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(Z)-1-(2,4-Dimethylphenyl)-3-phenyl-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-one

Rui-Zhu Mu

School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, People's Republic of China Correspondence e-mail: muruizhu@swu.edu.cn

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.113; data-to-parameter ratio = 13.0.

In the title compound, C₁₉H₁₇N₃O, the triazole and benzene rings adopt a Z configuration with respect to the C=C bond. The phenyl and benzene rings form dihedral angles of 66.20 (9) and 14.36 (9) $^{\circ}$, respectively, with the triazole ring. The dihedral angle between the phenyl and benzene rings is 52.64 (8)°.

Related literature

For the synthesis, see: Wang et al. (2009). For the pharmacological activity of triazole derivatives, see: Zhou & Wang (2012). For related structures, see: Wang et al. (2009); Yan et al. (2009).



Experimental

Crystal data C19H17N3O

 $M_r = 303.36$

Monoclinic, $P2_1/n$ a = 12.8499 (3) Å b = 7.8836 (2) Å c = 16.5274 (4) Å $\beta = 108.376 \ (1)^{\circ}$ V = 1588.91 (7) Å³

Data collection

Bruker SMART CCD	11768 measured reflections
diffractometer	2796 independent reflections
Absorption correction: multi-scan	2369 reflections with $I > 2\sigma(I)$
(SADABS; Sheldrick, 1996)	$R_{\rm int} = 0.025$
$T_{\min} = 0.984, \ T_{\max} = 0.986$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of
$wR(F^2) = 0.113$	independent and constrained
S = 1.04	refinement
2796 reflections	$\Delta \rho_{\rm max} = 0.18 \ {\rm e} \ {\rm \AA}^{-3}$
215 parameters	$\Delta \rho_{\rm min} = -0.15 \text{ e } \text{\AA}^{-3}$

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5401).

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Z = 4

Mo $K\alpha$ radiation

 $0.20 \times 0.20 \times 0.18 \; \mathrm{mm}$

 $I > 2\sigma(I)$

 $\mu = 0.08 \text{ mm}^-$

T = 296 K

supplementary materials

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(Z)-1-(2,4-Dimethylphenyl)-3-phenyl-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-one

R.-Z. Mu

Comment

Chalcones are an important type of biologically active compounds with a diaryl enone structural unit. Triazole compounds exhibit a broad bioactive spectrum (Zhou & Wang, 2012). Our interest is to develop novel triazole-derived chalcones as medicinal agents. Examples of related structures of triazolylchalcones have been reported (Wang *et al.*, 2009; Yan *et al.*, 2009). Herein, the crystal structure of the title compound (I) is reported.

In the molecular structure of (I) (Fig. 1) the triazole and benzene rings adopt a *Z* configuration with respect to the C=C bond. The phenyl (C3-C8) and benzene (C12-C17) rings form dihedral angles of 66.20 (9) and 14.36 (9)°, respectively with the triazole ring (N1-N3/C1/C2). The dihedral angle between the phenyl and benzene rings is 52.64 (8)Å.

Experimental

The title compound was prepared according to the procedure of Wang *et al.* (2009). A mixture of 1-(2,4-dimethylphenyl)-2-(1H-1,2,4-triazol-1-yl) ethanone (1.08 g, 5.0 mmol) and benzaldehyde (0.74 g, 7.0 mmol) in toluene (30 mL) in the presence of glacial acetic acid (0.08 mL, 1.4 mmol) and piperidine (0.08 mL, 1.4 mmol) as catalyst was refluxed. After the reaction was completed (monitored by TLC, petroleum ether/ethyl acetate, 3/1, V/V), the solvent was removed. The residue was dissolved in dichloromethane (30 mL) and washed with water (3x30 mL). The resulting phase was dried over anhydrous sodium sulfate, concentrated under reduced pressure and then purified by silica gel column chromatography eluting with petroleum ether/ethyl acetate (10/1-2/1, V/V) to give the title compound (I) (0.923 g) as solid. Mp.396-397K. A crystal of (I) suitable for X-ray analysis was grown from a mixed solution of ethyl acetate and petroleum ether by slow evaporation at room temperature.

Refinement

H atoms were placed in calculated positions with C—H = 0.93Å (aromatic) and 0.96Å (methyl). The U_{iso} (H) values were set equal to $1.2U_{eq}$ (C_{aromatic}) and $1.5U_{eq}$ (C_{methyl}). The H atom bonded to C9 was refined independently with an isotropic displacement paramemeter.

Figures



Fig. 1. The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

(Z)-1-(2,4-Dimethylphenyl)-3-phenyl-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-one

Crystal data

C ₁₉ H ₁₇ N ₃ O	F(000) = 640
$M_r = 303.36$	$D_{\rm x} = 1.268 {\rm ~Mg} {\rm ~m}^{-3}$
Monoclinic, $P2_1/n$	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4934 reflections
a = 12.8499 (3) Å	$\theta = 2.4 - 27.1^{\circ}$
<i>b</i> = 7.8836 (2) Å	$\mu = 0.08 \text{ mm}^{-1}$
c = 16.5274 (4) Å	T = 296 K
$\beta = 108.376 (1)^{\circ}$	Block, colorless
V = 1588.91 (7) Å ³	$0.20\times0.20\times0.18~mm$
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2796 independent reflections
Radiation source: fine-focus sealed tube	2369 reflections with $I > 2\sigma(I)$
graphite	$R_{\rm int} = 0.025$
ϕ and ω scans	$\theta_{\text{max}} = 25.0^{\circ}, \ \theta_{\text{min}} = 1.8^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 9$
$T_{\min} = 0.984, T_{\max} = 0.986$	$k = -8 \rightarrow 9$
11768 measured reflections	$l = -17 \rightarrow 19$

Refinement

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
$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0517P)^{2} + 0.3715P]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
$(\Delta/\sigma)_{\rm max} = 0.004$
$\Delta \rho_{max} = 0.18 \text{ e } \text{\AA}^{-3}$
$\Delta \rho_{min} = -0.15 \text{ e } \text{\AA}^{-3}$
Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), Fc [*] =kFc[1+0.001xFc ² λ^3 /sin(20)] ^{-1/4}

Primary atom site location: structure-invariant direct Extinction coefficient: 0.017 (2)

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 (A^2)

