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1-Acetyl-3-(4-bromophenyl)-5-(2-furyl)-2-pyrazoline

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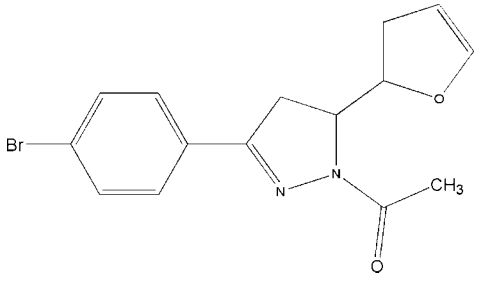
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 13.5.

The pyrazoline ring in the title compound, $C_{15}H_{13}BrN_2O_2$, is approximately perpendicular to the furan ring, forming a dihedral angle of 88.0 (2)°. Weak intermolecular C—H···O contacts help to stabilize the crystal structure.

Related literature

For related literature, see: Dhal *et al.* (1975); Fahrni *et al.* (2003); Guo *et al.* (2007); Kimura *et al.* (1977); Lombardino & Ottemes (1981); Manna *et al.* (2002); Rawal *et al.* (1963).



Experimental

Crystal data

$C_{15}H_{13}BrN_2O_2$
M_r = 333.18
Monoclinic, $P2_1/c$
a = 8.1417 (17) Å
b = 26.757 (6) Å
c = 7.0974 (15) Å
β = 115.587 (2)°
V = 1394.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.95 mm^{-1}
T = 298 (2) K
0.49 × 0.36 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.326, T_{max} = 0.757
5796 measured reflections
2461 independent reflections
1948 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.05
2461 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2^{i}	0.98	2.29	3.148 (4)	146

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2160).

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supplementary materials

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1-Acetyl-3-(4-bromophenyl)-5-(2-furyl)-2-pyrazoline

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Comment

Pyrazoline and its derivatives are important and useful five-membered heterocyclic compounds which possess anti-viral (Rawal *et al.*, 1963), anti-fungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Ottemes, 1981) activities. Further, 1-acetyl-3,5-diaryl-2-pyrazoline has been found to inhibit monoamine oxidases (Manna *et al.*, 2002). As part of our on-going investgation of pyrazolines and their metal complexes, we report here the crystal structure of the title compound (I).

In the structure of (I) (Fig. 1), all bond lengths and angles fall in the normal range (Fahrni *et al.*, 2003; Kimura *et al.*, 1977; Guo *et al.*, 2007). The dihedral angles formed by the pyrazolinyl ring with the phenyl and furan rings are 11.3 (2) and 88.0 (2)°, respectively. There are some intermolecular C—H···O contacts (Table 1) which stabilize the structure.

Experimental

1-(*p*-Bromophenyl)-3-furan-2-propenyl-1-ketone (0.02 mol) and hydrazine (0.02 mol) were mixed and stirred in refluxing 99.5% acetic acid (40 ml) for 6 h. The mixture was poured into ice-water to afford colourless solids. The solids were filtered and washed with water until the pH of solution was about to 7.0.at room temperature. Single crystals of (I) suitable for the X-ray study were obtained by recrystallization from an ethanol solution of (I) held at room temperature; m. pt. 329.9 − 330.3 K.

Refinement

H atoms were fixed geometrically and allowed to ride on their parent atoms with C—H distances = 0.93–0.96 Å, and with U_{iso} = 1.2–1.5U_{eq} of the parent atoms.

