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(5E)-1-Benzyl-5-(3,3,3-trichloro-2-oxo-propylidene)pyrrolidin-2-oneAlex Fabiani Claro Flores,^{a*} Darlene Correia Flores,^a Juliano Rosa de Menezes Vicenti,^a Lucas Pizzuti^b and Patrick Teixeira Campos^c^aEscola de Química e Alimentos, Universidade Federal do Rio Grande, Av. Itália, km 08, Campus Carreiros, 96203-900, Rio Grande, RS, Brazil, ^bUniversidade Federal da Grande Dourados, UFGD, CEP 79825-070, Dourados, MS, Brazil, and ^cInstituto Federal Farroupilha, Campus Júlio de Castilhos, CEP 98130-000, Júlio de Castilhos, RS, Brazil

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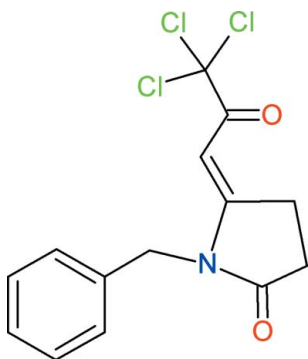
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.054; wR factor = 0.217; data-to-parameter ratio = 28.0.

In the crystal structure of the title compound, $\text{C}_{14}\text{H}_{12}\text{Cl}_3\text{NO}_2$, no classical hydrogen-bonding interactions are observed. The methylene fragments of the benzyl groups participate in non-classic hydrogen-bond interactions with the carbonyl O atoms of neighboring molecules, generating co-operative centrosymmetric dimers with $R_5^5(10)$ ring motifs. The overall molecular arrangement in the unit cell seems to be highly influenced by secondary non-covalent weak $\text{C}-\text{Cl}\cdots\pi$ [$\text{Cl}\cdots\text{Cg}(\text{phenyl ring}) = 3.732$ (2) Å] and $\text{C}-\text{O}\cdots\pi$ [$\text{O}\cdots\text{Cg}(\text{pyrrolidine ring}) = 2.985$ (2) Å] contacts.

Related literature

For the synthesis of the title compound, see: Flores *et al.* (2008). For pharmacological effects, see: Van der Schyf *et al.* (2006). For non-classical weak contacts, see: Irving & Irving (1994); Bissantz *et al.* (2010). For related structures, see: Bandeira *et al.* (2013); de Oliveira *et al.* (2012); de Bittencourt *et al.* (2014).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{Cl}_3\text{NO}_2$
 $M_r = 332.60$
 Monoclinic, $P2_1/n$
 $a = 15.7822$ (5) Å
 $b = 5.8465$ (2) Å
 $c = 17.4107$ (5) Å
 $\beta = 105.885$ (1)°
 $V = 1545.15$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.59$ mm⁻¹
 $T = 293$ K
 $0.83 \times 0.23 \times 0.19$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: gaussian (XPREF; Bruker, 2009)
 $T_{\min} = 0.814$, $T_{\max} = 1.000$
 21458 measured reflections
 5069 independent reflections
 2436 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.217$
 $S = 1.00$
 5069 reflections
 181 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.43$ e Å⁻³
 $\Delta\rho_{\min} = -0.51$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H82}\cdots\text{O71}^1$	0.97	2.38	3.292 (3)	156

Symmetry code: (i) $-x + 1, -y + 1, -z + 2$.

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: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZQ2220).

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supplementary materials

Acta Cryst. (2014). E70, o629–o630 [doi:10.1107/S160053681400751X]

(5E)-1-Benzyl-5-(3,3,3-trichloro-2-oxopropylidene)pyrrolidin-2-one

Alex Fabiani Claro Flores, Darlene Correia Flores, Juliano Rosa de Menezes Vicenti, Lucas Pizzuti and Patrick Teixeira Campos

