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(4*Z*)-4-[(Cyclopropylamino)(phenyl)-methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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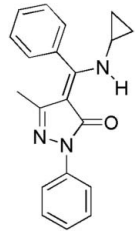
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.104; data-to-parameter ratio = 14.7.

In the title compound, $C_{20}H_{19}N_3O$, the dihedral angles formed by the pyrazolone ring with the two phenyl rings are 64.27 (6) and 17.00 (6)°. The molecular structure is stabilized by intramolecular N—H···O and C—H···O hydrogen bonds. In the crystal, the molecules are linked into chains along the b axis by intermolecular C—H···O hydrogen bonds.

Related literature

For the antibacterial, biological and analgesic activity of metal complexes of 1-phenyl-3-methyl-4-benzoylpyrazolon-5-one, see: Li *et al.* (1997); Liu *et al.* (1980); Zhou *et al.* (1999). For a related structure, see: Wang *et al.* (2003).



Experimental

Crystal data

$C_{20}H_{19}N_3O$ M_r = 317.38
Orthorhombic, *Pbca*
a = 8.9790 (18) Å
b = 18.500 (4) Å
c = 20.050 (4) Å
V = 3330.5 (12) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 113 K
0.24 × 0.21 × 0.20 mm

Data collection

Rigaku Saturn70 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.863, T_{max} = 0.884
34928 measured reflections
3262 independent reflections
2946 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.104
S = 1.06
3262 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1···O1	0.92 (2)	1.88 (2)	2.6726 (15)	143 (2)
C20—H20···O1	0.95	2.36	2.9453 (16)	120
C10—H10···O1^{i}	0.95	2.30	3.1809 (17)	154

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2005); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5077).

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supporting information

Acta Cryst. (2010). E**66**, o1123 [https://doi.org/10.1107/S1600536810013723]

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Hai-Zhen Xu, Yan-Xia Yang and You-Quan Zhu

S1. Comment

1-Phenyl-3-methyl-4-benzoylpyrazolon-5-one (HPMBP), an effective *β*-diketonate, is widely used and well known for its extractive ability. In recent years, HPMBP and its metal complexes have also been found to have good antibacterial and biological properties. Its metal complexes have analgesic activity (Liu *et al.*, 1980; Li *et al.*, 1997; Zhou *et al.*, 1999). In order to develop new medicines, we have synthesized the title compound and its crystal structure is reported here.

The structure of the title molecule is shown in Fig. 1. The dihedral angles formed by the pyrazolone ring with the C6–C11 and C15–C20 phenyl rings and cyclopropane ring are 64.27 (6)°, 17.00 (6)° and 71.28 (11)°, respectively. The O atom of the 3-methyl-1-phenylpyrazol-5-one moiety and the N atom of the amino group are available for coordination with metals. Atoms O1, C1, C2, C5 and N3 are coplanar (r.m.s. deviation = 0.028 Å). The dihedral angle between this plane and the pyrazoline ring is 4.34 (7)°, close to the value of 3.56 (3)° found in 4-{[3,4-dihydro-5-methyl-3-oxo-2-phenyl-2*H*-pyrazol-4-ylidene(phenyl) methylamino}-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Wang *et al.*, 2003). The bond lengths within this part of the molecule lie between classical single- and double-bond lengths, indicating extensive conjugation. A strong intramolecular N3—H1···O1 hydrogen bond (Table 1) is observed, leading to a keto-enamine form. The molecule is further stabilized by a C—H···O weak intramolecular hydrogen bond (Table 1).

The crystal structure also involves weak intermolecular C—H···O hydrogen-bond interactions (Fig. 2).

S2. Experimental

The title compound was synthesized by refluxing a mixture of 1-phenyl-3- methyl-4-benzoylpyrazol-5-one (10 mmol) and cyclopropanamine (10 mmol) in ethanol (80 ml) over a steam bath for about 16 h. Excess solvent was removed by evaporation and the solution was cooled to room temperature. After 2 d, a colourless solid was obtained and this was dried in air. The product was recrystallized from ethanol, to afford colourless crystals of the title compound suitable for X-ray analysis.

