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2-Amino-5-nitrophenyl 2-chlorophenyl ketone

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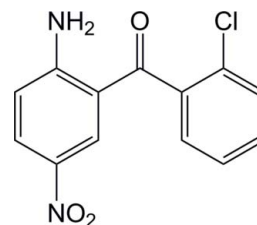
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Key indicators: single-crystal X-ray study; $T = 110$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 24.0.

In the title compound, $\text{C}_{13}\text{H}_9\text{ClN}_2\text{O}_3$, an intramolecular hydrogen bond between the carbonyl O and an amine H atom from the 2-aminobenzoyl group stabilizes the molecule, keeping these two groups nearly in the same plane [dihedral angle $14.6(6)^\circ$]. The dihedral angle between the mean planes of the planar 2-aminobenzoyl and 2-chlorobenzoyl groups is $73.8(6)^\circ$. The crystal packing is stabilized by a collection of intermediate hydrogen-bonding interactions which forms an infinite $\text{N}-\text{H}\cdots\text{O}\cdots\text{H}-\text{N}-\text{H}\cdots\text{O}$ hydrogen-bonded chain along the c axis in concert with weak $\text{N}-\text{H}\cdots\text{Cl}$ interactions in the same direction, producing a two-dimensional intermolecular bonding network parallel to (001). Additional weak $\text{C}-\text{Cl}\cdots\text{Cg}$ [$\text{Cl}\cdots\text{Cg} = 3.858(3)$ Å] and $\text{N}-\text{O}\cdots\text{Cg}$ [$\text{O}\cdots\text{Cg} = 3.574(1)$ and $3.868(6)$ Å] π -ring interactions provide added support to the crystal stability. A MOPAC computational calculation gives support to these observations.

Related literature

For related structures, see: Cox *et al.* (1997, 2008); Harrison *et al.* (2005); Malathy Sony *et al.* (2005); Prasanna & Guru Row (2000); Xing *et al.* (2005). For background to benzophenone derivatives, see: Colpaert *et al.* (2004); Deleu *et al.* (1992); Duncan *et al.* (2004); Evans *et al.* (1987); Ottosen *et al.* (2003); Revesz *et al.* (2004); Sieroń *et al.* (2004); Wiesner *et al.* (2002). For a description of the Cambridge Structural Database, see: Allen (2002). For MOPAC AM1 computational calculations, see: Schmidt & Polik (2007).



Experimental

Crystal data

 $\text{C}_{13}\text{H}_9\text{ClN}_2\text{O}_3$ $M_r = 276.67$ Monoclinic, $P2_1/c$ $a = 10.6120(3)$ Å $b = 11.3314(3)$ Å $c = 10.8456(3)$ Å $\beta = 108.399(3)^\circ$ $V = 1237.50(6)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.31$ mm⁻¹ $T = 110$ K $0.47 \times 0.36 \times 0.28$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer

Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007) $T_{\min} = 0.868$, $T_{\max} = 0.916$

8758 measured reflections

4131 independent reflections

3069 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.021$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$ $wR(F^2) = 0.099$ $S = 1.04$

4131 reflections

172 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O3}^i$	0.88	2.22	3.0733 (12)	164
$\text{N1}-\text{H1B}\cdots\text{O3}$	0.88	2.07	2.7176 (12)	130
$\text{N1}-\text{H1B}\cdots\text{Cl}^{\text{ii}}$	0.88	2.71	3.4848 (10)	148
$\text{Cl1}-\text{H13A}\cdots\text{O2}^{\text{iii}}$	0.95	2.46	3.1862 (14)	133

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2123).

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supporting information

Acta Cryst. (2009). E65, o1908–o1909 [doi:10.1107/S160053680902755X]

