

A second polymorphic form of *N,N'*-diphenyl-1,4-phenylenediamine

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Received 28 February 2000

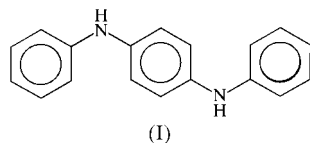
Accepted 2 March 2000

Data validation number: IUC0000062

A new triclinic polymorphic form of *N,N'*-diphenyl-1,4-phenylenediamine ($C_{18}H_{16}N_2$) has been obtained through appropriate recrystallization of the orthorhombic form. It crystallized in the centrosymmetric space group $P\bar{1}$, with two half molecules as the asymmetric unit.

Comment

Recent research in the conducting-polymer field pointed out the importance of preliminary studies on some related oligomers. It is now well established that conformational characteristics of the polyaniline polymer play a crucial role for its physical properties, including transport characteristics. The structure determination of *N,N'*-diphenyl-1,4-phenylenediamine, (I), an oligomer of polyaniline, is part of that research development.



The new triclinic polymorphic form of *N,N'*-diphenyl-1,4-phenylenediamine crystallized in the centrosymmetric space group $P\bar{1}$, with two half molecules as the asymmetric unit. It differs from the orthorhombic form (Povet'eva *et al.*, 1976) not only by its molecular packing, but also by its torsion angles. Analyzed with the three Euler angles, the torsion of the two independent molecules of the triclinic form (respectively $\omega = 140^\circ$, $\chi = 42^\circ$, $\varphi = 38^\circ$ and $\omega = 133^\circ$, $\chi = 28^\circ$, $\varphi = 43^\circ$) is much more pronounced than that of the unique molecule of the orthorhombic form ($\omega = 135^\circ$, $\chi = 4^\circ$, $\varphi = 30^\circ$).

Experimental

N,N'-Diphenyl-1,4-phenylenediamine (Aldrich 98%) was purified through three successive recrystallizations from toluene. Some gray crystals were obtained, with the structure corresponding to that

already published (Povet'eva *et al.*, 1976). The compound was then subsequently sublimed under vacuum at 413 K, giving rise to new transparent crystals.

Crystal data

$C_{18}H_{16}N_2$	$Z = 2$
$M_r = 260.3$	$D_x = 1.28 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.911 (2) \text{ \AA}$	Cell parameters from 1631 reflections
$b = 8.984 (2) \text{ \AA}$	$\theta = 2-24^\circ$
$c = 11.133 (3) \text{ \AA}$	$\mu = 0.076 \text{ mm}^{-1}$
$\alpha = 108.56 (3)^\circ$	$T = 150 \text{ K}$
$\beta = 94.60 (3)^\circ$	Plate, colourless
$\gamma = 112.38 (3)^\circ$	$0.30 \times 0.25 \times 0.08 \text{ mm}$
$V = 675.0 (4) \text{ \AA}^3$	

Data collection

Stoe IPDS diffractometer	$R_{\text{int}} = 0.057$
ω scans	$\theta_{\text{max}} = 23.95^\circ$
7072 measured reflections	$h = -8 \rightarrow 8$
1931 independent reflections	$k = -10 \rightarrow 8$
1450 reflections with $F^2 > 2\sigma(F^2)$	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(I) + 0.0016I^2]$
$R(F) = 0.030$	$(\Delta/\sigma)_{\text{max}} = 0.0001$
$wR(F^2) = 0.069$	$\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$
$S = 1.09$	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
1931 reflections	Extinction correction: B—C type 1,
189 parameters	Lorentzian isotropic
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.9 (1)

H atoms bonded to C atoms were placed at calculated positions. H atoms bonded to N were located from difference Fourier syntheses and their positions refined. A unique atomic displacement parameter was refined for all H atoms.

Data collection: *EXPOSE* (Stoe & Cie, 1996); cell refinement: *CELL* (Stoe & Cie, 1996); data reduction: *INTEGRATE* (Stoe & Cie, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1997); program(s) used to refine structure: *JANA98* (Petricek & Dusek, 1998); software used to prepare material for publication: *JANA98*.

The authors wish to acknowledge F. Guillet-Lary for her help in growing the crystals.

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