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

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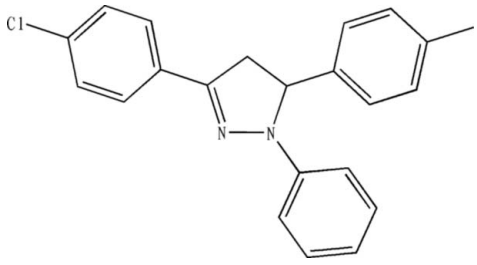
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.055; wR factor = 0.145; data-to-parameter ratio = 16.4.

The title compound, $C_{22}H_{19}ClN_2$, was prepared by the reaction of phenylhydrazine and 1-(4-chlorophenyl)-3-(4-methylphenyl)prop-2-en-1-one. The pyrazoline ring forms dihedral angles of 1.50 (5)° with the phenyl ring, 8.44 (2)° with the chlorophenyl ring and 80.07 (1)° with the tolyl ring.

Related literature

For related literature, see: Dhal *et al.* (1975); Fahrni *et al.* (2003); Ge (2006); Guo *et al.* (2006); Kimura *et al.* (1977); Lombardino & Ottemes (1981); Rawal *et al.* (1963); Rurack *et al.* (2000); Manna *et al.* (2002).



Experimental

Crystal data

$C_{22}H_{19}ClN_2$
M_r = 346.84
Monoclinic, $C2$
a = 23.614 (11) Å
b = 5.698 (3) Å
c = 14.232 (6) Å
β = 96.557 (8)°
V = 1902.6 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 294 (2) K
0.36 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.929, T_{max} = 0.960
5424 measured reflections
3715 independent reflections
2190 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.145
S = 0.98
3715 reflections
227 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 1575 Friedel Pairs
Flack parameter: −0.03 (10)

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: BT2344).

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supplementary materials

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

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Comment

Pyrazoline and its derivatives are important and useful five-membered heterocyclic compounds, which are 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 have been found to inhibit monoamine oxidases (Manna *et al.*, 2002). As part of our ongoing investgation of pyrazolines and their metal complexes, we report here the crystal structure of the title compound. In the structure of the title compound, all bond lengthes and bond angles fall in the normal range (Rurack *et al.*, 2000; Fahrni *et al.*, 2003; Ge, 2006; Guo *et al.*, 2006; Kimura *et al.*, 1977). The pyrazoline ring forms dihedral angles of 1.50 (5)° with the phenyl ring, 8.44 (2)° with the chlorophenyl ring and 80.07 (1)° with the tolyl ring.

Experimental

1-(4-chlorophenyl)-3-(4-methylphenyl)-2-propenyl-1-ketone (0.02 mol) and phenylhydrazine (0.02 mol) were mixed in acetic acid (40 ml) and stirred under reflux for 6 h. Then, the mixture was poured into ice-water to afford a light yellow solid which was filtrated and washed with water until the pH of the solution was about 7.0. Finally, the yellow solid was dry 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 geometrically positioned and allowed to ride on their parent atoms with C—H distances ranging from 0.93 to 0.96 Å, and with U_{iso}=1.2U_{eq}(C) or U_{iso}=1.5U_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip.

Figures

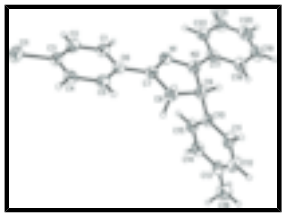


Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

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

Crystal data

$C_{22}H_{19}ClN_2$	F_{000} = 728
M_r = 346.84	D_x = 1.211 Mg m^{-3}

Monoclinic, *C*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 1354 reflections
a = 23.614 (11) Å	θ = 2.4–20.7º
b = 5.698 (3) Å	μ = 0.21 mm^{-1}
c = 14.232 (6) Å	*T* = 294 (2) K
β = 96.557 (8)º	Block, yellow
V = 1902.6 (15) $Å^3$	0.36 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3715 independent reflections
Radiation source: fine-focus sealed tube	2190 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
T = 294(2) K	θ_{max} = 26.5º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	*h* = −29→14
T_{min} = 0.929, T_{max} = 0.960	*k* = −7→7
5424 measured reflections	*l* = −14→17

