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Crystal structure of cyprodinil

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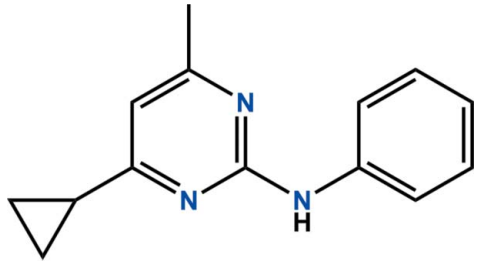
In the title compound, $C_{14}H_{15}N_3$ (systematic name: 4-cyclopropyl-6-methyl-*N*-phenylpyrimidin-2-amine), which is the anilinopyrimidine fungicide cyprodinil, the dihedral angles between the planes of the central pyrimidine ring and the terminal phenyl ring and the mean plane of the cyclopropane ring system are 14.52 (11) and 88.79 (10)°, respectively. In the crystal, weak π–π interactions [3.8551 (11) Å] connect the dimers into chains along the *b*-axis direction.

Keywords: crystal structure; cyprodinil; pyrimidin-2-amine; fungicide; hydrogen bonding; π–π interactions.

CCDC reference: 1035821

1. Related literature

For information on the fungicidal properties of the title compound, see: Sapp *et al.* (2003). For a related crystal structure, see: Kang *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_{14}H_{15}N_3$
M_r = 225.29
Monoclinic, $P2_1/c$
a = 13.1920 (6) Å
b = 5.3176 (2) Å
c = 16.8641 (7) Å
β = 100.288 (2)°
V = 1163.99 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 K
0.45 × 0.22 × 0.18 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.965, T_{max} = 0.986
18116 measured reflections
2864 independent reflections
2463 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.166
S = 1.14
2864 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5422).

References

Brandenburg, K. (2010). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kang, G., Jeon, Y., Lee, S. & Kim, T. H. (2014). *Acta Cryst.* E**70**, o1265.
Sapp, M., Ertunc, T., Bringmann, I., Schaffer, A. & Schmidt, S. (2003). *Pest Manag. Sci.* **60**, 65–74.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2015). E**71**, o5 [https://doi.org/10.1107/S2056989014025742]

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S1. Comment

Cyprodinil, $C_{14}H_{15}N_3$, is a systemic pyrimidine fungicide for foliar applications on cereals and strawberries against plant pathogenic fungi (Sapp *et al.*, 2003). Its crystal structure is reported herein. In this compound (Scheme 1, Fig. 1), the dihedral angles between the central pyrimidine ring and the terminal phenyl ring and mean plane of cyclopropane ring system are 14.52 (11) and 88.79 (10)°. All bond lengths and bond angles are normal and comparable to those observed in the crystal structure of a similar compound (Kang *et al.*, 2014).

In the crystal structure (Fig. 2), The crystal structure is stabilized by weak intermolecular π–π interaction between the pyrimidine ring and terminal phenyl ring systems [*C*g1···*C*g2^{ii}, 3.8552 (11) Å] are present (*C*g1 and *C*g2 are the centroids of the C1—C6 and C7—N2—C8—C9—C10—N3 rings, respectively) [for symmetry codes: (ii), *x*, *y* - 1, *z*].

S2. Experimental

The title compound was purchased from the Chem Servies Company. Slow evaporation of a solution in CH_2Cl_2 gave single crystals suitable for X-ray analysis.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(N—H) = 0.88 Å, U_{iso} = 1.2U_{eq}(C) for amine group, d(C—H) = 0.98 Å, U_{iso} = 1.5U_{eq}(C) for methyl group, d(C—H) = 0.99 Å, U_{iso} = 1.2U_{eq}(C) for Csp^3—H, d(C—H) = 1.00 Å, U_{iso} = 1.2U_{eq}(C) for Csp^3—H, and d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for aromatic C—H.

