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2-(1*H*-Imidazol-1-yl)-4,6-dimethylpyrimidine

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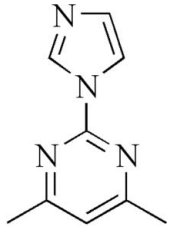
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.064; wR factor = 0.197; data-to-parameter ratio = 12.9.

The asymmetric unit of the title compound, $C_9H_{10}N_4$, consists of two molecules in which the dihedral angles between the planes of the imidazole and pyrimidine rings are 4.8 (1) and 2.1 (1)°.

Related literature

For related pyrimidine derivatives, see: Wu *et al.* (2008); Cetina *et al.* (2005); Liu *et al.* (2007).



Experimental

Crystal data

$C_9H_{10}N_4$ M_r = 174.21
Monoclinic, $P2_1/c$
a = 9.304 (5) Å
b = 26.756 (5) Å
c = 7.129 (5) Å
β = 91.259 (5)°
V = 1774.2 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART diffractometer
11971 measured reflections
3091 independent reflections
2365 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.197
S = 1.14
3091 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: NG5247).

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supporting information

Acta Cryst. (2011). E**67**, o3111 [doi:10.1107/S1600536811044357]

2-(1*H*-Imidazol-1-yl)-4,6-dimethylpyrimidine

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S1. Comment

In recent years,pyrimidine-based materials had been widely investigated for their high electron affinity in the area of nonlinear optical materials (Liu *et al.*, 2007); the crystal structures of a small number of pyrimidine derivatives have been widely reported (Wu *et al.*, 2008; Cetina *et al.*, 2005). The title molecule is a contribution to this topic. In (I), (Fig.1), the dihedral angles between imidazole and pyrimidine rings of the two molecules are only 4.8 (1) and 2.1 (1) °, which indicate that the molecules are almost co-planar. In the crystal structure, neighboring molecules are connected through weak intermolecular C—H···N interactions (Fig. 2).

S2. Experimental

CuI (0.19 g,1 mmol), 1,10-phenanthroline (0.6 g,3 mmol) and DMF (5 ml) were added to a three-necked flask equipped with a magnetic stirrer and a reflux condenser. The reaction mixture turned brown and was kept stirred for 5 min. Then, *t*-BuOK (1.12 g,10 mmol), imidazole (1.36 g, 20 mmol), 2-iodo-4,6-dimethylpyrimidine (0.46 g, 2 mmol) and a catalytic amount of 18-crown-6 were added in sequentially. After complete addition, the mixture was heated under nitrogen for about 2 h, then cooled to room temperature. The residue was extracted with 200 ml of dichloromethane, washed four times with distilled water, and dried with anhydrous $MgSO_4$. Then it was filtered and concentrated and purified by flash column- chromatography on silica. Elution with petroleum/ethyl acetate (2:1) gave colorless crystals. Yield: 0.2 g (60%).

S3. Refinement

All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93–0.96 Å, U_{iso}(H) = 1.2 - 1.5U_{eq}(C).