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.055	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.145	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.98	$\Delta\rho_{max}$ = 0.16 e $Å^{-3}$
3715 reflections	$\Delta\rho_{min}$ = −0.22 e $Å^{-3}$
227 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1575 Friedel Pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.03 (10)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$sigma(F^2) is used only for calculat-

ing 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}
Cl1	0.73839 (4)	−0.3110 (2)	−0.21682 (6)	0.0832 (4)
N1	0.57116 (11)	−0.0088 (5)	0.12353 (18)	0.0557 (7)
N2	0.54873 (12)	−0.0243 (6)	0.2088 (2)	0.0673 (9)
C1	0.63565 (14)	−0.0426 (6)	−0.0378 (2)	0.0546 (9)
H1	0.6129	0.0899	−0.0347	0.066*
C2	0.66528 (15)	−0.0759 (7)	−0.1148 (2)	0.0584 (9)
H2	0.6622	0.0336	−0.1636	0.070*
C3	0.69960 (13)	−0.2719 (7)	−0.1199 (2)	0.0542 (9)
C4	0.70369 (13)	−0.4384 (6)	−0.0491 (2)	0.0549 (9)
H4	0.7262	−0.5709	−0.0534	0.066*
C5	0.67375 (13)	−0.4067 (6)	0.0290 (2)	0.0526 (8)
H5	0.6766	−0.5190	0.0768	0.063*
C6	0.63962 (13)	−0.2088 (6)	0.0365 (2)	0.0461 (8)
C7	0.60807 (13)	−0.1782 (6)	0.1194 (2)	0.0497 (8)
C8	0.61383 (13)	−0.3355 (7)	0.2059 (2)	0.0596 (9)
H8A	0.6533	−0.3478	0.2334	0.071*
H8B	0.5991	−0.4915	0.1906	0.071*
C9	0.57695 (13)	−0.2056 (7)	0.2740 (2)	0.0581 (9)
H9	0.5483	−0.3128	0.2943	0.070*
C10	0.61184 (14)	−0.0972 (6)	0.3604 (2)	0.0527 (9)
C11	0.61394 (16)	−0.1990 (7)	0.4492 (3)	0.0687 (10)
H11	0.5935	−0.3359	0.4568	0.082*
C12	0.64627 (17)	−0.0988 (8)	0.5272 (3)	0.0758 (12)
H12	0.6469	−0.1711	0.5859	0.091*
C13	0.67719 (14)	0.1039 (7)	0.5199 (3)	0.0641 (10)
C14	0.67548 (15)	0.2027 (8)	0.4303 (3)	0.0713 (10)
H14	0.6964	0.3383	0.4225	0.086*
C15	0.64357 (14)	0.1053 (7)	0.3523 (3)	0.0634 (10)
H15	0.6434	0.1768	0.2935	0.076*
C16	0.71137 (17)	0.2189 (10)	0.6050 (3)	0.0929 (13)
H16A	0.7087	0.1247	0.6603	0.139*
H16B	0.6963	0.3724	0.6146	0.139*
H16C	0.7506	0.2318	0.5938	0.139*
C17	0.50758 (12)	0.1382 (7)	0.2305 (2)	0.0576 (9)
C18	0.48671 (14)	0.1344 (9)	0.3186 (3)	0.0790 (12)
H18	0.4996	0.0222	0.3635	0.095*
C19	0.44610 (16)	0.3015 (10)	0.3387 (3)	0.0926 (15)
H19	0.4323	0.2994	0.3973	0.111*
C20	0.42645 (17)	0.4677 (9)	0.2732 (4)	0.0899 (14)
H20	0.3998	0.5783	0.2879	0.108*
C21	0.44620 (16)	0.4709 (9)	0.1856 (3)	0.0837 (13)
H21	0.4325	0.5828	0.1411	0.100*

