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(E)-N-[(5-Methyl-2-furyl)methylene]-3-nitroaniline

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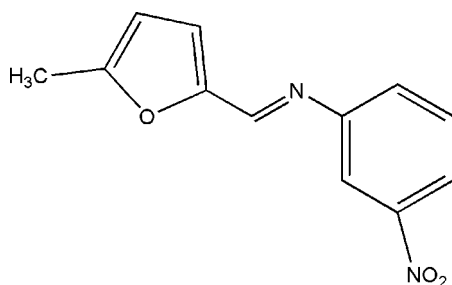
Received 21 February 2009; accepted 26 February 2009

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.045; wR factor = 0.127; data-to-parameter ratio = 6.5.

The asymmetric unit of the title compound, $\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}_3$, contains two crystallographically independent molecules, in which the furan and benzene rings are oriented at dihedral angles of $46.09(3)$ and $39.98(3)^\circ$. In the crystal structure, weak intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules into chains running nearly parallel to the a axis.

Related literature

For general background, see: Li & Zhang (2005); Antal *et al.* (1991); Basta & El-Saied (2003). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}_3$
 $M_r = 230.22$

 Orthorhombic, $Pca2_1$
 $a = 21.634(2)$ Å

 $b = 3.8286(9)$ Å

 $c = 26.660(2)$ Å

 $V = 2208.2(6)$ Å³
 $Z = 8$

 Mo $K\alpha$ radiation

 $\mu = 0.10$ mm⁻¹
 $T = 298$ K

 $0.42 \times 0.39 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Siemens, 1996)

 $T_{\min} = 0.959$, $T_{\max} = 0.980$

8789 measured reflections

2002 independent reflections

 1331 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.127$
 $S = 1.06$

2002 reflections

307 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C23}-\text{H23}\cdots\text{N1}^{\dagger}$	0.93	2.51	3.429 (3)	172

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; 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 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXTL.

The author gratefully acknowledges support from a research project (grant No. 05jk136) of the Education Department of Shaanxi Province.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2629).

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supplementary materials

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(*E*)-*N*-[(5-Methyl-2-furyl)methylene]-3-nitroaniline

Y.-N. Guo

Comment

Schiff base complexes are of great interests for inorganic and bioinorganic chemists. To the best of our knowledge, in the past two decades, Schiff base complexes derived from furaldehydes have been less reported (Li & Zhang, 2005). Furaldehydes are raw materials used for preparing many medicines and industrial products, and some of furfural derivatives have a strong bactericidal ability and their antibacterial activities are fairly broad (Antal *et al.*, 1991; Basta & El-Saied, 2003). As an extension of our work on the structural characterizations of Schiff bases of furaldehyde derivatives, we report herein the crystal structure of the title compound.

The asymmetric unit of the title compound contains two crystallographically independent molecules (Fig. 1), in which the bond lengths (Allen *et al.*, 1987) and angles are generally within normal ranges. Rings A (O1/C2-C5), B (C7-C12) and C (O4/C14-C17), D (C19-C24) are, of course, planar, and they are oriented at dihedral angles of A/B = 46.09 (3) and C/D = 39.98 (3) °.

In the crystal structure, weak intermolecular C-H...N hydrogen bonds (Table 1) link the molecules into chains nearly parallel to the *a*-axis (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, 5-methyl-2-furaldehyde (11.0 mg, 0.1 mmol) and 3-nitrobenzenamine (13.8 mg, 0.1 mmol) were dissolved in methanol (10 ml). The mixture was stirred for 1 h at room temperature, and then filtered. After allowing the filtrate to stand in air for 7 d, yellow block-shaped crystals of the title compound were obtained. They were collected, washed with methanol and dried in a vacuum desiccator using anhydrous CaCl₂ (yield; 60%).

Refinement

H atoms were positioned geometrically, with C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms. Friedel pairs were merged.

Figures

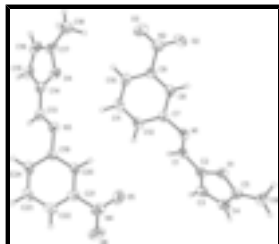


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

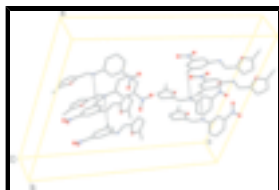


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding are omitted.

