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3-(4-Chlorophenyl)-5-(4-fluorophenyl)-1-phenyl-2-pyrazoline

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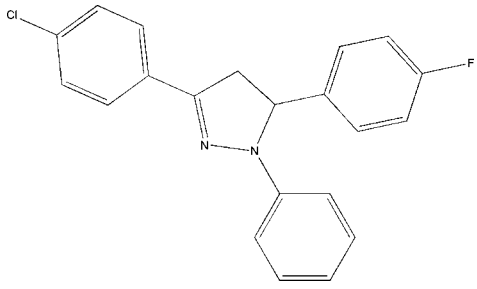
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.111; data-to-parameter ratio = 13.4.

In the title compound, $C_{21}H_{16}ClFN_2$, the pyrazoline ring forms dihedral angles of 14.88 (11)° with the phenyl ring, 74.59 (11)° with the fluorophenyl ring and 7.16 (10)° with the chlorophenyl ring.

Related literature

For related literature, see: Dhal *et al.* (1975); Fahrni *et al.* (2003); Foces-Foces, Jagerovic & Elguero (2001); Guo *et al.* (2006); Lombardino & Ottemes (1981); Rawal *et al.* (1963); Rurack *et al.* (2000); Wiley *et al.* (1958).



Experimental

Crystal data

$C_{21}H_{16}ClFN_2$
M_r = 350.81
Monoclinic, $P2_1/c$
a = 14.675 (3) Å
b = 11.271 (2) Å
c = 11.086 (2) Å
β = 109.818 (2)°
V = 1725.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 298 (2) K
0.48 × 0.47 × 0.23 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: none
7111 measured reflections
3044 independent reflections
2319 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.03
3044 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2131).

References

Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Versions 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Dhal, P. N., Acharya, T. E. & Nayak, A. (1975). *J. Indian Chem. Soc.* **52**, 1196–1200.
Fahrni, C. J., Yang, L. C. & VanDerveer, D. G. (2003). *J. Am. Chem. Soc.* **125**, 3799–3812.
Foces-Foces, C., Jagerovic, N. & Elguero, J. (2001). *Z. Kristallogr.* **216**, 240–244.
Guo, H.-M., Jian, F.-F., Zhou, L.-Y., Zhao, P.-S. & Zheng, J. (2006). *Acta Cryst.* E**62**, o4337–o4338.
Lombardino, G. & Ottemes, I. G. (1981). *J. Med. Chem.* **24**, 830–834.
Rawal, A. A., Thakor, V. M. & Shah, N. M. (1963). *J. Indian Chem. Soc.* **40**, 323–326.
Rurack, K., Bricks, J. L., Schulz, B., Maus, M., Reck, G. & Resch-Genger, U. (2000). *J. Phys. Chem. A*, **104**, 6171–6174.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wiley, R. H., Jarboe, C. H., Hayes, F. N., Hansbury, E., Nielsen, J. T., Callahan, P. X. & Sellars, M. (1958). *J. Org. Chem.* **23**, 732–738.

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supplementary materials

Acta Cryst. (2007). E**63**, o3318 [**doi:10.1107/S160053680703022X**]

3-(4-Chlorophenyl)-5-(4-fluorophenyl)-1-phenyl-2-pyrazoline

H.-M. Guo

Comment

As important and useful five-membered heterocyclic compounds, pyrazoline and its derivatives were found to possess anti-viral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Ottemes, 1981) activities. Several 1,3,5-triaryl-2-pyrazolines were also used as scintillation solutes (Wiley *et al.*, 1958).

In the structure of the title compound (Fig. 1), all of the bond lengths and angles fall in the normal range (Rurack *et al.*, 2000; Fahrni *et al.*, 2003; Guo, *et al.*, 2006; Foces-Foces *et al.*, 2001). The mean planes of the pyrazolinyl ring N1/N2/C7/C14/C15 and benzene ring C1—C6 and benzene ring C16—C21 and benzene ring C8—C13 make dihedral angles of 14.88 (11)°, 74.59 (11)° and 7.16 (10)°, respectively.

