Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-(Dicyanomethylene)-1,5-diphenylpenta-1,4-diyne

Peter G. Jones,[a]* Henning Hopf[b] and Martin Kreutzer[b]

[a]Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany, and [b]Institut für Organische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany

Correspondence e-mail:
jones@xray36.anchem.nat.tu-bs.de

Received 5 February 2002
Accepted 6 February 2002
Online 22 February 2002

Key indicators

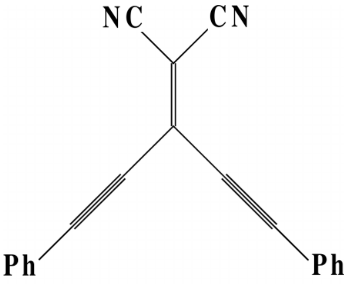
Single-crystal X-ray study
T = 178 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.138
Data-to-parameter ratio = 13.7

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

The molecule of the title compound, $C_{20}H_{10}N_2$, displays no imposed symmetry, but is largely planar [one phenyl ring is twisted by 10.4 (1)° out of the plane of the rest of the molecule]. The central C═C bond length is 1.371 (3) Å. The molecules are linked by a weak hydrogen bond of the form C—H···N.

Comment

Cross-conjugated enediynes are attracting increasing attention, since they can be used for the preparation of extended π-systems with novel electronic properties (Zhao *et al.*, 2002). We are interested in the synthesis of derivatives of 1,1-diethynylethene that bear polarizing functional groups (Hopf *et al.*, 1991). As a reference compound, we prepared the title compound, (I), by the condensation of 1,5-diphenylpenta-1,4-diyn-4-one with malonitrile in acetic acid/ethanol in the presence of β-alanine as catalyst (Kreutzer, 1993); we report here its crystal structure.



(I)

The molecule (Fig. 1) displays no imposed crystallographic symmetry. It is approximately planar; a closer analysis shows that the ring C9–14 is rotated by 10.4 (1)° from the rest of the molecule (mean deviations 0.004/0.033 Å, respectively, for these two parts). The molecular dimensions may be regarded as normal; the central double bond C3═C6 has a length of 1.371 (3) Å, and the angles subtended by each pair of substituents at this bond are slightly less than the ideal 120° [118.6 (2)° for the phenylethynyl and 117.4 (2)° for the cyano groups]. These values may be compared with the values of 1.378 (3)/1.373(3) Å and 116.8 (1)/118.2(2)° observed in two independent centrosymmetric molecules of tetrakis(phenylethynyl)ethene (Hopf *et al.*, 1991).

The molecules are connected by a weak C19—H19···N1 hydrogen bond by the 2_1 operator parallel to the b axis, forming a flattened herring-bone pattern (Fig. 2).

DOI: 10.1107/S1600536802002490

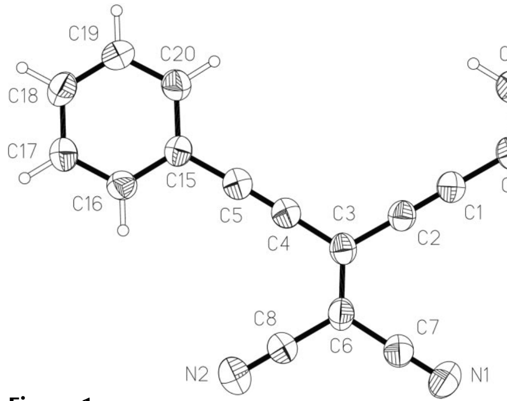


Figure 1
The molecule of the title compound in the crystal. Ellipsoids represent 50% probability levels.

Experimental

Crystals of (I) were grown by diffusion of pentane into a solution in chloroform.

