Schiff bases derivatives of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone (PMBP) and their metal complexes have been widely studied because of their high biological and pharmaceutical activities (Yang *et al.*, 2000; Wang *et al.*, 2005). For our interest in coordination chemistry, the crystal structure of the title compound was determined by X-ray diffraction analysis.

The asymmetric unit of the title compound contains a half of the molecule situated on a twofold rotational axis. In the independent part of the molecule, one amino group is involved in intramolecular N—H···O hydrogen bond (Table 1), and two phenyl rings are twisted from the plane of pyrazolone ring at 26.69 (10)° and 79.64 (8)°, respectively. The crystal packing exhibits no classical intermolecular contacts.

### S2. Experimental

The title compound was prepared according to the literature (Wang *et al.*, 2005). 1.1 g (4 mmol) of PMBP were dissolved in EtOH (50 ml), and the EtOH solution containing diethylenetriamine (0.2 g, 2 mmol) was added dropwise. The mixture refluxed on a water bath for 4 h, then part of the solvent was removed on a rotary evaporator. After cooling to 273 K, a large amount of yellow precipitate separated out. Yellow block crystals were obtained by slow evaporation of an ethanol /chloroform (1:1) solution.

### S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and were treated as riding, with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}$  of the parent atom.

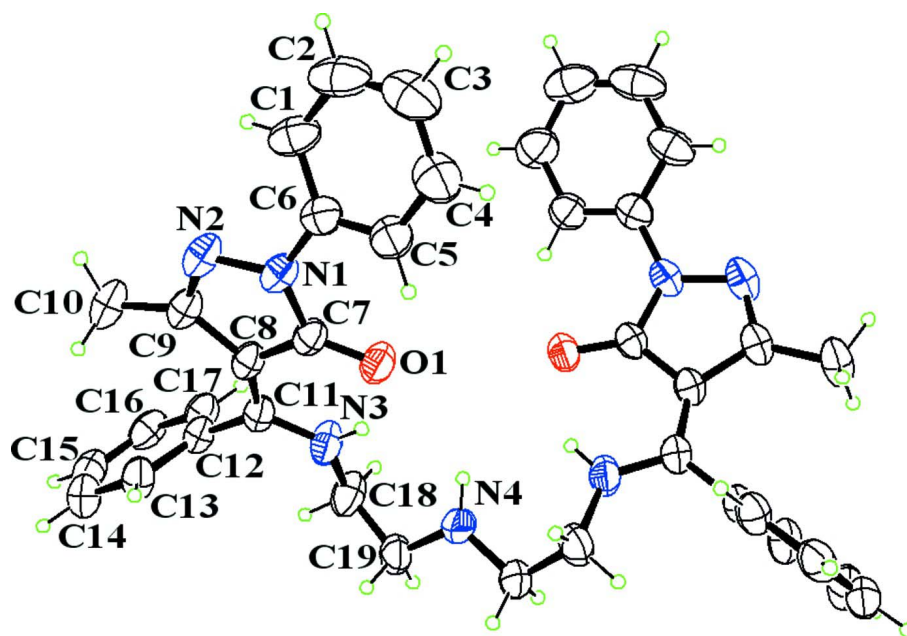


Figure 1

The molecular structure shown with 30% probability displacement ellipsoids. Unlabelled atoms are related with the labelled ones by symmetry operation  $(-x, y, -z+1/2)$ .

**(*E,E*)-3,3'-Dimethyl-1,1'-diphenyl-4,4'-[[3-azapentane-1,5-diylbis(azanediyl)]bis(phenylmethylidene)]di-1*H*-pyrazol-5(4*H*)-one**

*Crystal data*

$C_{38}H_{37}N_7O_2$

$M_r = 623.75$

Monoclinic,  $C2/c$

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$c = 20.5468$  (6) Å

$\beta = 106.748$  (2)°

$V = 3278.27$  (18) Å<sup>3</sup>

$Z = 4$

$F(000) = 1320$

$D_x = 1.264$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1721 reflections

$\theta = 2.5$ – $22.0$ °

$\mu = 0.08$  mm<sup>-1</sup>

$T = 296$  K

Block, yellow

$0.23 \times 0.21 \times 0.15$  mm

*Data collection*

Bruker SMART APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.982$ ,  $T_{\max} = 0.988$

8269 measured reflections

3765 independent reflections

1886 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 27.7$ °,  $\theta_{\min} = 2.1$ °

$h = -26 \rightarrow 20$

$k = -8 \rightarrow 10$

$l = -26 \rightarrow 25$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.054$  $wR(F^2) = 0.179$  $S = 1.01$ 

