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N′-[(*E*)-Furan-2-ylmethylidene]pyridine-3-carbohydrazide

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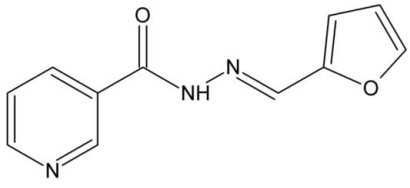
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.117; data-to-parameter ratio = 12.0.

The title compound, $C_{11}H_9N_3O_2$, exists in the *E* conformation with respect to the azomethane C=N bond, and has the keto form. There are two independent molecules in the asymmetric unit and each of these features a slight slanting of the pyridine and furan rings, which form a dihedral angle of 14.96 (10)° in one of the molecules and 5.53 (10)° in the other. The crystal structure is stabilized by N—H···O and N—H···N hydrogen bonds, weak C—H···O and C—H···N hydrogen bonds and C—H···π interactions and π–π interactions [shortest centroid–centroid distance = 3.7864 (15) Å].

Related literature

For applications of carbohydrazide in non-linear optics and molecular sensing, see: Bakir & Brown (2002). For the synthesis of related compounds, see: Fun *et al.* (2008); Neema & Kurup (2011). For similar structures, see: Nancy *et al.* (2011). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_9N_3O_2$
M_r = 215.21
Triclinic, $P\overline{1}$
a = 9.441 (2) Å
b = 10.237 (3) Å
c = 11.023 (2) Å
α = 75.10 (2)°
β = 85.413 (19)°
γ = 84.11 (2)°
V = 1022.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 150 K
0.26 × 0.21 × 0.18 mm

Data collection

Bruker P4 diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.975, T_{max} = 0.982
9430 measured reflections
3589 independent reflections
2702 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.117
S = 1.09
3589 reflections
298 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the O4/C19–C22 and O2/C8–C11 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···N1^{i}	0.86 (2)	2.10 (2)	2.944 (2)	169 (2)
N2—H2*N*···O3	0.89 (1)	2.08 (2)	2.9017 (19)	154 (2)
C21—H21···N3^{ii}	0.93	2.58	3.410 (3)	149
C16—H16···N1^{i}	0.93	2.53	3.370 (3)	150
C11—H11···O1^{iii}	0.93	2.51	3.365 (2)	153
C2—H2···O3^{iv}	0.93	2.49	3.116 (2)	125
C10—H10···*Cg*1^{v}	0.93	2.78	3.594 (2)	146
C12—H12···*Cg*2^{vi}	0.93	2.75	3.520 (2)	141

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y, -z+1$; (iv) $-x+1, -y, -z+2$; (v) $-x+2, -y+1, -z+1$; (vi) $x, y, z+1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5012).

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supplementary materials

Acta Cryst. (2011). E**67**, o3267 [**doi:10.1107/S1600536811046381**]

N'-[(*E*)-Furan-2-ylmethylidene]pyridine-3-carbohydrazide

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Comment

Derivatives of pyridine-3-carbohydrazide and their metal complexes possess pronounced biological activities. They also contain versatile binding properties and the presence of the carbonyl-O atom promotes the the formation of a chelate binding center (Neema & Kurup, 2011). Derivatives of pyridine-3-carbohydrazide and their metal complexes have received considerable attention during the last decade because of their versatile applications in nonlinear optics and molecular sensing (Bakir & Brown, 2002). The present report is an extension of earlier studies in this area (Nancy *et al.*, 2011).

The title compound, (I), crystallizes in triclinic space group P$\bar{1}$.There are two independent molecules (Fig. 1) in the asymmetric unit with almost the same bond length and bond angle, and therefore the detailed description can be limited to one of these molecules. The molecule adopts an *E* configuration with respect to C7═N3 bond and it exists in the keto form with C6═O1 bond length of 1.226 (2) Å which is very close to a formal C═O bond length [1.21 Å] (Allen *et al.*, 1987). The dihedral angle between pyridine and furan rings is 14.96 (10)°. The O1 and N3 atoms are *syn* with respect to the C6—N2 bond having a torsion angle of -2.0 (3)°. The molecule is almost planar with maximum deviation of 0.265 (2) Å for atom C2; the other molecule has the maximum deviation of 0.212 (1) Å for the atom O3 from its least-squares plane.

