Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6,8-Dichloro-*N*-methyl-3-nitro-4-nitromethyl-4*H*-chromen-2-amine

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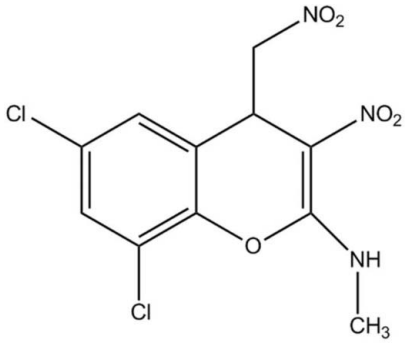
Received 10 February 2011; accepted 11 March 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.110; data-to-parameter ratio = 12.5.

In the title compound, $C_{11}H_9Cl_2N_3O_5$, the dihydropyran ring adopts a near-half-chair conformation. The benzene ring makes a torsion angle of 5.02 (5)° with the dihydropyran ring. Adjacent molecules are interlinked through intermolecular C—H···O, N—H···O and C—Cl···π [3.4743 (9) Å] interactions. The intermolecular N—H···O hydrogen bond generates an $R_2^2(12)$ motif, which is observed to contribute to the crystal packing stability. Moreover, the molecular structure displays an $S(6)$ motif formed by intramolecular N—H···O hydrogen bonding.

Related literature

For related structures, see: Gayathri *et al.* (2006); Bhaskaran *et al.* (2006). For the biological importance of 4*H*-chromene derivatives, see: Cai (2007, 2008); Cai *et al.* (2006); Gabor (1988); Brooks (1998); Valenti *et al.* (1993); Hyana & Saimoto (1987); Tang *et al.* (2007). For ring-puckering analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{11}H_9Cl_2N_3O_5$
M_r = 334.11
Triclinic, $P\overline{1}$
a = 8.7426 (7) Å
b = 9.2727 (7) Å
c = 9.3420 (7) Å
α = 70.017 (7)°
β = 72.609 (7)°
γ = 87.579 (6)°
V = 677.68 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.50 mm^{-1}
T = 293 K
0.4 × 0.35 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.792, T_{max} = 1.000
15150 measured reflections
2385 independent reflections
2072 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.110
S = 1.01
2385 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	2.00	2.613 (2)	128
N1—H1···O2^{i}	0.86	2.12	2.881 (2)	147
C7—H7···O3^{ii}	0.98	2.50	3.1944 (19)	128
C11—H11*B*···O3^{ii}	0.97	2.54	3.103 (2)	117

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

RK, JM and MK thank the Centre for Bioinformatics (funded by the Department of Biotechnology and the Department of Information Technology, New Delhi, India), Pondicherry University for providing the computational facilities to carry out this research work. MK also thanks the University Grants Commission (UGC) for a Rajiv Gandhi National Fellowship. AP thanks Pondicherry University for a fellowship. HSPR thanks UGC for the SAP and the Department of Science and Technology (DST) for the FIST.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2089).

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supporting information

Acta Cryst. (2011). E**67**, o898–o899 [doi:10.1107/S1600536811009366]

6,8-Dichloro-*N*-methyl-3-nitro-4-nitromethyl-4*H*-chromen-2-amine

J. Muthukumaran, A. Parthiban, M. Kannan, H. Surya Prakash Rao and R. Krishna

S1. Comment

4*H*-Chromenes are biologically important compounds used as synthetic ligands for drug designing and discovery process. They exhibit numerous biological and pharmacological properties such as anti-viral, anti-fungal, anti-inflammatory, anti-diabetic, cardionthonic, anti-anaphylactic and anti-cancer activity (Cai, 2008; Cai, 2007; Cai *et al.*, 2006; Gabor *et al.*, 1988; Brooks, 1998; Valenti *et al.*, 1993; Hyana & Saimoto, 1987; Tang *et al.*, 2007). In view of the growing medicinal importance of 4*H*-chromene derivatives, a single-crystal X-ray diffraction study on the title compound was carried out and analyzed.