(*E*)-*N*-[(5-Methyl-2-furyl)methylene]-3-nitroaniline

Crystal data

$C_{12}H_{10}N_2O_3$

$M_r = 230.22$

Orthorhombic, $Pca2_1$

Hall symbol: P 2c -2ac

$a = 21.634$ (2) Å

$b = 3.8286$ (9) Å

$c = 26.660$ (2) Å

$V = 2208.2$ (6) Å³

$Z = 8$

$F_{000} = 960$

$D_x = 1.385$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1515 reflections

$\theta = 2.4$ – 20.5°

$\mu = 0.10$ mm⁻¹

$T = 298$ K

Block, yellow

$0.42 \times 0.39 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Siemens, 1996)

$T_{\min} = 0.959$, $T_{\max} = 0.980$

8789 measured reflections

2002 independent reflections

1331 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 1.5^\circ$

$h = -25 \rightarrow 24$

$k = -4 \rightarrow 4$

$l = -31 \rightarrow 23$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.045$$

$$wR(F^2) = 0.127$$

$$S = 1.06$$

2002 reflections

307 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2 + 0.7218P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.06199 (19)	0.3004 (10)	0.26104 (17)	0.0472 (11)
N2	0.0529 (3)	0.1073 (14)	0.4392 (2)	0.0681 (14)
N3	0.31807 (19)	0.9617 (11)	0.36859 (16)	0.0470 (11)
N4	0.2860 (3)	1.0358 (15)	0.19047 (19)	0.0657 (14)
O1	0.00925 (16)	0.2744 (9)	0.16401 (13)	0.0497 (9)
O2	0.0034 (2)	-0.0350 (15)	0.43257 (19)	0.0921 (16)
O3	0.0753 (3)	0.1515 (18)	0.48052 (16)	0.110 (2)
O4	0.27482 (18)	0.7909 (9)	0.46480 (13)	0.0520 (10)
O5	0.2380 (2)	0.8701 (14)	0.19661 (19)	0.0890 (16)
O6	0.3026 (3)	1.1466 (17)	0.14984 (17)	0.1053 (19)
C1	0.0915 (2)	0.1827 (14)	0.2234 (2)	0.0466 (13)
H1	0.1320	0.1096	0.2287	0.056*
C2	0.0677 (2)	0.1540 (14)	0.17390 (19)	0.0460 (13)
C3	0.0929 (3)	0.0267 (15)	0.1313 (2)	0.0586 (16)
H3	0.1321	-0.0699	0.1277	0.070*
C4	0.0488 (3)	0.0683 (15)	0.0937 (2)	0.0611 (16)
H4	0.0533	0.0052	0.0602	0.073*
C5	-0.0012 (3)	0.2153 (14)	0.1144 (2)	0.0526 (15)
C6	-0.0618 (3)	0.3237 (16)	0.0943 (2)	0.0646 (17)
H6A	-0.0631	0.2783	0.0589	0.097*
H6B	-0.0677	0.5688	0.1001	0.097*

