Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Acetyl-5-(4-fluorophenyl)-3-(4-methylphenyl)-2-pyrazoline

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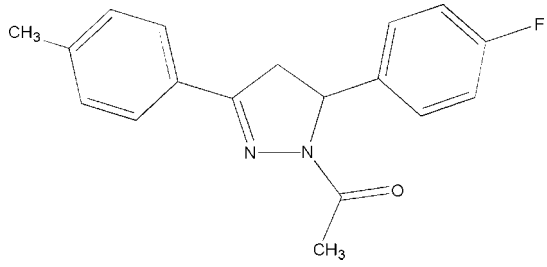
Received 2 June 2007; accepted 6 August 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 13.3.

In the title compound, $C_{18}H_{17}FN_2O$, all bond lengths and angles show normal values. The mean plane of pyrazoline ring makes dihedral angles of 83.33 (9) and 17.03 (9)° with the benzene rings; the two benzene rings make a dihedral angle of 76.01 (5)°. The H atoms of both methyl groups are disordered over two positions by rotation about their C—C σ bonds, with occupancies of 0.52 (3) and 0.48 (3) for the methyl of the tolyl group, and 0.62 (2) and 0.38 (2) for the methyl belonging to the acetyl group. Weak intermolecular C—H···F hydrogen bonds connect molecules into centrosymmetric dimers in the crystal structure.

Related literature

For related pyrazoline derivatives, see: Fahrni *et al.* (2003); Guo *et al.* (2007); Jian *et al.* (2006); Kimura *et al.* (1977); Manna *et al.* (2002); For biological properties, see: Rawal *et al.* (1963); Dhal *et al.* (1975); Lombardino & Otterness (1981).



Experimental

Crystal data

$C_{18}H_{17}FN_2O$
M_r = 296.34
Monoclinic, $P2_1/c$
a = 14.521 (3) Å
b = 11.405 (2) Å
c = 9.719 (2) Å
β = 108.368 (3)°
V = 1527.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.48 × 0.25 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
6307 measured reflections
2690 independent reflections
2015 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
S = 1.02
2690 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14E···F1^{i}	0.96	2.37	3.314 (2)	166

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2115).

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 doi:10.1107/S1600536807038810

supplementary materials

Acta Cryst. (2007). E**63**, o3779 [**doi:10.1107/S1600536807038810**]

1-Acetyl-5-(4-fluorophenyl)-3-(4-methylphenyl)-2-pyrazoline

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Comment

Pyrazoline and its derivatives are important and useful five-membered heterocyclic compounds, which possess antiviral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Otterness, 1981) activities. 1-Acetyl-3,5-diaryl-2-pyrazoline have also been found to inhibit the monoamine oxidases (Manna *et al.*, 2002). As part of our ongoing investigations on 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 ranges (Fahrni *et al.*, 2003; Kimura *et al.*, 1977; Guo *et al.*, 2007; Jian *et al.*, 2006). The dihedral angles formed by pyrazolinyl ring with aromatic groups at positions 3 and 5 are 17.03 (1) and 83.33 (2)°, respectively. A weak C—H···F hydrogen bond stabilizes the crystal structure of (I), forming centrosymmetric dimers in the cell.

Experimental

1-(*p*-Methylphenyl)-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 refluxed for 6 h. Then, the mixture was poured into ice–water to afford colourless solids. The solids were filtrated and washed with water, until the pH of the solution reached 7.0. Finally, the solid product was dried at room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

Refinement

In the case of methyl groups, a difference map revealed that H atoms are disordered over two positions, by rotation about the C—C bonds. In the last refinement cycles, corresponding H positions were regularized, with C—H bond lengths set to 0.96 Å. Site occupation factors of H atoms were refined to 0.52 (3)/0.48 (3) for the methyl of the tolyl group and 0.62 (2)/0.38 (2) for the methyl belonging to the acetyl group. Other H atoms were placed geometrically and allowed to ride on their parent atoms, with C—H distances set to 0.93 (aromatic CH), 0.97 (methylene CH_2) and 0.98 Å (methine CH). In all cases, isotropic displacement parameters for H atoms were set to $U_{iso}(H) = xU_{eq}$(carrier C atom), with $x = 1.5$ for methyl groups and $x = 1.2$ otherwise.

