organic papers

Tris(4-acetylphenyl)amine

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Key indicators

The crystal structure of the title compound, $C_{24}H_{21}NO_3$, is stabilized by weak C—H···π interactions.

Comment

Triphenylamine is of current research interest due to its potential application in a number of new areas. Most commonly, triphenylamine has been used as a hole-transporting layer (HTL) in the preparation of organic light-emitting diodes (OLEDs) (Li *et al.*, 2005). Recently, many triphenylamine derivatives have been reported (Yan *et al.*, 2004). In this paper, the synthesis and crystal structure of a new triphenylamine derivative are reported.

(I)
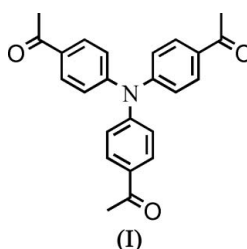
The molecular structure of (I) is shown in Fig. 1 and a packing diagram of the compound is given in Fig. 2. The N atom is in an essentially trigonally planar geometry, the bond angles around it ranging from 118.7 (3) to 120.9 (4)°. The C=O distances range from 1.208 (7) to 1.276 (6) Å. The dihedral angles between the benzene rings C3–C8 and C11–C16, C3–C8 and C19–C24, and C19–C24 and C11–C16 are 69.4 (2), 63.1 (1) and 63.7 (2)°, respectively. In the crystal
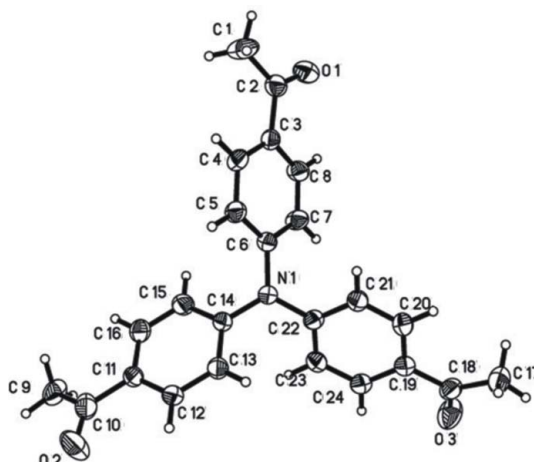
Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids.
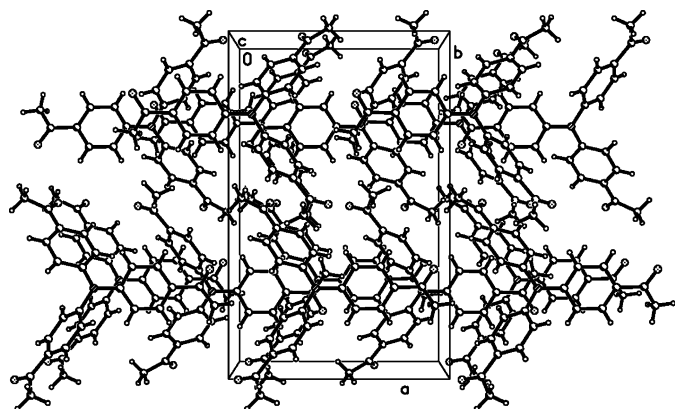
Figure 2
The packing of the title compound.

structure, the molecules are stacked in pairs through C—H···π interactions, with an H-to-centroid distance of 3.847 (2) Å.

Experimental

For the preparation of tris(4-acetylphenyl)amine: a flask was charged with a mixture of triphenylamines (1.486 g, 4 mmol) and acetyl chloride (0.552 g, 0.5 ml) in dichloromethane in ice–water, refluxed for 24 h and then poured into ice–water and stirred vigorously for 30 min. The resulting yellow solid was filtered and air-dried. The residue was purified by flash column chromatography to give the product as a yellow solid 1.22 g (yield: 80%). Single crystals of (I) were grown by slow evaporation of an ethyl acetate/petroleum ether (1:5) solution.

Crystal data

$C_{24}H_{21}NO_3$	Mo $K\alpha$ radiation
$M_r = 371.42$	Cell parameters from 1315
Orthorhombic, $Pna2_1$	reflections
$a = 18.697$ (4) Å	$\theta = 2.8$–20.2°
$b = 11.899$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 8.722$ (2) Å	$T = 298$ (2) K
$V = 1940.5$ (8) Å^3	Thick plate, yellow
$Z = 4$	$0.45 \times 0.38 \times 0.19$ mm
$D_x = 1.271$ Mg m^{-3}	

Data collection

Bruker SMART CCD area-detector diffractometer	1839 independent reflections
	1070 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.071$
Absorption correction: multi-scan	$\theta_{max} = 25.0°$
SADABS (Sheldrick, 1996)	$h = -22 \rightarrow 22$
$T_{min} = 0.963$, $T_{max} = 0.984$	$k = -11 \rightarrow 14$
9882 measured reflections	$l = -9 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$+ 0.5204P]$
$wR(F^2) = 0.126$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
1839 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C22	1.410 (6)	C1—C2	1.484 (8)
N1—C14	1.412 (5)	C2—C3	1.491 (7)
N1—C6	1.434 (5)	C9—C10	1.443 (7)
O1—C2	1.218 (6)	C17—C18	1.489 (7)
O2—C10	1.276 (6)	C18—C19	1.467 (7)
O3—C18	1.208 (7)		
C22—N1—C14	120.9 (4)	O1—C2—C3	119.5 (5)
C22—N1—C6	118.7 (3)	O2—C10—C11	119.9 (5)
C14—N1—C6	119.6 (4)	O3—C18—C17	120.5 (6)

In the absence of significant anomalous scattering effects, Friedel pairs were averaged. All H atoms were placed in geometrically idealized positions, with C—H = 0.93 or 0.96 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

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