2-Amino-5-nitrophenyl 2-chlorophenyl ketone

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S1. Comment

Benzophenone derivatives are widely used in sunscreen lotions for UVA protection (Deleu *et al.*, 1992). Benzophenone and related analogues have been reported to act as antiallergic, anti-inflammatory, antiasthmatic, antimalarial, antimicrobial and antianaphylactic agents (Evans *et al.*, 1987; Wiesner *et al.*, 2002; Sieroń *et al.*, 2004). The competence of benzophenones as chemotherapeutic agents, especially as inhibitors of HIV-1 reverse transcriptase RT, cancer and inflammation, is well established and their chemistry has been studied extensively (Revesz *et al.*, 2004). Phenylmethanones are a class of compounds having many pharmacological properties. 4-Aminobenzophenones have high anti-inflammatory activity (Ottosen *et al.*, 2003), a benzophenyl cyano derivative acts as a vasorelaxant (Duncan *et al.*, 2004) and the piperidiny derivative produces analgesia (Colpaert *et al.*, 2004). The crystal structures of some related compounds, viz., N-(2-benzoyl-4-chlorophenyl)-2-chloroacetamide (Malathy Sony *et al.*, 2005), 2-chloroacetamido-5-chlorobenzophenone and 2-chloroacetamido-5-chloro-2'-fluorobenzophenone (Prasanna & Guru Row, 2000), 2-methylamino-5-chlorobenzophenone (Cox *et al.*, 1997), 2-amino-2'-chloro-5-methylbenzophenone (Xing *et al.*, 2005) and 3-chloro-4-hydroxy-4'-methylbenzophenone (Harrison *et al.*, 2005) have been reported. Over 450 crystal structures of benzophenone derivatives in the Cambridge Structural Database (CSD, Version 5.26; Allen, 2002) highlight the importance of structural studies on such pharmaceutically useful compounds. The title compound, C₁₃H₉ClN₂O₃, is an intermediate in the synthesis of certain anxiolytic, anticonvulsant and sedative drugs. The title compound is also a starting material for the synthesis of diazepam and other benzodiazepines. In view of the importance of the title compound, the present paper describes its crystal structure.

The title compound, C₁₃H₉ClN₂O₃, crystallizes with one molecule in the asymmetric unit with $Z = 4$. An intramolecular hydrogen bond between the carbonyl oxygen (O3) and an amine hydrogen atom (H1B) from the 2-amino-5-nitrobenzoyl group keeps these two groups nearly in the same plane relative to each other (Fig. 1). The dihedral angle between the mean planes of the carbonyl group (-C6-C7(O3)-C8-) and the mean planes of the 2-amino and 2'-chlorobenzoyl planar groups is 14.6 (6)° and 66.2 (9)°, respectively. The C5-C6-C7-O3 torsion angle (164.45 (11)°) supports this observation. The nitro group is twisted slightly away from the plane of the 2-amino-benzoyl group (O2-N2-C4-C3 torsion angle = 178.46 (11)°). The dihedral angle between the mean planes of the 2-aminobenzoyl and 2'-chlorobenzoyl planar groups is 73.8 (6)°. This value lies between the large twist angle of 83.72 (6)° as seen in 2-amino and 2'-chlorobenzophenone, C₁₃H₉Cl₂NO, (Cox *et al.*, 2008) and 64.66 (8)° observed in 4-chloro-4'-hydroxybenzophenone, C₁₃H₉ClO₂ (Cox *et al.*, 2008). Crystal packing is supported by a collection of intermediate N1-H1A...O3, N1-H1B...O3, C13-H13A...O2 hydrogen bonds and weak N1-H1B...Cl intermolecular interactions (see Table 1) which produces an infinite, two-dimensional N-H...O...H-N-H...O bonding network parallel to the (001) plane of the unit cell (Fig. 2). Additional weak C9-Cl...Cg(2) [Cl...Cg(2) = 3.858 (3)Å], N2-O1...Cg(2) [O1...Cg(2) = 3.574 (1)Å] and N2-O2...Cg(1) [O2...Cg(1) = 3.868 (6)Å] π -ring interactions (-x, 1-y, -x; x, 1/2-y, 1/2+z; 1-x, 1-y, 1-z; Cg(1) = C1-C6 and Cg(2) = C8-C13 centroids, respectively) collectively provide added support to crystal stability.

After a MOPAC AM1 computational calculation (Schmidt & Polik, 2007), the nitro group now lies in the plane of the 2-aminobenzoyl group. The dihedral angle between the mean planes of the 2-aminobenzoyl and 2'-chlorobenzoyl planar groups becomes $88.6(1)^\circ$ while the dihedral angle between the mean planes of the carbonyl group (-C6-C7(O3)-C8-) and the mean planes of the 2-amino and 2'-chlorobenzoyl planar groups becomes $19.7(3)^\circ$ and $81.7(1)^\circ$, respectively. This supports the observation of a collective action of intermediate N-H \cdots O, C-H \cdots O hydrogen bonds, weak N-H \cdots Cl intermolecular interactions and weak C-Cl \cdots Cg, N-O \cdots Cg π -ring interactions influencing crystal packing stability.