Figures

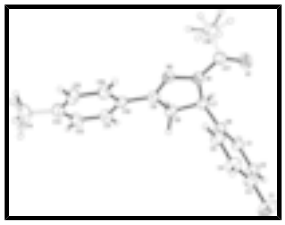


Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

1-Acetyl-5-(4-fluorophenyl)-3-(4-methylphenyl)-2-pyrazoline

Crystal data

$C_{18}H_{17}FN_2O$	F_{000} = 624
M_r = 296.34	D_x = 1.288 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2013 reflections
a = 14.521 (3) Å	θ = 2.3–24.1º
b = 11.405 (2) Å	μ = 0.09 mm^{-1}
c = 9.719 (2) Å	T = 298 (2) K
β = 108.368 (3)º	Prism, colourless
V = 1527.6 (5) Å^3	0.48 × 0.25 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2015 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.023
Monochromator: graphite	θ_{max} = 25.0º
T = 298(2) K	θ_{min} = 2.3º
φ and ω scans	h = −12→17
Absorption correction: none	k = −13→13
6307 measured reflections	l = −10→11
2690 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.1686P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001

2690 reflections	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
203 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.37035 (11)	0.47632 (13)	1.46974 (16)	0.0490 (4)	
H1	0.4222	0.4248	1.5039	0.059*	
C2	0.32733 (13)	0.52340 (14)	1.56553 (17)	0.0558 (4)	
H2	0.3493	0.5039	1.6634	0.067*	
C3	0.25217 (14)	0.59881 (15)	1.51273 (19)	0.0586 (4)	
C4	0.21734 (13)	0.63002 (16)	1.36947 (19)	0.0643 (5)	
H4	0.1657	0.6820	1.3365	0.077*	
C5	0.26131 (12)	0.58203 (15)	1.27545 (18)	0.0575 (4)	
H5	0.2391	0.6023	1.1778	0.069*	
C6	0.33761 (11)	0.50461 (13)	1.32401 (15)	0.0461 (4)	
C7	0.38072 (11)	0.44494 (14)	1.21964 (15)	0.0496 (4)	
H7	0.4468	0.4182	1.2709	0.059*	
C8	0.31881 (12)	0.34222 (14)	1.13874 (16)	0.0522 (4)	
H8A	0.3588	0.2750	1.1347	0.063*	
H8B	0.2709	0.3192	1.1840	0.063*	
C9	0.27163 (11)	0.39268 (13)	0.99076 (16)	0.0463 (4)	
C10	0.19172 (11)	0.33801 (13)	0.87748 (16)	0.0471 (4)	
C11	0.16780 (12)	0.22164 (15)	0.89026 (19)	0.0569 (4)	
H11	0.2009	0.1794	0.9729	0.068*	
C12	0.09508 (13)	0.16799 (15)	0.7811 (2)	0.0624 (5)	
H12	0.0806	0.0897	0.7915	0.075*	
C13	0.04356 (12)	0.22696 (16)	0.65762 (19)	0.0592 (5)	
C14	−0.03119 (15)	0.16550 (18)	0.5358 (2)	0.0848 (6)	
H14A	−0.0819	0.1358	0.5701	0.127*	0.52 (3)
H14B	−0.0013	0.1016	0.5016	0.127*	0.52 (3)
H14C	−0.0582	0.2198	0.4581	0.127*	0.52 (3)
H14D	−0.0060	0.1538	0.4566	0.127*	0.48 (3)
H14E	−0.0889	0.2125	0.5040	0.127*	0.48 (3)
H14F	−0.0464	0.0909	0.5691	0.127*	0.48 (3)
C15	0.06540 (13)	0.34419 (16)	0.64840 (18)	0.0622 (5)	
H15	0.0299	0.3871	0.5677	0.075*	
C16	0.13788 (12)	0.39907 (15)	0.75489 (17)	0.0561 (4)	
H16	0.1511	0.4778	0.7449	0.067*	
C17	0.44121 (12)	0.61308 (14)	1.10642 (18)	0.0518 (4)	
C18	0.43325 (13)	0.67838 (15)	0.96995 (19)	0.0650 (5)	
H18A	0.4675	0.6365	0.9155	0.098*	0.62 (2)
H18B	0.4609	0.7551	0.9935	0.098*	0.62 (2)
H18C	0.3662	0.6855	0.9131	0.098*	0.62 (2)
H18D	0.4966	0.7028	0.9706	0.098*	0.38 (2)
H18E	0.3927	0.7460	0.9635	0.098*	0.38 (2)

