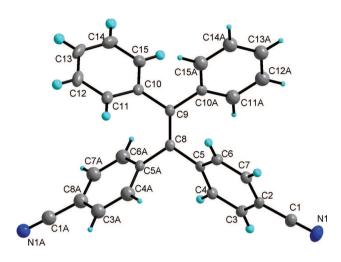
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# Crystal structure of 1,1-di(4-cyanophenyl)-2, 2-diphenylethene, $C_{28}H_{18}N_2$



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## Abstract

 $C_{28}H_{18}N_2$ , orthorhombic, Pccn (no. 56), a = 9.8955(6) Å, b = 11.0163(6) Å, c = 19.9752(14) Å, V = 2177.5(2) Å<sup>3</sup>, Z = 4,  $R_{gt}(F) = 0.0402$ ,  $wR_{ref}(F^2) = 0.1012$ , T = 123(2) K.

**CCDC no.:** 1840632

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

# Source of materials

1,1-Di(4-bromophenyl)-2,2-diphenylethene was synthesized according to the literature [4]. All other chemicals were purchased and used as received. A mixture of 1,1-di(4-bromophenyl)-2,2-diphenylethene (1.471 g, 3 mmol) and CuCN (0.717 g, 8 mmol) in dry DMF (45 mL) was heated at

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Table 1: Crystal collection and handling.

Crystal:	block, yellow		
size:	$0.16\times0.10\times0.06~\text{mm}$		
Wavelength:	Mo $K_{\alpha}$ radiation ( $\lambda = 0.71073 \text{ Å}$ )		
μ:	$0.068 \; \mathrm{mm}^{-1}$		
Diffractometer, scan mode:	Bruker APEX II, $oldsymbol{\phi}$ and $\omega$ -scans		
$\theta_{\sf max}$ , completeness:	26.4°, >99%		
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}, R_{\text{int}}$ :	20003, 2229, 0.0446		
Criterion for $I_{obs}$ , $N(hkl)_{gt}$ :	$I_{\rm obs} > 2\sigma(I_{\rm obs})$ , 1949		
N(param) <sub>refined</sub> :	137		
Programs:	Bruker programs [1], SHELX [2], PLATON [3]		

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\mathring{A}^2$ ).

Atom	х	у	z	U <sub>iso</sub> */U <sub>eq</sub>
N1	0.55161(13)	0.76255(11)	0.50231(6)	0.0376(3)
C1	0.57888(14)	0.67316(12)	0.47676(7)	0.0274(3)
C2	0.61666(13)	0.56147(11)	0.44331(6)	0.0228(3)
C3	0.73620(13)	0.50308(11)	0.46132(6)	0.0249(3)
Н3	0.7888	0.5332	0.4962	0.030
C4	0.77618(12)	0.39994(11)	0.42703(6)	0.0224(3)
H4	0.8548	0.3598	0.4398	0.027
C5	0.69997(12)	0.35547(10)	0.37361(6)	0.0189(3)
C6	0.57695(12)	0.41189(11)	0.35840(6)	0.0216(3)
H6	0.5227	0.3802	0.3246	0.026
C7	0.53510(12)	0.51390(11)	0.39279(6)	0.0234(3)
H7	0.4531	0.5506	0.3823	0.028
C8	0.7500	0.2500	0.33368(8)	0.0191(3)
C9	0.7500	0.2500	0.26570(9)	0.0206(4)
C10	0.78197(13)	0.13901(11)	0.22566(6)	0.0224(3)
C11	0.72256(13)	0.02739(11)	0.24041(7)	0.0260(3)
H11	0.6598	0.0218	0.2749	0.031
C12	0.75656(15)	-0.07574(12)	0.20389(7)	0.0333(3)
H12	0.7172	-0.1499	0.2146	0.040
C13	0.84816(16)	-0.06912(13)	0.15191(8)	0.0377(4)
H13	0.8714	-0.1386	0.1281	0.045
C14	0.90509(17)	0.04175(14)	0.13558(7)	0.0380(4)
H14	0.9656	0.0471	0.1001	0.046
C15	0.87219(15)	0.14520(13)	0.17196(7)	0.0303(3)
H15	0.9107	0.2193	0.1604	0.036

reflux under nitrogen for three days. A mixture of ethylenediamine (10 mL) and water (15 mL) was added after the mixture had cooled to 90 °C. The resulting mixture was stirred at 90 °C for 3 h and then cooled to room temperature. The

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product was extracted with dichloromethane three times and the organic layer dried over magnesium sulfate, filtered, and evaporated. A quantity of 0.802 g (70% yield) of C<sub>28</sub>H<sub>18</sub>N<sub>2</sub> was isolated as yellow crystals. <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>)  $\delta$  7.71 (d, J = 8.1 Hz, 2H), 7.16 (t, J = 7.9 Hz, 3H), 7.08 (d, J = 8.0 Hz, 2H), 7.04···6.96 (m, 2H). **MALDI-TOF MS**: m/z calculated for  $C_{28}H_{18}N_2$  382.4560, found 382.4321 [M]<sup>+</sup>. **Elemental analysis** calculated for C<sub>28</sub>H<sub>18</sub>N<sub>2</sub>: C, 87.93; H, 4.74; N, 7.33%; found: C, 87.80, H, 4.63; N, 7.27%.

Yellow block crystals were obtained by slow evaporation of methanol/methylene dichloride solution.

# **Experimental details**

All H atoms bond to C atoms were introduced using the HFIX command in the SHELXL program [2]. All H atoms were treated as riding atoms with  $U_{iso}(H) = 1.2 U_{eq}(C)$  for hydrogen atoms. The structure was checked using PLATON [3]. There is a void in the unit cell, which has a volume of 32  $Å^3$ .

### Comment

Aggregation-induced emission (AIE) phenomenon of fluorescent solid materials have attracted significant attention because of their wide applications such as organic lightemitting diodes (OLEDs), solar cells, bioimaging, optoelectronic, optomechanical switching and storage devices [5–10]. As an iconic AIE molecule, tetraphenylethylene (TPE) and derivatives have been used to develop new fluorescent materials, such as highly solid fluorescence quantum yield owing to their rich electrochemical and excited state properties [11-13]. It is well known that the electronic structures and optoelectronic properties of TPE can be facilely modulated through tuning the electron donor and acceptor groups. Amongst various strong electron acceptor groups, the cyano group is the special one: solid fluorescence quantum vield of TPE derivatives with cyano group has increased rather than decreased. TPE derivatives with cyano groups show special characteristic such as highly solid fluorescence quantum yield, intriguing TADF properties, multicolor mechanochromism, and so on [14-16]. Up to now, a few TPE derivatives directly connected cyano group were obtained because of its symmetrical structure and active positions [17].

The crystal structure analysis agrees with expected structure of the title compound. The molecular structure has almost axial symmetry. The cyano groups are at the expected sites. The C-N bond length is 1.1414(18) Å, which is the typical bond distance. The molecular structure displays twisted paddle-like conformation. As expected, there are no intermolecular  $\pi$ - $\pi$  interactions. However, there exist weak intermolecular  $C-H\cdots\pi$  and  $C-H\cdots N$  interactions. C-H··· N interactions link molecules into a ladder-like

one-dimensional structure. These are linked by  $C-H\cdots\pi$ interactions, giving a three-dimensional structure.

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