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1-(3-Chloro-4-methylphenyl)-3-pyrroline-2,5-dione

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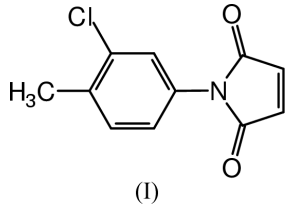
The structure of the title compound, $C_{11}H_8ClNO_2$, (I), comprises a twisted molecule with the dihedral angle between the two rings being 49.9 (2)°. Several C—H···*X* short contacts exist to both O atoms, but not to the Cl atom. The resultant structure packs in a noncentrosymmetric space group ($Pna2_1$) and the bulk material exhibits a second harmonic signal of I/I_{urea} = 0.09.

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.131
Data-to-parameter ratio = 15.2

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



(I)

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from an acetone solution.

Crystal data

$C_{11}H_8ClNO_2$
M_r = 221.63
Orthorhombic, $Pna2_1$
a = 10.473 (2) Å
b = 24.303 (5) Å
c = 3.8594 (8) Å
V = 982.3 (3) Å^3
Z = 4
D_x = 1.499 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 4247 reflections
θ = 2.9–39.4°
μ = 0.36 mm^{-1}
T = 150 (2) K
Needle, yellow
0.55 × 0.05 × 0.05 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.825, T_{max} = 0.982
6579 measured reflections
2076 independent reflections
1583 reflections with $I > 2\sigma(I)$
R_{int} = 0.091
θ_{max} = 27.5°
h = 0 → 13
k = 0 → 31
l = −4 → 4

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.131
S = 1.00
2076 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.28 (11)

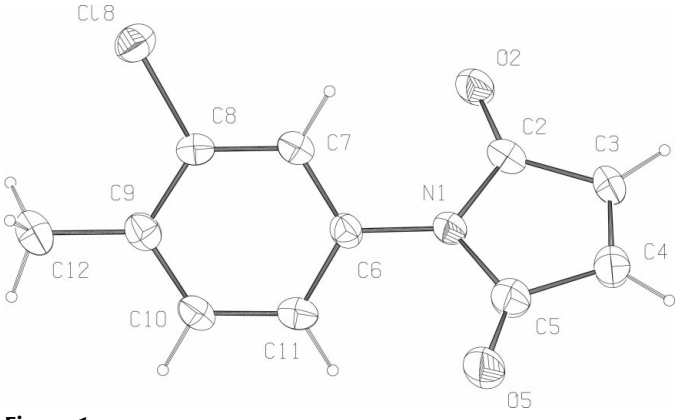


Figure 1
The molecular configuration and atom numbering scheme for (I), showing 50% probability ellipsoids.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.95	2.52	3.150 (4)	124
C7—H7···O2^{ii}	0.95	2.59	3.325 (4)	135
C10—H10···O5^{iii}	0.95	2.57	3.480 (4)	160

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

All H atoms were included in the refinement at calculated positions as riding models with C—H set to 0.95 (Ar-H) and 0.98 Å (CH_3). The number of Friedel pairs is 560.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1990); software used to prepare material for publication: *SHELXL*97.

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