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
C1	0.20259 (13)	1.1290 (2)	0.85885 (11)	0.0604 (5)
H1	0.1666	1.2043	0.8842	0.072*
C2	0.23209 (14)	0.9674 (3)	0.77106 (11)	0.0636 (5)
H2	0.2254	0.9031	0.7225	0.076*
C3	0.29220 (13)	0.6718 (2)	0.94192 (10)	0.0531 (4)
Н3	0.2511	0.7004	0.8865	0.064*
C4	0.24256 (14)	0.5912 (2)	0.99443 (12)	0.0634 (5)
H4	0.1685	0.5637	0.9736	0.076*
C5	0.30203 (15)	0.5514 (2)	1.07733 (11)	0.0615 (5)
Н5	0.2679	0.4990	1.1126	0.074*
C6	0.41158 (15)	0.5892 (2)	1.10754 (10)	0.0578 (4)
H6	0.4518	0.5634	1.1636	0.069*
C7	0.46229 (13)	0.6653 (2)	1.05485 (9)	0.0479 (4)
H7	0.5372	0.6870	1.0753	0.057*
C8	0.40332 (11)	0.71002 (18)	0.97182 (9)	0.0413 (3)
С9	0.46292 (12)	0.78548 (19)	0.91780 (9)	0.0428 (4)
C10	0.42801 (11)	0.89791 (19)	0.85496 (9)	0.0417 (3)
C11	0.48890 (13)	0.9480 (2)	0.79522 (10)	0.0486 (4)
C12	0.60794 (12)	0.90705 (19)	0.81731 (9)	0.0450 (4)
C13	0.67846 (13)	0.9510 (2)	0.89704 (10)	0.0511 (4)
H13	0.6502	1.0017	0.9365	0.061*
C14	0.78937 (13)	0.9210 (2)	0.91891 (11)	0.0566 (4)
H14	0.8351	0.9543	0.9723	0.068*
C15	0.83373 (13)	0.8419 (2)	0.86257 (11)	0.0543 (4)
C16	0.76298 (13)	0.7989 (2)	0.78301 (10)	0.0531 (4)
H16	0.7918	0.7458	0.7446	0.064*
C17	0.65123 (12)	0.8313 (2)	0.75783 (10)	0.0481 (4)
C18	0.58064 (16)	0.7803 (3)	0.67006 (11)	0.0724 (6)
H18A	0.6255	0.7291	0.6400	0.109*
H18B	0.5449	0.8788	0.6396	0.109*
H18C	0.5264	0.7003	0.6746	0.109*
C19	0.95482 (15)	0.8037 (3)	0.88741 (15)	0.0825 (6)
H19A	0.9910	0.8916	0.8663	0.124*

supplementary materials

H19B	0.9656	0.6968	0.8633	0.124*
H19C	0.9849	0.7983	0.9484	0.124*
H1M	0.5369 (13)	0.746 (2)	0.9311 (9)	0.045 (4)*
N1	0.15299 (12)	1.0603 (2)	0.78249 (9)	0.0674 (4)
N2	0.30462 (10)	1.08424 (18)	0.89592 (8)	0.0542 (4)
N3	0.32284 (9)	0.97702 (16)	0.83766 (7)	0.0434 (3)
01	0.43871 (10)	1.0182 (2)	0.72867 (8)	0.0757 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0483 (9)	0.0687 (12)	0.0681 (10)	0.0169 (8)	0.0240 (8)	0.0059 (9)
C2	0.0531 (10)	0.0799 (13)	0.0503 (9)	0.0104 (9)	0.0054 (7)	-0.0035 (8)
C3	0.0446 (9)	0.0601 (10)	0.0544 (9)	-0.0009 (8)	0.0151 (7)	0.0054 (8)
C4	0.0486 (10)	0.0656 (12)	0.0804 (12)	-0.0063 (8)	0.0267 (9)	0.0067 (9)
C5	0.0705 (12)	0.0555 (10)	0.0703 (11)	0.0024 (9)	0.0390 (9)	0.0125 (8)
C6	0.0705 (12)	0.0536 (10)	0.0511 (9)	0.0068 (8)	0.0219 (8)	0.0097 (7)
C7	0.0460 (9)	0.0442 (9)	0.0527 (8)	0.0036 (7)	0.0144 (7)	0.0023 (7)
C8	0.0418 (8)	0.0375 (8)	0.0479 (8)	0.0051 (6)	0.0188 (6)	0.0002 (6)
C9	0.0380 (8)	0.0447 (8)	0.0482 (8)	0.0046 (7)	0.0174 (6)	-0.0012 (6)
C10	0.0368 (7)	0.0458 (8)	0.0449 (7)	0.0032 (6)	0.0166 (6)	-0.0011 (6)
C11	0.0487 (9)	0.0509 (9)	0.0509 (8)	0.0026 (7)	0.0225 (7)	0.0035 (7)
C12	0.0467 (8)	0.0428 (8)	0.0525 (8)	-0.0021 (7)	0.0259 (7)	0.0016 (7)
C13	0.0521 (9)	0.0533 (10)	0.0552 (9)	-0.0002 (7)	0.0272 (7)	-0.0055 (7)
C14	0.0488 (9)	0.0617 (11)	0.0599 (9)	-0.0061 (8)	0.0182 (7)	-0.0072 (8)
C15	0.0474 (9)	0.0499 (10)	0.0720 (10)	-0.0020 (7)	0.0280 (8)	-0.0005 (8)
C16	0.0565 (10)	0.0478 (9)	0.0672 (10)	-0.0023 (8)	0.0372 (8)	-0.0056 (8)
C17	0.0507 (9)	0.0455 (9)	0.0561 (9)	-0.0066 (7)	0.0284 (7)	-0.0030(7)
C18	0.0682 (12)	0.0892 (15)	0.0663 (11)	-0.0097 (10)	0.0308 (9)	-0.0223 (10)
C19	0.0525 (11)	0.0907 (16)	0.1073 (16)	0.0077 (11)	0.0292 (11)	-0.0055 (13)
N1	0.0491 (8)	0.0839 (11)	0.0649 (9)	0.0173 (8)	0.0117 (7)	0.0101 (8)
N2	0.0462 (8)	0.0604 (9)	0.0585 (8)	0.0086 (6)	0.0201 (6)	-0.0077 (6)
N3	0.0397 (7)	0.0489 (7)	0.0427 (6)	0.0051 (5)	0.0145 (5)	0.0015 (5)
01	0.0634 (8)	0.1056 (11)	0.0651 (8)	0.0179 (7)	0.0302 (6)	0.0344 (7)

Geometric parameters (Å, °)

