Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-(*p*-Fluorophenyl)-1,3-diphenyl-2-pyrazoline

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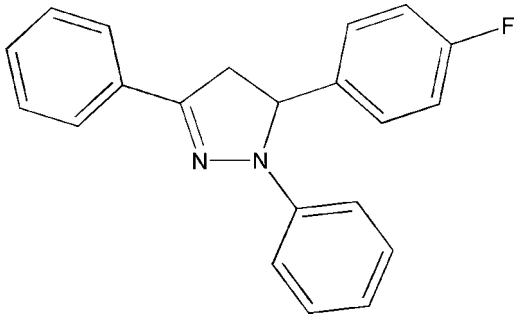
Received 31 May 2007; accepted 1 June 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.101; data-to-parameter ratio = 13.6.

The title compound, $C_{21}H_{17}FN_2$, was prepared from phenylhydrazine and 1-phenyl-3-(*p*-fluorophenyl)-2-propenyl-1-ketone. The pyrazolinyl ring forms dihedral angles of 11.87 (12), 8.30 (12) and 65.89 (12)° with phenyl rings at the 1 and 3 positions and the fluorophenyl ring, respectively.

Related literature

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



Experimental

Crystal data

$C_{21}H_{17}FN_2$
M_r = 316.37
Monoclinic, $P2_1/c$
a = 11.476 (5) Å
b = 13.389 (5) Å
c = 11.774 (4) Å
β = 111.653 (6)°
V = 1681.4 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.982, T_{max} = 0.989
7071 measured reflections
2958 independent reflections
1473 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.101
S = 1.02
2958 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 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*.

The authors thank the Natural Science Foundation of Shandong Province (grant No. Y2005B04) and the Doctoral Fund of Qingdao University of Science and Technology.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2315).

References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. 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. & Van Derveer, D. G. (2003). *J. Am. Chem. Soc.* **125**, 3799–3812.
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.
Orzeszka, A., Kaminsaka, B., Orzesko, G. & Stareerciak, J. (2000). *Farmaco*, **55**, 619–623.
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.

  doi:10.1107/S1600536807026840

supplementary materials

Acta Cryst. (2007). E**63**, o3280 [**doi:10.1107/S1600536807026840**]

5-(*p*-Fluorophenyl)-1,3-diphenyl-2-pyrazoline

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Comment

As important and useful five-membered heterocyclic compounds, pyrazoline and its derivatives were found to possess antiviral (Rawal *et al.* 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino *et al.*,1981) activities. Several 1,3,5-triaryl-2-pyrazolines were also used as scintillation solutes (Wiley *et al.*,1958). Here, we report the crystal strucutre of the title compound (I).

In the structure of (I) (Fig. 1), all of the bond lengths and bond angles fall in the normal range (Rurack *et al.*, 2000; Fahrni *et al.*, 2003; Guo *et al.*, 2006). The mean plane of pyrazolinyl ring N1/N2/C7—C9 make dihedral angles of 11.87 (12), 8.30 (12) and 65.89 (12)°, with the benzene rings C16—C21, C1—C6 and C10—C15 respectively.

Experimental

1-Phenyl-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 red solid crystals were dried 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 = 0.93–0.98 Å, and with U_{iso}=1.2–1.5U_{eq} of the parent atoms.

Figures

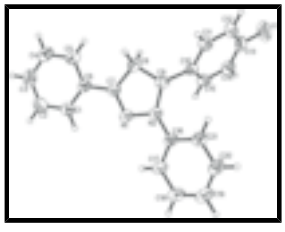


Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

5-(*p*-Fluorophenyl)-1,3-diphenyl-2-pyrazoline

Crystal data

$C_{21}H_{17}FN_2$ F_{000} = 664

M_r = 316.37	D_x = 1.250 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1142 reflections
a = 11.476 (5) Å	θ = 2.4–20.0º
b = 13.389 (5) Å	μ = 0.08 mm^{-1}
c = 11.774 (4) Å	T = 294 (2) K
β = 111.653 (6)º	Bar, yellow
V = 1681.4 (11) Å^3	0.22 × 0.20 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2958 independent reflections
Radiation source: fine-focus sealed tube	1473 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −13→13
T_{min} = 0.982, T_{max} = 0.989	k = −7→15
7071 measured reflections	l = −14→10

