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2-Acetylpyrrole

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The title molecule, C_6H_7NO, forms centrosymmetric dimers in the solid state, through N—H···O hydrogen bonds involving amine and carbonyl groups. The resulting $R_2^2(10)$ hydrogen-bond pattern is close to that observed in 2-formyl-3-methylpyrrole, an isomeric pyrrole derivative.

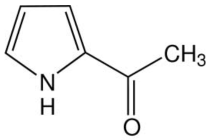
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.039
wR factor = 0.111
Data-to-parameter ratio = 11.8

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

Comment

The title pyrrole, (I), is a volatile compound naturally occurring in foods which have undergone some degree of either thermal treatment or microbial activity (Maga, 1981). For example, a concentration of 10 µg kg^{-1} has been found in popcorn (Buttery *et al.*, 1997). It has potent organoleptic properties, and is perceived to have a flavour associated with nuts, walnuts, and bread. It belongs to the GRAS (Generally Recognized As Safe) list of the Food and Drug Administration and is used in flavouring formulations in the low p.p.m. range (< 50 p.p.m.). Its current applications include roasted food and tobacco. Compound (I) has also been claimed to possess hepatoprotective properties (Ito *et al.*, 1991). The corresponding anion, 2-acetylpyrrolate, has been used, although to a limited extent, as a ligand in transition metal complexes (*e.g.* Reardon *et al.*, 2002; Jazzar *et al.*, 2006).



(I)

Because of the delocalization between the acetyl and pyrrole groups, the molecule is almost planar, the dihedral angle between these groups being 1.3 (2)°. The mean deviation from the least-squares plane including all non-H atoms is 0.007 Å. A notable feature of the acetyl functionality is disorder affecting the H atoms of the methyl group, due to a degree of rotation of *ca* 60° about the C6—C8 σ bond (see *Experimental* and Fig. 1). However, the more populated conformation is very close to the *MM2*-minimized structure (Acree & Arn, 2004).

Rather strong N—H···O hydrogen bonds (Table 1) assemble molecules into centrosymmetric dimers in the crystal structure (Fig. 1). Interestingly, an isographic $R_2^2(10)$ intramolecular hydrogen-bonding scheme (Etter *et al.*, 1990; Bernstein *et al.*, 1995) was previously observed for an isomeric pyrrole system, namely 2-formyl-3-methylpyrrole (Smith *et al.*, 1985). This compound crystallizes in the space group $P2_1/n$, as does (I), and the unit-cell parameters for both crystal structures compare well. Melting points are also very close, 362.97±0.02 K for (I) *versus* 364–365 K for 2-formyl-3-methylpyrrole. The hydrogen-bond pattern thus seems to determine many solid-state properties for these pyrrole derivatives.

Experimental

The title compound was purchased from Sigma–Aldrich and recrystallized three times from ethanol. The melting point was determined on the basis of seven measurements by differential scanning calorimetry (TA Instrument 2010) in an unsealed Al crucible under an N_2 atmosphere.

Crystal data

C_6H_7NO
$M_r = 109.13$
Monoclinic, $P2_1/n$
$a = 9.762$ (2) Å
$b = 5.172$ (2) Å
$c = 11.731$ (3) Å
$\beta = 90.158$ (5)°
$V = 592.3$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 296$ (1) K
0.60 × 0.18 × 0.12 mm

Data collection

Bruker P4 diffractometer
Absorption correction: none
4203 measured reflections
1362 independent reflections
1002 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
3 standard reflections
every 97 reflections
intensity decay: 4.5%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.111$
$S = 1.04$
1362 reflections
115 parameters
All H-atom parameters refined
$\Delta\rho_{\rm max} = 0.13$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.12$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O7$^{\rm i}$	0.912 (17)	1.985 (18)	2.8628 (17)	161.0 (14)

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

Single crystals systematically decomposed on contact with all available glues we attempted. A single crystal was then transferred in a capillary tube and the data collected without special precautions regarding the atmosphere around the sample. H atoms were found in a difference map and refined isotropically with free coordinates [C—H = 0.93 (5)–1.13 (7) Å]. The C8 methyl group is clearly disordered over two positions. Complementary site occupation factors for H atoms were refined. Occupation factors converged to 0.61 (6) and 0.39 (6) for H81*A*/H82*A*/H83*A* and H81*B*/H82*B*/H83*B*, respectively.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL-Plus*.

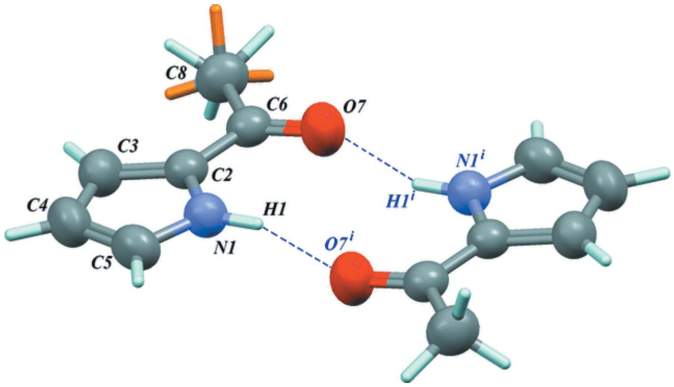


Figure 1
The structure of the dimer found in the crystal structure of (I), with displacement ellipsoids for non-H atoms drawn at the 50% probability level. The left-hand molecule corresponds to the selected asymmetric unit and is shown with disordered sites for methyl H atoms [light-blue: site occupancy = 0.61 (6); orange: site occupancy = 0.39 (6)]. The right-hand molecule is linked through hydrogen bonds (dashed lines) and only the main component of the methyl group is shown. [Symmetry code: (i) $1-x, -y, 2-z$.]

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