C1—N2	1.308 (2)	C10—C11	1.4933 (19)
C1—N1	1.336 (2)	C11—O1	1.2186 (18)
C1—H1	0.9300	C11—C12	1.492 (2)
C2—N1	1.314 (2)	C12—C13	1.387 (2)
C2—N3	1.330 (2)	C12—C17	1.406 (2)
С2—Н2	0.9300	C13—C14	1.376 (2)
C3—C4	1.383 (2)	C13—H13	0.9300
C3—C8	1.389 (2)	C14—C15	1.384 (2)
С3—Н3	0.9300	C14—H14	0.9300
C4—C5	1.378 (2)	C15—C16	1.384 (2)
C4—H4	0.9300	C15—C19	1.509 (2)
C5—C6	1.370 (2)	C16—C17	1.387 (2)

C6-C7 $1.379(2)$ C17-C18 $1.503(2)$ C6-H6 0.9300 C18-H18A 0.9600 C7-C8 $1.388(2)$ C18-H18B 0.9600 C7-C7 0.9300 C18-H18D 0.9600 C8-C9 $1.4727(19)$ C19-H19A 0.9600 C9-C10 $1.312(2)$ C19-H19B 0.9600 C9-H1M 0.958(15) C19-H19C 0.9600 C10-N3 $1.4330(18)$ N2-N3 $1.3560(17)$ N2-C1-H1 116.25(15) C13-C12-C11 119.40(13) N1-C2-N3 111.45(16) C14-C13-H13 119.4 N1-C2-H2 124.3 C13-C14-H14 119.6 C4-C3-C4 120.15(15) C13-C14-H14 119.6 C4-C3-C4 120.50(16) C14-C15-C19 120.99(16) C4-C4-C3 120.50(16) C14-C15-C19 120.4(16) C3-C4-H4 119.7 C16-C17 123.1(14) C6-C5-C4 120.0 C17-C18-H18 19.55(14) C4-C3-H5 120.1 C16-C1	С5—Н5	0.9300	С16—Н16	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—C7	1.379 (2)	C17—C18	1.503 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С6—Н6	0.9300	C18—H18A	0.9600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С7—С8	1.388 (2)	C18—H18B	0.9600
C8 L 4727 (19) C19—H19A 0.9600 C9—C10 1.331 (2) C19—H19B 0.9600 C9—H1M 0.958 (15) C19—H19C 0.9600 C10—N3 1.4330 (18) N2—N3 1.3560 (17) N2=C1—N1 116.25 (15) C13—C12=C11 119.40 (13) N2=C1—H1 121.9 C14—C13—C12 121.27 (14) N1=C2=N3 111.45 (16) C14—C13—H13 119.4 N1=C2=H2 124.3 C13—C14—C15 120.85 (15) C4=C3=C8 120.15 (15) C13—C14—C15 120.85 (15) C4=C3=H3 119.9 C14—C15—C16 117.57 (15) C5=C4=C3 120.50 (16) C14—C15—C19 120.99 (16) C5=C4=H4 119.7 C16—C15—C19 121.44 (16) C5=C4 119.79 (15) C15—C16—H16 118.4 C6=C5=H5 120.1 C16—C17—C12 17.96 (14) C5=C6=C7 120.03 (15) C16—C17—C18 19.53 (14) C5=C6=C7 120.03 (15) C16—C17=C18 19.53 (14) C5=	С7—Н7	0.9300	C18—H18C	0.9600
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C8—C9	1.4727 (19)	С19—Н19А	0.9600
C9-H1M 0.958 (15) C19-H19C 0.9600 C10-N3 1.4330 (18) N2-N3 1.3560 (17) N2-C1-N1 116.25 (15) C13-C12-C11 121.46 (14) N1-C1-H1 121.9 C17-C12-C11 121.46 (14) N1-C2-H1 121.9 C14-C13-H13 119.4 N1-C2-H2 124.3 C13-C14-C15 120.88 (15) C4-C3-C8 120.15 (15) C13-C14-H14 119.6 C4-C3-H3 119.9 C14-C15-C16 17.57 (15) C5-C4-C3 120.50 (16) C14-C15-C19 120.99 (16) C5-C4-H4 119.7 C16-C16-C17 123.21 (14) C6-C5-C4 119.79 (15) C15-C16-H16 118.4 C6-C5-C4 119.79 (15) C15-C16-H16 118.4 C6-C5-C4 119.79 (15) C15-C16-H16 118.4 C6-C7 120.03 (15) C16-C17-C12 117.96 (14) C5-C6-C7 120.03 (15) C16-C17-C18 122.48 (14) C7-C6-H6 120.0 C17-C18-H18B 109.5 C6-C	C9—C10	1.331 (2)	С19—Н19В	0.9600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С9—Н1М	0.958 (15)	С19—Н19С	0.9600
$\begin{split} & \text{N2} = \text{C1} = \text{N1} & 116.25 (15) & \text{C1} = \text{C1} = \text{C1} & 119.40 (13) \\ & \text{N1} = \text{C1} = \text{H1} & 121.9 & \text{C1} = \text{C1} = \text{C1} & 121.46 (14) \\ & \text{N1} = \text{C2} = \text{N3} & 111.45 (16) & \text{C1} = \text{C1} = \text{C1} & 121.31 & 119.4 \\ & \text{N1} = \text{C2} = \text{N3} & 111.45 (16) & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 113 & 119.4 \\ & \text{N1} = \text{C2} = \text{N2} & 124.3 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 113 & 119.4 \\ & \text{N3} = \text{C2} = \text{H2} & 124.3 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 113 & 119.4 \\ & \text{N3} = \text{C2} = \text{H2} & 124.3 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114 & 119.6 \\ & \text{C4} = \text{C3} = \text{H3} & 119.9 & \text{C1} = \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114 & 119.6 \\ & \text{C4} = \text{C3} = \text{H3} & 119.9 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114 & 119.6 \\ & \text{C3} = \text{C3} = \text{C3} & 120.50 (16) & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114.44 & 119.6 \\ & \text{C3} = \text{C4} = \text{C3} & 120.50 (16) & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114.44 & 119.6 \\ & \text{C3} = \text{C4} = \text{H4} & 119.7 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114.44 & (16) \\ & \text{C3} = \text{C4} = \text{H4} & 119.7 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114.44 & (16) \\ & \text{C3} = \text{C4} = \text{H4} & 119.7 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 114.44 & (16) \\ & \text{C3} = \text{C4} = \text{H4} & 119.7 & \text{C1} = \text{C1} = \text{C1} = \text{C1} & 118.44 & (16) \\ & \text{C4} = \text{C5} = \text{H5} & 120.1 & \text{C1} = \text{C1} = \text{C1} = \text{H1} & \text{H1} & 