

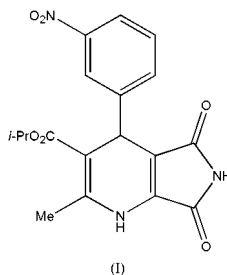
Viktor Vrábek,^{a*}
Štefan Marchalín^b and
Jozef Kožišek^c^aDepartment of Analytical Chemistry, Faculty of Chemical Technology, Slovak Technical University, Radlinskeho 9, Bratislava, Slovak Republic 81237, ^bDepartment of Organic Chemistry, Faculty of Chemical Technology, Slovak Technical University, Radlinskeho 9, Bratislava, Slovak Republic 81237, and ^cDepartment of Physical Chemistry, Faculty of Chemical Technology, Slovak Technical University, Radlinskeho 9, Bratislava, Slovak Republic 81237

Correspondence e-mail: vrabel@cvt.stuba.sk

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.060
 wR factor = 0.083
Data-to-parameter ratio = 16.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Isopropyl 2-methyl-4-(3-nitrophenyl)-5,7-dioxo-4,5,6,7-tetrahydro-1H-pyrrolo-[3,4-*b*]pyridine-3-carboxylateThe crystal structure of the title compound, $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_6$, is formed by single molecules linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into planar sheets. The dihedral angle between the mean planes of the pyridine and substituted phenyl rings is $84.2(1)^\circ$. The 3-nitro substituent on the phenyl ring is rotated from coplanarity with the ring by only $3.7(2)^\circ$.

Comment

The molecules of the title compound, (I), are linked by two $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds. The imino atom N1 (Fig. 1) acts as a donor, *via* H1, to nitro atom O41 of the neighbouring molecule at $(x, y, z - 1)$ [$\text{H1}\cdots\text{O41} = 2.11\text{ \AA}$ and $\text{N1}-\text{H1}\cdots\text{O41} = 173^\circ$]. The other imino atom N6 acts as donor, *via* H6, to carbonyl atom O31 of the adjacent molecule at $(x, y - 1, z)$ [$\text{H6}\cdots\text{O31} = 1.89\text{ \AA}$ and $\text{N6}-\text{H6}\cdots\text{O31} = 173^\circ$]. Each molecule is hydrogen bonded to four others, forming two-dimensional sheets. The sheets are nearly planar and lie parallel to (011). Hydrogen bonds of this kind are similar to those observed in another pyrrolopyridine derivative (Low *et al.*, 2001) and in 1,4-dihydropyridine (Kooijman *et al.*, 2002). There are aromatic $\pi-\pi$ stacking interactions between phenyl rings in adjacent sheets. The molecule at (x, y, z) forms a $\pi-\pi$ stacking interaction with the molecule at $(1 - x, -y, 2 - z)$, which forms part of an adjacent sheet. The shortest intermolecular distance of $3.155(4)\text{ \AA}$ is for $\text{C43}\cdots\text{C45}(1 - x, -y, 2 - z)$. Propagation of this $\pi-\pi$ interaction by the space group symmetry serves to link the sheets into a single three-dimensional framework. The pyrrolopyridine rings of (I) are essentially planar, except for the ester group, which is significantly twisted out of the ring planes (Fig. 1). The ester group has *cis-cis* geometry with respect to the ring double bonds and is rotated slightly out of the pyridine plane, with a $\text{C2}-\text{C3}-\text{C31}-\text{O32}$ torsion angle of $-172.2(3)^\circ$.

Experimental

Full details of the synthetic procedure have been published by Chudik *et al.* (2000). Yellow prismatic single crystals were prepared by recrystallization from ethanol.

