IUCrData

ISSN 2414-3146

1-Methyl-3-(2-methylphenyl)-4-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidine

Mohamed El Hafi,[a]* Mohammed Boulhaoua,[a] Youssef Ramli,[b] Mohammed Benchidmi,[a] El Mokhtar Essassi[a] and Joel T. Mague[c]

[a]Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche Des Sciences des Médicaments, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco, [b]Laboratory of Medicinal Chemistry, Faculty of Medicine and Pharmacy, Mohammed V University, Rabat, Morocco, and [c]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: elhafi.mohamed1@gmail.com

Received 23 September 2017
Accepted 24 September 2017

Edited by L. Van Meervelt, Katholieke Universiteit Leuven, Belgium

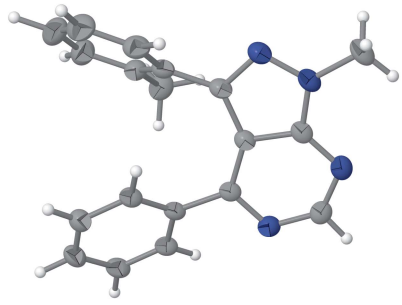
Keywords: crystal structure; pyrimidine; π-stacking; pyrazolo[3,4-*d*]pyrimidine.

CCDC reference: 1576254

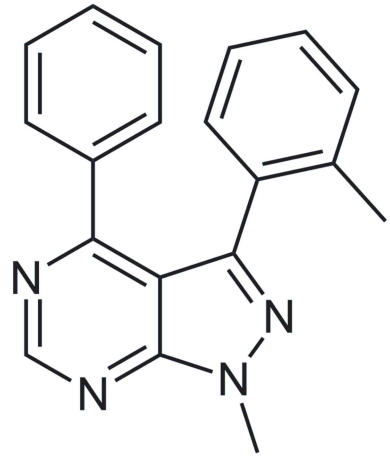
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{16}N_4$, the pyrazolopyrimidine unit is slightly twisted. A combination of π-stacking and offset π-stacking interactions forms columns along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Among the various classes of nitrogen containing heterocyclic compounds, pyrazolo-[3,4-*d*]pyrimidine derivatives display a broad spectrum of biological activities, because of their structural resemblance to purine nucleobases. In recent years, researchers have reported the use of purine derivatives of pyrazolo[3,4-*d*]pyrimidine as kinase inhibitors (Diner *et al.*, 2012), antiviral agents (Bektemirov *et al.*, 2010) and antitubercular agents (Trivedi *et al.*, 2012). The present paper is a continuation of our research work devoted to the development of pyrazolo[3,4-*d*]pyrimidine derivatives with potential pharmacological activities (El Fal *et al.*, 2013).

In the title compound, the pyrazolopyrimidine moiety is slightly twisted, as indicated by the dihedral angle of 3.19 (6)° between the mean planes through the five- and six-membered rings (Fig. 1). The *o*-tolyl ring is inclined to the pyrazole ring by 57.26 (6)°, while the phenyl ring is inclined to the pyrimidine ring by 33.04 (6)°. In the crystal, π-stacking interactions between pyrimidine rings form centrosymmetric dimers [centroid–centroid = 3.5178 (6) Å], which are formed into stacks along the *b*-axis direction by offset π-stacking interactions between the C2/N2/C3/N3 portions of the centrosymmetrically related dimers [interplanar spacing = 3.1850 (4) Å; Figs. 2 and 3].

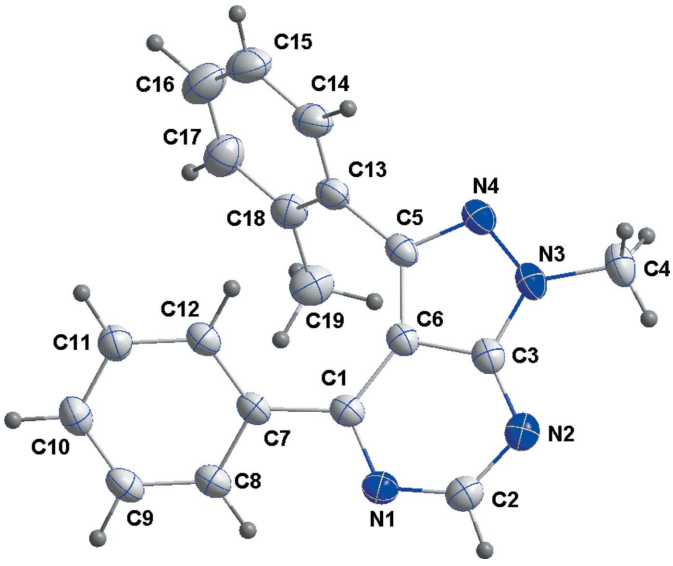


Figure 1
The molecular structure of the title molecule, with the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level.

