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5-(4-Fluorophenyl)-3-(4-methylphenyl)-1-phenyl-2-pyrazoline

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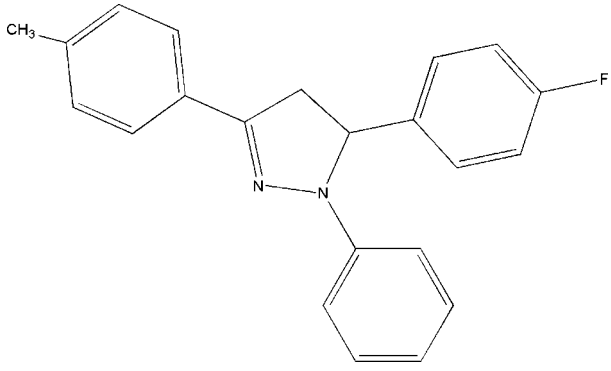
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.133; data-to-parameter ratio = 13.5.

In the title compound, $C_{22}H_{19}FN_2$, the mean plane of the pyrazoline ring forms dihedral angles of 18.52 (10)° with the phenyl ring, 71.69 (10)° with the fluorophenyl ring and 4.82 (10)° with the *p*-tolyl ring.

Related literature

For related literature, see: Guo *et al.* (2006); Manna *et al.* (2002); Wiley *et al.* (1958).



Experimental

Crystal data

$C_{22}H_{19}FN_2$
M_r = 330.39
Monoclinic, $P2_1/c$
a = 14.854 (3) Å
b = 11.429 (2) Å
c = 10.833 (2) Å
β = 109.090 (3)°
V = 1738.0 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.50 × 0.45 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
7135 measured reflections
3066 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.133
S = 1.01
3066 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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: AT2325).

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supplementary materials

Acta Cryst. (2007). E**63**, o3223 [**doi:10.1107/S1600536807028711**]

5-(4-Fluorophenyl)-3-(4-methylphenyl)-1-phenyl-2-pyrazoline

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Comment

Pyrazolines are important and useful five-membered heterocyclic compounds. 1-Acetyl-3,5-diaryl-2-pyrazolines have been found to inhibit the monoamine oxidases (Manna *et al.*, 2002). 1,3,5-Triaryl-2-pyrazolines were also used as scintillation solutes (Wiley *et al.*, 1958). Here, we report the crystal structure of the title compound (I).

In the structure of (I) (Fig. 1), the values of the bond lengths and bond angles arel in the normal range (Guo *et al.*, 2006). The mean plane of pyrazolinyl ring forms a dihedral angle of 18.52 (10)° with the phenyl ring, 71.69 (10)° with the fluorophenyl ring and 4.82 (10)° with the *p*-tolyl ring.

Experimental

1-(*p*-Methylphenyl)-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 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 = 0.93–0.96 Å and with U_{iso}(H) = 1.2U_{eq} or1.5U_{eq} of the parent atoms.