The title compound (Fig. 1) contains the 4*H*-chromene moiety with four different substituents [–Cl_2, –NO_2, –CH_2NO_2 and –$NHCH_3$]. The Cl1 group attached to C2 by an (+) anti-periplanar conformation with the torsion angle (Cl1/C2/C3/C4) of 178.76 (14) °, whereas another chlorine attached to C4 with the torsion angle (Cl2/C4/C3/C2) of -176.94 (14) °, which oriented in (-) anti-periplanar conformations. From the puckering analysis (Cremer & Pople, 1975), the fused dihydropyran ring (O1/C1/C6/C7/C8/C9) of 4*H*-chromene is very similar to half chair (H form) conformation with puckering parameters of Q = 0.1772 (17) Å, θ = 104.5 (5) ° and Φ = 11.6 (6) °. The molecular structure is stabilized by intramolecular N—H···O and C—H···O interactions. The intramolecular N1—H1···O2 interaction generates a graph-set motif *S* (6) (Fig. 2) with a *D*···*A* bond distance of 2.613 (2) Å. The crystal packing of the molecule (Fig. 3) is stabilized by intermolecular N1—H1···O2 (symmetry code: -*x* + 2, -*y* + 1, -*z* + 1), C7—H7···O3 (symmetry code: -*x* + 2, -*y* + 2, -*z*), C11—H11B···O3 (symmetry code:-*x* + 2, -*y* + 2, -*z*) and C—Cl··· π (symmetry code: 1 - *x*, 1 - *y*, -*z*) interactions (Fig. 4). The intermolecular N1—H1···O2 interaction generates a ring of graph-set R^2_2 (12) with the bond distance of 2.881 (2) Å (Fig. 5).

S2. Experimental

(E)-2,4-Dichloro-6-(2-nitrovinyl)phenol (100 mg, 0.427 mmol) was taken in a 25 ml round bottom flask in methanol (4 ml). To this solution, 1,8-diazabicyclo[5.4.0] undec-7-ene (DBU) (8 mg, 0.042 mmol) was added and stirred thoroughly for 10 minutes at room temperature. To this stirred solution, NMSM ((*E*) *N*-methyl-1-(methylthio)-2-nitroethenamine) was added and stirred for 10 h for completion (TLC, hexane: EtoAc, 3:2, R_f of I = 0.3). The reaction mixture was then kept in a refrigerator for 2 h to afford racemic mixture of the product (I), white precipitate, which was filtered. Good crystals were obtained by recrystallization with a solution of dichloromethane: hexane (9:3 *v*/*v*).

S3. Refinement

All hydrogen atoms were placed in calculated positions, with N—H=0.86 and C—H=0.97 and included in the final cycles of refinement using a riding model with U_{iso}(H) = 1.2 U_{eq}(*C*).

