organic compounds

4-[(5-Chloro-3-methyl-1-phenyl-1H-pyrazol-4-yl)methylideneamino]-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one

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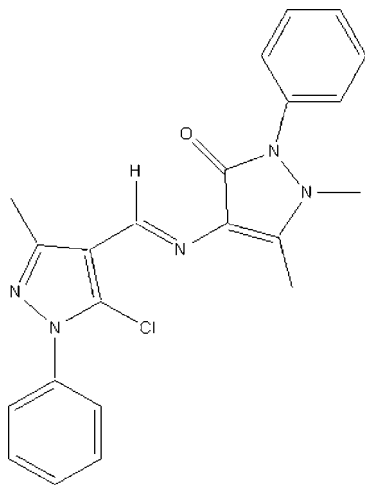Correspondence e-mail: zhuhualing2004@126.com

In the molecule of the title compound, $C_{22}H_{20}ClN_5O$, the atoms of the two pyrazole rings and the –C=N– group which joins them are essentially coplanar, with an r.m.s. deviation of 0.054 (2) Å. The phenyl rings form dihedral angles of 41.24 (5) and 55.53 (5)° with this plane. The crystal structure is stabilized by weak intermolecular π–π interactions, with centroid-to-centroid distances of 3.6179 (13) Å between the imidazole rings.

Related literature

For our previous work in this area, see: Zhu *et al.* (2005, 2010*a*,*b*,*c*). For a related crystal structure, see: Shi *et al.* (2005).

Experimental

Crystal data

$C_{22}H_{20}ClN_5O$	$V = 1935.4\ (7)$ Å^3
$M_r = 405.88$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.3982\ (17)$ Å	$\mu = 0.22$ mm^{-1}
$b = 9.5204\ (19)$ Å	$T = 113$ K
$c = 24.401\ (5)$ Å	$0.20 \times 0.18 \times 0.10$ mm
$\beta = 97.24\ (3)°$	

Data collection

Rigaku Saturn CCD diffractometer	15458 measured reflections
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)	3397 independent reflections
	2871 reflections with $I > 2\sigma(I)$
$T_{min} = 0.957$, $T_{max} = 0.978$	$R_{int} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	266 parameters
$wR(F^2) = 0.105$	H-atom parameters constrained
$S = 1.08$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
3397 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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supplementary materials

4-[(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

H. Zhu, J. Zhu, L. Ban, P. Zhang and M. Zhang

Comment

As part of our ongoing studies (Zhu *et al.*, 2005, 2010*a,b,c*) of pyrazolone derivatives as potential ligands (Shi *et al.*, 2005) we report the crystal structure of the title compound (I).

The molecular structure of the title compound is shown in Fig. 1. Atoms C11 and N3 and the two pyrazole rings are essentially coplplanar with the largest deviation being 0.0543 (18) Å for atom C13. The crystal structure is stabilized by weak intermolecular π–π interactions with ring centroid to ring centroid distances of 3.6179 (13) Å between the imidazole rings (see Fig. 2).

Experimental

The title compound was synthesized by refluxing a mixture of 4-formacyl-5-methyl-3-chloro-2-phenyl-2*H*-pyrazole (15*m* mol) and 4-antipyrine (15 mmol) in ethanol (100 ml) over a steam bath for about 4 h. The solution was then cooled to room temperature. After one day, pale-yellow blocks wre obtained and they were dried in air. Recrystallization of a solution of the title compound in ethanol afforded pale-yellow crystals suitable for X-ray analysis.

Refinement

H atoms were placed in calculated positions with C—H = 0.95 and 0.98 Å and included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl})$.
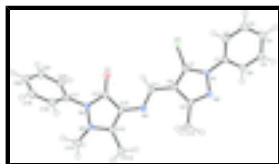
Figures

Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.
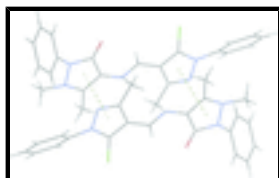

Fig. 2. Part of the crystal structure showing intermolecular π–π interactions as dashed lines.

supplementary materials

4-[(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylideneamino]- 1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

Crystal data

$C_{22}H_{20}ClN_5O$	$F(000) = 848$
$M_r = 405.88$	$D_x = 1.393$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4998 reflections
$a = 8.3982$ (17) Å	$\theta = 1.7$–$27.9°$
$b = 9.5204$ (19) Å	$\mu = 0.22$ mm^{-1}
$c = 24.401$ (5) Å	$T = 113$ K
$\beta = 97.24$ (3)°	Block, pale yellow
$V = 1935.4$ (7) Å^3	$0.20 \times 0.18 \times 0.10$ mm
$Z = 4$	