Experimental

1-(*p*-Chlorophenyl)-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 at reflux for 6 h. Then the mixture was poured into ice-water to afford yellow solids. The solids were filtered and washed with water until the pH of solution was about 7.0. Finally, the red solid crystals were 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

H atoms were fixed geometrically and allowed to ride on their parent atoms, C—H distances 0.93–0.96 Å, and with U_{iso} = 1.2–1.5U_{eq} of the parent atoms.

Figures

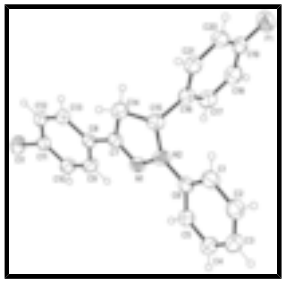


Fig. 1. The molecular structure and atom-labeling scheme with displacement ellipsoids drawn at the 30% probability level.

3-(4-Chlorophenyl)-5-(4-fluorophenyl)-1-phenyl-2-pyrazoline

Crystal data

$C_{21}H_{16}ClFN_2$	F_{000} = 728
M_r = 350.81	D_x = 1.351 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3206 reflections
a = 14.675 (3) Å	θ = 2.3–25.0º
b = 11.271 (2) Å	μ = 0.24 mm^{-1}
c = 11.086 (2) Å	T = 298 (2) K
β = 109.818 (2)º	Plate, yellow
V = 1725.0 (5) Å^3	0.48 × 0.47 × 0.23 mm
Z = 4	

Data collection

Bruker SMART 1000 diffractometer	2319 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.020
Monochromator: graphite	θ_{max} = 25.0º
T = 298(2) K	θ_{min} = 2.3º
φ and ω scans	h = −17→14
Absorption correction: none	k = −13→11
7111 measured reflections	l = −13→13
3044 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.3475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.111	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
3044 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
227 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: 0.0162 (16)
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	0.16149 (15)	1.01229 (18)	0.5524 (2)	0.0695 (5)
H1	0.1676	0.9390	0.5928	0.083*
C2	0.10157 (15)	1.0974 (2)	0.5741 (2)	0.0761 (6)
H2	0.0678	1.0812	0.6297	0.091*
C3	0.09107 (16)	1.2057 (2)	0.5150 (2)	0.0802 (6)
H3	0.0513	1.2634	0.5309	0.096*
C4	0.14050 (15)	1.2278 (2)	0.4311 (2)	0.0764 (6)
H4	0.1330	1.3007	0.3894	0.092*
C5	0.20035 (13)	1.14404 (17)	0.4084 (2)	0.0657 (5)
H5	0.2327	1.1600	0.3511	0.079*
C6	0.21268 (13)	1.03529 (16)	0.47079 (18)	0.0589 (5)
C7	0.40002 (13)	0.89975 (15)	0.39970 (17)	0.0555 (4)
C8	0.46938 (12)	0.90608 (15)	0.33153 (17)	0.0536 (4)
C9	0.45956 (14)	0.99101 (18)	0.2369 (2)	0.0647 (5)
H9	0.4078	1.0438	0.2166	0.078*
C10	0.52438 (15)	0.99847 (18)	0.1732 (2)	0.0672 (5)
H10	0.5169	1.0563	0.1107	0.081*
C11	0.60067 (13)	0.92043 (17)	0.20149 (19)	0.0615 (5)
C12	0.61265 (13)	0.83497 (18)	0.2935 (2)	0.0660 (5)
H12	0.6643	0.7821	0.3122	0.079*
C13	0.54739 (13)	0.82807 (16)	0.35827 (19)	0.0619 (5)
H13	0.5556	0.7703	0.4209	0.074*
C14	0.39643 (14)	0.80659 (18)	0.4945 (2)	0.0707 (6)
H14A	0.4533	0.8101	0.5713	0.085*
H14B	0.3913	0.7278	0.4577	0.085*
C15	0.30424 (14)	0.83989 (17)	0.52346 (19)	0.0645 (5)
H15	0.3206	0.8545	0.6155	0.077*
C16	0.22526 (13)	0.74734 (16)	0.48031 (17)	0.0543 (4)
C17	0.15803 (16)	0.74724 (19)	0.35858 (19)	0.0694 (5)
H17	0.1586	0.8079	0.3020	0.083*
C18	0.08956 (15)	0.6581 (2)	0.3194 (2)	0.0772 (6)
H18	0.0443	0.6582	0.2369	0.093*
C19	0.08968 (15)	0.57080 (18)	0.4032 (2)	0.0705 (6)

