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N-(4-Chlorophenyl)maleimide

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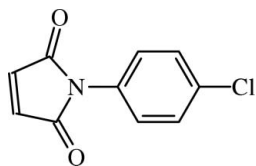
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.043; wR factor = 0.116; data-to-parameter ratio = 12.9.

In the title compound, $\text{C}_{10}\text{H}_6\text{ClNO}_2$, the dihedral angle between the benzene and maleimide rings is $47.54(9)^\circ$. Molecules form centrosymmetric dimers through $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, resulting in rings of graph-set motif $R_2^2(8)$ and chains in the [100] direction. Molecules are also linked by $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds along [001]. In this same direction, molecules are connected to other neighbouring molecules by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming edge-fused $R_4^4(24)$ rings.

Related literature

For general background, see: Etter (1990); Howell & Zhang (2006); Miller *et al.* (2000, 2001); Moreno-Fuquen, Valencia, Abonia, Kennedy & Graham (2003); Nardelli (1995); Sarma & Desiraju (1986).



Experimental

Crystal data

$\text{C}_{10}\text{H}_6\text{ClNO}_2$
 $M_r = 207.61$
 Monoclinic, $P2_1/c$
 $a = 10.6504(7)$ Å
 $b = 3.8589(2)$ Å
 $c = 22.0308(14)$ Å
 $\beta = 100.741(3)^\circ$
 $V = 889.57(9)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.40$ mm⁻¹
 $T = 150$ K
 $0.18 \times 0.04 \times 0.03$ mm

Data collection

Bruker-Nonius KappaCCD diffractometer
 Absorption correction: multi-scan (*DENZO*; Otwinowski & Minor, 1997)
 $T_{\min} = 0.951$, $T_{\max} = 0.982$
 11729 measured reflections
 1646 independent reflections
 1231 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.089$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.116$
 $S = 1.07$
 1646 reflections
 128 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{C8}-\text{H8}\cdots\text{O1}^{\text{i}}$ | 0.93 | 2.58 | 3.493 (3) | 169 |
| $\text{C2}-\text{H2}\cdots\text{O1}^{\text{ii}}$ | 0.93 | 2.77 | 3.659 (3) | 161 |
| $\text{C5}-\text{H5}\cdots\text{O2}^{\text{iii}}$ | 0.93 | 2.58 | 3.319 (3) | 137 |
| $\text{C9}-\text{H9}\cdots\text{O2}^{\text{iv}}$ | 0.93 | 2.64 | 3.326 (3) | 131 |
| $\text{C9}-\text{H9}\cdots\text{Cl1}^{\text{v}}$ | 0.93 | 2.89 | 3.551 (3) | 129 |

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

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 2000); cell refinement: *DENZO*; data reduction: *DENZO*; 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); software used to prepare material for publication: *PARST95* (Nardelli, 1995).

RMF dedicates this work to the memory of Professor J. Valderrama. RMF is grateful to the Instituto de Química Física Rocasolano, CSIC, Spain, for the use of the license of Cambridge Structural Database System (Allen, 2002). This work was partially supported by the Universidad del Valle, Colombia.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2150).

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supporting information

Acta Cryst. (2008). E64, o1991 [doi:10.1107/S160053680803016X]