Data collection

Rigaku Saturn CCD diffractometer	3397 independent reflections
Radiation source: rotating anode confocal	2871 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.046$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
ω and φ scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)	$k = -11 \rightarrow 11$
$T_{min} = 0.957$, $T_{max} = 0.978$	$l = -29 \rightarrow 29$
15458 measured 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
$wR(F^2) = 0.105$	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.6515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
3397 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
266 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0242 (16)

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 $F^2 > \sigma(F^2)$ 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	$U_{iso}*/U_{eq}$
Cl1	0.56582 (6)	0.05661 (6)	0.08916 (2)	0.02960 (19)
O1	0.75786 (16)	0.36105 (15)	−0.04914 (6)	0.0251 (4)
N1	0.80398 (18)	−0.09683 (17)	0.14372 (6)	0.0175 (4)
N2	0.96786 (17)	−0.11576 (16)	0.14899 (6)	0.0172 (4)
N3	1.03166 (18)	0.19175 (16)	0.02437 (6)	0.0181 (4)
N4	0.98109 (19)	0.45266 (17)	−0.08446 (6)	0.0196 (4)
N5	1.14617 (18)	0.42156 (17)	−0.07913 (6)	0.0201 (4)
C1	0.7142 (2)	−0.1746 (2)	0.17966 (8)	0.0181 (4)
C2	0.5695 (2)	−0.2379 (2)	0.16005 (8)	0.0206 (4)
H2	0.5247	−0.2262	0.1226	0.025*
C3	0.4910 (2)	−0.3182 (2)	0.19566 (9)	0.0246 (5)
H3	0.3912	−0.3610	0.1826	0.030*
C4	0.5566 (2)	−0.3368 (2)	0.25005 (9)	0.0263 (5)
H4	0.5026	−0.3927	0.2742	0.032*
C5	0.7015 (2)	−0.2736 (2)	0.26924 (8)	0.0254 (5)
H5	0.7469	−0.2867	0.3066	0.031*
C6	0.7808 (2)	−0.1913 (2)	0.23432 (8)	0.0213 (5)
H6	0.8794	−0.1468	0.2477	0.026*
C7	0.7592 (2)	0.0000 (2)	0.10393 (8)	0.0186 (4)
C8	0.8934 (2)	0.04644 (19)	0.08215 (8)	0.0164 (4)
C9	1.0207 (2)	−0.0306 (2)	0.11224 (7)	0.0163 (4)
C10	1.1952 (2)	−0.0254 (2)	0.10710 (8)	0.0209 (4)
H10A	1.2521	−0.0946	0.1321	0.031*
H10B	1.2366	0.0688	0.1168	0.031*
H10C	1.2119	−0.0470	0.0690	0.031*
C11	0.8978 (2)	0.14939 (19)	0.03858 (8)	0.0174 (4)
H11	0.8001	0.1860	0.0203	0.021*
C12	1.0353 (2)	0.2915 (2)	−0.01714 (8)	0.0178 (4)
C13	1.1767 (2)	0.3331 (2)	−0.03503 (7)	0.0189 (4)
C14	1.3431 (2)	0.2994 (2)	−0.01061 (8)	0.0265 (5)
H14A	1.4097	0.2833	−0.0402	0.040*
H14B	1.3425	0.2145	0.0121	0.040*
H14C	1.3871	0.3779	0.0124	0.040*