Figures

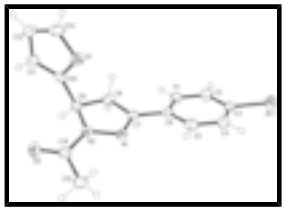

Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

1-Acetyl-3-(4-bromophenyl)-5-(2-furyl)-2-pyrazoline

Crystal data

$C_{15}H_{13}BrN_2O_2$	F_{000} = 672
M_r = 333.18	D_x = 1.587 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2387 reflections
$a = 8.1417\ (17)$ Å	$\theta = 2.3–25.3°$
$b = 26.757\ (6)$ Å	$\mu = 2.95$ mm^{-1}
$c = 7.0974\ (15)$ Å	$T = 298\ (2)$ K
$\beta = 115.587\ (2)°$	Plan, colourless
$V = 1394.5\ (5)$ Å^3	0.49 × 0.36 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2461 independent reflections
Radiation source: fine-focus sealed tube	1948 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.044$
$T = 298(2)$ K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -9\rightarrow9$
$T_{min} = 0.326$, $T_{max} = 0.757$	$k = -21\rightarrow31$
5796 measured reflections	$l = -8\rightarrow7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.5202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
2461 reflections	$\Delta\rho_{max} = 0.70$ e Å^{-3}
182 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.0947 (5)	0.41162 (13)	0.4859 (5)	0.0419 (8)
H1	0.0257	0.3832	0.4279	0.050*
C2	0.1101 (5)	0.44764 (14)	0.3554 (6)	0.0456 (9)
H2	0.0527	0.4436	0.2112	0.055*
C3	0.2128 (5)	0.48981 (13)	0.4436 (5)	0.0385 (8)
C4	0.2965 (5)	0.49611 (14)	0.6560 (6)	0.0486 (9)
H4	0.3645	0.5248	0.7129	0.058*
C5	0.2800 (5)	0.45990 (14)	0.7856 (6)	0.0455 (9)
H5	0.3361	0.4643	0.9297	0.055*
C6	0.1790 (4)	0.41671 (13)	0.7003 (5)	0.0336 (7)
C7	0.1609 (4)	0.37748 (12)	0.8347 (5)	0.0331 (7)
C8	0.0343 (5)	0.33378 (13)	0.7547 (5)	0.0398 (8)
H8A	0.0735	0.3112	0.6752	0.048*
H8B	−0.0891	0.3447	0.6675	0.048*
C9	0.0472 (4)	0.30873 (13)	0.9553 (5)	0.0373 (8)
H9	0.0792	0.2734	0.9553	0.045*
C10	−0.1191 (4)	0.31280 (12)	0.9911 (5)	0.0355 (8)
C11	−0.2383 (5)	0.27922 (15)	0.9944 (6)	0.0470 (9)
H11	−0.2315	0.2448	0.9813	0.056*
C12	−0.3780 (5)	0.30560 (16)	1.0217 (6)	0.0535 (10)
H12	−0.4796	0.2920	1.0306	0.064*
C13	−0.3341 (5)	0.35353 (17)	1.0319 (6)	0.0521 (10)
H13	−0.4020	0.3794	1.0501	0.063*
C14	0.3013 (5)	0.32032 (15)	1.3154 (6)	0.0440 (9)
C15	0.4664 (5)	0.34952 (16)	1.4508 (6)	0.0531 (10)
H15A	0.5274	0.3332	1.5835	0.080*
H15B	0.4309	0.3825	1.4712	0.080*
H15C	0.5472	0.3517	1.3847	0.080*
N1	0.2571 (4)	0.37738 (10)	1.0338 (4)	0.0350 (7)
N2	0.2051 (4)	0.33615 (10)	1.1156 (4)	0.0367 (7)
O1	−0.1747 (3)	0.35984 (9)	1.0122 (4)	0.0475 (6)
O2	0.2510 (4)	0.28316 (11)	1.3765 (5)	0.0643 (8)
Br1	0.23278 (6)	0.540128 (15)	0.26614 (7)	0.0570 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.041 (2)	0.042 (2)	0.040 (2)	−0.0056 (16)	0.0150 (17)	−0.0054 (15)
C2	0.049 (2)	0.055 (2)	0.033 (2)	0.0008 (18)	0.0177 (18)	−0.0001 (16)
C3	0.0306 (18)	0.044 (2)	0.045 (2)	0.0050 (15)	0.0202 (17)	0.0076 (15)
C4	0.045 (2)	0.046 (2)	0.050 (2)	−0.0078 (18)	0.0164 (19)	−0.0002 (17)
C5	0.045 (2)	0.049 (2)	0.036 (2)	−0.0021 (17)	0.0113 (18)	0.0000 (16)
C6	0.0237 (16)	0.0426 (19)	0.0336 (18)	0.0033 (14)	0.0115 (14)	−0.0002 (14)
C7	0.0257 (17)	0.0385 (19)	0.036 (2)	0.0038 (14)	0.0138 (15)	−0.0005 (14)

