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1-Acetyl-3-(2,5-dichlorophenyl)-5-(4-fluorophenyl)-2-pyrazoline

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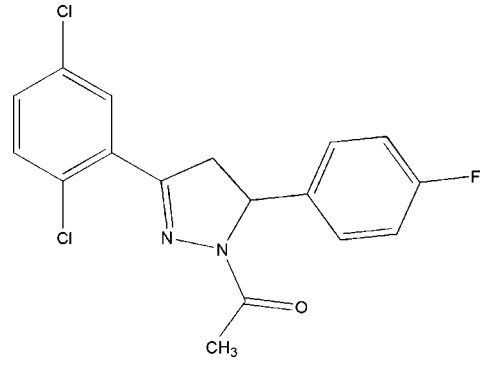
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.098; data-to-parameter ratio = 13.7.

The title compound, $C_{17}H_{13}Cl_2FN_2O$, was prepared by the reaction of hydrazine and 1-(2,5-dichlorophenyl)-3-(4-fluorophenyl)-2-propenyl-1-ketone. In the molecule, the dihedral angle between the two benzene rings is 66.63 (9)°. In the crystal structure, weak intermolecular C—H···Cl hydrogen bonds connect molecules into centrosymmetric dimers.

Related literature

The medicinal and biological properties of pyrazoline derivatives have been reported previously (Rawal *et al.*, 1963; Dhal *et al.*, 1975; Lombardino & Ottemes, 1981; Manna *et al.*, 2002). The bond lengths and angles in the title compound are similar to those in related structures (Fahrni *et al.*, 2003; Kimura *et al.*, 1977; Guo *et al.*, 2007).



Experimental

Crystal data

$C_{17}H_{13}Cl_2FN_2O$
M_r = 351.19
Monoclinic, $C2/c$
a = 21.263 (3) Å
b = 9.7330 (15) Å
c = 14.946 (2) Å
β = 90.188 (2)°
V = 3093.1 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 298 (2) K
0.50 × 0.44 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.812, T_{max} = 0.958
7879 measured reflections
2874 independent reflections
2510 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.098
S = 1.04
2874 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···Cl1^{i}	0.97	2.76	3.697 (3)	163

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2418).

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supplementary materials

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1-Acetyl-3-(2,5-dichlorophenyl)-5-(4-fluorophenyl)-2-pyrazoline

Y.-C. Zhang

Comment

Pyrazoline and its derivatives are useful compounds found to possess antiviral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Ottemes, 1981) activities. 1-Acetyl-3,5-diaryl-2-pyrazoline has been found to inhibit the monoamine oxidases (Manna *et al.*, 2002). As part of our ongoing investgation of pyrazolines and their metal complexes, we report here the crystal strucutre of the title compound.

In the molecule (Fig. 1), all of the bond lengthes and bond angles fall in the normal ranges (Fahrni *et al.*, 2003; Kimura *et al.*, 1977; Guo *et al.*, 2007). The dihedral angles formed by pyrazolinyl ring with phenyl groups at positions 3 and 5 of the pyrazoline are 33.79 (9) and 80.16 (9)°, respectively. Intermolecular C—H···Cl hydrogen bonds form centrosymmetric dimers.

Experimental

1-(2,5-dichlorophenyl)-3-(*p*-fluorophenyl)-2-propenyl-1-ketone (0.02 mol) and hydrazine (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 a colourless solid. The solid was filtered and washed with water until the pH of solution reached *ca* 7.0. Finally, the 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, C—H distances 0.93–0.96 Å,respectively, and with U_{iso} = 1.2–1.5U_{eq} of the parent atoms.

