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m-Cyanophenol

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m-Cyanophenol, NC—C_6H_4—OH or C_7H_5NO, crystallizes as chains of molecules held together by O—H···NC hydrogen bonds, with an O···N distance of 2.847 (2) Å.

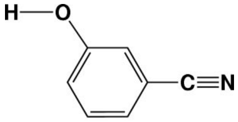
Key indicators

Single-crystal X-ray study
T = 174 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.107
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The crystal structures of *p*-cyanophenol (Higashi & Osaki, 1977) and *o*-cyanophenol (Beswick *et al.*, 1996) both contain O—H···NC hydrogen bonds as the dominant intermolecular interactions. The structure of *m*-cyanophenol, (I), is reported here to complete the series.


(I)

The bond lengths and angles in (I) (Fig. 1) are normal. The molecule is close to planar, with the CN group bent 0.49 (11)° out of the plane of the ring and a dihedral angle between the ring and the C1—O9—H9 plane of 4.9 (11)°. As is usual in phenols, the exocyclic ring angles at the OH group differ: O9—C1—C2 (*trans* to HO) is 117.33 (10)° and O9—C1—C6 is 122.55 (10)°.

The packing in (I) is shown in Fig. 2. As with the *ortho*- and *para*-isomers, there is an O—H···NC hydrogen bond. The geometric data for these bonds for all three isomers are compared in Table 1. It can be seen that all of these bonds are close to the ideal of linear interactions for both O—H···N and H···N≡C. The bonds are similar, but there is a significant lengthening on going from the two bonds in the *ortho*-isomer to the bonds in the *meta*-isomer; the data for the *para*-isomer are too imprecise to make a comparison.

The molecules of (I) assemble in linear chains, graph set *C*(7) (Etter *et al.*, 1990; Bernstein *et al.*, 1995). These chains

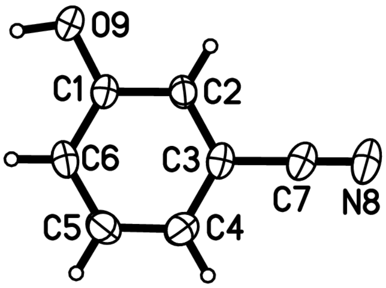


Figure 1
A view of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

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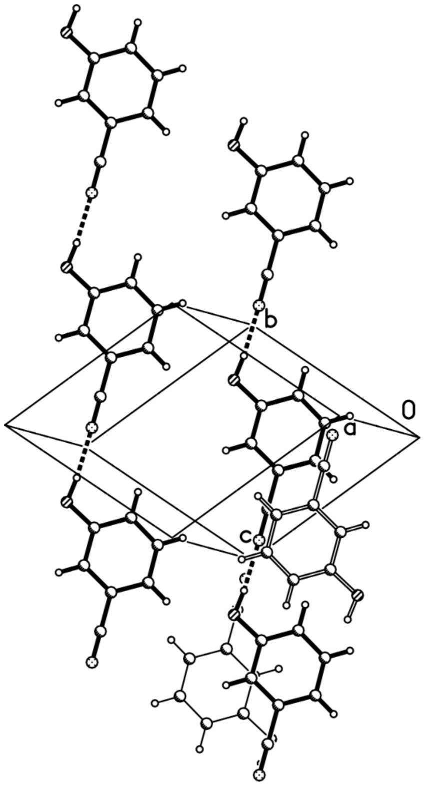

Figure 2
A view of the structure of (I), viewed normal to (100). Hydrogen bonds are shown as dashed lines. A molecule from the layer above is shown with open bonds and a molecule from the layer below with lighter bonds.

come together to form an approximately planar sheet parallel to (100); the molecules are tilted by 13.2 (1)° with respect to the sheet. All of the ring H atoms point in the general direction of N or O atoms of adjacent molecules, but in no case is the H···N (or O) distance less than 2.6 Å.

There is very little π overlap in the structure of (I) (see Fig. 2). The interplanar distance to the molecule in the layer above in Fig. 2 is 3.377 (1) Å and that to the molecule in the layer below is 3.437 (1) Å.

Experimental

The title compound was obtained from the Aldrich Chemical Company Inc. Satisfactory crystals of (I) grew as needles from the slow evaporation of an acetonitrile solution of the compound.

Crystal data

C_7H_5NO
$M_r = 119.12$
Triclinic, $P\overline{1}$
$a = 6.828$ (2) Å
$b = 7.197$ (3) Å
$c = 7.384$ (3) Å
$\alpha = 70.22$ (1)°
$\beta = 74.28$ (1)°
$\gamma = 65.70$ (1)°
$V = 307.5$ (2) Å^3
$Z = 2$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2621 reflections
$\theta = 2.4$–27.4°
$\mu = 0.09$ mm^{-1}
$T = 174$ (2) K
Elongated prism, colorless
0.50 × 0.40 × 0.35 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
3440 measured reflections
1329 independent reflections
1172 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 27.0°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.107$
$S = 1.12$
1329 reflections
87 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.044P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.010$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 1997)
Extinction coefficient: 0.12 (2)

Table 1
Distances and angles (Å,°) for the O—H···NC hydrogen bonds in *m*-, *p*- and *o*-cyanophenol.

O—H···N	O—H	O—H···N	H···N	H···N—C	O···N
O9—H9···N8$^{\rm i}$†	0.94	174	1.91	170	2.847 (2)
O1*A*—H1*A*···N9*B*$^{\rm ii}$‡	0.91	167	1.92	174	2.82 (5)
O1*B*—H1*B*···H9*A*$^{\rm iii}$‡	0.88	170	1.97	166	2.84 (5)
O1*A*—H1*A*···N21*B*$^{\rm iv}$§	0.92	173	1.88	170	2.795 (2)
O1*B*—H1*B*···N21*A*§	0.91	172	1.90	158	2.798 (2)

Symmetry codes: (i) $x, y+1, z-1$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, -z$; (iii) $-x, y, z-\frac{1}{2}$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$. † *m*-Cyanophenol (this work). ‡ *p*-Cyanophenol (Higashi & Osaki, 1977). § *o*-Cyanophenol (Beswick *et al.*, 1996).

C-bound H atoms were constrained in the riding-model approximation, with C—H = 0.95 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The hydroxy H atom was refined without constraint; O—H = 0.94 (2) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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