C22	0.48642 (14)	0.3075 (8)	0.1636 (3)	0.0677 (10)
H22	0.4994	0.3103	0.1043	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0870 (6)	0.1050 (9)	0.0608 (6)	−0.0051 (7)	0.0219 (5)	−0.0197 (6)
N1	0.0523 (16)	0.0607 (19)	0.0538 (17)	0.0134 (15)	0.0050 (14)	0.0023 (15)
N2	0.0647 (18)	0.081 (2)	0.0590 (18)	0.0284 (18)	0.0186 (15)	0.0098 (18)
C1	0.062 (2)	0.047 (2)	0.055 (2)	0.0068 (18)	0.0068 (17)	0.0026 (18)
C2	0.073 (2)	0.052 (2)	0.049 (2)	−0.006 (2)	0.0048 (18)	0.0021 (18)
C3	0.0514 (18)	0.065 (2)	0.0471 (18)	−0.0036 (19)	0.0083 (15)	−0.0104 (19)
C4	0.0518 (19)	0.052 (2)	0.060 (2)	0.0076 (16)	0.0026 (17)	−0.0105 (19)
C5	0.0538 (17)	0.048 (2)	0.055 (2)	0.0078 (17)	0.0040 (16)	0.0055 (17)
C6	0.0452 (16)	0.0459 (19)	0.0458 (18)	0.0002 (16)	−0.0005 (14)	0.0012 (15)
C7	0.0474 (17)	0.050 (2)	0.0506 (19)	0.0046 (17)	0.0007 (15)	−0.0014 (17)
C8	0.0660 (19)	0.058 (2)	0.0562 (19)	0.009 (2)	0.0112 (16)	0.0097 (19)
C9	0.0570 (19)	0.058 (2)	0.061 (2)	0.0067 (18)	0.0129 (17)	0.010 (2)
C10	0.0565 (19)	0.050 (2)	0.055 (2)	0.0079 (16)	0.0212 (17)	0.0109 (17)
C11	0.092 (3)	0.055 (2)	0.063 (2)	−0.016 (2)	0.023 (2)	0.008 (2)
C12	0.104 (3)	0.073 (3)	0.052 (2)	−0.008 (3)	0.015 (2)	0.005 (2)
C13	0.066 (2)	0.060 (3)	0.069 (3)	0.001 (2)	0.0210 (19)	−0.005 (2)
C14	0.067 (2)	0.058 (2)	0.092 (3)	−0.003 (2)	0.021 (2)	0.012 (3)
C15	0.065 (2)	0.060 (2)	0.067 (2)	−0.006 (2)	0.0146 (19)	0.020 (2)
C16	0.100 (3)	0.091 (3)	0.086 (3)	−0.002 (3)	0.007 (2)	−0.017 (3)
C17	0.0423 (16)	0.065 (2)	0.065 (2)	0.0058 (18)	0.0028 (16)	−0.007 (2)
C18	0.062 (2)	0.099 (3)	0.080 (3)	0.011 (2)	0.026 (2)	−0.002 (3)
C19	0.062 (2)	0.126 (4)	0.095 (3)	0.010 (3)	0.031 (2)	−0.019 (3)
C20	0.062 (2)	0.096 (4)	0.113 (4)	0.025 (3)	0.011 (3)	−0.021 (3)
C21	0.066 (2)	0.090 (3)	0.093 (3)	0.025 (2)	0.000 (2)	−0.016 (3)
C22	0.0519 (19)	0.081 (3)	0.067 (2)	0.011 (2)	−0.0046 (18)	−0.013 (2)

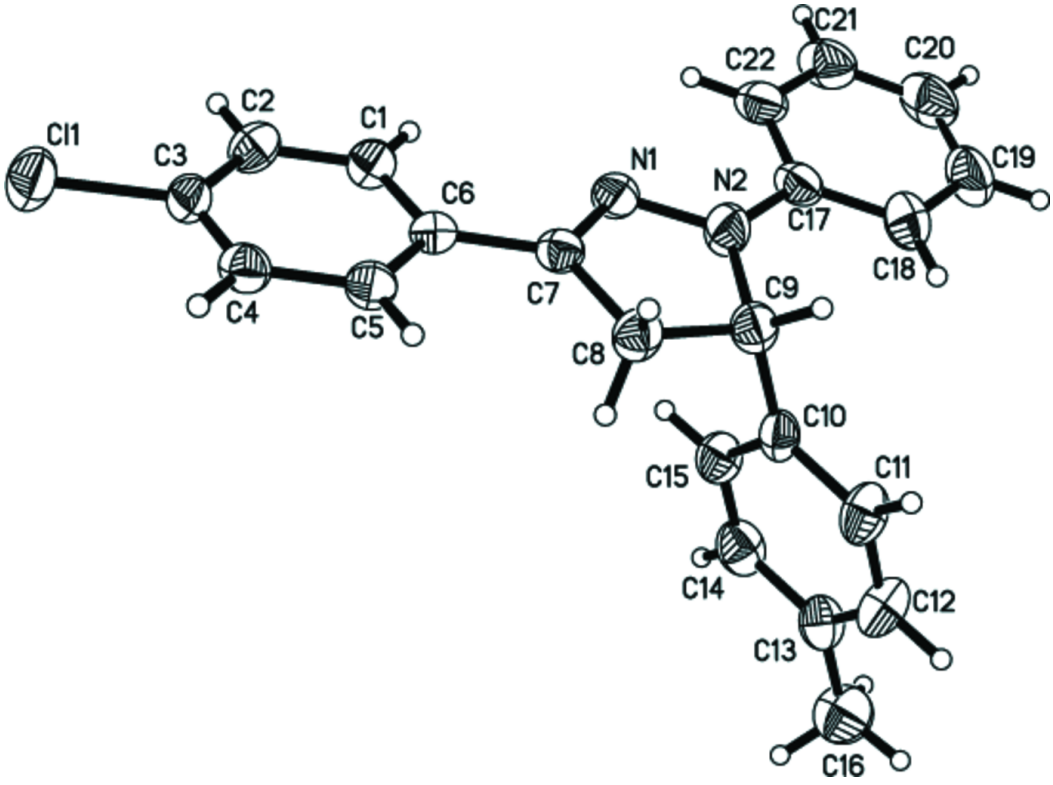
Geometric parameters (Å, °)