Synthesis and crystallization

Under an atmosphere of argon, a mixture of 1-methyl-4-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidine (0.1 g, 0.47 mmol), 2-iodotoluene (0.12 ml, 0.94 mmol), Cs_2CO_3 (0.46 g, 1.42 mmol), K_3PO_4 (0.25 g, 1.18 mmol), 1,10-phenanthroline (0.034 g, 0.19 mmol) and $Pd(OAc)_2$ (0.021 g, 0.094 mmol) in DMA (3 ml) was flushed with argon and heated to 438 K for 48 h. After completion of the reaction, the mixture was allowed to cool to room temperature and the solvent was removed under reduced pressure. Water (15 ml) was added and the resulting aqueous phase was extracted with CH_2Cl_2 (3 × 15 ml). The combined organic layers were dried with $MgSO_4$ and concentrated under vacuum. The residue was purified by column chromatography on silica gel (EtOAc/petroleum ether). The title compound was recrystallized from ethanol at room temperature, giving colourless crystals (yield 63%; m.p. 405–407 K).

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{16}N_4$
M_r	300.36
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	25.8546 (6), 6.9306 (2), 19.6783 (5)
β (°)	118.658 (1)
V (Å^3)	3094.16 (14)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.62
Crystal size (mm)	0.29 × 0.15 × 0.11
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.85, 0.94
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11463, 3124, 2874
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.100, 1.04
No. of reflections	3124
No. of parameters	273
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.20

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

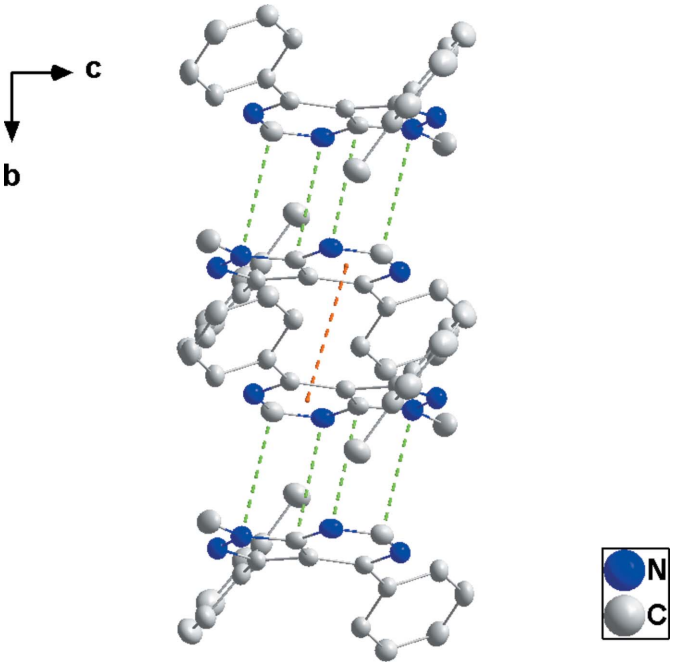


Figure 2
Detail of the π-stacking (orange dashed line) and the offset π-stacking (green dashed lines) viewed along the *a*-axis direction. H atoms have been omitted for clarity.

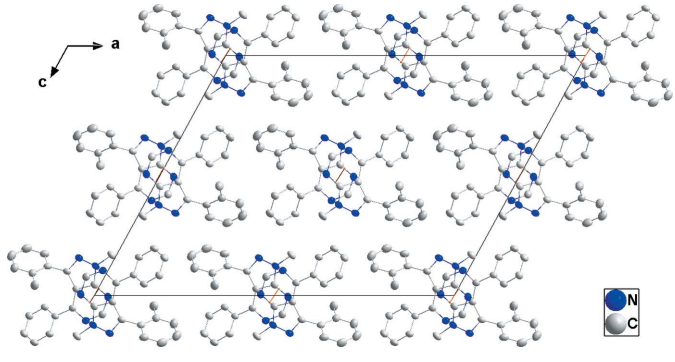


Figure 3
Packing viewed along the *b*-axis direction, with the π-stacking interactions shown as orange dashed lines. H atoms have been omitted for clarity.