H18F	0.4053	0.6282	0.8881	0.098*	0.38 (2)
F1	0.20957 (9)	0.64612 (10)	1.60668 (12)	0.0882 (4)	
N1	0.38063 (10)	0.52101 (11)	1.09674 (13)	0.0512 (3)	
N2	0.30906 (9)	0.49040 (12)	0.96894 (13)	0.0502 (3)	
O1	0.50015 (9)	0.63776 (11)	1.22326 (13)	0.0713 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0485 (9)	0.0517 (9)	0.0431 (9)	0.0004 (7)	0.0090 (7)	0.0043 (7)
C2	0.0667 (11)	0.0571 (10)	0.0416 (9)	−0.0045 (9)	0.0145 (8)	0.0023 (8)
C3	0.0710 (12)	0.0565 (10)	0.0538 (10)	0.0029 (9)	0.0274 (9)	−0.0033 (8)
C4	0.0642 (11)	0.0663 (11)	0.0613 (11)	0.0185 (9)	0.0183 (9)	0.0058 (9)
C5	0.0570 (10)	0.0689 (11)	0.0430 (9)	0.0092 (9)	0.0104 (8)	0.0071 (8)
C6	0.0433 (8)	0.0507 (9)	0.0406 (8)	−0.0009 (7)	0.0080 (7)	0.0030 (7)
C7	0.0454 (9)	0.0598 (10)	0.0407 (9)	0.0043 (8)	0.0095 (7)	0.0087 (7)
C8	0.0573 (10)	0.0528 (9)	0.0480 (9)	0.0041 (8)	0.0186 (8)	0.0047 (7)
C9	0.0483 (9)	0.0502 (9)	0.0432 (9)	0.0041 (7)	0.0185 (7)	0.0014 (7)
C10	0.0474 (9)	0.0511 (9)	0.0464 (9)	0.0032 (7)	0.0197 (7)	−0.0005 (7)
C11	0.0540 (10)	0.0548 (10)	0.0621 (11)	0.0051 (8)	0.0187 (9)	0.0057 (8)
C12	0.0562 (10)	0.0511 (10)	0.0810 (13)	−0.0020 (9)	0.0234 (10)	−0.0063 (9)
C13	0.0483 (10)	0.0639 (11)	0.0646 (11)	0.0041 (9)	0.0168 (9)	−0.0152 (9)
C14	0.0695 (13)	0.0827 (14)	0.0901 (15)	−0.0002 (11)	0.0077 (11)	−0.0286 (11)
C15	0.0625 (11)	0.0651 (11)	0.0519 (10)	0.0084 (9)	0.0079 (9)	−0.0009 (8)
C16	0.0630 (11)	0.0519 (9)	0.0503 (10)	0.0017 (8)	0.0134 (9)	−0.0004 (8)
C17	0.0482 (9)	0.0555 (10)	0.0525 (10)	0.0011 (8)	0.0170 (8)	−0.0013 (8)
C18	0.0724 (12)	0.0603 (11)	0.0666 (11)	−0.0068 (9)	0.0280 (10)	0.0060 (9)
F1	0.1181 (10)	0.0863 (8)	0.0758 (7)	0.0254 (7)	0.0528 (7)	−0.0003 (6)
N1	0.0514 (8)	0.0606 (8)	0.0396 (7)	−0.0064 (7)	0.0115 (6)	0.0041 (6)
N2	0.0498 (8)	0.0596 (8)	0.0400 (7)	−0.0037 (7)	0.0125 (6)	0.0015 (6)
O1	0.0626 (8)	0.0786 (9)	0.0624 (8)	−0.0137 (7)	0.0051 (7)	−0.0010 (6)

Geometric parameters (Å, °)

C1—C2	1.383 (2)	C10—C16	1.389 (2)
C1—C6	1.383 (2)	C11—C12	1.382 (2)
C1—H1	0.9300	C11—H11	0.9300
C2—C3	1.357 (2)	C12—C13	1.373 (2)
C2—H2	0.9300	C12—H12	0.9300
C3—F1	1.3651 (19)	C13—C15	1.383 (2)
C3—C4	1.370 (2)	C13—C14	1.504 (2)
C4—C5	1.382 (2)	C15—C16	1.373 (2)
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.379 (2)	C16—H16	0.9300
C5—H5	0.9300	C17—O1	1.2201 (19)
C6—C7	1.511 (2)	C17—N1	1.354 (2)
C7—N1	1.4760 (19)	C17—C18	1.494 (2)
C7—C8	1.534 (2)	N1—N2	1.3897 (17)
C7—H7	0.9800	C14—H14A	0.9600