Conventional N—H···O,N hydrogen bonds are present, Table 1, Moreover, there are non-conventional intermolecular interactions present in the crystal structure, Table 1, which contribute to the formation of a 3-D network.

Fig. 2 shows a partial packing diagram. The molecules shown participate in C–H···π interactions formed between the H atoms attached at the C10 and C12 atoms and the furan rings, Table 1. The presence of π–π interactions, with centroid-centroid distances of 3.7864 (15), 3.7864 (15), 3.7274 (15) and 3.7273 (15) Å between the rings, is also noted.

Experimental

The title compound, (I), was prepared by adapting a reported procedure (Fun *et al.*, 2008) by refluxing a mixture of a methanol solutions of furan-2-carboxaldehyde (0.960 g, 10 mmol) and pyridine-3-carbohydrazide (1.370 g, 10 mmol) for 3 h. The formed crystals were collected and recrystallized from a mixture of ethanol and dimethylformamide (1:1 *v*/*v*). Light-green crystals were obtained.

Refinement

All C-bound H atoms were placed in calculated positions with C—H = 0.93 Å, and with U_{iso}=1.2U_{eq}(C). The N-bound H atoms were refined with N—H = 0.88±0.1 Å and free U_{iso}.

Figures

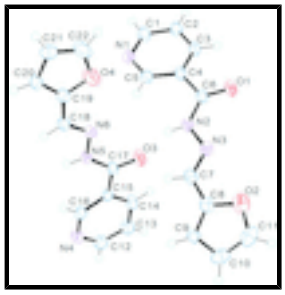

Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

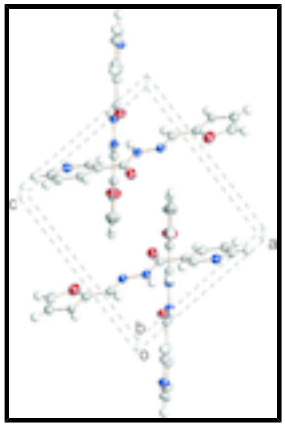

Fig. 2. A view of the unit cell for (I).

N'-[(*E*)-Furan-2-ylmethylidene]pyridine-3-carbohydrazide

Crystal data

$C_{11}H_9N_3O_2$	$Z = 4$
$M_r = 215.21$	$F(000) = 448$
Triclinic, $P\overline{1}$	$D_x = 1.398$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.441$ (2) Å	Cell parameters from 2702 reflections
$b = 10.237$ (3) Å	$\theta = 3.0$–$25.0°$
$c = 11.023$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 75.10$ (2)°	$T = 150$ K
$\beta = 85.413$ (19)°	Block, light-green
$\gamma = 84.11$ (2)°	0.26 × 0.21 × 0.18 mm
$V = 1022.5$ (4) Å^3	

Data collection

Bruker P4 diffractometer	3589 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2702 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
ω scans	$h = -11 \rightarrow 11$

Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)

T_{min} = 0.975, T_{max} = 0.982

9430 measured reflections

$k = -12 \rightarrow 11$

$l = -12 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.117$

$S = 1.09$

3589 reflections

298 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.0667P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.22$ e Å^{-3}

$\Delta\rho_{min} = -0.29$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.008 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.61774 (13)	−0.01358 (13)	0.71738 (12)	0.0408 (4)
O2	1.11415 (15)	0.10175 (14)	0.58530 (13)	0.0488 (4)
O3	0.76963 (14)	0.26997 (12)	0.97572 (11)	0.0373 (3)
O4	0.43780 (16)	0.54591 (14)	0.67271 (14)	0.0557 (4)
N1	0.32366 (15)	0.25812 (14)	0.94601 (14)	0.0331 (4)
N2	0.71582 (15)	0.15648 (15)	0.76984 (13)	0.0293 (4)
N3	0.84450 (15)	0.13134 (15)	0.70761 (13)	0.0306 (4)
N4	1.00763 (16)	0.47023 (16)	1.23845 (14)	0.0368 (4)
N5	0.70930 (14)	0.49236 (15)	0.96475 (13)	0.0268 (3)
N6	0.62315 (15)	0.50278 (15)	0.86641 (13)	0.0283 (3)
C1	0.2301 (2)	0.16377 (19)	0.97664 (17)	0.0355 (4)

