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Isopropyl 4-chloro-3,5-dinitrobenzoate

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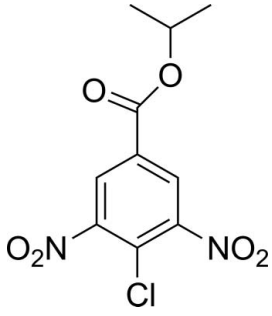
Key indicators: single-crystal X-ray study; T = 103 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.114; data-to-parameter ratio = 15.5.

In the title compound, $C_{10}H_9ClN_2O_6$, the two nitro groups and the ester group are oriented with respect to the benzene ring at dihedral angles of 49.42 (13)/87.61 (13) and 9.10 (10)°, respectively. In the crystal structure, a weak C—H···O interaction is present. A short Cl···O contact of 2.972 (2) Å is also observed in the crystal structure.

Related literature

For the application of the title compound as a herbicide and fungicide, see: Akira *et al.* (1978); Ferenc *et al.* (1984).



Experimental

Crystal data

$C_{10}H_9ClN_2O_6$
M_r = 288.64
Triclinic, $P\overline{1}$
a = 4.703 (2) Å
b = 10.783 (5) Å
c = 12.734 (5) Å
α = 69.483 (12)°
β = 87.75 (2)°
γ = 89.61 (2)°
V = 604.3 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 103 K
0.57 × 0.22 × 0.10 mm

Data collection

Rigaku SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.830, T_{max} = 0.967
5643 measured reflections
2689 independent reflections
1756 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 1.00
2689 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.95	2.35	3.178 (3)	146

Symmetry code: (i) $-x+1, -y+1, -z+2$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5065).

References

Akira, S., Shoji, K. & Kenichi, S. (1978). Jpn. Patent No. 53101528.
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Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
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supplementary materials

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Isopropyl 4-chloro-3,5-dinitrobenzoate

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Comment

Isopropyl 4-chloro-3,5-dinitrobenzoate (Fig. 1) is a useful herbicide and fungicide (Akira *et al.*, 1978; Ferenc *et al.*, 1984). It was used as the acid compounds to combat fungal diseases and weeds. We report here the crystal structure of the title compound. Two nitro groups (O3/ N1/O4 and O5/N2/O6) attached at C2 and C4, the ester group (O1/C7/O2) attached at C6 form dihedral angles of 49.4 (1)°, 87.6 (1)° and 9.1 (1)° with the mean plane of the C1-benzene ring, respectively. In the crystal structure, adjacent molecules are linked together by the weak C—H···O hydrogen bonds (Table 1).

Experimental

Commercial isopropyl 4-chloro-3,5-dinitrobenzoate was recrystallized by slow evaporation of methanol solution. Colourless single crystals were formed after several weeks.

Refinement

H atoms were placed in calculated positions and were allowed to ride on the parent C atoms with C—H distances of 0.95 (aromatic), 0.98 (methyl) and 1.00 Å (methine); U_{iso}(H) = 1.5U$_{eq}$(C) for methyl H atoms and 1.2U$_{eq}$(C) for the others.

Figures

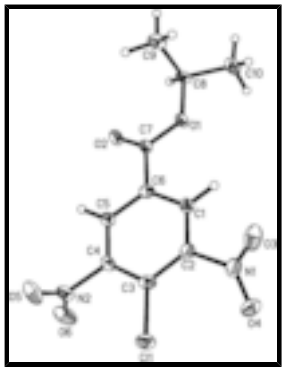

Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 50% probability level.

Isopropyl 4-chloro-3,5-dinitrobenzoate

Crystal data

$C_{10}H_9ClN_2O_6$	$Z = 2$
$M_r = 288.64$	$F(000) = 296$
Triclinic, $P\overline{1}$	$D_x = 1.586$ Mg m^{-3}

Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.703$ (2) Å	Cell parameters from 1327 reflections
$b = 10.783$ (5) Å	$\theta = 3.1–27.5°$
$c = 12.734$ (5) Å	$\mu = 0.34$ mm^{-1}
$\alpha = 69.483$ (12)°	$T = 103$ K
$\beta = 87.75$ (2)°	Prism, colourless
$\gamma = 89.61$ (2)°	0.57 × 0.22 × 0.10 mm
$V = 604.3$ (5) Å^3	

