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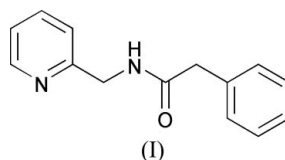
Key indicators

Single-crystal X-ray study
 $T = 97\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.033
 wR factor = 0.089
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2-Phenyl-*N*-(2-pyridylmethyl)acetamideThe geometrical parameters for the title compound, $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}$, are normal. There are two molecules in the asymmetric unit. The molecules assemble *via* $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into one-dimensional chains.

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Comment

Recently, we reported the synthesis and copper coordination chemistry of a family of pyridyl amide ligands (Klein *et al.*, 2004, Mondal *et al.*, 2004, Michels *et al.*, 2005, Pal Chaudhuri *et al.*, 2006). While these pyridyl amide compounds possess varied and versatile coordination properties as ligands with transition metal ions, we are also interested in their hydrogen-bonding behavior. Here we present the crystal structure of the phenylmethyl-substituted title compound, (I). In the following paper (Whiteaker *et al.*, 2006), we present the related triphenylmethyl-substituted pyridyl amide, $\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}$, (II).

Compound (I) possesses normal geometric parameters. There are two molecules in the asymmetric unit. Inter-

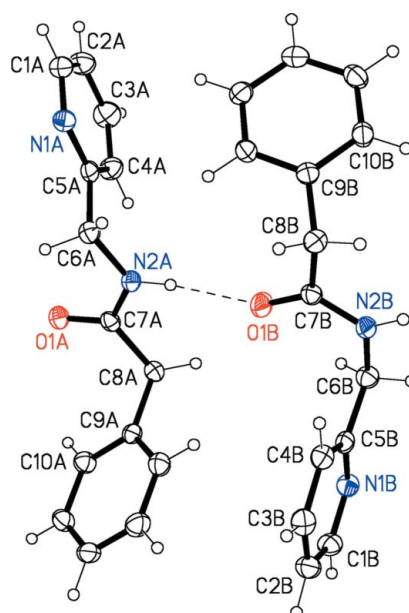


Figure 1

The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms). The dashed line indicates a hydrogen bond.

molecular N—H···O hydrogen bonding (Table 1) in (I) results in the formation of one-dimensional chains along the crystallographic *c* axis. The structure is further stabilized by C—H··· π interactions involving the phenyl groups in one chain of molecules and the pyridyl groups of an adjacent chain. The average distance between the least squares plane of the pyridyl ring and the edge of the phenyl ring (C13–C14) is 3.61 Å.

The intermolecular hydrogen bonding in (II) is different and involves inversion-symmetry-generated dimers linked by pairs of N—H···N(pyridine) hydrogen bonds. The difference may arise from steric factors; the bulky triphenylmethyl group in (II) prevents the amide groups from getting close enough to an adjacent C=O unit to form the chains of N—H···O hydrogen bonds that occur in (I).

Experimental

Compound (I) was synthesized according to previously reported procedures (Pal Chaudhuri *et al.*, 2006). X-ray quality crystals were grown by slow evaporation of a water–acetonitrile (1:1) solution.

Crystal data

| | |
|--------------------------------|---|
| $C_{14}H_{14}N_2O$ | $Z = 8$ |
| $M_r = 226.27$ | $D_x = 1.273 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 13.414 (2) \text{ \AA}$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $b = 9.2478 (14) \text{ \AA}$ | $T = 97 (2) \text{ K}$ |
| $c = 19.280 (3) \text{ \AA}$ | Block, colorless |
| $\beta = 99.106 (5)^\circ$ | $0.81 \times 0.41 \times 0.40 \text{ mm}$ |
| $V = 2361.5 (6) \text{ \AA}^3$ | |

Data collection

| | |
|---|--|
| Bruker APEX CCD diffractometer | 24749 measured reflections |
| ω scans | 4628 independent reflections |
| Absorption correction: multi-scan SADABS (Sheldrick, 2002) | 4394 reflections with $I > 2\sigma(I)$ |
| $T_{\min} = 0.937$, $T_{\max} = 0.968$ | $R_{\text{int}} = 0.021$ |
| | $\theta_{\text{max}} = 26.0^\circ$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.8P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.033$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.089$ | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| $S = 1.00$ | $\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$ |
| 4628 reflections | $\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$ |
| 313 parameters | |
| H atoms treated by a mixture of independent and constrained refinement | |

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------|------------|-------------|-------------|---------------|
| $N2A-H2A\cdots O1B$ | 0.893 (13) | 2.001 (14) | 2.8850 (12) | 170.0 (11) |
| $N2B-H2B\cdots O1A^i$ | 0.888 (14) | 1.964 (14) | 2.8483 (12) | 174.0 (12) |

Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

The C-bound H atoms were placed in idealized locations (C—H = 0.95–0.99 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The N-bound H atoms were located in a difference map and their positions were refined freely, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

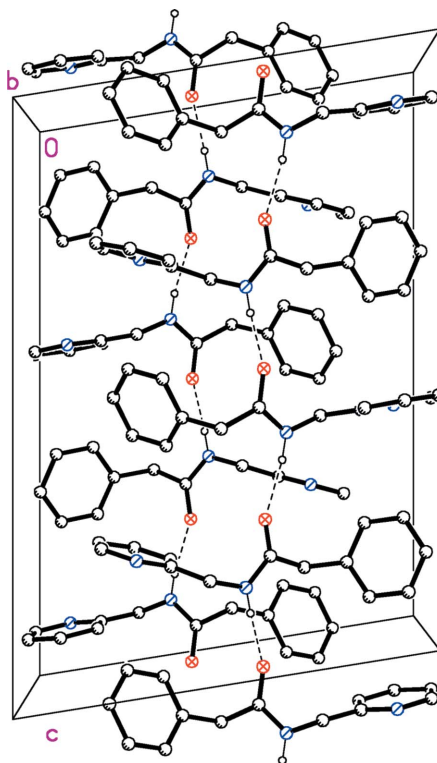


Figure 2

The molecular packing of (I), viewed along the *b* axis. H atoms have been omitted for clarity, except for those involved in hydrogen bonds (dashed lines).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2002); software used to prepare material for publication: *SHELXTL*.

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