S3. Refinement

C-bonded H atoms were positioned geometrically, with C–H = 0.95–1.00 Å and the amine H atom (H1) was found in a difference map. The amine H atom was refined freely, while C-bonded H atoms were included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(CH_2 and CH) or 1.5U_{eq}(CH_3).

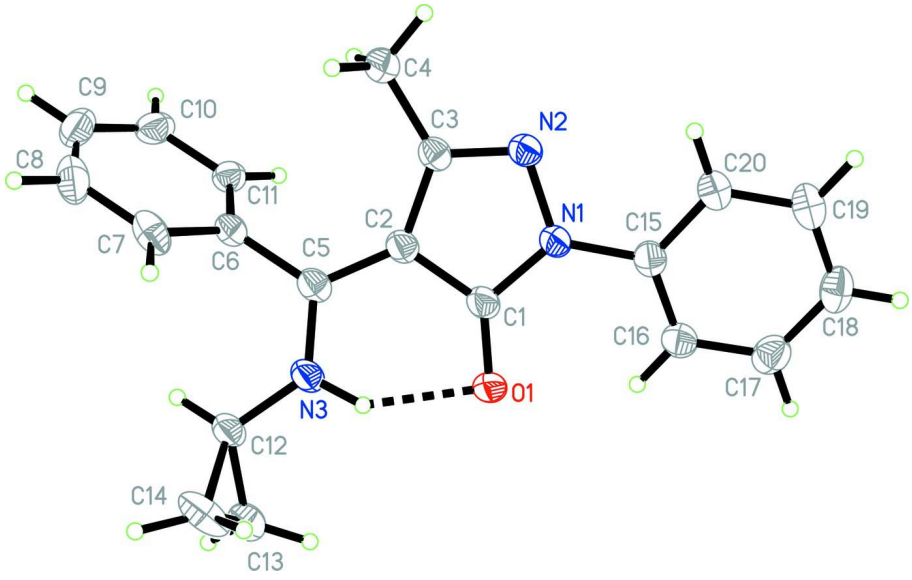

Figure 1

Molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

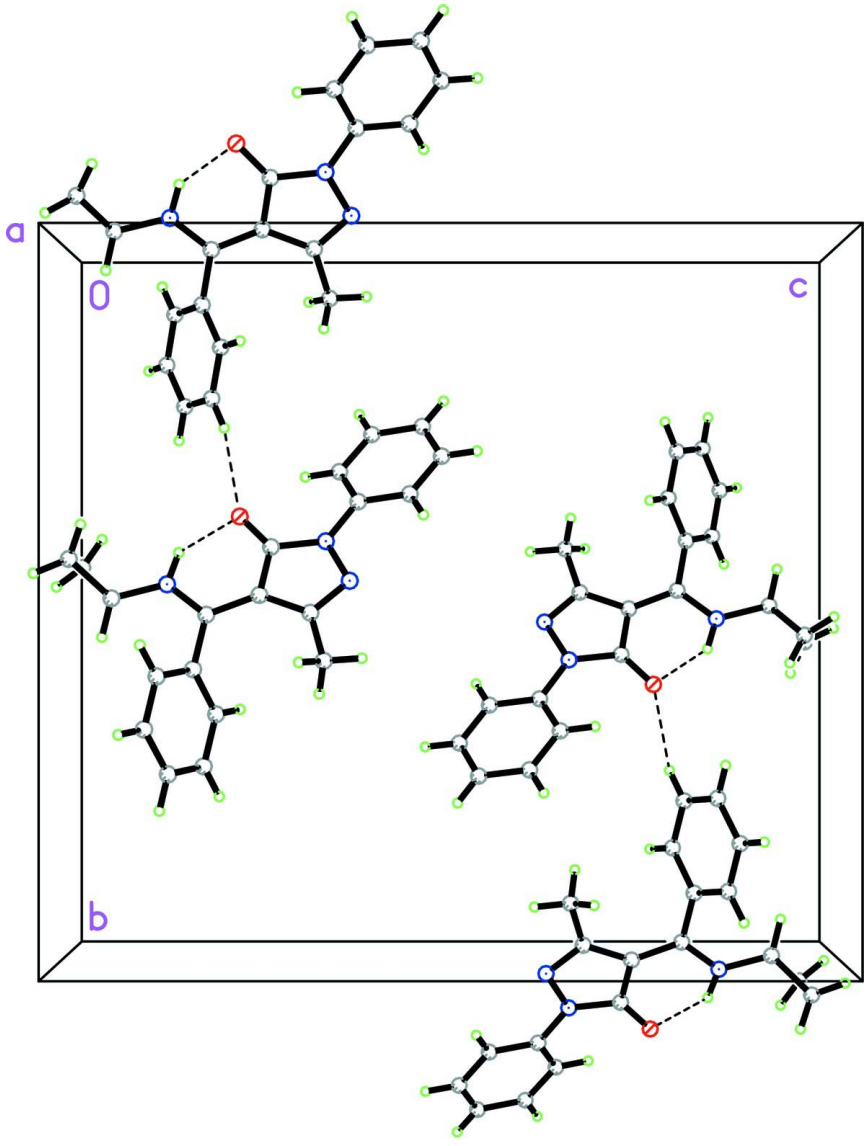

Figure 2

Part of hydrogen-bonded (dashed line) chains in the title compound.

(4*Z*)-4-[(Cyclopropylamino)(phenyl)methylene]-3-methyl-1-phenyl- 1*H*-pyrazol-5(4*H*)-one

Crystal data

$C_{20}H_{19}N_3O$
$M_r = 317.38$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 8.9790\ (18)$ Å
$b = 18.500\ (4)$ Å
$c = 20.050\ (4)$ Å
$V = 3330.5\ (12)$ Å^3
$Z = 8$
$F(000) = 1344$
$D_x = 1.266$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54187$ Å
Cell parameters from 2126 reflections
$\theta = 2.2–45.5°$
$\mu = 0.63$ mm^{-1}
$T = 113$ K
Prism, colourless
0.24 × 0.21 × 0.20 mm

Data collection

Rigaku Saturn70 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.863, T_{max} = 0.884
34928 measured reflections
3262 independent reflections