Refinement

Crystal data, data collection and structure refinement details are presented in Table 1.

Acknowledgements

Tulane University is gratefully acknowledged for support of the Tulane Crystallography Laboratory.

Funding information

Funding for this research was provided by: NSF–MRI (grant No. 1228232), for the purchase of the diffractometer.

References

Bektemirov, T. A., Chekunova, E. V., Korbukh, I. A., Bulychev, Y. N., Cosimelli, N. G. & Greco, G. (2010). *J. Med. Chem.* **53**, 3954–3963.

Brandenburg, K. & Putz, H. (2012). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Diner, P., Alao, J. P., Soderlund, J., Sunnerhagen, P. & Grotli, M. (2012). *J. Med. Chem.* **55**, 4872–4876.

El Fal, M., Ramli, Y., Essassi, E. M., Saadi, M. & El Ammari, L. (2013). *Acta Cryst.* E**69**, o1650.

Sheldrick, G. M. (2008). *Acta Cryst*. A**64**, 112–122.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Trivedi, A. R., Dholariya, B. H., Vakhariya, C. P., Dodiya, D. K., Ram, H. K., Kataria, V. B., Siddiqui, A. B. & Shah, V. H. (2012). *Med. Chem. Res.* **21**, 1887–1891.

full crystallographic data

IUCrData (2017). **2**, x171370 [https://doi.org/10.1107/S2414314617013700]

1-Methyl-3-(2-methylphenyl)-4-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidine

Mohamed El Hafi, Mohammed Boulhaoua, Youssef Ramli, Mohammed Benchidmi, El Mokhtar Essassi and Joel T. Mague

1-Methyl-3-(2-methylphenyl)-4-phenyl-1*H*-pyrazolo[3,4-d]pyrimidine

Crystal data

$C_{19}H_{16}N_4$
M_r = 300.36
Monoclinic, *C*2/*c*
a = 25.8546 (6) Å
b = 6.9306 (2) Å
c = 19.6783 (5) Å
β = 118.658 (1)°
V = 3094.16 (14) Å^3
Z = 8
F(000) = 1264
D_x = 1.290 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 9566 reflections
θ = 5.1–74.5°
μ = 0.62 mm^{-1}
T = 150 K
Column, colourless
0.29 × 0.15 × 0.11 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC I*μ*S micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.85, T_{max} = 0.94
11463 measured reflections
3124 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 74.5°, θ_{min} = 5.1°
h = −31→31
k = −8→8
l = −24→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.04
3124 reflections
273 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 1.7251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL2016* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00168 (14)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.51451 (4)	0.28267 (14)	0.60439 (5)	0.0309 (2)
N2	0.54018 (4)	0.19678 (13)	0.50584 (6)	0.0315 (2)
N3	0.45894 (4)	0.22510 (14)	0.37751 (6)	0.0312 (2)
N4	0.40026 (4)	0.26735 (14)	0.34325 (6)	0.0319 (2)
C1	0.45863 (5)	0.32694 (15)	0.55272 (6)	0.0264 (2)
C2	0.55098 (5)	0.21902 (17)	0.57827 (7)	0.0320 (3)
C3	0.48400 (5)	0.23908 (15)	0.45530 (6)	0.0277 (2)
H3	0.5903 (6)	0.187 (2)	0.6178 (8)	0.031 (3)*
C4	0.48669 (7)	0.1722 (2)	0.33122 (8)	0.0384 (3)
H4A	0.4883 (9)	0.281 (3)	0.3029 (12)	0.076 (6)*
H4B	0.5266 (8)	0.130 (3)	0.3651 (10)	0.053 (5)*
H4C	0.4639 (8)	0.067 (3)	0.2960 (11)	0.062 (5)*
C5	0.38752 (5)	0.31035 (16)	0.39930 (6)	0.0281 (2)
C6	0.43977 (5)	0.29888 (15)	0.47323 (6)	0.0262 (2)
C7	0.42235 (5)	0.40674 (16)	0.58573 (6)	0.0270 (2)
C8	0.43410 (5)	0.34806 (18)	0.65990 (6)	0.0315 (3)
H8	0.4642 (6)	0.250 (2)	0.6866 (8)	0.039 (4)*
C9	0.40480 (6)	0.43019 (19)	0.69569 (7)	0.0361 (3)
H9	0.4154 (7)	0.390 (2)	0.7493 (9)	0.046 (4)*
C10	0.36296 (6)	0.5724 (2)	0.65802 (7)	0.0372 (3)
H10	0.3424 (7)	0.628 (2)	0.6850 (9)	0.047 (4)*
C11	0.35024 (5)	0.63067 (18)	0.58415 (7)	0.0337 (3)
H11	0.3201 (7)	0.728 (2)	0.5559 (9)	0.046 (4)*
C12	0.37979 (5)	0.54851 (16)	0.54796 (6)	0.0291 (3)
H12	0.3720 (6)	0.593 (2)	0.4963 (8)	0.031 (3)*
C13	0.32570 (5)	0.35885 (17)	0.37772 (6)	0.0306 (3)
C14	0.29848 (6)	0.51143 (19)	0.32611 (7)	0.0387 (3)
H14	0.3218 (6)	0.577 (2)	0.3046 (8)	0.039 (4)*
C15	0.24060 (7)	0.5620 (2)	0.30375 (8)	0.0486 (4)
H15	0.2227 (8)	0.669 (3)	0.2667 (10)	0.060 (5)*
C16	0.20979 (6)	0.4615 (2)	0.33326 (9)	0.0512 (4)
H16	0.1656 (8)	0.497 (3)	0.3175 (10)	0.062 (5)*
C17	0.23610 (6)	0.3093 (2)	0.38378 (9)	0.0443 (3)
H17	0.2145 (7)	0.234 (3)	0.4087 (10)	0.056 (5)*
C18	0.29390 (5)	0.25321 (18)	0.40601 (7)	0.0340 (3)

