Table 2. *Selected geometric parameters (Å, °) for (2)*

F1—C2	1.352 (2)	O2—C3	1.506 (2)
F2—C2	1.349 (2)	C1—C2	1.514 (3)
O1—C1	1.187 (2)	C2—C3	1.526 (2)
O2—C1	1.352 (2)		
C1—O2—C3	93.92 (12)	C1—C2—C3	86.96 (13)
O2—C1—C2	92.3 (2)	O2—C3—C2	86.03 (12)

For (1), a hemisphere of data was collected (1321 frames, 0.3° scan in ω). The first 50 frames were remeasured at the end of data collection to monitor instrument and crystal stability. The full data set has a 97.1% coverage and a range of 2.7 to 3.8 redundancy. For (2), data were collected by ω scans over 1.2° using 3–6° min^{-1} scan speeds depending on intensity. Attempts were made to solve the structure of (1) in both centrosymmetric and non-centrosymmetric space groups *Pnma* and *Pna*2₁. A solution, followed by successful refinement, was only obtained in space group *Pna*2_1. Examination of the crystal packing revealed the presence of a pseudo-center of inversion in the lattice but no mirror-plane symmetry which is a requirement for the centrosymmetric space group *Pnma*. Since *XL* in *SHELXTL5* (Sheldrick, 1995) automatically generates origin restraints for polar space groups (floating origin restraint), no z coordinate of an atom has to be fixed for space group *Pna*2_1. The H atoms were placed in idealized positions and were refined riding on their parent atoms. C—H distances of 0.97 and 0.93 Å were used for methylene and aromatic C atoms, respectively. The displacement parameters of the H atoms were set at $1.2U_{eq}$ of the parent C atoms. The absolute configuration of the title compounds is undetermined.

Data collection: *SMART* (Siemens, 1995) for (1); *P3/PC Diffractometer Program* (Siemens, 1989) for (2). Cell refinement: *SMART* and *SAINT* (Siemens, 1995) for (1); *P3/PC Diffractometer Program* for (2). Data reduction: *SHELXTL5* (Sheldrick, 1995) for (1); *SHELXTL-Plus* (Sheldrick, 1990) for (2). For both compounds, program(s) used to solve structures: *SHELXTL5*; program(s) used to refine structures: *SHELXTL5*; molecular graphics: *SHELXTL5*; software used to prepare material for publication: *SHELXTL5*.

KAA wishes to acknowledge the National Science Foundation and the University of Florida for funding allowing the purchase of the X-ray equipment.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BS1033). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1997). C**53**, 1926–1927

2-Acetyl-3-(5-cyano-2-furyl)propenenitrile

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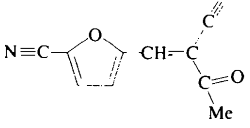
(*Received 26 March 1997; accepted 31 July 1997*)

Abstract

The crystal structure of the title compound, $C_{10}H_6N_2O_2$, consists of relatively isolated molecules, the shortest intermolecular contacts [C—H···O 2.51 (2); C—H···N 2.50 (1) and 2.60 (2) Å] indicate the presence of weak hydrogen bonding. As indicated by the planarity of the molecule and the pattern of bond lengths, the π-electron delocalization extends over the whole molecule.

Comment

The title compound, (I), belongs to a series of large conjugated molecules with potential use as organic dyes (Vrábel *et al.*, 1994; Lokaj *et al.*, 1990). The molecules absorb in the near ultraviolet and visible regions of the spectrum and exhibit pronounced colour changes depending on the nature of the substituents attached to the ethylene C atom and the furan ring. We report here on the crystal structure on the cyano–acetyl derivative, (I).