***N*-(4-Chlorophenyl)maleimide**

Rodolfo Moreno-Fuquen, Zulay Pardo-Botero and Javier Ellena

S1. Comment

It is known that cyclic unsaturated dicarbonyl compounds such as *N*-substituted maleimides can be used in free-radical-initiated polymerization processes upon exposure to light (Howell & Zhang, 2006). In order to study the possible application of *N*-(*p*-chlorophenylmaleimide) (I) in polymerization processes, and to explain its hydrogen bonding patterns, the synthesis and the study of the crystal structure are reported in this work. *N*-(*p*-nitrophenylmaleimide) (4NPMI) (Moreno-Fuquen *et al.*, 2003), *N*-(*o*-chlorophenylmaleimide) (2CIPMI) systems (Miller *et al.*, 2001) show a close analogy to the title compounds and are thus employed as a basic reference for comparison. Perspective view of (I), showing the atomic numbering scheme, can be seen in Fig.1. In the arylmaleimide systems the value of the dihedral angle between the benzene and imidic rings influences on the polymerization process, and the presence of different substituents in the benzene ring change the value of this angle (Miller *et al.*, 2000). The photochemical properties of arylmaleimide systems depend on the value of this angle. The dihedral angle between benzene and maleimide planes is 42.98 (5)° for 4NPMI, 66.10 (4)° for 2CIPMI and 47.54 (9)° for (I). The chlorine atoms, which are pending on the aromatic nucleus, tend to steer the crystal structure to a state characterized by a short axis (Sarma & Desiraju, 1986). For (I), the *b* axis has a small value [3.8589 (2) Å] and a Cl...Cl nonbonded contact is observed at the same distance. The crystal structure of (I) is stabilized by weak intermolecular C—H...O and C—H...Cl hydrogen-bonds (Nardelli, 1995) (Table 1). The molecules of (I) are linked into a three-dimensional framework by a combination of C—H...O and C—H...Cl hydrogen bonds. The formation of the framework can be explained in terms of three-one substructures. In the first substructure, atom C8 in the molecule at (*x,y,z*) acts as a hydrogen-bond donor to maleimidic atom O1 in the molecule at (-*x*,1 - *y*,1 - *z*) and atom C9 in the molecule at (*x,y,z*) acts as a hydrogen-bond donor to maleimidic atom O2 in the molecule at (1 - *x*,1 - *y*,1 - *z*). Both interactions generate dimers containing centrosymmetric rings with graph motif $R_2^2(8)$ (Etter, 1990) (Fig. 2, supp. material). These dimers are linked by C(5) chains which are running parallel to [100] direction. In the second substructure, atom C9 in the molecule at (*x*,1/2 - *y*,-1/2 + *z*) acts as a hydrogen-bond donor to atom C11 in the molecule at (*x,y,z*), similarly, atom C5 in the molecule at (*x,y,z*) acts as a hydrogen-bond donor to maleimidic atom O2 in the molecule at (*x*,1 + *y*,*z*) so generating a chain of edge-fused $R_4^4(24)$ rings along [001] (Fig. 3, supp. material). The third one-dimensional substructure is built by C—H...O hydrogen bonds. Atom C2 in the molecule at (*x,y,z*) acts as hydrogen bond donor to maleimidic O1 in the molecule at (-*x*,-1/2 + *y*,1/2 - *z*) so generating a C(7) chains in the [010] direction (Fig.4, supp. material). The low value of the dihedral angle between benzene and maleimide planes, allows to conclude that (I) is not a good candidate to use in a photopolymerization process.

S2. Experimental

All reagents (purchased from Aldrich) and solvents were used as received. Column chromatography was performed using silica gel H60 to purify the intermediates and final products. Thin layer chromatography (TLC) was used to confirm the structure of the individual compounds.

S3. Refinement

The space group $P 2_1/c$ for (I) was uniquely assigned from the systematic absences. All H-atoms were located from difference maps and then treated as riding atoms [$C-H = 0.93 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(C)$].

