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# 3-Carbazoyl-5-methylpyridazin-6(1*H*)-one

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.039
$wR$ factor = 0.102
Data-to-parameter ratio = 11.7

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



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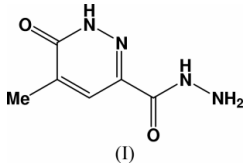
All the non-hydrogen atoms of the title compound, $C_6H_8N_4O_2$, are almost coplanar, except for the $-NH-NH_2$ moiety of the carbazoyl group, forming a conjugated system. There are $\pi$–$\pi$ interactions between neighboring parallel aromatic rings, and intermolecular N—H···N and N—H···O hydrogen bonds lead to a three-dimensional framework.

## Comment

Pyridazinone derivatives have been found to possess widespread pharmacological applications (Hamad *et al.*, 2000; Ingec *et al.*, 2000; Nabaweya, 1999). Some pyridazinones can be used as insecticides in vegetable, melon and other crops (Zou *et al.*, 2002). In order to better understand the structural characteristics of these pyridazinone derivatives, we have synthesized the title compound, (I), and investigated its crystal structure.




(I)

Except for atoms N3 and N4, all the non-H atoms of (I) are almost coplanar, forming a conjugated system (Fig. 1). The N1—N2 and N3—N4 bond lengths are 1.3362 (18) and 1.4054 (19) Å, respectively (Table 1). This means that N3—N4 is a single bond and N1═N2 has double-bond character as a result of the conjugation. There are $\pi$–$\pi$ interactions between adjacent molecules, the distance between neighboring parallel aromatic ring planes being 3.26 (1) Å. There are also N—H···N and N—H···O intermolecular hydrogen bonds (Table 2), which lead to a three-dimensional framework (Fig. 2).

## Experimental

The title compound, (I), was prepared from hydrazine and pyruvic acid by a one-step reaction. Hydrazine (1 mmol) was added slowly to pyruvic acid (1 mmol) and the resulting solution stirred at room temperature for 4 h. After cooling, the product was kept at room temperature and crystals of (I) suitable for single-crystal X-ray diffraction analysis appeared after several days.

*Crystal data*

$C_6H_8N_4O_2$
$M_r$ = 168.16
Monoclinic, $P2_1/c$
$a$ = 7.359 (1) Å
$b$ = 10.261 (1) Å
$c$ = 10.005 (1) Å
$\beta$ = 101.30 (1)°
$V$ = 740.84 (15) Å$^3$
$Z$ = 4
$D_x$ = 1.508 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2289 reflections
$\theta$ = 2.9–27.9°
$\mu$ = 0.12 mm$^{-1}$
$T$ = 293 (2) K
Block, colourless
0.3 × 0.2 × 0.2 mm

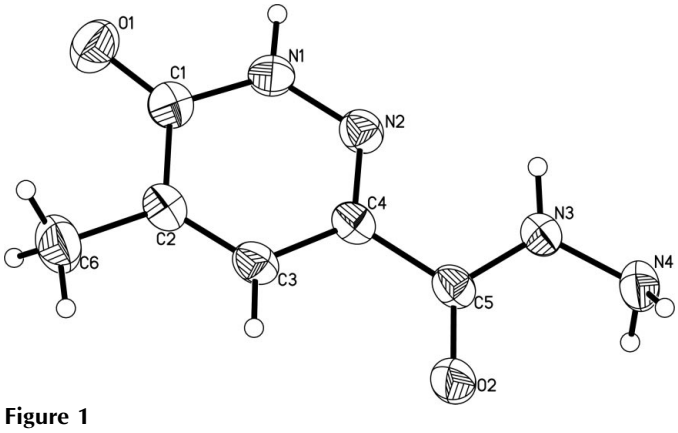



**Figure 1**
View of the title compound, (I), with ellipsoids at the 50% probability level.

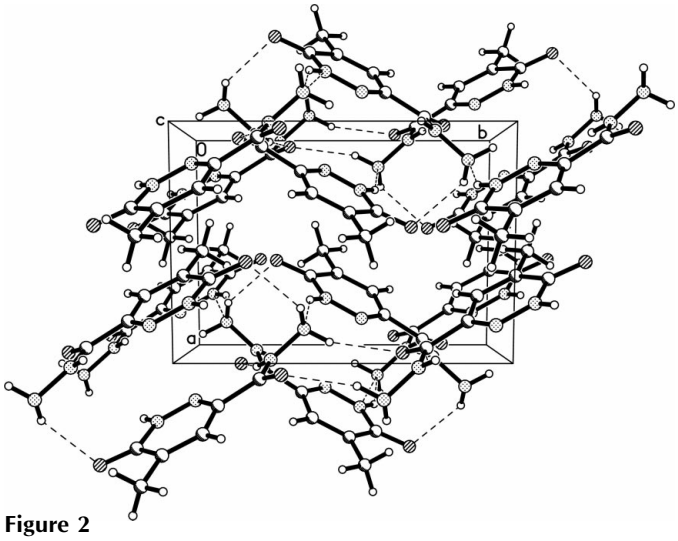



**Figure 2**
A view of the crystal packing of (I). Hydrogen bonds are indicated by dashed lines.

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 1190 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.037$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 25.0^\circ$ |
| Absorption correction: none | $h = -8 \rightarrow 8$ |
| 3540 measured reflections | $k = -12 \rightarrow 8$ |
| 1288 independent reflections | $l = -11 \rightarrow 11$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | |
| $wR(F^2) = 0.102$ | |
| $S = 1.09$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1288 reflections | $\Delta\rho_{max} = 0.19$ e Å$^{-3}$ |
| 110 parameters | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |
| H-atom parameters constrained | |

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

| | | | |
|---|---|---|---|
| C1—O1 | 1.2275 (19) | C4—C5 | 1.490 (2) |
| C1—N1 | 1.3711 (19) | C5—O2 | 1.2286 (18) |
| C1—C2 | 1.450 (2) | C5—N3 | 1.3281 (19) |
| C2—C3 | 1.348 (2) | N1—N2 | 1.3362 (18) |
| C3—C4 | 1.420 (2) | N3—N4 | 1.4054 (19) |
| C4—N2 | 1.2972 (19) | | |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N4$^{i}$ | 0.86 | 2.14 | 2.8794 (17) | 144 |
| N3—H3$A$···O2$^{ii}$ | 0.86 | 2.21 | 3.0171 (17) | 156 |
| N4—H4$A$···O2$^{iii}$ | 0.89 | 2.29 | 3.1452 (19) | 161 |
| N4—H4$C$···O1$^{iv}$ | 0.89 | 2.31 | 3.037 (2) | 139 |

Symmetry codes: (i) $2-x, \frac{1}{2}+y, \frac{5}{2}-z$; (ii) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (iii) $2-x, 1-y, 2-z$; (iv) $2-x, 2-y, 2-z$.

The positions of all H atoms were fixed geometrically (C—H = 0.93 and 0.96 Å, and N—H = 0.86 and 0.89 Å).

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

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