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# (4-Acetylphenyl)diphenylamine

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In the title compound, $C_{20}H_{17}NO$, the bond lengths are normal. The crystal packing is stabilized by van der Waals forces.

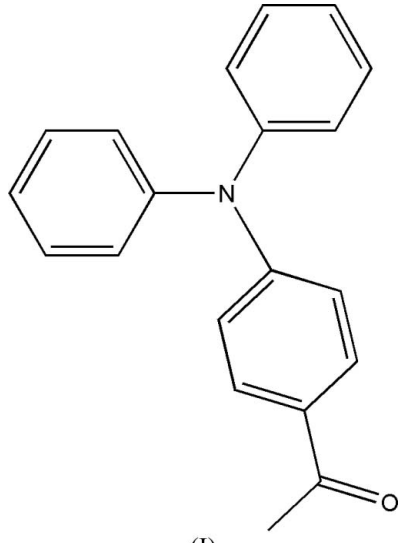
**Key indicators**

Single-crystal X-ray study
$T$ = 292 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.054
$wR$ factor = 0.142
Data-to-parameter ratio = 17.5

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

## Comment

Arylamine derivatives are common as intermediates in the synthesis of many compounds and polymers (Yao *et al.*, 2006; Beller, 1995). We became interested in using a Friedel–Crafts reaction to obtain the title compound, (I), which is a good intermediate for several compounds (Chiang *et al.*, 2002). In the structure of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Wang *et al.*, 2006) (Table 1).




(I)

## Experimental

Triphenylamine (4.42 g, 0.018 mole), zinc chloride (2.45 g, 0.018 mol) and dichloromethane (36 ml) were added slowly to a solution of acetyl chloride (1.42 g, 1.3 ml, 0.018 mol) in dichloromethane (4 ml) with vigorous stirring at room temperature over 5 min. The mixture was refluxed for 20 h; after cooling to room temperature, it was poured into aqueous HCl (2 *M*, 150 ml). The dichloromethane layer was separated and washed with water to pH 7. The dichloromethane was removed using a rotary evaporator and the residue purified by column chromatography over a silica gel column using petroleum ether/chloroform (*v*/*v*, 3:1) as eluent to afford (I) as yellow crystals (4.9 g, 95% yield; m.p. 416–418 K). Crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

*Crystal data*

$C_{20}H_{17}NO$
$M_r$ = 287.35
Monoclinic, $P2_1/c$
$a$ = 12.4246 (15) Å
$b$ = 11.6657 (14) Å
$c$ = 10.7149 (13) Å
$\beta$ = 95.692 (2)°
$V$ = 1545.4 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 292 (2) K
0.40 × 0.20 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{min}$ = 0.970, $T_{max}$ = 0.993
13015 measured reflections
3501 independent reflections
2405 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.142
$S$ = 1.04
3501 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C6—N1 | 1.425 (2) | C19—O1 | 1.217 (2) |
| C13—N1 | 1.4086 (19) | C19—C20 | 1.491 (3) |
| C16—C19 | 1.487 (2) | | |
| C13—N1—C6 | 119.98 (13) | C6—N1—C7 | 118.79 (12) |
| C13—N1—C7 | 120.21 (13) | | |

H were placed in geometrically idealized positions (C—H = 0.96 Å for methyl and 0.93 Å for aromatic) and refined using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C) or $U_{iso}$(H) = 1.5$U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

## References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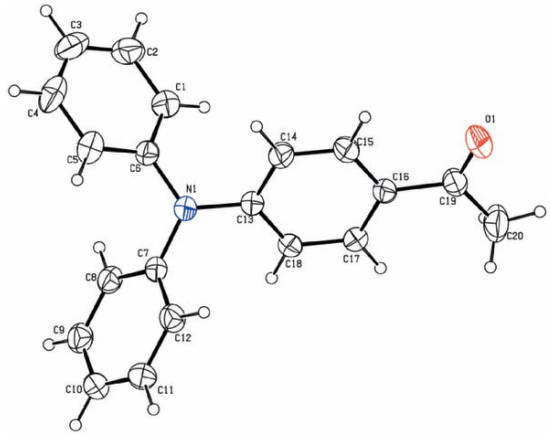


**Figure 1**
**Author: please supply ellipsoid plot. State probability level in caption.**

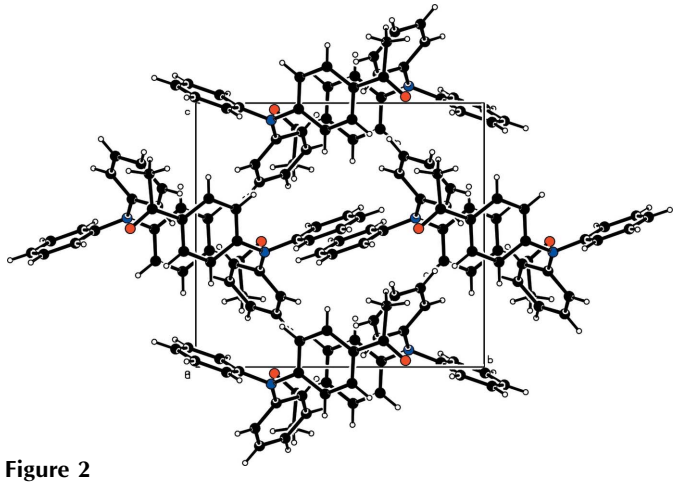

**Figure 2**
View of the packing of (I).


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