C20	0.15420 (16)	0.56749 (18)	0.5242 (2)	0.0722 (6)
H20	0.1526	0.5066	0.5801	0.087*
C21	0.22215 (14)	0.65665 (17)	0.56219 (19)	0.0629 (5)
H21	0.2669	0.6556	0.6450	0.076*
Cl1	0.68197 (4)	0.93159 (6)	0.11870 (6)	0.0864 (2)
F1	0.02159 (10)	0.48410 (12)	0.36443 (17)	0.1071 (5)
N1	0.33374 (11)	0.97931 (13)	0.38178 (15)	0.0591 (4)
N2	0.27689 (12)	0.95195 (14)	0.45308 (18)	0.0706 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0769 (13)	0.0621 (12)	0.0773 (14)	−0.0086 (10)	0.0365 (11)	−0.0067 (10)
C2	0.0720 (13)	0.0861 (16)	0.0797 (15)	−0.0070 (11)	0.0383 (12)	−0.0169 (12)
C3	0.0695 (13)	0.0755 (15)	0.1011 (17)	0.0093 (11)	0.0359 (13)	−0.0130 (13)
C4	0.0676 (13)	0.0669 (13)	0.0992 (17)	0.0087 (10)	0.0342 (12)	0.0036 (11)
C5	0.0599 (11)	0.0627 (12)	0.0792 (14)	−0.0012 (9)	0.0298 (10)	−0.0011 (10)
C6	0.0572 (10)	0.0545 (11)	0.0680 (12)	−0.0062 (8)	0.0249 (9)	−0.0094 (9)
C7	0.0544 (10)	0.0519 (10)	0.0564 (11)	−0.0036 (8)	0.0138 (8)	−0.0067 (8)
C8	0.0488 (9)	0.0511 (10)	0.0563 (10)	−0.0045 (8)	0.0117 (8)	−0.0077 (8)
C9	0.0606 (11)	0.0622 (12)	0.0727 (13)	0.0122 (9)	0.0244 (10)	0.0037 (10)
C10	0.0691 (12)	0.0646 (12)	0.0726 (13)	0.0062 (10)	0.0301 (10)	0.0064 (10)
C11	0.0521 (10)	0.0639 (12)	0.0673 (12)	−0.0030 (9)	0.0186 (9)	−0.0095 (10)
C12	0.0476 (10)	0.0629 (12)	0.0828 (14)	0.0039 (9)	0.0162 (10)	−0.0053 (10)
C13	0.0543 (10)	0.0564 (11)	0.0702 (12)	0.0003 (9)	0.0149 (9)	0.0018 (9)
C14	0.0655 (12)	0.0653 (12)	0.0826 (14)	0.0041 (10)	0.0267 (11)	0.0095 (10)
C15	0.0737 (12)	0.0590 (11)	0.0644 (12)	−0.0008 (10)	0.0281 (10)	0.0020 (9)
C16	0.0621 (11)	0.0526 (10)	0.0534 (11)	0.0058 (8)	0.0261 (9)	0.0030 (8)
C17	0.0821 (13)	0.0694 (12)	0.0580 (12)	0.0037 (11)	0.0253 (11)	0.0081 (10)
C18	0.0697 (13)	0.0881 (16)	0.0673 (13)	0.0072 (12)	0.0146 (11)	−0.0094 (12)
C19	0.0580 (11)	0.0613 (12)	0.1002 (17)	−0.0005 (10)	0.0375 (12)	−0.0121 (12)
C20	0.0762 (13)	0.0593 (12)	0.0931 (17)	0.0044 (11)	0.0444 (13)	0.0142 (11)
C21	0.0656 (11)	0.0675 (12)	0.0584 (11)	0.0066 (10)	0.0245 (9)	0.0102 (9)
Cl1	0.0664 (3)	0.1100 (5)	0.0926 (4)	0.0053 (3)	0.0396 (3)	−0.0006 (3)
F1	0.0793 (8)	0.0874 (9)	0.1598 (14)	−0.0181 (7)	0.0471 (9)	−0.0274 (9)
N1	0.0639 (9)	0.0518 (9)	0.0673 (10)	−0.0021 (7)	0.0295 (8)	−0.0041 (7)
N2	0.0801 (11)	0.0528 (9)	0.0963 (13)	0.0052 (8)	0.0525 (10)	0.0086 (8)

