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Key indicators

Single-crystal X-ray study

T = 193 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.047

wR factor = 0.112

Data-to-parameter ratio = 13.4

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

1-Methyl-4-nitro-2-(trichloroacetyl)pyrrole

The crystal structure of the title compound, $\text{C}_7\text{H}_5\text{Cl}_3\text{N}_2\text{O}_3$, has been determined in the orthorhombic space group *Pbca*. The CNO skeleton is essentially planar, except for the carbonyl O atom, which deviates by $0.217(3) \text{ \AA}$. There is a strong interaction between one of the nitro O atoms and a Cl atom of a neighbouring molecule.

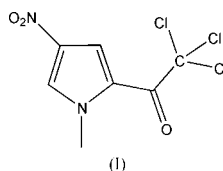
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Comment

In the past decade, Dervan and co-workers have discovered that polyamides with certain numbers of *N*-methylpyrrole carboxamides and *N*-methylimidazole carboxamides can recognize and bind in the minor groove of predetermined DNA sequences with high affinity and specificity, comparable to naturally occurring DNA-binding proteins, and further regulate gene expression (Dervan & Bürl, 1999; Simon *et al.*, 2000). These properties stimulated our interest in this field. Crystals of the title compound, (I), were obtained as an intermediate in our synthetic investigations of polyamides.



The molecular structure and a packing diagram of (I) are illustrated in Figs. 1 and 2, respectively. Selected geometric parameters of (I) are listed in Table 1. Inspection of these values indicates that there is delocalization of the π -electron

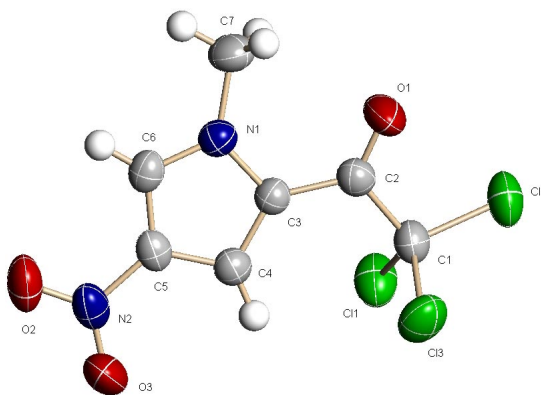


Figure 1

The structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

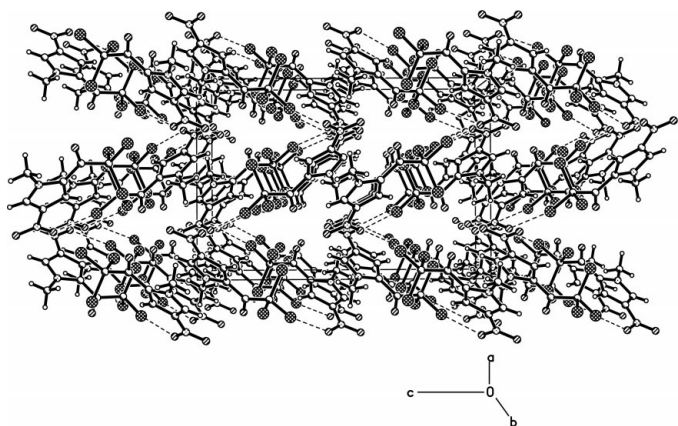


Figure 2

A packing diagram of (I), viewed along the *b* axis. The strong intermolecular O...Cl interactions are shown as dashed lines.

density in the pyrrole ring. Furthermore, there are no significant differences from the geometry found in a similar pyrrole (Lu *et al.*, 2003). The 12 atoms N1–N2, O1–O3 and C1–C7 are essentially coplanar, the r.m.s. deviation being 0.088 Å and the maximum deviation from the plane 0.217 (3) Å for O1. There is a strong interaction between O3 and Cl2(1 – *x*, –1 – *y*, 1 – *z*), with an O3...Cl2A distance of 3.015 (2) Å.

Experimental

The title compound, (I), was synthesized according to a literature procedure (Nishiwaki *et al.*, 1988), with minor modification. The product was dissolved in CHCl₃ and the solution was set aside at room temperature. As the solvent slowly evaporated, crystals of (I) were formed.

Crystal data

C₇H₅Cl₃N₂O₃
M_r = 271.48
 Orthorhombic, *Pbca*
a = 11.590 (4) Å
b = 10.603 (3) Å
c = 16.935 (5) Å
V = 2081.2 (11) Å³
Z = 8
D_x = 1.733 Mg m^{–3}

Mo *K*α radiation
 Cell parameters from 3073 reflections
 $\theta = 2.9\text{--}27.2^\circ$
 $\mu = 0.87\text{ mm}^{-1}$
T = 193 (2) K
 Block, yellow
 0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
 ω scans
 Absorption correction: none
 7949 measured reflections
 1837 independent reflections

1574 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -13 \rightarrow 12$
 $k = -11 \rightarrow 12$
 $l = -18 \rightarrow 20$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.112$
 $S = 1.09$
 1837 reflections
 137 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.8439P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.33\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.19\text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

O2–N2	1.224 (3)	N2–O3	1.217 (3)
Cl1–C1	1.769 (3)	N2–C5	1.421 (4)
Cl2–C1	1.762 (3)	N1–C6	1.331 (3)
Cl3–C1	1.769 (3)	N1–C7	1.465 (4)
C3–C4	1.371 (4)	C2–O1	1.199 (3)
C3–N1	1.393 (3)	C2–C1	1.556 (4)
C3–C2	1.457 (4)	C5–C6	1.372 (4)
C4–C5	1.394 (4)		
C4–C3–N1	107.8 (2)	C6–C5–C4	108.8 (2)
C4–C3–C2	131.3 (2)	C6–C5–N2	125.5 (3)
N1–C3–C2	120.8 (2)	C4–C5–N2	125.7 (3)
C3–C4–C5	106.3 (2)	C2–C1–Cl2	109.0 (2)
O3–N2–C5	118.4 (3)	C2–C1–Cl1	111.87 (19)
O2–N2–C5	118.1 (3)	Cl2–C1–Cl1	107.77 (16)
C6–N1–C3	109.1 (2)	C2–C1–Cl3	108.8 (2)
O1–C2–C3	124.0 (3)	Cl2–C1–Cl3	109.01 (16)
O1–C2–C1	118.0 (3)	Cl1–C1–Cl3	110.32 (17)
C3–C2–C1	118.0 (2)	N1–C6–C5	108.0 (2)
N1–C3–C4–C5	–0.2 (3)	N1–C3–C2–O1	9.0 (4)
C2–C3–C4–C5	177.0 (3)	C4–C3–C2–C1	10.9 (4)
C4–C3–N1–C6	–0.2 (3)	N1–C3–C2–C1	–172.1 (2)
C2–C3–N1–C6	–177.8 (2)	C3–C4–C5–C6	0.5 (3)
C4–C3–N1–C7	–175.1 (3)	C3–C4–C5–N2	179.0 (2)
C2–C3–N1–C7	7.3 (4)	C3–N1–C6–C5	0.5 (3)
C4–C3–C2–O1	–168.0 (3)		

H atoms attached to C atoms were placed in geometrically idealized positions, with $Csp^2\text{--H} = 0.93\text{ \AA}$ and $Csp^3\text{--H} = 0.96\text{ \AA}$, and were constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{C})$, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2000); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2000); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

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