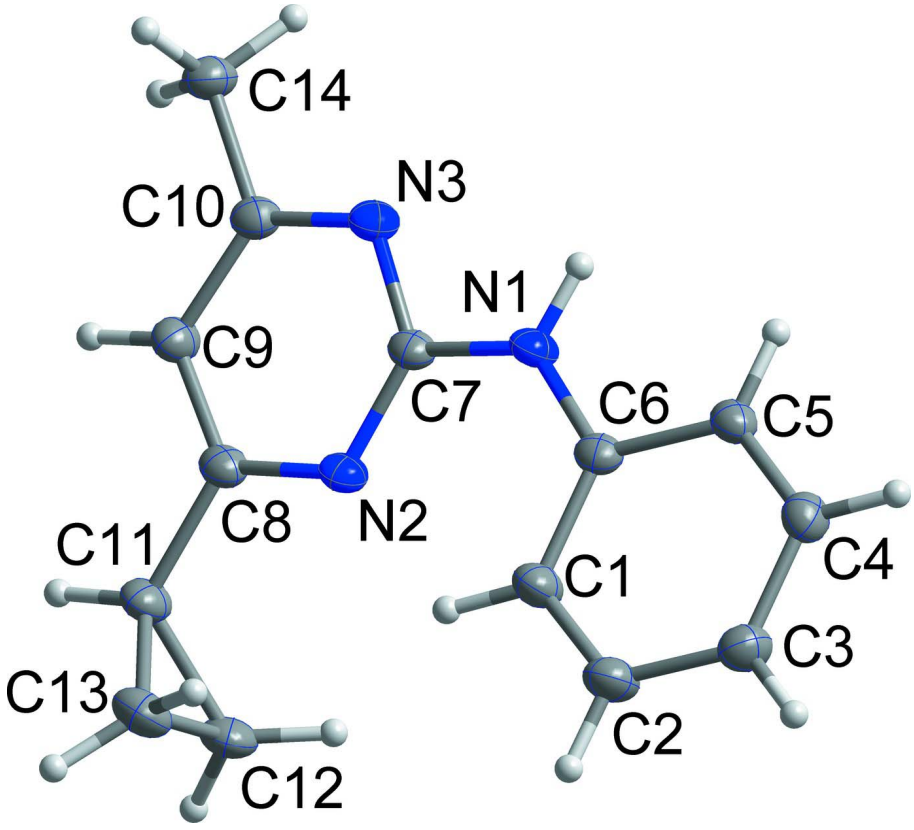

Figure 1

The asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

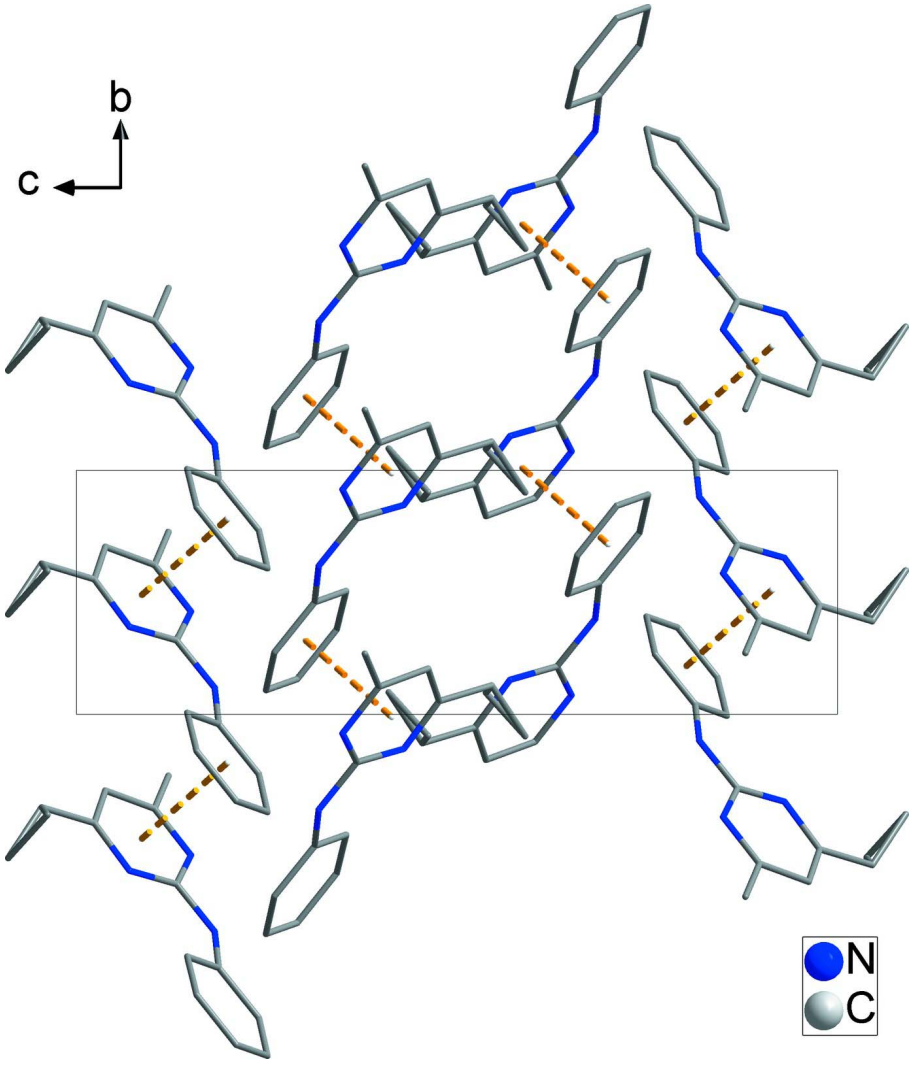

Figure 2

Crystal packing viewed along the *a* axis. The weak π–π interactions are shown as dashed lines.

