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# Pentafluorobenzonitrile

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**Key indicators**

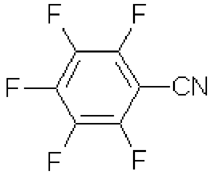
Single-crystal X-ray study
$T$ = 180 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.036
$wR$ factor = 0.108
Data-to-parameter ratio = 12.0

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

The crystal structure of pentafluorobenzonitrile, $C_7F_5N$, has been determined by *in-situ* crystal growth from the liquid at 268 K. The structure is identical to that of the isocyanide, crystallizing in *Cmca* with the molecule lying on a mirror plane bisecting the $C_6F_5$ ring and the cyano group. CN$\cdots$F interactions are not observed in the structure.

## Comment

Halogen–cyano interactions have been utilized in supramolecular synthons for crystal engineering (Desiraju & Harlow, 1989). For the heavier halogens ($X$ = I, Br) the CN$\cdots X$ interaction is strongly structure-directing. We have recently investigated a series of perfluoro-aromatics of general formula, *para*-$XC_6F_4CN$. For the heavier halogens ($X$ = Cl, Br, I), the compounds are solids at room temperature, whereas $C_6F_5CN$, (I), is a liquid (m.p. = 275.4 K; Fluorochem). A crystal of (I) was grown in a 0.4 mm capillary tube (GLAS) at 268 K, cooled with an Oxford Cryosystems Cryostream cooler (Cosier & Glazer, 1986), and cooled further to 180 K for data collection.



(I)

Compound (I) is isostructural with the isocyanide, $C_6F_5NC$ (Lentz & Preugschat, 1993), crystallizing in the orthorhombic space group *Cmca* with the molecule lying on a mirror plane bisecting the $C_6F_5$ ring and the cyano group (Fig. 2). Compound (I) does not exhibit CN$\cdots$F-type interactions. Instead, neighbouring molecules adopt a coplanar arrangement in which the F atom *para* to the cyano group is located over the centroid of the adjacent aromatic ring [$d$(F$\cdots$centroid) = 3.263 Å]. The cyanide group aproaches the opposite face in a direction approximately perpendicular to the plane of the aromatic ring [$d$(N$\cdots$centroid) = 3.071 Å] (Fig. 3). This interaction with the $\pi$-electron density of the phenyl ring presumably accommodates the complementary electronic demands of both the electronegative F and *sp*-hybridized N atoms.

It is interesting to note that the melting point of the isocyanide, $C_6F_5NC$, is some 10° higher than that of (I) (m.p. = 286 K) (Lentz & Preugschat, 1993). This suggests that the

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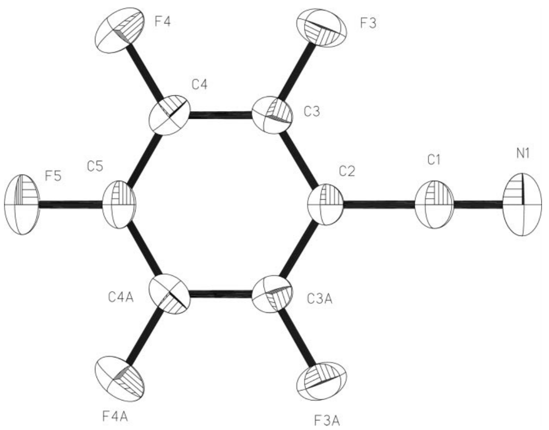