Data collection

Rigaku SPIDER diffractometer	2689 independent reflections
Radiation source: Rotating Anode	1756 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.030$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.8°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -6\rightarrow6$
$T_{min} = 0.830$, $T_{max} = 0.967$	$k = -14\rightarrow13$
5643 measured reflections	$l = -16\rightarrow15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.114$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.219P]$ where $P = (F_o^2 + 2F_c^2)/3$
2689 reflections	$(\Delta/\sigma)_{max} < 0.001$
174 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.35262 (13)	0.43193 (6)	0.65836 (5)	0.02487 (18)
O1	0.4518 (3)	0.85871 (15)	0.76139 (13)	0.0185 (4)
O2	0.3137 (3)	0.67501 (15)	0.90566 (13)	0.0208 (4)
O3	1.2776 (4)	0.83028 (19)	0.51714 (14)	0.0338 (5)
O4	1.1930 (4)	0.66488 (19)	0.46231 (15)	0.0359 (5)
O5	1.2157 (4)	0.31097 (18)	0.93908 (16)	0.0343 (5)
O6	0.8756 (4)	0.24121 (18)	0.86381 (17)	0.0364 (5)
N1	1.1805 (4)	0.7201 (2)	0.53094 (17)	0.0240 (5)
N2	1.0218 (4)	0.3277 (2)	0.87522 (18)	0.0226 (5)
C1	0.8350 (5)	0.7223 (2)	0.67783 (18)	0.0170 (5)
H1	0.7969	0.8119	0.6342	0.020*
C2	1.0341 (5)	0.6512 (2)	0.64011 (18)	0.0182 (5)
C3	1.1009 (5)	0.5203 (2)	0.7020 (2)	0.0187 (5)
C4	0.9569 (5)	0.4649 (2)	0.80468 (19)	0.0170 (5)
C5	0.7538 (5)	0.5317 (2)	0.8453 (2)	0.0177 (5)
H5	0.6590	0.4898	0.9161	0.021*
C6	0.6914 (5)	0.6612 (2)	0.78022 (19)	0.0165 (5)
C7	0.4638 (5)	0.7312 (2)	0.82410 (19)	0.0160 (5)
C8	0.2407 (5)	0.9393 (2)	0.7970 (2)	0.0188 (5)
H8	0.0665	0.8848	0.8302	0.023*
C9	0.3717 (6)	0.9834 (3)	0.8837 (2)	0.0288 (6)
H9A	0.4320	0.9057	0.9461	0.043*
H9B	0.2316	1.0332	0.9117	0.043*
H9C	0.5372	1.0401	0.8500	0.043*
C10	0.1679 (6)	1.0513 (2)	0.6922 (2)	0.0290 (6)
H10A	0.3399	1.1034	0.6591	0.043*
H10B	0.0261	1.1082	0.7108	0.043*
H10C	0.0902	1.0155	0.6383	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0219 (3)	0.0263 (3)	0.0289 (3)	0.0080 (2)	−0.0003 (2)	−0.0129 (3)
O1	0.0203 (9)	0.0125 (8)	0.0194 (8)	0.0043 (6)	0.0027 (7)	−0.0019 (7)
O2	0.0215 (9)	0.0166 (8)	0.0197 (9)	0.0035 (7)	0.0035 (7)	−0.0011 (7)
O3	0.0334 (11)	0.0378 (12)	0.0238 (10)	−0.0102 (9)	0.0041 (8)	−0.0030 (9)
O4	0.0432 (12)	0.0413 (12)	0.0239 (10)	0.0147 (9)	0.0041 (9)	−0.0130 (9)
O5	0.0284 (11)	0.0266 (10)	0.0409 (11)	0.0075 (8)	−0.0108 (9)	−0.0020 (9)
O6	0.0382 (12)	0.0172 (9)	0.0545 (13)	−0.0016 (8)	−0.0044 (10)	−0.0131 (9)
N1	0.0205 (11)	0.0307 (12)	0.0175 (10)	0.0076 (9)	−0.0001 (8)	−0.0049 (9)
N2	0.0201 (11)	0.0172 (11)	0.0291 (11)	0.0044 (8)	0.0030 (9)	−0.0068 (9)
C1	0.0176 (12)	0.0161 (12)	0.0170 (12)	0.0022 (9)	−0.0039 (9)	−0.0050 (10)
C2	0.0174 (12)	0.0212 (12)	0.0155 (12)	0.0012 (9)	−0.0005 (9)	−0.0057 (10)
C3	0.0149 (11)	0.0200 (12)	0.0248 (13)	0.0037 (9)	−0.0022 (10)	−0.0122 (10)

C4	0.0172 (12)	0.0125 (11)	0.0210 (12)	0.0014 (9)	−0.0049 (9)	−0.0049 (9)
C5	0.0182 (12)	0.0155 (12)	0.0193 (12)	0.0002 (9)	0.0000 (9)	−0.0059 (10)
C6	0.0155 (11)	0.0169 (11)	0.0184 (12)	−0.0007 (9)	−0.0007 (9)	−0.0078 (10)
C7	0.0183 (12)	0.0128 (11)	0.0162 (11)	0.0021 (9)	−0.0039 (9)	−0.0041 (9)
C8	0.0190 (12)	0.0140 (11)	0.0243 (13)	0.0043 (9)	0.0013 (10)	−0.0081 (10)
C9	0.0336 (15)	0.0229 (14)	0.0324 (14)	0.0073 (11)	−0.0029 (12)	−0.0128 (12)
C10	0.0358 (16)	0.0197 (13)	0.0272 (14)	0.0096 (11)	−0.0017 (12)	−0.0029 (11)