C15	0.9051 (2)	0.3662 (2)	−0.04929 (8)	0.0191 (4)
C16	1.2558 (2)	0.5346 (2)	−0.09045 (9)	0.0277 (5)
H16A	1.2703	0.5994	−0.0590	0.042*
H16B	1.2106	0.5856	−0.1237	0.042*
H16C	1.3598	0.4944	−0.0962	0.042*
C17	0.9040 (2)	0.5093 (2)	−0.13518 (8)	0.0194 (4)
C18	0.9457 (2)	0.4650 (2)	−0.18560 (8)	0.0231 (5)
H18	1.0276	0.3968	−0.1870	0.028*
C19	0.8665 (2)	0.5215 (2)	−0.23385 (8)	0.0257 (5)
H19	0.8960	0.4932	−0.2685	0.031*
C20	0.7448 (2)	0.6188 (2)	−0.23199 (8)	0.0250 (5)
H20	0.6897	0.6560	−0.2652	0.030*
C21	0.7038 (2)	0.6615 (2)	−0.18128 (9)	0.0256 (5)
H21	0.6198	0.7278	−0.1799	0.031*
C22	0.7844 (2)	0.6082 (2)	−0.13259 (8)	0.0235 (5)
H22	0.7578	0.6393	−0.0979	0.028*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0146 (3)	0.0348 (3)	0.0391 (3)	0.0050 (2)	0.0026 (2)	0.0133 (2)
O1	0.0202 (8)	0.0284 (8)	0.0269 (8)	0.0014 (6)	0.0035 (6)	0.0068 (6)
N1	0.0137 (8)	0.0208 (9)	0.0185 (8)	−0.0001 (7)	0.0033 (6)	0.0039 (7)
N2	0.0132 (8)	0.0197 (9)	0.0187 (8)	0.0005 (7)	0.0021 (6)	0.0010 (7)
N3	0.0204 (9)	0.0170 (9)	0.0169 (8)	−0.0018 (7)	0.0024 (7)	0.0003 (6)
N4	0.0204 (8)	0.0215 (9)	0.0171 (8)	0.0023 (7)	0.0031 (7)	0.0051 (7)
N5	0.0189 (9)	0.0227 (9)	0.0185 (8)	−0.0020 (7)	0.0012 (7)	0.0040 (7)
C1	0.0181 (10)	0.0162 (10)	0.0213 (10)	0.0016 (8)	0.0073 (8)	0.0021 (8)
C2	0.0198 (10)	0.0218 (11)	0.0209 (10)	0.0011 (8)	0.0049 (8)	−0.0013 (8)
C3	0.0223 (11)	0.0198 (11)	0.0330 (12)	−0.0023 (8)	0.0087 (9)	−0.0020 (9)
C4	0.0305 (12)	0.0190 (11)	0.0324 (12)	0.0012 (9)	0.0155 (10)	0.0055 (9)
C5	0.0308 (12)	0.0253 (12)	0.0213 (10)	0.0037 (9)	0.0075 (9)	0.0055 (9)
C6	0.0211 (10)	0.0213 (11)	0.0215 (10)	−0.0002 (8)	0.0028 (8)	0.0018 (8)
C7	0.0152 (10)	0.0192 (11)	0.0208 (10)	0.0022 (8)	0.0006 (8)	0.0016 (8)
C8	0.0154 (9)	0.0168 (10)	0.0166 (9)	−0.0007 (8)	0.0010 (8)	−0.0004 (8)
C9	0.0170 (9)	0.0172 (10)	0.0148 (9)	−0.0010 (8)	0.0024 (8)	−0.0014 (8)
C10	0.0158 (10)	0.0248 (11)	0.0220 (10)	0.0005 (8)	0.0030 (8)	0.0026 (8)
C11	0.0192 (10)	0.0160 (10)	0.0166 (10)	0.0021 (8)	0.0001 (8)	0.0021 (8)
C12	0.0218 (10)	0.0162 (10)	0.0154 (9)	−0.0008 (8)	0.0021 (8)	0.0000 (8)
C13	0.0239 (10)	0.0199 (11)	0.0127 (9)	−0.0014 (8)	0.0012 (8)	−0.0008 (8)
C14	0.0213 (11)	0.0367 (13)	0.0217 (11)	−0.0007 (9)	0.0035 (9)	0.0048 (9)
C15	0.0231 (11)	0.0174 (11)	0.0169 (10)	−0.0015 (8)	0.0028 (8)	−0.0001 (8)
C16	0.0283 (12)	0.0251 (12)	0.0305 (12)	−0.0043 (9)	0.0072 (9)	0.0051 (9)
C17	0.0233 (10)	0.0162 (10)	0.0182 (10)	−0.0040 (8)	0.0001 (8)	0.0033 (8)
C18	0.0275 (11)	0.0207 (11)	0.0215 (10)	0.0009 (9)	0.0054 (9)	0.0028 (8)
C19	0.0334 (12)	0.0276 (12)	0.0160 (10)	−0.0055 (10)	0.0030 (9)	0.0006 (9)
C20	0.0279 (11)	0.0231 (12)	0.0219 (10)	−0.0055 (9)	−0.0048 (9)	0.0046 (9)
C21	0.0239 (11)	0.0221 (11)	0.0293 (12)	0.0015 (9)	−0.0025 (9)	0.0016 (9)