H1	0.1473	0.1808	1.0237	0.043*
C2	0.24961 (19)	0.04281 (18)	0.94233 (17)	0.0329 (4)
H2	0.1806	−0.0191	0.9640	0.039*
C3	0.37305 (18)	0.01569 (17)	0.87553 (16)	0.0307 (4)
H3	0.3890	−0.0656	0.8516	0.037*
C4	0.47390 (18)	0.10983 (17)	0.84378 (15)	0.0267 (4)
C5	0.44343 (18)	0.23048 (17)	0.88037 (16)	0.0300 (4)
H5	0.5096	0.2951	0.8581	0.036*
C6	0.60870 (18)	0.07795 (17)	0.77142 (16)	0.0288 (4)
C7	0.94024 (19)	0.21070 (18)	0.71100 (16)	0.0316 (4)
H7	0.9194	0.2776	0.7546	0.038*
C8	1.07818 (19)	0.19826 (19)	0.64918 (16)	0.0337 (4)
C9	1.18880 (17)	0.27331 (18)	0.64346 (15)	0.0294 (4)
H9	1.1906	0.3450	0.6806	0.035*
C10	1.3003 (2)	0.2241 (2)	0.57180 (17)	0.0404 (5)
H10	1.3897	0.2571	0.5519	0.049*
C11	1.2542 (2)	0.1210 (2)	0.53733 (18)	0.0458 (5)
H11	1.3072	0.0695	0.4886	0.055*
C12	1.0577 (2)	0.3466 (2)	1.30061 (17)	0.0386 (5)
H12	1.1209	0.3400	1.3629	0.046*
C13	1.0218 (2)	0.2281 (2)	1.27846 (18)	0.0397 (5)
H13	1.0602	0.1442	1.3241	0.048*
C14	0.92747 (19)	0.23689 (18)	1.18683 (16)	0.0340 (4)
H14	0.9003	0.1585	1.1706	0.041*
C15	0.87333 (17)	0.36337 (17)	1.11913 (15)	0.0262 (4)
C16	0.91764 (18)	0.47580 (18)	1.14965 (16)	0.0318 (4)
H16	0.8819	0.5611	1.1048	0.038*
C17	0.77872 (18)	0.37120 (17)	1.01468 (15)	0.0267 (4)
C18	0.57217 (18)	0.62304 (18)	0.81434 (16)	0.0293 (4)
H18	0.5977	0.6954	0.8421	0.035*
C19	0.47684 (18)	0.64921 (18)	0.71446 (16)	0.0316 (4)
C20	0.41102 (18)	0.76644 (18)	0.65139 (15)	0.0302 (4)
H20	0.4195	0.8518	0.6636	0.036*
C21	0.32700 (19)	0.7377 (2)	0.56365 (17)	0.0369 (5)
H21	0.2697	0.7994	0.5068	0.044*
C22	0.3457 (2)	0.6057 (2)	0.5781 (2)	0.0546 (6)
H22	0.3028	0.5586	0.5312	0.066*
H2N	0.7125 (19)	0.2127 (17)	0.8202 (16)	0.035 (5)*
H5N	0.713 (2)	0.5638 (17)	0.9912 (18)	0.043 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0418 (8)	0.0409 (8)	0.0502 (8)	−0.0061 (6)	0.0002 (6)	−0.0300 (7)
O2	0.0606 (9)	0.0428 (9)	0.0435 (8)	−0.0036 (7)	−0.0011 (7)	−0.0126 (7)
O3	0.0526 (8)	0.0267 (7)	0.0372 (7)	−0.0020 (6)	−0.0121 (6)	−0.0139 (6)
O4	0.0671 (10)	0.0386 (9)	0.0648 (10)	−0.0073 (7)	−0.0282 (8)	−0.0108 (7)
N1	0.0369 (9)	0.0286 (9)	0.0363 (9)	0.0003 (7)	−0.0034 (7)	−0.0137 (7)