3765 reflections

214 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0884P)^2 + 0.1149P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$ *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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.06573 (8)	0.23883 (18)	0.35444 (8)	0.0809 (5)
N1	0.14838 (9)	0.0606 (2)	0.41990 (8)	0.0707 (5)
C7	0.12657 (11)	0.1980 (3)	0.38051 (10)	0.0645 (6)
C12	0.25215 (10)	0.4844 (3)	0.32781 (11)	0.0661 (6)
N2	0.21985 (10)	0.0439 (3)	0.43823 (10)	0.0819 (6)
N3	0.12874 (9)	0.4629 (2)	0.29494 (10)	0.0833 (6)
H3A	0.0927	0.4145	0.2992	0.100*
C11	0.18821 (10)	0.4066 (3)	0.33364 (11)	0.0657 (6)
N4	0.0000	0.6106 (3)	0.2500	0.0898 (9)
H4	0.0000	0.5057	0.2500	0.108*
C8	0.18835 (10)	0.2749 (3)	0.37639 (10)	0.0635 (6)
C6	0.10856 (13)	-0.0732 (3)	0.42954 (10)	0.0719 (6)
C17	0.27276 (12)	0.4657 (3)	0.27000 (11)	0.0738 (6)
H17	0.2456	0.4070	0.2333	0.089*
C9	0.24330 (11)	0.1713 (3)	0.41344 (10)	0.0715 (6)
C19	0.06028 (11)	0.7026 (3)	0.25289 (12)	0.0802 (7)
H19A	0.0749	0.7608	0.2958	0.096*
H19B	0.0500	0.7825	0.2165	0.096*
C15	0.37336 (13)	0.6229 (3)	0.32006 (17)	0.0930 (8)
H15	0.4144	0.6685	0.3174	0.112*
C13	0.29269 (12)	0.5747 (3)	0.38196 (12)	0.0822 (7)
H13	0.2791	0.5876	0.4212	0.099*
C16	0.33348 (14)	0.5339 (3)	0.26650 (14)	0.0840 (7)
H16	0.3476	0.5196	0.2277	0.101*
C5	0.04144 (14)	-0.0517 (3)	0.42877 (12)	0.0830 (7)

H5	0.0224	0.0524	0.4239	0.100*
C18	0.11649 (12)	0.5955 (3)	0.24635 (13)	0.0913 (8)
H18A	0.1048	0.5511	0.2007	0.110*
H18B	0.1582	0.6592	0.2535	0.110*
C14	0.35261 (13)	0.6447 (3)	0.37766 (15)	0.0951 (8)
H14	0.3792	0.7068	0.4136	0.114*
C10	0.31871 (12)	0.1867 (4)	0.42487 (13)	0.0961 (8)
H10A	0.3412	0.0905	0.4472	0.144*
H10B	0.3354	0.2803	0.4528	0.144*
H10C	0.3281	0.1991	0.3820	0.144*
C1	0.13730 (17)	-0.2275 (3)	0.43868 (12)	0.0930 (8)
H1	0.1832	-0.2428	0.4409	0.112*
C2	0.0968 (2)	-0.3578 (4)	0.44439 (14)	0.1196 (12)
H2	0.1156	-0.4621	0.4496	0.144*
C4	0.00213 (17)	-0.1842 (4)	0.43516 (14)	0.1080 (9)
H4A	-0.0435	-0.1692	0.4344	0.130*
C3	0.0297 (3)	-0.3380 (5)	0.44262 (15)	0.1220 (12)
H3	0.0030	-0.4276	0.4464	0.146*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0582 (10)	0.0849 (11)	0.0935 (11)	0.0105 (8)	0.0123 (8)	0.0203 (9)
N1	0.0691 (12)	0.0775 (12)	0.0639 (11)	0.0186 (10)	0.0165 (9)	0.0105 (10)
C7	0.0633 (14)	0.0714 (13)	0.0550 (11)	0.0118 (11)	0.0113 (10)	0.0031 (11)
C12	0.0527 (12)	0.0789 (14)	0.0630 (13)	0.0104 (10)	0.0106 (10)	0.0064 (11)
N2	0.0710 (13)	0.1030 (15)	0.0698 (12)	0.0299 (11)	0.0171 (9)	0.0151 (11)
N3	0.0534 (11)	0.0994 (14)	0.0904 (14)	0.0020 (10)	0.0098 (9)	0.0312 (12)
C11	0.0534 (12)	0.0782 (14)	0.0613 (12)	0.0071 (11)	0.0099 (9)	-0.0004 (11)
N4	0.0586 (17)	0.0646 (15)	0.141 (3)	0.000	0.0209 (16)	0.000
C8	0.0578 (13)	0.0768 (14)	0.0529 (11)	0.0114 (11)	0.0109 (9)	0.0040 (11)
C6	0.0888 (17)	0.0736 (15)	0.0502 (11)	0.0087 (13)	0.0153 (11)	0.0050 (11)
C17	0.0676 (15)	0.0905 (16)	0.0623 (13)	0.0129 (12)	0.0171 (11)	0.0103 (12)
C9	0.0635 (14)	0.0937 (16)	0.0556 (12)	0.0222 (13)	0.0144 (10)	0.0047 (12)
C19	0.0640 (15)	0.0849 (15)	0.0790 (15)	-0.0046 (13)	0.0001 (11)	0.0105 (13)
C15	0.0587 (15)	0.0976 (19)	0.118 (2)	0.0060 (14)	0.0185 (15)	0.0314 (18)
C13	0.0626 (14)	0.1095 (18)	0.0691 (14)	0.0038 (14)	0.0101 (11)	-0.0065 (14)
C16	0.0793 (18)	0.0950 (17)	0.0848 (17)	0.0241 (14)	0.0348 (14)	0.0294 (15)
C5	0.0876 (18)	0.0819 (16)	0.0771 (15)	-0.0009 (14)	0.0201 (13)	0.0111 (13)
C18	0.0667 (15)	0.1080 (18)	0.0938 (17)	0.0109 (14)	0.0146 (12)	0.0381 (15)
C14	0.0646 (17)	0.110 (2)	0.101 (2)	-0.0025 (14)	0.0075 (14)	-0.0023 (16)
C10	0.0650 (16)	0.134 (2)	0.0863 (16)	0.0318 (15)	0.0163 (12)	0.0204 (16)
C1	0.136 (2)	0.0787 (17)	0.0666 (14)	0.0274 (17)	0.0325 (15)	0.0120 (13)
C2	0.205 (4)	0.074 (2)	0.0774 (19)	0.014 (2)	0.037 (2)	0.0158 (15)
C4	0.119 (2)	0.105 (2)	0.0920 (19)	-0.020 (2)	0.0188 (16)	0.0229 (17)
C3	0.182 (4)	0.100 (3)	0.0778 (18)	-0.037 (3)	0.026 (2)	0.0155 (17)