C22	0.0277 (11)	0.0228 (11)	0.0198 (10)	−0.0011 (9)	0.0019 (9)	−0.0013 (8)

Geometric parameters (Å, °)

Cl1—C7	1.7064 (19)	C8—C11	1.450 (3)
O1—C15	1.238 (2)	C9—C10	1.487 (3)
N1—C7	1.357 (2)	C10—H10A	0.9800
N1—N2	1.378 (2)	C10—H10B	0.9800
N1—C1	1.433 (2)	C10—H10C	0.9800
N2—C9	1.326 (2)	C11—H11	0.9500
N3—C11	1.282 (2)	C12—C13	1.374 (3)
N3—C12	1.392 (2)	C12—C15	1.449 (3)
N4—C15	1.400 (2)	C13—C14	1.484 (3)
N4—N5	1.408 (2)	C14—H14A	0.9800
N4—C17	1.428 (2)	C14—H14B	0.9800
N5—C13	1.365 (2)	C14—H14C	0.9800
N5—C16	1.465 (3)	C16—H16A	0.9800
C1—C2	1.386 (3)	C16—H16B	0.9800
C1—C6	1.389 (3)	C16—H16C	0.9800
C2—C3	1.385 (3)	C17—C22	1.384 (3)
C2—H2	0.9500	C17—C18	1.387 (3)
C3—C4	1.383 (3)	C18—C19	1.385 (3)
C3—H3	0.9500	C18—H18	0.9500
C4—C5	1.385 (3)	C19—C20	1.385 (3)
C4—H4	0.9500	C19—H19	0.9500
C5—C6	1.388 (3)	C20—C21	1.387 (3)
C5—H5	0.9500	C20—H20	0.9500
C6—H6	0.9500	C21—C22	1.387 (3)
C7—C8	1.378 (3)	C21—H21	0.9500
C8—C9	1.422 (3)	C22—H22	0.9500
C7—N1—N2	109.82 (14)	H10B—C10—H10C	109.5
C7—N1—C1	132.03 (16)	N3—C11—C8	121.01 (17)
N2—N1—C1	118.13 (15)	N3—C11—H11	119.5
C9—N2—N1	105.80 (15)	C8—C11—H11	119.5
C11—N3—C12	120.78 (16)	C13—C12—N3	121.80 (17)
C15—N4—N5	109.84 (15)	C13—C12—C15	108.06 (17)
C15—N4—C17	124.14 (16)	N3—C12—C15	130.13 (17)
N5—N4—C17	119.57 (15)	N5—C13—C12	110.13 (17)
C13—N5—N4	106.72 (14)	N5—C13—C14	121.60 (17)
C13—N5—C16	122.81 (16)	C12—C13—C14	128.17 (18)
N4—N5—C16	117.58 (15)	C13—C14—H14A	109.5
C2—C1—C6	120.76 (18)	C13—C14—H14B	109.5
C2—C1—N1	121.27 (17)	H14A—C14—H14B	109.5
C6—C1—N1	117.88 (17)	C13—C14—H14C	109.5
C3—C2—C1	119.28 (19)	H14A—C14—H14C	109.5
C3—C2—H2	120.4	H14B—C14—H14C	109.5
C1—C2—H2	120.4	O1—C15—N4	123.90 (17)
C4—C3—C2	120.61 (19)	O1—C15—C12	131.67 (18)
C4—C3—H3	119.7	N4—C15—C12	104.43 (16)