Figures

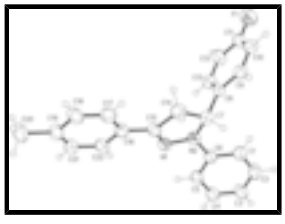


Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

5-(4-Fluorophenyl)-3-(4-methylphenyl)-1-phenyl-2-pyrazoline

Crystal data

$C_{22}H_{19}FN_2$	F_{000} = 696
M_r = 330.39	D_x = 1.263 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2776 reflections
$a = 14.854$ (3) Å	$\theta = 2.3$–24.0°
$b = 11.429$ (2) Å	$\mu = 0.08$ mm^{-1}
$c = 10.833$ (2) Å	$T = 298$ (2) K
$\beta = 109.090$ (3)º	Block, yellow
$V = 1738.0$ (6) Å^3	0.50 × 0.45 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2155 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.020$
Monochromator: graphite	$\theta_{max} = 25.0^\circ$
$T = 298(2)$ K	$\theta_{min} = 2.3^\circ$
φ and ω scans	$h = -17 \rightarrow 16$
Absorption correction: none	$k = -12 \rightarrow 13$
7135 measured reflections	$l = -11 \rightarrow 12$
3066 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
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.1146P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.003$
3066 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
227 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.84586 (13)	1.01263 (17)	−0.0443 (2)	0.0773 (5)
H1	0.8430	0.9388	−0.0814	0.093*
C2	0.90293 (14)	1.09809 (18)	−0.07041 (19)	0.0812 (5)
H2	0.9379	1.0814	−0.1255	0.097*
C3	0.90851 (13)	1.20709 (18)	−0.0161 (2)	0.0848 (6)
H3	0.9460	1.2650	−0.0351	0.102*
C4	0.85805 (13)	1.22952 (17)	0.0669 (2)	0.0845 (6)
H4	0.8625	1.3029	0.1055	0.101*
C5	0.80102 (12)	1.14601 (16)	0.09424 (19)	0.0739 (5)
H5	0.7677	1.1628	0.1514	0.089*
C6	0.79317 (12)	1.03656 (15)	0.03659 (17)	0.0650 (4)
C7	0.70449 (13)	0.84353 (15)	−0.01505 (18)	0.0730 (5)
H7	0.6890	0.8604	−0.1084	0.088*
C8	0.78013 (12)	0.75006 (14)	0.02456 (16)	0.0616 (4)
C9	0.77887 (13)	0.65943 (16)	−0.06012 (17)	0.0711 (5)
H9	0.7329	0.6593	−0.1426	0.085*
C10	0.84354 (14)	0.56954 (17)	−0.0260 (2)	0.0791 (5)
H10	0.8420	0.5090	−0.0840	0.095*
C11	0.90948 (13)	0.57141 (17)	0.0943 (2)	0.0755 (5)
C12	0.91423 (13)	0.65768 (19)	0.18137 (19)	0.0817 (6)
H12	0.9604	0.6563	0.2636	0.098*
C13	0.84913 (14)	0.74803 (17)	0.14589 (17)	0.0756 (5)
H13	0.8519	0.8083	0.2047	0.091*
C14	0.61277 (13)	0.81138 (17)	0.0143 (2)	0.0825 (6)
H14A	0.5578	0.8123	−0.0647	0.099*
H14B	0.6180	0.7348	0.0545	0.099*
C15	0.60609 (11)	0.90527 (14)	0.10650 (16)	0.0612 (4)
C16	0.53417 (11)	0.91201 (14)	0.17113 (16)	0.0617 (4)
C17	0.46009 (12)	0.83265 (16)	0.14551 (19)	0.0753 (5)
H17	0.4552	0.7736	0.0846	0.090*
C18	0.39311 (12)	0.83949 (18)	0.2089 (2)	0.0812 (6)
H18	0.3444	0.7844	0.1900	0.097*
C19	0.39667 (12)	0.92547 (16)	0.29887 (19)	0.0737 (5)
C20	0.32370 (13)	0.9332 (2)	0.3669 (2)	0.0968 (7)
H20A	0.2669	0.8930	0.3163	0.145*
H20B	0.3091	1.0138	0.3764	0.145*
H20C	0.3484	0.8976	0.4516	0.145*
C21	0.47016 (14)	1.00439 (18)	0.3234 (2)	0.0862 (6)
H21	0.4746	1.0637	0.3838	0.103*
C22	0.53736 (13)	0.99869 (17)	0.2615 (2)	0.0810 (6)
H22	0.5859	1.0541	0.2808	0.097*
F1	0.97450 (8)	0.48320 (11)	0.13006 (15)	0.1102 (5)
N1	0.67233 (10)	0.98251 (12)	0.12690 (13)	0.0657 (4)
N2	0.73301 (11)	0.95237 (12)	0.06048 (16)	0.0777 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0876 (12)	0.0718 (11)	0.0851 (13)	0.0018 (9)	0.0454 (11)	0.0045 (10)
C2	0.0812 (12)	0.0913 (14)	0.0851 (13)	0.0026 (10)	0.0462 (10)	0.0124 (11)
C3	0.0767 (11)	0.0812 (13)	0.1082 (16)	−0.0091 (10)	0.0461 (11)	0.0126 (12)
C4	0.0788 (12)	0.0689 (11)	0.1175 (16)	−0.0094 (9)	0.0480 (12)	−0.0024 (11)
C5	0.0719 (10)	0.0672 (11)	0.0941 (13)	−0.0009 (9)	0.0430 (10)	0.0006 (10)
C6	0.0659 (9)	0.0604 (10)	0.0760 (11)	0.0025 (8)	0.0331 (9)	0.0074 (8)
C7	0.0870 (11)	0.0666 (11)	0.0736 (11)	−0.0032 (9)	0.0376 (9)	−0.0034 (9)
C8	0.0734 (10)	0.0604 (9)	0.0608 (10)	−0.0114 (8)	0.0354 (9)	−0.0045 (8)
C9	0.0782 (11)	0.0760 (11)	0.0635 (11)	−0.0098 (10)	0.0293 (9)	−0.0112 (9)
C10	0.0902 (13)	0.0680 (12)	0.0921 (14)	−0.0091 (10)	0.0476 (12)	−0.0156 (10)
C11	0.0734 (11)	0.0673 (11)	0.0992 (15)	−0.0039 (9)	0.0467 (11)	0.0090 (11)
C12	0.0800 (12)	0.0912 (14)	0.0733 (12)	−0.0115 (11)	0.0242 (10)	0.0079 (11)
C13	0.0938 (12)	0.0746 (12)	0.0628 (11)	−0.0103 (11)	0.0315 (10)	−0.0103 (9)
C14	0.0778 (11)	0.0760 (12)	0.0999 (14)	−0.0071 (9)	0.0377 (10)	−0.0111 (11)
C15	0.0616 (9)	0.0561 (9)	0.0644 (10)	0.0025 (8)	0.0187 (8)	0.0083 (8)
C16	0.0553 (9)	0.0582 (9)	0.0702 (11)	0.0039 (7)	0.0187 (8)	0.0115 (8)
C17	0.0630 (10)	0.0696 (11)	0.0913 (13)	−0.0031 (9)	0.0225 (9)	−0.0051 (10)
C18	0.0544 (9)	0.0796 (13)	0.1092 (15)	−0.0072 (9)	0.0261 (10)	0.0081 (12)
C19	0.0603 (10)	0.0727 (11)	0.0917 (13)	0.0054 (9)	0.0297 (9)	0.0128 (10)
C20	0.0713 (12)	0.1072 (16)	0.1243 (18)	−0.0014 (11)	0.0491 (12)	0.0124 (13)
C21	0.0844 (12)	0.0781 (12)	0.1126 (16)	−0.0115 (10)	0.0550 (12)	−0.0112 (11)
C22	0.0751 (11)	0.0708 (12)	0.1084 (15)	−0.0156 (9)	0.0454 (11)	−0.0075 (11)
F1	0.0939 (8)	0.0929 (8)	0.1555 (12)	0.0150 (7)	0.0567 (8)	0.0225 (8)
N1	0.0708 (9)	0.0589 (8)	0.0762 (9)	0.0022 (7)	0.0361 (7)	0.0072 (7)
N2	0.0917 (10)	0.0588 (8)	0.1033 (12)	−0.0085 (7)	0.0600 (9)	−0.0090 (8)

