Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

Crystal structure of 1-{3-(4-methylphenyl)-5-[(*E*)-2-phenylethenyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethan-1-one

Farook Adam,[a]* Kanathur Smitha,[b] Sharath Poojary Charishma,[b] Seranthimata Samshuddin[b] and Nadiah Ameram[a]

[a]School of Chemical Sciences, Universiti Sains Malaysia, 11800, Pulau Pinang, Malaysia, and [b]Department of PG Studies in Chemistry, Alva's College, Moodbidri, Karnataka 574 227, India. *Correspondence e-mail: farook@usm.my/farookdr@gmail.com

Received 21 November 2015; accepted 24 December 2015

Edited by S. V. Lindeman, Marquette University, USA

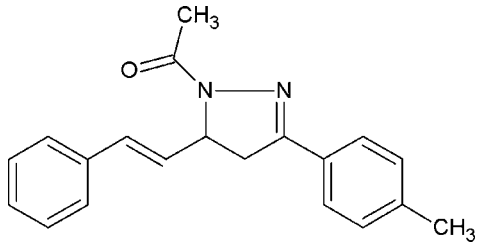
The title compound, $C_{20}H_{20}N_2O$, was studied as a part of our work on pyrazoline derivatives. It represents a *trans*-isomer. The central pyrazoline ring adopts an envelope conformation with the asymmetric C atom having the largest deviation of 0.107 (1) Å from the mean plane. It forms dihedral angles of 6.2 (1) and 86.4 (1)° with the adjacent *p*-tolyl and styrene groups, respectively. In the crystal, C—H···O interactions link molecules into infinite chains along the *c* axis.

Keywords: crystal structure; synthesis; pyrazoline; pharmacological properties.

CCDC reference: 1444202

1. Related literature

For background to pyrazoles, see: Samshuddin *et al.* (2012); Wiley *et al.* (1958); Sarojini *et al.* (2010); Lu *et al.*(1999). For crystal structures of pyrazoline-derived chalcones, see: Jasinski *et al.* (2012); Baktır *et al.* (2011). For stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



2. Experimental

2.1. Crystal data

$C_{20}H_{20}N_2O$
M_r = 304.38
Orthorhombic, *Pccn*
a = 19.872 (2) Å
b = 20.304 (2) Å
c = 8.2924 (8) Å
V = 3345.9 (6) Å^3
Z = 8
Mo *Kα* radiation
μ = 0.08 mm^{-1}
T = 100 K
0.38 × 0.31 × 0.17 mm

2.2. Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.914, T_{max} = 0.960
60332 measured reflections
5482 independent reflections
4234 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.146
S = 1.04
5482 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19*C*···O1^{i}	0.98	2.51	3.4416 (18)	158

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Acknowledgements

FA would like to thank University Sains Malaysia for the RU research Grant (No. PKIMIA/846017 and 1001/PKIMIA/811269) which partly supported the work. SS thanks to Alva's Education Foundation, Moodbidri, for the research facilities.

Supporting information for this paper is available from the IUCr electronic archives (Reference: LD2138).

References

Baktır, Z., Akkurt, M., Samshuddin, S., Narayana, B. & Yathirajan, H. S. (2011). *Acta Cryst.* E**67**, o1292–o1293.

Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.

Jasinski, J. P., Golen, J. A., Samshuddin, S., Narayana, B. & Yathirajan, H. S. (2012). *Crystals*, **2**, 1108–1115.

Lu, Z. Y., Zhu, W. G., Jiang, Q. & Xie, M. G. (1999). *Chin. Chem. Lett.* **10**, 679–682.

Samshuddin, S., Narayana, B., Sarojini, B. K., Khan, M. T. H., Yathirajan, H. S., Raj, C. G. D. & Raghavendra, R. (2012). *Med. Chem. Res.* **21**, 2012–2022.

Sarojini, B. K., Vidyagayatri, M., Darshanraj, C. G., Bharath, B. R. & Manjunatha, H. (2010). *Lett. Drug. Des. Discov.* **7**, 214–224.