N2	0.0332 (8)	0.0302 (9)	0.0293 (8)	−0.0044 (7)	−0.0002 (6)	−0.0158 (7)
N3	0.0342 (8)	0.0318 (9)	0.0273 (8)	−0.0021 (7)	−0.0019 (6)	−0.0105 (6)
N4	0.0373 (9)	0.0377 (10)	0.0394 (9)	−0.0021 (7)	−0.0085 (7)	−0.0152 (8)
N5	0.0296 (8)	0.0256 (9)	0.0286 (8)	−0.0016 (6)	−0.0047 (6)	−0.0126 (7)
N6	0.0290 (8)	0.0300 (9)	0.0282 (8)	−0.0037 (6)	−0.0042 (6)	−0.0105 (6)
C1	0.0370 (10)	0.0353 (11)	0.0354 (10)	−0.0026 (9)	0.0004 (8)	−0.0118 (9)
C2	0.0356 (10)	0.0267 (10)	0.0360 (10)	−0.0059 (8)	−0.0032 (8)	−0.0057 (8)
C3	0.0394 (10)	0.0224 (10)	0.0327 (10)	−0.0017 (8)	−0.0051 (8)	−0.0107 (8)
C4	0.0340 (10)	0.0250 (9)	0.0230 (9)	−0.0010 (7)	−0.0075 (7)	−0.0081 (7)
C5	0.0325 (10)	0.0282 (10)	0.0317 (10)	−0.0041 (8)	−0.0060 (8)	−0.0102 (8)
C6	0.0351 (10)	0.0265 (10)	0.0272 (9)	−0.0011 (8)	−0.0061 (7)	−0.0102 (8)
C7	0.0375 (10)	0.0317 (10)	0.0282 (10)	−0.0046 (8)	−0.0023 (8)	−0.0110 (8)
C8	0.0403 (11)	0.0367 (11)	0.0250 (9)	−0.0016 (8)	−0.0045 (8)	−0.0090 (8)
C9	0.0281 (9)	0.0377 (11)	0.0271 (9)	−0.0072 (8)	−0.0001 (7)	−0.0151 (8)
C10	0.0329 (10)	0.0528 (13)	0.0329 (10)	−0.0011 (9)	−0.0028 (8)	−0.0065 (9)
C11	0.0503 (13)	0.0470 (13)	0.0343 (11)	0.0125 (10)	0.0017 (9)	−0.0076 (10)
C12	0.0370 (11)	0.0459 (13)	0.0347 (11)	0.0010 (9)	−0.0094 (8)	−0.0132 (9)
C13	0.0501 (12)	0.0345 (11)	0.0344 (10)	0.0041 (9)	−0.0126 (9)	−0.0084 (8)
C14	0.0433 (11)	0.0295 (11)	0.0319 (10)	−0.0020 (8)	−0.0030 (8)	−0.0127 (8)
C15	0.0268 (9)	0.0270 (10)	0.0262 (9)	−0.0006 (7)	0.0017 (7)	−0.0105 (7)
C16	0.0348 (10)	0.0290 (10)	0.0329 (10)	−0.0011 (8)	−0.0060 (8)	−0.0098 (8)
C17	0.0309 (9)	0.0252 (10)	0.0256 (9)	−0.0040 (7)	0.0025 (7)	−0.0101 (7)
C18	0.0313 (9)	0.0289 (11)	0.0292 (10)	−0.0036 (8)	0.0001 (7)	−0.0103 (8)
C19	0.0312 (10)	0.0342 (11)	0.0302 (10)	−0.0073 (8)	0.0014 (7)	−0.0086 (8)
C20	0.0329 (10)	0.0320 (10)	0.0276 (9)	0.0022 (8)	−0.0036 (7)	−0.0125 (8)
C21	0.0351 (11)	0.0438 (13)	0.0311 (10)	−0.0036 (9)	−0.0056 (8)	−0.0067 (9)
C22	0.0612 (15)	0.0515 (15)	0.0581 (14)	−0.0118 (11)	−0.0262 (11)	−0.0167 (11)

