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1,2-Diphenyl-2-(*m*-tolylamino)ethanone[1]

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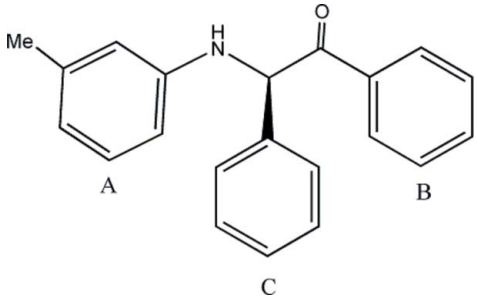
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.137; data-to-parameter ratio = 13.3.

The title compound, $C_{21}H_{19}NO$, belongs to the family of α-aminoketones. The structure contains three benzene rings, two of which [the phenyl ring in the 1-position (*B*) and the methylaniline ring (*A*)] are nearly coplanar [dihedral angle = 5.4 (1)°], whereas the phenyl ring in the 2-position (*C*) is nearly normal to them [dihedral angles = 81.8 (1) and 87.0 (1)° for *A*/*C* and *B*/*C*, respectively]. The conformation of the N—H bond is *syn* to the C=O bond, favouring the formation of a centrosymmetric dimer of molecules in the crystal structure. The molecular packing is consolidated by this N—H···O hydrogen-bonding network.

Related literature

For the structure of alpha-aminoketones, see: Batsanov *et al.* (2006). For the crystal structure of 1,2-diphenyl-2-(*p*-tolylamino)ethanone, see: Au & Tafeenko (1986).



Experimental

Crystal data

$C_{21}H_{19}NO$
M_r = 301.37
Triclinic, $P\overline{1}$
a = 6.0510 (3) Å
b = 11.5745 (4) Å
c = 12.9458 (7) Å
α = 112.542 (5)°
β = 97.396 (4)°
γ = 99.960 (4)°
V = 805.62 (8) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 293 K
0.34 × 0.12 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur Gemini S diffractometer
Absorption correction: refined from ΔF [cubic fit to sin(theta)/lambda - 24 parameters; Parkin *et al.* (1995)]
T_{min} = 0.919, T_{max} = 0.960
8027 measured reflections
2833 independent reflections
2174 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.137
S = 1.09
2833 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H22···O1^{i}	0.859 (17)	2.660 (17)	3.3913 (17)	143.8 (15)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

Financial support by the Agencia Española de Cooperación Internacional y Desarrollo (AECID), FEDER funding, the Spanish MICINN (MAT2006–01997 and Factoría de Cristalización Consolider Ingenio 2010) and the Gobierno del Principado de Asturias (PCTI) is acknowledged. Special acknowledgements go to Professor José Manuel Concellón for his support and scientific advice.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2170).

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[1] Dedicated to the memory of Professor José Manuel Concellón.

supporting information

Acta Cryst. (2010). E**66**, o1107 [https://doi.org/10.1107/S1600536810013371]

1,2-Diphenyl-2-(*m*-tolylamino)ethanone

Rafael Mendoza Meroño, Felix Nápoles Esculary, Laura Menéndez Taboada and Santiago García-Granda

S1. Comment

The structure of various members of the alpha-aminoketone family have been extensively studied (Batsanov *et al.*, 2006). These compounds can be used as intermediates to synthesize other biologically active compounds like thio-semicarbazones. Alpha-aminoketones also exhibit biological activity but are less active than the thiosemicarbazones. They are generally synthesised by the reaction of an alpha-hydroxiketone with an amine.

The molecular structure of the title molecule is illustrated in Fig. 1. According to the dihedral angles between the benzene rings planes, two benzene rings are nearly coplanar whereas the central ring is almost normal to them (5.3 (1)° for A/B, 81.8 (1)° for A/C and 87.0 (1)° for B/C). Comparing these values with those in the similar structure where the methyl subtitutent is in the para position (5.1° for A/B, 86.28° for A/C and 84.19° for B/C), there are no noticeable differences (Au & Tafeenko, 1986).

