Liping Lu, Chengyong Zhou, Guocai Zhang, Miaoli Zhu and Pin Yang*

Institute of Molecular Science, University of Shanxi, Taiyuan, Shanxi 030006, People’s Republic of China

Correspondence e-mail: yangpin@sxu.edu.cn

Key indicators

Single-crystal X-ray study

T = 193 K

Mean σ(C-C) = 0.004 Å

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.

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

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 & Bühr, 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 \( \pi \)-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.
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 0.08 Å and the maximum deviation from the plane 0.217 (3) Å for O1. There is a strong interaction between O3 and C12(1 − χ, −1 − χ, 1 − χ), with an O3···C12A 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

Mᵣ = 271.48

Orthorhombic, Pnca

a = 11.590 (4) Å

b = 10.603 (3) Å

c = 16.935 (5) Å

V = 2081.2 (11) Å³

Z = 8

Dᵣ = 1.733 Mg m⁻³

**Data collection**

Mo Kα radiation

Cell parameters from 3073 reflections

θ = 2.9–27.2°

μ = 0.87 mm⁻¹

T = 193 (2) K

Block, yellow

0.20 × 0.20 × 0.20 mm

1574 reflections with I > 2σ(I)

Refinement

Refinement on F²

R[F² > 2σ(F²)] = 0.047

wR[F²] = 0.112

S = 1.09

1837 reflections

137 parameters

H-atom parameters constrained


### Table 1

<table>
<thead>
<tr>
<th>Bond</th>
<th>Distance (Å)</th>
</tr>
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<tbody>
<tr>
<td>O2···N2</td>
<td>1.224 (3)</td>
</tr>
<tr>
<td>N2···O3</td>
<td>1.217 (3)</td>
</tr>
<tr>
<td>C1···C1</td>
<td>1.769 (3)</td>
</tr>
<tr>
<td>C1···C2</td>
<td>1.762 (3)</td>
</tr>
<tr>
<td>C2···C3</td>
<td>1.769 (3)</td>
</tr>
<tr>
<td>C3···C4</td>
<td>1.37 (4)</td>
</tr>
<tr>
<td>C4···C5</td>
<td>1.394 (4)</td>
</tr>
<tr>
<td>C1···N1</td>
<td>1.393 (3)</td>
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<tr>
<td>C2···C1</td>
<td>1.457 (4)</td>
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<td>1.180 (3)</td>
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<tr>
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<td>1.180 (3)</td>
</tr>
<tr>
<td>C6···C2</td>
<td>1.180 (3)</td>
</tr>
</tbody>
</table>

H atoms attached to C atoms were placed in geometrically idealized positions, with Csp²–H = 0.93 Å and Csp³–H = 0.96 Å, and were constrained to ride on their parent atoms, with Uiso(H) = 1.2Ueq(C) and 1.5Ueq(C), respectively.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; 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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**References**