1. Comment

Pyrrolidin-2-ones have received considerable attention due to their activity in *CNS* as nootropic drugs. Piracetam-like nootropics revert amnesia induced by scopolamine and other amnesing drugs, electroconvulsive shock and hypoxia with an unknown mechanism. In general, they show no affinity for the most important central receptors, but are able to modulate the action of these most important central neurotransmitters, in particular acetylcholine and glutamate. Extensive study of the modes of action of the 2-pyrrolidinones has revealed various pharmacological effects, with striking differences between drugs (Van der Schyf *et al.*, 2006). This work is a continuation of the research on the synthesis of 1-[alkyl(aryl)]-5-(3,3,3-trihalo-2-oxopropylidene)pyrrolidin-2-ones (Flores *et al.*, 2008). In the crystal structure of the title compound, C₁₄H₁₂O₂NCl₃ (Fig. 1), no classic hydrogen bonds are observed. There is a non-classic intramolecular hydrogen bond with a distance C8—H82ⁱⁱ⋯O71 of 2.442 Å, generating a *S*(5) ring motif (de Bittencourt *et al.*, 2014). The molecule possesses two sites revealing an interesting geometric conformation: the plane defined by the aromatic ring (r.m.s. of 0.0032 Å) revealed a dihedral angle of 87.03 (8)° with respect to the second plane formed by C1/C2/O21/C3/C4/C5/C6/C7/N1/C8/O71 atoms (r.m.s. of 0.0978 Å; Bandeira *et al.*, 2013; de Oliveira *et al.*, 2012). This almost orthogonal configuration (Fig. 2) seems to be related with the crystal packing. In this context, the CH₂ fragment of the benzyl group participates in non-classic hydrogen bonding with carbonyl oxygen of the neighbor molecules. This feature generates co-operative centrosymmetric dimers related through inversion centers, displaying C8ⁱⁱ—H82ⁱⁱ⋯O71ⁱ distances of 2.382 Å in a *R*_s⁵(10) ring fashion (de Bittencourt *et al.*, 2014). The overall molecular arrangement in the unit cell (Fig. 3) seems to be highly influenced by weak interactions, where O21ⁱⁱⁱ are clearly pointing to C(1) (2.985 Å), related to the centroid of the neighbor ring formed by C4ⁱⁱ/C5ⁱⁱ/C6ⁱⁱ/C7ⁱⁱ/N1ⁱⁱ atoms. Similarly, the centroid C(2) of the ring formed by C9^{iv}/C10^{iv}/C11^{iv}/C12^{iv}/C13^{iv}/C14^{iv} atoms from the benzyl fragment presented directional long range interactions with adjacent C11ⁱⁱ atoms (Irving & Irving, 1994; Bissantz *et al.*, 2010), with distances of 3.732 Å (symmetry codes: (i) $-x + 3/2, y + 1/2, -z + 3/2$; (ii) $x + 1/2, -y + 3/2, z - 1/2$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $x, y + 1, z - 1$).

2. Experimental

To a stirred solution of methyl 7,7,7-trichloro-4-methoxy-6-oxo-3-heptenoate (5 mmol, 1.52 g) in CHCl₃ (5 ml) kept at 25 °C, was added benzylamine (Aldrich, 185701, 5.1 mmol, 0.58 ml) in CHCl₃ (5 ml). The mixture was stirred at 25 °C for 2 h. Then the solvent was evaporated and residue was dried under vacuum. The brown amorphous solid was recrystallized in hexane to furnish yellowish needles with 94% yield. *M.p.* 88 - 89°C. ¹H NMR (400 MHz, CDCl₃/TMS): δ 2.72 (m, 2H, H3), 3.34 (m, 2H, H4), 4.8 (s, 2H, H9), 6.2 (s, 1H, H6), 7.3 (m, 5H, Ph) p.p.m. ¹³C NMR (100 MHz, CDCl₃): 26.1, 27.5, 44.6, 91.7, 97.1, 127.6, 128.1, 128.9, 134.1, 166.4, 177.1, 180 p.p.m. Crystals were grown from a diluted hexane solution at room temperature.

3. Refinement

All H atoms attached to C atoms were positioned with idealized geometry and were refined isotropic with $U_{\text{eq}}(\text{H})$ set to 1.2 times of the $U_{\text{eq}}(\text{C})$. It was used a riding model with C—H = 0.97 Å for CH₂ and C—H = 0.93 Å for CH. Reflection (101) was omitted due to the large difference observed between F_o^2 and F_c^2 . The crystals were relatively weak in terms of intensity of diffraction, prompting us to select a big crystal for the measurement and consequently a collimator with a larger diameter (0.6 mm) than in routine studies.