In the crystal structure, the molecular packing is made up of a network of weak hydrogen-bonding interactions (Fig. 2 & Table 1), favouring the formation of centrosymmetric dimers. Such conformations bring the C═O and N—H bonds into a syn orientation. The intermolecular distance between the centroids of the parallel benzene rings is ca. 3.77 Å. This value suggests the absence of any relevant π-stacking interactions.

S2. Experimental

0.0235 mol benzoin, 0.0235 mol 3-methylaniline and 0.0235 mol boric acid were added to 10 ml of ethyleneglycol. The mixture was heated to reflux for 1 h, then 15 ml of ethanol were added and the mixture cooled to RT. The reaction was followed using TLC. The yellow precipitate obtained was washed with cold water and ethanol (yield 85%). Yellow needle-like crystals, suitable for x-ray diffraction analysis, were obtained after a week by slow evaporation of a solution in ethanol.

S3. Refinement

The NH H-atom was located in difference electron-density map and was freely refined: N-H = 0.858 (17) Å. The C-bound H-atoms were included in calculated positions and treated as riding atoms: C-H = 0.98 Å, 0.93 Å and 0.96 Å for tertiary CH, aromatic CH and CH_3 H-atoms, respectively, with $U_{iso}(H) = k \times U_{eq}(C)$, where k = 1.2 for CH H-atoms, and 1.5 for CH_3 H-atoms.

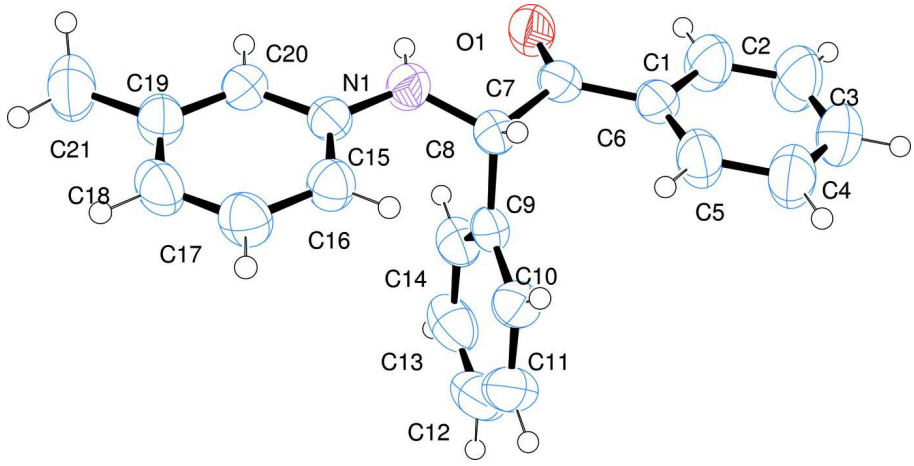

Figure 1

A view of the molecular structure of the title molecule showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