(I)

Acta Crystallographica Section C
ISSN 0108-2701 © 1997

As shown in Fig. 1, the furyl and acetyl groups are *trans* positioned on the C2═C3 double bond. This bond in the title structure [1.341 (2) Å] is considerably longer than that reported for unsubstituted ethylene [1.314 (6) Å] (van Nes & Vos, 1977). The furan ring is approximately planar [maximum deviation of the C6 atom from the least-squares plane is 0.003 (3) Å]. The extensive conjugation in the molecule is also observed in the C1—C2, C3—C4 and C7—C8 bond distances which are all significantly shorter than the normal value of 1.487 Å reported for the C_{sp^2}—C_{sp^2} single bond (Shmueli *et al.*, 1973). The planarity of the whole molecule is also manifested in the small dihedral angles between the planes of the furan and propenenitrile moieties [5.79 (9)°].

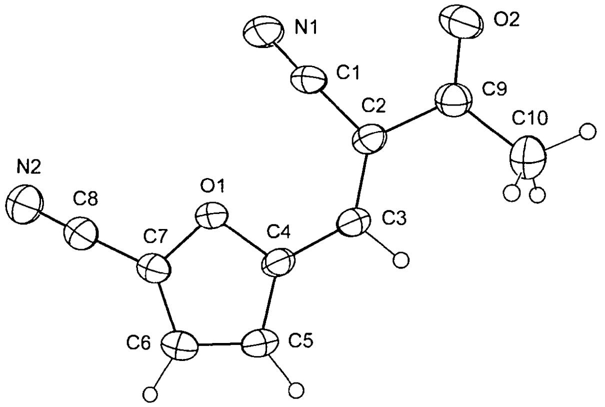


Fig. 1. View of the title molecule showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level; H atoms are drawn as small circles of arbitrary radii.

Experimental

Full details of the synthetic procedure have been published by Marchalín *et al.*, (1993). Single crystals were prepared by crystallization from ethanol.

Crystal data

$C_{10}H_6N_2O_2$
M_r = 186.17
Triclinic
$P\overline{1}$
a = 7.634 (4) Å
b = 8.243 (9) Å
c = 8.507 (7) Å
α = 69.10 (8)°
β = 64.97 (5)°
γ = 72.96 (7)°
V = 446.7 (7) Å^3
Z = 2
D_x = 1.384 Mg m^{-3}
D_m = 1.39 (1) Mg m^{-3}
D_m measured by flotation in bromoform–hexane

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 15 reflections
θ = 12.4–28.6°
μ = 0.100 mm^{-1}
T = 293 (2) K
Prism
0.4 × 0.3 × 0.2 mm
Light yellow

Data collection

Syntex $P2_1$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2062 measured reflections
2062 independent reflections
1161 reflections with $I > 2\sigma(I)$

$\theta_{\max}$ = 27.56°
$h = 0 \rightarrow 9$
$k = -9 \rightarrow 10$
$l = -9 \rightarrow 10$
2 standard reflections frequency: 100 min intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.038
$wR(F^2)$ = 0.090
S = 1.196
2062 reflections
152 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.003

$\Delta\rho_{\max}$ = 0.140 e Å^{-3}
$\Delta\rho_{\min}$ = −0.138 e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.029 (7)
Scattering factors from *International Tables for Crystallography* (Vol. C)

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

O1—C7	1.350 (2)	C2—C3	1.341 (2)
O1—C4	1.364 (2)	C3—C4	1.418 (3)
O2—C9	1.208 (2)	C4—C5	1.352 (2)
N1—C1	1.130 (2)	C5—C6	1.396 (3)
N2—C8	1.129 (2)	C6—C7	1.343 (2)
C1—C2	1.429 (2)	C7—C8	1.416 (3)
C7—O1—C4	105.95 (13)	C5—C4—O1	109.6 (2)
N1—C1—C2	177.66 (15)	O1—C4—C3	119.12 (13)
C3—C2—C9	123.80 (15)	C4—C5—C6	107.2 (2)
C1—C2—C9	113.92 (14)	C6—C7—O1	111.2 (2)

Non-H atoms were refined anisotropically, H atoms were located from a difference Fourier map and all parameters were refined isotropically.

Data collection: Syntex $P2_1$ software. Cell refinement: syntex $P2_1$ software. Data reduction: *XP*21 (Pavelčík, 1987). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93 and *PARST* (Nardelli, 1983).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AB1486). Services for accessing these data are described at the back of the journal.

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