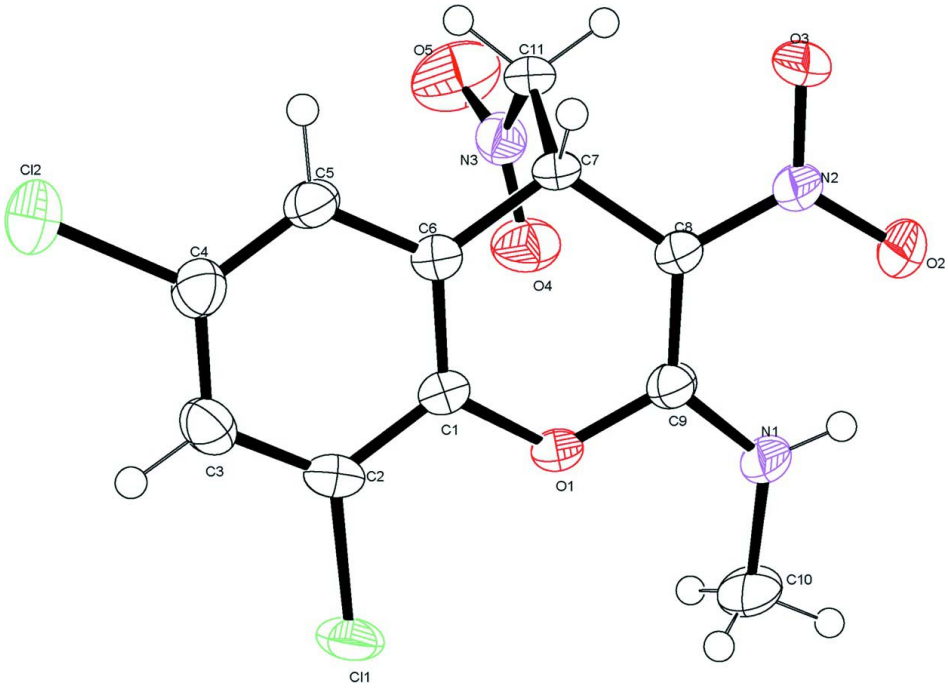

Figure 1

The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

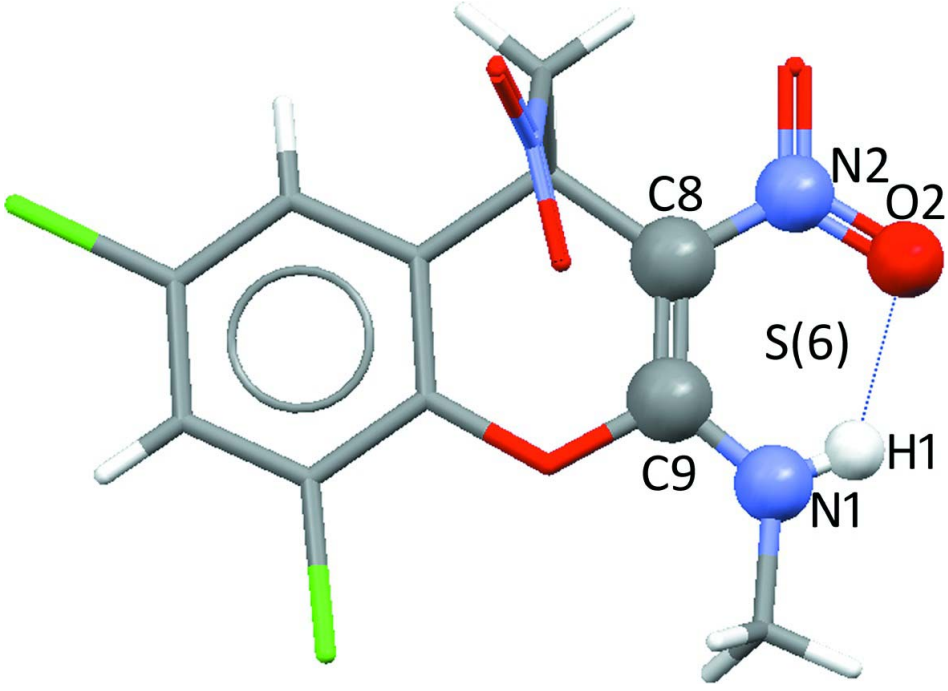

Figure 2

A view of intramolecular motif *S* (6) formed by N—H···O interaction in (I). The motif forming atoms are shown in ball and stick model and the Hydrogen bond are shown in blue dashed lines.