119.6 & (14) \\ & \text{C5} = \text{C6} = \text{C7} & 120.03 (15) & \text{C1} = \text{C1} = \text{C1} & \text{M1} & 119.53 & (14) \\ & \text{C5} = \text{C6} = \text{C6} & 120.0 & \text{C1} = \text{C1} = \text{H1} & \text{H3} & 109.5 & (16) \\ & \text{C6} = \text{C7} = \text{C8} & 121.04 & (15) & \text{C1} = \text{C1} = \text{H1} & \text{H8} & 109.5 & (16) \\ & \text{C6} = \text{C7} = \text{C8} & 120.40 & (15) & \text{C1} = \text{C1} = \text{H1} & \text{H3} & 109.5 & (16) \\ & \text{C6} = \text{C7} = \text{C8} & 120.07 & (14) & \text{C1} = \text{C1} = \text{H1} & \text{H3} & 109.5 & (16) \\ & \text{C6} = \text{C7} = \text{C8} & 120.40 & (15) & \text{C1} = \text{C1} = \text{H1} & \text{M1} & 109.5 & (16) \\ & \text{C6} = \text{C7} = \text{C8} & 120.40 & (15) & \text{C1} = \text{C1} = \text{H1} & \text{H3} & 109.5 & (16) \\ & \text{C6} = \text{C7} = \text{C8} & 118.42 & (13) & \text{H1} & \text{M2} = \text{C1} = \text{H1} & \text{H1} & 109.5 & (16) \\ & \text{C6} = \text$	C10—N3	1.4330 (18)	N2—N3	1.3560 (17)
$\begin{split} & \text{N2}-\text{C1}-\text{H1} & \text{121.9} & \text{C1}7-\text{C1}2-\text{C11} & \text{121.46} (\text{H}) \\ & \text{N1}-\text{C1}-\text{H1} & \text{121.9} & \text{C1}4-\text{C1}3-\text{C12} & \text{121.27} (\text{H}) \\ & \text{N1}-\text{C2}-\text{N3} & \text{111.45} (\text{16}) & \text{C1}4-\text{C1}3-\text{H13} & \text{119.4} \\ & \text{N3}-\text{C2}-\text{H2} & \text{124.3} & \text{C1}3-\text{C1}3-\text{H13} & \text{119.4} \\ & \text{N3}-\text{C2}-\text{H2} & \text{124.3} & \text{C1}3-\text{C1}4-\text{C15} & \text{120.85} (\text{15}) \\ & \text{C4}-\text{C3}-\text{C8} & \text{120.15} (\text{15}) & \text{C1}3-\text{C1}4-\text{H14} & \text{119.6} \\ & \text{C4}-\text{C3}-\text{C8} & \text{120.50} (\text{16}) & \text{C1}5-\text{C16} & \text{117.57} (\text{15}) \\ & \text{C5}-\text{C4}-\text{C3} & \text{120.50} (\text{16}) & \text{C1}4-\text{C15}-\text{C16} & \text{117.57} (\text{15}) \\ & \text{C5}-\text{C4}-\text{C3} & \text{120.50} (\text{16}) & \text{C1}4-\text{C15}-\text{C16} & \text{117.57} (\text{15}) \\ & \text{C5}-\text{C4}-\text{C3} & \text{120.50} (\text{16}) & \text{C1}5-\text{C16}-\text{C17} & \text{123.21} (\text{14}) \\ & \text{C6}-\text{C5}-\text{C4} & \text{119.79} (\text{15}) & \text{C15}-\text{C16}-\text{C17} & \text{123.21} (\text{14}) \\ & \text{C6}-\text{C5}-\text{C4} & \text{119.79} (\text{15}) & \text{C15}-\text{C16}-\text{C17} & \text{123.21} (\text{14}) \\ & \text{C6}-\text{C5}-\text{C4} & \text{120.1} & \text{C17}-\text{C16}-\text{H16} & \text{118.4} \\ & \text{C6}-\text{C5}-\text{H5} & \text{120.1} & \text{C1}7-\text{C18} & \text{119.53} (\text{14}) \\ & \text{C5}-\text{C6}-\text{C7} & \text{120.03} (\text{15}) & \text{C1}-\text{C17}-\text{C18} & \text{119.53} (\text{14}) \\ & \text{C5}-\text{C6}-\text{C7} & \text{120.03} (\text{15}) & \text{C1}7-\text{C18} & \text{118.8} & \text{109.5} \\ & \text{C6}-\text{C7}-\text{C8} & \text{121.04} (\text{15}) & \text{C1}7-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C6}-\text{C7}-\text{C8} & \text{121.04} (\text{15}) & \text{C1}7-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C6}-\text{C7}-\text{H7} & \text{119.5} & \text{H18A}-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C6}-\text{C7}-\text{H7} & \text{119.5} & \text{C1}7-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C6}-\text{C7}-\text{H7} & \text{119.5} & \text{C1}7-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C}7-\text{C8}-\text{C9} & \text{13.34} (\text{13}) & \text{H18A}-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C7}-\text{C8}-\text{C9} & \text{13.34} (\text{13}) & \text{H18A}-\text{C18}-\text{H18B} & \text{109.5} \\ & \text{C1}-\text{C9}-\text{C1}-\text{H1} & \text{113.3} (\text{9}) & \text{C1}5-\text{C1}-\text{H19A} & \text{109.5} \\ & \text{C1}-\text{C1}-\text{C1}-\text{H19A} & \text{109.5} \\ & \text{C1}-\text{C1}-\text{C1}-\text{H19B} & \text{109.5} \\ & \text{C1}-\text{C1}-\text{C1}-\text{H19B} & \text{109.5} \\ & \text{C1}-\text{C1}-\text{C1}-\text{H19B} & \text{109.5} \\ & \text{C1}-\text{C1}-\text{C1}-\text{C1} & \text{C1}-C$	N2—C1—N1	116.25 (15)	C13—C12—C11	119.40 (13)