Figures

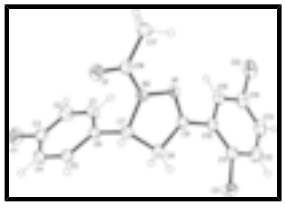


Fig. 1. The molecular structure and atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

1-Acetyl-3-(2,5-dichlorophenyl)-5-(4-fluorophenyl)-2-pyrazoline

Crystal data

$C_{17}H_{13}Cl_2FN_2O$ F_{000} = 1440

M_r = 351.19	D_x = 1.508 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4395 reflections
a = 21.263 (3) Å	θ = 2.3–27.9º
b = 9.7330 (15) Å	μ = 0.44 mm^{-1}
c = 14.946 (2) Å	T = 298 (2) K
β = 90.188 (2)º	Prism, colourless
V = 3093.1 (8) Å^3	0.50 × 0.44 × 0.10 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	2874 independent reflections
Radiation source: fine-focus sealed tube	2510 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 298(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→21
T_{min} = 0.812, T_{max} = 0.958	k = −10→11
7879 measured reflections	l = −18→13

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 1.9032P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.098	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
2874 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
210 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0041 (4)
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 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	0.08006 (9)	0.13527 (18)	0.79684 (12)	0.0476 (4)
H1	0.0845	0.2242	0.7750	0.057*
C2	0.08279 (9)	0.0262 (2)	0.73842 (13)	0.0534 (5)
H2	0.0886	0.0403	0.6775	0.064*
C3	0.07675 (8)	−0.10387 (18)	0.77260 (13)	0.0505 (5)
C4	0.06837 (8)	−0.12930 (17)	0.86159 (14)	0.0497 (4)
H4	0.0649	−0.2188	0.8828	0.060*
C5	0.06521 (8)	−0.01852 (16)	0.91935 (12)	0.0412 (4)
H5	0.0592	−0.0336	0.9802	0.049*
C6	0.07087 (7)	0.11499 (16)	0.88765 (11)	0.0374 (4)
C7	0.06956 (8)	0.23354 (16)	0.95263 (11)	0.0399 (4)
H7	0.0489	0.2051	1.0081	0.048*
C8	0.13482 (8)	0.29360 (17)	0.97412 (13)	0.0460 (4)
H8A	0.1414	0.3009	1.0382	0.055*
H8B	0.1680	0.2378	0.9485	0.055*
C9	0.13231 (7)	0.43332 (16)	0.93100 (10)	0.0360 (3)
C10	0.18616 (7)	0.52742 (16)	0.91690 (11)	0.0389 (4)
C11	0.23777 (8)	0.53748 (17)	0.97440 (13)	0.0461 (4)
C12	0.28884 (8)	0.6198 (2)	0.95410 (16)	0.0577 (5)
H12	0.3232	0.6228	0.9927	0.069*
C13	0.28910 (9)	0.6967 (2)	0.87754 (16)	0.0595 (6)
H13	0.3237	0.7510	0.8634	0.071*
C14	0.23750 (9)	0.69286 (18)	0.82176 (13)	0.0510 (5)
