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N,*N*-Dimethyl-4-[5-(5-methyl-1-phenyl-1*H*-pyrazol-4-yl)-1,3,4-oxadiazol-2-yl]-aniline

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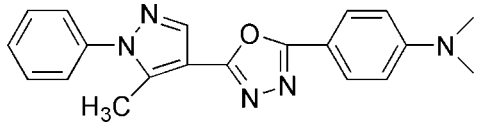
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 13.0.

In the molecule of the title compound, $C_{20}H_{19}N_5O$, the pyrazole and oxadiazole rings are not completely conjugated, the dihedral angle between them being 7.97 (6)°. The pyrazole and oxadiazole rings form dihedral angles of 42.74 (6) and 4.35 (5)° with the attached phenyl and benzene rings, respectively.

Related literature

For related literature, see: Ashton *et al.* (1993); Charles *et al.* (2004); Coswami *et al.* (1984); Wang *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{19}N_5O$
M_r = 345.40
Monoclinic, $P2_1/c$
a = 17.746 (7) Å
b = 6.942 (3) Å
c = 14.474 (6) Å
β = 99.738 (5)°
V = 1757.6 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.28 × 0.20 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.993
9198 measured reflections
3096 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.04
3096 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); 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: RZ2184).

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supporting information

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N,*N*-Dimethyl-4-[5-(5-methyl-1-phenyl-1*H*-pyrazol-4-yl)-1,3,4-oxadiazol-2-yl]aniline

Shu-Wen Wang, Zheng-Quan Zuo and Wen-Long Yang

S1. Comment

In recent years, 1,3,4-oxadiazole derivatives have been extensively studied due to their broad biological activities, such as herbicidal, insecticidal and fungicidal activities (Coswami *et al.*, 1984). Pyrazoles, as an important class of compounds in medicinal chemistry, constitute the basic framework of drugs in many pharmacological and medicinal applications (Ashton *et al.*, 1993). Bis-heterocycles with high bioactivity have been reported in literature (Charles *et al.*, 2004). In a continuation of our study on structure-activity relationship (Wang *et al.*, 2006), we report here the crystal structure of the title compound (Fig.1), which was synthesized from *N*′-(4-(dimethylamino)benzylidene)-5-methyl-1-phenyl-1*H*-pyrazole-4 -carbohydrazide.

Most bond lengths and angles in the title compound are as expected for this type of compounds. The N4—C12 bond length (1.290 (2) Å) in the oxadiazole ring is shorter than the N2—C9 bond length (1.311 (2) Å) in the pyrazole ring, while the N3—N4 bond length (1.4140 (19) Å) is longer than the N1—N2 bond distance (1.3701 (18) Å). This could be ascribed to the strong electron withdrawing effect of the oxygen atom in the oxadiazole ring. In addition, because of the conjugated effect among oxygen and the two C=N bonds, the C—O bond lengths are shorter than the normal C—O single bond (1.42–1.46 Å). The pyrazole and oxadiazole rings are not completely conjugated, the dihedral angle between them being 7.97 (6)°. The dihedral angles formed by the pyrazole and oxadiazole rings with the attached phenyl and benzene rings are 42.74 (6) and 4.35 (5)° respectively.

S2. Experimental

A mixture of *N*′-(4-(dimethylamino)benzylidene)-5-methyl-1-phenyl-1*H*-pyrazole -4-carbohydrazide (0.694 g, 2 mmol), obtained according to a previously reported procedure (Wang *et al.*, 2006), iodosobenzene diacetate (0.644 g, 2 mmol) and anhydrous ethanol (50 ml) was stirred in a 100 ml flask at room temperature for 2 h. The solid product formed was then filtered and washed with anhydrous ethanol. Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (m.p. 488 K).

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93–0.96 A%, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for methyl groups.

