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2-[(4-Chlorophenyl)aminomethyl]phenol

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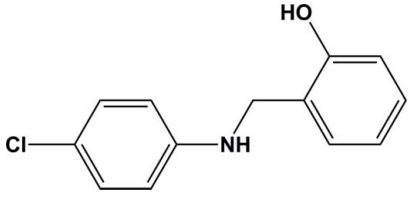
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.068; wR factor = 0.187; data-to-parameter ratio = 18.2.

In the title molecule, $C_{13}H_{12}ClNO$, the two benzene rings are twisted from each other by a dihedral angle of 68.60 (8)°. In the crystal structure, the hydroxy and amino H atoms are involved in intermolecular hydrogen bonds, O—H···N and N—H···O, respectively, resulting in $R_4^4(8)$ loops about inversion centers.

Related literature

For the properties and structures of related amino compounds, see: Fu *et al.* (2007, 2008, 2009); Fu & Xiong (2008). For a description of ring motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_{12}ClNO$
M_r = 233.69
Triclinic, $P\overline{1}$
a = 5.5842 (11) Å
b = 7.9485 (16) Å
c = 13.023 (3) Å
α = 86.87 (3)°
β = 89.12 (3)°
γ = 88.65 (3)°
V = 577.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 298 K
0.10 × 0.03 × 0.03 mm

Data collection

Mercury2 (2×2 bin mode) diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
5968 measured reflections
2637 independent reflections
1383 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.187
S = 0.98
2637 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.97	2.780 (3)	171
N1—H1A···O1^{ii}	0.89	2.17	3.037 (3)	165

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x-1, y, z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: PV2434).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Fu, D.-W., Ge, J.-Z., Dai, J., Ye, H.-Y. & Qu, Z.-R. (2009). *Inorg. Chem. Commun.* **12**, 994–997.
Fu, D.-W., Song, Y.-M., Wang, G.-X., Ye, Q., Xiong, R.-G., Akutagawa, T., Nakamura, T., Chan, P. W. H. & Huang, S. P. D. (2007). *J. Am. Chem. Soc.* **129**, 5346–5347.
Fu, D.-W. & Xiong, R.-G. (2008). *Dalton Trans.* **30**, 3946–3948.
Fu, D.-W., Zhang, W. & Xiong, R.-G. (2008). *Cryst. Growth Des.* **8**, 3461–3464.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o2364 [doi:10.1107/S1600536811032557]

2-[(4-Chlorophenyl)aminomethyl]phenol

Jie Xu

S1. Comment

Organic amino compounds have attracted much attention as phase transition dielectric materials for their application in memory storage (Fu *et al.*, 2007; Fu & Xiong 2008; Fu *et al.*, 2008; Fu *et al.*, 2009). With the purpose of obtaining phase transition crystals of amino compounds, various amines have been studied and we have developed a series of new organic molecules. In this article, we describe the crystal structure of the title compound.

In the title molecule (Fig. 1), the two benzene rings are twisted from each other by a dihedral angle of 68.60 (8)°. In the crystal structure, the hydroxyl and amino H atoms are involved in intermolecular hydrogen bonds, O1—H1···N1 and N1—H1A···O1, respectively, resulting in a $R^4_4(8)$ ring motif (Bernstein *et al.*, 1995) about inversion centers, which plays an important role in stabilizing the crystal structure. The $R^4_4(8)$ motif units are further linked into a one-dimentional chain along the *b* axis (Table 1 and Fig. 2).

S2. Experimental

The commercial 2-((4-chlorophenylamino)methyl)phenol (3 mmol) was dissolved in water/EtOH (1:1 *v*/*v*) solution. The solvent was slowly evaporated in air affording colourless block-shaped crystals of the title compound suitable for X-ray analysis.

S3. Refinement

The H atoms were fixed geometrically and treated as riding with N–H = 0.89), O–H = 0.82 and C–H = 0.93 and 0.97 Å for aryl and methylene H-atoms, respectively, in riding mode on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C/N/O).

