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1,5-Dichloro-2,4-dinitrobenzene

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.061
wR factor = 0.163
Data-to-parameter ratio = 13.6

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

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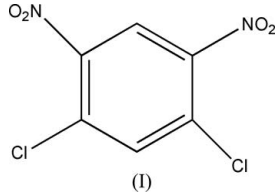
In the title compound, $C_6H_2Cl_2N_2O$, the two nitro groups are twisted away from the plane of the aromatic ring. Intermolecular short Cl···O and Cl···Cl contacts are observed in the crystal structure.

Comment

1,5-Dichloro-2,4-dinitrobenzene, (I), is an important intermediate which can be used for the syntheses of dyes and pesticides (Lv, 1995). We report here the crystal structure of (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The O—N—C—C torsion angles (Table 1) indicate that the two nitro groups are twisted away from the plane of the attached ring.

Short intermolecular Cl···O [Cl1···O4($2-x, 2-y, 1-z$) = 3.158 (5) Å] and Cl···Cl [Cl2···Cl2($1-x, -y, 1-z$) = 3.261 (2) Å] contacts are observed in the crystal structure.

Experimental

Compound (I) was prepared according to the reported procedure of Lv (1995). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol (50 ml) solution of (I) (1.0 g).

Crystal data

$C_6H_2Cl_2N_2O_4$
M_r = 237.00
Monoclinic, $P2_1/c$
a = 9.5900 (19) Å
b = 6.5860 (13) Å
c = 14.751 (3) Å
β = 106.86 (3)°
V = 891.6 (3) Å^3
Z = 4
D_x = 1.766 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 298 (2) K
Block, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.814, T_{max} = 0.932
1845 measured reflections
1739 independent reflections
1065 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.8029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.061$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.163$	$\Delta\rho_{max} = 0.39$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
1739 reflections	Extinction correction: *SHELXL97* (Sheldrick, 1997)
128 parameters	Extinction coefficient: 0.081 (7)
H-atom parameters constrained	

Table 1
Selected torsion angles (°).

O4—N2—C2—C3	−135.2 (5)	O2—N1—C4—C3	−33.8 (6)
O3—N2—C2—C3	42.0 (7)	O1—N1—C4—C3	144.9 (4)
O4—N2—C2—C1	45.8 (7)	O2—N1—C4—C5	145.8 (4)
O3—N2—C2—C1	−137.0 (5)	O1—N1—C4—C5	−35.6 (6)

H atoms were positioned geometrically (C—H = 0.93 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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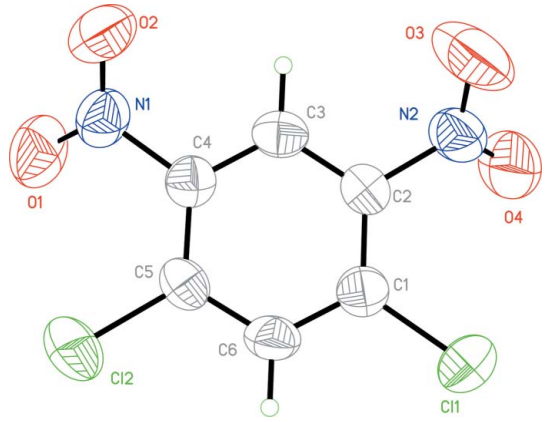

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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