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1-(1*H*-Imidazol-1-yl)ethanone

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.001 Å
R factor = 0.037
wR factor = 0.099
Data-to-parameter ratio = 14.2

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

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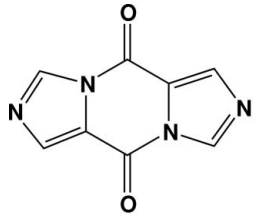
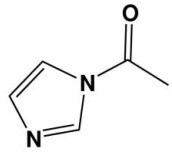
The title compound, $C_5H_6N_2O$, was obtained as a side product during the synthesis of diimidazo[1,5-*a*;1′,5′-*d*]pyrazine-5,10-dione. The molecule is almost planar with the acetyl group inclined to the mean plane of the imidazole ring by 1.52 (12)°. In the crystal structure, molecules are linked by C—H···O and C—H···N hydrogen bonds, forming a sheet-like structure.

Comment

In the preceding paper we describe the crystal structure of diimidazo[1,5-*a*;1′,5′-*d*]pyrazine-5,10-dione, (I) (Castillejo Merchán & Stoeckli-Evans, 2007), which was prepared by the reaction of 4,5-imidazoldicarboxylic acid with an excess of acetic anhydride. During the isolation process to obtain compound (I) it was noticed that, on evaporation of the excess acetic anhydride, a white crystalline solid formed on the walls of an enlargement device, which had been inserted between the solution flask and the vacuum pump. The crystal structure analysis of this compound showed it to be the title compound, (II) (Fig. 1).



(I)



(II)

Compound (II) has been known since (Boyer, 1955) reported the first synthesis. The drying process of compound (I) required delicate handling due to its thermosensitivity and it is believed that compound (II) is a degradation product of compound (I). The bond lengths and angles in (II) are close to the corresponding values reported for compound (I) and similar structures, as found during a search of the Cambridge Structural Database (Version 1.8, last update November 2006; Allen, 2002). The molecule is almost planar, with the acetyl group (atoms O1, C4 and C5) inclined to the mean plane through the imidazole ring [planar to within 0.0015 (6) Å] at an angle of only 1.52 (12)°.

In the crystal structure of (II), adjacent molecules are linked by C—H···O and C—H···N hydrogen bonds, forming a sheet-like structure (Table 1 and Fig. 2). An inter-sheet C4═O4···π interaction occurs: the O···Cg^{i} separation is 3.269 (1) Å, and the C═O···Cg^{i} angle is 91.73 (6)° [*Cg* is the centroid of the imidazole ring; symmetry code: (i) $1-x, -y, 1-z$].

Experimental

Compound (II) was obtained as a secondary product during the synthesis of compound (I). The latter was synthesized according to the procedure described by Kasina & Nematollahi (1975). During the evaporation of the excess of the acetic anhydride used in the synthesis of (I), an enlargement device was inserted between the solution flask and the vacuum pump. A white crystalline solid formed on the walls of this device and was recovered. Recrystallization from acetone gave X-ray quality crystals of compound (II) (yield 0.11 g, 8%).

Crystal data

$C_5H_6N_2O$
M_r = 110.12
Monoclinic, $P2_1/n$
a = 7.5263 (8) Å
b = 7.5835 (10) Å
c = 9.0853 (10) Å
β = 100.361 (8)°
V = 510.09 (10) Å^3
Z = 4
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 (2) K
Block, colourless
0.50 × 0.34 × 0.23 mm

Data collection

Stoe IPDS-2 diffractometer
ω and φ scans
Absorption correction: none
6541 measured reflections
1380 independent reflections
1208 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 29.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.08
1380 reflections
97 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1063P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.964 (15)	2.446 (15)	3.3826 (13)	163.9 (12)
C3—H3···N2^{ii}	0.940 (15)	2.597 (15)	3.5252 (14)	169.7 (12)

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

H atoms were located in difference Fourier maps and their positions and U_{iso} values freely refined; the C—H bond lengths vary between 0.940 (16) and 0.967 (15) Å.

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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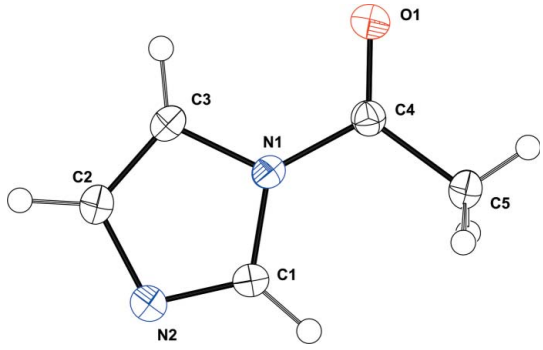

Figure 1
The molecular structure of (II), showing displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

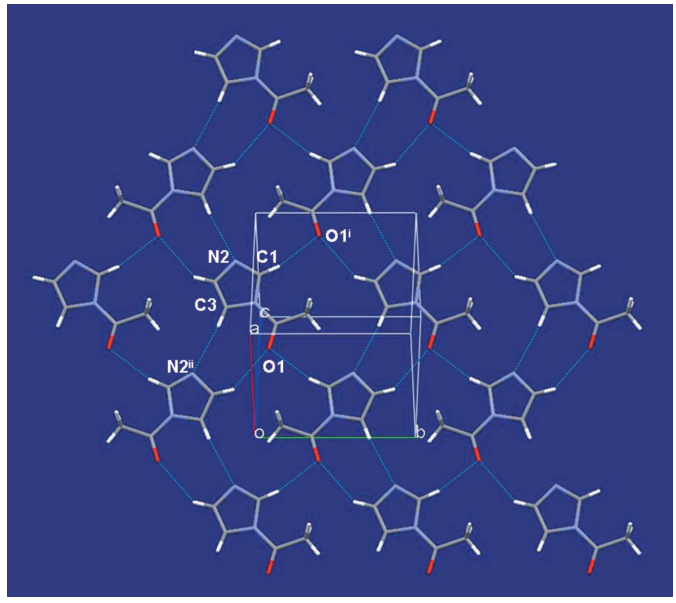

Figure 2
Crystal packing of compound (II), viewed perpendicular to the plane of the hydrogen-bonded sheets. The C—H···O and C—H···N hydrogen bonds are shown as dashed lines; symmetry codes correspond to those in Table 2.

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