*Geometric parameters (Å, °)*

O1—C7	1.243 (2)	C19—H19A	0.9700
N1—C7	1.383 (3)	C19—H19B	0.9700
N1—N2	1.398 (2)	C15—C16	1.374 (4)
N1—C6	1.411 (3)	C15—C14	1.378 (4)
C7—C8	1.429 (3)	C15—H15	0.9300
C12—C17	1.377 (3)	C13—C14	1.372 (3)
C12—C13	1.391 (3)	C13—H13	0.9300
C12—C11	1.483 (3)	C16—H16	0.9300
N2—C9	1.310 (3)	C5—C4	1.377 (4)
N3—C11	1.324 (3)	C5—H5	0.9300
N3—C18	1.448 (3)	C18—H18A	0.9700
N3—H3A	0.8600	C18—H18B	0.9700
C11—C8	1.392 (3)	C14—H14	0.9300
N4—C19	1.425 (3)	C10—H10A	0.9600
N4—C19 <sup>i</sup>	1.425 (3)	C10—H10B	0.9600
N4—H4	0.8600	C10—H10C	0.9600
C8—C9	1.435 (3)	C1—C2	1.375 (4)
C6—C5	1.371 (3)	C1—H1	0.9300
C6—C1	1.384 (3)	C2—C3	1.362 (5)
C17—C16	1.375 (3)	C2—H2	0.9300
C17—H17	0.9300	C4—C3	1.370 (5)
C9—C10	1.487 (3)	C4—H4A	0.9300
C19—C18	1.477 (3)	C3—H3	0.9300
C7—N1—N2	111.73 (18)	C16—C15—H15	120.0
C7—N1—C6	127.98 (19)	C14—C15—H15	120.0
N2—N1—C6	118.64 (18)	C14—C13—C12	120.2 (2)
O1—C7—N1	125.6 (2)	C14—C13—H13	119.9
O1—C7—C8	129.6 (2)	C12—C13—H13	119.9
N1—C7—C8	104.77 (18)	C15—C16—C17	120.3 (2)
C17—C12—C13	119.5 (2)	C15—C16—H16	119.8
C17—C12—C11	120.9 (2)	C17—C16—H16	119.8
C13—C12—C11	119.66 (19)	C6—C5—C4	120.0 (3)
C9—N2—N1	106.44 (17)	C6—C5—H5	120.0
C11—N3—C18	128.4 (2)	C4—C5—H5	120.0
C11—N3—H3A	115.8	N3—C18—C19	111.5 (2)
C18—N3—H3A	115.8	N3—C18—H18A	109.3
N3—C11—C8	119.03 (19)	C19—C18—H18A	109.3
N3—C11—C12	118.1 (2)	N3—C18—H18B	109.3
C8—C11—C12	122.84 (18)	C19—C18—H18B	109.3
C19—N4—C19 <sup>i</sup>	116.1 (3)	H18A—C18—H18B	108.0
C19—N4—H4	122.0	C13—C14—C15	119.9 (3)
C19 <sup>i</sup> —N4—H4	122.0	C13—C14—H14	120.1
C11—C8—C7	122.52 (18)	C15—C14—H14	120.1
C11—C8—C9	130.9 (2)	C9—C10—H10A	109.5
C7—C8—C9	105.7 (2)	C9—C10—H10B	109.5