S2. Experimental

The title compound was obtained as a gift sample from *R. L. Fine Chem*, Bangalore, India. The compound was used without further purification. Pale yellow crystals (m.p. 378–380 K) were obtained by slow evaporation from acetonitrile solution.

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with N—H = 0.88, C—H = 0.95 Å, and with $U_{\text{iso}}(\text{H}) = 1.18\text{--}1.21 U_{\text{eq}}(\text{C}, \text{N})$.

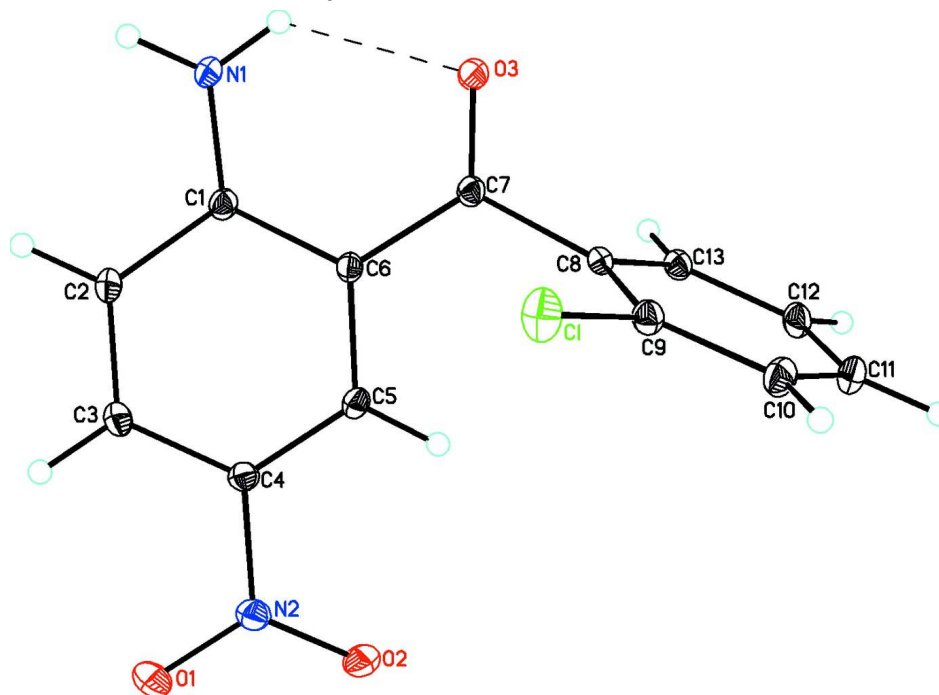
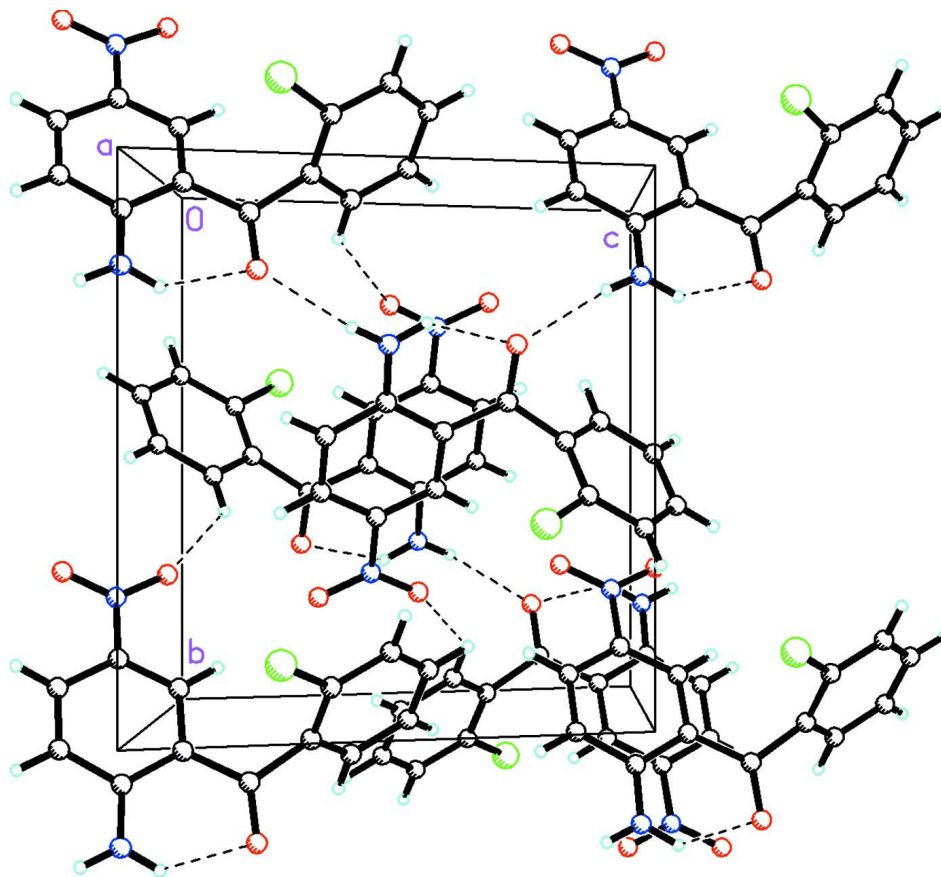


