Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4,6-Trichlorophenol

Sandra Patricia González Martínez[a] and Sylvain Bernès[b]*

[a]Preparatoria 3, UANL, Félix U. Gómez y Madero, Monterrey, NL, Mexico, and [b]DEP Facultad de Ciencias Químicas, UANL, Guerrero y Progreso S/N, Col. Treviño, 64570 Monterrey, NL, Mexico
Correspondence e-mail: sylvain_bernes@hotmail.com

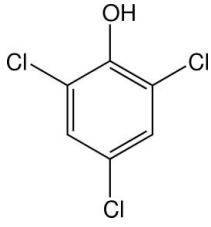
Received 23 August 2007; accepted 28 August 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.109; data-to-parameter ratio = 15.7.

In the title compound, $C_6H_3Cl_3O$, the molecular geometry approximates C_{2v} symmetry. The hydroxyl H atom lies in the plane of the ring; the closest approach between the centroids of aromatic rings of symmetry-related molecules exceeds 3.8 Å.

Related literature

For the carcinogenicity of the title molecule, see US Department of Health and Human Services (2005). For the polymorphism observed for a related molecule, pentafluorophenol, see Das *et al.* (2006). Metal-ion complexes including the phenolate ion of the title compound as ligand have been reported; see Gökaugaç *et al.* (1999); Wesolek *et al.* (1994); Zechmann *et al.* (2000).



Experimental

Crystal data

$C_6H_3Cl_3O$
M_r = 197.43
Monoclinic, $P2_1/c$
a = 3.8181 (18) Å
b = 15.742 (7) Å
c = 12.127 (6) Å
β = 95.05 (4)°
V = 726.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 297 (1) K
0.60 × 0.20 × 0.04 mm

Data collection

Siemens P4 diffractometer
Absorption correction: Gaussian (*XSCANS*; Siemens, 1999)
T_{min} = 0.792, T_{max} = 0.954
2445 measured reflections
1427 independent reflections
1086 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
3 standard reflections
every 97 reflections
intensity decay: 1.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.109
S = 1.08
1427 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Data collection: *XSCANS* (Siemens, 1999); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL-Plus*.

Support by PROVERICyT (IX Verano de la Investigación Científica y Tecnológica UANL) is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2314).

References

Das, D., Banerjee, D., Mondal, R., Howard, J. A. K., Boese, R. & Desiraju, G. R. (2006). *Chem. Commun.* pp. 555–557.
Gökaugaç, G., Tatar, L., Kisakürek, D. & Ülkü, D. (1999). *Acta Cryst.* C**55**, 1413–1416.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Sheldrick, G. M. (1998). *SHELXTL-Plus*. Release 5.10. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1999). *XSCANS*. Version 2.31. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
US Department of Health and Human Services (2005). *Report on Carcinogens*, 11th ed. http://ntp.niehs.nih.gov/ntp/roc/eleventh/profiles/s181trcp.pdf.
Wesolek, M., Meyer, D., Osborn, J. A., De Cian, A., Fischer, J., Derory, A., Legoll, P. & Drillo, M. (1994). *Angew. Chem. Int. Ed. Engl.* **33**, 1592–1594.
Zechmann, C. A., Boyle, T. J., Rodriguez, M. A. & Kemp, R. A. (2000). *Polyhedron*, **19**, 2557–2564.

 doi:10.1107/S1600536807042080

supplementary materials

Acta Cryst. (2007). E**63**, o3947 [**doi:10.1107/S1600536807042080**]

2,4,6-Trichlorophenol

S. P. González Martínez and S. Bernès

Comment

The title molecule has been used in the past as an antiseptic, a pesticide for wood, leather and glue preservation, and also as an antimildew treatment for textiles. However, production was discontinued in the 1980 s and the molecule is no longer used in the USA, mainly because its production process systematically affords small quantities of dioxins and dibenzofurans. This molecule is currently listed as "*reasonably anticipated to be a human carcinogen*" (US Department of Health and Human Services, 2005). The corresponding phenolate has been used as a ligand for transition and non-transition metal ions, *e.g.* Cu^{II} (Gökaugaç *et al.*, 1999), Mn^{III} (Wesolek *et al.*, 1994), or Mg^{II} (Zechmann *et al.*, 2000).