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

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Wiley, R. H., Jarboe, C. H., Hayes, F. N., Hansbury, E., Nielsen, J. T., Callahan, P. X. & Sellars, M. (1958). *J. Org. Chem.* **23**, 732–738.

supporting information

Acta Cryst. (2015). E**71**, o1095–o1096 [https://doi.org/10.1107/S2056989015024792]

Crystal structure of 1-{3-(4-methylphenyl)-5-[(*E*)-2-phenylethenyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethan-1-one

Farook Adam, Kanathur Smitha, Sharath Poojary Charishma, Seranthimata Samshuddin and Nadiah Ameram

S1. Introduction

Pyrazoline derivatives exhibit numerous pharmacological activities including antioxidant, antiamoebic, anti-inflammatory, analgesic, antimicrobial, anti depressant and anticancer activities (Sarojini *et al.*, 2010; Samshuddin *et al.*, 2012). Many 1,3,5-triaryl-2-pyrazolines were used as scintillation solutes (Wiley *et al.* ,1958) and as fluorescent agents (Lu *et al.*, 1999). The crystal structures of some pyrazolines containing *N*-alkyl chain *viz*., 3,5-bis(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbaldehyde (Baktir *et al.*, 2011), 3,5-bis(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carboxamide and 3,5-bis(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbothioamide (Jasinski *et al.*, 2012) had been reported. In view of the importance of pyrazolines, the title compound (I) is prepared and its crystal structure is reported.

S2. Experimental

A mixture of (2*E*,4*E*)-1-(4-methylphenyl)-5-phenylpenta-2,4-dien-1-one (2.48 g, 0.01 mol) and hydrazine hydrate (1 ml) in 30 ml acetic acid was refluxed for 6 h.The reaction mixture was cooled and poured into 100 ml ice-cold water. The precipitate was collected by filtration and purified by recrystallization from ethanol.

S2.1. Synthesis and crystallization

Single crystals were grown from ethanol by slow evaporation method. m.p.: 386-390 K .Yield: 71 %.

S2.2. Refinement

All H atoms were placed in calculated positions and refined with riding model [U_{iso} (H) = 1.2 × U_{eq}(C methylene or methine) or 1.5 × U_{eq} (C methyl), C—H = 0.95 Å, 0.98 Å, 0.99 Å and 1.00 Å]. A rotating group model (AFIX 137) is applied to methyl groups.

S3. related literature

For background of pyrazoles, see: Samshuddin *et al.* (2012); Wiley *et al.* (1958); Sarojini *et al.* (2010); Lu *et al.* (1999). For crystal structures of pyrazoline derived chalcone, see: Jasinski *et al.* (2012); Baktir *et al.* (2011). For stability of the temperature controller used for data collection, see: Cosier & Glazer (1986). For ring conformations, see: Cremer & Pople (1975).

S4. Results and discussion

The asymmetric unit of (I) consists of a single crystallographic independent molecule as shown in Fig. 1. The C6/C7/C8/C9 carbon chains adopts a *trans* configuration with respect to C7—C8 double bond. The pyrazoline ring (N1/N2/C9/C10/C11) adopts an envelope conformation on atom C9 [Q2 = 0.1772 (12) Å and φ2 = 317.3 (4)°] with

maximum deviation of 0.107 (1) Å from its mean plane. The *p*-tolyl ring and styrene group make dihedral angles of 6.19 (7)° and 86.39 (7)° with central pyrazoline ring. In crystal, molecules are connected by weak C—H···O hydrogen bond into one-dimensional chains (Fig. 2), propagating along crystallographic *c*-axis.

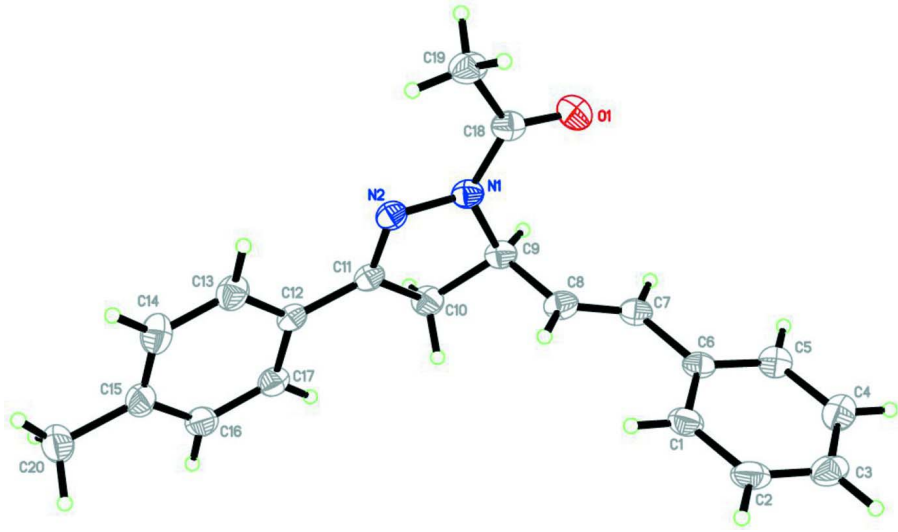


Figure 1

The molecular structure of title compound (I) with atom labels and 50% probability displacement ellipsoids.