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.101	$(\Delta/\sigma)_{max} < 0.001$
S = 1.02	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
2958 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
218 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0084 (9)
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}
F1	0.10006 (15)	0.46529 (10)	0.77127 (14)	0.1173 (6)
N1	0.29414 (16)	−0.06861 (13)	0.87003 (15)	0.0592 (5)
N2	0.33402 (16)	0.02657 (13)	0.85440 (15)	0.0621 (5)
C1	0.2031 (2)	−0.24652 (19)	0.9413 (2)	0.0727 (7)
H1	0.2442	−0.2529	0.8868	0.087*
C2	0.1559 (3)	−0.3302 (2)	0.9768 (3)	0.0946 (9)
H2	0.1651	−0.3925	0.9461	0.113*
C3	0.0953 (2)	−0.3221 (2)	1.0573 (3)	0.0904 (8)
H3	0.0643	−0.3789	1.0819	0.108*
C4	0.0806 (2)	−0.2304 (2)	1.1013 (2)	0.0783 (7)
H4	0.0383	−0.2245	1.1548	0.094*
C5	0.1288 (2)	−0.14629 (18)	1.06592 (19)	0.0643 (6)
H5	0.1196	−0.0841	1.0968	0.077*
C6	0.19058 (19)	−0.15360 (17)	0.98517 (18)	0.0534 (6)
C7	0.24386 (19)	−0.06540 (16)	0.95107 (18)	0.0522 (6)
C8	0.2448 (2)	0.03719 (15)	1.00217 (19)	0.0651 (6)
H8A	0.2823	0.0368	1.0907	0.078*
H8B	0.1607	0.0643	0.9769	0.078*
C9	0.3251 (2)	0.09683 (15)	0.94696 (18)	0.0557 (6)
H9	0.4086	0.1076	1.0094	0.067*
C10	0.26740 (18)	0.19610 (15)	0.89596 (19)	0.0485 (5)
C11	0.2857 (2)	0.27606 (18)	0.9737 (2)	0.0626 (6)
H11	0.3369	0.2688	1.0555	0.075*
C12	0.2297 (2)	0.36675 (18)	0.9326 (3)	0.0768 (7)
H12	0.2416	0.4205	0.9857	0.092*
C13	0.1567 (2)	0.37566 (19)	0.8128 (3)	0.0705 (7)
C14	0.1370 (2)	0.2999 (2)	0.7326 (2)	0.0673 (7)
H14	0.0870	0.3085	0.6507	0.081*
C15	0.1930 (2)	0.20892 (16)	0.7753 (2)	0.0597 (6)
H15	0.1801	0.1556	0.7213	0.072*
C16	0.41798 (19)	0.03619 (17)	0.79499 (18)	0.0553 (6)
C17	0.4340 (2)	−0.04195 (18)	0.72432 (19)	0.0665 (6)
H17	0.3910	−0.1017	0.7191	0.080*
C18	0.5140 (2)	−0.0304 (2)	0.6621 (2)	0.0785 (7)
H18	0.5244	−0.0828	0.6149	0.094*
C19	0.5786 (2)	0.0571 (2)	0.6685 (2)	0.0803 (8)
H19	0.6327	0.0638	0.6265	0.096*
C20	0.5625 (2)	0.1340 (2)	0.7375 (2)	0.0722 (7)
H20	0.6055	0.1936	0.7417	0.087*
C21	0.4835 (2)	0.12442 (17)	0.80117 (19)	0.0629 (6)