C8—C9	1.499 (2)	C14—H14B	0.9600
C8—H8A	0.9700	C14—H14C	0.9600
C8—H8B	0.9700	C18—H18A	0.9600
C9—N2	1.2865 (19)	C18—H18B	0.9600
C9—C10	1.464 (2)	C18—H18C	0.9600
C10—C11	1.387 (2)		
C2—C1—C6	121.11 (15)	C10—C9—C8	124.91 (14)
C2—C1—H1	119.4	C11—C10—C16	117.86 (15)
C6—C1—H1	119.4	C11—C10—C9	120.11 (14)
C3—C2—C1	118.15 (15)	C16—C10—C9	122.02 (14)
C3—C2—H2	120.9	C12—C11—C10	120.47 (16)
C1—C2—H2	120.9	C12—C11—H11	119.8
C2—C3—F1	118.53 (15)	C10—C11—H11	119.8
C2—C3—C4	122.97 (16)	C13—C12—C11	121.89 (17)
F1—C3—C4	118.50 (16)	C13—C12—H12	119.1
C3—C4—C5	118.00 (16)	C11—C12—H12	119.1
C3—C4—H4	121.0	C12—C13—C15	117.20 (16)
C5—C4—H4	121.0	C12—C13—C14	121.25 (17)
C6—C5—C4	121.08 (15)	C15—C13—C14	121.53 (17)
C6—C5—H5	119.5	C16—C15—C13	121.92 (16)
C4—C5—H5	119.5	C16—C15—H15	119.0
C5—C6—C1	118.68 (15)	C13—C15—H15	119.0
C5—C6—C7	121.12 (13)	C15—C16—C10	120.59 (16)
C1—C6—C7	120.07 (14)	C15—C16—H16	119.7
N1—C7—C6	112.55 (13)	C10—C16—H16	119.7
N1—C7—C8	100.55 (11)	O1—C17—N1	119.57 (15)
C6—C7—C8	112.84 (13)	O1—C17—C18	123.15 (16)
N1—C7—H7	110.2	N1—C17—C18	117.27 (15)
C6—C7—H7	110.2	C17—N1—N2	122.92 (13)
C8—C7—H7	110.2	C17—N1—C7	124.39 (13)
C9—C8—C7	102.44 (12)	N2—N1—C7	112.67 (12)
C9—C8—H8A	111.3	C9—N2—N1	107.82 (12)
C7—C8—H8A	111.3	C13—C14—H14A	109.5
C9—C8—H8B	111.3	C13—C14—H14B	109.5
C7—C8—H8B	111.3	C13—C14—H14C	109.5
H8A—C8—H8B	109.2	C17—C18—H18A	109.5
N2—C9—C10	121.40 (14)	C17—C18—H18B	109.5
N2—C9—C8	113.67 (13)	C17—C18—H18C	109.5
C6—C1—C2—C3	−0.3 (2)	C16—C10—C11—C12	2.5 (2)
C1—C2—C3—F1	−179.69 (15)	C9—C10—C11—C12	−177.35 (15)
C1—C2—C3—C4	0.0 (3)	C10—C11—C12—C13	−0.6 (3)
C2—C3—C4—C5	0.0 (3)	C11—C12—C13—C15	−1.9 (3)
F1—C3—C4—C5	179.70 (16)	C11—C12—C13—C14	176.26 (16)
C3—C4—C5—C6	0.3 (3)	C12—C13—C15—C16	2.5 (3)
C4—C5—C6—C1	−0.6 (2)	C14—C13—C15—C16	−175.68 (17)
C4—C5—C6—C7	175.26 (15)	C13—C15—C16—C10	−0.6 (3)
C2—C1—C6—C5	0.6 (2)	C11—C10—C16—C15	−1.9 (2)
C2—C1—C6—C7	−175.30 (14)	C9—C10—C16—C15	177.90 (15)