Cl1—C3	1.755 (3)	C11—C12	1.396 (5)
N1—C7	1.306 (4)	C11—H11	0.9300
N1—N2	1.382 (4)	C12—C13	1.377 (5)
N2—C17	1.402 (4)	C12—H12	0.9300
N2—C9	1.493 (4)	C13—C14	1.390 (5)
C1—C2	1.379 (4)	C13—C16	1.525 (5)
C1—C6	1.415 (4)	C14—C15	1.384 (5)
C1—H1	0.9300	C14—H14	0.9300
C2—C3	1.387 (5)	C15—H15	0.9300
C2—H2	0.9300	C16—H16A	0.9600
C3—C4	1.379 (5)	C16—H16B	0.9600
C4—C5	1.396 (4)	C16—H16C	0.9600
C4—H4	0.9300	C17—C18	1.399 (5)
C5—C6	1.398 (4)	C17—C22	1.407 (5)
C5—H5	0.9300	C18—C19	1.404 (6)

C6—C7	1.476 (4)	C18—H18	0.9300
C7—C8	1.517 (4)	C19—C20	1.372 (7)
C8—C9	1.561 (4)	C19—H19	0.9300
C8—H8A	0.9700	C20—C21	1.380 (6)
C8—H8B	0.9700	C20—H20	0.9300
C9—C10	1.530 (5)	C21—C22	1.391 (5)
C9—H9	0.9800	C21—H21	0.9300
C10—C11	1.386 (5)	C22—H22	0.9300
C10—C15	1.388 (5)		
C7—N1—N2	108.5 (3)	C10—C11—C12	120.9 (3)
N1—N2—C17	119.7 (3)	C10—C11—H11	119.5
N1—N2—C9	113.6 (2)	C12—C11—H11	119.5
C17—N2—C9	126.3 (3)	C13—C12—C11	121.9 (4)
C2—C1—C6	120.4 (3)	C13—C12—H12	119.0
C2—C1—H1	119.8	C11—C12—H12	119.0
C6—C1—H1	119.8	C12—C13—C14	116.7 (4)
C1—C2—C3	120.3 (3)	C12—C13—C16	122.5 (4)
C1—C2—H2	119.8	C14—C13—C16	120.8 (4)
C3—C2—H2	119.8	C15—C14—C13	121.9 (4)
C4—C3—C2	120.6 (3)	C15—C14—H14	119.0
C4—C3—Cl1	119.2 (3)	C13—C14—H14	119.0
C2—C3—Cl1	120.2 (3)	C14—C15—C10	121.1 (3)
C3—C4—C5	119.5 (3)	C14—C15—H15	119.4
C3—C4—H4	120.2	C10—C15—H15	119.4
C5—C4—H4	120.2	C13—C16—H16A	109.5
C4—C5—C6	120.9 (3)	C13—C16—H16B	109.5
C4—C5—H5	119.5	H16A—C16—H16B	109.5
C6—C5—H5	119.5	C13—C16—H16C	109.5
C5—C6—C1	118.2 (3)	H16A—C16—H16C	109.5
C5—C6—C7	120.3 (3)	H16B—C16—H16C	109.5
C1—C6—C7	121.5 (3)	C18—C17—N2	120.7 (3)
N1—C7—C6	121.5 (3)	C18—C17—C22	118.9 (3)
N1—C7—C8	113.5 (3)	N2—C17—C22	120.4 (3)
C6—C7—C8	124.9 (3)	C17—C18—C19	119.4 (4)
C7—C8—C9	102.6 (3)	C17—C18—H18	120.3
C7—C8—H8A	111.2	C19—C18—H18	120.3
C9—C8—H8A	111.2	C20—C19—C18	121.1 (4)
C7—C8—H8B	111.2	C20—C19—H19	119.4
C9—C8—H8B	111.2	C18—C19—H19	119.4
H8A—C8—H8B	109.2	C19—C20—C21	120.0 (4)
N2—C9—C10	112.4 (3)	C19—C20—H20	120.0
N2—C9—C8	100.6 (2)	C21—C20—H20	120.0
C10—C9—C8	113.7 (3)	C20—C21—C22	120.3 (4)
N2—C9—H9	109.9	C20—C21—H21	119.8
C10—C9—H9	109.9	C22—C21—H21	119.8
C8—C9—H9	109.9	C21—C22—C17	120.3 (4)
C11—C10—C15	117.4 (4)	C21—C22—H22	119.8
C11—C10—C9	121.6 (3)	C17—C22—H22	119.8
C15—C10—C9	121.0 (3)		