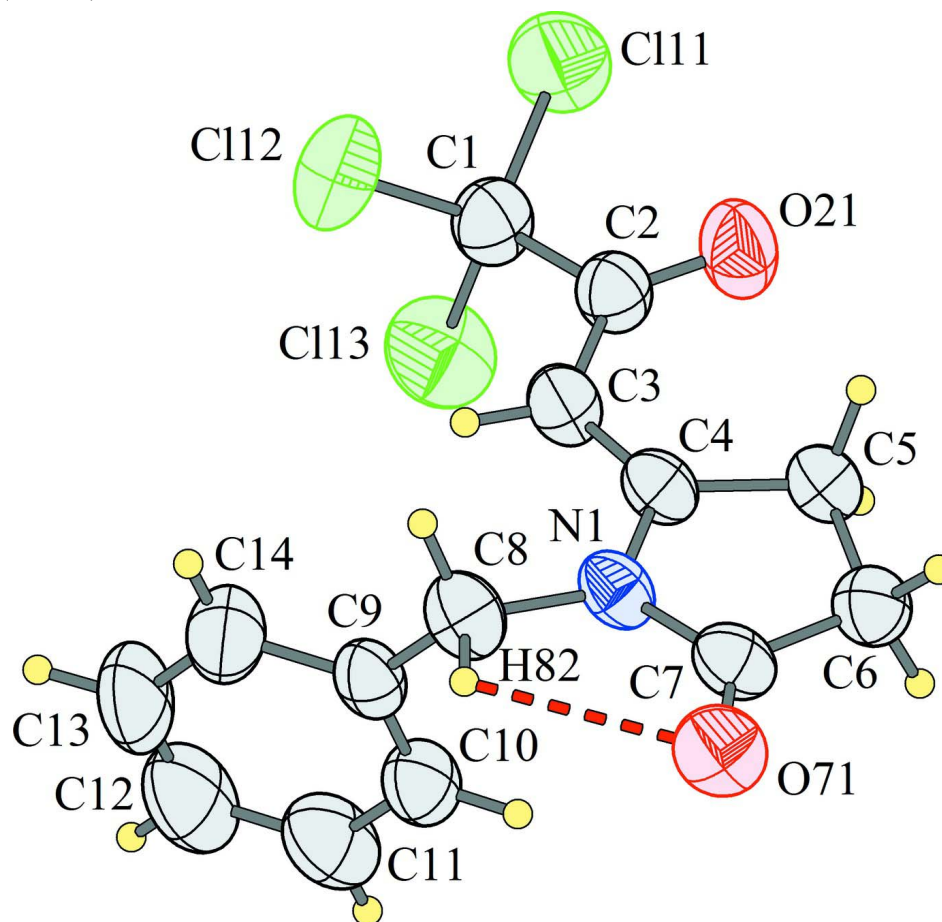


Figure 1

Asymmetric unit of the title compound showing an intramolecular hydrogen bond interaction represented with red dashed lines. Ellipsoid probability: 50%.

