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3-(4-Chlorophenyl)-5-(2-furyl)-1-phenyl-2-pyrazoline

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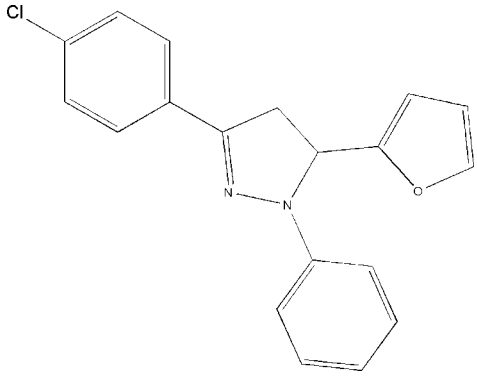
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.126; data-to-parameter ratio = 13.8.

The title compound, $C_{19}H_{15}ClN_2O$, was prepared from phenylhydrazine and 1-(4-chlorophenyl)-3-(2-furyl)-2-propenyl-1-ketone. The pyrazoline ring forms a dihedral angle of 11.09 (10)° with the phenyl ring, 89.23 (1)° with the furan ring and 7.58 (10)° with the chlorophenyl ring.

Related literature

For related literature, see: Dhal *et al.* (1975); Fahrni *et al.* (2003); Guo *et al.* (2006); Lombardino & Ottemes (1981); Orzeszka *et al.* (2000); Rawal *et al.* (1963); Rurack *et al.* (2000); Wiley *et al.* (1958).



Experimental

Crystal data

$C_{19}H_{15}ClN_2O$
M_r = 322.78
Triclinic, $P\overline{1}$
a = 5.9247 (14) Å
b = 8.482 (2) Å
c = 16.284 (4) Å
α = 101.424 (3)°
β = 90.909 (3)°
γ = 99.468 (3)°
V = 790.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 298 (2) K
0.50 × 0.27 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4160 measured reflections
2886 independent reflections
2425 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.05
2886 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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: AT2318).

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supplementary materials

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3-(4-Chlorophenyl)-5-(2-furyl)-1-phenyl-2-pyrazoline

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Comment

As important and useful five-membered heterocyclic compounds, pyrazoline and its derivatives were found to possess anti-viral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Ottemes, 1981) activities. Several 1,3,5-triaryl-2-pyrazolines were also used as scintillation solutes (Wiley *et al.*,1958). We report herein the crystal structure of the title compound (I).

In the structure of (I) (Fig. 1), all of the bond lengths and bond angles fall in the normal range (Rurack, *et al.*, 2000; Fahrni *et al.*, 2003; Guo *et al.*, 2006). The mean plane of pyrazolinyl ring N1/N2/C7/C12/C13 makes dihedral angles of 11.09 (10), 7.58 (10) and 89.23 (1)°, with phenyl ring C1—C6 and benzene ring C14—C19 and furan ring O1/C8—C11, respectively.

Experimental

1-(*p*-Chloromophenyl)-3-(*p*-fluorophenyl)-2-propenyl-1-ketone (0.02 mol) and phenylhydrazine (0.02 mol) were mixed in 99.5% acetic acid (40 ml) and stirred in refluxing for 6 h, then the mixture was poured into ice-water to afford yellow solids·The solids were filtrated and washed with water until the pH of solution is about to 7.0. Finally, the red solid crystals were dry under room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

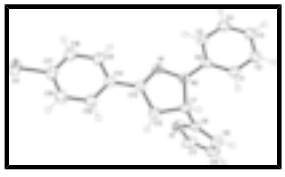


Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

3-(4-Chlorophenyl)-5-(2-furyl)-1-phenyl-2-pyrazoline

Crystal data

$C_{19}H_{15}ClN_2O$	$Z = 2$
$M_r = 322.78$	$F_{000} = 336$
Triclinic, $P\overline{1}$	$D_x = 1.357$ Mg m^{-3}

Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 5.9247 (14) Å	Cell parameters from 2279 reflections
b = 8.482 (2) Å	θ = 2.5–27.7º
c = 16.284 (4) Å	μ = 0.25 mm^{-1}
α = 101.424 (3)º	T = 298 (2) K
β = 90.909 (3)º	Bar, colourless
γ = 99.468 (3)º	0.50 × 0.27 × 0.24 mm
V = 790.2 (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2425 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.019
Monochromator: graphite	θ_{max} = 25.5º
T = 298(2) K	θ_{min} = 2.5º
φ and ω scans	$h = -6 \rightarrow 7$
Absorption correction: none	$k = -9 \rightarrow 10$
4160 measured reflections	$l = -19 \rightarrow 10$
2886 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.1935P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.126	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
2886 reflections	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
209 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.050 (6)
Secondary atom site location: difference Fourier map	

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 calculat-

ing *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	0.2263 (3)	0.3482 (2)	0.90901 (11)	0.0489 (4)
H1	0.3316	0.4297	0.9427	0.059*
C2	0.0290 (4)	0.2820 (2)	0.94263 (13)	0.0580 (5)
H2	0.0029	0.3190	0.9988	0.070*
C3	−0.1287 (4)	0.1619 (3)	0.89393 (14)	0.0641 (6)
H3	−0.2612	0.1172	0.9167	0.077*
C4	−0.0881 (3)	0.1084 (2)	0.81056 (13)	0.0574 (5)
H4	−0.1951	0.0276	0.7773	0.069*
C5	0.1076 (3)	0.1722 (2)	0.77587 (11)	0.0458 (4)
H5	0.1325	0.1341	0.7197	0.055*
C6	0.2692 (3)	0.29446 (19)	0.82523 (10)	0.0403 (4)
C7	0.6222 (3)	0.5127 (2)	0.83136 (11)	0.0431 (4)
H7	0.6803	0.5025	0.8864	0.052*
C8	0.5065 (3)	0.6574 (2)	0.84082 (11)	0.0436 (4)
C9	0.4495 (4)	0.7644 (2)	0.90572 (13)	0.0587 (5)
H9	0.4799	0.7668	0.9622	0.070*
C10	0.3343 (4)	0.8731 (2)	0.87274 (16)	0.0645 (6)
H10	0.2742	0.9602	0.9031	0.077*
C11	0.3291 (4)	0.8265 (3)	0.79033 (16)	0.0649 (6)
H11	0.2633	0.8773	0.7527	0.078*
C12	0.8169 (3)	0.5140 (2)	0.77046 (11)	0.0475 (4)
H12A	0.8497	0.6174	0.7524	0.057*
H12B	0.9555	0.4930	0.7957	0.057*
C13	0.7202 (3)	0.3770 (2)	0.69861 (11)	0.0430 (4)
C14	0.8373 (3)	0.3343 (2)	0.62124 (11)	0.0448 (4)
C15	0.7365 (4)	0.2127 (3)	0.55436 (13)	0.0589 (5)
H15	0.5882	0.1587	0.5580	0.071*
C16	0.8527 (4)	0.1711 (3)	0.48325 (13)	0.0668 (6)
H16	0.7838	0.0894	0.4390	0.080*
C17	1.0720 (4)	0.2513 (3)	0.47784 (12)	0.0567 (5)
C18	1.1761 (4)	0.3720 (3)	0.54203 (13)	0.0597 (5)
H18	1.3242	0.4256	0.5377	0.072*
C19	1.0582 (3)	0.4134 (3)	0.61333 (12)	0.0542 (5)
H19	1.1281	0.4958	0.6570	0.065*
Cl1	1.21959 (12)	0.20021 (9)	0.38763 (4)	0.0841 (3)
N1	0.5275 (2)	0.29548 (17)	0.71306 (9)	0.0448 (4)
N2	0.4665 (3)	0.36129 (17)	0.79203 (9)	0.0483 (4)
O1	0.4334 (2)	0.69357 (17)	0.76793 (8)	0.0591 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.0487 (11)	0.0472 (10)	0.0446 (10)	−0.0019 (8)	−0.0019 (8)	0.0034 (7)
C2	0.0607 (12)	0.0584 (11)	0.0483 (11)	0.0001 (9)	0.0108 (9)	0.0025 (9)
C3	0.0523 (12)	0.0603 (12)	0.0695 (13)	−0.0068 (9)	0.0150 (10)	0.0015 (10)
C4	0.0471 (11)	0.0499 (10)	0.0644 (12)	−0.0053 (8)	−0.0007 (9)	−0.0028 (9)
C5	0.0475 (10)	0.0405 (9)	0.0463 (9)	0.0073 (7)	−0.0009 (7)	0.0015 (7)
C6	0.0406 (9)	0.0358 (8)	0.0450 (9)	0.0072 (7)	−0.0002 (7)	0.0087 (7)
C7	0.0410 (9)	0.0421 (9)	0.0416 (9)	0.0009 (7)	−0.0040 (7)	0.0031 (7)
C8	0.0376 (9)	0.0432 (9)	0.0449 (9)	−0.0022 (7)	−0.0002 (7)	0.0050 (7)
C9	0.0664 (13)	0.0514 (11)	0.0528 (11)	0.0085 (9)	0.0049 (9)	−0.0016 (9)
C10	0.0569 (13)	0.0439 (10)	0.0876 (16)	0.0103 (9)	0.0074 (11)	−0.0006 (10)
C11	0.0594 (13)	0.0516 (11)	0.0845 (16)	0.0141 (10)	−0.0090 (11)	0.0135 (11)
C12	0.0397 (10)	0.0479 (10)	0.0514 (10)	0.0059 (7)	0.0004 (7)	0.0033 (8)
C13	0.0403 (10)	0.0449 (9)	0.0433 (9)	0.0084 (7)	−0.0022 (7)	0.0075 (7)
C14	0.0428 (10)	0.0480 (9)	0.0439 (9)	0.0094 (7)	−0.0006 (7)	0.0087 (7)
C15	0.0549 (12)	0.0607 (12)	0.0527 (11)	−0.0011 (9)	0.0036 (9)	0.0006 (9)
C16	0.0686 (14)	0.0691 (13)	0.0532 (12)	0.0028 (11)	0.0055 (10)	−0.0029 (10)
C17	0.0634 (13)	0.0652 (12)	0.0452 (10)	0.0201 (10)	0.0083 (9)	0.0119 (9)
C18	0.0464 (11)	0.0729 (13)	0.0593 (12)	0.0070 (9)	0.0086 (9)	0.0144 (10)
C19	0.0473 (11)	0.0626 (11)	0.0479 (10)	0.0052 (9)	0.0006 (8)	0.0032 (9)
Cl1	0.0923 (5)	0.1062 (5)	0.0554 (4)	0.0281 (4)	0.0260 (3)	0.0092 (3)
N1	0.0462 (9)	0.0446 (8)	0.0409 (8)	0.0060 (7)	0.0013 (6)	0.0036 (6)
N2	0.0503 (9)	0.0426 (8)	0.0441 (8)	−0.0021 (6)	0.0059 (6)	−0.0024 (6)
O1	0.0660 (9)	0.0584 (8)	0.0532 (8)	0.0172 (7)	−0.0056 (6)	0.0072 (6)