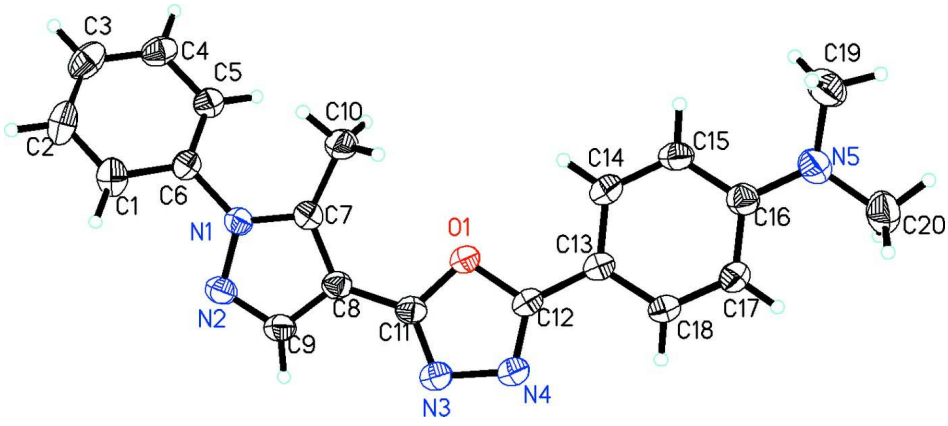

Figure 1

View of the title compound with 35% probability ellipsoid.

N,*N*-Dimethyl-4-[5-(5-methyl-1-phenyl-1*H*-pyrazol-4-yl)-1,3,4-oxadiazol- 2-yl]aniline

Crystal data

$C_{20}H_{19}N_5O$
$M_r = 345.40$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.746\ (7)$ Å
$b = 6.942\ (3)$ Å
$c = 14.474\ (6)$ Å
$\beta = 99.738\ (5)°$
$V = 1757.6\ (12)$ Å^3
$Z = 4$
$F(000) = 728$
$D_x = 1.305$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2162 reflections
$\theta = 2.3–23.1°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Plate, colourless
0.28 × 0.20 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.976$, $T_{max} = 0.993$
9198 measured reflections
3096 independent reflections
2212 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -21\rightarrow20$
$k = -7\rightarrow8$
$l = -15\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.108$
$S = 1.04$
3096 reflections
238 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.1148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.23457 (6)	0.46275 (15)	0.97159 (7)	0.0441 (3)
N1	0.36081 (7)	0.98159 (18)	0.95277 (9)	0.0419 (3)
N2	0.35181 (8)	1.0599 (2)	1.03710 (9)	0.0519 (4)
N3	0.22892 (9)	0.5614 (2)	1.11520 (10)	0.0546 (4)
N4	0.18766 (9)	0.3870 (2)	1.09869 (10)	0.0554 (4)
N5	0.07036 (9)	−0.3315 (2)	0.82215 (11)	0.0683 (5)
C1	0.46094 (10)	1.2036 (2)	0.92564 (13)	0.0560 (5)
H1	0.4814	1.1998	0.9892	0.067*
C2	0.49418 (11)	1.3160 (3)	0.86493 (16)	0.0666 (6)
H2	0.5375	1.3882	0.8878	0.080*
C3	0.46404 (12)	1.3224 (3)	0.77106 (16)	0.0659 (6)
H3	0.4869	1.3984	0.7307	0.079*
C4	0.40026 (11)	1.2166 (2)	0.73698 (13)	0.0560 (5)
H4	0.3802	1.2199	0.6733	0.067*
C5	0.36550 (9)	1.1050 (2)	0.79661 (11)	0.0465 (4)
H5	0.3214	1.0361	0.7736	0.056*
C6	0.39648 (9)	1.0964 (2)	0.89030 (11)	0.0412 (4)
C7	0.32987 (9)	0.8024 (2)	0.93957 (10)	0.0400 (4)
C8	0.29830 (9)	0.7646 (2)	1.01870 (10)	0.0420 (4)
C9	0.31435 (10)	0.9277 (2)	1.07553 (12)	0.0516 (4)
H9	0.3000	0.9408	1.1341	0.062*
C10	0.33531 (11)	0.6795 (3)	0.85662 (12)	0.0558 (5)
H10A	0.2911	0.6998	0.8094	0.084*
H10B	0.3379	0.5465	0.8750	0.084*
H10C	0.3805	0.7130	0.8319	0.084*
C11	0.25474 (9)	0.5991 (2)	1.03925 (11)	0.0428 (4)
C12	0.19272 (9)	0.3352 (2)	1.01439 (11)	0.0427 (4)
C13	0.16085 (9)	0.1674 (2)	0.96261 (11)	0.0430 (4)
C14	0.17535 (9)	0.1234 (2)	0.87380 (12)	0.0471 (4)
H14	0.2054	0.2063	0.8450	0.057*
C15	0.14621 (9)	−0.0402 (3)	0.82743 (12)	0.0501 (4)
H15	0.1573	−0.0663	0.7681	0.060*
C16	0.10020 (9)	−0.1681 (2)	0.86788 (12)	0.0484 (4)
C17	0.08488 (10)	−0.1211 (3)	0.95697 (12)	0.0539 (5)
H17	0.0540	−0.2020	0.9856	0.065*