Geometric parameters (Å, °)

O1—C6	1.2258 (19)	C5—H5	0.9300
O2—C8	1.356 (2)	C7—C8	1.430 (2)
O2—C11	1.398 (2)	C7—H7	0.9300
O3—C17	1.2325 (19)	C8—C9	1.347 (2)
O4—C19	1.350 (2)	C9—C10	1.396 (2)
O4—C22	1.388 (3)	C9—H9	0.9300
N1—C1	1.337 (2)	C10—C11	1.333 (3)
N1—C5	1.338 (2)	C10—H10	0.9300
N2—C6	1.351 (2)	C11—H11	0.9300
N2—N3	1.381 (2)	C12—C13	1.377 (3)
N2—H2N	0.893 (14)	C12—H12	0.9300
N3—C7	1.285 (2)	C13—C14	1.379 (3)
N4—C12	1.333 (2)	C13—H13	0.9300
N4—C16	1.333 (2)	C14—C15	1.387 (2)
N5—C17	1.346 (2)	C14—H14	0.9300
N5—N6	1.383 (2)	C15—C16	1.390 (2)
N5—H5N	0.858 (15)	C15—C17	1.494 (2)
N6—C18	1.279 (2)	C16—H16	0.9300
C1—C2	1.376 (2)	C18—C19	1.432 (3)

C1—H1	0.9300	C18—H18	0.9300
C2—C3	1.371 (2)	C19—C20	1.340 (2)
C2—H2	0.9300	C20—C21	1.403 (2)
C3—C4	1.385 (2)	C20—H20	0.9300
C3—H3	0.9300	C21—C22	1.314 (3)
C4—C5	1.391 (2)	C21—H21	0.9300
C4—C6	1.499 (2)	C22—H22	0.9300
C8—O2—C11	105.59 (15)	C11—C10—C9	106.90 (17)
C19—O4—C22	105.42 (15)	C11—C10—H10	126.6
C1—N1—C5	117.26 (15)	C9—C10—H10	126.6
C6—N2—N3	119.18 (14)	C10—C11—O2	109.84 (16)
C6—N2—H2N	121.8 (12)	C10—C11—H11	125.1
N3—N2—H2N	117.9 (12)	O2—C11—H11	125.1
C7—N3—N2	114.99 (14)	N4—C12—C13	124.17 (18)
C12—N4—C16	116.25 (16)	N4—C12—H12	117.9
C17—N5—N6	118.33 (14)	C13—C12—H12	117.9
C17—N5—H5N	124.5 (14)	C12—C13—C14	118.32 (18)
N6—N5—H5N	117.2 (14)	C12—C13—H13	120.8
C18—N6—N5	115.34 (14)	C14—C13—H13	120.8
N1—C1—C2	123.62 (17)	C13—C14—C15	119.56 (17)
N1—C1—H1	118.2	C13—C14—H14	120.2
C2—C1—H1	118.2	C15—C14—H14	120.2
C3—C2—C1	118.45 (17)	C14—C15—C16	116.92 (16)
C3—C2—H2	120.8	C14—C15—C17	118.80 (15)
C1—C2—H2	120.8	C16—C15—C17	124.18 (16)
C2—C3—C4	119.73 (15)	N4—C16—C15	124.78 (17)
C2—C3—H3	120.1	N4—C16—H16	117.6
C4—C3—H3	120.1	C15—C16—H16	117.6
C3—C4—C5	117.67 (15)	O3—C17—N5	122.79 (16)
C3—C4—C6	118.95 (14)	O3—C17—C15	119.94 (15)
C5—C4—C6	123.37 (15)	N5—C17—C15	117.25 (14)
N1—C5—C4	123.25 (16)	N6—C18—C19	121.73 (16)
N1—C5—H5	118.4	N6—C18—H18	119.1
C4—C5—H5	118.4	C19—C18—H18	119.1
O1—C6—N2	123.49 (16)	C20—C19—O4	109.62 (16)
O1—C6—C4	120.77 (15)	C20—C19—C18	130.05 (17)
N2—C6—C4	115.74 (14)	O4—C19—C18	120.31 (16)
N3—C7—C8	121.36 (16)	C19—C20—C21	107.93 (17)
N3—C7—H7	119.3	C19—C20—H20	126.0
C8—C7—H7	119.3	C21—C20—H20	126.0
C9—C8—O2	109.95 (15)	C22—C21—C20	106.02 (18)
C9—C8—C7	128.47 (17)	C22—C21—H21	127.0
O2—C8—C7	121.59 (16)	C20—C21—H21	127.0
C8—C9—C10	107.72 (16)	C21—C22—O4	111.01 (18)
C8—C9—H9	126.1	C21—C22—H22	124.5
C10—C9—H9	126.1	O4—C22—H22	124.5
C6—N2—N3—C7	−179.93 (16)	C8—O2—C11—C10	0.4 (2)
C17—N5—N6—C18	−172.91 (14)	C16—N4—C12—C13	−0.2 (3)