Crystal data

$C_{20}H_{10}N_2$
$M_r = 278.30$
Monoclinic, $P2_1/c$
$a = 12.138$ (4) Å
$b = 15.279$ (4) Å
$c = 8.763$ (3) Å
$\beta = 107.24$ (3)°
$V = 1552.1$ (8) Å^3
$Z = 4$

$D_x = 1.191$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 50 reflections
$\theta = 10$–12.5°
$\mu = 0.07$ mm^{-1}
$T = 178$ (2) K
Prism, yellow
0.70 × 0.20 × 0.15 mm

Data collection

Nicolet *R*3 diffractometer
ω scans
Absorption correction: none
2909 measured reflections
2722 independent reflections
1498 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.050$

$\theta_{\rm max} = 25.0°$
$h = -13 \rightarrow 14$
$k = -18 \rightarrow 0$
$l = -10 \rightarrow 0$
3 standard reflections
every 147 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.138$
$S = 0.90$
2722 reflections
199 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.15$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.198 (3)	C5—C15	1.429 (3)
C1—C9	1.426 (3)	C6—C8	1.425 (3)
C2—C3	1.424 (3)	C6—C7	1.433 (3)
C3—C6	1.371 (3)	C7—N1	1.145 (3)
C3—C4	1.419 (3)	C8—N2	1.152 (3)
C4—C5	1.199 (3)		
C2—C1—C9	179.4 (2)	C4—C5—C15	177.2 (2)
C1—C2—C3	178.8 (3)	C3—C6—C8	121.53 (19)
C6—C3—C4	120.44 (19)	C3—C6—C7	121.1 (2)
C6—C3—C2	120.98 (19)	C8—C6—C7	117.4 (2)
C4—C3—C2	118.6 (2)	N1—C7—C6	179.1 (3)
C5—C4—C3	179.0 (2)	N2—C8—C6	179.5 (3)
C4—C3—C6—C8	−1.4 (3)	C2—C3—C6—C7	−1.8 (3)

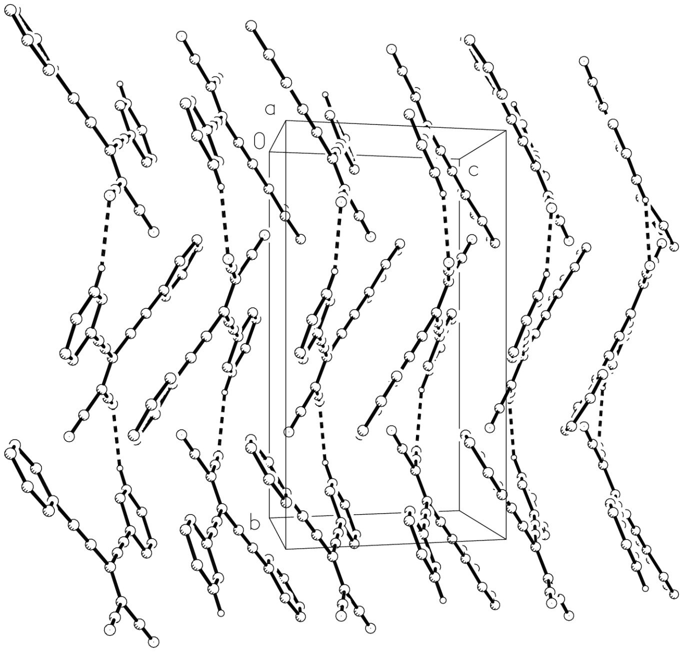


Figure 2
Packing diagram of the title compound with view direction slightly rotated from the *a* axis. Hydrogen bonds are indicated by dashed lines. Radii are arbitrary.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···N1$^{\rm i}$	0.95	2.61	3.436 (3)	145

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

H atoms were included using a riding model, starting from idealized positions.

Data collection: *P*3 (Nicolet, 1987); cell refinement: *P*3; data reduction: *XDISK* (Nicolet, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

Financial support from the Fonds der Chemischen Industrie is gratefully acknowledged. We thank Mr A. Weinkauf for technical assistance.

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