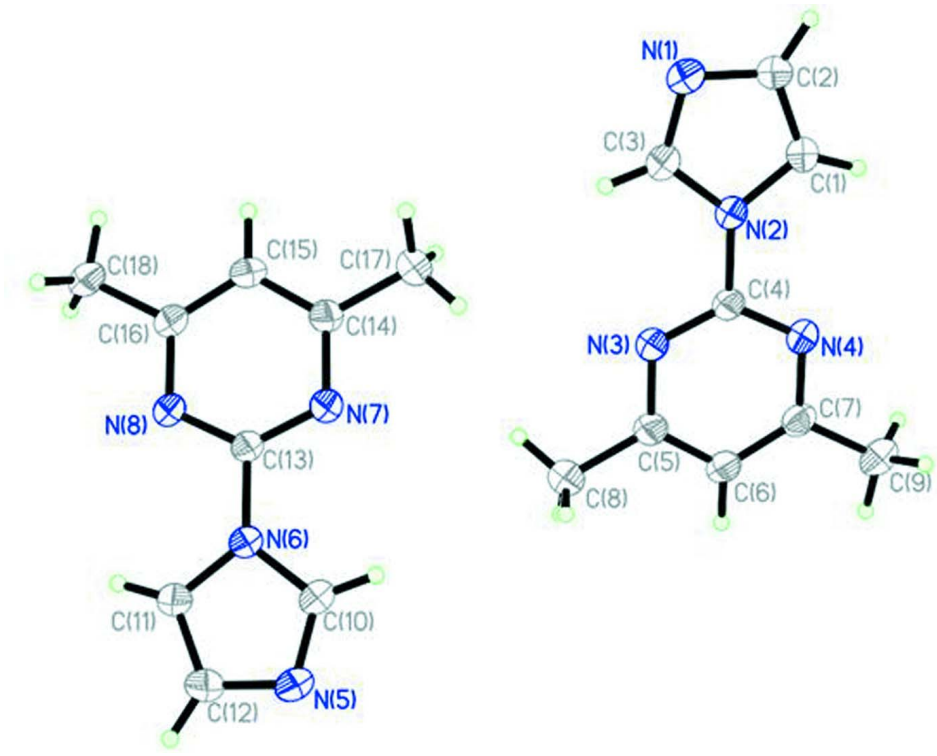

Figure 1

The molecular structure of the title molecule(I) showing 30% probability displacement ellipsoids.

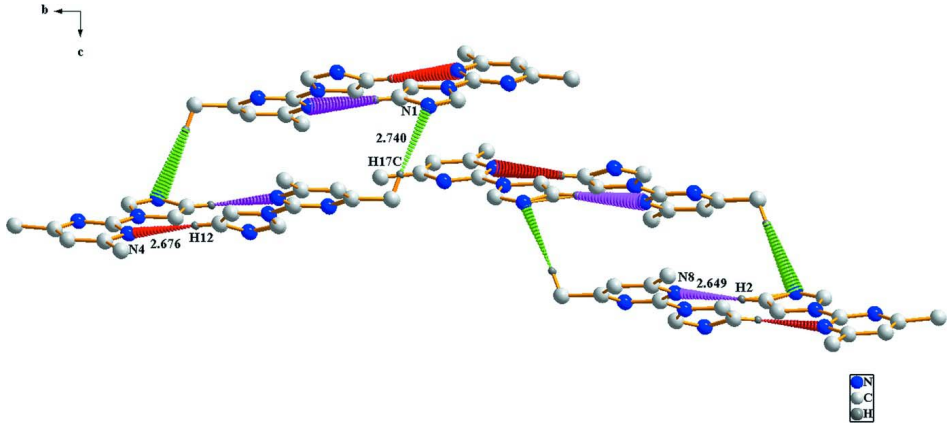

Figure 2

The packing diagram of the title compound(I). H atoms not involved in hydrogen bonds are omitted.

2-(1*H*-Imidazol-1-yl)-4,6-dimethylpyrimidine

Crystal data

$C_9H_{10}N_4$
M_r = 174.21
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 9.304 (5) Å
b = 26.756 (5) Å
c = 7.129 (5) Å
β = 91.259 (5)°
V = 1774.2 (16) Å^3
Z = 8
F(000) = 736
D_x = 1.304 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 3786 reflections
θ = 2.7–25.4°
μ = 0.09 mm^{-1}
T = 296 K
Needle, white
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART diffractometer
Radiation source: sealed tube
Graphite monochromator
ω scans
11971 measured reflections
3091 independent reflections
2365 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.0°, θ_{min} = 1.5°
h = −11→10
k = −26→31
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.197
S = 1.14
3091 reflections
240 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
$w = 1/[\sigma^2(F_o^2) + (0.0895P)^2 + 0.9302P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.008 (2)

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}
N7	0.3875 (2)	0.45208 (8)	0.7788 (3)	0.0472 (6)
N2	0.1912 (2)	0.21267 (8)	0.6762 (3)	0.0493 (6)
N4	−0.0469 (2)	0.22566 (9)	0.5881 (3)	0.0483 (6)
N8	0.5461 (2)	0.52131 (8)	0.7336 (3)	0.0461 (6)
N6	0.3095 (2)	0.53376 (8)	0.8162 (3)	0.0465 (6)
C13	0.4215 (3)	0.50025 (10)	0.7736 (4)	0.0420 (6)
C14	0.4946 (3)	0.42061 (10)	0.7404 (4)	0.0471 (7)
N3	0.1114 (2)	0.29410 (9)	0.6535 (3)	0.0513 (6)
C15	0.6291 (3)	0.43849 (11)	0.6982 (4)	0.0517 (7)
H15	0.7034	0.4164	0.6727	0.062*
C4	0.0780 (3)	0.24630 (10)	0.6363 (4)	0.0453 (7)
N5	0.0973 (3)	0.56080 (10)	0.9067 (4)	0.0649 (8)

