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2-Bromobenzaldehyde cyanohydrin

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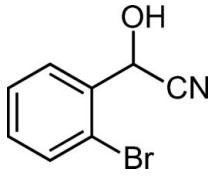
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.083; data-to-parameter ratio = 18.1.

The title compound [alternatively called (2-bromophenyl)(hydroxy)acetonitrile], C_8H_6BrNO, is the reaction product of 2-bromobenzaldehyde and hydrogen cyanide. Bond lengths and angles are normal. In the crystal structure, an intermolecular hydrogen bond between the hydroxy group and the nitrile N atom is established. In agreement with bonding considerations, a linear C—N···H acceptor geometry is observed. Each molecule is a single donor and a single acceptor; extended hydrogen-bonded chains are formed along [100].

Related literature

For the synthesis of the title compound, see: Becker *et al.* (2001). For the crystal structure of a related compound, see: Flores-Morales *et al.* (2003). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

C_8H_6BrNO
M_r = 212.05
Orthorhombic, *Pbca*
a = 8.0538 (3) Å
b = 13.9970 (5) Å
c = 14.2969 (5) Å
V = 1611.68 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 5.04 mm^{-1}
T = 200 (2) K
0.14 × 0.09 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.624, T_{max} = 0.86
19593 measured reflections
1844 independent reflections
1351 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.083
S = 1.02
1844 reflections
102 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H82···N^{i}	0.84	2.01	2.844 (3)	170

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

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

The authors thank Dr Peter Mayer and Sandra Albrecht for professional support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2526).

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supporting information

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S1. Comment

The title compound was prepared as in intermediate in the synthesis of 2-bromomandelic acid.

In the title compound a phenyl moiety, a hydroxy group and a cyano group are bonded to one C atom. The aromatic moiety bears a Br atom in 2- position to this C atom (Fig. 1). Bond lengths and angles show no significant deviations from values apparent in the literature for similar bonds (Allen *et al.*, 1987).

In the crystal structure, hydrogen bonds between the hydroxy groups and the N atom result in the formation of infinite chains along [100]. The aromatic moieties are arranged parallel to each other (Fig. 2).

S2. Experimental

The title compound was obtained as an intermediate in the synthesis of 2-bromomandelic acid according to a published procedure (Becker *et al.*, 2001) upon addition of 2-bromobenzaldehyde to an acidified aqueous solution of potassium cyanide. After workup, crystals suitable for X-ray analysis were obtained upon free evaporation of a solution of the compound in diethylether.

S3. Refinement

All H atoms were located in a difference map and refined as riding on their parent atoms. One common isotropic displacement parameter for all H atoms was refined.

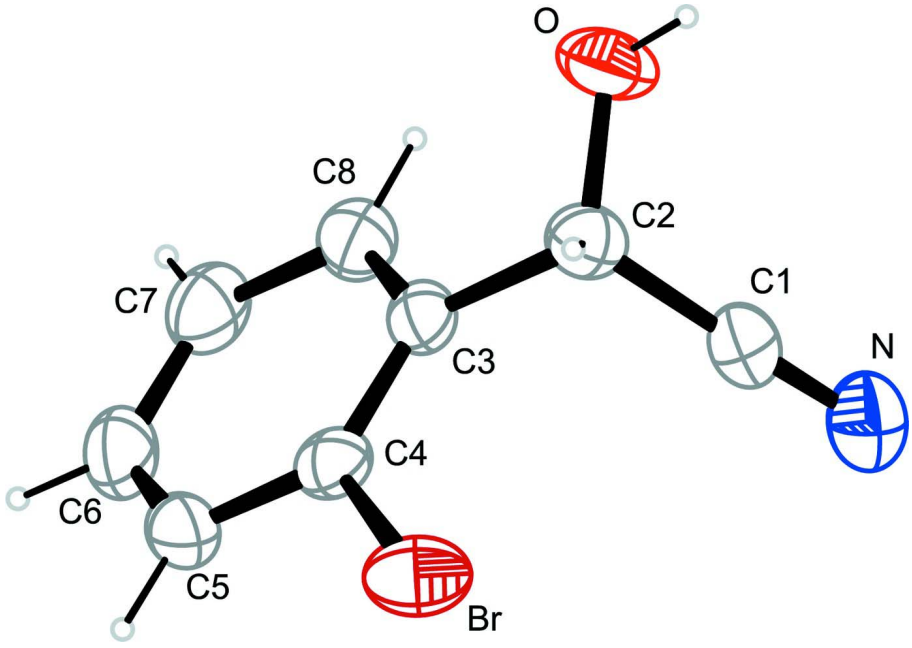

Figure 1

The molecular structure with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