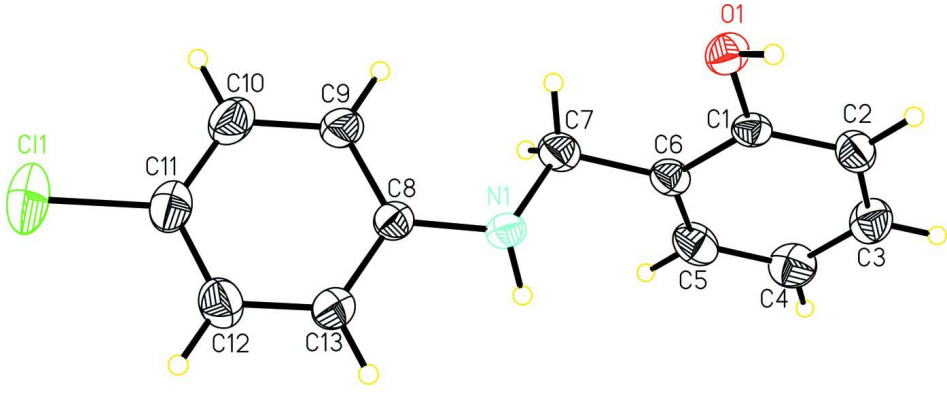

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

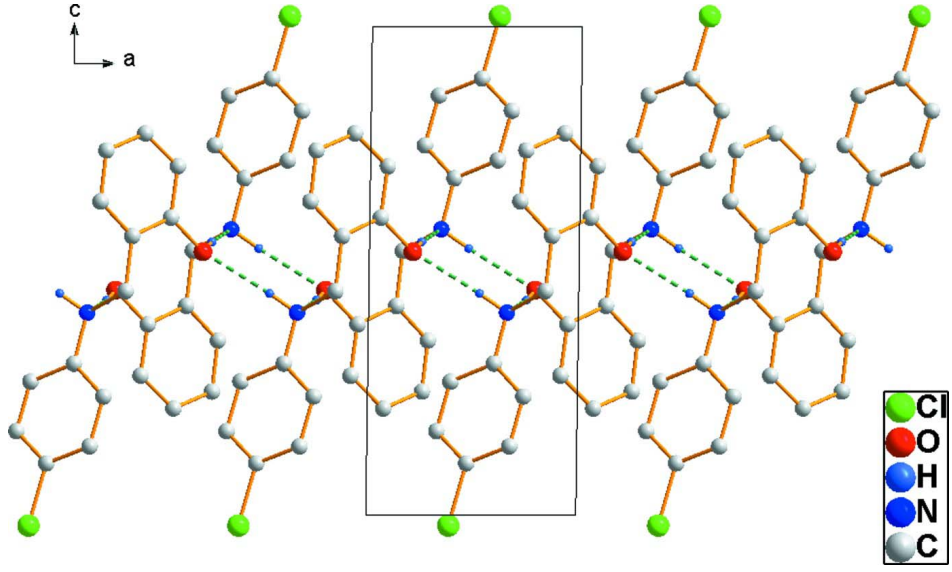

Figure 2

The crystal packing of the title compound, showing the one-dimensional chain. H atoms not involved in hydrogen bonding (dashed line) have been omitted for clarity.

2-[(4-Chlorophenyl)aminomethyl]phenol

Crystal data

$C_{13}H_{12}ClNO$
$M_r = 233.69$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.5842$ (11) Å
$b = 7.9485$ (16) Å
$c = 13.023$ (3) Å
$\alpha = 86.87$ (3)°
$\beta = 89.12$ (3)°
$\gamma = 88.65$ (3)°
$V = 577.0$ (2) Å^3
$Z = 2$
$F(000) = 244$
$D_x = 1.345$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2637 reflections
$\theta = 3.2$–27.5°
$\mu = 0.31$ mm^{-1}
$T = 298$ K
Block, colorless
0.10 × 0.03 × 0.03 mm