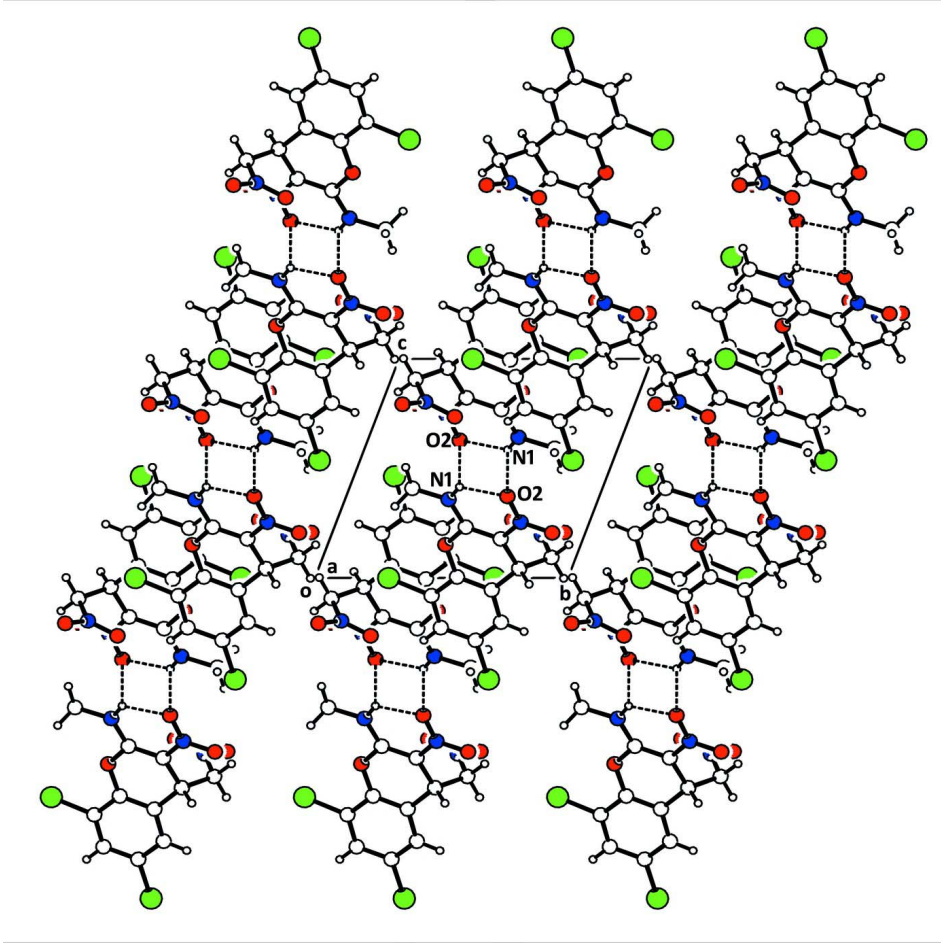

Figure 3

The crystal packing of (I) viewed down the *XO*-axis, showing intermolecular hydrogen bonding interactions as dashed lines.

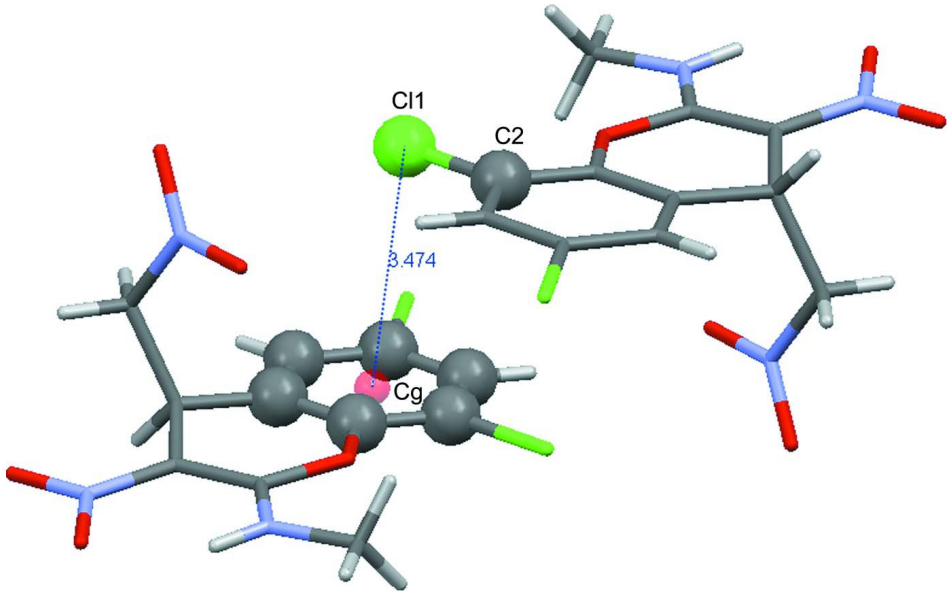

Figure 4

The molecular interaction showing the weak C—Cl···pi interaction in (I). *Cg* is a centroid of C1—C6 ring in 4*H*-chromene moiety.

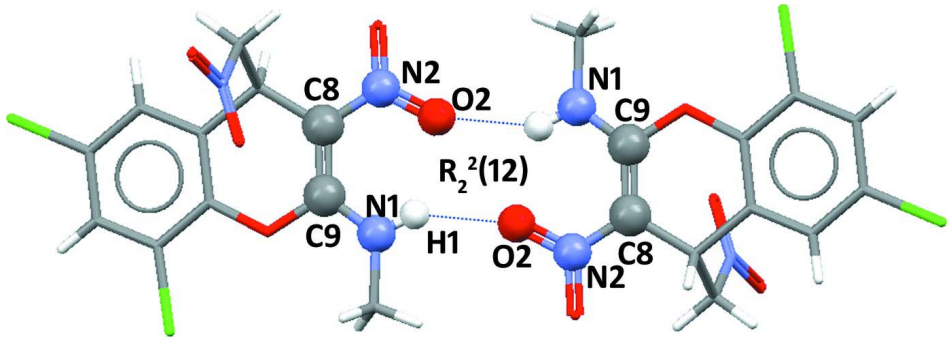

Figure 5

A view of intermolecular ring motif R_2^2 (12) formed by N—H···O interaction in (I). The motif forming atoms are shown in ball and stick model and the hydrogen bond are shown in blue dashed lines.

