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# A phenyl-end-capped tetramer of aniline

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**Key indicators**

Single-crystal X-ray study
$T$ = 300 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.049
$wR$ factor = 0.113
Data-to-parameter ratio = 14.4

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



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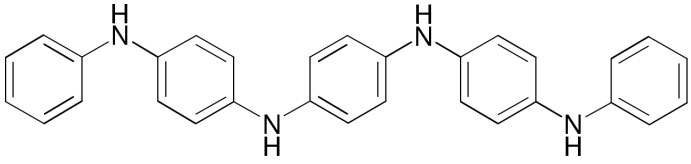
The title compound, *N*,*N*′-bis[4-(phenylamino)phenyl]-1,4-phenylenediamine, $C_6H_5(NHC_6H_4)_3NHC_6H_5$ or $C_{30}H_{26}N_4$, has been obtained as large single crystals through sublimation under a static secondary vacuum, allowing for its structure determination. As in the phenyl-end-capped dimer, the (CNC) inter-ring links lie within a plane. The molecules have crystallographic twofold rotation symmetry, two half molecules making up the asymmetric unit.

## Comment

Recently, many oligoanilines have received particular attention due to their interesting physical properties. Indeed, their various methods of processing (crystal growth, ordered thin films, powders or solutions) make them good candidates for electronic devices. Several papers have already reported some of their potential applications, such as gas sensors (Feng & MacDiarmid, 1999) or FET transistor devices (Kuo & Weng, 2000). In the course of our work on those oligoanilines, we obtained the phenyl-end-capped tetramer aniline, (I), and show that it resembles its phenyl-end-capped dimer counterpart (Boyer *et al.*, 2000).



(I)

The crystal structure consists of two half molecules in the asymmetric unit (Fig. 1). Since, within each molecule, the (C—N—C) inter-ring links lie in the same plane, both molecules can easily be described in terms of torsion angles between rings. The departure of the rings from that plane are 44.07 (12) [C1*a* through C3*a*], 13.05 (7) [C4*a* through C9*a*] and 44.39 (7)° [C10*a* through C15*a*] in molecule *A*, and 32.08 (13) [C1*b* through C3*b*], 22.66 (8) [C4*b* through C9*b*] and 28.96 (7)° [C10*b* through C15*b*] in molecule *B*.

## Experimental

The title compound was prepared according to a new synthetic route for oligoanilines developed by Wang & MacDiarmid (2002). The phenyl-end tetramer of aniline in the reduced oxidation state is prepared from a reaction of dianiline(*N*-phenyl-1,4-phenylenediamine) with hydroquinone, using titanium(IV) *n*-butoxide as condensing reagent. A light-violet powder was obtained and recrystallized through sublimation under a static secondary vacuum. Colourless crystals were grown at *ca* 483 K.

*Crystal data*

| | |
|---|---|
| $C_{30}H_{26}N_4$ | $Z = 2$ |
| $M_r = 442.6$ | $D_x = 1.287$ Mg m$^{-3}$ |
| Triclinic, $P\overline{1}$ | Cell parameters from 23 907 reflections |
| $a = 5.7328$ (1) Å | $\theta = 4.1$–$26.4°$ |
| $b = 8.8866$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $c = 22.6889$ (6) Å | $T = 300$ K |
| $\alpha = 82.7481$ (8)° | Plate, colourless |
| $\beta = 84.5281$ (8)° | 0.25 × 0.10 × 0.02 mm |
| $\gamma = 88.4739$ (11)° | |
| $V = 1141.29$ (4) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD diffractometer | $R_{int} = 0.047$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 26.3°$ |
| 23 907 measured reflections | $h = -7 \rightarrow 7$ |
| 4616 independent reflections | $k = -11 \rightarrow 10$ |
| 3022 reflections with $I > 2\sigma(I)$ | $l = -28 \rightarrow 28$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(I) + 0.001024I^2]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.049$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.113$ | $\Delta\rho_{max} = 0.24$ e Å$^{-3}$ |
| $S = 1.54$ | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |
| 4616 reflections | Extinction correction: B–C type 1 Gaussian isotropic (Becker & Coppens, 1974) |
| 320 parameters | Extinction coefficient: 1.21 (18) |
| H atoms treated by a mixture of independent and constrained refinement | |

H atoms bonded to C atoms were placed at calculated positions. H atoms bonded to N atoms were located from difference Fourier syntheses and their positions refined. Riding isotropic displacement parameters were used for all H atoms.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1995); program(s) used to refine structure: *JANA*2000 (Petricek & Dusek, 2000); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *JANA*2000.

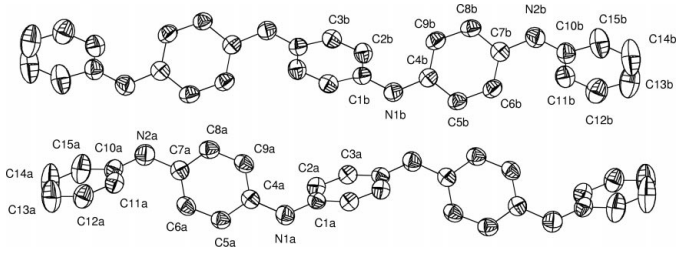



**Figure 1**
The molecular structure of (I) showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

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