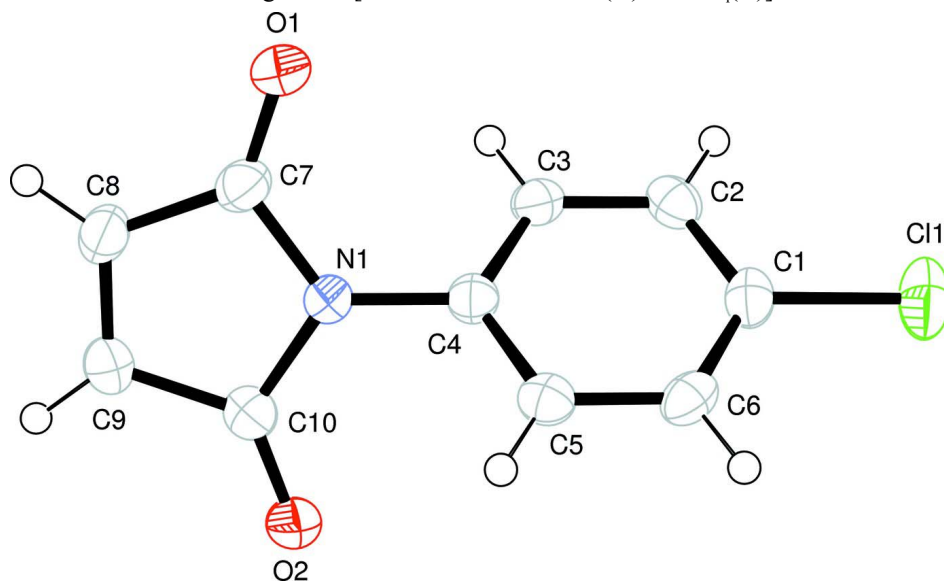
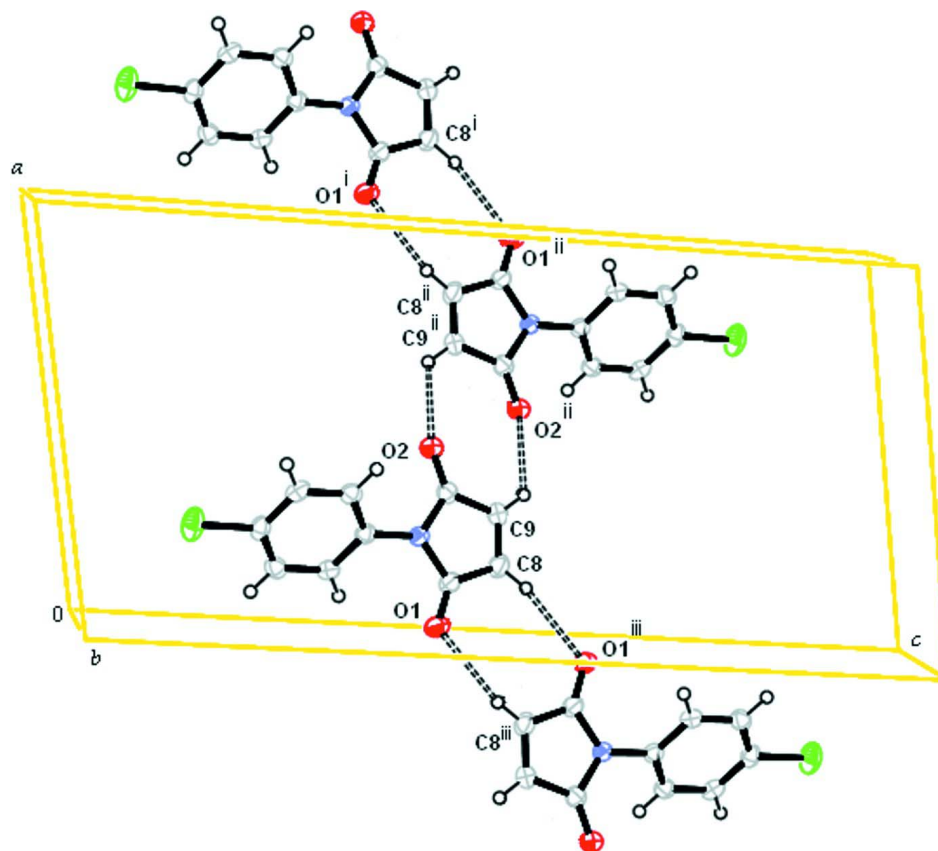
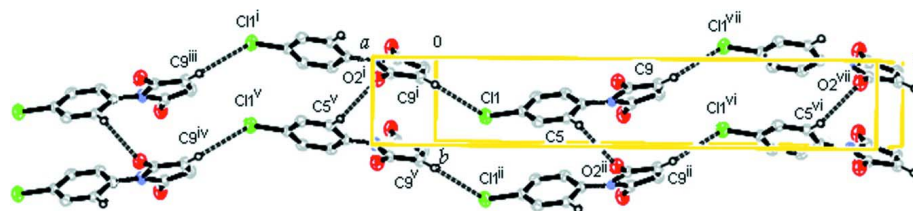


Figure 1

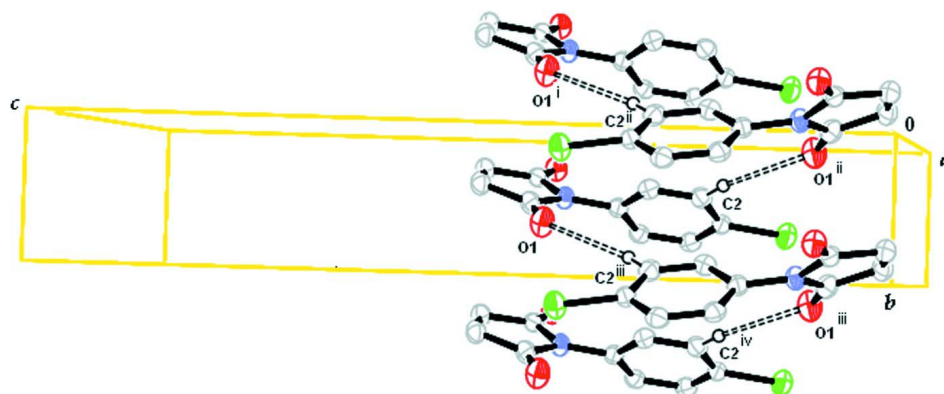
An ORTEP-3 (Farrugia, 1997) plot of the (I) compound, with the atomic labelling scheme. The shapes of the ellipsoids correspond to 50% probability contours of atomic displacement and, for the sake of clarity, H atoms are shown as spheres of arbitrary radius.