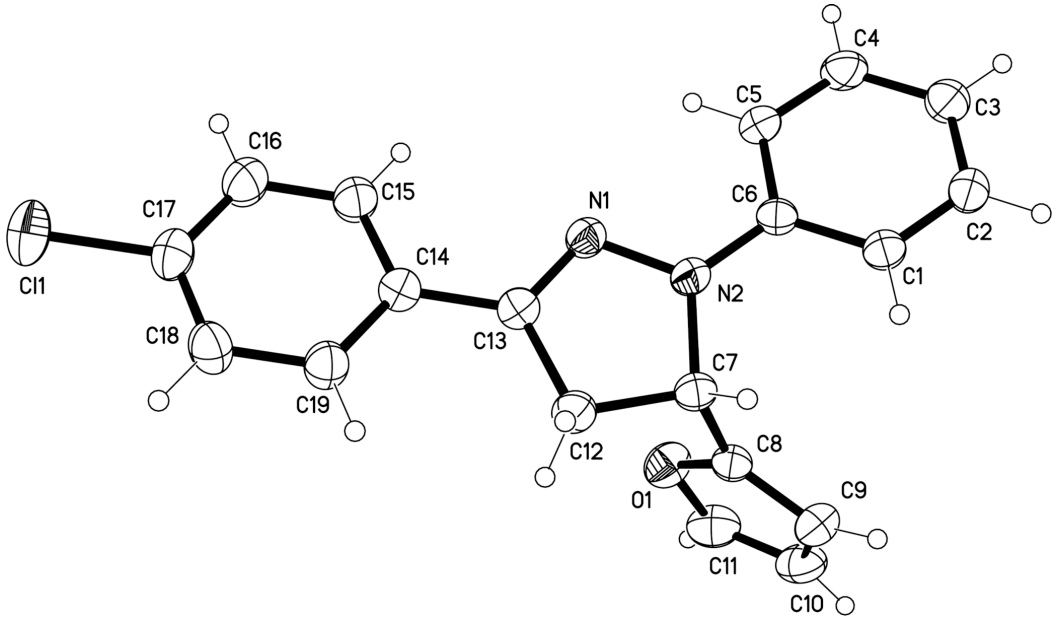
Geometric parameters (Å, °)