C18	0.11459 (10)	0.0419 (3)	1.00279 (12)	0.0519 (4)
H18	0.1036	0.0691	1.0620	0.062*
C19	0.09588 (13)	−0.4001 (3)	0.73912 (15)	0.0736 (6)
H19A	0.0894	−0.3005	0.6924	0.110*
H19B	0.0664	−0.5109	0.7155	0.110*
H19C	0.1489	−0.4349	0.7539	0.110*
C20	0.02076 (12)	−0.4574 (3)	0.86451 (16)	0.0731 (6)
H20A	0.0480	−0.5061	0.9228	0.110*
H20B	0.0047	−0.5631	0.8230	0.110*
H20C	−0.0233	−0.3866	0.8758	0.110*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0498 (6)	0.0455 (6)	0.0386 (6)	−0.0029 (5)	0.0125 (5)	0.0024 (5)
N1	0.0463 (8)	0.0422 (8)	0.0365 (8)	−0.0030 (6)	0.0049 (6)	−0.0006 (6)
N2	0.0677 (9)	0.0506 (8)	0.0369 (8)	−0.0056 (7)	0.0077 (7)	−0.0051 (6)
N3	0.0693 (10)	0.0535 (9)	0.0438 (9)	−0.0081 (8)	0.0180 (7)	−0.0004 (7)
N4	0.0689 (10)	0.0561 (9)	0.0450 (9)	−0.0106 (8)	0.0205 (7)	−0.0011 (7)
N5	0.0716 (11)	0.0739 (11)	0.0617 (10)	−0.0230 (9)	0.0175 (8)	−0.0193 (8)
C1	0.0505 (10)	0.0482 (10)	0.0648 (12)	−0.0017 (8)	−0.0034 (9)	0.0090 (9)
C2	0.0499 (11)	0.0521 (11)	0.0978 (17)	−0.0068 (9)	0.0128 (11)	0.0138 (11)
C3	0.0708 (14)	0.0469 (11)	0.0880 (16)	0.0084 (10)	0.0362 (12)	0.0188 (10)
C4	0.0711 (13)	0.0479 (10)	0.0527 (11)	0.0103 (9)	0.0217 (9)	0.0107 (8)
C5	0.0489 (10)	0.0443 (9)	0.0468 (10)	0.0035 (8)	0.0094 (8)	0.0035 (8)
C6	0.0415 (9)	0.0371 (9)	0.0453 (10)	0.0027 (7)	0.0079 (7)	0.0052 (7)
C7	0.0410 (9)	0.0387 (9)	0.0395 (9)	0.0031 (7)	0.0045 (7)	0.0005 (7)
C8	0.0458 (9)	0.0429 (9)	0.0367 (9)	0.0017 (7)	0.0054 (7)	0.0032 (7)
C9	0.0653 (11)	0.0541 (11)	0.0359 (9)	−0.0042 (9)	0.0102 (8)	0.0012 (8)
C10	0.0702 (12)	0.0481 (10)	0.0536 (11)	−0.0042 (9)	0.0239 (9)	−0.0066 (8)
C11	0.0469 (9)	0.0444 (9)	0.0367 (9)	0.0044 (7)	0.0060 (7)	0.0023 (7)
C12	0.0431 (9)	0.0465 (9)	0.0405 (9)	0.0017 (7)	0.0124 (7)	0.0081 (7)
C13	0.0439 (9)	0.0466 (9)	0.0396 (9)	0.0023 (7)	0.0103 (7)	0.0043 (7)
C14	0.0442 (9)	0.0541 (10)	0.0457 (10)	0.0002 (8)	0.0148 (7)	0.0077 (8)
C15	0.0495 (10)	0.0626 (11)	0.0399 (10)	0.0008 (9)	0.0127 (8)	−0.0014 (8)
C16	0.0435 (9)	0.0570 (10)	0.0440 (10)	−0.0014 (8)	0.0052 (7)	−0.0016 (8)
C17	0.0548 (10)	0.0601 (11)	0.0494 (11)	−0.0138 (9)	0.0163 (8)	0.0006 (9)
C18	0.0590 (11)	0.0586 (11)	0.0418 (10)	−0.0081 (9)	0.0192 (8)	−0.0008 (8)
C19	0.0827 (14)	0.0702 (13)	0.0685 (14)	−0.0006 (11)	0.0145 (11)	−0.0198 (11)
C20	0.0697 (13)	0.0660 (13)	0.0822 (15)	−0.0179 (11)	0.0089 (11)	−0.0085 (11)