$\begin{split} & \text{N1}-\text{C1}-\text{H1} & 121.9 & \text{C1}4-\text{C1}3-\text{C1}2 & 121.27 (14) \\ & \text{N1}-\text{C2}-\text{N3} & 111.45 (16) & \text{C1}4-\text{C1}3-\text{H1}3 & 119.4 \\ & \text{N1}-\text{C2}-\text{H2} & 124.3 & \text{C1}3-\text{C1}3-\text{H1}3 & 119.4 \\ & \text{N3}-\text{C2}-\text{H2} & 124.3 & \text{C1}3-\text{C1}4-\text{C1}5 & 120.85 (15) \\ & \text{C4}-\text{C3}-\text{C8} & 120.15 (15) & \text{C1}3-\text{C1}4-\text{H1}4 & 119.6 \\ & \text{C4}-\text{C3}-\text{H3} & 119.9 & \text{C1}5-\text{C1}4-\text{H1}4 & 119.6 \\ & \text{C4}-\text{C3}-\text{H3} & 119.9 & \text{C1}5-\text{C1}6-\text{C1}6 & 117.57 (15) \\ & \text{C5}-\text{C4}-\text{C3} & 120.50 (16) & \text{C1}4-\text{C1}5-\text{C1}6 & 117.57 (15) \\ & \text{C5}-\text{C4}-\text{C3} & 120.50 (16) & \text{C1}4-\text{C1}5-\text{C1}9 & 120.99 (16) \\ & \text{C5}-\text{C4}-\text{C3} & 120.50 (16) & \text{C1}4-\text{C1}5-\text{C1}9 & 123.21 (14) \\ & \text{C6}-\text{C5}-\text{C4} & 119.79 (15) & \text{C1}5-\text{C1}6-\text{C1}7 & 123.21 (14) \\ & \text{C6}-\text{C5}-\text{H5} & 120.1 & \text{C1}6-\text{C1}7-\text{C1}8 & 119.53 (14) \\ & \text{C5}-\text{C6}-\text{C7} & 120.03 (15) & \text{C1}6-\text{C1}7-\text{C1}8 & 119.53 (14) \\ & \text{C5}-\text{C6}-\text{C6} & 120.0 & \text{C1}2-\text{C1}7-\text{C1}8 & 119.53 (14) \\ & \text{C5}-\text{C6}-\text{H6} & 120.0 & \text{C1}2-\text{C1}7-\text{C1}8 & 119.53 (14) \\ & \text{C5}-\text{C6}-\text{C7} & 120.03 (15) & \text{C1}6-\text{C1}7-\text{C1}8 & 109.5 \\ & \text{C6}-\text{C7}-\text{H7} & 119.5 & \text{H18}-\text{C18}-\text{H18}8 & 109.5 \\ & \text{C6}-\text{C7}-\text{H7} & 119.5 & \text{C1}7-\text{C18}-\text{H18}8 & 109.5 \\ & \text{C6}-\text{C7}-\text{H7} & 119.5 & \text{C1}7-\text{C18}-\text{H18}8 & 109.5 \\ & \text{C7}-\text{C8}-\text{C9} & 118.45 (13) & \text{H18}-\text{C18}-\text{H18}C & 109.5 \\ & \text{C7}-\text{C8}-\text{C9} & 123.01 (13) & \text{C1}5-\text{C1}9-\text{H19}A & 109.5 \\ & \text{C1}0-\text{C9}-\text{H1}M & 117.6 (9) & \text{H19}A-\text{C1}9-\text{H19}B & 109.5 \\ & \text{C1}0-\text{C9}-\text{H1}M & 117.6 (9) & \text{H19}A-\text{C1}9-\text{H19}B & 109.5 \\ & \text{C1}0-\text{C9}-\text{H1}M & 117.6 (9) & \text{H19}A-\text{C1}9-\text{H19}B & 109.5 \\ & \text{C1}0-\text{C1}-\text{H1}M & 117.6 (9) & \text{H19}A-\text{C1}9-\text{H19}B & 109.5 \\ & \text{C1}0-\text{C1}-\text{H1}M & 117.6 (9) & \text{H19}A-\text{C1}9-\text{H19}B & 109.5 \\ & \text{C3}-\text{C6}-\text{C7} & 123.01 (13) & \text{C1}5-\text{C1}9-\text{H1}9B & 109.5 \\ & \text{C3}-\text{C6}-\text{C1}1 & 114.25 (12) & \text{C2}-\text{N1}-\text{C1} & 101.62 (14) \\ & \text{O1}-51-\text{C1}0 & 119.55 (13) & \text{C1}-\text{C1}9-\text{H1}9B & 109.5 \\ & \text{C3}-\text{C6}-\text{C1}1 & 119.29 (13) & \text{C1}-\text{C1}9-\text{H1}9B & 109.5 \\ & \text{C3}-\text{C1}$	N2—C1—H1	121.9	C17—C12—C11	121.46 (14)
N1-C2-N3 111.45 (16) C14-C13-H13 119.4 N1-C2-H2 124.3 C12-C13-H13 119.4 N3-C2-H2 124.3 C13-C14-C15 120.85 (15) C4-C3-C8 120.15 (15) C13-C14-H14 119.6 C4-C3-H3 119.9 C15-C14-H14 119.6 C5-C4-H4 119.7 C16-C15-C19 120.90 (16) C5-C4-H4 119.7 C15-C16-H16 118.4 C6-C5-C4 119.79 (15) C15-C16-H16 118.4 C6-C5-C4 119.79 (15) C15-C16-H16 118.4 C4-C5-H5 120.1 C16-C17-C12 17.96 (14) C5-C6-H5 120.1 C16-C17-C18 119.53 (14) C5-C6-H6 120.0 C17-C18-H18 109.5 C6-C7-C8 121.04 (15) C17-C18-H18 109.5 C6-C7-H7 119.5 H18A-C18-H18 109.5 C6-C7-C8 121.04 (15) C17-C18-H18 109.5 C6-C7-C7 12.03 (13) C15-C19-H19A 109.5 C6-C7-C8 121.04 (15) H18A-C18-H18C 109.5 C7-C8-C9 118.42 (13)<	N1—C1—H1	121.9	C14—C13—C12	121.27 (14)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N1—C2—N3	111 45 (16)	C14—C13—H13	119.4
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N1—C2—H2	124.3	C12—C13—H13	119.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N3—C2—H2	124.3	C13—C14—C15	120.85 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4-C3-C8	120.15 (15)	C13—C14—H14	119.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4-C3-H3	119.9	C15 - C14 - H14	119.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8_C3_H3	119.9	C_{14} C_{15} C_{16}	117.57 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{5} - C_{4} - C_{3}$	120 50 (16)	$C_{14} = C_{15} = C_{10}$	120.99 (16)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{5} = C_{4} = C_{5}$	110.7	$C_{14} = C_{15} = C_{19}$	120.99(10)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_3 = C_4 = H_4$	119.7	$C_{10} = C_{13} = C_{13}$	121.44(10) 122.21(14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C_{5}	119.7	$C_{15} = C_{16} = C_{17}$	123.21 (14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_0 = C_3 = C_4$	119.79 (13)	C13-C16-H16	118.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Со-Со-Но	120.1	C1/-C16-H16	118.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С4—С5—Н5	120.1	C16-C17-C12	117.96 (14)
