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4-Chloro-2,6-dinitrophenol

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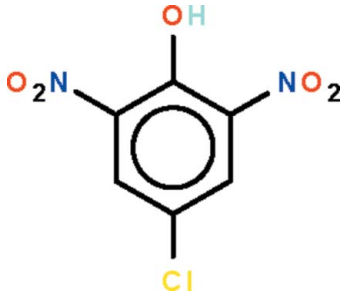
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.051; wR factor = 0.098; data-to-parameter ratio = 10.9.

The aromatic ring of the title compound, $C_6H_3ClN_2O_5$, is almost planar (r.m.s. deviation = 0.007 Å); one nitro substituent is nearly coplanar with the ring [dihedral angle = 3(1)°], whereas the other is twisted [dihedral angle = 36 (1)°]. The phenol OH group is intramolecularly hydrogen bonded to the nitro group that is coplanar with the ring, generating an S(6) graph-set motif.

Related literature

For the crystal structure of picric acid, see: Duesler *et al.* (1978); Soriano-Garcia *et al.* (1980).



Experimental

Crystal data

$C_6H_3ClN_2O_5$
M_r = 218.55
Monoclinic, $P2_1$
a = 7.4700 (19) Å
b = 5.8973 (15) Å
c = 9.952 (2) Å
β = 109.939 (6)°
V = 412.13 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 293 K
0.24 × 0.21 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.897, T_{max} = 0.922
3209 measured reflections
1434 independent reflections
816 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.098
S = 1.01
1434 reflections
131 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 640 Friedel pairs
Flack parameter: 0.14 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.84 (6)	1.82 (4)	2.563 (6)	146 (7)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

I thank Professor Shan Gao of Heilongjiang University for the diffraction measurements, and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2748).

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supplementary materials

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4-Chloro-2,6-dinitrophenol

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Comment

2,4,6-Trinitrophenol (picric acid) is a strong oxygen acid that dissociates in water. In the solid state, the molecule is nearly flat (Duesler *et al.*, 1978; Soriano-Garcia *et al.*, 1980). 4-Chloro-2,6-dinitrophenol (Scheme I) is also a similarly strong oxygen acid as it dissociates in water completely in water. In the crystal structure, the aromatic ring is nearly co-planar with one nitro substituent (dihedral angle 3(1) °) whereas it is twisted with respect to the other (dihedral angle 36 (1) °) (Fig. 1). The phenolic group is intra-molecularly hydrogen bonded to the nitro group that is co-planar with the ring.

Experimental

Commercially available 4-chloro-2,6-dinitrophenol was recrystallized from methanol to yield colorless prisms.

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C). The hydroxy H-atom was located in a difference Fourier map, and was refined with a distance restraint of O–H 0.84±0.01 Å.

Figures

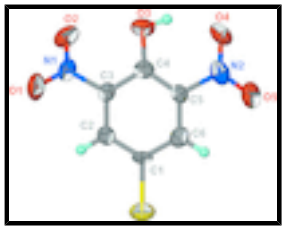

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of 4-chloro-2,6-dinitrophenol at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-Chloro-2,6-dinitrophenol

Crystal data

$C_6H_3ClN_2O_5$	F(000) = 220
M_r = 218.55	D_x = 1.761 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 1662 reflections
a = 7.4700 (19) Å	θ = 4.1–27.4°
b = 5.8973 (15) Å	μ = 0.46 mm^{-1}
c = 9.952 (2) Å	T = 293 K

β = 109.939 (6)°	Prism, colorless
V = 412.13 (18) Å^3	0.24 × 0.21 × 0.18 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	1434 independent reflections
Radiation source: fine-focus sealed tube	816 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.067
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 25.0°, θ_{min} = 4.1°
ω scans	h = −8→8
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	k = −7→7
T_{min} = 0.897, T_{max} = 0.922	l = −11→11
3209 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
1434 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
131 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
2 restraints	Absolute structure: Flack (1983), 640 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.14 (14)

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.4887 (2)	0.0000 (3)	0.86383 (14)	0.0688 (5)
O1	0.3354 (6)	0.5743 (6)	0.4395 (4)	0.0733 (13)
O2	0.2527 (5)	0.8807 (6)	0.5218 (4)	0.0721 (13)
O3	−0.0108 (6)	0.7765 (6)	0.6318 (4)	0.0604 (12)
H3	−0.101 (7)	0.774 (12)	0.664 (7)	0.10 (3)*
O4	−0.1986 (6)	0.6424 (8)	0.7898 (4)	0.0729 (14)
O5	−0.1056 (7)	0.3531 (8)	0.9292 (5)	0.0845 (14)
N1	0.2807 (6)	0.6773 (8)	0.5258 (5)	0.0497 (12)
N2	−0.0885 (7)	0.4861 (11)	0.8388 (5)	0.0594 (13)
C1	0.3379 (8)	0.2247 (7)	0.7937 (5)	0.0383 (13)
C2	0.3679 (7)	0.3605 (9)	0.6918 (6)	0.0430 (13)
H2	0.4672	0.3293	0.6582	0.052*