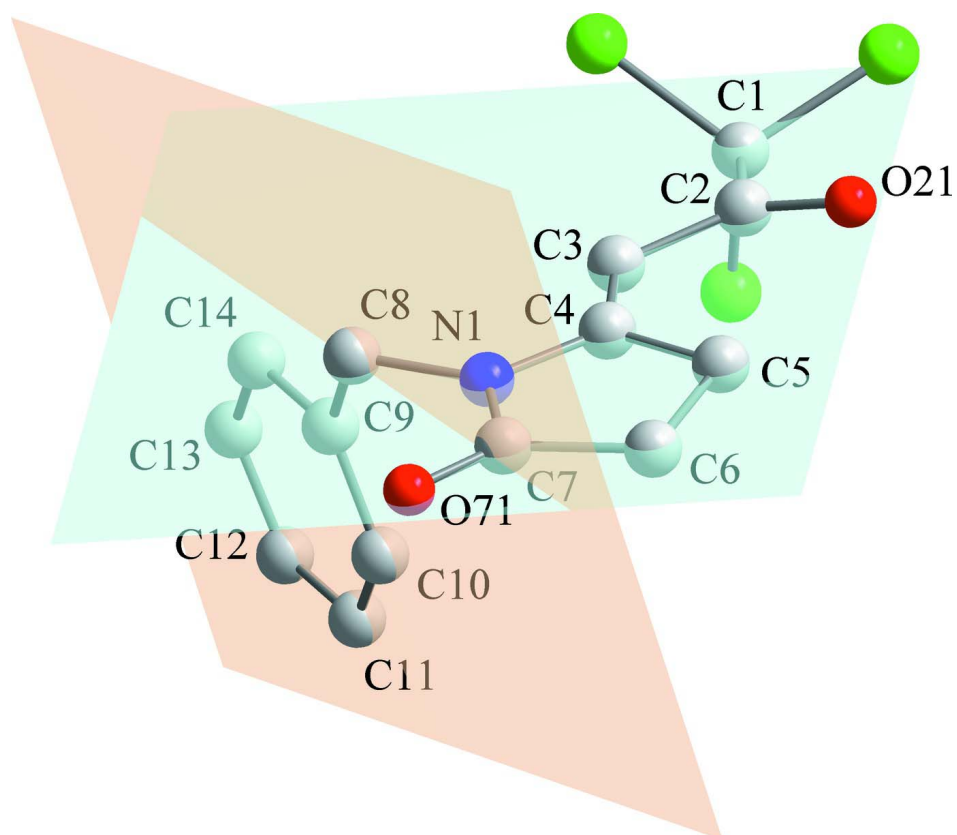
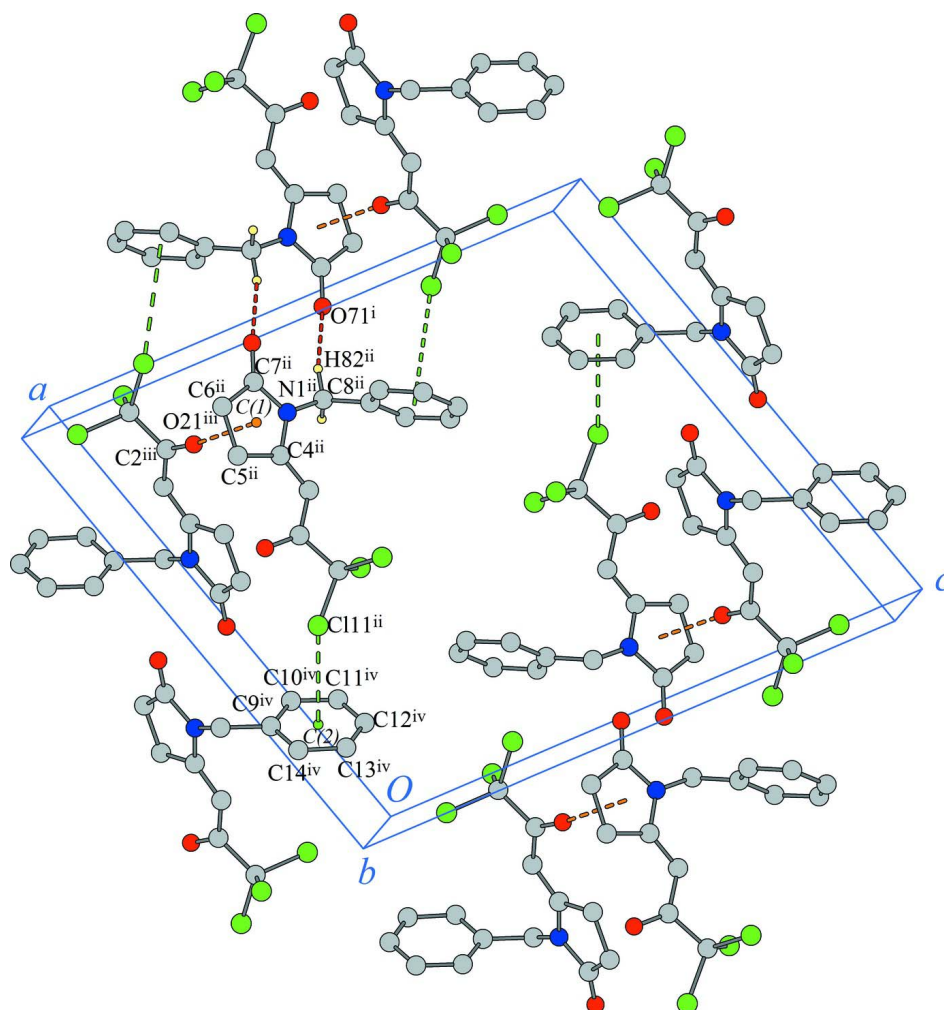


Figure 2

Representation of the two mean planes traced through non-hydrogenoid atoms considered for dihedral angle calculation.