**Figure 1**
The molecular unit showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993).

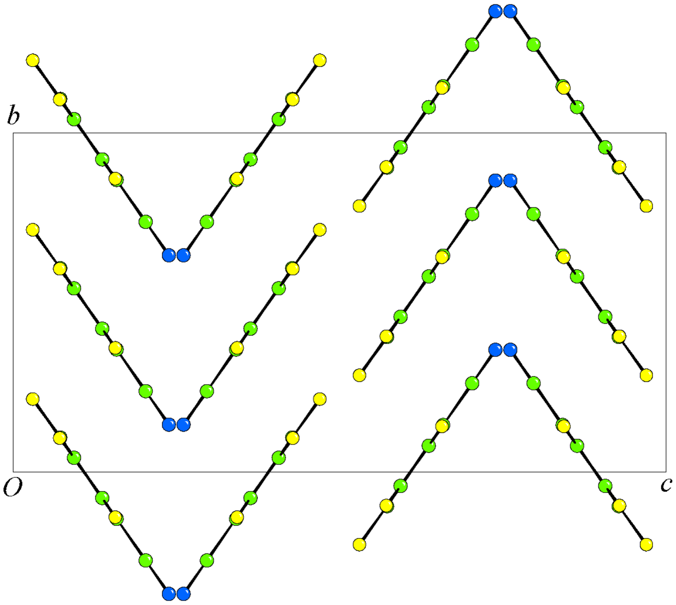

**Figure 2**
Projection on to (100) showing the overall packing arrangement in (I) (*CAMERON*; Watkin *et al.*, 1996).

NC$\cdots\pi$ interactions in the isocyanide are stronger than the CN$\cdots\pi$ interactions in (I).

## Experimental

Pentafluorobenzonitrile was obtained from Lancaster Synthesis and crystallized in a 0.4 mm capillary tube at 268 K, cooled with an Oxford Cryosystems Cryostream cooler.

*Crystal data*

$C_7F_5N$
$M_r = 193.08$
Orthorhombic, *Cmca*
$a = 7.6864\ (5)$ Å
$b = 9.5175\ (3)$ Å
$c = 18.3480\ (12)$ Å
$V = 1342.25\ (13)$ Å$^3$
$Z = 8$
$D_x = 1.911$ Mg m$^{-3}$

Mo $K\alpha$ radiation
Cell parameters from 2861 reflections
$\theta = 1.0–27.5°$
$\mu = 0.21$ mm$^{-1}$
$T = 180\ (2)$ K
Cylinder, colourless
0.35 mm (radius)

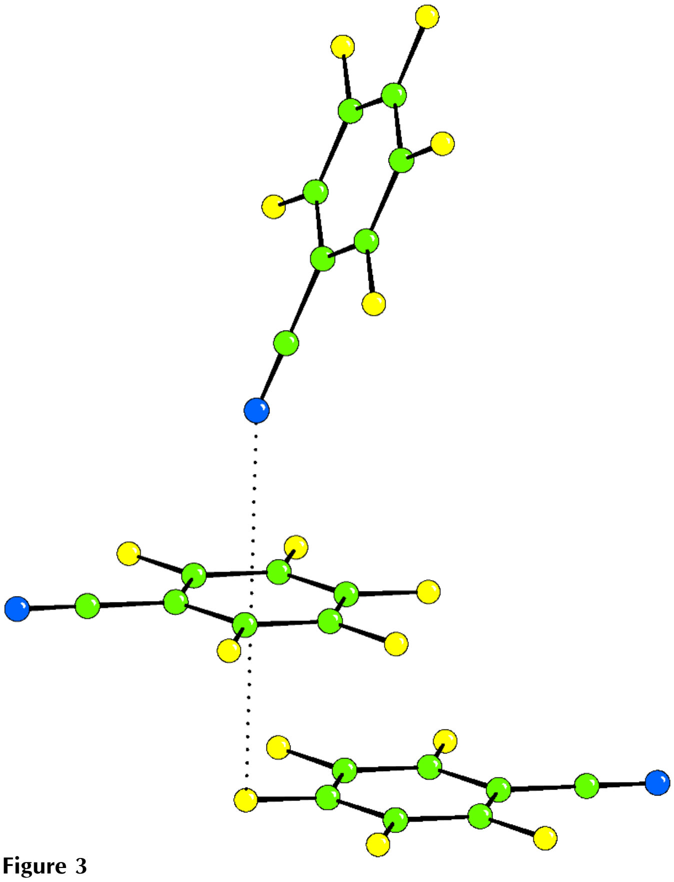

**Figure 3**
The structural motif observed in (I) (*CAMERON*; Watkin *et al.*, 1996). F$\cdots\pi$ and CN$\cdots\pi$ interactions are indicated by dotted lines.

*Data collection*

Nonius KappaCCD diffractometer
$\omega$ and $\varphi$ scans
4072 measured reflections
820 independent reflections
732 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.052$
$\theta_{\rm max} = 27.5°$
$h = 0 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -23 \rightarrow 23$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.108$
$S = 1.15$
819 reflections
68 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.5299P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -0.24$ e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.016 (4)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1999); data reduction: *HKL DENZO and SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL*97.

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