2946 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 72.5°, θ_{min} = 4.4°
h = −8→10
k = −22→22
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.104
S = 1.06
3262 reflections
222 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
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
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.7718P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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.

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 $F^2 > 2$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}
O1	0.67690 (13)	0.11712 (5)	0.26555 (4)	0.0415 (3)
N1	0.73850 (11)	0.08273 (5)	0.15606 (5)	0.0274 (2)
N2	0.82349 (11)	0.02871 (5)	0.12501 (5)	0.0262 (2)
N3	0.79592 (14)	0.02403 (5)	0.35244 (5)	0.0336 (3)
C1	0.73711 (15)	0.07497 (6)	0.22477 (6)	0.0299 (3)
C2	0.82015 (14)	0.00961 (6)	0.23704 (5)	0.0266 (3)
C3	0.87030 (13)	−0.01421 (6)	0.17276 (5)	0.0248 (2)
C4	0.96427 (14)	−0.07788 (7)	0.15470 (6)	0.0313 (3)
H4A	0.9070	−0.1224	0.1613	0.038*
H4B	1.0531	−0.0789	0.1831	0.038*
H4C	0.9944	−0.0742	0.1079	0.038*
C5	0.84118 (13)	−0.01694 (6)	0.30210 (5)	0.0260 (3)
C6	0.90512 (12)	−0.08952 (6)	0.31601 (5)	0.0246 (2)
C7	1.03261 (14)	−0.09759 (8)	0.35553 (6)	0.0344 (3)
H7	1.0806	−0.0562	0.3736	0.041*