CS-C6-H6120.0C12-C17-C18122.48 (14)C7-C6-H6120.0C17-C18-H18A109.5C6-C7-C8121.04 (15)C17-C18-H18B109.5C6-C7-H7119.5H18A-C18-H18B109.5C8-C7-H7119.5C17-C18-H18C109.5C7-C8-C3118.45 (13)H18A-C18-H18C109.5C7-C8-C9118.42 (13)H18B-C18-H18C109.5C10-C9-C8129.07 (14)C15-C19-H19A109.5C10-C9-H1M117.6 (9)H19A-C19-H19B109.5C8-C9-H1M113.3 (9)C15-C19-H19C109.5C9-C10-N3120.68 (13)H19A-C19-H19C109.5C9-C10-C11125.02 (13)H19A-C19-H19C109.5C9-C10-C11125.02 (13)H19A-C19-H19C109.5C10-C21-C12121.95 (13)C1-N2-N3101.96 (13)O1-C11-C12121.95 (13)C1-N2-N3101.96 (13)O1-C11-C10118.58 (14)C2-N3-N2108.70 (13)C12-C11-C10119.45 (13)C2-N3-C10119.52 (11)C8-C3-C4-C51.4 (3)C12-C13-C14-C15-1.6 (3)C3-C4-C5-C6-1.1 (3)C13-C14-C15-C161.8 (3)C4-C5-C6-C7-0.6 (3)C13-C14-C15-C16-1.78.00 (17)C5-C6-C7-C82.2 (3)C14-C15-C16-C170.0 (3)C6-C7-C8-C3-1.9 (2)C19-C15-C16-C17179.80 (16)	C5—C6—C7	120.03 (15)	C16—C17—C18	119.53 (14)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С5—С6—Н6	120.0	C12—C17—C18	122.48 (14)
C6-C7-C8 $121.04 (15)$ $C17-C18-H18B$ 109.5 $C6-C7-H7$ 119.5 $H18A-C18-H18B$ 109.5 $C8-C7-H7$ 119.5 $C17-C18-H18C$ 109.5 $C7-C8-C3$ $118.45 (13)$ $H18A-C18-H18C$ 109.5 $C7-C8-C9$ $118.42 (13)$ $H18B-C18-H18C$ 109.5 $C3-C8-C9$ $123.01 (13)$ $C15-C19-H19A$ 109.5 $C10-C9-C8$ $129.07 (14)$ $C15-C19-H19B$ 109.5 $C10-C9-H1M$ $117.6 (9)$ $H19A-C19-H19B$ 109.5 $C9-C10-M3$ $120.68 (13)$ $H19A-C19-H19C$ 109.5 $C9-C10-C11$ $125.02 (13)$ $H19B-C19-H19C$ 109.5 $N3-C10-C11$ $114.25 (12)$ $C2-N1-C1$ $101.62 (14)$ $O1-C11-C12$ $121.95 (13)$ $C1-N2-N3$ $101.96 (13)$ $O1-C11-C10$ $118.58 (14)$ $C2-N3-N2$ $108.70 (13)$ $C12-C17$ $119.09 (14)$ $N2-N3-C10$ $119.52 (11)$ $C8-C3-C4-C5$ $1.4 (3)$ $C12-C13-C14-C15$ $-1.6 (3)$ $C3-C4-C5-C6$ $-1.1 (3)$ $C13-C14-C15-C16$ $1.8 (3)$ $C4-C5-C6-C7$ $-0.6 (3)$ $C13-C14-C15-C16$ $1.8 (3)$ $C4-C5-C6-C7-C8$ $2.2 (3)$ $C14-C15-C16-C17$ $0.0 (3)$ $C6-C7-C8-C3$ $-1.9 (2)$ $C19-C15-C16-C17$ $179.80 (16)$	С7—С6—Н6	120.0	C17—C18—H18A	109.5
C6-C7-H7119.5H18A-C18-H18B109.5 $C8-C7-H7$ 119.5 $C17-C18-H18C$ 109.5 $C7-C8-C3$ 118.45 (13)H18A-C18-H18C109.5 $C7-C8-C9$ 118.42 (13)H18B-C18-H18C109.5 $C3-C8-C9$ 123.01 (13) $C15-C19-H19A$ 109.5 $C10-C9-C8$ 129.07 (14) $C15-C19-H19B$ 109.5 $C10-C9-H1M$ 117.6 (9)H19A-C19-H19B109.5 $C9-C10-N3$ 120.68 (13)H19A-C19-H19C109.5 $C9-C10-C11$ 125.02 (13)H19B-C19-H19C109.5 $N3-C10-C11$ 114.25 (12) $C2-N1-C1$ 101.62 (14) $O1-C11-C12$ 121.95 (13) $C1-N2-N3$ 101.96 (13) $O1-C11-C10$ 118.58 (14) $C2-N3-N2$ 108.70 (13) $C12-C11-C10$ 119.45 (13) $C2-N3-C10$ 131.78 (13) $C13-C12-C17$ 119.09 (14)N2-N3-C10119.52 (11) $C8-C3-C4-C5$ 1.4 (3) $C12-C13-C14-C15$ -1.6 (3) $C3-C4-C5-C6$ -1.1 (3) $C13-C14-C15-C16$ 1.8 (3) $C4-C5-C6-C7$ -0.6 (3) $C13-C14-C15-C16-C17$ 0.0 (3) $C6-C7-C8-C3$ -1.9 (2) $C19-C15-C16-C17$ 179.80 (16)	C6—C7—C8	121.04 (15)	C17—C18—H18B	109.5
C8-C7-H7119.5C17-C18-H18C109.5C7-C8-C3118.45 (13)H18A-C18-H18C109.5C7-C8-C9118.42 (13)H18B-C18-H18C109.5C3-C8-C9123.01 (13)C15-C19-H19A109.5C10-C9-C8129.07 (14)C15-C19-H19B109.5C10-C9-H1M117.6 (9)H19A-C19-H19B109.5C8-C9-H1M113.3 (9)C15-C19-H19C109.5C9-C10-N3120.68 (13)H19A-C19-H19C109.5C9-C10-C11125.02 (13)H19B-C19-H19C109.5N3-C10-C11114.25 (12)C2-N1-C1101.62 (14)O1-C11-C12121.95 (13)C1-N2-N3101.96 (13)O1-C11-C10118.58 (14)C2-N3-N2108.70 (13)C12-C17119.09 (14)N2-N3-C10131.78 (13)C13-C12-C17119.09 (14)N2-N3-C10119.52 (11)C8-C3-C4-C51.4 (3)C12-C13-C14-C15-1.6 (3)C3-C4-C5-C6-1.1 (3)C13-C14-C15-C161.8 (3)C4-C5-C6-C7-0.6 (3)C13-C14-C15-C161.8 (3)C4-C5-C6-C7-C82.2 (3)C14-C15-C16-C170.0 (3)C6-C7-C8-C3-1.9 (2)C19-C15-C16-C17179.80 (16)	С6—С7—Н7	119.5	H18A—C18—H18B	109.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С8—С7—Н7	119.5	C17—C18—H18C	109.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7—C8—C3	118.45 (13)	H18A—C18—H18C	109.5
C3—C8—C9123.01 (13)C15—C19—H19A109.5C10—C9—C8129.07 (14)C15—C19—H19B109.5C10—C9—H1M117.6 (9)H19A—C19—H19B109.5C8—C9—H1M113.3 (9)C15—C19—H19C109.5C9—C10—N3120.68 (13)H19A—C19—H19C109.5C9—C10—C11125.02 (13)H19B—C19—H19C109.5N3—C10—C11114.25 (12)C2—N1—C1101.62 (14)O1—C11—C12121.95 (13)C1—N2—N3101.96 (13)O1—C11—C10118.58 (14)C2—N3—N2108.70 (13)C13—C12—C17119.09 (14)N2—N3—C10119.52 (11)C8—C3—C4—C51.4 (3)C12—C13—C14—C15-1.6 (3)C3—C4—C5—C6-1.1 (3)C13—C14—C15—C161.8 (3)C4—C5—C6—C7-0.6 (3)C13—C14—C15—C19-178.00 (17)C5—C6—C7—C82.2 (3)C14—C15—C16—C170.0 (3)C6—C7—C8—C3-1.9 (2)C19—C15—C16—C17179.80 (16)	C7—C8—C9	118.42 (13)	H18B—C18—H18C	109.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—C8—C9	123.01 (13)	С15—С19—Н19А	109.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10—C9—C8	129.07 (14)	C15—C19—H19B	109.5