Data collection

Mercury2 (2x2 bin mode) diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.910$, $T_{max} = 1.000$
5968 measured reflections
2637 independent reflections
1383 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.187$
$S = 0.98$
2637 reflections
145 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.082P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.22$ e Å^{-3}
	$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.3943 (2)	0.26250 (15)	−0.02082 (7)	0.1028 (5)
O1	1.2067 (3)	0.3735 (2)	0.53925 (13)	0.0478 (5)
H1	1.2487	0.4639	0.5596	0.057*
N1	0.6595 (4)	0.3048 (2)	0.41481 (16)	0.0425 (6)
H1A	0.5273	0.3047	0.4539	0.051*
C1	1.0518 (4)	0.2978 (3)	0.60896 (19)	0.0394 (6)
C6	0.8691 (4)	0.2033 (3)	0.5715 (2)	0.0430 (7)
C8	0.5997 (4)	0.2890 (3)	0.3104 (2)	0.0420 (6)
C2	1.0819 (5)	0.3070 (3)	0.7143 (2)	0.0503 (7)
H2A	1.2081	0.3667	0.7391	0.060*
C7	0.8410 (5)	0.1848 (3)	0.4587 (2)	0.0499 (7)
H7A	0.9936	0.2038	0.4239	0.060*
H7B	0.7942	0.0706	0.4472	0.060*
C5	0.7158 (5)	0.1240 (4)	0.6422 (3)	0.0593 (8)
H5A	0.5925	0.0603	0.6186	0.071*
C13	0.3944 (5)	0.3687 (4)	0.2737 (2)	0.0519 (7)
H13A	0.2966	0.4278	0.3183	0.062*
C9	0.7429 (5)	0.2015 (4)	0.2432 (2)	0.0544 (8)
H9A	0.8824	0.1468	0.2666	0.065*
C11	0.4753 (6)	0.2735 (4)	0.1065 (2)	0.0612 (8)
C12	0.3308 (6)	0.3628 (4)	0.1723 (2)	0.0620 (8)
H12A	0.1924	0.4182	0.1484	0.074*
C3	0.9239 (5)	0.2273 (4)	0.7814 (2)	0.0588 (8)
H3A	0.9423	0.2353	0.8518	0.071*
C10	0.6794 (6)	0.1947 (4)	0.1411 (2)	0.0642 (9)
H10A	0.7768	0.1361	0.0961	0.077*
C4	0.7407 (6)	0.1367 (4)	0.7467 (2)	0.0632 (9)
H4A	0.6338	0.0841	0.7929	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1312 (10)	0.1295 (10)	0.0494 (6)	−0.0067 (7)	−0.0159 (6)	−0.0148 (6)
O1	0.0486 (11)	0.0435 (11)	0.0524 (12)	−0.0078 (9)	0.0067 (9)	−0.0115 (9)
N1	0.0386 (12)	0.0443 (13)	0.0451 (13)	0.0034 (10)	0.0031 (10)	−0.0089 (10)
C1	0.0347 (13)	0.0364 (14)	0.0470 (16)	0.0056 (11)	0.0013 (12)	−0.0042 (12)
C6	0.0387 (14)	0.0374 (14)	0.0533 (17)	0.0010 (12)	−0.0030 (12)	−0.0050 (13)
C8	0.0392 (14)	0.0426 (15)	0.0447 (16)	−0.0073 (12)	0.0031 (12)	−0.0065 (12)
C2	0.0465 (16)	0.0529 (18)	0.0519 (18)	0.0009 (13)	−0.0075 (13)	−0.0044 (14)
C7	0.0443 (15)	0.0446 (16)	0.0619 (19)	0.0037 (13)	−0.0050 (13)	−0.0134 (14)
C5	0.0491 (17)	0.0526 (18)	0.077 (2)	−0.0091 (14)	−0.0073 (16)	−0.0022 (16)
C13	0.0522 (17)	0.0561 (18)	0.0474 (17)	0.0055 (14)	0.0029 (13)	−0.0063 (14)
C9	0.0459 (16)	0.0616 (18)	0.0575 (19)	0.0015 (14)	0.0018 (14)	−0.0215 (15)
C11	0.069 (2)	0.068 (2)	0.0470 (18)	−0.0101 (18)	−0.0010 (16)	−0.0071 (16)
C12	0.0618 (19)	0.069 (2)	0.0548 (19)	0.0018 (16)	−0.0088 (15)	0.0042 (16)
C3	0.067 (2)	0.064 (2)	0.0447 (18)	0.0054 (17)	−0.0007 (15)	0.0034 (15)
C10	0.068 (2)	0.070 (2)	0.057 (2)	−0.0048 (17)	0.0071 (16)	−0.0235 (17)
C4	0.062 (2)	0.066 (2)	0.059 (2)	−0.0058 (17)	0.0084 (16)	0.0117 (17)