C8	1.08875 (16)	−0.16611 (9)	0.36826 (7)	0.0454 (4)
H8	1.1754	−0.1715	0.3950	0.054*
C9	1.01929 (17)	−0.22661 (8)	0.34232 (7)	0.0465 (4)
H9	1.0586	−0.2733	0.3512	0.056*
C10	0.89239 (16)	−0.21934 (7)	0.30344 (6)	0.0379 (3)
H10	0.8443	−0.2610	0.2860	0.045*
C11	0.83581 (13)	−0.15080 (6)	0.29005 (6)	0.0269 (3)
H11	0.7495	−0.1458	0.2631	0.032*
C12	0.78672 (15)	0.00510 (6)	0.42190 (6)	0.0319 (3)
H12	0.7987	−0.0472	0.4331	0.038*
C13	0.84272 (17)	0.05784 (9)	0.47193 (6)	0.0446 (4)
H13A	0.8899	0.0384	0.5128	0.053*
H13B	0.8863	0.1035	0.4552	0.053*
C14	0.68020 (16)	0.04703 (8)	0.46359 (6)	0.0378 (3)
H14A	0.6226	0.0860	0.4417	0.045*
H14B	0.6263	0.0209	0.4993	0.045*
C15	0.67274 (13)	0.13754 (6)	0.11655 (6)	0.0269 (3)
C16	0.72259 (13)	0.14729 (6)	0.05108 (6)	0.0290 (3)
H16	0.8004	0.1180	0.0338	0.035*
C17	0.65736 (14)	0.20020 (7)	0.01143 (6)	0.0346 (3)
H17	0.6903	0.2064	−0.0332	0.042*
C18	0.54501 (15)	0.24393 (7)	0.03623 (7)	0.0369 (3)
H18	0.5017	0.2803	0.0090	0.044*
C19	0.49628 (15)	0.23398 (7)	0.10137 (7)	0.0364 (3)
H19	0.4194	0.2639	0.1185	0.044*
C20	0.55835 (14)	0.18084 (6)	0.14184 (6)	0.0322 (3)
H20	0.5234	0.1741	0.1861	0.039*
H1	0.7554 (18)	0.0673 (10)	0.3395 (8)	0.048 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0784 (7)	0.0231 (4)	0.0230 (4)	0.0114 (4)	0.0030 (4)	−0.0021 (3)
N1	0.0387 (6)	0.0230 (5)	0.0204 (5)	0.0014 (4)	−0.0011 (4)	−0.0008 (3)
N2	0.0302 (5)	0.0259 (5)	0.0226 (5)	−0.0004 (4)	−0.0001 (4)	−0.0016 (4)
N3	0.0610 (7)	0.0201 (5)	0.0197 (5)	−0.0004 (4)	−0.0005 (4)	0.0003 (4)
C1	0.0472 (7)	0.0215 (5)	0.0210 (5)	−0.0018 (5)	−0.0007 (5)	−0.0012 (4)
C2	0.0376 (6)	0.0207 (5)	0.0216 (6)	−0.0036 (4)	−0.0013 (4)	−0.0009 (4)
C3	0.0266 (6)	0.0253 (5)	0.0225 (5)	−0.0039 (4)	−0.0013 (4)	−0.0006 (4)
C4	0.0315 (6)	0.0358 (6)	0.0267 (6)	0.0052 (5)	0.0025 (5)	0.0019 (5)
C5	0.0341 (6)	0.0221 (5)	0.0217 (5)	−0.0075 (4)	−0.0014 (4)	−0.0011 (4)
C6	0.0268 (6)	0.0264 (5)	0.0204 (5)	−0.0019 (4)	0.0012 (4)	0.0017 (4)
C7	0.0273 (6)	0.0524 (8)	0.0235 (5)	−0.0080 (5)	−0.0008 (5)	0.0058 (5)
C8	0.0305 (7)	0.0732 (10)	0.0325 (7)	0.0154 (6)	0.0044 (5)	0.0204 (7)
C9	0.0528 (9)	0.0464 (8)	0.0403 (7)	0.0257 (7)	0.0173 (6)	0.0171 (6)
C10	0.0528 (8)	0.0255 (6)	0.0353 (6)	0.0064 (5)	0.0129 (6)	0.0016 (5)
C11	0.0297 (6)	0.0241 (5)	0.0269 (6)	−0.0004 (4)	0.0018 (4)	−0.0016 (4)
C12	0.0509 (8)	0.0256 (6)	0.0191 (5)	−0.0011 (5)	0.0004 (5)	0.0013 (4)