C5	0.0032 (3)	0.32600 (11)	0.6131 (4)	0.0539 (8)
C16	0.6525 (3)	0.48921 (11)	0.6942 (4)	0.0474 (7)
C7	−0.1541 (3)	0.25785 (11)	0.5495 (4)	0.0494 (7)
C6	−0.1306 (3)	0.30860 (11)	0.5581 (4)	0.0550 (8)
H6	−0.2041	0.3309	0.5271	0.066*
C10	0.1743 (3)	0.52165 (12)	0.8750 (4)	0.0552 (8)
H10	0.1420	0.4890	0.8903	0.066*
N1	0.4063 (3)	0.18529 (10)	0.7662 (5)	0.0728 (9)
C11	0.3144 (3)	0.58522 (11)	0.8102 (4)	0.0548 (8)
H11	0.3914	0.6051	0.7755	0.066*
C9	−0.2980 (3)	0.23589 (13)	0.4997 (5)	0.0647 (9)
H9A	−0.2873	0.2114	0.4027	0.097*
H9B	−0.3615	0.2619	0.4560	0.097*
H9C	−0.3373	0.2203	0.6086	0.097*
C3	0.3271 (3)	0.22439 (12)	0.7368 (5)	0.0622 (9)
H3	0.3593	0.2570	0.7551	0.075*
C18	0.7944 (3)	0.51142 (13)	0.6463 (5)	0.0625 (9)
H18A	0.7812	0.5352	0.5464	0.094*
H18B	0.8582	0.4854	0.6070	0.094*
H18C	0.8351	0.5279	0.7546	0.094*
C17	0.4608 (4)	0.36581 (11)	0.7441 (5)	0.0664 (9)
H17A	0.3708	0.3607	0.8044	0.100*
H17B	0.5356	0.3484	0.8123	0.100*
H17C	0.4545	0.3533	0.6180	0.100*
C1	0.1867 (3)	0.16122 (11)	0.6687 (5)	0.0629 (9)
H1	0.1088	0.1413	0.6328	0.076*
C12	0.1844 (3)	0.60062 (12)	0.8651 (5)	0.0647 (9)
H12	0.1569	0.6339	0.8738	0.078*
C8	0.0358 (4)	0.38062 (12)	0.6319 (6)	0.0768 (11)
H8A	0.0052	0.3923	0.7520	0.115*
H8B	−0.0143	0.3987	0.5344	0.115*
H8C	0.1374	0.3859	0.6214	0.115*
C2	0.3180 (3)	0.14584 (13)	0.7239 (6)	0.0734 (10)
H2	0.3456	0.1125	0.7323	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N7	0.0400 (13)	0.0420 (13)	0.0596 (14)	−0.0005 (10)	−0.0030 (10)	−0.0009 (10)
N2	0.0380 (13)	0.0443 (14)	0.0659 (15)	−0.0011 (10)	0.0068 (11)	0.0059 (11)
N4	0.0401 (13)	0.0492 (14)	0.0559 (14)	−0.0035 (10)	0.0065 (10)	0.0015 (10)
N8	0.0342 (12)	0.0457 (14)	0.0583 (14)	−0.0013 (10)	−0.0026 (10)	−0.0007 (10)
N6	0.0354 (12)	0.0439 (13)	0.0601 (14)	0.0023 (10)	−0.0018 (10)	−0.0037 (10)
C13	0.0358 (14)	0.0414 (15)	0.0485 (15)	0.0028 (11)	−0.0041 (11)	−0.0017 (11)
C14	0.0433 (15)	0.0424 (15)	0.0553 (16)	0.0035 (12)	−0.0057 (12)	−0.0024 (12)
N3	0.0425 (13)	0.0436 (14)	0.0681 (15)	−0.0002 (11)	0.0125 (11)	0.0031 (11)
C15	0.0395 (15)	0.0509 (18)	0.0645 (18)	0.0094 (13)	−0.0011 (13)	−0.0025 (13)
C4	0.0387 (15)	0.0454 (16)	0.0522 (16)	0.0021 (12)	0.0109 (12)	0.0040 (12)