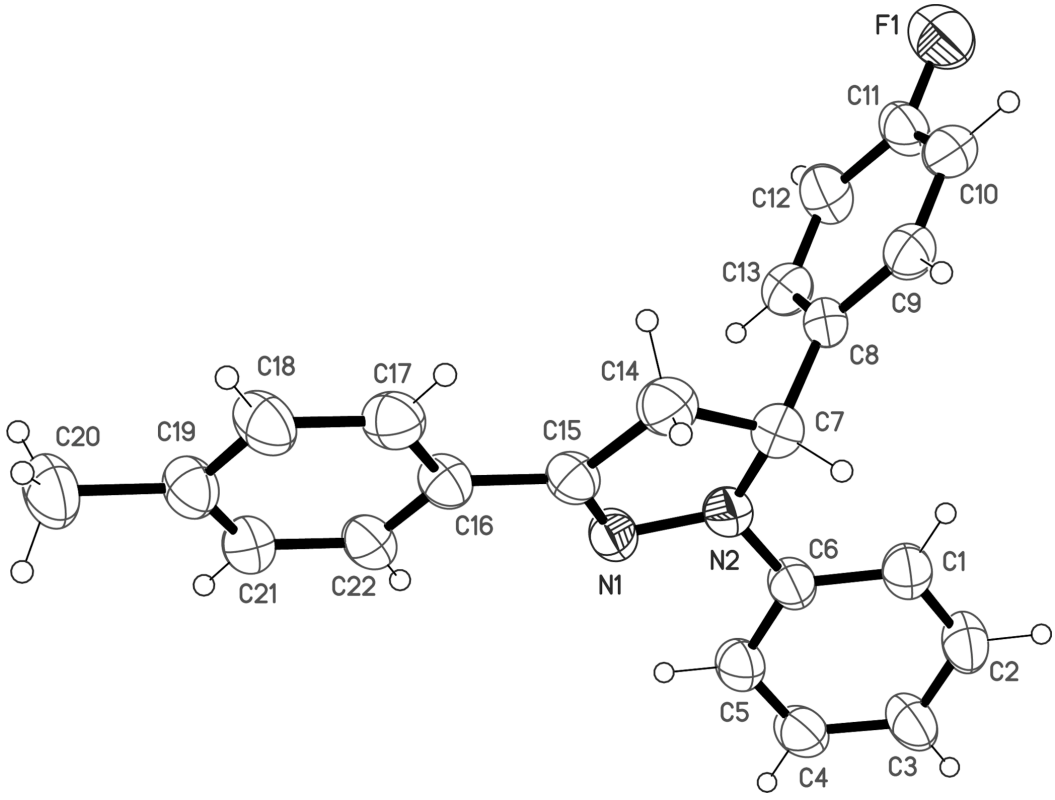
Geometric parameters (Å, °)