Figure 2

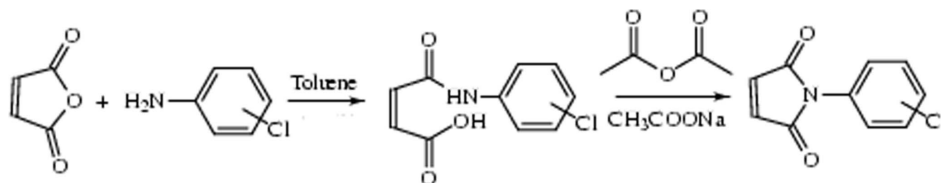
Part of the crystal structure of (I) showing the formation of centrosymmetric $R_2^2(8)$ dimers rings and C(4) chains which are running parallel to the [100] direction. [Symmetry codes: (i) $1 + x, y + z$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $-x, 1 - y, 1 - z$].


Figure 3

Part of the crystal structure of (I) showing the formation of C(9) chains and edge-fused $R_4^4(24)$ rings along [001]. [Symmetry codes: (i) $x, 1/2 - y, -1/2 + z$; (ii) $x, 1 + y, z$; (iii) $x, y, -1 + z$; (iv) $x, 1 + y, -1 + z$; (v) $x, 3/2 - y, -1/2 + z$; (vi) $x, 1/2 - y, 1/2 + z$; (vii) $x, 1/2 - y, 1/2 + z$].


Figure 4

Part of the crystal structure of (I) showing the formation of C(7) chains along [010]. [Symmetry codes: (i) $x, -1 + y, z$; (ii) $-x, -1/2 + y, 1/2 + z$; (iii) $-x, 1/2 + y, 1/2 - z$; (iv) $x, 1 + y, z$].


Figure 5

The formation of the title compound.

N-(4-Chlorophenyl)maleimide

Crystal data

$C_{10}H_6ClNO_2$

$M_r = 207.61$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 10.6504\ (7)\ \text{\AA}$

$b = 3.8589\ (2)\ \text{\AA}$

$c = 22.0308\ (14)\ \text{\AA}$

$\beta = 100.741\ (3)^\circ$

$V = 889.57\ (9)\ \text{\AA}^3$

$Z = 4$

$F(000) = 424$

$D_x = 1.550\ \text{Mg m}^{-3}$

Melting point: $384(1)\ \text{K}$

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

Cell parameters from 11729 reflections

$\theta = 2.9\text{--}25.4^\circ$

$\mu = 0.40\ \text{mm}^{-1}$

$T = 150\ \text{K}$

Needle, pale-yellow

$0.18 \times 0.04 \times 0.03\ \text{mm}$

Data collection

Bruker–Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*DENZO*; Otwinowski & Minor, 1997)

$T_{\min} = 0.951$, $T_{\max} = 0.982$

11729 measured reflections

1646 independent reflections

1231 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.089$

$\theta_{\max} = 25.4^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -12 \rightarrow 12$