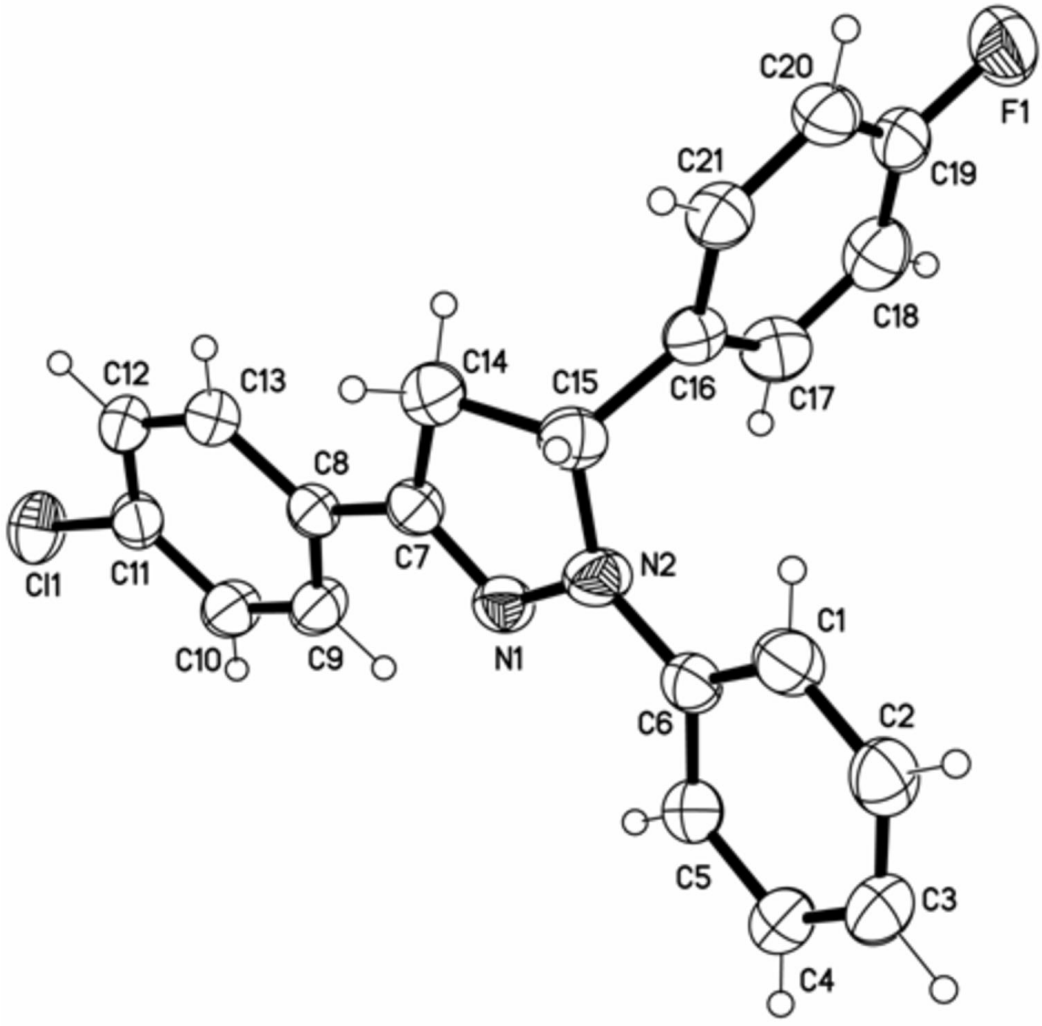
Geometric parameters (Å, °)

