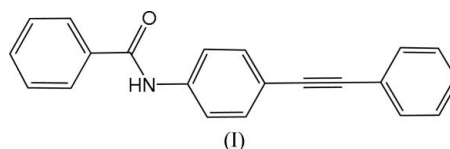


***N*-[4-(Phenylethynyl)phenyl]benzamide**Guodong Yin,<sup>a</sup> Shengli Hu,<sup>b</sup>  
Yitao Li<sup>a</sup> and Anxin Wu<sup>a\*</sup><sup>a</sup>Key Laboratory of Pesticides and Chemical Biology of the Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and <sup>b</sup>Department of Chemistry & Environmental Engineering, Hubei Normal University, Huangshi 435002, People's Republic of ChinaCorrespondence e-mail:  
chwuax@mail.ccnu.edu.cn**Key indicators**Single-crystal X-ray study  
*T* = 292 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
*R* factor = 0.045  
*wR* factor = 0.133  
Data-to-parameter ratio = 8.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In the title molecule,  $\text{C}_{21}\text{H}_{15}\text{NO}$ , the two ethynyl-bridged six-membered rings are almost coplanar, making a dihedral angle of  $3.3 (2)^\circ$ . The dihedral angle between the two terminal phenyl rings is  $62.9 (2)^\circ$ . The crystal packing is stabilized by weak intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.**Comment**The low-temperature luminescence of the title compound, (I), in non-polar solvents has been studied by Frederick & Liu (1999). In this paper, we report the crystal structure of (I). In the molecule (Fig. 1), the bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The two ethynyl-bridged six-membered rings are almost coplanar, making a dihedral angle of  $3.3 (2)^\circ$ . The dihedral angle between the two terminal phenyl rings is  $62.9 (2)^\circ$ . The  $\text{C}12-\text{N}1-\text{C}15-\text{C}16$  torsion angle is  $178.8 (2)^\circ$ . The crystal packing (Fig. 2) is stabilized by weak intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 1), which link the molecules into chains along the *b* axis. The intermolecular  $\text{N}\cdots\text{O}$  distance of  $3.252 (3) \text{ \AA}$  is slightly longer than that in benzanilide [ $3.141 (4) \text{ \AA}$ ; Bowes *et al.*, 2003].**Experimental**

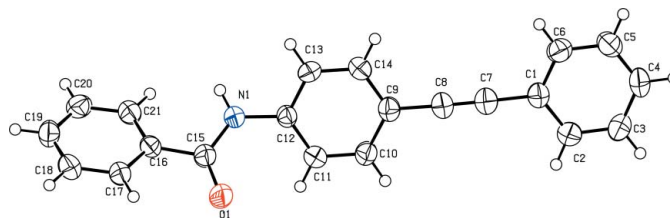
The title compound was synthesized according to the literature method of Frederick &amp; Liu (1999). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution in DMF–MeOH (1:1).

*Crystal data* $\text{C}_{21}\text{H}_{15}\text{NO}$   
 $M_r = 297.34$   
Monoclinic, *Cc*  
 $a = 36.589 (5) \text{ \AA}$   
 $b = 5.3932 (7) \text{ \AA}$   
 $c = 7.9572 (11) \text{ \AA}$   
 $\beta = 96.689 (2)^\circ$   
 $V = 1559.5 (4) \text{ \AA}^3$   
 $Z = 4$  $D_x = 1.266 \text{ Mg m}^{-3}$   
Mo  $K\alpha$  radiation  
Cell parameters from 1147 reflections  
 $\theta = 2.2-23.6^\circ$   
 $\mu = 0.08 \text{ mm}^{-1}$   
 $T = 292 (2) \text{ K}$   
Block, colourless  
 $0.30 \times 0.20 \times 0.10 \text{ mm}$ *Data collection*Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.977$ ,  $T_{\max} = 0.992$   
4343 measured reflections1690 independent reflections  
1360 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\text{max}} = 27.0^\circ$   
 $h = -35 \rightarrow 46$   
 $k = -6 \rightarrow 6$   
 $l = -10 \rightarrow 8$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.133$   
 $S = 1.08$   
 1690 reflections  
 208 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0786P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{Å}^{-3}$



**Figure 1**  
View of (I), showing the atom-labelling scheme and 50% probability displacement ellipsoids.

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O1^i$	0.86	2.42	3.250 (4)	163

Symmetry code: (i)  $x, y + 1, z$ .

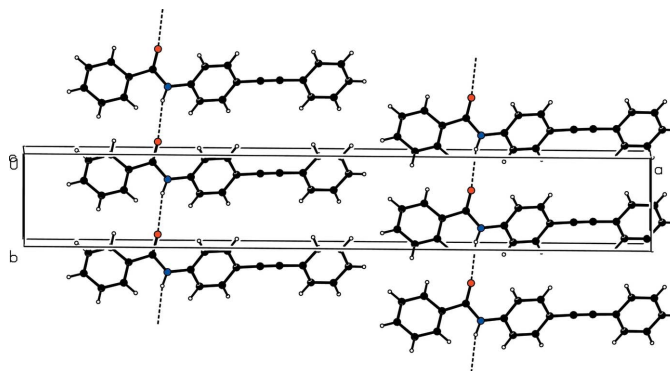
After their location on a difference Fourier map, H atoms were placed in calculated positions and refined as riding with  $C-H = 0.93-0.97 \text{ Å}$ ,  $N-H = 0.86 \text{ Å}$ , and  $U_{\text{iso}} = 1.2$  or  $1.5$  times  $U_{\text{eq}}$  of the parent atom. Owing to the absence of any significant anomalous scatterers in the molecule, the Friedel pairs were merged before the final refinement.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Central China Normal University, the National Natural Science Foundation of China (No.20472022), and the Hubei Province Natural Science Fund (Nos. 2004ABA085 and 2004ABC002) for financial support.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.



**Figure 2**  
The crystal packing, viewed approximately along the  $c$  axis. Inter-molecular  $N-H\cdots O$  hydrogen bonds are shown as dashed lines.

Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (1999). *SAINTE*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Frederick, D. L. & Liu, W. (1999). *J. Phys. Chem. A*, **103**, 9678–9686.  
 Bowes, K. F., Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2003). *Acta Cryst.* **C59**, o1–o3.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.