C15	0.18688 (8)	0.60848 (17)	0.83969 (12)	0.0434 (4)
H15	0.1530	0.6055	0.8001	0.052*
C16	−0.02538 (7)	0.36318 (16)	0.90137 (10)	0.0375 (4)
C17	−0.05060 (8)	0.49241 (19)	0.86017 (13)	0.0474 (4)
H17A	−0.0432	0.4910	0.7968	0.071*
H17B	−0.0298	0.5704	0.8862	0.071*
H17C	−0.0950	0.4986	0.8711	0.071*
Cl1	0.23910 (2)	0.45553 (6)	1.07729 (4)	0.06206 (19)
Cl2	0.23626 (3)	0.79727 (6)	0.72775 (4)	0.0752 (2)
F1	0.07820 (6)	−0.21172 (12)	0.71487 (10)	0.0747 (4)
N1	0.07803 (6)	0.46514 (13)	0.89974 (9)	0.0367 (3)
N2	0.03744 (6)	0.35574 (13)	0.91536 (10)	0.0393 (3)
O1	−0.05868 (6)	0.26601 (13)	0.92112 (9)	0.0510 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0561 (10)	0.0350 (9)	0.0518 (10)	−0.0013 (8)	0.0062 (8)	0.0052 (7)
C2	0.0576 (11)	0.0549 (11)	0.0478 (10)	0.0016 (9)	0.0035 (8)	−0.0039 (8)
C3	0.0443 (10)	0.0414 (10)	0.0657 (12)	0.0023 (8)	−0.0036 (8)	−0.0146 (8)
C4	0.0450 (10)	0.0295 (9)	0.0746 (13)	0.0000 (7)	−0.0008 (9)	0.0025 (8)
C5	0.0375 (8)	0.0347 (8)	0.0515 (10)	0.0012 (7)	0.0007 (7)	0.0072 (7)
C6	0.0333 (8)	0.0310 (8)	0.0478 (9)	−0.0008 (6)	0.0013 (6)	0.0031 (7)
C7	0.0405 (9)	0.0319 (8)	0.0474 (9)	0.0023 (6)	0.0007 (7)	0.0047 (7)
C8	0.0439 (9)	0.0354 (9)	0.0586 (11)	0.0036 (7)	−0.0072 (8)	−0.0003 (7)
C9	0.0355 (8)	0.0323 (8)	0.0402 (8)	0.0024 (6)	0.0015 (6)	−0.0058 (6)
C10	0.0321 (8)	0.0335 (8)	0.0512 (10)	0.0012 (6)	0.0032 (7)	−0.0102 (7)
C11	0.0374 (9)	0.0410 (9)	0.0598 (11)	0.0066 (7)	−0.0025 (8)	−0.0127 (8)
C12	0.0317 (9)	0.0556 (12)	0.0858 (15)	0.0013 (8)	−0.0046 (9)	−0.0199 (11)
C13	0.0370 (10)	0.0519 (11)	0.0898 (16)	−0.0094 (8)	0.0158 (10)	−0.0195 (11)
C14	0.0496 (10)	0.0429 (10)	0.0607 (11)	−0.0063 (8)	0.0181 (9)	−0.0113 (8)
C15	0.0399 (9)	0.0391 (9)	0.0512 (10)	−0.0044 (7)	0.0058 (7)	−0.0083 (7)
C16	0.0355 (8)	0.0371 (8)	0.0399 (8)	0.0002 (7)	0.0040 (6)	−0.0053 (7)
C17	0.0386 (9)	0.0481 (10)	0.0556 (10)	0.0063 (7)	0.0004 (8)	0.0026 (8)
Cl1	0.0583 (3)	0.0617 (3)	0.0661 (3)	0.0081 (2)	−0.0211 (2)	−0.0039 (2)
Cl2	0.0900 (4)	0.0650 (4)	0.0708 (4)	−0.0253 (3)	0.0261 (3)	0.0020 (3)
F1	0.0812 (9)	0.0544 (7)	0.0886 (9)	0.0047 (6)	−0.0089 (7)	−0.0312 (6)
N1	0.0344 (7)	0.0296 (7)	0.0462 (8)	−0.0017 (5)	0.0037 (6)	−0.0014 (5)
N2	0.0346 (7)	0.0280 (7)	0.0554 (8)	−0.0008 (5)	0.0008 (6)	0.0034 (6)
O1	0.0399 (7)	0.0480 (7)	0.0652 (8)	−0.0094 (5)	0.0035 (6)	0.0038 (6)