C8—C9—H1M113.3 (9)C15—C19—H19C109.5C9—C10—N3120.68 (13)H19A—C19—H19C109.5C9—C10—C11125.02 (13)H19B—C19—H19C109.5N3—C10—C11114.25 (12)C2—N1—C1101.62 (14)O1—C11—C12121.95 (13)C1—N2—N3101.96 (13)O1—C11—C10118.58 (14)C2—N3—N2108.70 (13)C12—C11—C10119.45 (13)C2—N3—C10131.78 (13)C13—C12—C17119.09 (14)N2—N3—C10119.52 (11)C8—C3—C4—C51.4 (3)C12—C13—C14—C15-1.6 (3)C3—C4—C5—C6-1.1 (3)C13—C14—C15—C161.8 (3)C4—C5—C6—C7-0.6 (3)C13—C14—C15—C161.8 (3)C4—C5—C6—C7-0.6 (3)C14—C15—C16—C170.0 (3)C5—C6—C7—C82.2 (3)C14—C15—C16—C170.0 (3)C6—C7—C8—C3-1.9 (2)C19—C15—C16—C17179.80 (16)	C10—C9—H1M	117.6 (9)	H19A—C19—H19B	109.5
C9—C10—N3120.68 (13)H19A—C19—H19C109.5C9—C10—C11125.02 (13)H19B—C19—H19C109.5N3—C10—C11114.25 (12)C2—N1—C1101.62 (14)O1—C11—C12121.95 (13)C1—N2—N3101.96 (13)O1—C11—C10118.58 (14)C2—N3—N2108.70 (13)C12—C11—C10119.45 (13)C2—N3—C10131.78 (13)C13—C12—C17119.09 (14)N2—N3—C10119.52 (11)C8—C3—C4—C51.4 (3)C12—C13—C14—C15-1.6 (3)C3—C4—C5—C6-1.1 (3)C13—C14—C15—C161.8 (3)C4—C5—C6—C7-0.6 (3)C13—C14—C15—C19-178.00 (17)C5—C6—C7—C82.2 (3)C14—C15—C16—C170.0 (3)C6—C7—C8—C3-1.9 (2)C19—C15—C16—C17179.80 (16)	C8—C9—H1M	113.3 (9)	С15—С19—Н19С	109.5
C9—C10—C11125.02 (13)H19B—C19—H19C109.5N3—C10—C11114.25 (12)C2—N1—C1101.62 (14)O1—C11—C12121.95 (13)C1—N2—N3101.96 (13)O1—C11—C10118.58 (14)C2—N3—N2108.70 (13)C12—C11—C10119.45 (13)C2—N3—C10131.78 (13)C13—C12—C17119.09 (14)N2—N3—C10119.52 (11)C8—C3—C4—C51.4 (3)C12—C13—C14—C15-1.6 (3)C3—C4—C5—C6-1.1 (3)C13—C14—C15—C161.8 (3)C4—C5—C6—C7-0.6 (3)C13—C14—C15—C19-178.00 (17)C5—C6—C7—C82.2 (3)C14—C15—C16—C170.0 (3)C6—C7—C8—C3-1.9 (2)C19—C15—C16—C17179.80 (16)	C9—C10—N3	120.68 (13)	H19A—C19—H19C	109.5
N3-C10-C11114.25 (12)C2-N1-C1101.62 (14)O1-C11-C12121.95 (13)C1-N2-N3101.96 (13)O1-C11-C10118.58 (14)C2-N3-N2108.70 (13)C12-C11-C10119.45 (13)C2-N3-C10131.78 (13)C13-C12-C17119.09 (14)N2-N3-C10119.52 (11)C8-C3-C4-C51.4 (3)C12-C13-C14-C15-1.6 (3)C3-C4-C5-C6-1.1 (3)C13-C14-C15-C161.8 (3)C4-C5-C6-C7-0.6 (3)C13-C14-C15-C19-178.00 (17)C5-C6-C7-C82.2 (3)C14-C15-C16-C170.0 (3)C6-C7-C8-C3-1.9 (2)C19-C15-C16-C17179.80 (16)	C9—C10—C11	125.02 (13)	H19B—C19—H19C	109.5
01C11C12 $121.95 (13)$ $C1N2N3$ $101.96 (13)$ $01C11C10$ $118.58 (14)$ $C2N3N2$ $108.70 (13)$ $C12C11C10$ $119.45 (13)$ $C2N3C10$ $131.78 (13)$ $C13C12C17$ $119.09 (14)$ $N2N3C10$ $119.52 (11)$ $C8C3C4C5$ $1.4 (3)$ $C12C13C14C15$ $-1.6 (3)$ $C3C4C5C6$ $-1.1 (3)$ $C13C14C15C16$ $1.8 (3)$ $C4C5C6C7$ $-0.6 (3)$ $C13C14C15C16$ $1.8 (3)$ $C4C5C6C7$ $-0.6 (3)$ $C13C14C15C16$ $1.8 (3)$ $C5C6C7C8$ $2.2 (3)$ $C14C15C16C17$ $0.0 (3)$ $C6C7C8C3$ $-1.9 (2)$ $C19C15C16C17$ $179.80 (16)$	N3—C10—C11	114.25 (12)	C2—N1—C1	101.62 (14)
O1-C11-C10 $118.58 (14)$ $C2-N3-N2$ $108.70 (13)$ $C12-C11-C10$ $119.45 (13)$ $C2-N3-C10$ $131.78 (13)$ $C13-C12-C17$ $119.09 (14)$ $N2-N3-C10$ $119.52 (11)$ $C8-C3-C4-C5$ $1.4 (3)$ $C12-C13-C14-C15$ $-1.6 (3)$ $C3-C4-C5-C6$ $-1.1 (3)$ $C13-C14-C15-C16$ $1.8 (3)$ $C4-C5-C6-C7$ $-0.6 (3)$ $C13-C14-C15-C19$ $-178.00 (17)$ $C5-C6-C7-C8$ $2.2 (3)$ $C14-C15-C16-C17$ $0.0 (3)$ $C6-C7-C8-C3$ $-1.9 (2)$ $C19-C15-C16-C17$ $179.80 (16)$	O1—C11—C12	121.95 (13)	C1—N2—N3	101.96 (13)
C12—C11—C10119.45 (13)C2—N3—C10131.78 (13)C13—C12—C17119.09 (14)N2—N3—C10119.52 (11)C8—C3—C4—C51.4 (3)C12—C13—C14—C15 $-1.6 (3)$ C3—C4—C5—C6 $-1.1 (3)$ C13—C14—C15—C161.8 (3)C4—C5—C6—C7 $-0.6 (3)$ C13—C14—C15—C19 $-178.00 (17)$ C5—C6—C7—C82.2 (3)C14—C15—C16—C170.0 (3)C6—C7—C8—C3 $-1.9 (2)$ C19—C15—C16—C17179.80 (16)	O1—C11—C10	118.58 (14)	C2—N3—N2	108.70 (13)
C13—C12—C17119.09 (14)N2—N3—C10119.52 (11)C8—C3—C4—C51.4 (3)C12—C13—C14—C15 $-1.6 (3)$ C3—C4—C5—C6 $-1.1 (3)$ C13—C14—C15—C161.8 (3)C4—C5—C6—C7 $-0.6 (3)$ C13—C14—C15—C19 $-178.00 (17)$ C5—C6—C7—C82.2 (3)C14—C15—C16—C170.0 (3)C6—C7—C8—C3 $-1.9 (2)$ C19—C15—C16—C17179.80 (16)	C12-C11-C10	119.45 (13)	C2—N3—C10	131.78 (13)
C8-C3-C4-C5 $1.4 (3)$ $C12-C13-C14-C15$ $-1.6 (3)$ $C3-C4-C5-C6$ $-1.1 (3)$ $C13-C14-C15-C16$ $1.8 (3)$ $C4-C5-C6-C7$ $-0.6 (3)$ $C13-C14-C15-C19$ $-178.00 (17)$ $C5-C6-C7-C8$ $2.2 (3)$ $C14-C15-C16-C17$ $0.0 (3)$ $C6-C7-C8-C3$ $-1.9 (2)$ $C19-C15-C16-C17$ $179.80 (16)$	C13—C12—C17	119.09 (14)	N2—N3—C10	119.52 (11)
C3-C4-C5-C6 -1.1 (3)C13-C14-C15-C16 1.8 (3)C4-C5-C6-C7 -0.6 (3)C13-C14-C15-C19 -178.00 (17)C5-C6-C7-C8 2.2 (3)C14-C15-C16-C17 0.0 (3)C6-C7-C8-C3 -1.9 (2)C19-C15-C16-C17 179.80 (16)	C8—C3—C4—C5	1.4 (3)	C12—C13—C14—C15	-1.6 (3)
C4—C5—C6—C7 -0.6 (3) C13—C14—C15—C19 -178.00 (17) C5—C6—C7—C8 2.2 (3) C14—C15—C16—C17 0.0 (3) C6—C7—C8—C3 -1.9 (2) C19—C15—C16—C17 179.80 (16)	C3—C4—C5—C6	-1.1 (3)	C13-C14-C15-C16	1.8 (3)
C5-C6-C7-C8 2.2 (3) C14-C15-C16-C17 0.0 (3) C6-C7-C8-C3 -1.9 (2) C19-C15-C16-C17 179.80 (16)	C4—C5—C6—C7	-0.6 (3)	C13—C14—C15—C19	-178.00 (17)
C6-C7-C8-C3 -1.9 (2) C19-C15-C16-C17 179.80 (16)	C5—C6—C7—C8	2.2 (3)	C14—C15—C16—C17	0.0 (3)
	C6—C7—C8—C3	-1.9 (2)	C19—C15—C16—C17	179.80 (16)