Figure 1

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

**Figure 2**

Packing diagram of the title compound, viewed down the *a* axis. Dashed lines indicate intramolecular N-H...O and intermediate intermolecular N-H...O and C-H...O hydrogen bonds in concert with weak N-H...Cl interactions in the same direction producing an infinite, 2-dimensional intermolecular bonding network parallel to the (001) plane of the unit cell.

2-Amino-5-nitrophenyl 2-chlorophenyl ketone

Crystal data

$C_{13}H_9ClN_2O_3$

$M_r = 276.67$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.6120(3) \text{ \AA}$

$b = 11.3314(3) \text{ \AA}$

$c = 10.8456(3) \text{ \AA}$

$\beta = 108.399(3)^\circ$

$V = 1237.50(6) \text{ \AA}^3$

$Z = 4$

$F(000) = 568$

$D_x = 1.485 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4505 reflections

$\theta = 4.7\text{--}32.6^\circ$

$\mu = 0.31 \text{ mm}^{-1}$

$T = 110 \text{ K}$

Chunk, colorless

$0.47 \times 0.36 \times 0.28 \text{ mm}$

Data collection

Oxford Diffraction Gemini R CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $10.5081 \text{ pixels mm}^{-1}$

φ and ω scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2007)

$T_{\min} = 0.868$, $T_{\max} = 0.916$

8758 measured reflections

4131 independent reflections
 3069 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 32.7^\circ$, $\theta_{\text{min}} = 4.7^\circ$

$h = -15 \rightarrow 16$
 $k = -13 \rightarrow 16$
 $l = -16 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.099$
 $S = 1.04$
 4131 reflections
 172 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-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0548P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.42 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl	0.96431 (3)	0.63182 (3)	0.78827 (3)	0.02769 (10)
O1	0.48712 (10)	0.77733 (9)	0.32532 (9)	0.0350 (2)
O2	0.50201 (9)	0.76958 (8)	0.52898 (8)	0.0271 (2)
O3	0.82129 (9)	0.31290 (8)	0.73196 (7)	0.02303 (19)
N1	0.82197 (10)	0.31577 (9)	0.48161 (9)	0.0214 (2)
H1A	0.8367	0.2872	0.4120	0.026*
H1B	0.8515	0.2779	0.5561	0.026*
N2	0.52756 (10)	0.73094 (9)	0.43331 (9)	0.0211 (2)
C1	0.75466 (11)	0.41681 (10)	0.47433 (10)	0.0162 (2)
C2	0.70760 (12)	0.47688 (11)	0.35352 (10)	0.0197 (2)
H2A	0.7267	0.4453	0.2802	0.024*
C3	0.63591 (12)	0.57843 (11)	0.33976 (10)	0.0202 (2)
H3A	0.6049	0.6169	0.2579	0.024*
C4	0.60840 (11)	0.62550 (10)	0.44837 (10)	0.0169 (2)
C5	0.65568 (10)	0.57301 (10)	0.56856 (10)	0.0157 (2)
H5A	0.6376	0.6076	0.6410	0.019*
C6	0.73013 (10)	0.46916 (10)	0.58484 (10)	0.0148 (2)
C7	0.77971 (11)	0.41506 (10)	0.71401 (10)	0.0159 (2)
C8	0.77845 (11)	0.48654 (10)	0.83067 (9)	0.0154 (2)
C9	0.85984 (11)	0.58380 (11)	0.87385 (10)	0.0184 (2)
C10	0.86275 (12)	0.64296 (11)	0.98728 (11)	0.0228 (3)