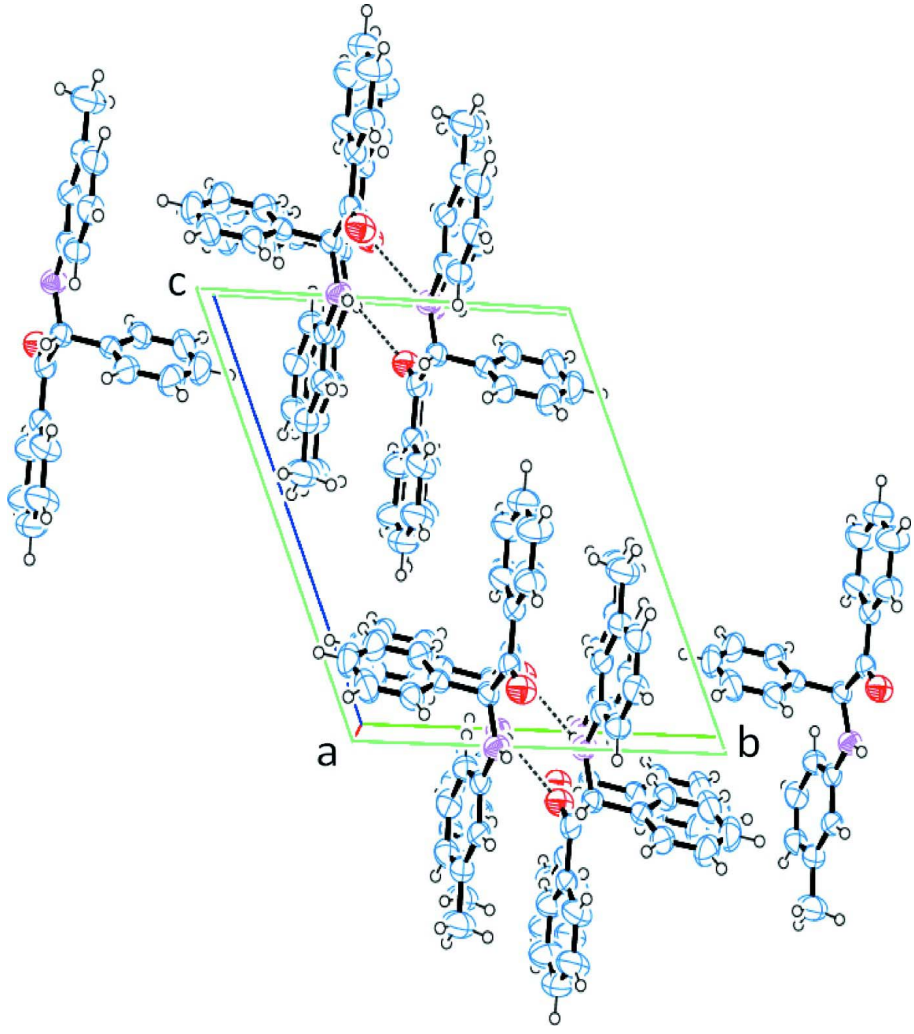

Figure 2

A view along the a-axis of the crystal packing of the title compound. Hydrogen bonds are indicated by dashed lines (see Table 1 for details).

1,2-Diphenyl-2-(*m*-tolylamino)ethanone

Crystal data

$C_{21}H_{19}NO$
$M_r = 301.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.0510\ (3)$ Å
$b = 11.5745\ (4)$ Å
$c = 12.9458\ (7)$ Å
$\alpha = 112.542\ (5)°$
$\beta = 97.396\ (4)°$
$\gamma = 99.960\ (4)°$
$V = 805.62\ (8)$ Å^3

$Z = 2$
$F(000) = 320$
$D_x = 1.242$ Mg m^{-3}
Melting point: 385.14 K
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 4346 reflections
$\theta = 3.8–66.7°$
$\mu = 0.59$ mm^{-1}
$T = 293$ K
Needle, yellow
0.34 × 0.12 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur Gemini S diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0827 pixels mm^{-1}
ω scans
Absorption correction: part of the refinement model (ΔF)
[cubic fit to sin(theta)/lambda - 24 parameters; Parkin *et al.* (1995)]
T_{min} = 0.919, T_{max} = 0.960
8027 measured reflections
2833 independent reflections
2174 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 66.7°, θ_{min} = 3.8°
h = −6→7
k = −10→13
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.137
S = 1.09
2833 reflections
213 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
$w = 1/[\sigma^2(F_o^2) + (0.0863P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0041 (11)

Special details

Experimental. 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 > 2sigma(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.

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.52659 (18)	0.50924 (11)	0.14596 (9)	0.0662 (4)
N1	0.1300 (2)	0.38301 (13)	0.00199 (11)	0.0529 (4)
C1	0.6200 (3)	0.63202 (19)	0.38272 (15)	0.0714 (6)
C2	0.6620 (4)	0.6946 (2)	0.50033 (17)	0.0880 (8)
C3	0.4898 (4)	0.6891 (2)	0.55688 (17)	0.0847 (8)
C4	0.2717 (4)	0.6232 (2)	0.49658 (17)	0.0863 (8)
C5	0.2260 (3)	0.56261 (18)	0.37817 (15)	0.0707 (6)
C6	0.4006 (3)	0.56467 (14)	0.31949 (13)	0.0497 (5)
C7	0.3671 (2)	0.49865 (14)	0.19224 (13)	0.0480 (5)
C8	0.1322 (2)	0.41085 (13)	0.12058 (12)	0.0452 (4)