Geometric parameters (Å, °)

C1—C2	1.376 (3)	C9—C10	1.482 (2)
C1—C6	1.386 (2)	C10—C11	1.395 (2)
C1—H1	0.9300	C10—C15	1.398 (2)
C2—C3	1.371 (3)	C11—C12	1.384 (3)
C2—H2	0.9300	C11—Cl1	1.733 (2)
C3—F1	1.359 (2)	C12—C13	1.368 (3)
C3—C4	1.365 (3)	C12—H12	0.9300
C4—C5	1.383 (2)	C13—C14	1.376 (3)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.388 (2)	C14—C15	1.381 (2)
C5—H5	0.9300	C14—Cl2	1.734 (2)
C6—C7	1.509 (2)	C15—H15	0.9300
C7—N2	1.479 (2)	C16—O1	1.2183 (19)
C7—C8	1.539 (2)	C16—N2	1.353 (2)
C7—H7	0.9800	C16—C17	1.499 (2)
C8—C9	1.506 (2)	C17—H17A	0.9600
C8—H8A	0.9700	C17—H17B	0.9600
C8—H8B	0.9700	C17—H17C	0.9600
C9—N1	1.282 (2)	N1—N2	1.3909 (18)

C2—C1—C6	121.19 (16)	C10—C9—C8	126.35 (14)
C2—C1—H1	119.4	C11—C10—C15	117.26 (15)
C6—C1—H1	119.4	C11—C10—C9	124.22 (16)
C3—C2—C1	118.15 (18)	C15—C10—C9	118.48 (15)
C3—C2—H2	120.9	C12—C11—C10	121.45 (18)
C1—C2—H2	120.9	C12—C11—Cl1	116.78 (15)
F1—C3—C4	118.80 (17)	C10—C11—Cl1	121.67 (14)
F1—C3—C2	118.30 (18)	C13—C12—C11	120.38 (18)
C4—C3—C2	122.89 (17)	C13—C12—H12	119.8
C3—C4—C5	118.26 (16)	C11—C12—H12	119.8
C3—C4—H4	120.9	C12—C13—C14	119.11 (17)
C5—C4—H4	120.9	C12—C13—H13	120.4
C4—C5—C6	120.81 (17)	C14—C13—H13	120.4
C4—C5—H5	119.6	C13—C14—C15	121.27 (19)
C6—C5—H5	119.6	C13—C14—Cl2	118.99 (15)
C1—C6—C5	118.69 (15)	C15—C14—Cl2	119.74 (16)
C1—C6—C7	121.63 (14)	C14—C15—C10	120.44 (17)
C5—C6—C7	119.63 (15)	C14—C15—H15	119.8
N2—C7—C6	112.46 (14)	C10—C15—H15	119.8
N2—C7—C8	100.84 (12)	O1—C16—N2	119.67 (15)
C6—C7—C8	113.98 (13)	O1—C16—C17	122.93 (15)
N2—C7—H7	109.7	N2—C16—C17	117.39 (14)
C6—C7—H7	109.7	C16—C17—H17A	109.5
C8—C7—H7	109.7	C16—C17—H17B	109.5
C9—C8—C7	102.89 (13)	H17A—C17—H17B	109.5
C9—C8—H8A	111.2	C16—C17—H17C	109.5
C7—C8—H8A	111.2	H17A—C17—H17C	109.5
C9—C8—H8B	111.2	H17B—C17—H17C	109.5
C7—C8—H8B	111.2	C9—N1—N2	108.20 (13)
H8A—C8—H8B	109.1	C16—N2—N1	123.08 (13)
N1—C9—C10	119.61 (14)	C16—N2—C7	123.74 (13)
N1—C9—C8	113.88 (14)	N1—N2—C7	113.12 (12)
C6—C1—C2—C3	−0.6 (3)	C15—C10—C11—Cl1	173.58 (12)
C1—C2—C3—F1	178.74 (17)	C9—C10—C11—Cl1	−8.7 (2)
C1—C2—C3—C4	−0.2 (3)	C10—C11—C12—C13	1.8 (3)
F1—C3—C4—C5	−178.22 (15)	Cl1—C11—C12—C13	−174.68 (15)
C2—C3—C4—C5	0.7 (3)	C11—C12—C13—C14	1.0 (3)
C3—C4—C5—C6	−0.5 (3)	C12—C13—C14—C15	−2.8 (3)
C2—C1—C6—C5	0.8 (3)	C12—C13—C14—Cl2	176.69 (14)
C2—C1—C6—C7	178.31 (17)	C13—C14—C15—C10	1.9 (3)
C4—C5—C6—C1	−0.3 (2)	Cl2—C14—C15—C10	−177.67 (12)
C4—C5—C6—C7	−177.83 (15)	C11—C10—C15—C14	0.9 (2)
C1—C6—C7—N2	38.3 (2)	C9—C10—C15—C14	−176.98 (14)
C5—C6—C7—N2	−144.20 (15)	C10—C9—N1—N2	175.10 (13)
C1—C6—C7—C8	−75.7 (2)	C8—C9—N1—N2	−0.65 (18)
C5—C6—C7—C8	101.81 (17)	O1—C16—N2—N1	−175.94 (14)
N2—C7—C8—C9	−9.30 (16)	C17—C16—N2—N1	5.0 (2)
C6—C7—C8—C9	111.43 (15)	O1—C16—N2—C7	1.1 (2)