C8	0.038 (2)	0.042 (2)	0.041 (2)	−0.0011 (16)	0.0185 (17)	−0.0042 (15)
C9	0.0318 (19)	0.0380 (19)	0.042 (2)	−0.0008 (15)	0.0159 (16)	−0.0005 (15)
C10	0.0321 (18)	0.0379 (19)	0.0329 (18)	0.0024 (15)	0.0105 (15)	0.0013 (14)
C11	0.038 (2)	0.042 (2)	0.061 (3)	−0.0017 (17)	0.0208 (19)	0.0065 (17)
C12	0.035 (2)	0.069 (3)	0.059 (3)	0.000 (2)	0.0223 (19)	0.013 (2)
C13	0.038 (2)	0.072 (3)	0.053 (2)	0.013 (2)	0.0256 (19)	−0.0008 (19)
C14	0.0339 (19)	0.057 (2)	0.042 (2)	0.0057 (17)	0.0179 (17)	0.0104 (17)
C15	0.035 (2)	0.076 (3)	0.040 (2)	−0.0051 (19)	0.0084 (18)	0.0077 (19)
N1	0.0277 (15)	0.0415 (17)	0.0363 (17)	0.0012 (12)	0.0142 (13)	0.0030 (12)
N2	0.0264 (14)	0.0425 (17)	0.0372 (17)	−0.0024 (13)	0.0098 (13)	0.0052 (13)
O1	0.0433 (15)	0.0425 (15)	0.0624 (17)	0.0000 (12)	0.0282 (13)	−0.0055 (12)
O2	0.0591 (19)	0.072 (2)	0.0582 (18)	−0.0086 (15)	0.0221 (15)	0.0243 (15)
Br1	0.0593 (3)	0.0572 (3)	0.0622 (3)	0.0015 (2)	0.0335 (2)	0.01656 (19)

Geometric parameters (Å, °)

C1—C2	1.379 (5)	C9—N2	1.490 (4)
C1—C6	1.380 (5)	C9—H9	0.9800
C1—H1	0.9300	C10—C11	1.330 (5)
C2—C3	1.383 (5)	C10—O1	1.367 (4)
C2—H2	0.9300	C11—C12	1.421 (5)
C3—C4	1.370 (5)	C11—H11	0.9300
C3—Br1	1.898 (3)	C12—C13	1.325 (6)
C4—C5	1.382 (5)	C12—H12	0.9300
C4—H4	0.9300	C13—O1	1.375 (4)
C5—C6	1.396 (5)	C13—H13	0.9300
C5—H5	0.9300	C14—O2	1.224 (4)
C6—C7	1.467 (5)	C14—N2	1.358 (5)
C7—N1	1.287 (4)	C14—C15	1.492 (5)
C7—C8	1.499 (5)	C15—H15A	0.9600
C8—C9	1.535 (5)	C15—H15B	0.9600
C8—H8A	0.9700	C15—H15C	0.9600
C8—H8B	0.9700	N1—N2	1.395 (4)
C9—C10	1.486 (5)		
C2—C1—C6	121.7 (3)	C10—C9—H9	109.4
C2—C1—H1	119.1	N2—C9—H9	109.4
C6—C1—H1	119.1	C8—C9—H9	109.4
C1—C2—C3	118.6 (3)	C11—C10—O1	110.0 (3)
C1—C2—H2	120.7	C11—C10—C9	132.8 (3)
C3—C2—H2	120.7	O1—C10—C9	117.1 (3)
C4—C3—C2	121.0 (3)	C10—C11—C12	107.4 (4)
C4—C3—Br1	119.9 (3)	C10—C11—H11	126.3
C2—C3—Br1	119.1 (3)	C12—C11—H11	126.3
C3—C4—C5	120.0 (3)	C13—C12—C11	106.0 (3)
C3—C4—H4	120.0	C13—C12—H12	127.0
C5—C4—H4	120.0	C11—C12—H12	127.0
C4—C5—C6	120.0 (3)	C12—C13—O1	111.0 (3)
C4—C5—H5	120.0	C12—C13—H13	124.5
C6—C5—H5	120.0	O1—C13—H13	124.5