C19	0.31878 (6)	0.0783 (2)	0.45680 (9)	0.0425 (3)
H19A	0.3415 (12)	0.112 (4)	0.5138 (16)	0.110 (8)*
H19B	0.3482 (10)	0.005 (4)	0.4467 (13)	0.098 (7)*
H19C	0.2857 (10)	−0.014 (4)	0.4487 (13)	0.098 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0322 (5)	0.0299 (5)	0.0291 (5)	−0.0016 (4)	0.0136 (4)	0.0013 (4)
N2	0.0344 (5)	0.0257 (5)	0.0387 (5)	−0.0015 (4)	0.0211 (4)	0.0020 (4)
N3	0.0407 (5)	0.0301 (5)	0.0301 (5)	−0.0013 (4)	0.0228 (4)	−0.0008 (4)
N4	0.0387 (5)	0.0320 (5)	0.0278 (5)	−0.0010 (4)	0.0183 (4)	0.0003 (4)
C1	0.0314 (5)	0.0228 (5)	0.0253 (5)	−0.0030 (4)	0.0137 (4)	0.0008 (4)
C2	0.0314 (6)	0.0288 (6)	0.0354 (6)	−0.0009 (4)	0.0157 (5)	0.0031 (5)
C3	0.0358 (6)	0.0213 (5)	0.0307 (6)	−0.0023 (4)	0.0196 (5)	0.0007 (4)
C4	0.0526 (8)	0.0377 (7)	0.0385 (7)	−0.0001 (6)	0.0329 (6)	−0.0021 (6)
C5	0.0356 (6)	0.0262 (5)	0.0239 (5)	−0.0015 (4)	0.0154 (4)	0.0008 (4)
C6	0.0323 (5)	0.0225 (5)	0.0261 (5)	−0.0012 (4)	0.0160 (4)	0.0010 (4)
C7	0.0308 (5)	0.0272 (5)	0.0231 (5)	−0.0043 (4)	0.0130 (4)	−0.0022 (4)
C8	0.0351 (6)	0.0337 (6)	0.0242 (5)	−0.0016 (5)	0.0129 (4)	0.0004 (4)
C9	0.0418 (6)	0.0436 (7)	0.0250 (5)	−0.0040 (5)	0.0177 (5)	−0.0004 (5)
C10	0.0423 (7)	0.0422 (7)	0.0337 (6)	−0.0018 (5)	0.0236 (5)	−0.0053 (5)
C11	0.0368 (6)	0.0332 (6)	0.0333 (6)	0.0011 (5)	0.0186 (5)	−0.0003 (5)
C12	0.0340 (6)	0.0290 (5)	0.0251 (5)	−0.0030 (4)	0.0148 (4)	−0.0002 (4)
C13	0.0338 (6)	0.0311 (6)	0.0234 (5)	−0.0003 (4)	0.0110 (4)	−0.0028 (4)
C14	0.0435 (7)	0.0380 (7)	0.0291 (6)	0.0029 (5)	0.0129 (5)	0.0030 (5)
C15	0.0474 (8)	0.0447 (8)	0.0405 (7)	0.0126 (6)	0.0106 (6)	0.0076 (6)
C16	0.0358 (7)	0.0515 (8)	0.0560 (9)	0.0066 (6)	0.0137 (6)	−0.0006 (7)
C17	0.0358 (7)	0.0452 (7)	0.0501 (8)	−0.0010 (6)	0.0192 (6)	−0.0023 (6)
C18	0.0327 (6)	0.0351 (6)	0.0319 (6)	−0.0017 (5)	0.0137 (5)	−0.0025 (5)
C19	0.0400 (7)	0.0402 (7)	0.0482 (8)	−0.0028 (6)	0.0218 (6)	0.0081 (6)