C3	0.2500 (6)	0.5442 (8)	0.6390 (5)	0.0376 (13)
C4	0.0974 (7)	0.5968 (8)	0.6866 (6)	0.0425 (13)
C5	0.0733 (7)	0.4491 (8)	0.7875 (5)	0.0387 (14)
C6	0.1891 (8)	0.2652 (9)	0.8411 (6)	0.0479 (15)
H6	0.1666	0.1703	0.9083	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0706 (9)	0.0606 (9)	0.0678 (10)	0.0225 (9)	0.0142 (8)	0.0110 (9)
O1	0.098 (3)	0.069 (3)	0.075 (3)	−0.012 (2)	0.058 (3)	0.002 (2)
O2	0.090 (3)	0.050 (3)	0.075 (3)	−0.002 (2)	0.027 (3)	0.018 (2)
O3	0.055 (3)	0.048 (2)	0.077 (3)	0.011 (2)	0.021 (3)	0.008 (2)
O4	0.063 (3)	0.083 (3)	0.084 (3)	0.023 (3)	0.038 (3)	0.001 (3)
O5	0.093 (3)	0.093 (3)	0.092 (4)	0.009 (3)	0.062 (3)	0.012 (3)
N1	0.052 (3)	0.055 (3)	0.043 (3)	−0.011 (2)	0.017 (3)	0.003 (3)
N2	0.062 (4)	0.065 (3)	0.057 (3)	−0.005 (3)	0.028 (3)	−0.019 (3)
C1	0.037 (3)	0.027 (3)	0.044 (3)	0.011 (2)	0.005 (3)	0.003 (2)
C2	0.039 (3)	0.047 (3)	0.044 (3)	0.000 (3)	0.016 (3)	−0.001 (3)
C3	0.034 (3)	0.042 (4)	0.034 (3)	−0.009 (3)	0.009 (2)	−0.002 (2)
C4	0.037 (3)	0.042 (3)	0.044 (3)	−0.001 (3)	0.007 (3)	−0.003 (3)
C5	0.037 (3)	0.041 (4)	0.040 (3)	−0.002 (3)	0.016 (3)	−0.005 (3)
C6	0.055 (4)	0.048 (3)	0.037 (3)	−0.004 (3)	0.012 (3)	−0.002 (3)

Geometric parameters (Å, °)

Cl1—C1	1.725 (4)	C1—C6	1.369 (7)
O1—N1	1.230 (5)	C1—C2	1.369 (6)
O2—N1	1.216 (5)	C2—C3	1.382 (7)
O3—C4	1.332 (6)	C2—H2	0.9300
O3—H3	0.84 (6)	C3—C4	1.410 (6)
O4—N2	1.221 (6)	C4—C5	1.387 (6)
O5—N2	1.233 (6)	C5—C6	1.376 (7)
N1—C3	1.454 (6)	C6—H6	0.9300
N2—C5	1.480 (6)		
C4—O3—H3	107 (5)	C2—C3—C4	121.9 (5)
O2—N1—O1	124.0 (5)	C2—C3—N1	118.0 (4)
O2—N1—C3	119.2 (5)	C4—C3—N1	120.1 (5)
O1—N1—C3	116.9 (5)	O3—C4—C5	125.9 (5)
O4—N2—O5	123.3 (5)	O3—C4—C3	119.0 (5)
O4—N2—C5	119.5 (5)	C5—C4—C3	115.1 (4)
O5—N2—C5	117.3 (6)	C6—C5—C4	123.8 (4)
C6—C1—C2	120.7 (5)	C6—C5—N2	117.5 (5)
C6—C1—Cl1	119.3 (4)	C4—C5—N2	118.7 (5)
C2—C1—Cl1	120.0 (4)	C1—C6—C5	118.7 (5)
C1—C2—C3	119.7 (4)	C1—C6—H6	120.6
C1—C2—H2	120.1	C5—C6—H6	120.6
C3—C2—H2	120.1		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4	0.84 (6)	1.82 (4)	2.563 (6)	146 (7)

Fig. 1