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Crystal structure of 1-(5-(4-chlorophenyl)-3-(2-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-1-yl)ethan-1-one, C₁₇H₁₄N₂OCl

Abstract

C₁₇H₁₄N₂OCl, triclinic, $P\bar{1}$ (no. 2), $a = 8.2387(19)$ Å, $b = 9.764(2)$ Å, $c = 10.644(3)$ Å, $\alpha = 72.023(4)^\circ$, $\beta = 72.770(4)^\circ$, $\gamma = 78.581(4)^\circ$, $V = 772.5(3)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0444$, $wR_{\text{ref}}(F^2) = 0.1099$, $T = 294.15$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.24 × 0.22 × 0.18 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.26 mm ⁻¹
Diffractometer, scan mode:	Enraf-Nonius CAD-4, ω
θ_{max} , completeness:	25.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	4480, 2719, 0.024
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1757
$N(\text{param})_{\text{refined}}$:	200
Programs:	CAD-4 [1], XCAD4 [2], Olex2 [3]

Source of material

A mixture of 3-(4-chlorophenyl)-1-(6-fluorophenyl)prop-2-en-1-one (2.60 g, 0.01 mol) and hydrazine hydrate (0.5 g, 0.01 mol) were mixed in acetic acid (40 mL) and stirred under reflux for 6 h. The reaction mixture was cooled and poured into 50 mL ice-cold water. The precipitate was collected by filtration and crystals of the title compound were obtained from ethanol.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Pyrazoline systems are well known nitrogen-containing heterocyclic compounds which play an important role in

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cl1	1.34455(10)	1.11044(8)	0.26098(8)	0.0903(3)
F1	0.36321(18)	0.76185(18)	0.66293(16)	0.0881(5)
O1	1.0005(2)	0.68137(19)	0.09072(16)	0.0704(5)
N1	0.7716(2)	0.5526(2)	0.43074(18)	0.0506(5)
N2	0.8347(2)	0.64340(19)	0.30306(18)	0.0524(5)
C1	0.4290(3)	0.6254(3)	0.7203(3)	0.0636(6)
C2	0.3515(3)	0.5608(4)	0.8539(3)	0.0748(8)
H2	0.2589(3)	0.6102(4)	0.9033(3)	0.0898(10)*
C3	0.4131(4)	0.4234(4)	0.9120(3)	0.0842(9)
H3	0.3624(4)	0.3784(4)	1.0022(3)	0.1010(11)*
C4	0.5495(4)	0.3505(3)	0.8388(3)	0.0836(9)
H4	0.5897(4)	0.2558(3)	0.8787(3)	0.1003(11)*
C5	0.6266(3)	0.4183(3)	0.7057(3)	0.0669(7)
H5	0.7206(3)	0.3689(3)	0.6576(3)	0.0802(9)*
C6	0.5675(3)	0.5583(3)	0.6417(2)	0.0513(6)
C7	0.6536(3)	0.6281(3)	0.5002(2)	0.0496(6)
C8	0.6195(3)	0.7829(3)	0.4217(2)	0.0607(7)
H8a	0.5097(3)	0.8011(3)	0.3997(2)	0.0729(8)*
H8b	0.6219(3)	0.8491(3)	0.4726(2)	0.0729(8)*
C9	0.7677(3)	0.7979(2)	0.2916(2)	0.0544(6)
H9	0.7234(3)	0.8396(2)	0.2102(2)	0.0653(7)*
C10	0.9057(3)	0.8818(2)	0.2864(2)	0.0501(6)
C11	0.9914(3)	0.8396(3)	0.3894(2)	0.0590(7)
H11	0.9586(3)	0.7619(3)	0.4642(2)	0.0708(8)*
C12	1.1234(3)	0.9102(3)	0.3831(2)	0.0599(7)
H12	1.1794(3)	0.8805(3)	0.4528(2)	0.0718(8)*
C13	1.1715(3)	1.0250(3)	0.2726(3)	0.0588(6)
C14	1.0870(4)	1.0719(3)	0.1710(3)	0.0706(8)
H14	1.1191(4)	1.1508(3)	0.0972(3)	0.0847(9)*
C15	0.9542(4)	1.0006(3)	0.1797(2)	0.0643(7)
H15	0.8955(4)	1.0336(3)	0.1116(2)	0.0772(8)*
C16	0.9535(3)	0.5953(3)	0.2012(2)	0.0535(6)
C17	1.0209(3)	0.4387(3)	0.2323(3)	0.0652(7)
H17a	1.052(2)	0.4071(5)	0.1505(4)	0.0978(11)*
H17b	1.1195(13)	0.4245(4)	0.2674(16)	0.0978(11)*
H17c	0.9342(8)	0.3835(3)	0.2992(13)	0.0978(11)*

pharmaceuticals as well as medicinal chemistry because they possess a broad spectrum of biological activities [4–6]. As a result, a great deal of attention has been paid to the investigation on the structure and property of pyrazolines [7–9]. Continuing our previous work related to 1,3,5-triaryl-2-pyrazoline [10], we report herein the crystal structure of the title compound.

The molecular structure of the title compound is shown in the figure. Bond lengths and angles are within normal ranges [11]. The dihedral angles between the mean plane of the pyrazolinyl ring with the mean planes of the phenyl rings at positions 3 and 5 of the pyrazoline are 84.9(2)° and 10.2(3)°, respectively.

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