C9	0.0958 (2)	0.28933 (13)	0.14383 (11)	0.0454 (4)
C10	−0.0802 (3)	0.25707 (16)	0.19337 (14)	0.0586 (5)
C11	−0.1102 (3)	0.14576 (19)	0.21171 (17)	0.0757 (7)
C12	0.0364 (4)	0.06604 (19)	0.18093 (18)	0.0819 (7)
C13	0.2102 (3)	0.09623 (17)	0.13051 (17)	0.0742 (7)
C14	0.2411 (3)	0.20731 (15)	0.11226 (14)	0.0574 (5)
C15	−0.0560 (2)	0.30252 (13)	−0.08485 (12)	0.0452 (4)
C16	−0.2728 (3)	0.26933 (15)	−0.06433 (14)	0.0540 (5)
C17	−0.4522 (3)	0.18600 (16)	−0.15360 (14)	0.0597 (6)
C18	−0.4218 (3)	0.13398 (16)	−0.26408 (15)	0.0633 (6)
C19	−0.2086 (3)	0.16684 (16)	−0.28761 (14)	0.0578 (5)
C20	−0.0286 (3)	0.25155 (14)	−0.19799 (13)	0.0510 (5)
C21	−0.1709 (4)	0.1084 (2)	−0.40766 (16)	0.0896 (8)
H1	0.74080	0.63510	0.34540	0.0860*
H2	0.81000	0.74100	0.54130	0.1060*
H3	0.52000	0.73000	0.63640	0.1020*
H4	0.15330	0.61900	0.53520	0.1040*
H5	0.07610	0.52010	0.33780	0.0850*
H8	0.01180	0.45580	0.14410	0.0540*
H10	−0.17960	0.31080	0.21460	0.0700*
H11	−0.22970	0.12480	0.24490	0.0910*
H12	0.01770	−0.00810	0.19430	0.0980*
H13	0.30790	0.04160	0.10850	0.0890*
H14	0.36020	0.22730	0.07850	0.0690*
H16	−0.29700	0.30340	0.00980	0.0650*
H17	−0.59640	0.16470	−0.13870	0.0720*
H18	−0.54410	0.07680	−0.32300	0.0760*
H20	0.11400	0.27500	−0.21360	0.0610*
H21A	−0.31250	0.05270	−0.45850	0.1340*
H21B	−0.05730	0.05940	−0.40990	0.1340*
H21C	−0.11860	0.17570	−0.43120	0.1340*
H22	0.262 (3)	0.4037 (17)	−0.0130 (15)	0.062 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0533 (7)	0.0727 (8)	0.0548 (7)	−0.0058 (6)	0.0118 (5)	0.0167 (6)
N1	0.0473 (7)	0.0602 (8)	0.0438 (7)	0.0004 (6)	0.0051 (6)	0.0207 (6)
C1	0.0584 (10)	0.0864 (13)	0.0546 (10)	0.0023 (9)	0.0014 (8)	0.0235 (9)
C2	0.0714 (12)	0.1108 (17)	0.0540 (11)	−0.0008 (11)	−0.0099 (10)	0.0220 (11)
C3	0.1014 (16)	0.0868 (14)	0.0459 (10)	0.0088 (12)	0.0028 (10)	0.0164 (10)
C4	0.0896 (14)	0.0886 (14)	0.0559 (11)	0.0028 (12)	0.0230 (10)	0.0096 (10)
C5	0.0637 (10)	0.0698 (11)	0.0536 (10)	0.0000 (9)	0.0116 (8)	0.0066 (9)
C6	0.0528 (8)	0.0442 (8)	0.0467 (8)	0.0051 (6)	0.0043 (7)	0.0180 (7)
C7	0.0482 (8)	0.0424 (8)	0.0495 (9)	0.0043 (6)	0.0072 (7)	0.0189 (7)
C8	0.0449 (7)	0.0435 (7)	0.0419 (8)	0.0067 (6)	0.0063 (6)	0.0148 (6)
C9	0.0449 (7)	0.0429 (8)	0.0373 (7)	0.0024 (6)	−0.0008 (6)	0.0114 (6)
C10	0.0547 (9)	0.0597 (9)	0.0553 (10)	0.0018 (7)	0.0080 (7)	0.0239 (8)