C7—N1—N2—C17	−179.7 (3)	N2—C9—C10—C11	142.3 (3)
C7—N1—N2—C9	6.6 (4)	C8—C9—C10—C11	−104.2 (4)
C6—C1—C2—C3	−0.4 (5)	N2—C9—C10—C15	−39.0 (4)
C1—C2—C3—C4	1.3 (5)	C8—C9—C10—C15	74.5 (4)
C1—C2—C3—Cl1	−178.7 (3)	C15—C10—C11—C12	0.8 (5)
C2—C3—C4—C5	−1.1 (5)	C9—C10—C11—C12	179.6 (3)
Cl1—C3—C4—C5	178.9 (2)	C10—C11—C12—C13	0.1 (6)
C3—C4—C5—C6	0.1 (5)	C11—C12—C13—C14	−1.0 (6)
C4—C5—C6—C1	0.8 (4)	C11—C12—C13—C16	178.3 (4)
C4—C5—C6—C7	179.8 (3)	C12—C13—C14—C15	1.1 (6)
C2—C1—C6—C5	−0.6 (4)	C16—C13—C14—C15	−178.2 (3)
C2—C1—C6—C7	−179.6 (3)	C13—C14—C15—C10	−0.2 (6)
N2—N1—C7—C6	−179.9 (3)	C11—C10—C15—C14	−0.7 (5)
N2—N1—C7—C8	0.9 (4)	C9—C10—C15—C14	−179.6 (3)
C5—C6—C7—N1	−172.5 (3)	N1—N2—C17—C18	−176.2 (3)
C1—C6—C7—N1	6.5 (5)	C9—N2—C17—C18	−3.3 (5)
C5—C6—C7—C8	6.7 (5)	N1—N2—C17—C22	4.0 (5)
C1—C6—C7—C8	−174.3 (3)	C9—N2—C17—C22	176.9 (3)
N1—C7—C8—C9	−7.2 (4)	N2—C17—C18—C19	179.1 (4)
C6—C7—C8—C9	173.6 (3)	C22—C17—C18—C19	−1.1 (5)
N1—N2—C9—C10	110.9 (3)	C17—C18—C19—C20	0.2 (6)
C17—N2—C9—C10	−62.4 (4)	C18—C19—C20—C21	0.7 (7)
N1—N2—C9—C8	−10.4 (4)	C19—C20—C21—C22	−0.6 (7)
C17—N2—C9—C8	176.3 (3)	C20—C21—C22—C17	−0.3 (6)
C7—C8—C9—N2	9.7 (3)	C18—C17—C22—C21	1.2 (5)
C7—C8—C9—C10	−110.7 (3)	N2—C17—C22—C21	−179.1 (3)

Fig. 1


C21
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