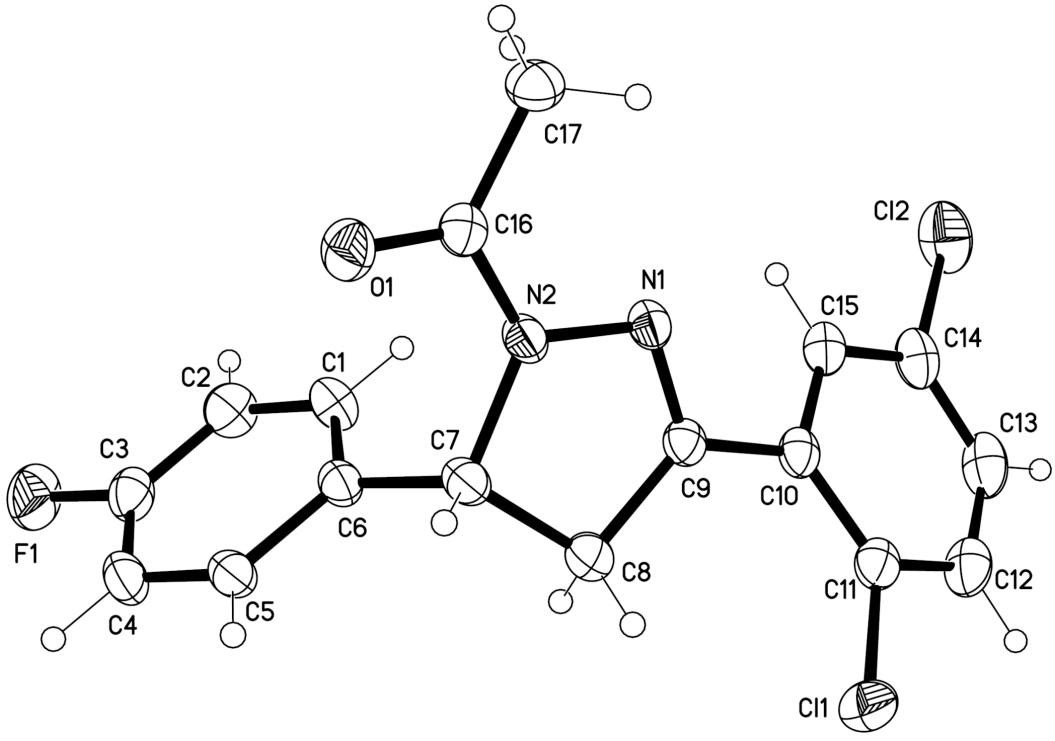
C7—C8—C9—N1	6.82 (19)	C17—C16—N2—C7	−177.93 (15)
C7—C8—C9—C10	−168.60 (15)	C9—N1—N2—C16	170.90 (15)
N1—C9—C10—C11	152.10 (15)	C9—N1—N2—C7	−6.41 (18)
C8—C9—C10—C11	−32.7 (2)	C6—C7—N2—C16	70.98 (19)
N1—C9—C10—C15	−30.2 (2)	C8—C7—N2—C16	−167.22 (15)
C8—C9—C10—C15	144.99 (16)	C6—C7—N2—N1	−111.73 (15)
C15—C10—C11—C12	−2.7 (2)	C8—C7—N2—N1	10.07 (17)
C9—C10—C11—C12	175.05 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8B···Cl1^{i}	0.97	2.76	3.697 (3)	163

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

Fig. 1


C17
C16
O1
N2
N1
Cl2
C15
C14
C13
C1
C2
C3
C7
C9
C10
F1
C6
C8
C11
C12
C4
C5
Cl1