6,8-dichloro-*N*-methyl-3-nitro-4-nitromethyl-4*H*-chromen-2-amine

Crystal data

$C_{11}H_9Cl_2N_3O_5$
M_r = 334.11
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.7426 (7) Å
b = 9.2727 (7) Å
c = 9.3420 (7) Å
α = 70.017 (7)°
β = 72.609 (7)°
γ = 87.579 (6)°
V = 677.68 (9) Å^3

Z = 2
F(000) = 340
D_x = 1.637 Mg m^{-3}
Melting point: 485.65 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8735 reflections
θ = 2.7–29.2°
μ = 0.50 mm^{-1}
T = 293 K
Block, colourless
0.4 × 0.35 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9821 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.792, T_{max} = 1.000

15150 measured reflections
2385 independent reflections
2072 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.0°, θ_{min} = 2.7°
h = −10→10
k = −11→11
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.110
S = 1.01
2385 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.091P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.046
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.66030 (6)	0.29149 (5)	−0.00059 (6)	0.04277 (19)
Cl2	0.68824 (8)	0.83939 (6)	−0.46350 (6)	0.0599 (2)
O1	0.77375 (15)	0.46548 (12)	0.15081 (14)	0.0344 (3)
C6	0.79885 (19)	0.71693 (18)	−0.05514 (19)	0.0273 (4)
O3	1.02216 (15)	0.86894 (13)	0.20553 (15)	0.0389 (3)
N2	0.98248 (17)	0.72806 (15)	0.25417 (16)	0.0321 (3)
O2	1.01949 (18)	0.63676 (15)	0.37199 (16)	0.0494 (4)
O4	0.55005 (17)	0.69199 (16)	0.26437 (17)	0.0502 (4)
C1	0.7612 (2)	0.55977 (18)	0.00458 (19)	0.0283 (4)
C5	0.7793 (2)	0.80191 (19)	−0.20214 (19)	0.0312 (4)
H5	0.8046	0.9075	−0.2450	0.037*
C7	0.8539 (2)	0.79260 (17)	0.04217 (19)	0.0275 (4)
H7	0.9526	0.8554	−0.0288	0.033*
N1	0.8653 (2)	0.40896 (17)	0.35814 (18)	0.0383 (4)
H1	0.9139	0.4331	0.4152	0.046*
C3	0.6865 (2)	0.5726 (2)	−0.2272 (2)	0.0365 (4)