**Figure 3**

Packing diagram showing the molecular arrangement in the unit cell. Non-classic hydrogen bond interactions are represented with red dashed lines, meanwhile other weak non-covalent contacts are represented with orange and green dashed lines. Most of the hydrogen atoms were omitted for clarity. Symmetry codes: (i) $-x + 3/2, y + 1/2, -z + 3/2$; (ii) $x + 1/2, -y + 3/2, z - 1/2$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $x, y + 1, z - 1$.

(E)-1-Benzyl-5-(3,3,3-trichloro-2-oxopropylidene)pyrrolidin-2-one

Crystal data

$C_{14}H_{12}Cl_3NO_2$

$M_r = 332.60$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1/n$

$a = 15.7822$ (5) Å

$b = 5.8465$ (2) Å

$c = 17.4107$ (5) Å

$\beta = 105.885$ (1)°

$V = 1545.15$ (8) Å³

$Z = 4$

$F(000) = 680$

$D_x = 1.430$ Mg m⁻³

Melting point: 361 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3113 reflections

$\theta = 2.4$ – 21.5 °

$\mu = 0.59$ mm⁻¹

$T = 293$ K

Block, yellow

$0.83 \times 0.23 \times 0.19$ mm

Data collection

Bruker APEXII CCD diffractometer	21458 measured reflections
Radiation source: fine-focus sealed tube	5069 independent reflections
Graphite monochromator	2436 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.033$
Absorption correction: gaussian (XPREP; Bruker, 2009)	$\theta_{\text{max}} = 31.5^\circ$, $\theta_{\text{min}} = 2.7^\circ$
$T_{\text{min}} = 0.814$, $T_{\text{max}} = 1$	$h = -23 \rightarrow 23$
	$k = -8 \rightarrow 3$
	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.217$	$w = 1/[\sigma^2(F_o^2) + (0.1095P)^2 + 0.2217P]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
5069 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
181 parameters	$\Delta\rho_{\text{max}} = 0.43 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.51 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. Gaussian absorption correction based on the face-indexed crystal size

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl11	-0.04344 (5)	-0.0759 (2)	0.73859 (6)	0.0958 (3)
Cl12	0.01375 (6)	0.32178 (15)	0.83385 (6)	0.0921 (3)
Cl13	0.03185 (7)	-0.11995 (17)	0.90926 (6)	0.0955 (3)
O71	0.50426 (12)	0.2290 (4)	0.95046 (11)	0.0688 (5)
N1	0.35352 (12)	0.2022 (3)	0.92101 (10)	0.0485 (5)
O21	0.13827 (13)	-0.1294 (4)	0.75824 (13)	0.0766 (6)
C9	0.30299 (15)	0.3271 (4)	1.03807 (14)	0.0517 (6)
C4	0.28593 (15)	0.0825 (4)	0.87105 (13)	0.0473 (5)
C2	0.13065 (16)	-0.0046 (4)	0.81150 (14)	0.0541 (6)
C3	0.20017 (17)	0.1159 (4)	0.86770 (14)	0.0537 (6)
H3	0.1858	0.2195	0.9027	0.064*
C8	0.34165 (19)	0.3933 (4)	0.97121 (15)	0.0573 (6)
H81	0.3035	0.5058	0.9379	0.069*
H82	0.3984	0.4653	0.9939	0.069*
C6	0.42339 (17)	-0.0584 (5)	0.85719 (15)	0.0584 (6)
H62	0.4489	-0.1974	0.8843	0.070*