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H6C	-0.0940	0.1944	0.1107	0.097*
C7	0.0929 (2)	0.3138 (12)	0.3078 (2)	0.0409 (12)
C8	0.0596 (2)	0.2124 (14)	0.3490 (2)	0.0447 (13)
H8	0.0189	0.1385	0.3459	0.054*
C9	0.0879 (3)	0.2223 (15)	0.39510 (19)	0.0494 (14)
C10	0.1472 (3)	0.3357 (16)	0.4017 (2)	0.0592 (15)
H10	0.1653	0.3391	0.4334	0.071*
C11	0.1794 (3)	0.4448 (15)	0.3600 (2)	0.0609 (16)
H11	0.2196	0.5280	0.3635	0.073*
C12	0.1525 (2)	0.4314 (13)	0.3136 (2)	0.0499 (14)
H12	0.1749	0.5026	0.2856	0.060*
C13	0.3537 (3)	0.8338 (15)	0.4012 (2)	0.0511 (14)
H13	0.3951	0.8058	0.3929	0.061*
C14	0.3343 (3)	0.7292 (14)	0.4502 (2)	0.0490 (13)
C15	0.3657 (3)	0.5765 (16)	0.4878 (2)	0.0621 (16)
H15	0.4070	0.5101	0.4873	0.075*
C16	0.3243 (3)	0.5366 (16)	0.5277 (2)	0.0672 (18)
H16	0.3329	0.4364	0.5587	0.081*
C17	0.2701 (3)	0.6692 (14)	0.5130 (2)	0.0569 (16)
C18	0.2091 (3)	0.7113 (18)	0.5369 (2)	0.078 (2)
H18A	0.2017	0.9543	0.5434	0.117*
H18B	0.2082	0.5841	0.5679	0.117*
H18C	0.1776	0.6229	0.5149	0.117*
C19	0.3425 (2)	1.0521 (13)	0.32122 (18)	0.0421 (12)
C20	0.3048 (2)	1.0067 (12)	0.27975 (19)	0.0422 (12)
H20	0.2651	0.9172	0.2836	0.051*
C21	0.3259 (3)	1.0933 (14)	0.23347 (19)	0.0484 (13)
C22	0.3846 (3)	1.2301 (14)	0.2259 (2)	0.0589 (16)
H22	0.3984	1.2841	0.1937	0.071*
C23	0.4218 (3)	1.2838 (15)	0.2669 (3)	0.0568 (15)
H23	0.4611	1.3780	0.2629	0.068*
C24	0.4007 (2)	1.1980 (13)	0.3141 (2)	0.0542 (14)
H24	0.4259	1.2383	0.3417	0.065*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.040 (2)	0.046 (3)	0.055 (3)	0.002 (2)	0.007 (2)	0.003 (2)
N2	0.060 (4)	0.085 (4)	0.059 (4)	0.005 (3)	0.004 (3)	0.008 (3)
N3	0.047 (3)	0.047 (3)	0.047 (3)	0.000 (2)	-0.002 (2)	-0.003 (2)
N4	0.065 (4)	0.083 (4)	0.048 (3)	0.019 (3)	0.004 (3)	-0.002 (3)
O1	0.050 (2)	0.050 (2)	0.049 (2)	0.0024 (17)	0.0033 (17)	-0.0044 (17)
O2	0.060 (3)	0.141 (5)	0.076 (3)	-0.015 (3)	0.015 (2)	0.016 (3)
O3	0.116 (4)	0.164 (6)	0.052 (3)	-0.029 (4)	-0.012 (3)	0.018 (3)
O4	0.059 (3)	0.053 (2)	0.044 (2)	0.0019 (18)	-0.0083 (17)	0.0021 (18)
O5	0.063 (3)	0.132 (5)	0.072 (3)	-0.004 (3)	-0.013 (2)	-0.014 (3)
O6	0.128 (5)	0.140 (5)	0.048 (3)	0.002 (4)	0.006 (3)	0.007 (3)
C1	0.033 (3)	0.050 (3)	0.057 (4)	-0.001 (2)	0.006 (3)	0.006 (3)