Geometric parameters (Å, º)

N1—C1	1.3440 (14)	C9—C10	1.3861 (19)
N1—C2	1.3462 (16)	C9—H9	0.993 (16)
N2—C2	1.3235 (16)	C10—C11	1.3879 (17)
N2—C3	1.3412 (15)	C10—H10	0.991 (16)
N3—C3	1.3496 (15)	C11—C12	1.3919 (16)
N3—N4	1.3642 (14)	C11—H11	0.978 (16)
N3—C4	1.4510 (15)	C12—H12	0.987 (14)
N4—C5	1.3277 (14)	C13—C14	1.3998 (17)
C1—C6	1.4109 (15)	C13—C18	1.4004 (17)
C1—C7	1.4806 (15)	C14—C15	1.387 (2)
C2—H3	0.964 (14)	C14—H14	0.998 (15)
C3—C6	1.4111 (15)	C15—C16	1.379 (2)
C4—H4A	0.95 (2)	C15—H15	0.984 (19)
C4—H4B	0.967 (18)	C16—C17	1.384 (2)

C4—H4C	0.982 (19)	C16—H16	1.061 (17)
C5—C6	1.4363 (15)	C17—C18	1.3961 (18)
C5—C13	1.4820 (16)	C17—H17	1.043 (18)
C7—C12	1.3943 (16)	C18—C19	1.5053 (18)
C7—C8	1.4009 (15)	C19—H19A	1.01 (3)
C8—C9	1.3805 (17)	C19—H19B	1.01 (3)
C8—H8	0.977 (15)	C19—H19C	1.02 (3)