C1—C2	1.381 (3)	C10—H10	0.9300
C1—C6	1.392 (2)	C11—O1	1.364 (2)
C1—H1	0.9300	C11—H11	0.9300
C2—C3	1.372 (3)	C12—C13	1.506 (2)
C2—H2	0.9300	C12—H12A	0.9700
C3—C4	1.382 (3)	C12—H12B	0.9700
C3—H3	0.9300	C13—N1	1.285 (2)
C4—C5	1.375 (3)	C13—C14	1.459 (2)
C4—H4	0.9300	C14—C19	1.389 (3)
C5—C6	1.399 (2)	C14—C15	1.393 (3)
C5—H5	0.9300	C15—C16	1.372 (3)
C6—N2	1.380 (2)	C15—H15	0.9300
C7—N2	1.475 (2)	C16—C17	1.377 (3)
C7—C8	1.485 (2)	C16—H16	0.9300
C7—C12	1.533 (2)	C17—C18	1.367 (3)
C7—H7	0.9800	C17—Cl1	1.739 (2)
C8—C9	1.337 (3)	C18—C19	1.380 (3)
C8—O1	1.365 (2)	C18—H18	0.9300
C9—C10	1.412 (3)	C19—H19	0.9300
C9—H9	0.9300	N1—N2	1.376 (2)
C10—C11	1.320 (3)		
C2—C1—C6	120.70 (17)	C10—C11—H11	124.7
C2—C1—H1	119.6	O1—C11—H11	124.7