C2	0.044 (3)	0.048 (3)	0.047 (3)	0.003 (2)	0.006 (3)	0.001 (2)
C3	0.058 (4)	0.055 (4)	0.062 (4)	0.003 (3)	0.014 (3)	-0.002 (3)
C4	0.075 (4)	0.058 (4)	0.050 (3)	-0.007 (3)	0.014 (3)	-0.010 (3)
C5	0.063 (4)	0.048 (3)	0.047 (4)	-0.009 (3)	0.003 (3)	-0.004 (3)
C6	0.076 (5)	0.062 (4)	0.055 (4)	0.000 (3)	-0.007 (3)	-0.002 (3)
C7	0.036 (3)	0.035 (3)	0.051 (3)	0.004 (2)	-0.002 (3)	-0.003 (2)
C8	0.034 (3)	0.045 (3)	0.055 (3)	0.002 (2)	-0.001 (3)	-0.002 (3)
C9	0.049 (3)	0.052 (4)	0.046 (3)	0.002 (3)	0.002 (3)	0.002 (3)
C10	0.054 (4)	0.064 (4)	0.060 (4)	0.002 (3)	-0.016 (3)	-0.005 (3)
C11	0.040 (3)	0.061 (4)	0.082 (5)	-0.010 (3)	-0.009 (3)	-0.002 (3)
C12	0.041 (3)	0.042 (3)	0.067 (4)	-0.006 (2)	0.005 (3)	0.007 (3)
C13	0.051 (4)	0.050 (3)	0.052 (4)	-0.002 (3)	-0.007 (3)	-0.007 (3)
C14	0.051 (3)	0.043 (3)	0.052 (3)	0.003 (3)	-0.007 (3)	-0.008 (3)
C15	0.066 (4)	0.053 (4)	0.067 (4)	-0.001 (3)	-0.025 (3)	-0.004 (3)
C16	0.097 (5)	0.060 (4)	0.045 (4)	-0.002 (4)	-0.020 (4)	0.002 (3)
C17	0.087 (5)	0.044 (3)	0.040 (3)	-0.009 (3)	-0.003 (3)	-0.003 (3)
C18	0.097 (5)	0.072 (5)	0.064 (4)	-0.011 (4)	0.016 (4)	0.000 (3)
C19	0.041 (3)	0.039 (3)	0.046 (3)	-0.004 (2)	0.007 (2)	-0.001 (2)
C20	0.033 (3)	0.043 (3)	0.051 (3)	0.000 (2)	0.005 (2)	-0.002 (3)
C21	0.053 (3)	0.044 (3)	0.048 (3)	0.007 (3)	0.007 (3)	0.002 (3)
C22	0.062 (4)	0.044 (3)	0.071 (4)	0.002 (3)	0.027 (4)	0.010 (3)
C23	0.039 (3)	0.049 (4)	0.083 (4)	-0.008 (2)	0.014 (3)	0.000 (3)
C24	0.046 (3)	0.044 (3)	0.073 (4)	0.000 (2)	0.002 (3)	-0.010 (3)

Geometric parameters (Å, °)

N1—C1	1.273 (6)	C8—H8	0.9300
N1—C7	1.415 (6)	C9—C10	1.366 (7)
N2—O2	1.215 (7)	C10—C11	1.376 (8)
N2—O3	1.216 (6)	C10—H10	0.9300
N2—C9	1.465 (7)	C11—C12	1.369 (8)
N3—C13	1.260 (6)	C11—H11	0.9300
N3—C19	1.412 (6)	C12—H12	0.9300
N4—O6	1.218 (7)	C13—C14	1.429 (8)
N4—O5	1.229 (6)	C13—H13	0.9300
N4—C21	1.452 (7)	C14—C15	1.345 (8)
O1—C5	1.359 (6)	C15—C16	1.400 (9)
O1—C2	1.371 (6)	C15—H15	0.9300
O4—C14	1.364 (7)	C16—C17	1.335 (8)
O4—C17	1.372 (6)	C16—H16	0.9300
C1—C2	1.420 (7)	C17—C18	1.474 (9)
C1—H1	0.9300	C18—H18A	0.9600
C2—C3	1.352 (7)	C18—H18B	0.9600
C3—C4	1.393 (9)	C18—H18C	0.9600
C3—H3	0.9300	C19—C20	1.385 (7)
C4—C5	1.339 (8)	C19—C24	1.391 (7)
C4—H4	0.9300	C20—C21	1.357 (7)
C5—C6	1.477 (8)	C20—H20	0.9300
C6—H6A	0.9600	C21—C22	1.387 (8)