H21	0.4740	0.1772	0.8483	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1337 (13)	0.0680 (10)	0.1532 (14)	0.0224 (9)	0.0564 (11)	0.0353 (9)
N1	0.0616 (12)	0.0649 (13)	0.0596 (12)	0.0006 (10)	0.0325 (10)	−0.0002 (10)
N2	0.0717 (13)	0.0592 (12)	0.0714 (13)	0.0028 (10)	0.0450 (11)	−0.0017 (10)
C1	0.0777 (17)	0.0666 (17)	0.0866 (18)	0.0077 (14)	0.0454 (14)	0.0027 (15)
C2	0.101 (2)	0.0677 (19)	0.131 (3)	0.0109 (16)	0.062 (2)	0.0078 (17)
C3	0.082 (2)	0.086 (2)	0.113 (2)	0.0033 (16)	0.0477 (18)	0.0298 (18)
C4	0.0665 (16)	0.105 (2)	0.0722 (18)	−0.0017 (17)	0.0361 (14)	0.0099 (17)
C5	0.0588 (15)	0.0812 (18)	0.0568 (15)	−0.0060 (13)	0.0260 (13)	−0.0024 (13)
C6	0.0482 (13)	0.0652 (16)	0.0483 (14)	0.0054 (12)	0.0195 (11)	0.0047 (12)
C7	0.0497 (13)	0.0618 (16)	0.0462 (14)	0.0077 (12)	0.0190 (11)	0.0014 (12)
C8	0.0764 (16)	0.0677 (16)	0.0607 (15)	0.0142 (13)	0.0363 (13)	0.0108 (12)
C9	0.0563 (14)	0.0638 (15)	0.0474 (13)	0.0064 (12)	0.0197 (11)	−0.0004 (12)
C10	0.0442 (12)	0.0570 (15)	0.0443 (14)	−0.0027 (11)	0.0166 (11)	−0.0015 (12)
C11	0.0667 (15)	0.0632 (16)	0.0565 (15)	−0.0087 (13)	0.0210 (12)	−0.0052 (14)
C12	0.094 (2)	0.0542 (18)	0.088 (2)	−0.0121 (15)	0.0406 (17)	−0.0085 (15)
C13	0.0725 (18)	0.0514 (18)	0.095 (2)	0.0055 (14)	0.0396 (17)	0.0217 (17)
C14	0.0584 (15)	0.0815 (19)	0.0596 (17)	0.0032 (14)	0.0188 (13)	0.0134 (16)
C15	0.0573 (14)	0.0686 (17)	0.0514 (16)	0.0008 (13)	0.0179 (12)	−0.0053 (12)
C16	0.0490 (14)	0.0703 (17)	0.0505 (14)	0.0131 (13)	0.0228 (12)	0.0117 (12)
C17	0.0650 (16)	0.0815 (17)	0.0618 (15)	0.0022 (13)	0.0338 (13)	−0.0002 (13)
C18	0.0783 (18)	0.101 (2)	0.0682 (17)	0.0033 (16)	0.0412 (15)	−0.0076 (15)
C19	0.0631 (17)	0.118 (2)	0.0707 (18)	0.0049 (17)	0.0369 (14)	0.0097 (17)
C20	0.0483 (15)	0.094 (2)	0.0768 (18)	0.0042 (14)	0.0261 (14)	0.0210 (15)
C21	0.0526 (15)	0.0739 (18)	0.0638 (16)	0.0085 (13)	0.0233 (12)	0.0097 (12)