supplementary materials

C6—C7—C8—C9	-177.89 (14)	C15-C16-C17-C12	-1.9 (2)
C4—C3—C8—C7	0.1 (2)	C15-C16-C17-C18	179.96 (16)
C4—C3—C8—C9	175.91 (15)	C13—C12—C17—C16	2.1 (2)
C7—C8—C9—C10	-149.02 (16)	C11—C12—C17—C16	179.33 (14)
C3—C8—C9—C10	35.2 (2)	C13—C12—C17—C18	-179.86 (16)
C8—C9—C10—N3	7.0 (2)	C11-C12-C17-C18	-2.6 (2)
C8—C9—C10—C11	-170.43 (14)	N3—C2—N1—C1	1.4 (2)
C9—C10—C11—O1	162.17 (16)	N2-C1-N1-C2	-1.1 (2)
N3-C10-C11-O1	-15.4 (2)	N1—C1—N2—N3	0.3 (2)
C9—C10—C11—C12	-16.3 (2)	N1—C2—N3—N2	-1.3 (2)
N3-C10-C11-C12	166.14 (13)	N1-C2-N3-C10	179.01 (15)
O1—C11—C12—C13	131.04 (18)	C1—N2—N3—C2	0.56 (18)
C10-C11-C12-C13	-50.6 (2)	C1—N2—N3—C10	-179.71 (13)
O1-C11-C12-C17	-46.2 (2)	C9-C10-N3-C2	-113.9 (2)
C10-C11-C12-C17	132.18 (16)	C11—C10—N3—C2	63.8 (2)
C17—C12—C13—C14	-0.4 (2)	C9—C10—N3—N2	66.43 (19)
C11—C12—C13—C14	-177.68 (15)	C11—C10—N3—N2	-115.87 (15)



Fig. 1