Geometric parameters (Å, º)

Cl1—C11	1.733 (3)	C7—H7B	0.9700
O1—C1	1.369 (3)	C5—C4	1.380 (4)
O1—H1	0.8202	C5—H5A	0.9300
N1—C8	1.417 (3)	C13—C12	1.376 (4)
N1—C7	1.476 (3)	C13—H13A	0.9300
N1—H1A	0.8898	C9—C10	1.386 (4)
C1—C2	1.390 (3)	C9—H9A	0.9300
C1—C6	1.391 (4)	C11—C10	1.358 (4)
C6—C5	1.384 (4)	C11—C12	1.381 (4)
C6—C7	1.495 (4)	C12—H12A	0.9300
C8—C13	1.376 (4)	C3—C4	1.361 (4)
C8—C9	1.382 (4)	C3—H3A	0.9300
C2—C3	1.374 (4)	C10—H10A	0.9300
C2—H2A	0.9300	C4—H4A	0.9300
C7—H7A	0.9700		
C1—O1—H1	110.1	C4—C5—H5A	119.1
C8—N1—C7	117.0 (2)	C6—C5—H5A	119.1
C8—N1—H1A	110.1	C12—C13—C8	121.4 (3)
C7—N1—H1A	110.7	C12—C13—H13A	119.3
O1—C1—C2	121.5 (2)	C8—C13—H13A	119.3
O1—C1—C6	117.9 (2)	C8—C9—C10	120.2 (3)
C2—C1—C6	120.5 (2)	C8—C9—H9A	119.9
C5—C6—C1	117.8 (3)	C10—C9—H9A	119.9
C5—C6—C7	120.8 (2)	C10—C11—C12	120.4 (3)
C1—C6—C7	121.3 (2)	C10—C11—Cl1	120.1 (3)

C13—C8—C9	118.6 (3)	C12—C11—Cl1	119.5 (3)
C13—C8—N1	118.6 (2)	C13—C12—C11	119.1 (3)
C9—C8—N1	122.7 (3)	C13—C12—H12A	120.4
C3—C2—C1	119.5 (3)	C11—C12—H12A	120.4
C3—C2—H2A	120.3	C4—C3—C2	121.2 (3)
C1—C2—H2A	120.3	C4—C3—H3A	119.4
N1—C7—C6	111.5 (2)	C2—C3—H3A	119.4
N1—C7—H7A	109.3	C11—C10—C9	120.2 (3)
C6—C7—H7A	109.3	C11—C10—H10A	119.9
N1—C7—H7B	109.3	C9—C10—H10A	119.9
C6—C7—H7B	109.3	C3—C4—C5	119.1 (3)
H7A—C7—H7B	108.0	C3—C4—H4A	120.5
C4—C5—C6	121.9 (3)	C5—C4—H4A	120.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.97	2.780 (3)	171
N1—H1*A*···O1^{ii}	0.89	2.17	3.037 (3)	165

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