C5—N1—C1—C2	−1.3 (3)	N4—C12—C13—C14	−0.4 (3)
N1—C1—C2—C3	1.6 (3)	C12—C13—C14—C15	0.8 (3)
C1—C2—C3—C4	−0.4 (3)	C13—C14—C15—C16	−0.7 (2)
C2—C3—C4—C5	−0.9 (2)	C13—C14—C15—C17	176.09 (15)
C2—C3—C4—C6	179.60 (16)	C12—N4—C16—C15	0.4 (3)
C1—N1—C5—C4	−0.1 (3)	C14—C15—C16—N4	0.1 (3)
C3—C4—C5—N1	1.2 (3)	C17—C15—C16—N4	−176.49 (15)
C6—C4—C5—N1	−179.32 (16)	N6—N5—C17—O3	0.7 (2)
N3—N2—C6—O1	−2.0 (3)	N6—N5—C17—C15	178.83 (13)
N3—N2—C6—C4	178.51 (14)	C14—C15—C17—O3	−12.5 (2)
C3—C4—C6—O1	15.9 (2)	C16—C15—C17—O3	163.98 (16)
C5—C4—C6—O1	−163.54 (17)	C14—C15—C17—N5	169.29 (15)
C3—C4—C6—N2	−164.56 (15)	C16—C15—C17—N5	−14.2 (2)
C5—C4—C6—N2	16.0 (2)	N5—N6—C18—C19	−177.59 (14)
N2—N3—C7—C8	−179.07 (15)	C22—O4—C19—C20	1.1 (2)
C11—O2—C8—C9	−0.6 (2)	C22—O4—C19—C18	179.52 (16)
C11—O2—C8—C7	179.48 (16)	N6—C18—C19—C20	178.28 (17)
N3—C7—C8—C9	179.63 (18)	N6—C18—C19—O4	0.2 (2)
N3—C7—C8—O2	−0.5 (3)	O4—C19—C20—C21	−0.8 (2)
O2—C8—C9—C10	0.6 (2)	C18—C19—C20—C21	−179.05 (17)
C7—C8—C9—C10	−179.48 (18)	C19—C20—C21—C22	0.2 (2)
C8—C9—C10—C11	−0.4 (2)	C20—C21—C22—O4	0.5 (2)
C9—C10—C11—O2	0.0 (2)	C19—O4—C22—C21	−1.0 (2)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the O4/C19–C22 and O2/C8–C11 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···N1^{i}	0.86 (2)	2.10 (2)	2.944 (2)	169.(2)
N2—H2N···O3	0.89 (1)	2.08 (2)	2.9017 (19)	154.(2)
C21—H21···N3^{ii}	0.93	2.58	3.410 (3)	149.
C16—H16···N1^{i}	0.93	2.53	3.370 (3)	150.
C11—H11···O1^{iii}	0.93	2.51	3.365 (2)	153.
C2—H2···O3^{iv}	0.93	2.49	3.116 (2)	125.
C10—H10···Cg1^{v}	0.93	2.78	3.594 (2)	146
C12—H12···Cg2^{vi}	0.93	2.75	3.520 (2)	141