C11	0.0766 (12)	0.0717 (12)	0.0716 (13)	−0.0114 (10)	0.0029 (10)	0.0387 (10)
C12	0.0939 (14)	0.0551 (10)	0.0810 (14)	−0.0101 (10)	−0.0212 (11)	0.0360 (10)
C13	0.0802 (12)	0.0503 (10)	0.0758 (12)	0.0156 (9)	−0.0107 (10)	0.0177 (9)
C14	0.0583 (9)	0.0513 (9)	0.0527 (9)	0.0100 (7)	0.0032 (7)	0.0152 (7)
C15	0.0466 (8)	0.0422 (7)	0.0455 (8)	0.0090 (6)	0.0030 (6)	0.0199 (6)
C16	0.0487 (8)	0.0590 (9)	0.0502 (9)	0.0106 (7)	0.0078 (7)	0.0202 (7)
C17	0.0452 (8)	0.0632 (10)	0.0640 (11)	0.0057 (7)	0.0031 (7)	0.0253 (9)
C18	0.0583 (10)	0.0554 (9)	0.0591 (10)	0.0013 (8)	−0.0093 (8)	0.0178 (8)
C19	0.0662 (10)	0.0531 (9)	0.0479 (9)	0.0111 (7)	0.0037 (7)	0.0187 (7)
C20	0.0531 (8)	0.0517 (8)	0.0481 (9)	0.0092 (7)	0.0085 (7)	0.0230 (7)
C21	0.0968 (15)	0.0917 (15)	0.0515 (11)	0.0013 (12)	0.0072 (10)	0.0113 (10)

Geometric parameters (Å, º)

O1—C7	1.2123 (18)	C17—C18	1.374 (2)
N1—C8	1.4405 (19)	C18—C19	1.386 (3)
N1—C15	1.3810 (19)	C19—C20	1.388 (2)
N1—H22	0.862 (19)	C19—C21	1.505 (3)
C1—C6	1.383 (3)	C1—H1	0.9300
C1—C2	1.378 (3)	C2—H2	0.9300
C2—C3	1.355 (3)	C3—H3	0.9300
C3—C4	1.365 (3)	C4—H4	0.9300
C4—C5	1.385 (3)	C5—H5	0.9300
C5—C6	1.381 (3)	C8—H8	0.9800
C6—C7	1.495 (2)	C10—H10	0.9300
C7—C8	1.534 (2)	C11—H11	0.9300
C8—C9	1.534 (2)	C12—H12	0.9300
C9—C14	1.388 (2)	C13—H13	0.9300
C9—C10	1.381 (2)	C14—H14	0.9300
C10—C11	1.383 (3)	C16—H16	0.9300
C11—C12	1.375 (3)	C17—H17	0.9300
C12—C13	1.371 (3)	C18—H18	0.9300
C13—C14	1.380 (3)	C20—H20	0.9300
C15—C20	1.398 (2)	C21—H21A	0.9600
C15—C16	1.390 (2)	C21—H21B	0.9600
C16—C17	1.380 (2)	C21—H21C	0.9600
C8—N1—C15	122.36 (13)	C6—C1—H1	120.00
C8—N1—H22	115.3 (12)	C1—C2—H2	120.00
C15—N1—H22	120.7 (12)	C3—C2—H2	120.00
C2—C1—C6	120.89 (18)	C2—C3—H3	120.00
C1—C2—C3	120.6 (2)	C4—C3—H3	120.00
C2—C3—C4	119.66 (19)	C3—C4—H4	120.00
C3—C4—C5	120.3 (2)	C5—C4—H4	120.00
C4—C5—C6	120.71 (18)	C4—C5—H5	120.00
C1—C6—C7	118.15 (15)	C6—C5—H5	120.00
C1—C6—C5	117.76 (15)	N1—C8—H8	109.00
C5—C6—C7	124.08 (15)	C7—C8—H8	109.00