Received 16 September 2003

Accepted 17 September 2003

Online 30 September 2003

Crystal data

$C_{18}H_{17}N_3O_6$
 $M_r = 371.35$
 Triclinic, $P\bar{1}$
 $a = 8.555$ (3) Å
 $b = 9.445$ (2) Å
 $c = 11.322$ (4) Å
 $\alpha = 83.76$ (2)°
 $\beta = 72.52$ (3)°
 $\gamma = 77.18$ (2)°
 $V = 850.0$ (5) Å³

$Z = 2$
 $D_x = 1.451$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 6.8$ – 19.3 °
 $\mu = 0.11$ mm⁻¹
 $T = 293$ (2) K
 Prism, yellow
 $0.4 \times 0.3 \times 0.3$ mm

Data collection

Syntex $P2_1$ diffractometer
 θ – 2θ scans
 Absorption correction: none
 4128 measured reflections
 4128 independent reflections
 1439 reflections with $I > 2\sigma(I)$
 $\theta_{\max} = 28.0$ °

$h = 0 \rightarrow 11$
 $k = -12 \rightarrow 12$
 $l = -13 \rightarrow 14$
 2 standard reflections
 frequency: 100 min
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.083$
 $S = 0.88$
 4128 reflections
 248 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0121P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.18$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0111 (6)

Table 1

Selected geometric parameters (Å, °).

O31–C31	1.155 (3)	C2–C3	1.335 (3)
O41–N41	1.205 (3)	C3–C4	1.513 (3)
O42–N41	1.187 (3)	C4–C9	1.438 (3)
N1–C2	1.331 (3)	C5–C9	1.404 (3)
N6–C7	1.341 (3)	C7–C8	1.425 (3)
N6–C5	1.382 (3)	C9–C8	1.309 (3)
C8–N1–C2	116.4 (2)	C9–C4–C3	103.8 (2)
O42–N41–O41	122.2 (3)	C3–C4–C41	111.7 (2)
C7–N6–C5	114.0 (2)	C9–C8–C7	111.6 (3)
C8–N1–C2–C22	177.7 (3)	C2–C3–C31–O31	8.0 (5)
N1–C2–C3–C4	–3.7 (4)	C2–C3–C31–O32	–172.2 (3)
C2–C3–C4–C41	–112.6 (3)	C3–C4–C41–C46	48.7 (3)
C2–N1–C8–C7	–178.2 (3)		

All H atoms were positioned geometrically and these atoms were treated as riding atoms (N–H = 0.86 Å and C–H = 0.93–0.98 Å), with U_{iso} set at $1.2U_{\text{eq}}$ ($1.5U_{\text{eq}}$ for methyl) of the parent atom.

Data collection: *P2₁ Diffractometer Control Software* (Syntex, 1973; cell refinement: *P2₁ Diffractometer Control Software*; data reduction: *XP21* (Pavelčík, 1987); program(s) used to solve structure:

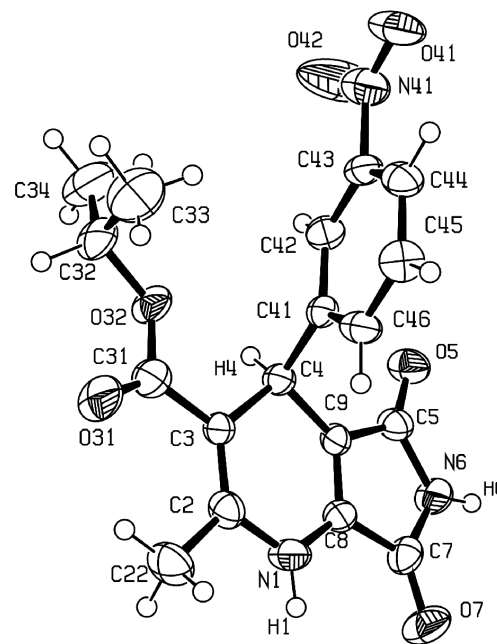


Figure 1

A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Grant Agency of the Slovak Republic (grant No. 1/9249/02 and 1/9255/02).

References

- Chudík, M., Marchalin, Š., Daich, A. & Decroix, B. (2000). *Res. Adv. Synth. Org. Chem.* pp. 1–7.
 Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
 Kooijman, H., Spek, A. L., Sobolev, A., Jongejan, H. & Franssen, M. C. R. (2002). *Acta Cryst.* **E58**, o532–o534.
 Low, J. N., Cobo, J., Garcia, C., Melguizo, M., Noguera, M., Sánchez, A. & Glidewell, C. (2001). *Acta Cryst.* **C57**, 597–599.
 Pavelčík, F. (1987). *XP21*. Comenius University, Bratislava, Slovakia.
 Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
 Syntex (1973). *P2₁ Diffractometer Control Software*. Syntex Analytical Instruments, Cupertino, California, USA.