Geometric parameters (Å, º)

O1—C11	1.3656 (19)	C7—C10	1.489 (2)
O1—C12	1.3694 (18)	C8—C9	1.400 (2)
N1—C7	1.360 (2)	C8—C11	1.443 (2)
N1—N2	1.3701 (18)	C9—H9	0.9300
N1—C6	1.431 (2)	C10—H10A	0.9600

N2—C9	1.311 (2)	C10—H10B	0.9600
N3—C11	1.287 (2)	C10—H10C	0.9600
N3—N4	1.4140 (19)	C12—C13	1.447 (2)
N4—C12	1.290 (2)	C13—C14	1.387 (2)
N5—C16	1.374 (2)	C13—C18	1.390 (2)
N5—C19	1.435 (2)	C14—C15	1.375 (2)
N5—C20	1.448 (2)	C14—H14	0.9300
C1—C2	1.380 (3)	C15—C16	1.400 (2)
C1—C6	1.388 (2)	C15—H15	0.9300
C1—H1	0.9300	C16—C17	1.401 (2)
C2—C3	1.374 (3)	C17—C18	1.371 (2)
C2—H2	0.9300	C17—H17	0.9300
C3—C4	1.369 (3)	C18—H18	0.9300
C3—H3	0.9300	C19—H19A	0.9600
C4—C5	1.380 (2)	C19—H19B	0.9600
C4—H4	0.9300	C19—H19C	0.9600
C5—C6	1.376 (2)	C20—H20A	0.9600
C5—H5	0.9300	C20—H20B	0.9600
C7—C8	1.383 (2)	C20—H20C	0.9600

C11—O1—C12	102.73 (12)	C7—C10—H10C	109.5
C7—N1—N2	112.53 (13)	H10A—C10—H10C	109.5
C7—N1—C6	129.20 (13)	H10B—C10—H10C	109.5
N2—N1—C6	118.20 (13)	N3—C11—O1	112.53 (14)
C9—N2—N1	104.12 (13)	N3—C11—C8	128.20 (15)
C11—N3—N4	106.20 (14)	O1—C11—C8	119.24 (13)
C12—N4—N3	106.35 (13)	N4—C12—O1	112.19 (14)
C16—N5—C19	121.80 (16)	N4—C12—C13	129.10 (15)
C16—N5—C20	120.45 (16)	O1—C12—C13	118.71 (14)
C19—N5—C20	117.04 (16)	C14—C13—C18	117.70 (15)
C2—C1—C6	118.87 (18)	C14—C13—C12	122.67 (15)
C2—C1—H1	120.6	C18—C13—C12	119.63 (15)
C6—C1—H1	120.6	C15—C14—C13	121.40 (15)
C3—C2—C1	120.74 (19)	C15—C14—H14	119.3
C3—C2—H2	119.6	C13—C14—H14	119.3
C1—C2—H2	119.6	C14—C15—C16	121.18 (16)
C4—C3—C2	119.91 (18)	C14—C15—H15	119.4
C4—C3—H3	120.0	C16—C15—H15	119.4
C2—C3—H3	120.0	N5—C16—C15	121.80 (16)
C3—C4—C5	120.35 (18)	N5—C16—C17	121.12 (16)
C3—C4—H4	119.8	C15—C16—C17	117.07 (16)
C5—C4—H4	119.8	C18—C17—C16	121.26 (16)
C6—C5—C4	119.63 (17)	C18—C17—H17	119.4
C6—C5—H5	120.2	C16—C17—H17	119.4
C4—C5—H5	120.2	C17—C18—C13	121.39 (16)
C5—C6—C1	120.47 (15)	C17—C18—H18	119.3
C5—C6—N1	120.09 (14)	C13—C18—H18	119.3
C1—C6—N1	119.40 (15)	N5—C19—H19A	109.5

