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2,3,5,6-Tetrachloro-1,4-dicyanobenzene–anthracene (1/1)

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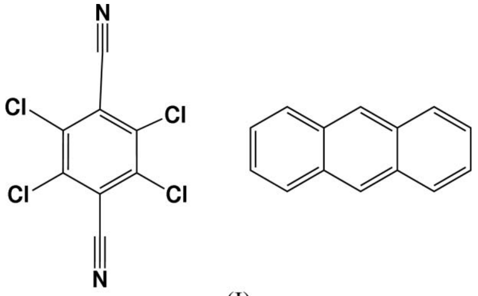
2,3,5,6-Tetrachloro-1,4-dicyanobenzene forms a 1:1 complex with anthracene, $C_8N_2Cl_4 \cdot C_{14}H_{10}$. The two molecules, which both lie on inversion centers, alternate in π stacks. There are no unusual intermolecular interactions.

Key indicators
Single-crystal X-ray study
T = 174 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.121
Data-to-parameter ratio = 14.6

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

Comment

In an earlier paper (Britton, 2002) the formation of two-dimensional arrays of the isomers of tetrachlorodicyanobenzene, TCDB, by formation of complexes with hexamethylbenzene, was described. At the same time, the possibility of forming similar arrangements, with other π bases replacing the hexamethylbenzene, was explored. While a number of complexes were formed, none of them had the desired layers of TCDB. The structure of one of these complexes, p-TCDB–anthracene (1/1), (I), is described here.



(I)

Fig. 1 shows the labeling and the anisotropic displacement ellipsoids. The bond lengths and angles are normal. Both

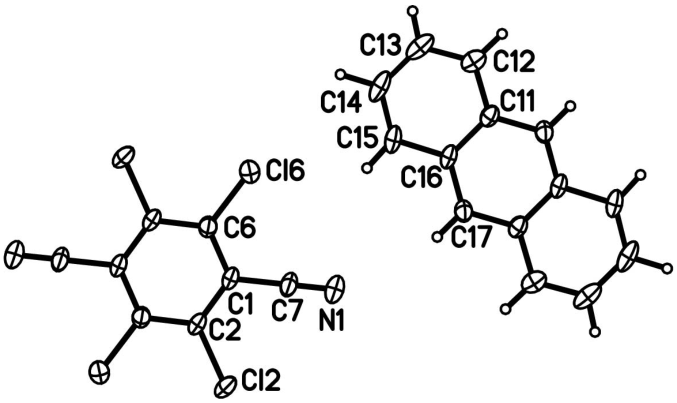


Figure 1
Both molecules in TCDB–anthracene (1/1). Displacement ellipsoids are shown at the 50% probability level. Only the independent atoms are labeled. The unlabeled atoms of the substituted benzene component are related to the labeled atoms by $(-x, 2-y, 1-z)$. The unlabeled atoms of the anthracene component are related to the labelled atoms by $(1-x, -y, 1-z)$.

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molecules lie on centers of symmetry.

Fig. 2 shows the packing. The molecules assemble in layers parallel to (210) with no contact distances within the layers shorter than the usual van der Waals distances. The two kinds of molecule alternate in π stacks parallel to the a axis. The average interplanar distance in the π stacks is 3.427 (3) Å. Adjacent molecules in the stack are tilted by 1.2 (1)° with respect to each other.

Experimental

The complex was prepared by dissolving an approximately equimolar mixture of the two components in a diethyl ether/acetonitrile mixture and allowing the solution to evaporate.

Crystal data

$C_8N_2Cl_4\cdot C_{14}H_{10}$
$M_r = 444.12$
Triclinic, $P\overline{1}$
$a = 7.294$ (2) Å
$b = 8.762$ (2) Å
$c = 8.891$ (2) Å
$\alpha = 64.87$ (1)°
$\beta = 70.10$ (1)°
$\gamma = 73.79$ (1)°
$V = 477.6$ (2) Å^3
$Z = 1$
$D_x = 1.544$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3062 reflections
$\theta = 2.6$–27.4°
$\mu = 0.63$ mm^{-1}
$T = 174$ (2) K
Prism, yellow
0.45 × 0.40 × 0.35 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{\min} = 0.77$, $T_{\max} = 0.80$
5418 measured reflections
2143 independent reflections
1739 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 27.6°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.121$
$S = 1.06$
2143 reflections
147 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.086P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.005$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.60$ e Å^{-3}

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*.

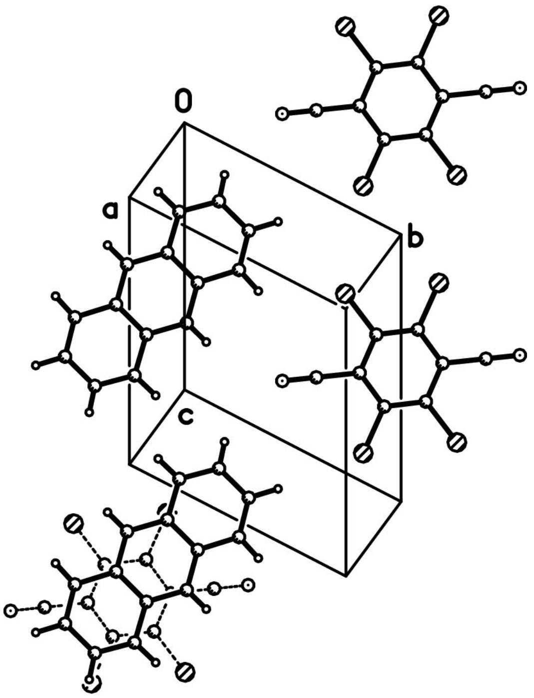

Figure 2
The packing in TCDB–anthracene (1/1), viewed normal to (210). The molecules in one layer are shown with heavy bonds. One molecule in a π-stacked layer is shown with dashed bonds.

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