H10A	0.9199	0.7088	1.0165	0.027*
C11	0.78122 (12)	0.60456 (12)	1.05687 (11)	0.0240 (3)
H11A	0.7827	0.6443	1.1345	0.029*
C12	0.69750 (12)	0.50870 (12)	1.01432 (10)	0.0214 (2)
H12A	0.6406	0.4839	1.0616	0.026*
C13	0.69720 (11)	0.44907 (10)	0.90242 (10)	0.0174 (2)
H13A	0.6413	0.3823	0.8744	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.02888 (16)	0.03213 (19)	0.02478 (15)	-0.01301 (13)	0.01233 (12)	-0.00264 (12)
O1	0.0449 (6)	0.0315 (6)	0.0230 (4)	0.0161 (5)	0.0026 (4)	0.0071 (4)
O2	0.0329 (5)	0.0238 (5)	0.0292 (4)	0.0088 (4)	0.0161 (4)	0.0015 (4)
O3	0.0372 (5)	0.0166 (4)	0.0187 (4)	0.0056 (4)	0.0137 (3)	0.0035 (3)
N1	0.0332 (5)	0.0174 (5)	0.0147 (4)	0.0061 (4)	0.0092 (4)	-0.0015 (4)
N2	0.0217 (5)	0.0192 (5)	0.0209 (5)	0.0027 (4)	0.0045 (4)	0.0014 (4)
C1	0.0192 (5)	0.0147 (5)	0.0147 (5)	-0.0015 (4)	0.0054 (4)	-0.0022 (4)
C2	0.0259 (6)	0.0212 (6)	0.0125 (4)	0.0014 (5)	0.0066 (4)	-0.0012 (4)
C3	0.0242 (5)	0.0220 (6)	0.0129 (5)	0.0015 (5)	0.0035 (4)	0.0013 (4)
C4	0.0180 (5)	0.0151 (6)	0.0172 (5)	0.0010 (4)	0.0047 (4)	-0.0006 (4)
C5	0.0179 (5)	0.0151 (6)	0.0149 (5)	-0.0023 (4)	0.0063 (4)	-0.0030 (4)
C6	0.0182 (5)	0.0139 (5)	0.0125 (4)	-0.0011 (4)	0.0052 (4)	-0.0006 (4)
C7	0.0194 (5)	0.0150 (5)	0.0148 (5)	-0.0009 (4)	0.0076 (4)	0.0005 (4)
C8	0.0201 (5)	0.0147 (5)	0.0115 (4)	0.0026 (4)	0.0051 (4)	0.0019 (4)
C9	0.0200 (5)	0.0193 (6)	0.0165 (5)	-0.0007 (4)	0.0066 (4)	0.0009 (4)
C10	0.0257 (6)	0.0220 (6)	0.0191 (5)	-0.0029 (5)	0.0047 (4)	-0.0050 (5)
C11	0.0290 (6)	0.0271 (7)	0.0155 (5)	0.0027 (5)	0.0067 (4)	-0.0047 (5)
C12	0.0247 (6)	0.0267 (7)	0.0149 (5)	0.0023 (5)	0.0091 (4)	0.0018 (4)
C13	0.0211 (5)	0.0163 (6)	0.0150 (5)	-0.0004 (4)	0.0060 (4)	0.0016 (4)

Geometric parameters (Å, °)

Cl—C9	1.7426 (12)	C5—C6	1.3972 (15)
O1—N2	1.2309 (13)	C5—H5A	0.9500
O2—N2	1.2326 (13)	C6—C7	1.4663 (15)
O3—C7	1.2322 (14)	C7—C8	1.5059 (15)
N1—C1	1.3385 (15)	C8—C9	1.3873 (16)
N1—H1A	0.8800	C8—C13	1.3975 (15)
N1—H1B	0.8800	C9—C10	1.3927 (16)
N2—C4	1.4498 (15)	C10—C11	1.3856 (18)
C1—C2	1.4201 (15)	C10—H10A	0.9500
C1—C6	1.4329 (14)	C11—C12	1.3868 (18)
C2—C3	1.3614 (17)	C11—H11A	0.9500
C2—H2A	0.9500	C12—C13	1.3882 (15)
C3—C4	1.4052 (15)	C12—H12A	0.9500
C3—H3A	0.9500	C13—H13A	0.9500
C4—C5	1.3754 (15)		