$k = -4 \rightarrow 4$

$l = -24 \rightarrow 26$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.116$
 $S = 1.07$
 1646 reflections
 128 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
 $w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.491P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|------------|--------------|----------------------------------|
| Cl1 | 0.26337 (8) | 0.6828 (2) | 0.13972 (3) | 0.0486 (3) |
| O1 | 0.04581 (16) | 0.6461 (5) | 0.40894 (8) | 0.0419 (5) |
| O2 | 0.45773 (15) | 0.2532 (5) | 0.43624 (8) | 0.0342 (5) |
| N1 | 0.25175 (18) | 0.4677 (5) | 0.40446 (9) | 0.0278 (5) |
| C1 | 0.2590 (2) | 0.6168 (6) | 0.21732 (11) | 0.0303 (6) |
| C2 | 0.1564 (2) | 0.4474 (7) | 0.23409 (11) | 0.0314 (6) |
| H2 | 0.0899 | 0.3657 | 0.2040 | 0.038* |
| C3 | 0.1537 (2) | 0.4004 (6) | 0.29608 (11) | 0.0282 (6) |
| H3 | 0.0852 | 0.2870 | 0.3081 | 0.034* |
| C4 | 0.2542 (2) | 0.5240 (6) | 0.34041 (11) | 0.0269 (6) |
| C5 | 0.3567 (2) | 0.6933 (6) | 0.32329 (12) | 0.0283 (6) |
| H5 | 0.4237 | 0.7748 | 0.3532 | 0.034* |
| C6 | 0.3585 (2) | 0.7399 (6) | 0.26132 (12) | 0.0303 (6) |
| H6 | 0.4266 | 0.8541 | 0.2492 | 0.036* |
| C7 | 0.1462 (2) | 0.5170 (7) | 0.43329 (12) | 0.0323 (6) |
| C8 | 0.1852 (2) | 0.3901 (7) | 0.49762 (11) | 0.0340 (6) |
| H8 | 0.1336 | 0.3862 | 0.5273 | 0.041* |
| C9 | 0.3057 (2) | 0.2833 (7) | 0.50601 (12) | 0.0317 (6) |
| H9 | 0.3524 | 0.1958 | 0.5427 | 0.038* |
| C10 | 0.3538 (2) | 0.3260 (6) | 0.44722 (11) | 0.0291 (6) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| Cl1 | 0.0730 (6) | 0.0459 (5) | 0.0305 (4) | 0.0071 (4) | 0.0186 (4) | 0.0053 (3) |
| O1 | 0.0297 (10) | 0.0600 (13) | 0.0376 (11) | 0.0126 (9) | 0.0101 (8) | 0.0056 (9) |
| O2 | 0.0285 (10) | 0.0420 (11) | 0.0320 (10) | 0.0049 (8) | 0.0055 (8) | -0.0004 (8) |
| N1 | 0.0251 (11) | 0.0339 (12) | 0.0249 (11) | 0.0031 (9) | 0.0061 (9) | 0.0013 (9) |
| C1 | 0.0401 (15) | 0.0260 (14) | 0.0262 (14) | 0.0073 (11) | 0.0102 (11) | 0.0018 (11) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C2 | 0.0325 (14) | 0.0296 (14) | 0.0304 (15) | 0.0052 (11) | 0.0009 (11) | -0.0018 (11) |
| C3 | 0.0242 (13) | 0.0275 (14) | 0.0337 (14) | 0.0016 (10) | 0.0074 (11) | 0.0025 (11) |
| C4 | 0.0274 (13) | 0.0262 (13) | 0.0277 (13) | 0.0047 (10) | 0.0064 (10) | 0.0008 (10) |
| C5 | 0.0278 (13) | 0.0252 (13) | 0.0316 (14) | 0.0035 (10) | 0.0045 (10) | -0.0025 (11) |
| C6 | 0.0301 (13) | 0.0260 (14) | 0.0382 (16) | 0.0034 (11) | 0.0151 (12) | 0.0020 (11) |
| C7 | 0.0286 (14) | 0.0368 (15) | 0.0329 (15) | 0.0005 (12) | 0.0097 (11) | -0.0052 (12) |
| C8 | 0.0361 (15) | 0.0392 (16) | 0.0288 (14) | -0.0014 (12) | 0.0121 (11) | -0.0005 (12) |
| C9 | 0.0346 (15) | 0.0338 (14) | 0.0260 (14) | -0.0009 (12) | 0.0036 (11) | -0.0013 (11) |
| C10 | 0.0311 (14) | 0.0261 (13) | 0.0292 (14) | 0.0017 (11) | 0.0036 (11) | -0.0025 (11) |