H3	0.6498	0.5253	−0.2850	0.044*
C8	0.8987 (2)	0.67447 (18)	0.17785 (19)	0.0285 (4)
C2	0.7067 (2)	0.48781 (19)	−0.0813 (2)	0.0316 (4)
C9	0.8488 (2)	0.51877 (19)	0.23183 (19)	0.0298 (4)
N3	0.56967 (19)	0.83127 (18)	0.19612 (18)	0.0373 (4)
C11	0.7329 (2)	0.90325 (17)	0.0935 (2)	0.0326 (4)
H11A	0.7759	0.9524	0.1510	0.039*
H11B	0.7223	0.9831	−0.0017	0.039*
C4	0.7221 (2)	0.7293 (2)	−0.2847 (2)	0.0355 (4)
C10	0.8075 (3)	0.2491 (2)	0.4088 (3)	0.0485 (5)
H10A	0.8584	0.2078	0.3263	0.073*
H10B	0.6932	0.2433	0.4287	0.073*
H10C	0.8325	0.1909	0.5049	0.073*
O5	0.4625 (2)	0.9172 (2)	0.2075 (2)	0.0744 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0508 (3)	0.0246 (3)	0.0566 (3)	−0.0001 (2)	−0.0175 (2)	−0.0172 (2)
Cl2	0.0942 (5)	0.0534 (4)	0.0365 (3)	0.0011 (3)	−0.0335 (3)	−0.0086 (2)
O1	0.0450 (7)	0.0202 (6)	0.0367 (6)	−0.0035 (5)	−0.0182 (5)	−0.0025 (5)
C6	0.0271 (8)	0.0246 (8)	0.0290 (8)	0.0025 (6)	−0.0077 (6)	−0.0084 (6)
O3	0.0469 (8)	0.0250 (7)	0.0444 (7)	−0.0074 (5)	−0.0186 (6)	−0.0064 (5)
N2	0.0362 (8)	0.0250 (8)	0.0314 (7)	−0.0018 (6)	−0.0139 (6)	−0.0018 (6)
O2	0.0678 (10)	0.0365 (8)	0.0478 (8)	−0.0027 (7)	−0.0388 (7)	−0.0004 (6)
O4	0.0407 (8)	0.0409 (8)	0.0602 (9)	−0.0049 (6)	−0.0082 (7)	−0.0117 (7)
C1	0.0295 (9)	0.0229 (8)	0.0299 (8)	0.0040 (6)	−0.0083 (7)	−0.0068 (6)
C5	0.0348 (9)	0.0245 (9)	0.0293 (8)	0.0015 (7)	−0.0071 (7)	−0.0053 (7)
C7	0.0308 (9)	0.0186 (8)	0.0295 (8)	−0.0006 (6)	−0.0096 (7)	−0.0030 (6)
N1	0.0483 (9)	0.0252 (8)	0.0387 (8)	−0.0021 (6)	−0.0221 (7)	0.0006 (6)
C3	0.0392 (10)	0.0387 (11)	0.0383 (10)	0.0041 (8)	−0.0126 (8)	−0.0208 (8)
C8	0.0309 (9)	0.0229 (8)	0.0307 (8)	0.0002 (7)	−0.0130 (7)	−0.0044 (6)
C2	0.0309 (9)	0.0238 (9)	0.0401 (9)	0.0028 (7)	−0.0077 (7)	−0.0136 (7)
C9	0.0296 (9)	0.0248 (9)	0.0322 (9)	0.0021 (7)	−0.0109 (7)	−0.0050 (7)
N3	0.0405 (9)	0.0388 (9)	0.0378 (8)	0.0085 (7)	−0.0150 (7)	−0.0177 (7)
C11	0.0397 (10)	0.0210 (8)	0.0383 (9)	0.0022 (7)	−0.0163 (7)	−0.0078 (7)
C4	0.0409 (10)	0.0369 (10)	0.0277 (8)	0.0045 (8)	−0.0101 (7)	−0.0106 (7)
C10	0.0579 (13)	0.0245 (10)	0.0514 (11)	−0.0055 (9)	−0.0192 (10)	0.0047 (8)
O5	0.0539 (10)	0.0656 (11)	0.0901 (13)	0.0263 (9)	−0.0061 (9)	−0.0262 (9)

Geometric parameters (Å, º)

Cl1—C2	1.7287 (16)	C7—H7	0.9800
Cl2—C4	1.7391 (17)	N1—C9	1.311 (2)
O1—C9	1.352 (2)	N1—C10	1.455 (2)
O1—C1	1.3812 (19)	N1—H1	0.8600
C6—C1	1.385 (2)	C3—C2	1.381 (2)
C6—C5	1.388 (2)	C3—C4	1.379 (2)

C6—C7	1.509 (2)	C3—H3	0.9300
O3—N2	1.2537 (17)	C8—C9	1.398 (2)
N2—O2	1.2593 (18)	N3—O5	1.208 (2)
N2—C8	1.370 (2)	N3—C11	1.492 (2)
O4—N3	1.222 (2)	C11—H11A	0.9700
C1—C2	1.392 (2)	C11—H11B	0.9700
C5—C4	1.383 (2)	C10—H10A	0.9600
C5—H5	0.9300	C10—H10B	0.9600
C7—C8	1.507 (2)	C10—H10C	0.9600
C7—C11	1.531 (2)		