H61	0.4507	-0.0263	0.8148	0.070*
C5	0.32443 (16)	-0.0833 (4)	0.82383 (14)	0.0507 (5)
H51	0.3062	-0.0455	0.7674	0.061*
H52	0.3060	-0.2384	0.8308	0.061*
C10	0.32564 (18)	0.1269 (5)	1.08009 (16)	0.0614 (7)
H10	0.3654	0.0275	1.0667	0.074*
C7	0.43644 (17)	0.1369 (4)	0.91455 (14)	0.0536 (6)
C11	0.2900 (2)	0.0712 (7)	1.14227 (18)	0.0810 (9)
H11	0.3059	-0.0653	1.1699	0.097*
C14	0.2441 (2)	0.4725 (6)	1.0591 (2)	0.0778 (8)
H14	0.2273	0.6087	1.0315	0.093*
C13	0.2094 (2)	0.4110 (8)	1.1238 (2)	0.0972 (12)
H13	0.1704	0.5088	1.1389	0.117*
C1	0.03650 (17)	0.0294 (5)	0.82250 (16)	0.0615 (6)
C12	0.2326 (2)	0.2126 (8)	1.1629 (2)	0.0930 (11)
H12	0.2089	0.1729	1.2044	0.112*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl11	0.0520 (4)	0.1369 (8)	0.0932 (6)	-0.0116 (4)	0.0110 (4)	-0.0291 (5)
Cl12	0.0838 (6)	0.0785 (6)	0.1221 (7)	0.0163 (4)	0.0416 (5)	-0.0080 (5)
Cl13	0.0997 (7)	0.1099 (7)	0.0892 (6)	-0.0161 (5)	0.0465 (5)	0.0130 (5)
O71	0.0531 (10)	0.0804 (13)	0.0728 (11)	-0.0168 (9)	0.0169 (9)	-0.0078 (10)
N1	0.0497 (10)	0.0571 (11)	0.0417 (9)	-0.0128 (8)	0.0175 (8)	-0.0064 (8)
O21	0.0558 (11)	0.0922 (15)	0.0809 (13)	-0.0063 (10)	0.0169 (10)	-0.0388 (11)
C9	0.0454 (12)	0.0599 (14)	0.0497 (12)	-0.0087 (10)	0.0130 (10)	-0.0156 (11)
C4	0.0522 (13)	0.0517 (12)	0.0396 (11)	-0.0085 (10)	0.0155 (9)	-0.0008 (9)
C2	0.0508 (13)	0.0580 (14)	0.0547 (14)	-0.0029 (11)	0.0166 (11)	-0.0057 (11)
C3	0.0545 (13)	0.0597 (14)	0.0491 (13)	-0.0055 (11)	0.0176 (11)	-0.0090 (10)
C8	0.0633 (15)	0.0533 (13)	0.0576 (14)	-0.0138 (11)	0.0205 (12)	-0.0080 (11)
C6	0.0532 (14)	0.0696 (16)	0.0537 (14)	0.0010 (11)	0.0167 (11)	-0.0030 (12)
C5	0.0551 (13)	0.0542 (13)	0.0441 (11)	-0.0039 (10)	0.0158 (10)	-0.0027 (10)
C10	0.0568 (15)	0.0748 (17)	0.0579 (14)	-0.0009 (12)	0.0245 (12)	-0.0040 (13)
C7	0.0545 (14)	0.0640 (14)	0.0433 (12)	-0.0096 (11)	0.0150 (10)	0.0011 (10)
C11	0.088 (2)	0.101 (2)	0.0599 (17)	-0.0077 (18)	0.0312 (16)	0.0037 (16)
C14	0.0735 (19)	0.081 (2)	0.082 (2)	0.0109 (15)	0.0257 (16)	-0.0153 (16)
C13	0.075 (2)	0.140 (4)	0.089 (2)	0.013 (2)	0.0438 (19)	-0.033 (2)
C1	0.0522 (14)	0.0691 (16)	0.0661 (16)	-0.0036 (12)	0.0208 (12)	-0.0052 (13)
C12	0.088 (2)	0.131 (3)	0.074 (2)	-0.013 (2)	0.0459 (19)	-0.012 (2)

Geometric parameters (\AA , $^\circ$)

Cl11—C1	1.760 (3)	C8—H82	0.9700
Cl12—C1	1.769 (3)	C6—C7	1.494 (3)
Cl13—C1	1.764 (3)	C6—C5	1.517 (4)
O71—C7	1.208 (3)	C6—H62	0.9700
N1—C4	1.370 (3)	C6—H61	0.9700
N1—C7	1.397 (3)	C5—H51	0.9700
N1—C8	1.462 (3)	C5—H52	0.9700

