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3-(5-Ethyl-2-methyl-4-nitro-2*H*-pyrazole-3-carbonyl)oxazolidin-2-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.064
wR factor = 0.193
Data-to-parameter ratio = 8.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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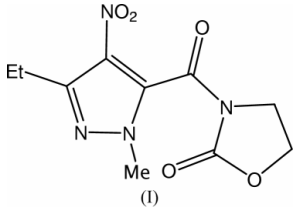
The title compound, $C_{10}H_{12}N_4O_5$, shows an orthogonal relationship between the five-membered rings.

Comment

Derivatives of pyrazolyl heterocycles have high potential for biological activity and, as such, these derivatives have been widely used as pesticides and fungicides (Grenda *et al.*, 1965). As a continuation of our work on the structure–activity relationship of pyrazolyl heterocycle derivatives, we have obtained a colourless crystalline compound that was the product of the condensation reaction of 3-ethyl-4-nitro-1-methyl-5-pyrazolecarboxylic acid chloride and 2-oxazolidinone.



(I)

The structural identity of the product, (I) (Fig. 1), has been established crystallographically. An inspection of the geometric parameters collected in Table 1 indicates that there is considerable delocalization of π-electron density over the pyrazole ring. This is also true, at least for the heteroatoms, in the oxazolidin-2-one moiety. However, this delocalization does not extend over the entire molecule, as seen in the dihedral angles formed between the central C5/C4/O3/N1 link and the five-membered pyrazole [planar to 0.014 (3) Å] and oxazolidin-2-one rings [planar to 0.079 (4) Å] of 89.2 (2) and 11.2 (2)°, respectively, and this fact is emphasized by the orthogonal relationship between the rings [dihedral angle = 90.0 (2)°].

Experimental

3-Ethyl-4-nitro-1-methyl-5-pyrazolecarboxylic acid chloride (2.4 g, 11 mmol; Okada *et al.*, 1989) was added dropwise to a dichloromethane solution (30 ml) containing 2-oxazolidinone (0.87 g, 10 mmol), prepared according to the procedure of Homeyer (1946), and thiethylamine (1.2 g, 12 mmol). The mixture was stirred for 6 h, poured into ice-water and extracted with dichloromethane. The dichloromethane layer was washed with an aqueous solution of sodium carbonate, water and a saturated aqueous solution of sodium chloride. After drying over anhydrous sodium sulfate, the solution was concentrated under reduced pressure. The residue was then recrystallized from ethanol, giving colorless blocks (m.p. 414–415 K).

Crystal data

$C_{10}H_{12}N_4O_5$	D_x = 1.446 Mg m^{-3}
M_r = 268.23	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 9126 reflections
a = 15.2175 (3) Å	θ = 1.7–27.5°
b = 5.2970 (1) Å	μ = 0.12 mm^{-1}
c = 15.8185 (3) Å	T = 293 (1) K
β = 104.893 (4)°	Block, colorless
V = 1232.25 (4) Å^3	0.30 × 0.24 × 0.14 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	1541 reflections with $F^2 > 2\sigma(F^2)$
ω scans	R_{int} = 0.068
Absorption correction: none	θ_{max} = 27.5°
10 185 measured reflections	$h = -19 \rightarrow 19$
2703 independent reflections	$k = -6 \rightarrow 6$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.064	$w = 1/[0.0074F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$wR(F^2)$ = 0.193	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
1541 reflections	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
184 parameters	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.210 (5)	N2—C5	1.337 (4)
O2—C1	1.338 (5)	N2—C10	1.462 (5)
O2—C2	1.448 (5)	N3—C7	1.345 (4)
O3—C4	1.211 (4)	N4—C6	1.434 (4)
O4—N4	1.234 (4)	C2—C3	1.486 (6)
O5—N4	1.225 (4)	C4—C5	1.511 (5)
N1—C1	1.383 (4)	C5—C6	1.373 (4)
N1—C3	1.464 (5)	C6—C7	1.406 (5)
N1—C4	1.373 (5)	C7—C8	1.504 (5)
N2—N3	1.365 (4)	C8—C9	1.526 (6)
C1—O2—C2	109.7 (3)	O1—C1—N1	127.5 (4)
C1—N1—C3	111.1 (3)	O2—C1—N1	109.3 (3)
N3—N2—C10	119.3 (3)	O3—C4—N1	121.2 (4)
N3—N2—C5	112.7 (2)	N1—C4—C5	117.0 (3)
C5—N2—C10	127.8 (3)	N2—C5—C6	105.7 (3)
N2—N3—C7	105.4 (3)	N4—C6—C5	124.3 (3)
O1—C1—O2	123.1 (3)	N4—C6—C7	128.3 (3)

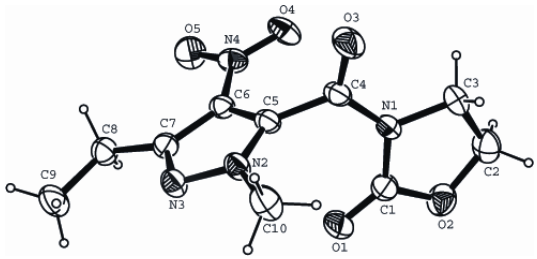


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids.

The H atoms were included in the riding-model approximation, with C—H = 0.96 and 0.97 Å for methyl and methylene H atoms, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku and Rigaku/MSC, 2000–2004); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP*-3 (Farrugia, 1999); software used to prepare material for publication: *CrystalStructure*.

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