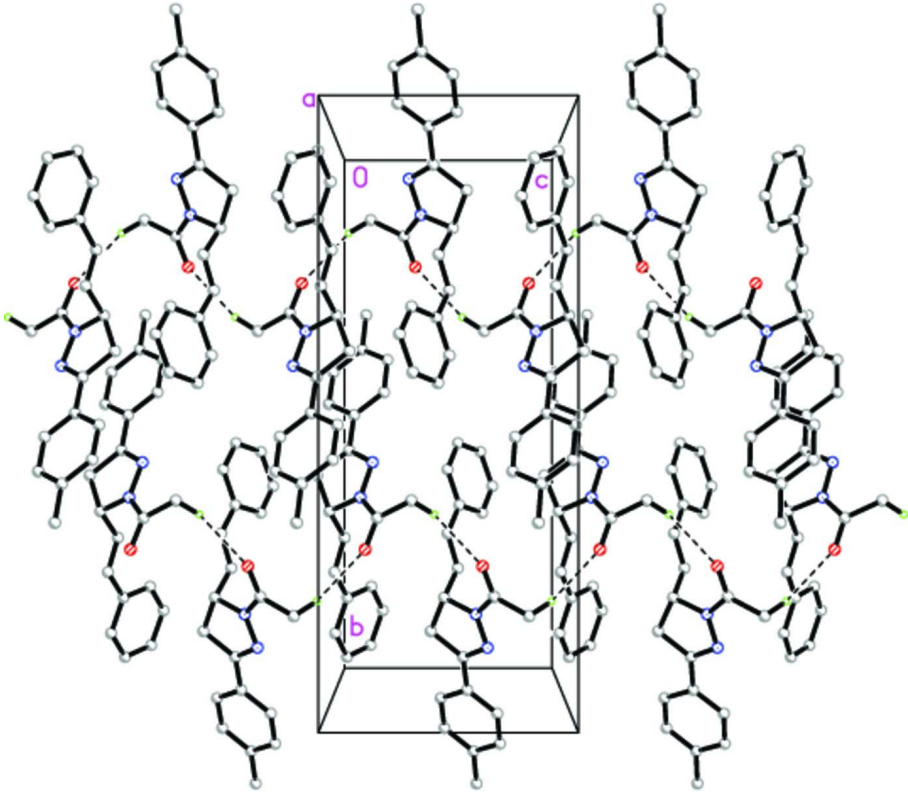


Figure 2

The crystal packing of title compound (I) viewed along the *a*-axis.

1-{3-(4-Methylphenyl)-5-[(*E*)-2-phenylethenyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethan-1-one

Crystal data

$C_{20}H_{20}N_2O$
$M_r = 304.38$
Orthorhombic, *Pccn*
$a = 19.872$ (2) Å
$b = 20.304$ (2) Å
$c = 8.2924$ (8) Å
$V = 3345.9$ (6) Å^3
$Z = 8$
$F(000) = 1296$
$D_x = 1.208$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9875 reflections
$\theta = 2.8$–$31.0°$
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Block, colourless
0.38 × 0.31 × 0.17 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.914$, $T_{max} = 0.960$
60332 measured reflections
5482 independent reflections
4234 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 31.4°$, $\theta_{min} = 1.4°$
$h = -28 \rightarrow 28$
$k = -29 \rightarrow 29$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.146$
$S = 1.04$
5482 reflections
210 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 1.4451P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.07312 (5)	0.73524 (5)	0.64575 (12)	0.0353 (2)
N1	−0.00679 (5)	0.64670 (5)	0.61909 (12)	0.0251 (2)
N2	0.01613 (5)	0.58545 (5)	0.66989 (12)	0.0240 (2)
C1	0.18906 (6)	0.81809 (7)	0.65242 (17)	0.0309 (3)
H1A	0.1938	0.7741	0.6900	0.037*
C2	0.23498 (6)	0.86562 (7)	0.70037 (18)	0.0347 (3)
H2A	0.2707	0.8541	0.7712	0.042*
C3	0.22917 (7)	0.92989 (7)	0.64565 (16)	0.0339 (3)
H3A	0.2610	0.9622	0.6780	0.041*
C4	0.17664 (7)	0.94670 (7)	0.54333 (16)	0.0332 (3)