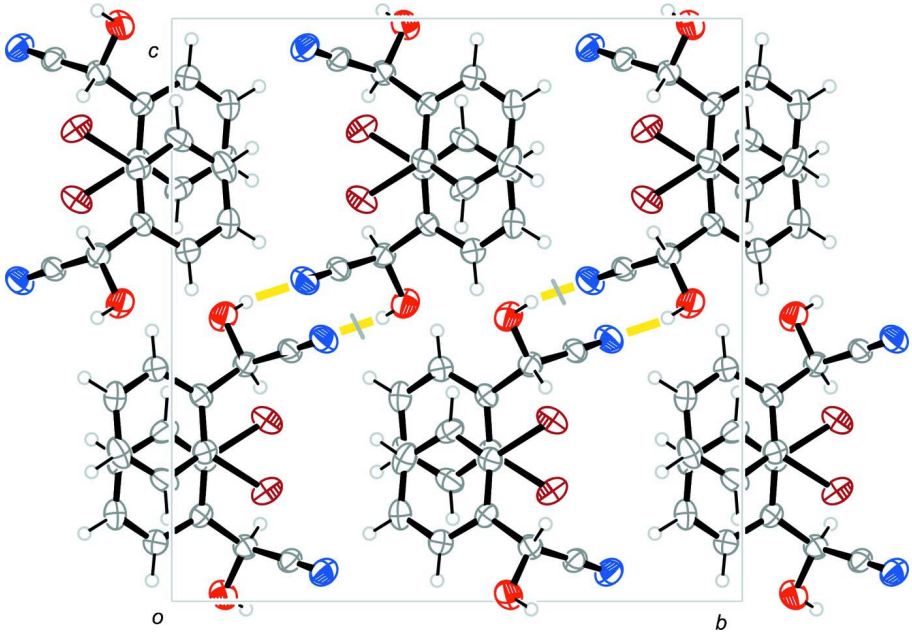

Figure 2

The packing of viewed along [-1 0 0]. Hydrogen bonds are drawn as yellow bars.

(2-bromophenyl)(hydroxy)acetonitrile

Crystal data

C_8H_6BrNO
$M_r = 212.05$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 8.0538$ (3) Å
$b = 13.9970$ (5) Å
$c = 14.2969$ (5) Å
$V = 1611.68$ (10) Å^3
$Z = 8$
$F(000) = 832$
$D_x = 1.748$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10818 reflections
$\theta = 3.1$–$27.5°$
$\mu = 5.04$ mm^{-1}
$T = 200$ K
Platelet, colourless
0.14 × 0.09 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
MONTEL, graded multilayered X-ray optics monochromator
CCD; rotation images; thick slices scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.624$, $T_{max} = 0.86$
19593 measured reflections
1844 independent reflections
1351 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -10 \rightarrow 10$
$k = -18 \rightarrow 15$
$l = -18 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.083$
$S = 1.02$
1844 reflections
102 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
Only H-atom displacement parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 1.1081P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br	0.25307 (3)	0.16689 (2)	0.310767 (19)	0.04887 (13)
O	0.1470 (3)	0.09045 (13)	0.01121 (14)	0.0533 (5)
H82	0.0823	0.1302	−0.0135	0.055 (3)*
N	0.4211 (3)	0.26649 (17)	0.05011 (16)	0.0501 (6)
C1	0.3312 (3)	0.20716 (18)	0.07017 (16)	0.0367 (5)
C2	0.2128 (3)	0.12902 (19)	0.09341 (17)	0.0364 (5)
H2	0.1206	0.1552	0.1327	0.055 (3)*
C3	0.3037 (3)	0.05167 (17)	0.14759 (16)	0.0309 (5)
C4	0.3299 (3)	0.05819 (17)	0.24325 (16)	0.0330 (5)
C5	0.4107 (3)	−0.01275 (19)	0.29246 (18)	0.0410 (6)
H5	0.4253	−0.0075	0.3582	0.055 (3)*
C6	0.4697 (4)	−0.09138 (18)	0.2449 (2)	0.0469 (7)
H6	0.5261	−0.1405	0.2779	0.055 (3)*