C1—C6	1.380 (2)	C12—C13	1.381 (3)
C1—C2	1.382 (3)	C12—H12	0.9300
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.369 (3)	C14—C15	1.492 (3)
C2—H2	0.9300	C14—H14A	0.9700
C3—C4	1.369 (3)	C14—H14B	0.9700
C3—H3	0.9300	C15—N1	1.2862 (19)
C4—C5	1.371 (2)	C15—C16	1.458 (2)
C4—H4	0.9300	C16—C17	1.382 (2)
C5—C6	1.386 (2)	C16—C22	1.383 (3)
C5—H5	0.9300	C17—C18	1.383 (3)
C6—N2	1.394 (2)	C17—H17	0.9300
C7—N2	1.473 (2)	C18—C19	1.373 (3)
C7—C8	1.507 (2)	C18—H18	0.9300
C7—C14	1.541 (2)	C19—C21	1.373 (3)
C7—H7	0.9800	C19—C20	1.500 (3)
C8—C13	1.377 (2)	C20—H20A	0.9600

C8—C9	1.380 (2)	C20—H20B	0.9600
C9—C10	1.372 (3)	C20—H20C	0.9600
C9—H9	0.9300	C21—C22	1.373 (3)
C10—C11	1.350 (3)	C21—H21	0.9300
C10—H10	0.9300	C22—H22	0.9300
C11—C12	1.350 (3)	N1—N2	1.3686 (19)
C11—F1	1.362 (2)		
C6—C1—C2	120.21 (18)	C8—C13—H13	119.6
C6—C1—H1	119.9	C12—C13—H13	119.6
C2—C1—H1	119.9	C15—C14—C7	102.92 (14)
C3—C2—C1	120.67 (18)	C15—C14—H14A	111.2
C3—C2—H2	119.7	C7—C14—H14A	111.2
C1—C2—H2	119.7	C15—C14—H14B	111.2
C2—C3—C4	118.92 (18)	C7—C14—H14B	111.2
C2—C3—H3	120.5	H14A—C14—H14B	109.1
C4—C3—H3	120.5	N1—C15—C16	121.38 (15)
C3—C4—C5	121.39 (19)	N1—C15—C14	113.20 (15)
C3—C4—H4	119.3	C16—C15—C14	125.41 (15)
C5—C4—H4	119.3	C17—C16—C22	116.93 (16)
C4—C5—C6	119.85 (17)	C17—C16—C15	121.94 (16)
C4—C5—H5	120.1	C22—C16—C15	121.14 (15)
C6—C5—H5	120.1	C16—C17—C18	121.18 (18)
C1—C6—C5	118.91 (16)	C16—C17—H17	119.4
C1—C6—N2	120.82 (16)	C18—C17—H17	119.4
C5—C6—N2	120.27 (16)	C19—C18—C17	121.72 (17)
N2—C7—C8	112.84 (15)	C19—C18—H18	119.1
N2—C7—C14	101.54 (14)	C17—C18—H18	119.1
C8—C7—C14	113.54 (15)	C18—C19—C21	116.80 (17)
N2—C7—H7	109.6	C18—C19—C20	121.65 (17)
C8—C7—H7	109.6	C21—C19—C20	121.55 (19)
C14—C7—H7	109.6	C19—C20—H20A	109.5
C13—C8—C9	117.76 (17)	C19—C20—H20B	109.5
C13—C8—C7	122.44 (16)	H20A—C20—H20B	109.5
C9—C8—C7	119.74 (16)	C19—C20—H20C	109.5
C10—C9—C8	121.78 (17)	H20A—C20—H20C	109.5
C10—C9—H9	119.1	H20B—C20—H20C	109.5
C8—C9—H9	119.1	C22—C21—C19	122.22 (19)
C11—C10—C9	118.13 (18)	C22—C21—H21	118.9
C11—C10—H10	120.9	C19—C21—H21	118.9
C9—C10—H10	120.9	C21—C22—C16	121.15 (17)
C12—C11—C10	122.76 (19)	C21—C22—H22	119.4
C12—C11—F1	118.17 (19)	C16—C22—H22	119.4
C10—C11—F1	119.07 (19)	C15—N1—N2	109.60 (14)
C11—C12—C13	118.69 (18)	N1—N2—C6	119.76 (14)
C11—C12—H12	120.7	N1—N2—C7	112.66 (13)
C13—C12—H12	120.7	C6—N2—C7	124.43 (15)
C8—C13—C12	120.87 (18)		
C6—C1—C2—C3	0.4 (3)	N1—C15—C16—C17	176.97 (15)