C1—N1—C2	118.79 (10)	C10—C9—H9	120.8 (9)
C2—N2—C3	111.54 (10)	C9—C10—C11	119.95 (11)
C3—N3—N4	111.12 (9)	C9—C10—H10	118.2 (9)
C3—N3—C4	128.11 (11)	C11—C10—H10	121.9 (9)
N4—N3—C4	120.76 (10)	C10—C11—C12	120.29 (12)
C5—N4—N3	107.33 (9)	C10—C11—H11	121.3 (9)
N1—C1—C6	118.80 (10)	C12—C11—H11	118.4 (9)
N1—C1—C7	115.52 (9)	C11—C12—C7	120.13 (10)
C6—C1—C7	125.67 (10)	C11—C12—H12	120.5 (8)
N2—C2—N1	128.65 (11)	C7—C12—H12	119.3 (8)
N2—C2—H3	116.0 (8)	C14—C13—C18	119.76 (11)
N1—C2—H3	115.4 (8)	C14—C13—C5	118.51 (11)
N2—C3—N3	125.83 (10)	C18—C13—C5	121.71 (10)
N2—C3—C6	126.73 (10)	C15—C14—C13	120.78 (13)
N3—C3—C6	107.40 (10)	C15—C14—H14	122.0 (8)
N3—C4—H4A	109.8 (12)	C13—C14—H14	117.2 (8)
N3—C4—H4B	109.2 (10)	C16—C15—C14	119.47 (13)
H4A—C4—H4B	108.1 (16)	C16—C15—H15	122.0 (11)
N3—C4—H4C	108.7 (10)	C14—C15—H15	118.5 (11)
H4A—C4—H4C	110.8 (16)	C15—C16—C17	120.23 (13)
H4B—C4—H4C	110.1 (15)	C15—C16—H16	121.3 (10)
N4—C5—C6	109.96 (10)	C17—C16—H16	118.5 (10)
N4—C5—C13	118.42 (10)	C16—C17—C18	121.40 (14)
C6—C5—C13	131.61 (10)	C16—C17—H17	122.0 (10)
C1—C6—C3	115.28 (10)	C18—C17—H17	116.5 (9)
C1—C6—C5	140.57 (10)	C17—C18—C13	118.31 (12)
C3—C6—C5	104.15 (9)	C17—C18—C19	119.00 (12)
C12—C7—C8	118.78 (10)	C13—C18—C19	122.66 (11)
C12—C7—C1	122.23 (10)	C18—C19—H19A	112.7 (16)
C8—C7—C1	118.83 (10)	C18—C19—H19B	113.5 (14)
C9—C8—C7	120.92 (11)	H19A—C19—H19B	104.1 (19)
C9—C8—H8	120.2 (8)	C18—C19—H19C	110.2 (13)
C7—C8—H8	118.8 (8)	H19A—C19—H19C	108.4 (19)
C8—C9—C10	119.92 (11)	H19B—C19—H19C	108 (2)
C8—C9—H9	119.2 (9)		

C3—N3—N4—C5	0.49 (13)	C6—C1—C7—C12	−34.01 (16)
C4—N3—N4—C5	−179.90 (10)	N1—C1—C7—C8	−30.76 (15)
C2—N1—C1—C6	2.10 (15)	C6—C1—C7—C8	150.72 (11)
C2—N1—C1—C7	−176.53 (10)	C12—C7—C8—C9	−0.82 (17)

C3—N2—C2—N1	−2.75 (17)	C1—C7—C8—C9	174.62 (11)
C1—N1—C2—N2	1.98 (18)	C7—C8—C9—C10	0.21 (19)
C2—N2—C3—N3	−177.90 (10)	C8—C9—C10—C11	0.56 (19)
C2—N2—C3—C6	−0.49 (16)	C9—C10—C11—C12	−0.70 (19)
N4—N3—C3—N2	176.18 (10)	C10—C11—C12—C7	0.09 (18)
C4—N3—C3—N2	−3.39 (19)	C8—C7—C12—C11	0.66 (17)
N4—N3—C3—C6	−1.64 (12)	C1—C7—C12—C11	−174.61 (10)
C4—N3—C3—C6	178.79 (11)	N4—C5—C13—C14	−56.95 (15)
N3—N4—C5—C6	0.86 (12)	C6—C5—C13—C14	123.35 (13)
N3—N4—C5—C13	−178.91 (9)	N4—C5—C13—C18	121.40 (12)
N1—C1—C6—C3	−4.64 (15)	C6—C5—C13—C18	−58.30 (17)
C7—C1—C6—C3	173.83 (10)	C18—C13—C14—C15	1.29 (19)
N1—C1—C6—C5	175.06 (13)	C5—C13—C14—C15	179.68 (12)
C7—C1—C6—C5	−6.5 (2)	C13—C14—C15—C16	0.5 (2)
N2—C3—C6—C1	4.03 (16)	C14—C15—C16—C17	−1.1 (2)
N3—C3—C6—C1	−178.17 (9)	C15—C16—C17—C18	−0.1 (2)
N2—C3—C6—C5	−175.77 (10)	C16—C17—C18—C13	1.9 (2)
N3—C3—C6—C5	2.02 (11)	C16—C17—C18—C19	−175.90 (13)
N4—C5—C6—C1	178.48 (13)	C14—C13—C18—C17	−2.47 (18)
C13—C5—C6—C1	−1.8 (2)	C5—C13—C18—C17	179.20 (11)
N4—C5—C6—C3	−1.79 (12)	C14—C13—C18—C19	175.27 (12)
C13—C5—C6—C3	177.93 (11)	C5—C13—C18—C19	−3.06 (18)
N1—C1—C7—C12	144.51 (11)		