N5	0.0360 (13)	0.0625 (17)	0.096 (2)	0.0053 (12)	0.0027 (13)	−0.0125 (14)
C5	0.0479 (17)	0.0472 (17)	0.0672 (18)	0.0042 (13)	0.0165 (14)	0.0047 (13)
C16	0.0366 (14)	0.0505 (17)	0.0548 (17)	0.0018 (12)	−0.0038 (12)	0.0009 (12)
C7	0.0404 (15)	0.0578 (18)	0.0504 (16)	0.0026 (13)	0.0092 (12)	0.0050 (13)
C6	0.0411 (16)	0.0547 (19)	0.0694 (19)	0.0047 (13)	0.0094 (14)	0.0074 (14)
C10	0.0357 (15)	0.0547 (18)	0.075 (2)	−0.0004 (13)	0.0035 (13)	−0.0041 (14)
N1	0.0422 (15)	0.0608 (18)	0.115 (2)	0.0029 (13)	0.0018 (15)	0.0157 (16)
C11	0.0427 (16)	0.0431 (16)	0.078 (2)	0.0040 (13)	0.0000 (14)	−0.0005 (14)
C9	0.0428 (17)	0.081 (2)	0.071 (2)	−0.0022 (16)	0.0011 (14)	−0.0004 (17)
C3	0.0402 (17)	0.0538 (19)	0.093 (2)	−0.0027 (14)	−0.0002 (15)	0.0081 (16)
C18	0.0376 (16)	0.064 (2)	0.086 (2)	0.0005 (14)	0.0039 (15)	0.0028 (16)
C17	0.0557 (19)	0.0439 (18)	0.100 (2)	−0.0009 (15)	0.0019 (17)	−0.0026 (16)
C1	0.0459 (17)	0.0442 (17)	0.099 (2)	−0.0030 (14)	0.0063 (16)	0.0055 (16)
C12	0.0490 (18)	0.0501 (19)	0.095 (2)	0.0104 (15)	−0.0030 (16)	−0.0094 (16)
C8	0.060 (2)	0.0479 (19)	0.124 (3)	0.0022 (16)	0.015 (2)	0.0013 (19)
C2	0.0458 (18)	0.0491 (19)	0.126 (3)	0.0060 (15)	0.0120 (18)	0.0158 (19)

Geometric parameters (Å, º)

N7—C13	1.328 (3)	C7—C9	1.497 (4)
N7—C14	1.337 (4)	C6—H6	0.9300
N2—C3	1.363 (4)	C10—H10	0.9300
N2—C1	1.378 (4)	N1—C3	1.294 (4)
N2—C4	1.410 (4)	N1—C2	1.367 (4)
N4—C4	1.325 (4)	C11—C12	1.344 (4)
N4—C7	1.342 (4)	C11—H11	0.9300
N8—C13	1.326 (3)	C9—H9A	0.9600
N8—C16	1.345 (3)	C9—H9B	0.9600
N6—C10	1.373 (4)	C9—H9C	0.9600
N6—C11	1.379 (4)	C3—H3	0.9300
N6—C13	1.413 (3)	C18—H18A	0.9600
C14—C15	1.379 (4)	C18—H18B	0.9600
C14—C17	1.500 (4)	C18—H18C	0.9600
N3—C4	1.321 (4)	C17—H17A	0.9600
N3—C5	1.347 (4)	C17—H17B	0.9600
C15—C16	1.375 (4)	C17—H17C	0.9600
C15—H15	0.9300	C1—C2	1.340 (5)
N5—C10	1.292 (4)	C1—H1	0.9300
N5—C12	1.375 (4)	C12—H12	0.9300
C5—C6	1.378 (4)	C8—H8A	0.9600
C5—C8	1.498 (4)	C8—H8B	0.9600
C16—C18	1.495 (4)	C8—H8C	0.9600
C7—C6	1.377 (4)	C2—H2	0.9300
C13—N7—C14	115.3 (2)	C12—C11—N6	105.5 (3)
C3—N2—C1	105.6 (2)	C12—C11—H11	127.3
C3—N2—C4	126.9 (3)	N6—C11—H11	127.3
C1—N2—C4	127.4 (2)	C7—C9—H9A	109.5