C6—C1—H1	119.6	C13—C12—C7	102.38 (14)
C3—C2—C1	120.57 (19)	C13—C12—H12A	111.3
C3—C2—H2	119.7	C7—C12—H12A	111.3
C1—C2—H2	119.7	C13—C12—H12B	111.3
C2—C3—C4	119.11 (18)	C7—C12—H12B	111.3
C2—C3—H3	120.4	H12A—C12—H12B	109.2
C4—C3—H3	120.4	N1—C13—C14	122.54 (16)
C5—C4—C3	121.30 (18)	N1—C13—C12	113.56 (15)
C5—C4—H4	119.3	C14—C13—C12	123.84 (16)
C3—C4—H4	119.3	C19—C14—C15	117.91 (17)
C4—C5—C6	119.85 (17)	C19—C14—C13	120.04 (16)
C4—C5—H5	120.1	C15—C14—C13	122.04 (17)
C6—C5—H5	120.1	C16—C15—C14	121.01 (19)
N2—C6—C1	120.40 (15)	C16—C15—H15	119.5
N2—C6—C5	121.13 (16)	C14—C15—H15	119.5
C1—C6—C5	118.47 (16)	C15—C16—C17	119.5 (2)
N2—C7—C8	111.74 (14)	C15—C16—H16	120.3
N2—C7—C12	101.52 (13)	C17—C16—H16	120.3
C8—C7—C12	114.22 (14)	C18—C17—C16	121.16 (19)
N2—C7—H7	109.7	C18—C17—Cl1	119.11 (17)
C8—C7—H7	109.7	C16—C17—Cl1	119.72 (16)
C12—C7—H7	109.7	C17—C18—C19	119.06 (19)
C9—C8—O1	109.14 (17)	C17—C18—H18	120.5
C9—C8—C7	135.12 (17)	C19—C18—H18	120.5
O1—C8—C7	115.72 (15)	C18—C19—C14	121.38 (18)
C8—C9—C10	107.40 (19)	C18—C19—H19	119.3
C8—C9—H9	126.3	C14—C19—H19	119.3
C10—C9—H9	126.3	C13—N1—N2	108.75 (14)
C11—C10—C9	106.41 (19)	N1—N2—C6	121.33 (14)
C11—C10—H10	126.8	N1—N2—C7	112.76 (13)
C9—C10—H10	126.8	C6—N2—C7	125.74 (14)
C10—C11—O1	110.64 (19)	C11—O1—C8	106.40 (16)
C6—C1—C2—C3	−0.1 (3)	C13—C14—C15—C16	−177.95 (19)
C1—C2—C3—C4	−0.2 (3)	C14—C15—C16—C17	−0.2 (3)
C2—C3—C4—C5	0.5 (3)	C15—C16—C17—C18	−0.2 (3)
C3—C4—C5—C6	−0.4 (3)	C15—C16—C17—Cl1	−179.60 (17)
C2—C1—C6—N2	179.94 (17)	C16—C17—C18—C19	0.1 (3)
C2—C1—C6—C5	0.2 (3)	Cl1—C17—C18—C19	179.52 (16)
C4—C5—C6—N2	−179.69 (16)	C17—C18—C19—C14	0.4 (3)
C4—C5—C6—C1	0.1 (3)	C15—C14—C19—C18	−0.7 (3)
N2—C7—C8—C9	115.2 (2)	C13—C14—C19—C18	177.90 (17)
C12—C7—C8—C9	−130.3 (2)	C14—C13—N1—N2	177.55 (15)
N2—C7—C8—O1	−63.19 (19)	C12—C13—N1—N2	0.4 (2)
C12—C7—C8—O1	51.3 (2)	C13—N1—N2—C6	−178.02 (15)
O1—C8—C9—C10	0.2 (2)	C13—N1—N2—C7	6.48 (19)
C7—C8—C9—C10	−178.27 (19)	C1—C6—N2—N1	171.10 (15)
C8—C9—C10—C11	−0.2 (2)	C5—C6—N2—N1	−9.1 (2)
C9—C10—C11—O1	0.2 (3)	C1—C6—N2—C7	−14.0 (3)
N2—C7—C12—C13	9.09 (16)	C5—C6—N2—C7	165.74 (16)

C8—C7—C12—C13	−111.32 (16)	C8—C7—N2—N1	112.14 (16)
C7—C12—C13—N1	−6.46 (19)	C12—C7—N2—N1	−10.00 (18)
C7—C12—C13—C14	176.41 (15)	C8—C7—N2—C6	−63.1 (2)
N1—C13—C14—C19	−171.77 (17)	C12—C7—N2—C6	174.74 (15)
C12—C13—C14—C19	5.1 (3)	C10—C11—O1—C8	−0.1 (2)
N1—C13—C14—C15	6.8 (3)	C9—C8—O1—C11	−0.1 (2)
C12—C13—C14—C15	−176.32 (18)	C7—C8—O1—C11	178.72 (15)
C19—C14—C15—C16	0.6 (3)		

Fig. 1


C4
C5
C3
C16
C15
C17
N1
C6
C2
C14
C1
Cl1
N2
C18
C13
C7
C19
C12
C8
O1
C9
C11
C10