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+2, −*y*, −*z*+1; (iv) −*x*+1, −*y*, −*z*+2; (v) −*x*+2, −*y*+1, −*z*+1; (vi) *x*, *y*, *z*+1.

Fig. 1

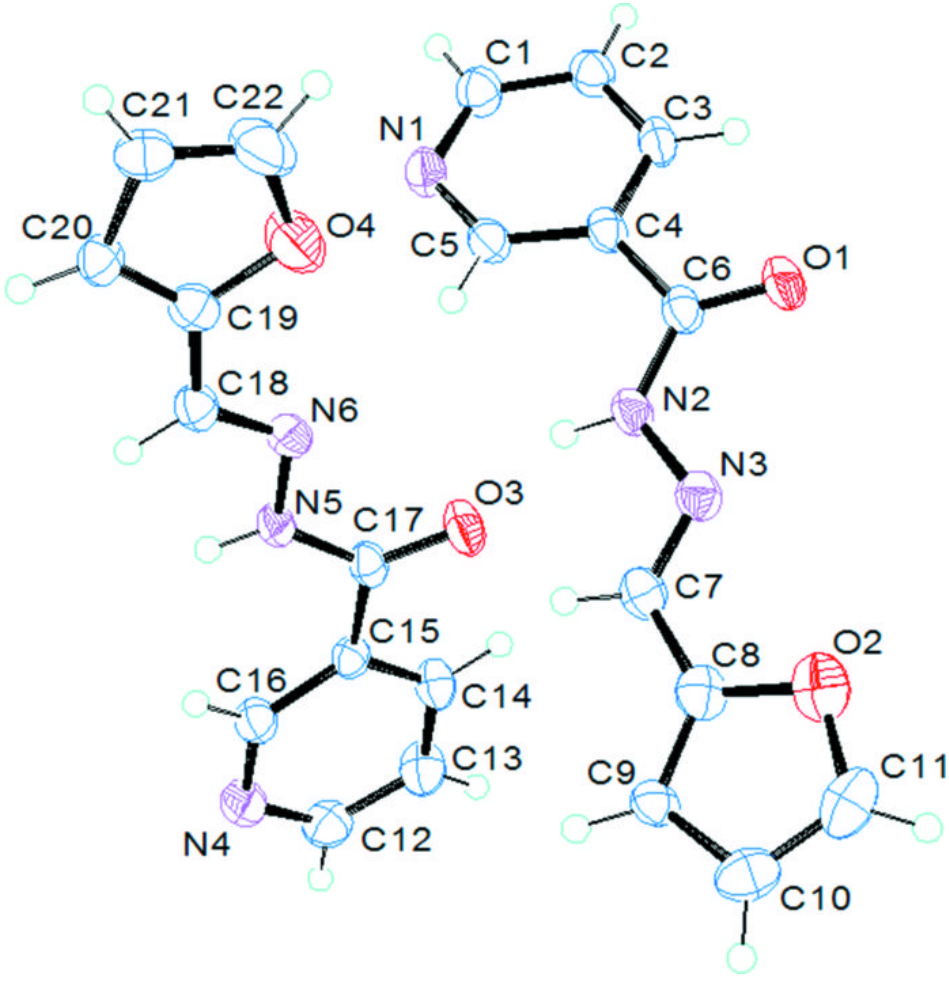
C1
C2
C3
N1
C4
C5
C6
O1
N2
N3
C7
C8
O2
C9
C11
C10
C21
C22
C20
O4
C19
C18
N6
N5
C17
O3
C15
C16
C14
C13
N4
C12

Fig. 2