O1—C7—C8	119.84 (13)	C9—C8—H8	109.00
O1—C7—C6	120.53 (14)	C9—C10—H10	120.00
C6—C7—C8	119.55 (13)	C11—C10—H10	120.00
N1—C8—C9	112.77 (13)	C10—C11—H11	120.00
C7—C8—C9	107.94 (12)	C12—C11—H11	120.00
N1—C8—C7	108.31 (12)	C11—C12—H12	120.00
C10—C9—C14	118.55 (16)	C13—C12—H12	120.00
C8—C9—C10	122.18 (13)	C12—C13—H13	120.00
C8—C9—C14	119.26 (13)	C14—C13—H13	120.00
C9—C10—C11	120.72 (17)	C9—C14—H14	120.00
C10—C11—C12	120.06 (19)	C13—C14—H14	120.00
C11—C12—C13	119.8 (2)	C15—C16—H16	120.00
C12—C13—C14	120.36 (19)	C17—C16—H16	120.00
C9—C14—C13	120.52 (16)	C16—C17—H17	119.00
C16—C15—C20	117.97 (14)	C18—C17—H17	119.00
N1—C15—C16	122.36 (13)	C17—C18—H18	120.00
N1—C15—C20	119.68 (13)	C19—C18—H18	120.00
C15—C16—C17	120.25 (15)	C15—C20—H20	119.00
C16—C17—C18	121.25 (17)	C19—C20—H20	119.00
C17—C18—C19	119.89 (17)	C19—C21—H21A	109.00
C18—C19—C20	118.88 (16)	C19—C21—H21B	109.00
C18—C19—C21	120.58 (17)	C19—C21—H21C	110.00
C20—C19—C21	120.51 (17)	H21A—C21—H21B	109.00
C15—C20—C19	121.73 (16)	H21A—C21—H21C	110.00
C2—C1—H1	120.00	H21B—C21—H21C	109.00

C15—N1—C8—C7	177.87 (14)	N1—C8—C9—C14	55.51 (17)
C15—N1—C8—C9	58.48 (18)	C7—C8—C9—C10	117.19 (14)
C8—N1—C15—C16	17.0 (2)	C7—C8—C9—C14	−64.09 (16)
C8—N1—C15—C20	−162.92 (15)	C8—C9—C10—C11	179.09 (15)
C6—C1—C2—C3	1.5 (4)	C14—C9—C10—C11	0.4 (2)
C2—C1—C6—C5	0.1 (3)	C8—C9—C14—C13	−178.99 (15)
C2—C1—C6—C7	−179.82 (19)	C10—C9—C14—C13	−0.2 (2)
C1—C2—C3—C4	−1.4 (4)	C9—C10—C11—C12	0.2 (3)
C2—C3—C4—C5	−0.3 (4)	C10—C11—C12—C13	−1.0 (3)
C3—C4—C5—C6	1.9 (4)	C11—C12—C13—C14	1.1 (3)
C4—C5—C6—C1	−1.8 (3)	C12—C13—C14—C9	−0.5 (3)
C4—C5—C6—C7	178.17 (19)	N1—C15—C16—C17	−178.40 (17)
C1—C6—C7—O1	−3.4 (3)	C20—C15—C16—C17	1.5 (3)
C1—C6—C7—C8	173.22 (17)	N1—C15—C20—C19	177.80 (17)
C5—C6—C7—O1	176.72 (18)	C16—C15—C20—C19	−2.2 (3)
C5—C6—C7—C8	−6.7 (3)	C15—C16—C17—C18	0.1 (3)
O1—C7—C8—N1	−16.0 (2)	C16—C17—C18—C19	−1.1 (3)
O1—C7—C8—C9	106.37 (17)	C17—C18—C19—C20	0.5 (3)
C6—C7—C8—N1	167.39 (14)	C17—C18—C19—C21	178.57 (19)
C6—C7—C8—C9	−70.22 (17)	C18—C19—C20—C15	1.1 (3)
N1—C8—C9—C10	−123.21 (14)	C21—C19—C20—C15	−176.92 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H22···O1^{i}	0.859 (17)	2.660 (17)	3.3913 (17)	143.8 (15)

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