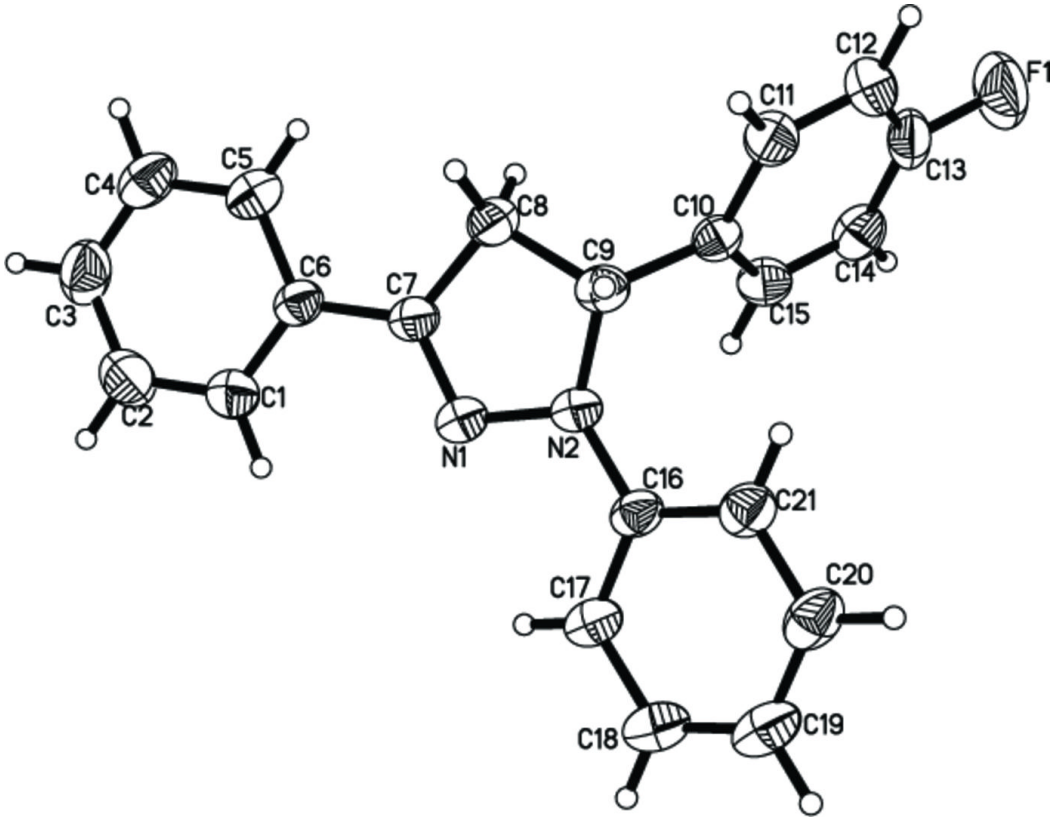
Geometric parameters (Å, °)

F1—C13	1.367 (2)	C9—H9	0.9800
N1—C7	1.285 (2)	C10—C15	1.372 (2)
N1—N2	1.389 (2)	C10—C11	1.373 (3)
N2—C16	1.390 (2)	C11—C12	1.376 (3)
N2—C9	1.472 (2)	C11—H11	0.9300
C1—C6	1.375 (3)	C12—C13	1.354 (3)
C1—C2	1.375 (3)	C12—H12	0.9300
C1—H1	0.9300	C13—C14	1.347 (3)
C2—C3	1.372 (3)	C14—C15	1.382 (3)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.367 (3)	C15—H15	0.9300
C3—H3	0.9300	C16—C21	1.387 (3)
C4—C5	1.385 (3)	C16—C17	1.391 (3)
C4—H4	0.9300	C17—C18	1.378 (3)
C5—C6	1.383 (3)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.373 (3)
C6—C7	1.453 (3)	C18—H18	0.9300