H4A	0.1724	0.9907	0.5055	0.040*
C5	0.13015 (7)	0.89918 (7)	0.49601 (15)	0.0285 (3)
H5A	0.0942	0.9112	0.4266	0.034*
C6	0.13563 (6)	0.83413 (6)	0.54917 (14)	0.0244 (2)
C7	0.08568 (6)	0.78511 (6)	0.49662 (14)	0.0248 (2)
H7A	0.0522	0.7998	0.4232	0.030*
C8	0.08281 (6)	0.72257 (7)	0.54150 (15)	0.0275 (2)
H8A	0.1151	0.7079	0.6180	0.033*
C9	0.03274 (6)	0.67307 (6)	0.48142 (14)	0.0258 (2)
H9A	0.0029	0.6922	0.3964	0.031*
C10	0.06773 (7)	0.61000 (6)	0.42244 (15)	0.0292 (3)
H10A	0.0456	0.5922	0.3247	0.035*
H10B	0.1159	0.6179	0.3993	0.035*
C11	0.05888 (6)	0.56455 (6)	0.56448 (14)	0.0232 (2)
C12	0.09411 (6)	0.50166 (6)	0.58275 (14)	0.0234 (2)
C13	0.08359 (7)	0.46040 (7)	0.71578 (16)	0.0311 (3)
H13A	0.0527	0.4731	0.7975	0.037*
C14	0.11770 (8)	0.40148 (7)	0.72904 (18)	0.0360 (3)
H14A	0.1093	0.3739	0.8194	0.043*
C15	0.16411 (7)	0.38152 (6)	0.61306 (18)	0.0315 (3)
C16	0.17496 (7)	0.42273 (7)	0.48225 (17)	0.0317 (3)
H16A	0.2068	0.4104	0.4023	0.038*
C17	0.14018 (6)	0.48161 (6)	0.46596 (16)	0.0288 (3)
H17A	0.1479	0.5086	0.3741	0.035*
C18	−0.05635 (6)	0.68098 (6)	0.69553 (15)	0.0276 (2)
C19	−0.08727 (7)	0.64978 (7)	0.84270 (17)	0.0339 (3)
H19A	−0.0718	0.6041	0.8519	0.051*
H19B	−0.1364	0.6505	0.8330	0.051*
H19C	−0.0737	0.6744	0.9390	0.051*
C20	0.20029 (8)	0.31682 (7)	0.6276 (2)	0.0421 (4)
H20A	0.1884	0.2959	0.7303	0.063*
H20B	0.2490	0.3243	0.6237	0.063*
H20C	0.1871	0.2880	0.5383	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0345 (5)	0.0360 (5)	0.0353 (5)	0.0065 (4)	−0.0006 (4)	0.0001 (4)
N1	0.0237 (5)	0.0295 (5)	0.0222 (5)	−0.0003 (4)	0.0008 (4)	0.0024 (4)
N2	0.0230 (4)	0.0269 (5)	0.0220 (4)	−0.0028 (4)	−0.0009 (4)	0.0010 (4)
C1	0.0213 (5)	0.0345 (6)	0.0368 (7)	0.0047 (5)	−0.0022 (5)	−0.0026 (5)
C2	0.0192 (5)	0.0454 (8)	0.0395 (7)	0.0026 (5)	−0.0021 (5)	−0.0081 (6)
C3	0.0270 (6)	0.0434 (7)	0.0313 (6)	−0.0069 (5)	0.0075 (5)	−0.0094 (5)
C4	0.0396 (7)	0.0344 (7)	0.0255 (6)	−0.0059 (5)	0.0057 (5)	−0.0008 (5)
C5	0.0307 (6)	0.0338 (6)	0.0211 (5)	0.0004 (5)	0.0010 (4)	0.0007 (5)
C6	0.0203 (5)	0.0321 (6)	0.0207 (5)	0.0016 (4)	0.0032 (4)	−0.0014 (4)
C7	0.0212 (5)	0.0323 (6)	0.0210 (5)	0.0016 (4)	−0.0009 (4)	0.0014 (4)
C8	0.0224 (5)	0.0358 (6)	0.0244 (5)	−0.0011 (5)	−0.0027 (4)	0.0053 (5)