C5—C6—C1	119.9 (2)	H10A—C10—H10B	109.5
C5—C6—N1	120.5 (2)	C9—C10—H10C	109.5
C1—C6—N1	119.6 (2)	H10A—C10—H10C	109.5
C16—C17—C12	120.0 (2)	H10B—C10—H10C	109.5
C16—C17—H17	120.0	C2—C1—C6	118.8 (3)
C12—C17—H17	120.0	C2—C1—H1	120.6
N2—C9—C8	111.3 (2)	C6—C1—H1	120.6
N2—C9—C10	118.7 (2)	C3—C2—C1	121.6 (3)
C8—C9—C10	130.0 (2)	C3—C2—H2	119.2
N4—C19—C18	111.1 (2)	C1—C2—H2	119.2
N4—C19—H19A	109.4	C3—C4—C5	120.4 (3)
C18—C19—H19A	109.4	C3—C4—H4A	119.8
N4—C19—H19B	109.4	C5—C4—H4A	119.8
C18—C19—H19B	109.4	C2—C3—C4	119.1 (3)
H19A—C19—H19B	108.0	C2—C3—H3	120.4
C16—C15—C14	120.1 (2)	C4—C3—H3	120.4
N2—N1—C7—O1	176.4 (2)	C11—C12—C17—C16	-177.64 (19)
C6—N1—C7—O1	11.4 (3)	N1—N2—C9—C8	-1.4 (2)
N2—N1—C7—C8	-2.4 (2)	N1—N2—C9—C10	-179.79 (19)
C6—N1—C7—C8	-167.39 (18)	C11—C8—C9—N2	-168.8 (2)
C7—N1—N2—C9	2.5 (2)	C7—C8—C9—N2	0.0 (2)
C6—N1—N2—C9	169.01 (18)	C11—C8—C9—C10	9.3 (4)
C18—N3—C11—C8	-178.9 (2)	C7—C8—C9—C10	178.1 (2)
C18—N3—C11—C12	-0.7 (3)	C19 <sup>i</sup> —N4—C19—C18	-172.3 (2)
C17—C12—C11—N3	-69.2 (3)	C17—C12—C13—C14	0.1 (4)
C13—C12—C11—N3	112.2 (2)	C11—C12—C13—C14	178.8 (2)
C17—C12—C11—C8	108.9 (2)	C14—C15—C16—C17	-0.1 (4)
C13—C12—C11—C8	-69.7 (3)	C12—C17—C16—C15	-1.0 (3)
N3—C11—C8—C7	-0.3 (3)	C1—C6—C5—C4	-1.8 (3)
C12—C11—C8—C7	-178.43 (19)	N1—C6—C5—C4	177.1 (2)
N3—C11—C8—C9	166.9 (2)	C11—N3—C18—C19	-135.6 (3)
C12—C11—C8—C9	-11.2 (3)	N4—C19—C18—N3	-52.7 (3)
O1—C7—C8—C11	-7.3 (4)	C12—C13—C14—C15	-1.3 (4)
N1—C7—C8—C11	171.45 (18)	C16—C15—C14—C13	1.3 (4)
O1—C7—C8—C9	-177.3 (2)	C5—C6—C1—C2	2.3 (3)
N1—C7—C8—C9	1.4 (2)	N1—C6—C1—C2	-176.6 (2)
C7—N1—C6—C5	-32.3 (3)	C6—C1—C2—C3	-1.3 (4)
N2—N1—C6—C5	163.56 (19)	C6—C5—C4—C3	0.3 (4)
C7—N1—C6—C1	146.5 (2)	C1—C2—C3—C4	-0.2 (5)
N2—N1—C6—C1	-17.5 (3)	C5—C4—C3—C2	0.7 (5)
C13—C12—C17—C16	1.0 (3)		

Symmetry code: (i)  $-x, y, -z+1/2$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3A $\cdots$ O1	0.86	2.00	2.722 (2)	140