C1—C2—C3—C4	1.3 (3)	C14—C15—C16—C17	−4.0 (3)
C2—C3—C4—C5	−1.3 (3)	N1—C15—C16—C22	−3.2 (2)
C3—C4—C5—C6	−0.5 (3)	C14—C15—C16—C22	175.91 (17)
C2—C1—C6—C5	−2.1 (3)	C22—C16—C17—C18	−0.7 (3)
C2—C1—C6—N2	177.96 (18)	C15—C16—C17—C18	179.21 (15)
C4—C5—C6—C1	2.2 (3)	C16—C17—C18—C19	0.5 (3)
C4—C5—C6—N2	−177.92 (17)	C17—C18—C19—C21	−0.2 (3)
N2—C7—C8—C13	23.6 (2)	C17—C18—C19—C20	179.66 (17)
C14—C7—C8—C13	−91.3 (2)	C18—C19—C21—C22	0.0 (3)
N2—C7—C8—C9	−159.53 (15)	C20—C19—C21—C22	−179.81 (19)
C14—C7—C8—C9	85.6 (2)	C19—C21—C22—C16	−0.2 (3)
C13—C8—C9—C10	0.1 (3)	C17—C16—C22—C21	0.5 (3)
C7—C8—C9—C10	−176.90 (16)	C15—C16—C22—C21	−179.36 (17)
C8—C9—C10—C11	0.1 (3)	C16—C15—N1—N2	176.66 (14)
C9—C10—C11—C12	−0.1 (3)	C14—C15—N1—N2	−2.50 (19)
C9—C10—C11—F1	−179.81 (15)	C15—N1—N2—C6	161.69 (15)
C10—C11—C12—C13	−0.2 (3)	C15—N1—N2—C7	0.88 (19)
F1—C11—C12—C13	179.52 (16)	C1—C6—N2—N1	−171.52 (16)
C9—C8—C13—C12	−0.4 (3)	C5—C6—N2—N1	8.6 (3)
C7—C8—C13—C12	176.52 (16)	C1—C6—N2—C7	−13.1 (3)
C11—C12—C13—C8	0.5 (3)	C5—C6—N2—C7	167.00 (16)
N2—C7—C14—C15	−2.16 (18)	C8—C7—N2—N1	−120.91 (15)
C8—C7—C14—C15	119.24 (16)	C14—C7—N2—N1	0.97 (19)
C7—C14—C15—N1	3.0 (2)	C8—C7—N2—C6	79.3 (2)
C7—C14—C15—C16	−176.13 (14)	C14—C7—N2—C6	−158.79 (16)

Fig. 1


F1
C11
C10
C12
C13
C9
C8
C14
C7
C18
C17
C15
C20
C19
C16
N2
C6
C1
N1
C21
C22
C2
C5
C3
C4