C9—O1—C1	120.56 (13)	N2—C8—C7	116.78 (13)
C1—C6—C5	118.53 (15)	C9—C8—C7	122.28 (14)
C1—C6—C7	119.89 (14)	C3—C2—C1	120.45 (15)
C5—C6—C7	121.54 (14)	C3—C2—Cl1	120.48 (13)
O3—N2—O2	120.24 (13)	C1—C2—Cl1	119.04 (13)
O3—N2—C8	119.38 (12)	N1—C9—O1	111.86 (15)
O2—N2—C8	120.38 (13)	N1—C9—C8	127.76 (16)
O1—C1—C6	123.02 (14)	O1—C9—C8	120.38 (14)
O1—C1—C2	116.01 (14)	O5—N3—O4	123.38 (17)
C6—C1—C2	120.97 (15)	O5—N3—C11	116.64 (16)
C4—C5—C6	119.86 (15)	O4—N3—C11	119.98 (14)
C4—C5—H5	120.1	N3—C11—C7	115.17 (13)
C6—C5—H5	120.1	N3—C11—H11A	108.5
C8—C7—C6	110.98 (13)	C7—C11—H11A	108.5
C8—C7—C11	114.16 (13)	N3—C11—H11B	108.5
C6—C7—C11	111.64 (13)	C7—C11—H11B	108.5
C8—C7—H7	106.5	H11A—C11—H11B	107.5
C6—C7—H7	106.5	C3—C4—C5	121.98 (15)
C11—C7—H7	106.5	C3—C4—Cl2	118.91 (13)
C9—N1—C10	124.73 (17)	C5—C4—Cl2	119.08 (13)
C9—N1—H1	117.6	N1—C10—H10A	109.5
C10—N1—H1	117.6	N1—C10—H10B	109.5
C2—C3—C4	118.19 (15)	H10A—C10—H10B	109.5
C2—C3—H3	120.9	N1—C10—H10C	109.5
C4—C3—H3	120.9	H10A—C10—H10C	109.5
N2—C8—C9	120.80 (14)	H10B—C10—H10C	109.5

C9—O1—C1—C6	−10.9 (2)	C4—C3—C2—Cl1	178.69 (13)
C9—O1—C1—C2	169.50 (14)	O1—C1—C2—C3	178.49 (15)
C5—C6—C1—O1	−178.84 (15)	C6—C1—C2—C3	−1.1 (2)
C7—C6—C1—O1	−1.1 (2)	O1—C1—C2—Cl1	0.0 (2)
C5—C6—C1—C2	0.8 (2)	C6—C1—C2—Cl1	−179.62 (13)
C7—C6—C1—C2	178.55 (15)	C10—N1—C9—O1	−1.3 (3)
C1—C6—C5—C4	0.5 (2)	C10—N1—C9—C8	178.82 (18)
C7—C6—C5—C4	−177.25 (15)	C1—O1—C9—N1	−172.63 (14)
C1—C6—C7—C8	14.2 (2)	C1—O1—C9—C8	7.2 (2)
C5—C6—C7—C8	−168.08 (15)	N2—C8—C9—N1	3.4 (3)

C1—C6—C7—C11	−114.39 (16)	C7—C8—C9—N1	−172.13 (17)
C5—C6—C7—C11	63.3 (2)	N2—C8—C9—O1	−176.45 (15)
O3—N2—C8—C9	−178.20 (15)	C7—C8—C9—O1	8.0 (2)
O2—N2—C8—C9	1.9 (2)	O5—N3—C11—C7	−163.02 (15)
O3—N2—C8—C7	−2.4 (2)	O4—N3—C11—C7	17.5 (2)
O2—N2—C8—C7	177.65 (15)	C8—C7—C11—N3	−65.94 (19)
C6—C7—C8—N2	166.39 (14)	C6—C7—C11—N3	60.95 (17)
C11—C7—C8—N2	−66.4 (2)	C2—C3—C4—C5	1.1 (3)
C6—C7—C8—C9	−17.9 (2)	C2—C3—C4—Cl2	−176.92 (14)
C11—C7—C8—C9	109.33 (17)	C6—C5—C4—C3	−1.4 (3)
C4—C3—C2—C1	0.2 (3)	C6—C5—C4—Cl2	176.55 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.00	2.613 (2)	128
N1—H1···O2^{i}	0.86	2.12	2.881 (2)	147
C7—H7···O3^{ii}	0.98	2.50	3.1944 (19)	128
C11—H11*B*···O3^{ii}	0.97	2.54	3.103 (2)	117

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+2, −*z*.