C13	0.0500 (8)	0.0613 (9)	0.0223 (6)	−0.0220 (7)	0.0007 (5)	−0.0058 (6)
C14	0.0435 (8)	0.0431 (7)	0.0268 (6)	0.0033 (6)	0.0029 (5)	0.0014 (5)
C15	0.0332 (6)	0.0225 (5)	0.0249 (5)	−0.0050 (4)	−0.0058 (4)	−0.0005 (4)
C16	0.0289 (6)	0.0309 (6)	0.0273 (6)	−0.0038 (4)	−0.0025 (4)	0.0033 (5)
C17	0.0336 (7)	0.0391 (7)	0.0310 (6)	−0.0064 (5)	−0.0050 (5)	0.0102 (5)
C18	0.0370 (7)	0.0328 (6)	0.0410 (7)	−0.0004 (5)	−0.0110 (5)	0.0084 (5)
C19	0.0372 (7)	0.0323 (6)	0.0397 (7)	0.0035 (5)	−0.0076 (5)	−0.0035 (5)
C20	0.0394 (7)	0.0293 (6)	0.0280 (6)	−0.0006 (5)	−0.0035 (5)	−0.0033 (5)

Geometric parameters (Å, º)

O1—C1	1.2525 (15)	C9—H9	0.95
N1—C1	1.3852 (15)	C10—C11	1.3921 (17)
N1—N2	1.4029 (13)	C10—H10	0.95
N1—C15	1.4158 (14)	C11—H11	0.95
N2—C3	1.3130 (15)	C12—C13	1.4869 (17)
N3—C5	1.3260 (15)	C12—C14	1.4885 (18)
N3—C12	1.4382 (15)	C12—H12	1.00
N3—H1	0.917 (18)	C13—C14	1.482 (2)
C1—C2	1.4417 (16)	C13—H13A	0.99
C2—C5	1.4066 (15)	C13—H13B	0.99
C2—C3	1.4345 (15)	C14—H14A	0.99
C3—C4	1.4935 (16)	C14—H14B	0.99
C4—H4A	0.98	C15—C20	1.3978 (17)
C4—H4B	0.98	C15—C16	1.3984 (17)
C4—H4C	0.98	C16—C17	1.3904 (17)
C5—C6	1.4868 (16)	C16—H16	0.95
C6—C11	1.3940 (16)	C17—C18	1.3854 (19)
C6—C7	1.4001 (16)	C17—H17	0.95
C7—C8	1.388 (2)	C18—C19	1.3898 (19)
C7—H7	0.95	C18—H18	0.95
C8—C9	1.383 (2)	C19—C20	1.3912 (17)
C8—H8	0.95	C19—H19	0.95
C9—C10	1.387 (2)	C20—H20	0.95
C1—N1—N2	111.86 (9)	C10—C11—C6	120.38 (12)
C1—N1—C15	128.83 (10)	C10—C11—H11	119.8
N2—N1—C15	119.26 (9)	C6—C11—H11	119.8
C3—N2—N1	106.35 (9)	N3—C12—C13	118.30 (11)
C5—N3—C12	127.99 (10)	N3—C12—C14	116.99 (11)
C5—N3—H1	113.9 (10)	C13—C12—C14	59.76 (9)
C12—N3—H1	117.6 (10)	N3—C12—H12	116.6
O1—C1—N1	126.06 (11)	C13—C12—H12	116.6
O1—C1—C2	129.34 (11)	C14—C12—H12	116.6
N1—C1—C2	104.59 (10)	C14—C13—C12	60.17 (9)
C5—C2—C3	133.14 (11)	C14—C13—H13A	117.8
C5—C2—C1	121.37 (10)	C12—C13—H13A	117.8
C3—C2—C1	105.47 (9)	C14—C13—H13B	117.8