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C6—H6B	0.9600	C22—C23	1.375 (8)
C6—H6C	0.9600	C22—H22	0.9300
C7—C8	1.370 (7)	C23—C24	1.377 (8)
C7—C12	1.375 (6)	C23—H23	0.9300
C8—C9	1.372 (7)	C24—H24	0.9300
C1—N1—C7	118.1 (4)	C12—C11—H11	119.9
O2—N2—O3	123.1 (6)	C10—C11—H11	119.9
O2—N2—C9	118.3 (5)	C11—C12—C7	120.9 (5)
O3—N2—C9	118.7 (6)	C11—C12—H12	119.6
C13—N3—C19	118.9 (5)	C7—C12—H12	119.6
O6—N4—O5	123.2 (6)	N3—C13—C14	124.0 (5)
O6—N4—C21	118.3 (6)	N3—C13—H13	118.0
O5—N4—C21	118.4 (5)	C14—C13—H13	118.0
C5—O1—C2	106.5 (4)	C15—C14—O4	109.8 (5)
C14—O4—C17	106.2 (4)	C15—C14—C13	130.9 (6)
N1—C1—C2	125.3 (5)	O4—C14—C13	119.3 (5)
N1—C1—H1	117.4	C14—C15—C16	106.9 (6)
C2—C1—H1	117.4	C14—C15—H15	126.6
C3—C2—O1	109.4 (5)	C16—C15—H15	126.6
C3—C2—C1	131.5 (5)	C17—C16—C15	107.3 (5)
O1—C2—C1	119.2 (4)	C17—C16—H16	126.3
C2—C3—C4	106.7 (5)	C15—C16—H16	126.3
C2—C3—H3	126.6	C16—C17—O4	109.8 (5)
C4—C3—H3	126.6	C16—C17—C18	134.5 (6)
C5—C4—C3	107.7 (5)	O4—C17—C18	115.7 (6)
C5—C4—H4	126.2	C17—C18—H18A	109.5
C3—C4—H4	126.2	C17—C18—H18B	109.5
C4—C5—O1	109.7 (5)	H18A—C18—H18B	109.5
C4—C5—C6	133.2 (6)	C17—C18—H18C	109.5
O1—C5—C6	117.1 (5)	H18A—C18—H18C	109.5
C5—C6—H6A	109.5	H18B—C18—H18C	109.5
C5—C6—H6B	109.5	C20—C19—C24	118.3 (5)
H6A—C6—H6B	109.5	C20—C19—N3	117.6 (4)
C5—C6—H6C	109.5	C24—C19—N3	124.0 (5)
H6A—C6—H6C	109.5	C21—C20—C19	119.8 (5)
H6B—C6—H6C	109.5	C21—C20—H20	120.1
C8—C7—C12	119.6 (5)	C19—C20—H20	120.1
C8—C7—N1	116.7 (4)	C20—C21—C22	122.2 (5)
C12—C7—N1	123.7 (5)	C20—C21—N4	118.7 (5)
C7—C8—C9	118.5 (5)	C22—C21—N4	119.1 (5)
C7—C8—H8	120.8	C23—C22—C21	118.4 (5)
C9—C8—H8	120.8	C23—C22—H22	120.8
C10—C9—C8	122.8 (5)	C21—C22—H22	120.8
C10—C9—N2	118.5 (5)	C22—C23—C24	119.9 (5)
C8—C9—N2	118.7 (5)	C22—C23—H23	120.1
C9—C10—C11	117.9 (5)	C24—C23—H23	120.1
C9—C10—H10	121.0	C23—C24—C19	121.4 (5)
C11—C10—H10	121.0	C23—C24—H24	119.3
C12—C11—C10	120.2 (5)	C19—C24—H24	119.3