Geometric parameters (Å, °)

| | | | |
|--------------|--------------|--------------|------------|
| Cl1—C1 | 1.738 (2) | C3—H3 | 0.9300 |
| O1—C7 | 1.210 (3) | C4—C5 | 1.384 (3) |
| O2—C10 | 1.209 (3) | C5—C6 | 1.380 (4) |
| N1—C7 | 1.404 (3) | C5—H5 | 0.9300 |
| N1—C10 | 1.410 (3) | C6—H6 | 0.9300 |
| N1—C4 | 1.433 (3) | C7—C8 | 1.484 (4) |
| C1—C6 | 1.380 (4) | C8—C9 | 1.327 (4) |
| C1—C2 | 1.381 (4) | C8—H8 | 0.9300 |
| C2—C3 | 1.383 (3) | C9—C10 | 1.489 (4) |
| C2—H2 | 0.9300 | C9—H9 | 0.9300 |
| C3—C4 | 1.392 (3) | | |
| C7—N1—C10 | 109.5 (2) | C4—C5—H5 | 120.4 |
| C7—N1—C4 | 126.0 (2) | C1—C6—C5 | 120.0 (2) |
| C10—N1—C4 | 124.3 (2) | C1—C6—H6 | 120.0 |
| C6—C1—C2 | 121.1 (2) | C5—C6—H6 | 120.0 |
| C6—C1—Cl1 | 118.86 (19) | O1—C7—N1 | 124.8 (2) |
| C2—C1—Cl1 | 120.01 (19) | O1—C7—C8 | 128.8 (2) |
| C1—C2—C3 | 119.3 (2) | N1—C7—C8 | 106.4 (2) |
| C1—C2—H2 | 120.4 | C9—C8—C7 | 109.1 (2) |
| C3—C2—H2 | 120.4 | C9—C8—H8 | 125.5 |
| C2—C3—C4 | 119.5 (2) | C7—C8—H8 | 125.5 |
| C2—C3—H3 | 120.2 | C8—C9—C10 | 109.0 (2) |
| C4—C3—H3 | 120.2 | C8—C9—H9 | 125.5 |
| C5—C4—C3 | 120.9 (2) | C10—C9—H9 | 125.5 |
| C5—C4—N1 | 120.0 (2) | O2—C10—N1 | 125.3 (2) |
| C3—C4—N1 | 119.1 (2) | O2—C10—C9 | 128.7 (2) |
| C6—C5—C4 | 119.2 (2) | N1—C10—C9 | 106.0 (2) |
| C6—C5—H5 | 120.4 | | |
| C6—C1—C2—C3 | 0.0 (4) | C10—N1—C7—O1 | 177.3 (3) |
| Cl1—C1—C2—C3 | -179.27 (18) | C4—N1—C7—O1 | -7.5 (4) |
| C1—C2—C3—C4 | -0.1 (4) | C10—N1—C7—C8 | -1.2 (3) |
| C2—C3—C4—C5 | 0.0 (4) | C4—N1—C7—C8 | 174.0 (2) |
| C2—C3—C4—N1 | -178.7 (2) | O1—C7—C8—C9 | -177.0 (3) |
| C7—N1—C4—C5 | 136.1 (3) | N1—C7—C8—C9 | 1.5 (3) |

| | | | |
|--------------|-------------|--------------|------------|
| C10—N1—C4—C5 | -49.4 (3) | C7—C8—C9—C10 | -1.1 (3) |
| C7—N1—C4—C3 | -45.1 (3) | C7—N1—C10—O2 | 179.8 (2) |
| C10—N1—C4—C3 | 129.4 (3) | C4—N1—C10—O2 | 4.4 (4) |
| C3—C4—C5—C6 | 0.1 (4) | C7—N1—C10—C9 | 0.6 (3) |
| N1—C4—C5—C6 | 178.9 (2) | C4—N1—C10—C9 | -174.7 (2) |
| C2—C1—C6—C5 | 0.2 (4) | C8—C9—C10—O2 | -178.8 (3) |
| C11—C1—C6—C5 | 179.46 (18) | C8—C9—C10—N1 | 0.3 (3) |
| C4—C5—C6—C1 | -0.3 (4) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C8—H8 \cdots O1 ⁱ | 0.93 | 2.58 | 3.493 (3) | 169 |
| C2—H2 \cdots O1 ⁱⁱ | 0.93 | 2.77 | 3.659 (3) | 161 |
| C5—H5 \cdots O2 ⁱⁱⁱ | 0.93 | 2.58 | 3.319 (3) | 137 |
| C9—H9 \cdots O2 ^{iv} | 0.93 | 2.64 | 3.326 (3) | 131 |
| C9—H9 \cdots C11 ^v | 0.93 | 2.89 | 3.551 (3) | 129 |

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