C7—C8	1.498 (2)	C19—C20	1.366 (3)
C8—C9	1.533 (3)	C19—H19	0.9300
C8—H8A	0.9700	C20—C21	1.379 (3)
C8—H8B	0.9700	C20—H20	0.9300
C9—C10	1.507 (3)	C21—H21	0.9300
C7—N1—N2	109.14 (17)	C15—C10—C11	118.4 (2)
N1—N2—C16	118.38 (18)	C15—C10—C9	122.46 (19)
N1—N2—C9	111.83 (16)	C11—C10—C9	119.0 (2)
C16—N2—C9	124.35 (19)	C10—C11—C12	121.2 (2)
C6—C1—C2	121.1 (2)	C10—C11—H11	119.4
C6—C1—H1	119.5	C12—C11—H11	119.4
C2—C1—H1	119.5	C13—C12—C11	118.2 (2)
C3—C2—C1	120.2 (3)	C13—C12—H12	120.9
C3—C2—H2	119.9	C11—C12—H12	120.9
C1—C2—H2	119.9	C14—C13—C12	122.9 (2)
C4—C3—C2	119.9 (2)	C14—C13—F1	118.4 (3)
C4—C3—H3	120.1	C12—C13—F1	118.7 (3)
C2—C3—H3	120.1	C13—C14—C15	118.3 (2)
C3—C4—C5	119.8 (2)	C13—C14—H14	120.9
C3—C4—H4	120.1	C15—C14—H14	120.9
C5—C4—H4	120.1	C10—C15—C14	121.0 (2)
C6—C5—C4	120.8 (2)	C10—C15—H15	119.5
C6—C5—H5	119.6	C14—C15—H15	119.5
C4—C5—H5	119.6	C21—C16—N2	121.0 (2)
C1—C6—C5	118.2 (2)	C21—C16—C17	118.9 (2)
C1—C6—C7	121.3 (2)	N2—C16—C17	120.0 (2)
C5—C6—C7	120.5 (2)	C18—C17—C16	119.6 (2)
N1—C7—C6	121.9 (2)	C18—C17—H17	120.2
N1—C7—C8	112.96 (19)	C16—C17—H17	120.2
C6—C7—C8	125.16 (19)	C19—C18—C17	121.2 (2)
C7—C8—C9	102.93 (17)	C19—C18—H18	119.4
C7—C8—H8A	111.2	C17—C18—H18	119.4
C9—C8—H8A	111.2	C20—C19—C18	119.1 (3)
C7—C8—H8B	111.2	C20—C19—H19	120.4
C9—C8—H8B	111.2	C18—C19—H19	120.4
H8A—C8—H8B	109.1	C19—C20—C21	120.9 (2)
N2—C9—C10	114.15 (16)	C19—C20—H20	119.5
N2—C9—C8	101.42 (16)	C21—C20—H20	119.5
C10—C9—C8	112.58 (17)	C20—C21—C16	120.2 (2)
N2—C9—H9	109.5	C20—C21—H21	119.9
C10—C9—H9	109.5	C16—C21—H21	119.9
C8—C9—H9	109.5		
C7—N1—N2—C16	164.09 (17)	C8—C9—C10—C15	−94.2 (2)
C7—N1—N2—C9	9.0 (2)	N2—C9—C10—C11	−161.80 (18)
C6—C1—C2—C3	−0.1 (4)	C8—C9—C10—C11	83.3 (2)
C1—C2—C3—C4	0.8 (4)	C15—C10—C11—C12	0.9 (3)
C2—C3—C4—C5	−1.1 (4)	C9—C10—C11—C12	−176.6 (2)
C3—C4—C5—C6	0.8 (3)	C10—C11—C12—C13	−0.7 (3)

C2—C1—C6—C5	−0.1 (3)	C11—C12—C13—C14	−0.1 (4)
C2—C1—C6—C7	178.0 (2)	C11—C12—C13—F1	179.6 (2)
C4—C5—C6—C1	−0.2 (3)	C12—C13—C14—C15	0.6 (3)
C4—C5—C6—C7	−178.33 (19)	F1—C13—C14—C15	−179.07 (19)
N2—N1—C7—C6	178.60 (17)	C11—C10—C15—C14	−0.4 (3)
N2—N1—C7—C8	−0.3 (2)	C9—C10—C15—C14	177.07 (19)
C1—C6—C7—N1	6.8 (3)	C13—C14—C15—C10	−0.4 (3)
C5—C6—C7—N1	−175.14 (19)	N1—N2—C16—C21	−164.84 (17)
C1—C6—C7—C8	−174.4 (2)	C9—N2—C16—C21	−13.1 (3)
C5—C6—C7—C8	3.6 (3)	N1—N2—C16—C17	17.6 (3)
N1—C7—C8—C9	−7.7 (2)	C9—N2—C16—C17	169.32 (18)
C6—C7—C8—C9	173.42 (18)	C21—C16—C17—C18	−0.1 (3)
N1—N2—C9—C10	−134.33 (17)	N2—C16—C17—C18	177.61 (18)
C16—N2—C9—C10	72.3 (2)	C16—C17—C18—C19	0.1 (3)
N1—N2—C9—C8	−13.0 (2)	C17—C18—C19—C20	−0.3 (4)
C16—N2—C9—C8	−166.37 (17)	C18—C19—C20—C21	0.6 (3)
C7—C8—C9—N2	11.62 (19)	C19—C20—C21—C16	−0.6 (3)
C7—C8—C9—C10	134.04 (18)	N2—C16—C21—C20	−177.35 (19)
N2—C9—C10—C15	20.8 (3)	C17—C16—C21—C20	0.3 (3)

Fig. 1


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