N2—C3—C2	111.64 (10)	C12—C13—H13B	117.8
N2—C3—C4	118.76 (10)	H13A—C13—H13B	114.9
C2—C3—C4	129.60 (10)	C13—C14—C12	60.07 (9)
C3—C4—H4A	109.5	C13—C14—H14A	117.8
C3—C4—H4B	109.5	C12—C14—H14A	117.8
H4A—C4—H4B	109.5	C13—C14—H14B	117.8
C3—C4—H4C	109.5	C12—C14—H14B	117.8
H4A—C4—H4C	109.5	H14A—C14—H14B	114.9
H4B—C4—H4C	109.5	C20—C15—C16	120.12 (11)
N3—C5—C2	117.73 (11)	C20—C15—N1	120.92 (10)
N3—C5—C6	119.45 (10)	C16—C15—N1	118.95 (11)
C2—C5—C6	122.76 (10)	C17—C16—C15	119.52 (12)
C11—C6—C7	119.31 (11)	C17—C16—H16	120.2
C11—C6—C5	119.47 (10)	C15—C16—H16	120.2
C7—C6—C5	121.21 (10)	C18—C17—C16	120.84 (12)
C8—C7—C6	119.90 (12)	C18—C17—H17	119.6
C8—C7—H7	120.0	C16—C17—H17	119.6
C6—C7—H7	120.0	C17—C18—C19	119.29 (11)
C9—C8—C7	120.41 (13)	C17—C18—H18	120.4
C9—C8—H8	119.8	C19—C18—H18	120.4
C7—C8—H8	119.8	C18—C19—C20	121.04 (12)
C8—C9—C10	120.22 (12)	C18—C19—H19	119.5
C8—C9—H9	119.9	C20—C19—H19	119.5
C10—C9—H9	119.9	C19—C20—C15	119.19 (12)
C9—C10—C11	119.77 (13)	C19—C20—H20	120.4
C9—C10—H10	120.1	C15—C20—H20	120.4
C11—C10—H10	120.1		

C1—N1—N2—C3	2.41 (13)	C2—C5—C6—C7	122.97 (13)
C15—N1—N2—C3	179.94 (10)	C11—C6—C7—C8	0.19 (17)
N2—N1—C1—O1	176.20 (12)	C5—C6—C7—C8	179.28 (11)
C15—N1—C1—O1	−1.0 (2)	C6—C7—C8—C9	−0.20 (19)
N2—N1—C1—C2	−3.16 (13)	C7—C8—C9—C10	−0.2 (2)
C15—N1—C1—C2	179.61 (11)	C8—C9—C10—C11	0.60 (19)
O1—C1—C2—C5	1.6 (2)	C9—C10—C11—C6	−0.61 (18)
N1—C1—C2—C5	−179.04 (10)	C7—C6—C11—C10	0.21 (17)
O1—C1—C2—C3	−176.70 (13)	C5—C6—C11—C10	−178.89 (11)
N1—C1—C2—C3	2.63 (13)	C5—N3—C12—C13	135.28 (14)
N1—N2—C3—C2	−0.57 (13)	C5—N3—C12—C14	−156.29 (13)
N1—N2—C3—C4	179.70 (10)	N3—C12—C13—C14	106.42 (13)
C5—C2—C3—N2	−179.36 (12)	N3—C12—C14—C13	−108.60 (13)
C1—C2—C3—N2	−1.32 (13)	C1—N1—C15—C20	−19.43 (18)
C5—C2—C3—C4	0.3 (2)	N2—N1—C15—C20	163.52 (10)
C1—C2—C3—C4	178.36 (11)	C1—N1—C15—C16	161.44 (12)
C12—N3—C5—C2	170.89 (12)	N2—N1—C15—C16	−15.61 (15)
C12—N3—C5—C6	−6.43 (19)	C20—C15—C16—C17	−0.12 (17)
C3—C2—C5—N3	170.75 (13)	N1—C15—C16—C17	179.02 (10)
C1—C2—C5—N3	−7.04 (17)	C15—C16—C17—C18	0.82 (18)

C3—C2—C5—C6	−12.0 (2)	C16—C17—C18—C19	−0.70 (19)
C1—C2—C5—C6	170.18 (11)	C17—C18—C19—C20	−0.11 (19)
N3—C5—C6—C11	119.23 (13)	C18—C19—C20—C15	0.80 (19)
C2—C5—C6—C11	−57.95 (16)	C16—C15—C20—C19	−0.68 (17)
N3—C5—C6—C7	−59.85 (16)	N1—C15—C20—C19	−179.80 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1···O1	0.92 (2)	1.88 (2)	2.6726 (15)	143 (2)
C20—H20···O1	0.95	2.36	2.9453 (16)	120
C10—H10···O1^{i}	0.95	2.30	3.1809 (17)	154

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