C9	0.0241 (5)	0.0320 (6)	0.0214 (5)	−0.0003 (4)	0.0001 (4)	0.0049 (4)
C10	0.0304 (6)	0.0334 (6)	0.0237 (5)	0.0011 (5)	0.0055 (5)	0.0045 (5)
C11	0.0209 (5)	0.0277 (5)	0.0212 (5)	−0.0043 (4)	−0.0013 (4)	0.0012 (4)
C12	0.0215 (5)	0.0255 (5)	0.0233 (5)	−0.0052 (4)	−0.0011 (4)	0.0002 (4)
C13	0.0363 (7)	0.0303 (6)	0.0267 (6)	−0.0032 (5)	0.0050 (5)	0.0017 (5)
C14	0.0461 (8)	0.0291 (6)	0.0327 (7)	−0.0024 (6)	0.0013 (6)	0.0054 (5)
C15	0.0290 (6)	0.0248 (6)	0.0406 (7)	−0.0038 (5)	−0.0060 (5)	−0.0015 (5)
C16	0.0260 (6)	0.0313 (6)	0.0378 (7)	−0.0027 (5)	0.0031 (5)	−0.0045 (5)
C17	0.0266 (6)	0.0305 (6)	0.0293 (6)	−0.0039 (5)	0.0040 (5)	0.0010 (5)
C18	0.0245 (5)	0.0341 (6)	0.0242 (5)	−0.0021 (5)	−0.0011 (4)	−0.0041 (5)
C19	0.0323 (6)	0.0402 (7)	0.0291 (6)	−0.0032 (5)	0.0081 (5)	−0.0042 (5)
C20	0.0385 (8)	0.0285 (6)	0.0593 (10)	0.0013 (6)	−0.0065 (7)	0.0007 (6)

Geometric parameters (Å, º)

O1—C18	1.2228 (16)	C10—C11	1.5066 (17)
N1—C18	1.3625 (16)	C10—H10A	0.9900
N1—N2	1.3898 (14)	C10—H10B	0.9900
N1—C9	1.4855 (15)	C11—C12	1.4642 (17)
N2—C11	1.2907 (15)	C12—C17	1.3934 (17)
C1—C2	1.3865 (19)	C12—C13	1.4008 (17)
C1—C6	1.4023 (17)	C13—C14	1.3795 (19)
C1—H1A	0.9500	C13—H13A	0.9500
C2—C3	1.386 (2)	C14—C15	1.393 (2)
C2—H2A	0.9500	C14—H14A	0.9500
C3—C4	1.388 (2)	C15—C16	1.387 (2)
C3—H3A	0.9500	C15—C20	1.5025 (19)
C4—C5	1.3923 (19)	C16—C17	1.3876 (19)
C4—H4A	0.9500	C16—H16A	0.9500
C5—C6	1.3967 (18)	C17—H17A	0.9500
C5—H5A	0.9500	C18—C19	1.5061 (18)
C6—C7	1.4717 (17)	C19—H19A	0.9800
C7—C8	1.3244 (17)	C19—H19B	0.9800
C7—H7A	0.9500	C19—H19C	0.9800
C8—C9	1.4995 (17)	C20—H20A	0.9800
C8—H8A	0.9500	C20—H20B	0.9800
C9—C10	1.5370 (18)	C20—H20C	0.9800
C9—H9A	1.0000		

C18—N1—N2	123.57 (10)	C9—C10—H10B	111.4
C18—N1—C9	123.76 (10)	H10A—C10—H10B	109.2
N2—N1—C9	112.47 (9)	N2—C11—C12	122.10 (11)
C11—N2—N1	107.73 (10)	N2—C11—C10	113.89 (11)
C2—C1—C6	120.78 (13)	C12—C11—C10	124.00 (10)
C2—C1—H1A	119.6	C17—C12—C13	118.08 (12)
C6—C1—H1A	119.6	C17—C12—C11	119.80 (11)
C3—C2—C1	120.43 (13)	C13—C12—C11	122.11 (11)
C3—C2—H2A	119.8	C14—C13—C12	120.53 (13)