C1—N1—H1A	120.0	C1—C6—C7	121.40 (10)
C1—N1—H1B	120.0	O3—C7—C6	123.11 (10)
H1A—N1—H1B	120.0	O3—C7—C8	118.06 (9)
O1—N2—O2	123.10 (11)	C6—C7—C8	118.83 (10)
O1—N2—C4	118.38 (10)	C9—C8—C13	118.76 (10)
O2—N2—C4	118.52 (9)	C9—C8—C7	122.77 (9)
N1—C1—C2	119.35 (10)	C13—C8—C7	118.36 (10)
N1—C1—C6	122.63 (10)	C8—C9—C10	121.23 (10)
C2—C1—C6	118.00 (10)	C8—C9—C1	120.08 (8)
C3—C2—C1	121.87 (10)	C10—C9—C1	118.67 (9)
C3—C2—H2A	119.1	C11—C10—C9	119.10 (11)
C1—C2—H2A	119.1	C11—C10—H10A	120.5
C2—C3—C4	119.06 (10)	C9—C10—H10A	120.5
C2—C3—H3A	120.5	C10—C11—C12	120.62 (11)
C4—C3—H3A	120.5	C10—C11—H11A	119.7
C5—C4—C3	121.35 (11)	C12—C11—H11A	119.7
C5—C4—N2	119.28 (10)	C11—C12—C13	119.78 (11)
C3—C4—N2	119.37 (10)	C11—C12—H12A	120.1
C4—C5—C6	120.43 (10)	C13—C12—H12A	120.1
C4—C5—H5A	119.8	C12—C13—C8	120.49 (11)
C6—C5—H5A	119.8	C12—C13—H13A	119.8
C5—C6—C1	119.20 (9)	C8—C13—H13A	119.8
C5—C6—C7	119.40 (9)		
N1—C1—C2—C3	178.41 (11)	C1—C6—C7—O3	-14.58 (17)
C6—C1—C2—C3	-2.95 (17)	C5—C6—C7—C8	-14.71 (16)
C1—C2—C3—C4	0.38 (18)	C1—C6—C7—C8	166.26 (10)
C2—C3—C4—C5	1.95 (18)	O3—C7—C8—C9	112.56 (13)
C2—C3—C4—N2	-177.50 (11)	C6—C7—C8—C9	-68.24 (14)
O1—N2—C4—C5	179.35 (11)	O3—C7—C8—C13	-63.73 (14)
O2—N2—C4—C5	-1.01 (16)	C6—C7—C8—C13	115.48 (12)
O1—N2—C4—C3	-1.19 (17)	C13—C8—C9—C10	0.79 (17)
O2—N2—C4—C3	178.46 (11)	C7—C8—C9—C10	-175.49 (11)
C3—C4—C5—C6	-1.56 (17)	C13—C8—C9—C1	179.06 (8)
N2—C4—C5—C6	177.89 (10)	C7—C8—C9—C1	2.79 (15)
C4—C5—C6—C1	-1.10 (16)	C8—C9—C10—C11	-0.93 (18)
C4—C5—C6—C7	179.85 (10)	C1—C9—C10—C11	-179.23 (10)
N1—C1—C6—C5	-178.14 (11)	C9—C10—C11—C12	-0.14 (19)
C2—C1—C6—C5	3.28 (16)	C10—C11—C12—C13	1.31 (19)
N1—C1—C6—C7	0.89 (17)	C11—C12—C13—C8	-1.45 (18)
C2—C1—C6—C7	-177.69 (10)	C9—C8—C13—C12	0.41 (17)
C5—C6—C7—O3	164.45 (11)	C7—C8—C13—C12	176.85 (10)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1A \cdots O3 ⁱ	0.88	2.22	3.0733 (12)	164

N1—H1B···O3	0.88	2.07	2.7176 (12)	130
N1—H1B···Cl ⁱⁱ	0.88	2.71	3.4848 (10)	148
C13—H13A···O2 ⁱⁱⁱ	0.95	2.46	3.1862 (14)	133

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (ii) $-x+2, y-1/2, -z+3/2$; (iii) $-x+1, y-1/2, -z+3/2$.