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## Key indicators

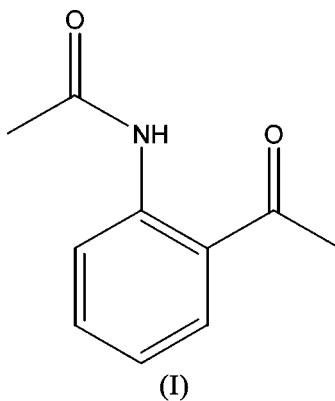
Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.048  
 $wR$  factor = 0.118  
Data-to-parameter ratio = 13.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.***N*-(2-Acetylphenyl)acetamide**

The title compound,  $\text{C}_{10}\text{H}_{11}\text{NO}_2$ , was synthesized from 2'-aminoacetophenone in acetic anhydride. In the molecular structure, an intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond [ $\text{H}\cdots\text{O} = 1.893(18)$  Å] appears to affect the overall planar conformation of the molecule.

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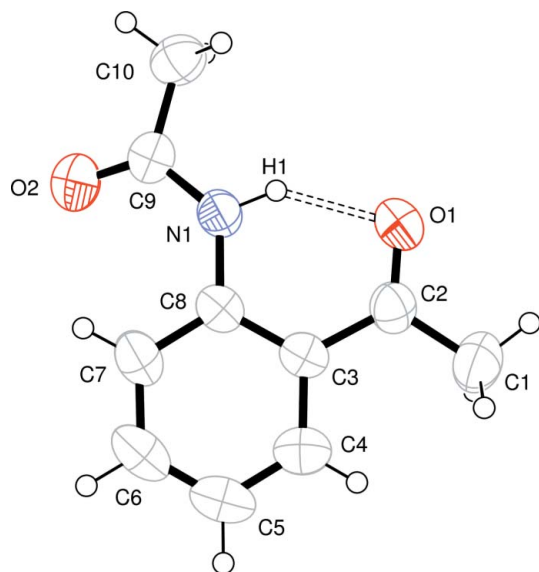
## Comment

Derivatives of acetophenone have been synthesized for many reasons: as precursors of indoles (Fuerstner *et al.*, 1991; Fuerstner & Jumbam, 1992) and quinolines (Curran & Kuo, 1984), in order to study their chemiluminescent properties (Pileni & Santus, 1977, Giraud *et al.*, 1977; Sugiyama & Akutagawa, 1967), as potential analgesic precursors (Giuliani *et al.*, 1983; Lembo *et al.*, 1983), and to study intramolecular hydrogen bonding (Appleton *et al.*, 1970; Hambly & Bonnyman, 1958). Our special interest in acetophenone derivatives results from their use in the synthesis of unsymmetrical Tröger's base analogs (Webb & Wilcox, 1990; Pardo *et al.*, 2001; Jensen *et al.*, 2002).



The title compound, (I) (Fig. 1), was synthesized as an intermediate in the total synthesis of 6-methyl-2-nitro-6*H*,12*H*-5,11-methanodibenzo[*b,f*][1,5]diazocine, an unsymmetrical Tröger's base compound. A key step in the synthesis involved Schiff base formation between the acetyl O atom of compound (I) and the amino N atom of *p*-nitroaniline. The imine product did not form, although several methodologies were attempted (Weingarten *et al.*, 1967). It is possible that the intramolecular hydrogen bond between the amide H atom and acetyl O atom somehow interferes with the condensation reaction.

The intramolecular hydrogen-bond distance between atoms O1 and H1 (on N1) of 1.893 (18) Å is consistent with other six-



**Figure 1**  
A view of (I) (Farrugia, 1997). Displacement ellipsoids are drawn at the 50% probability level. The intramolecular hydrogen bond between O1 and H1 (on N1) is indicated as a dashed line.

membered ring intramolecular hydrogen bonds [two recent examples have been reported by Manh *et al.* (1999) and Ando *et al.* (2004)]. The molecule of (I) is essentially planar, with an r.m.s. deviation of 0.0420 Å for atoms O1/N1/C1–C8, while atoms C9, C10 and O2 are displaced by 0.344 (2), 0.321 (3) and 0.645 (2) Å, respectively, from this plane.

## Experimental

The title compound, C<sub>10</sub>H<sub>11</sub>NO<sub>2</sub>, was synthesized according to a previously reported method (Leonard & Boyd, 1946). 2'-Aminoacetophenone (5 g, 37 mmol) was dissolved in acetic anhydride (10 ml) and stirred at room temperature for 3 h. The resulting clear solution was poured on to crushed ice (100 ml) and allowed to stand until all of the excess acetic anhydride had been hydrolyzed. The white precipitate which formed was filtered off and recrystallized from ethanol to yield 6.3 g (96%) of *N*-(2-acetylphenyl)acetamide.

### Crystal data

C<sub>10</sub>H<sub>11</sub>NO<sub>2</sub>  
*M<sub>r</sub>* = 177.20  
 Monoclinic, *P*<sub>2<sub>1</sub></sub>/*c*  
*a* = 7.765 (7) Å  
*b* = 8.699 (7) Å  
*c* = 15.805 (13) Å  
 β = 119.35 (7)°  
*V* = 930.6 (14) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.265 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 μ = 0.09 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Needle, orange  
 0.43 × 0.31 × 0.27 mm

### Data collection

Oxford Diffraction Sapphire3 diffractometer  
 ω scans  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2005)  
*T<sub>min</sub>* = 0.809, *T<sub>max</sub>* = 0.975

19878 measured reflections  
 1639 independent reflections  
 1019 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.036  
*θ<sub>max</sub>* = 25.0°

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.048  
*wR*(*F*<sup>2</sup>) = 0.118  
*S* = 0.93  
 1639 reflections  
 124 parameters

H atoms treated by a mixture of independent and constrained refinement  
*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0807*P*)<sup>2</sup>]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
 (Δ/σ)<sub>max</sub> < 0.001  
 Δρ<sub>max</sub> = 0.18 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.26 e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1···O1	0.888 (17)	1.893 (18)	2.657 (2)	143.1 (15)

H atoms bonded to C atoms were placed in calculated positions, with C–H = 0.93 Å, or 0.96 Å for methyl groups, and included in the refinement in a riding-model approximation, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C), or 1.5*U*<sub>eq</sub>(C) for methyl H atoms. The N-bound H atom was refined independently with an isotropic displacement parameter.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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