N1—C7—C8	105.52 (13)	N5—C19—H19B	109.5
N1—C7—C10	123.88 (14)	H19A—C19—H19B	109.5
C8—C7—C10	130.53 (15)	N5—C19—H19C	109.5
C7—C8—C9	105.22 (14)	H19A—C19—H19C	109.5
C7—C8—C11	128.89 (14)	H19B—C19—H19C	109.5
C9—C8—C11	125.83 (15)	N5—C20—H20A	109.5
N2—C9—C8	112.60 (15)	N5—C20—H20B	109.5
N2—C9—H9	123.7	H20A—C20—H20B	109.5
C8—C9—H9	123.7	N5—C20—H20C	109.5
C7—C10—H10A	109.5	H20A—C20—H20C	109.5
C7—C10—H10B	109.5	H20B—C20—H20C	109.5
H10A—C10—H10B	109.5		

C7—N1—N2—C9	−0.54 (17)	C12—O1—C11—N3	0.19 (16)
C6—N1—N2—C9	176.53 (13)	C12—O1—C11—C8	−178.00 (13)
C11—N3—N4—C12	0.29 (18)	C7—C8—C11—N3	176.18 (16)
C6—C1—C2—C3	0.1 (3)	C9—C8—C11—N3	−7.0 (3)
C1—C2—C3—C4	0.1 (3)	C7—C8—C11—O1	−5.9 (2)
C2—C3—C4—C5	0.7 (3)	C9—C8—C11—O1	170.91 (15)
C3—C4—C5—C6	−1.7 (2)	N3—N4—C12—O1	−0.18 (18)
C4—C5—C6—C1	2.0 (2)	N3—N4—C12—C13	−179.99 (15)
C4—C5—C6—N1	179.85 (14)	C11—O1—C12—N4	0.01 (16)
C2—C1—C6—C5	−1.2 (3)	C11—O1—C12—C13	179.84 (13)
C2—C1—C6—N1	−179.07 (16)	N4—C12—C13—C14	−175.58 (17)
C7—N1—C6—C5	41.8 (2)	O1—C12—C13—C14	4.6 (2)
N2—N1—C6—C5	−134.74 (15)	N4—C12—C13—C18	3.4 (3)
C7—N1—C6—C1	−140.34 (17)	O1—C12—C13—C18	−176.37 (14)
N2—N1—C6—C1	43.1 (2)	C18—C13—C14—C15	−1.1 (2)
N2—N1—C7—C8	0.98 (17)	C12—C13—C14—C15	177.95 (15)
C6—N1—C7—C8	−175.69 (14)	C13—C14—C15—C16	0.5 (2)
N2—N1—C7—C10	−176.36 (14)	C19—N5—C16—C15	12.1 (3)
C6—N1—C7—C10	7.0 (2)	C20—N5—C16—C15	−177.81 (17)
N1—C7—C8—C9	−0.98 (16)	C19—N5—C16—C17	−168.77 (18)
C10—C7—C8—C9	176.12 (17)	C20—N5—C16—C17	1.3 (3)
N1—C7—C8—C11	176.38 (15)	C14—C15—C16—N5	179.64 (16)
C10—C7—C8—C11	−6.5 (3)	C14—C15—C16—C17	0.5 (2)
N1—N2—C9—C8	−0.13 (19)	N5—C16—C17—C18	180.00 (17)
C7—C8—C9—N2	0.72 (19)	C15—C16—C17—C18	−0.8 (3)
C11—C8—C9—N2	−176.75 (14)	C16—C17—C18—C13	0.2 (3)
N4—N3—C11—O1	−0.30 (18)	C14—C13—C18—C17	0.7 (2)
N4—N3—C11—C8	177.69 (15)	C12—C13—C18—C17	−178.34 (16)