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2,5-Diphenylpentanenitrile

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Key indicators

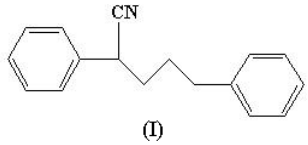
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.143
Data-to-parameter ratio = 17.4

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

This paper reports a new synthesis of the title compound, $C_{17}H_{17}N$, and its crystal structure. In the molecule, the two phenyl rings are approximately parallel. The cyano group is almost perpendicular to the two phenyl rings.

Comment

Freerksen *et al.* (1983) repeated the Watt procedure (Watt, 1974), obtaining the title compound, (I), in 56% yield. Masuko *et al.* (1985) synthesized (I) in 94% yield, starting from benzyl nitrile and phenylpropyl chloride. Similarly, Hino *et al.* (1988) prepared the compound using benzyl nitrile and 3-bromopropylbenzene. In these syntheses, expensive starting materials were used. We report our synthesis of this compound *via* a Friedel–Crafts reaction. The starting material, 5-chloro-2-phenylvaleronitrile was synthesized by reaction of benzyl nitrile and 1-bromo-3-chloropropane in the presence of NaOH and the phase-transfer catalyst benzyltrimethylammonium bromide. (I) was produced in 90% yield by refluxing a mixture of benzene, $AlCl_3$ and 5-chloro-2-phenylvaleronitrile.



(I)

The molecular structure is illustrated in Fig. 1. The two phenyl rings are approximately parallel, forming a dihedral angle of 7.9 (5)°. The angle N1—C5—C1 is 178.6 (2)°, indicating that atom C5 is *sp* hybridized. The angles between N1—C5—C1 and the two phenyl rings are 86.9 (5) and 92.7 (5)°, respectively, indicating that the cyano group is perpendicular

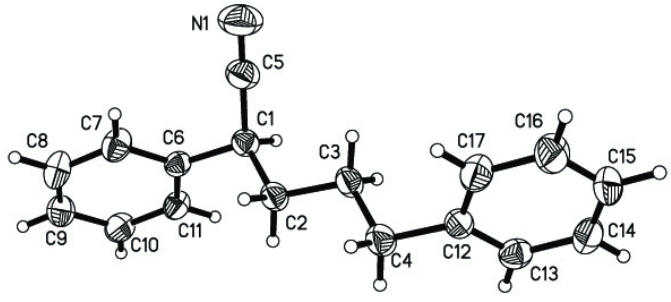


Figure 1
View of the molecular structure of (I), with 30% probability ellipsoids.

to the phenyl ring planes. Atoms, C1, C2, C3 and C4 are almost coplanar. The C5—N1 distance is 1.137 (3) Å, similar to the C—N bond length 1.134 (2) Å in bis(2-methylbenzyl cyanide) tetracyanobenzene (Hosomi *et al.*, 1997).

Experimental

5-Chloro-2-phenylvaleronitrile (4.3 g, 22.3 mmol) and benzene (20.0 ml) were heated in a 50 ml round-bottom flask, catalysed by $AlCl_3$ (4.0 g, 29.9 mmol). The reaction mixture was refluxed for 6 h, then poured into iced water and acidified with dilute HCl. The organic layer was separated and washed with water, dried and concentrated. Evaporation of the solvent and crystallization of the residue from toluene yielded (I), 4.733 g, 90%, m.p. 351–353 K (literature m.p. 349–351 K). Crystals were obtained by slow evaporation of a toluene solution. IR (KBr) 2235 (ms) cm^{-1}. ^1H NMR (400 $CDCl_3$) δ 3.75–3.78 (1*H*, m), 7.13–7.38 (10*H*, m) p.p.m.

Crystal data

$C_{17}H_{17}N$
M_r = 235.32
Orthorhombic, *Pbca*
a = 8.356 (3) Å
b = 17.406 (5) Å
c = 19.052 (6) Å
V = 2771.0 (15) Å^3
Z = 8
D_x = 1.128 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 897 reflections
θ = 2.6–22.7°
μ = 0.07 mm^{-1}
T = 293 (2) K
Block, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
14985 measured reflections
2843 independent reflections
1751 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 26.4°
$h = -6 \rightarrow 10$
$k = -21 \rightarrow 21$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.143
S = 1.04
2843 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.5892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C5	1.472 (3)	C1—C2	1.544 (2)
C1—C6	1.519 (2)		
C5—C1—C6	111.74 (15)	C11—C6—C1	119.22 (15)
C12—C4—C3	112.25 (15)	C17—C12—C4	120.62 (18)
C7—C6—C1	122.37 (16)	C13—C12—C4	121.70 (18)
C5—C1—C2—C3	−61.9 (2)	C3—C4—C12—C17	78.3 (2)
C5—C1—C6—C7	−31.9 (2)	C3—C4—C12—C13	−99.5 (2)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997) and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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