The molecular structure (Fig. 1) approximates a C_{2v} symmetry. However, the molecule is placed on a general position. The hydroxyl H atom lies in the plane of the aromatic ring and is oriented toward Cl6. The corresponding site oriented toward Cl2 is not available for hydroxyl H atom, as, due to crystal symmetry, it would give a short intermolecular H···H contact.

Interestingly, two polymorphs of pentafluorophenol have been reported (Das *et al.*, 2006). For the Z' = 1 polymorph, hydroxyl H atom is placed 0.36 Å above the aromatic ring. A second polymorph, with Z' = 3, shows a variety of hydroxyl conformations. Two molecules are almost planar, with H deviations of 0.10 and 0.04 Å, while the third one has O—H bond almost normal to the aromatic ring, with the H atom placed 0.66 Å out of the benzene mean plane. In the same way, the title compound could present a degree of free rotation about the C—O bond, allowing the stabilization of polymorphic phases.

Regarding the crystal structure, no significant π···π interactions are observed. The closest approach between centroids of aromatic rings of symmetry-related molecules is 3.818 Å.

Experimental

A sample of the title compound was donated by the Chemistry Stores at Universidad Autónoma de Nuevo León (UANL), and used without previous recrystallization.

Refinement

All H atoms were found in a difference map, but their positions regularized in order to get an idealized geometry for C—H and O—H groups. Constrained bond lengths: 0.82 (hydroxyl OH) and 0.93 Å (aromatic CH). Isotropic displacement parameters for H atoms were fixed to U_{iso}(H1) = 1.5 U_{eq}(O1); U_{iso}(H3) = 1.2 U_{eq}(C3); U_{iso}(H5) = 1.2 U_{eq}(C5).

Figures

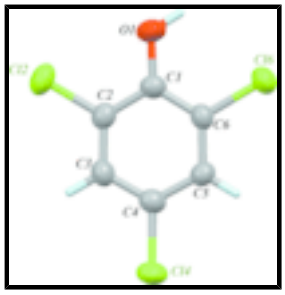


Fig. 1. The structure of the title molecule, with displacement ellipsoids at the 50% probability level for non-H atoms.

2,4,6-Trichlorophenol

Crystal data

$C_6H_3Cl_3O$	F_{000} = 392
M_r = 197.43	D_x = 1.806 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 342 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 3.8181 (18) Å	Cell parameters from 47 reflections
b = 15.742 (7) Å	θ = 6.0–12.4º
c = 12.127 (6) Å	μ = 1.18 mm^{-1}
β = 95.05 (4)º	T = 297 (1) K
V = 726.1 (6) Å^3	Plate, colourless
Z = 4	0.60 × 0.20 × 0.04 mm

Data collection

Siemens P4 diffractometer	R_{int} = 0.089
Monochromator: graphite	θ_{max} = 26.0º
T = 297(1) K	θ_{min} = 2.1º
2θ/ω scans	h = −4→2
Absorption correction: Gaussian (XSCANS; Siemens, 1999)	k = −19→1
T_{min} = 0.792, T_{max} = 0.954	l = −14→14
2445 measured reflections	3 standard reflections
1427 independent reflections	every 97 reflections
1086 reflections with $I > 2\sigma(I)$	intensity decay: 1.5%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained

$wR(F^2) = 0.109$	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.2366P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
1427 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
91 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Cl2	1.2802 (2)	0.10705 (5)	0.52181 (6)	0.0599 (3)
Cl4	0.6704 (3)	0.06153 (5)	0.11139 (7)	0.0627 (3)
Cl6	0.7136 (2)	0.37081 (5)	0.29722 (6)	0.0587 (3)
O1	1.1072 (7)	0.28196 (14)	0.48426 (17)	0.0594 (6)
H1	1.0670	0.3331	0.4822	0.089*
C1	0.9955 (8)	0.23290 (17)	0.3971 (2)	0.0414 (6)
C2	1.0664 (7)	0.14727 (19)	0.4024 (2)	0.0420 (6)
C3	0.9675 (8)	0.09404 (17)	0.3154 (2)	0.0445 (6)
H3	1.0169	0.0362	0.3200	0.053*
C4	0.7952 (8)	0.12773 (17)	0.2219 (2)	0.0437 (6)
C5	0.7129 (7)	0.21246 (18)	0.2133 (2)	0.0413 (6)
H5	0.5911	0.2343	0.1498	0.050*
C6	0.8167 (8)	0.26403 (17)	0.3019 (2)	0.0408 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl2	0.0671 (5)	0.0637 (5)	0.0464 (4)	0.0052 (4)	−0.0082 (3)	0.0143 (3)
Cl4	0.0876 (6)	0.0460 (4)	0.0519 (4)	−0.0112 (4)	−0.0086 (4)	−0.0119 (3)
Cl6	0.0812 (6)	0.0372 (4)	0.0559 (5)	0.0080 (4)	−0.0031 (4)	−0.0018 (3)
O1	0.0813 (15)	0.0537 (12)	0.0406 (11)	0.0020 (11)	−0.0093 (10)	−0.0117 (9)
C1	0.0489 (16)	0.0407 (14)	0.0347 (12)	−0.0026 (13)	0.0049 (12)	−0.0037 (11)
C2	0.0429 (15)	0.0453 (14)	0.0374 (13)	0.0012 (12)	0.0023 (11)	0.0040 (11)
C3	0.0533 (17)	0.0355 (13)	0.0447 (15)	0.0015 (13)	0.0033 (13)	0.0034 (11)
C4	0.0529 (16)	0.0389 (14)	0.0396 (14)	−0.0059 (13)	0.0059 (12)	−0.0031 (11)
C5	0.0465 (16)	0.0427 (14)	0.0338 (13)	−0.0015 (12)	−0.0010 (11)	0.0009 (10)
C6	0.0466 (15)	0.0337 (13)	0.0419 (13)	0.0032 (12)	0.0032 (12)	0.0016 (11)

Geometric parameters (Å, °)

Cl2—C2	1.719 (3)	C2—C3	1.374 (4)
Cl4—C4	1.731 (3)	C3—C4	1.366 (4)
Cl6—C6	1.726 (3)	C3—H3	0.9300
O1—C1	1.347 (3)	C4—C5	1.372 (4)
O1—H1	0.8200	C5—C6	1.377 (4)
C1—C2	1.375 (4)	C5—H5	0.9300
C1—C6	1.379 (4)		

C1—O1—H1	119.6	C3—C4—C5	122.1 (3)
O1—C1—C2	118.5 (3)	C3—C4—Cl4	119.2 (2)
O1—C1—C6	123.5 (3)	C5—C4—Cl4	118.7 (2)
C2—C1—C6	117.9 (2)	C4—C5—C6	117.7 (3)
C3—C2—C1	121.5 (3)	C4—C5—H5	121.1
C3—C2—Cl2	120.0 (2)	C6—C5—H5	121.1
C1—C2—Cl2	118.5 (2)	C5—C6—C1	122.1 (2)
C4—C3—C2	118.7 (3)	C5—C6—Cl6	120.0 (2)
C4—C3—H3	120.7	C1—C6—Cl6	117.9 (2)
C2—C3—H3	120.7		
O1—C1—C2—C3	−178.4 (3)	C3—C4—C5—C6	1.4 (4)
C6—C1—C2—C3	0.9 (4)	Cl4—C4—C5—C6	−179.6 (2)
O1—C1—C2—Cl2	2.2 (4)	C4—C5—C6—C1	−0.4 (4)
C6—C1—C2—Cl2	−178.5 (2)	C4—C5—C6—Cl6	−178.7 (2)
C1—C2—C3—C4	0.0 (4)	O1—C1—C6—C5	178.5 (3)
Cl2—C2—C3—C4	179.4 (2)	C2—C1—C6—C5	−0.7 (4)
C2—C3—C4—C5	−1.2 (4)	O1—C1—C6—Cl6	−3.1 (4)
C2—C3—C4—Cl4	179.8 (2)	C2—C1—C6—Cl6	177.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···Cl6	0.82	2.58	2.960 (3)	110
O1—H1···Cl4^{i}	0.82	2.81	3.418 (3)	132

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

Fig. 1