C1—C2	1.377 (3)	C11—Cl1	1.739 (2)
C1—C6	1.382 (3)	C12—C13	1.380 (3)
C1—H1	0.9300	C12—H12	0.9300
C2—C3	1.370 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.539 (3)
C3—C4	1.382 (3)	C14—H14A	0.9700
C3—H3	0.9300	C14—H14B	0.9700
C4—C5	1.370 (3)	C15—N2	1.467 (2)
C4—H4	0.9300	C15—C16	1.511 (3)

C5—C6	1.389 (3)	C15—H15	0.9800
C5—H5	0.9300	C16—C17	1.375 (3)
C6—N2	1.391 (2)	C16—C21	1.378 (3)
C7—N1	1.288 (2)	C17—C18	1.382 (3)
C7—C8	1.461 (3)	C17—H17	0.9300
C7—C14	1.499 (3)	C18—C19	1.353 (3)
C8—C9	1.391 (3)	C18—H18	0.9300
C8—C13	1.393 (2)	C19—C20	1.355 (3)
C9—C10	1.366 (3)	C19—F1	1.359 (2)
C9—H9	0.9300	C20—C21	1.377 (3)
C10—C11	1.374 (3)	C20—H20	0.9300
C10—H10	0.9300	C21—H21	0.9300
C11—C12	1.370 (3)	N1—N2	1.365 (2)
C2—C1—C6	120.3 (2)	C12—C13—H13	119.4
C2—C1—H1	119.8	C8—C13—H13	119.4
C6—C1—H1	119.8	C7—C14—C15	102.57 (15)
C3—C2—C1	120.8 (2)	C7—C14—H14A	111.3
C3—C2—H2	119.6	C15—C14—H14A	111.3
C1—C2—H2	119.6	C7—C14—H14B	111.3
C2—C3—C4	118.9 (2)	C15—C14—H14B	111.3
C2—C3—H3	120.5	H14A—C14—H14B	109.2
C4—C3—H3	120.5	N2—C15—C16	112.56 (16)
C5—C4—C3	121.0 (2)	N2—C15—C14	101.57 (15)
C5—C4—H4	119.5	C16—C15—C14	113.56 (16)
C3—C4—H4	119.5	N2—C15—H15	109.6
C4—C5—C6	120.00 (19)	C16—C15—H15	109.6
C4—C5—H5	120.0	C14—C15—H15	109.6
C6—C5—H5	120.0	C17—C16—C21	118.21 (18)
C1—C6—C5	118.92 (18)	C17—C16—C15	121.95 (17)
C1—C6—N2	120.68 (18)	C21—C16—C15	119.77 (17)
C5—C6—N2	120.38 (17)	C16—C17—C18	120.82 (19)
N1—C7—C8	120.56 (17)	C16—C17—H17	119.6
N1—C7—C14	113.05 (16)	C18—C17—H17	119.6
C8—C7—C14	126.39 (16)	C19—C18—C17	118.7 (2)
C9—C8—C13	117.54 (17)	C19—C18—H18	120.6
C9—C8—C7	120.77 (16)	C17—C18—H18	120.6
C13—C8—C7	121.69 (17)	C18—C19—C20	122.5 (2)
C10—C9—C8	121.34 (18)	C18—C19—F1	118.4 (2)
C10—C9—H9	119.3	C20—C19—F1	119.0 (2)
C8—C9—H9	119.3	C19—C20—C21	118.23 (19)
C9—C10—C11	119.90 (19)	C19—C20—H20	120.9
C9—C10—H10	120.0	C21—C20—H20	120.9
C11—C10—H10	120.0	C20—C21—C16	121.48 (19)
C12—C11—C10	120.61 (18)	C20—C21—H21	119.3
C12—C11—Cl1	120.39 (15)	C16—C21—H21	119.3
C10—C11—Cl1	118.99 (16)	C7—N1—N2	109.35 (15)
C11—C12—C13	119.36 (18)	N1—N2—C6	120.37 (15)
C11—C12—H12	120.3	N1—N2—C15	113.06 (14)
C13—C12—H12	120.3	C6—N2—C15	125.63 (16)