C2—C3—H3	119.7	N5—C16—H16A	109.5
C3—C4—C5	119.72 (19)	N5—C16—H16B	109.5
C3—C4—H4	120.1	H16A—C16—H16B	109.5
C5—C4—H4	120.1	N5—C16—H16C	109.5
C4—C5—C6	120.45 (19)	H16A—C16—H16C	109.5
C4—C5—H5	119.8	H16B—C16—H16C	109.5
C6—C5—H5	119.8	C22—C17—C18	120.90 (18)
C5—C6—C1	119.18 (18)	C22—C17—N4	118.02 (17)
C5—C6—H6	120.4	C18—C17—N4	121.07 (18)
C1—C6—H6	120.4	C19—C18—C17	119.21 (19)
N1—C7—C8	109.14 (16)	C19—C18—H18	120.4
N1—C7—Cl1	122.43 (14)	C17—C18—H18	120.4
C8—C7—Cl1	128.31 (15)	C20—C19—C18	120.59 (19)
C7—C8—C9	103.49 (16)	C20—C19—H19	119.7
C7—C8—C11	126.70 (17)	C18—C19—H19	119.7
C9—C8—C11	129.81 (17)	C19—C20—C21	119.54 (19)
N2—C9—C8	111.75 (16)	C19—C20—H20	120.2
N2—C9—C10	119.64 (17)	C21—C20—H20	120.2
C8—C9—C10	128.61 (17)	C20—C21—C22	120.50 (19)
C9—C10—H10A	109.5	C20—C21—H21	119.8
C9—C10—H10B	109.5	C22—C21—H21	119.8
H10A—C10—H10B	109.5	C17—C22—C21	119.24 (19)
C9—C10—H10C	109.5	C17—C22—H22	120.4
H10A—C10—H10C	109.5	C21—C22—H22	120.4
C7—N1—N2—C9	−0.2 (2)	C7—C8—C11—N3	175.01 (19)
C1—N1—N2—C9	−178.74 (16)	C9—C8—C11—N3	−5.4 (3)
C15—N4—N5—C13	−9.4 (2)	C11—N3—C12—C13	−176.57 (18)
C17—N4—N5—C13	−162.32 (16)	C11—N3—C12—C15	2.0 (3)
C15—N4—N5—C16	−152.04 (17)	N4—N5—C13—C12	8.4 (2)
C17—N4—N5—C16	55.0 (2)	C16—N5—C13—C12	148.65 (18)
C7—N1—C1—C2	44.7 (3)	N4—N5—C13—C14	−168.34 (17)
N2—N1—C1—C2	−137.15 (18)	C16—N5—C13—C14	−28.1 (3)
C7—N1—C1—C6	−138.7 (2)	N3—C12—C13—N5	174.47 (16)
N2—N1—C1—C6	39.5 (2)	C15—C12—C13—N5	−4.4 (2)
C6—C1—C2—C3	0.1 (3)	N3—C12—C13—C14	−9.1 (3)
N1—C1—C2—C3	176.61 (17)	C15—C12—C13—C14	172.05 (19)
C1—C2—C3—C4	−0.7 (3)	N5—N4—C15—O1	−172.85 (17)
C2—C3—C4—C5	0.5 (3)	C17—N4—C15—O1	−21.4 (3)
C3—C4—C5—C6	0.3 (3)	N5—N4—C15—C12	6.6 (2)
C4—C5—C6—C1	−0.9 (3)	C17—N4—C15—C12	158.02 (17)
C2—C1—C6—C5	0.7 (3)	C13—C12—C15—O1	177.9 (2)
N1—C1—C6—C5	−175.93 (17)	N3—C12—C15—O1	−0.8 (4)
N2—N1—C7—C8	0.1 (2)	C13—C12—C15—N4	−1.4 (2)
C1—N1—C7—C8	178.39 (18)	N3—C12—C15—N4	179.85 (18)
N2—N1—C7—Cl1	−176.18 (13)	C15—N4—C17—C22	67.4 (3)
C1—N1—C7—Cl1	2.1 (3)	N5—N4—C17—C22	−143.73 (18)
N1—C7—C8—C9	0.0 (2)	C15—N4—C17—C18	−111.6 (2)
Cl1—C7—C8—C9	176.01 (15)	N5—N4—C17—C18	37.3 (3)
N1—C7—C8—C11	179.71 (17)	C22—C17—C18—C19	0.3 (3)

Cl1—C7—C8—C11	−4.3 (3)	N4—C17—C18—C19	179.23 (18)
N1—N2—C9—C8	0.2 (2)	C17—C18—C19—C20	−1.4 (3)
N1—N2—C9—C10	−179.94 (16)	C18—C19—C20—C21	1.0 (3)
C7—C8—C9—N2	−0.1 (2)	C19—C20—C21—C22	0.4 (3)
C11—C8—C9—N2	−179.82 (18)	C18—C17—C22—C21	1.1 (3)
C7—C8—C9—C10	−179.97 (19)	N4—C17—C22—C21	−177.85 (17)
C11—C8—C9—C10	0.3 (3)	C20—C21—C22—C17	−1.5 (3)
C12—N3—C11—C8	−179.42 (16)		

Fig. 1

Fig. 2