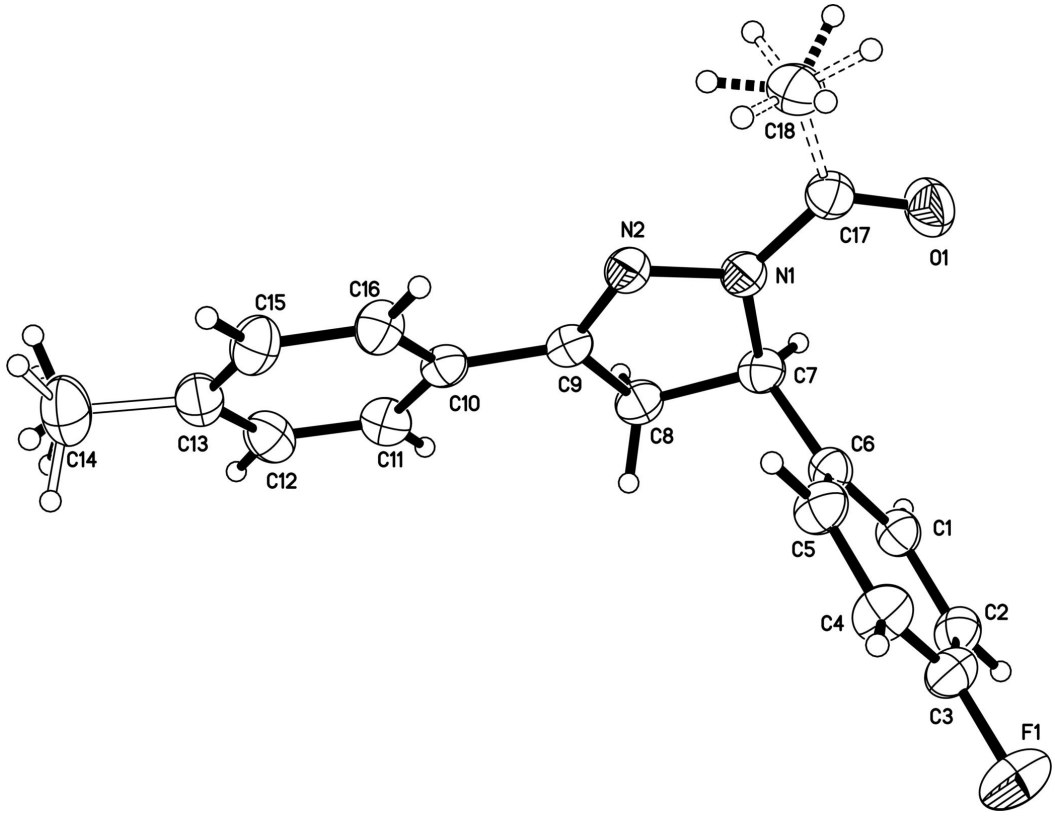
C5—C6—C7—N1	35.0 (2)	O1—C17—N1—N2	177.33 (14)
C1—C6—C7—N1	−149.18 (14)	C18—C17—N1—N2	−3.9 (2)
C5—C6—C7—C8	−77.93 (18)	O1—C17—N1—C7	−0.6 (2)
C1—C6—C7—C8	97.86 (17)	C18—C17—N1—C7	178.08 (14)
N1—C7—C8—C9	−15.53 (14)	C6—C7—N1—C17	73.61 (19)
C6—C7—C8—C9	104.59 (14)	C8—C7—N1—C17	−166.07 (14)
C7—C8—C9—N2	12.45 (17)	C6—C7—N1—N2	−104.54 (14)
C7—C8—C9—C10	−168.70 (14)	C8—C7—N1—N2	15.78 (16)
N2—C9—C10—C11	164.88 (15)	C10—C9—N2—N1	178.27 (13)
C8—C9—C10—C11	−13.9 (2)	C8—C9—N2—N1	−2.83 (18)
N2—C9—C10—C16	−14.9 (2)	C17—N1—N2—C9	172.91 (14)
C8—C9—C10—C16	166.30 (15)	C7—N1—N2—C9	−8.90 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14E···F1^{i}	0.96	2.37	3.314 (2)	166

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

Fig. 1


C18
C17
O1
N2
N1
C15
C16
C9
C10
C7
C8
C6
C13
C14
C12
C11
C1
C5
C4
C2
C3
F1