Geometric parameters (Å, °)

Cl1—C3	1.709 (2)	C3—C4	1.384 (3)
O1—C7	1.328 (3)	C4—C5	1.382 (3)
O1—C8	1.475 (3)	C5—C6	1.388 (3)
O2—C7	1.205 (3)	C5—H5	0.9500
O3—N1	1.227 (3)	C6—C7	1.505 (3)
O4—N1	1.217 (3)	C8—C9	1.500 (3)
O5—N2	1.216 (3)	C8—C10	1.503 (3)
O6—N2	1.215 (3)	C8—H8	1.0000
N1—C2	1.472 (3)	C9—H9A	0.9800
N2—C4	1.474 (3)	C9—H9B	0.9800
C1—C2	1.382 (3)	C9—H9C	0.9800
C1—C6	1.388 (3)	C10—H10A	0.9800
C1—H1	0.9500	C10—H10B	0.9800
C2—C3	1.395 (3)	C10—H10C	0.9800
C7—O1—C8	116.83 (18)	C1—C6—C7	121.8 (2)
O4—N1—O3	125.7 (2)	C5—C6—C7	117.9 (2)
O4—N1—C2	118.2 (2)	O2—C7—O1	125.9 (2)
O3—N1—C2	116.1 (2)	O2—C7—C6	122.6 (2)
O6—N2—O5	125.8 (2)	O1—C7—C6	111.5 (2)
O6—N2—C4	116.5 (2)	O1—C8—C9	107.98 (19)
O5—N2—C4	117.61 (19)	O1—C8—C10	105.83 (19)
C2—C1—C6	119.1 (2)	C9—C8—C10	113.8 (2)
C2—C1—H1	120.4	O1—C8—H8	109.7
C6—C1—H1	120.4	C9—C8—H8	109.7
C1—C2—C3	122.5 (2)	C10—C8—H8	109.7
C1—C2—N1	117.2 (2)	C8—C9—H9A	109.5
C3—C2—N1	120.3 (2)	C8—C9—H9B	109.5
C4—C3—C2	116.1 (2)	H9A—C9—H9B	109.5
C4—C3—Cl1	120.62 (18)	C8—C9—H9C	109.5
C2—C3—Cl1	123.26 (19)	H9A—C9—H9C	109.5
C5—C4—C3	123.4 (2)	H9B—C9—H9C	109.5
C5—C4—N2	117.8 (2)	C8—C10—H10A	109.5
C3—C4—N2	118.8 (2)	C8—C10—H10B	109.5
C4—C5—C6	118.5 (2)	H10A—C10—H10B	109.5
C4—C5—H5	120.7	C8—C10—H10C	109.5
C6—C5—H5	120.7	H10A—C10—H10C	109.5
C1—C6—C5	120.3 (2)	H10B—C10—H10C	109.5
C6—C1—C2—C3	−1.1 (3)	O6—N2—C4—C3	−92.1 (3)
C6—C1—C2—N1	179.8 (2)	O5—N2—C4—C3	87.7 (3)

O4—N1—C2—C1	−131.1 (2)	C3—C4—C5—C6	−0.3 (3)
O3—N1—C2—C1	48.2 (3)	N2—C4—C5—C6	179.6 (2)
O4—N1—C2—C3	49.9 (3)	C2—C1—C6—C5	2.0 (3)
O3—N1—C2—C3	−130.8 (2)	C2—C1—C6—C7	−177.5 (2)
C1—C2—C3—C4	−0.4 (3)	C4—C5—C6—C1	−1.3 (3)
N1—C2—C3—C4	178.6 (2)	C4—C5—C6—C7	178.3 (2)
C1—C2—C3—Cl1	−178.36 (18)	C8—O1—C7—O2	1.9 (3)
N1—C2—C3—Cl1	0.6 (3)	C8—O1—C7—C6	−178.73 (17)
C2—C3—C4—C5	1.2 (3)	C1—C6—C7—O2	170.8 (2)
Cl1—C3—C4—C5	179.18 (18)	C5—C6—C7—O2	−8.8 (3)
C2—C3—C4—N2	−178.78 (19)	C1—C6—C7—O1	−8.7 (3)
Cl1—C3—C4—N2	−0.8 (3)	C5—C6—C7—O1	171.78 (19)
O6—N2—C4—C5	87.9 (3)	C7—O1—C8—C9	84.7 (2)
O5—N2—C4—C5	−92.3 (3)	C7—O1—C8—C10	−153.16 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.95	2.35	3.178 (3)	146

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2.

Fig. 1