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2-[4-(Dimethylamino)phenyl]ethylene-1,1-dinitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.106
Data-to-parameter ratio = 8.9

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

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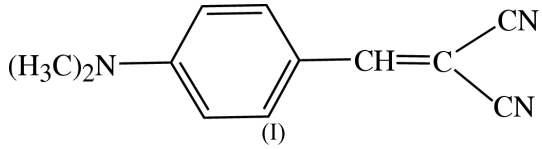
The determination of the crystal structure of the title compound, $C_{12}H_{11}N_3$, was carried out in order to explain its observed optical and electrical properties. Parallel and overlapping supramolecular packing was found in the crystal.

Comment

Organic compounds with a donor–π-acceptor structure have been drawing attention because of their being potent second-order non-linear optical materials which offer potential applications in optical signal processing, such as amplification, frequency conversion and modulation (Williams, 1984). Also, as one of the polynitrile π acceptors, the title compound, (I), has found application in electronic switching devices (Wang *et al.*, 1995; Li *et al.*, 2000). Parallel molecular arrangements in its vacuum-deposited film have been observed by scanning tunnel microscopy. The crystal structure determination of (I) has been undertaken in order to understand the relationship between its optical and electrical properties, and its structure.



(I)

The molecular structure with the atom labelling scheme of (I) is shown in Fig. 1. Mean values of six aromatic C—C bonds and two C≡N bond lengths are 1.395 (3) and 1.143 (3) Å, respectively. The mean C—CN bond length is 1.427 (10) Å. This bond length is intermediate between the expected value of 1.419 Å for sp–sp^2 C—C bond lengths and the value of 1.466 (10) Å for sp–sp^3 C—C bond lengths (Allen *et al.*, 1987), indicating strong intramolecular charge transfer (Janczak & Kubiak, 1995; Stoecheff, 1962). The mutual arrangement of the title compound is illustrated in Fig. 2. The structure is composed of linear stacks of parallel and overlapping molecules forming a supramolecular columnar aggregation. The mean distance between two successive packed benzene rings is 3.582 (2) Å. This value is a little larger than the van der Waals distance of 3.4 (4) Å for aromatic C atoms (Pauling, 1960). The non-H atoms of the molecule are almost coplanar; two least-squares planes defined by N1/N2/C1–C5 and N3/C4–C12 give r.m.s. deviations of 0.0079 (1) and 0.0173 (2) Å, respectively. The dihedral angle between the two planes is 6.65 (5)°. Here lies the basis for the supramolecular array of the molecules observed in the crystal.

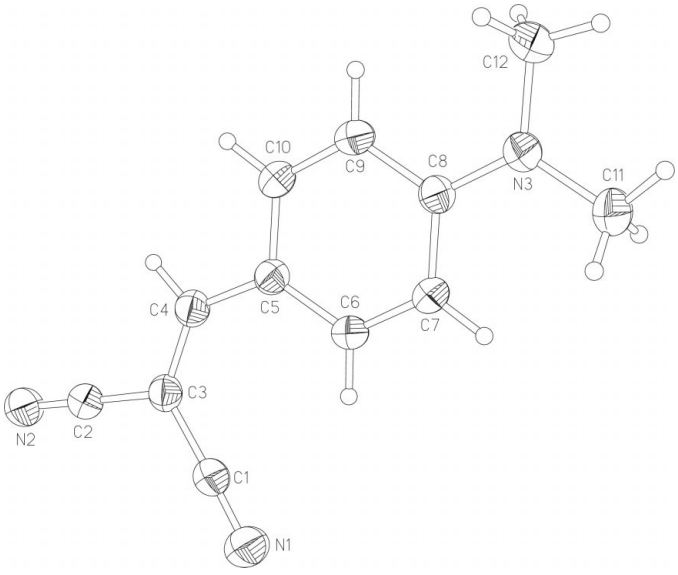


Figure 1
A view of (I) with the atomic numbering scheme.

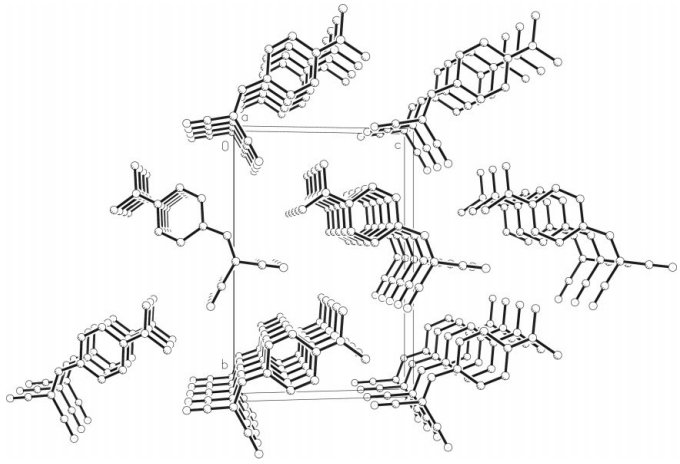


Figure 2
Packing diagram of the molecules of (I) in the crystal.

Experimental

The title compound was prepared according to the literature method of Wang *et al.* (1995). Crystals suitable for X-ray analysis were grown by slow evaporation of a 1:1 (*v*/*v*) CH_2Cl_2/C_2H_5OH solution at room temperature.

Crystal data

$C_{12}H_{11}N_3$
M_r = 197.24
Monoclinic, $P2_1$
a = 3.9972 (4) Å
b = 14.0618 (17) Å
c = 9.5477 (11) Å
β = 100.600 (7)°
V = 527.50 (10) Å^3
Z = 2
D_x = 1.242 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8650 reflections
θ = 4.3–27.5°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, orange
0.50 × 0.33 × 0.25 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
8650 measured reflections
1239 independent reflections
1067 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°
$h = -5 \rightarrow 5$
$k = -18 \rightarrow 18$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.06
1239 reflections
139 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 0.0411P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.18 (5)

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

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