C1—C6—C5	118.6 (3)	O2—C14—N2	119.5 (4)
C1—C6—C7	120.3 (3)	O2—C14—C15	122.9 (4)
C5—C6—C7	121.1 (3)	N2—C14—C15	117.5 (3)
N1—C7—C6	122.1 (3)	C14—C15—H15A	109.5
N1—C7—C8	114.0 (3)	C14—C15—H15B	109.5
C6—C7—C8	123.9 (3)	H15A—C15—H15B	109.5
C7—C8—C9	103.3 (3)	C14—C15—H15C	109.5
C7—C8—H8A	111.1	H15A—C15—H15C	109.5
C9—C8—H8A	111.1	H15B—C15—H15C	109.5
C7—C8—H8B	111.1	C7—N1—N2	108.0 (3)
C9—C8—H8B	111.1	C14—N2—N1	122.6 (3)
H8A—C8—H8B	109.1	C14—N2—C9	124.2 (3)
C10—C9—N2	112.5 (3)	N1—N2—C9	112.9 (3)
C10—C9—C8	115.1 (3)	C10—O1—C13	105.6 (3)
N2—C9—C8	100.6 (3)		
C6—C1—C2—C3	−0.1 (6)	C8—C9—C10—O1	−61.3 (4)
C1—C2—C3—C4	−0.6 (6)	O1—C10—C11—C12	−0.8 (4)
C1—C2—C3—Br1	−179.2 (3)	C9—C10—C11—C12	−175.8 (4)
C2—C3—C4—C5	0.4 (6)	C10—C11—C12—C13	0.3 (4)
Br1—C3—C4—C5	179.0 (3)	C11—C12—C13—O1	0.2 (5)
C3—C4—C5—C6	0.4 (6)	C6—C7—N1—N2	178.7 (3)
C2—C1—C6—C5	0.9 (5)	C8—C7—N1—N2	−2.5 (4)
C2—C1—C6—C7	−179.5 (3)	O2—C14—N2—N1	−178.3 (3)
C4—C5—C6—C1	−1.1 (5)	C15—C14—N2—N1	1.4 (5)
C4—C5—C6—C7	179.4 (3)	O2—C14—N2—C9	−5.3 (5)
C1—C6—C7—N1	170.1 (3)	C15—C14—N2—C9	174.3 (3)
C5—C6—C7—N1	−10.4 (5)	C7—N1—N2—C14	168.2 (3)
C1—C6—C7—C8	−8.5 (5)	C7—N1—N2—C9	−5.5 (4)
C5—C6—C7—C8	171.0 (3)	C10—C9—N2—C14	73.8 (4)
N1—C7—C8—C9	8.9 (4)	C8—C9—N2—C14	−163.2 (3)
C6—C7—C8—C9	−172.4 (3)	C10—C9—N2—N1	−112.6 (3)
C7—C8—C9—C10	110.6 (3)	C8—C9—N2—N1	10.4 (3)
C7—C8—C9—N2	−10.6 (3)	C11—C10—O1—C13	0.9 (4)
N2—C9—C10—C11	−132.1 (4)	C9—C10—O1—C13	176.8 (3)
C8—C9—C10—C11	113.5 (4)	C12—C13—O1—C10	−0.7 (4)
N2—C9—C10—O1	53.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{i}	0.98	2.29	3.148 (4)	146

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2.

Fig. 1