C7	0.4473 (3)	−0.09931 (18)	0.1491 (2)	0.0443 (6)
H7	0.4899	−0.1531	0.1164	0.055 (3)*
C8	0.3623 (3)	−0.02833 (17)	0.10115 (18)	0.0392 (6)
H8	0.3442	−0.0347	0.0358	0.055 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0455 (2)	0.0566 (2)	0.04446 (19)	0.00087 (13)	−0.00098 (12)	−0.01748 (11)
O	0.0627 (14)	0.0467 (11)	0.0505 (12)	0.0086 (9)	−0.0308 (10)	−0.0072 (9)
N	0.0567 (15)	0.0477 (14)	0.0458 (13)	−0.0024 (12)	0.0043 (11)	0.0100 (11)
C1	0.0415 (14)	0.0352 (13)	0.0334 (12)	0.0049 (12)	0.0002 (11)	0.0049 (10)
C2	0.0362 (13)	0.0366 (13)	0.0363 (12)	0.0030 (11)	−0.0045 (10)	−0.0020 (11)
C3	0.0259 (10)	0.0319 (11)	0.0350 (12)	−0.0025 (9)	−0.0007 (10)	0.0051 (10)
C4	0.0272 (12)	0.0357 (12)	0.0361 (12)	−0.0071 (10)	0.0011 (10)	−0.0009 (10)
C5	0.0396 (14)	0.0482 (15)	0.0352 (12)	−0.0121 (12)	−0.0060 (11)	0.0110 (11)
C6	0.0435 (16)	0.0375 (14)	0.0596 (18)	−0.0003 (12)	−0.0086 (14)	0.0154 (13)
C7	0.0455 (16)	0.0302 (13)	0.0573 (17)	0.0032 (11)	−0.0012 (13)	−0.0015 (12)
C8	0.0427 (14)	0.0371 (14)	0.0378 (12)	−0.0015 (11)	0.0004 (11)	0.0001 (10)

Geometric parameters (Å, º)

Br—C4	1.905 (2)	C4—C5	1.380 (3)
O—C2	1.398 (3)	C5—C6	1.379 (4)
O—H82	0.8400	C5—H5	0.9500
N—C1	1.138 (3)	C6—C7	1.386 (4)
C1—C2	1.489 (4)	C6—H6	0.9500
C2—C3	1.519 (3)	C7—C8	1.387 (4)
C2—H2	1.0000	C7—H7	0.9500
C3—C8	1.385 (3)	C8—H8	0.9500
C3—C4	1.387 (3)		
C2—O—H82	109.5	C3—C4—Br	120.18 (17)
N—C1—C2	178.3 (3)	C6—C5—C4	119.0 (2)
O—C2—C1	109.8 (2)	C6—C5—H5	120.5
O—C2—C3	109.6 (2)	C4—C5—H5	120.5
C1—C2—C3	109.2 (2)	C5—C6—C7	120.5 (2)
O—C2—H2	109.4	C5—C6—H6	119.8
C1—C2—H2	109.4	C7—C6—H6	119.8
C3—C2—H2	109.4	C6—C7—C8	119.7 (2)
C8—C3—C4	118.3 (2)	C6—C7—H7	120.2
C8—C3—C2	119.7 (2)	C8—C7—H7	120.2
C4—C3—C2	122.0 (2)	C3—C8—C7	120.7 (2)
C5—C4—C3	121.8 (2)	C3—C8—H8	119.6
C5—C4—Br	118.01 (19)	C7—C8—H8	119.6
O—C2—C3—C8	22.9 (3)	C3—C4—C5—C6	1.3 (4)
C1—C2—C3—C8	−97.4 (3)	Br—C4—C5—C6	−178.99 (19)

O—C2—C3—C4	−156.8 (2)	C4—C5—C6—C7	−0.4 (4)
C1—C2—C3—C4	82.9 (3)	C5—C6—C7—C8	−1.1 (4)
C8—C3—C4—C5	−0.6 (3)	C4—C3—C8—C7	−1.0 (4)
C2—C3—C4—C5	179.1 (2)	C2—C3—C8—C7	179.3 (2)
C8—C3—C4—Br	179.68 (18)	C6—C7—C8—C3	1.8 (4)
C2—C3—C4—Br	−0.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H82···N^{i}	0.84	2.01	2.844 (3)	170

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