C7—N1—C1—C2	-179.5 (5)	C19—N3—C13—C14	-179.4 (5)
C5—O1—C2—C3	0.6 (6)	C17—O4—C14—C15	-0.3 (6)
C5—O1—C2—C1	179.8 (5)	C17—O4—C14—C13	-179.1 (5)
N1—C1—C2—C3	-177.9 (6)	N3—C13—C14—C15	176.7 (6)
N1—C1—C2—O1	3.1 (8)	N3—C13—C14—O4	-4.8 (8)
O1—C2—C3—C4	-0.1 (6)	O4—C14—C15—C16	0.6 (7)
C1—C2—C3—C4	-179.2 (6)	C13—C14—C15—C16	179.2 (5)
C2—C3—C4—C5	-0.4 (7)	C14—C15—C16—C17	-0.7 (7)
C3—C4—C5—O1	0.7 (6)	C15—C16—C17—O4	0.5 (7)
C3—C4—C5—C6	179.7 (6)	C15—C16—C17—C18	-179.2 (6)
C2—O1—C5—C4	-0.8 (6)	C14—O4—C17—C16	-0.2 (6)
C2—O1—C5—C6	-180.0 (5)	C14—O4—C17—C18	179.6 (5)
C1—N1—C7—C8	-137.9 (5)	C13—N3—C19—C20	145.3 (5)
C1—N1—C7—C12	44.1 (7)	C13—N3—C19—C24	-37.8 (7)
C12—C7—C8—C9	-1.8 (7)	C24—C19—C20—C21	2.2 (7)
N1—C7—C8—C9	-179.9 (4)	N3—C19—C20—C21	179.3 (5)
C7—C8—C9—C10	1.4 (8)	C19—C20—C21—C22	-0.5 (8)
C7—C8—C9—N2	-178.8 (5)	C19—C20—C21—N4	178.6 (5)
O2—N2—C9—C10	-170.6 (6)	O6—N4—C21—C20	172.6 (6)
O3—N2—C9—C10	7.8 (9)	O5—N4—C21—C20	-9.2 (8)
O2—N2—C9—C8	9.5 (8)	O6—N4—C21—C22	-8.3 (8)
O3—N2—C9—C8	-172.1 (6)	O5—N4—C21—C22	169.9 (5)
C8—C9—C10—C11	0.2 (9)	C20—C21—C22—C23	-1.1 (8)
N2—C9—C10—C11	-179.7 (5)	N4—C21—C22—C23	179.9 (5)
C9—C10—C11—C12	-1.3 (9)	C21—C22—C23—C24	0.8 (8)
C10—C11—C12—C7	0.9 (8)	C22—C23—C24—C19	0.9 (8)
C8—C7—C12—C11	0.7 (8)	C20—C19—C24—C23	-2.4 (8)
N1—C7—C12—C11	178.6 (5)	N3—C19—C24—C23	-179.4 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C23—H23 \cdots N1 ⁱ	0.93	2.51	3.429 (3)	172

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

Fig. 1

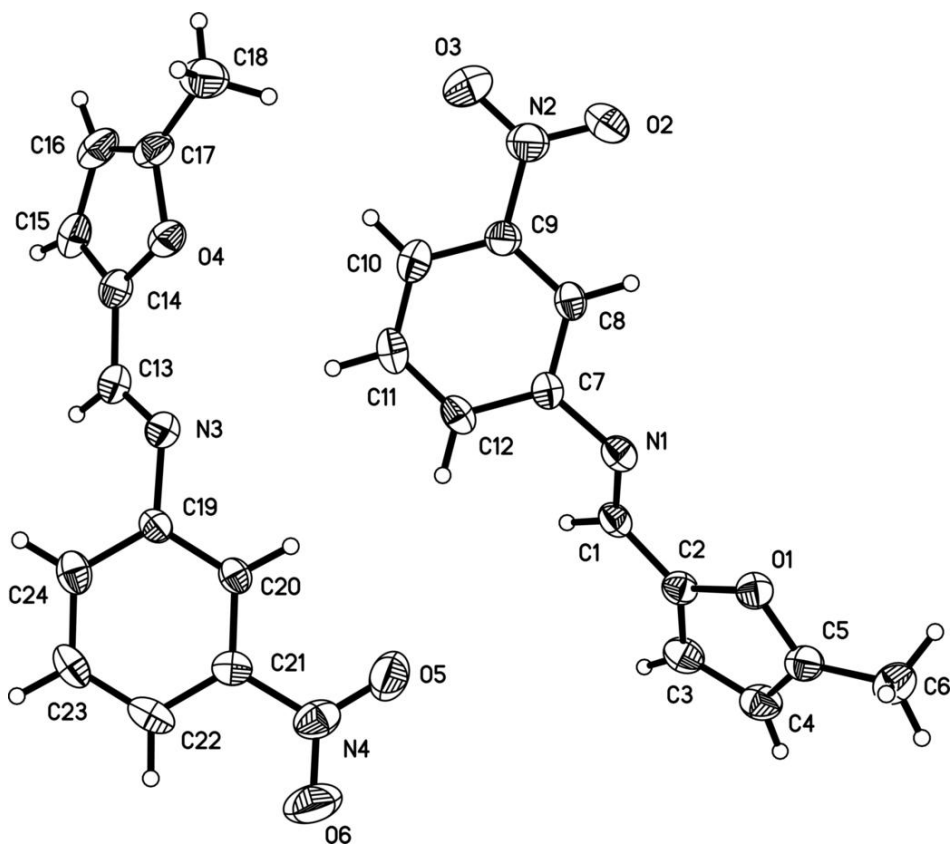


Fig. 2