C1—C2—H2A	119.8	C14—C13—H13A	119.7
C2—C3—C4	119.62 (13)	C12—C13—H13A	119.7
C2—C3—H3A	120.2	C13—C14—C15	121.52 (13)
C4—C3—H3A	120.2	C13—C14—H14A	119.2
C3—C4—C5	120.07 (13)	C15—C14—H14A	119.2
C3—C4—H4A	120.0	C16—C15—C14	117.87 (12)
C5—C4—H4A	120.0	C16—C15—C20	121.06 (13)
C4—C5—C6	120.97 (12)	C14—C15—C20	121.06 (13)
C4—C5—H5A	119.5	C15—C16—C17	121.24 (12)
C6—C5—H5A	119.5	C15—C16—H16A	119.4
C5—C6—C1	118.13 (12)	C17—C16—H16A	119.4
C5—C6—C7	119.57 (11)	C16—C17—C12	120.75 (12)
C1—C6—C7	122.29 (12)	C16—C17—H17A	119.6
C8—C7—C6	126.46 (11)	C12—C17—H17A	119.6
C8—C7—H7A	116.8	O1—C18—N1	120.02 (12)
C6—C7—H7A	116.8	O1—C18—C19	122.77 (12)
C7—C8—C9	125.30 (11)	N1—C18—C19	117.19 (12)
C7—C8—H8A	117.3	C18—C19—H19A	109.5
C9—C8—H8A	117.3	C18—C19—H19B	109.5
N1—C9—C8	109.70 (10)	H19A—C19—H19B	109.5
N1—C9—C10	100.58 (9)	C18—C19—H19C	109.5
C8—C9—C10	111.35 (10)	H19A—C19—H19C	109.5
N1—C9—H9A	111.6	H19B—C19—H19C	109.5
C8—C9—H9A	111.6	C15—C20—H20A	109.5
C10—C9—H9A	111.6	C15—C20—H20B	109.5
C11—C10—C9	102.04 (10)	H20A—C20—H20B	109.5
C11—C10—H10A	111.4	C15—C20—H20C	109.5
C9—C10—H10A	111.4	H20A—C20—H20C	109.5
C11—C10—H10B	111.4	H20B—C20—H20C	109.5

C18—N1—N2—C11	174.87 (11)	N1—N2—C11—C10	−2.35 (14)
C9—N1—N2—C11	−10.15 (13)	C9—C10—C11—N2	12.88 (14)
C6—C1—C2—C3	−0.6 (2)	C9—C10—C11—C12	−168.09 (11)
C1—C2—C3—C4	0.6 (2)	N2—C11—C12—C17	−179.52 (11)
C2—C3—C4—C5	0.0 (2)	C10—C11—C12—C17	1.53 (18)
C3—C4—C5—C6	−0.45 (19)	N2—C11—C12—C13	−0.05 (18)
C4—C5—C6—C1	0.41 (18)	C10—C11—C12—C13	−179.00 (12)
C4—C5—C6—C7	−179.89 (11)	C17—C12—C13—C14	−0.50 (19)
C2—C1—C6—C5	0.11 (19)	C11—C12—C13—C14	−179.97 (12)
C2—C1—C6—C7	−179.58 (12)	C12—C13—C14—C15	1.0 (2)
C5—C6—C7—C8	−177.26 (13)	C13—C14—C15—C16	−0.3 (2)
C1—C6—C7—C8	2.4 (2)	C13—C14—C15—C20	−179.17 (13)
C6—C7—C8—C9	−177.71 (11)	C14—C15—C16—C17	−0.8 (2)
C18—N1—C9—C8	74.84 (14)	C20—C15—C16—C17	178.07 (13)
N2—N1—C9—C8	−100.12 (12)	C15—C16—C17—C12	1.3 (2)
C18—N1—C9—C10	−167.76 (11)	C13—C12—C17—C16	−0.58 (18)
N2—N1—C9—C10	17.27 (12)	C11—C12—C17—C16	178.90 (11)
C7—C8—C9—N1	−120.45 (14)	N2—N1—C18—O1	178.64 (11)

C7—C8—C9—C10	129.11 (13)	C9—N1—C18—O1	4.22 (18)
N1—C9—C10—C11	−16.55 (11)	N2—N1—C18—C19	−0.05 (17)
C8—C9—C10—C11	99.63 (11)	C9—N1—C18—C19	−174.47 (11)
N1—N2—C11—C12	178.60 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19*C*···O1^{i}	0.98	2.51	3.4416 (18)	158

Symmetry code: (i) *x*, −*y*+3/2, *z*+1/2.