C12—C13—C8	121.25 (18)		
C6—C1—C2—C3	0.4 (3)	N2—C15—C16—C17	26.7 (2)
C1—C2—C3—C4	1.0 (3)	C14—C15—C16—C17	−88.0 (2)
C2—C3—C4—C5	−1.0 (3)	N2—C15—C16—C21	−156.32 (16)
C3—C4—C5—C6	−0.5 (3)	C14—C15—C16—C21	89.0 (2)
C2—C1—C6—C5	−1.9 (3)	C21—C16—C17—C18	−0.4 (3)
C2—C1—C6—N2	176.89 (19)	C15—C16—C17—C18	176.66 (18)
C4—C5—C6—C1	2.0 (3)	C16—C17—C18—C19	0.1 (3)
C4—C5—C6—N2	−176.86 (19)	C17—C18—C19—C20	0.2 (3)
N1—C7—C8—C9	−6.4 (3)	C17—C18—C19—F1	179.38 (17)
C14—C7—C8—C9	174.00 (18)	C18—C19—C20—C21	−0.2 (3)
N1—C7—C8—C13	173.63 (16)	F1—C19—C20—C21	−179.45 (16)
C14—C7—C8—C13	−6.0 (3)	C19—C20—C21—C16	0.0 (3)
C13—C8—C9—C10	−0.5 (3)	C17—C16—C21—C20	0.3 (3)
C7—C8—C9—C10	179.47 (17)	C15—C16—C21—C20	−176.80 (17)
C8—C9—C10—C11	0.5 (3)	C8—C7—N1—N2	178.28 (15)
C9—C10—C11—C12	−0.1 (3)	C14—C7—N1—N2	−2.0 (2)
C9—C10—C11—Cl1	179.85 (16)	C7—N1—N2—C6	167.07 (17)
C10—C11—C12—C13	−0.2 (3)	C7—N1—N2—C15	−2.5 (2)
Cl1—C11—C12—C13	179.79 (15)	C1—C6—N2—N1	−173.95 (17)
C11—C12—C13—C8	0.2 (3)	C5—C6—N2—N1	4.9 (3)
C9—C8—C13—C12	0.2 (3)	C1—C6—N2—C15	−5.8 (3)
C7—C8—C13—C12	−179.84 (17)	C5—C6—N2—C15	173.00 (18)
N1—C7—C14—C15	5.3 (2)	C16—C15—N2—N1	−116.27 (17)
C8—C7—C14—C15	−175.02 (16)	C14—C15—N2—N1	5.5 (2)
C7—C14—C15—N2	−5.97 (19)	C16—C15—N2—C6	74.8 (2)
C7—C14—C15—C16	115.13 (18)	C14—C15—N2—C6	−163.37 (19)

Fig. 1


C20
F1
C21
C19
C18
C12
C13
C14
C15
C16
C17
C8
C7
N2
Cl1
C11
C1
C10
C9
N1
C6
C2
C5
C3
C4