C4—N4—C7	115.4 (2)	C7—C9—H9B	109.5
C13—N8—C16	115.1 (2)	H9A—C9—H9B	109.5
C10—N6—C11	106.0 (2)	C7—C9—H9C	109.5
C10—N6—C13	126.9 (2)	H9A—C9—H9C	109.5
C11—N6—C13	127.0 (2)	H9B—C9—H9C	109.5
N8—C13—N7	128.9 (2)	N1—C3—N2	112.7 (3)
N8—C13—N6	115.4 (2)	N1—C3—H3	123.6
N7—C13—N6	115.6 (2)	N2—C3—H3	123.6
N7—C14—C15	120.7 (3)	C16—C18—H18A	109.5
N7—C14—C17	117.0 (3)	C16—C18—H18B	109.5
C15—C14—C17	122.3 (3)	H18A—C18—H18B	109.5
C4—N3—C5	114.8 (3)	C16—C18—H18C	109.5
C16—C15—C14	119.5 (3)	H18A—C18—H18C	109.5
C16—C15—H15	120.3	H18B—C18—H18C	109.5
C14—C15—H15	120.3	C14—C17—H17A	109.5
N3—C4—N4	129.1 (3)	C14—C17—H17B	109.5
N3—C4—N2	115.2 (2)	H17A—C17—H17B	109.5
N4—C4—N2	115.7 (2)	C14—C17—H17C	109.5
C10—N5—C12	105.0 (3)	H17A—C17—H17C	109.5
N3—C5—C6	120.9 (3)	H17B—C17—H17C	109.5
N3—C5—C8	116.8 (3)	C2—C1—N2	105.5 (3)
C6—C5—C8	122.4 (3)	C2—C1—H1	127.2
N8—C16—C15	120.6 (2)	N2—C1—H1	127.2
N8—C16—C18	116.9 (2)	C11—C12—N5	111.3 (3)
C15—C16—C18	122.6 (3)	C11—C12—H12	124.3
N4—C7—C6	120.5 (3)	N5—C12—H12	124.3
N4—C7—C9	116.9 (3)	C5—C8—H8A	109.5
C6—C7—C9	122.6 (3)	C5—C8—H8B	109.5
C7—C6—C5	119.2 (3)	H8A—C8—H8B	109.5
C7—C6—H6	120.4	C5—C8—H8C	109.5
C5—C6—H6	120.4	H8A—C8—H8C	109.5
N5—C10—N6	112.2 (3)	H8B—C8—H8C	109.5
N5—C10—H10	123.9	C1—C2—N1	111.6 (3)
N6—C10—H10	123.9	C1—C2—H2	124.2
C3—N1—C2	104.5 (3)	N1—C2—H2	124.2

C16—N8—C13—N7	−0.5 (4)	C13—N8—C16—C18	179.4 (3)
C16—N8—C13—N6	179.7 (2)	C14—C15—C16—N8	0.9 (4)
C14—N7—C13—N8	0.9 (4)	C14—C15—C16—C18	−178.9 (3)
C14—N7—C13—N6	−179.3 (2)	C4—N4—C7—C6	1.0 (4)
C10—N6—C13—N8	−175.0 (3)	C4—N4—C7—C9	−178.3 (2)
C11—N6—C13—N8	3.8 (4)	N4—C7—C6—C5	−2.2 (4)
C10—N6—C13—N7	5.2 (4)	C9—C7—C6—C5	177.1 (3)
C11—N6—C13—N7	−176.0 (3)	N3—C5—C6—C7	1.7 (4)
C13—N7—C14—C15	−0.3 (4)	C8—C5—C6—C7	−178.0 (3)
C13—N7—C14—C17	−179.9 (3)	C12—N5—C10—N6	0.7 (4)
N7—C14—C15—C16	−0.6 (4)	C11—N6—C10—N5	−0.5 (4)
C17—C14—C15—C16	179.0 (3)	C13—N6—C10—N5	178.5 (3)

C5—N3—C4—N4	−1.2 (4)	C10—N6—C11—C12	0.1 (3)
C5—N3—C4—N2	179.3 (2)	C13—N6—C11—C12	−178.9 (3)
C7—N4—C4—N3	0.8 (4)	C2—N1—C3—N2	−0.3 (4)
C7—N4—C4—N2	−179.7 (2)	C1—N2—C3—N1	0.3 (4)
C3—N2—C4—N3	2.8 (4)	C4—N2—C3—N1	178.3 (3)
C1—N2—C4—N3	−179.7 (3)	C3—N2—C1—C2	−0.2 (4)
C3—N2—C4—N4	−176.8 (3)	C4—N2—C1—C2	−178.1 (3)
C1—N2—C4—N4	0.8 (4)	N6—C11—C12—N5	0.3 (4)
C4—N3—C5—C6	−0.1 (4)	C10—N5—C12—C11	−0.6 (4)
C4—N3—C5—C8	179.6 (3)	N2—C1—C2—N1	0.0 (4)
C13—N8—C16—C15	−0.4 (4)	C3—N1—C2—C1	0.2 (4)