O21—C2	1.212 (3)	C10—C11	1.389 (4)
C9—C10	1.375 (4)	C10—H10	0.9300
C9—C14	1.381 (4)	C11—C12	1.345 (5)
C9—C8	1.505 (3)	C11—H11	0.9300
C4—C3	1.353 (3)	C14—C13	1.426 (5)
C4—C5	1.503 (3)	C14—H14	0.9300
C2—C3	1.439 (4)	C13—C12	1.345 (6)
C2—C1	1.562 (3)	C13—H13	0.9300
C3—H3	0.9300	C12—H12	0.9300
C8—H81	0.9700		
C4—N1—C7	113.14 (19)	C6—C5—H51	110.8
C4—N1—C8	124.4 (2)	C4—C5—H52	110.8
C7—N1—C8	122.2 (2)	C6—C5—H52	110.8
C10—C9—C14	118.6 (2)	H51—C5—H52	108.8
C10—C9—C8	121.9 (2)	C9—C10—C11	120.8 (3)
C14—C9—C8	119.4 (3)	C9—C10—H10	119.6
C3—C4—N1	123.4 (2)	C11—C10—H10	119.6
C3—C4—C5	128.2 (2)	O71—C7—N1	123.6 (2)
N1—C4—C5	108.4 (2)	O71—C7—C6	128.8 (2)
O21—C2—C3	126.8 (2)	N1—C7—C6	107.6 (2)
O21—C2—C1	117.9 (2)	C12—C11—C10	120.7 (4)
C3—C2—C1	115.4 (2)	C12—C11—H11	119.7
C4—C3—C2	121.8 (2)	C10—C11—H11	119.7
C4—C3—H3	119.1	C9—C14—C13	119.1 (3)
C2—C3—H3	119.1	C9—C14—H14	120.5
N1—C8—C9	114.3 (2)	C13—C14—H14	120.5
N1—C8—H81	108.7	C12—C13—C14	120.5 (3)
C9—C8—H81	108.7	C12—C13—H13	119.8
N1—C8—H82	108.7	C14—C13—H13	119.8
C9—C8—H82	108.7	C2—C1—C11	110.10 (18)
H81—C8—H82	107.6	C2—C1—C13	107.82 (19)
C7—C6—C5	105.6 (2)	C11—C1—C13	110.45 (15)
C7—C6—H62	110.6	C2—C1—C12	111.45 (18)
C5—C6—H62	110.6	C11—C1—C12	108.04 (16)
C7—C6—H61	110.6	C13—C1—C12	109.00 (15)
C5—C6—H61	110.6	C13—C12—C11	120.3 (3)
H62—C6—H61	108.8	C13—C12—H12	119.8
C4—C5—C6	104.88 (19)	C11—C12—H12	119.8
C4—C5—H51	110.8		
C7—N1—C4—C3	179.4 (2)	C8—N1—C7—O71	1.3 (4)
C8—N1—C4—C3	-5.8 (3)	C4—N1—C7—C6	-3.7 (3)
C7—N1—C4—C5	-0.5 (3)	C8—N1—C7—C6	-178.6 (2)
C8—N1—C4—C5	174.3 (2)	C5—C6—C7—O71	-173.7 (3)
N1—C4—C3—C2	176.7 (2)	C5—C6—C7—N1	6.2 (3)
C5—C4—C3—C2	-3.4 (4)	C9—C10—C11—C12	-0.2 (5)
O21—C2—C3—C4	-6.5 (4)	C10—C9—C14—C13	0.4 (4)
C1—C2—C3—C4	172.5 (2)	C8—C9—C14—C13	-178.5 (3)

C4—N1—C8—C9	67.9 (3)	C9—C14—C13—C12	-1.0 (6)
C7—N1—C8—C9	-117.8 (2)	O21—C2—C1—C11	-13.2 (3)
C10—C9—C8—N1	38.3 (3)	C3—C2—C1—C11	167.62 (19)
C14—C9—C8—N1	-142.8 (3)	O21—C2—C1—C13	107.3 (3)
C3—C4—C5—C6	-175.6 (2)	C3—C2—C1—C13	-71.8 (3)
N1—C4—C5—C6	4.3 (2)	O21—C2—C1—C12	-133.1 (2)
C7—C6—C5—C4	-6.3 (2)	C3—C2—C1—C12	47.8 (3)
C14—C9—C10—C11	0.2 (4)	C14—C13—C12—C11	1.0 (6)
C8—C9—C10—C11	179.1 (3)	C10—C11—C12—C13	-0.4 (6)
C4—N1—C7—O71	176.2 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H82...O71 ⁱ	0.97	2.38	3.292 (3)	156

Symmetry code: (i) $-x+1, -y+1, -z+2$.