4-Cyclopropyl-6-methyl-*N*-phenylpyrimidin-2-amine

Crystal data

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Monoclinic, $P2_1/c$
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$\beta = 100.288\ (2)°$
$V = 1163.99\ (8)$ Å^3
$Z = 4$

$F(000) = 480$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8168 reflections
$\theta = 2.5$–$28.2°$
$\mu = 0.08$ mm^{-1}
$T = 173$ K
Block, colourless
0.45 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.965, T_{max} = 0.986
18116 measured reflections
2864 independent reflections
2463 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 28.3°, θ_{min} = 1.6°
h = −17→17
k = −7→7
l = −21→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.166
S = 1.14
2864 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 1.3715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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}
N1	0.64381 (12)	0.1086 (3)	0.81833 (9)	0.0210 (3)
H1N	0.5882	0.0697	0.7834	0.025*
N2	0.70730 (12)	0.3584 (3)	0.93020 (9)	0.0201 (3)
N3	0.53921 (12)	0.4215 (3)	0.84955 (9)	0.0206 (3)
C1	0.83033 (14)	0.0059 (4)	0.85440 (11)	0.0246 (4)
H1	0.8436	0.1437	0.8906	0.030*
C2	0.90995 (15)	−0.1513 (4)	0.84207 (12)	0.0277 (4)
H2	0.9778	−0.1183	0.8700	0.033*
C3	0.89324 (15)	−0.3555 (4)	0.79011 (12)	0.0256 (4)
H3	0.9486	−0.4621	0.7827	0.031*
C4	0.79368 (15)	−0.4010 (4)	0.74907 (11)	0.0241 (4)
H4	0.7808	−0.5396	0.7131	0.029*
C5	0.71331 (14)	−0.2457 (4)	0.76022 (11)	0.0208 (4)
H5	0.6458	−0.2787	0.7318	0.025*
C6	0.73029 (14)	−0.0402 (4)	0.81301 (10)	0.0195 (4)
C7	0.63140 (14)	0.3035 (4)	0.86853 (10)	0.0189 (4)

C8	0.69016 (14)	0.5539 (4)	0.97648 (10)	0.0208 (4)
C9	0.59859 (15)	0.6871 (4)	0.96202 (11)	0.0233 (4)
H9	0.5873	0.8251	0.9951	0.028*
C10	0.52353 (14)	0.6127 (4)	0.89742 (11)	0.0209 (4)
C11	0.77222 (15)	0.6184 (4)	1.04550 (11)	0.0246 (4)
H11	0.7567	0.7622	1.0796	0.029*
C12	0.83749 (15)	0.4101 (4)	1.08962 (12)	0.0276 (4)
H12A	0.8585	0.4258	1.1488	0.033*
H12B	0.8239	0.2360	1.0698	0.033*
C13	0.88371 (16)	0.5880 (4)	1.03804 (12)	0.0300 (5)
H13A	0.8989	0.5239	0.9863	0.036*
H13B	0.9334	0.7136	1.0653	0.036*
C14	0.42255 (15)	0.7483 (4)	0.87894 (12)	0.0255 (4)
H14A	0.4283	0.8895	0.8427	0.038*
H14B	0.4043	0.8118	0.9291	0.038*
H14C	0.3690	0.6324	0.8530	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0185 (7)	0.0259 (8)	0.0165 (7)	0.0004 (6)	−0.0023 (5)	−0.0027 (6)
N2	0.0205 (7)	0.0238 (8)	0.0145 (7)	0.0001 (6)	−0.0009 (5)	0.0008 (6)
N3	0.0196 (7)	0.0250 (8)	0.0164 (7)	0.0014 (6)	0.0010 (5)	0.0005 (6)
C1	0.0218 (9)	0.0278 (10)	0.0221 (9)	−0.0006 (8)	−0.0016 (7)	−0.0040 (8)
C2	0.0209 (9)	0.0329 (11)	0.0270 (9)	0.0014 (8)	−0.0016 (7)	−0.0027 (8)
C3	0.0242 (9)	0.0279 (10)	0.0243 (9)	0.0047 (8)	0.0031 (7)	0.0001 (8)
C4	0.0290 (10)	0.0234 (10)	0.0194 (8)	−0.0003 (8)	0.0027 (7)	−0.0025 (7)
C5	0.0226 (9)	0.0220 (9)	0.0166 (8)	−0.0016 (7)	0.0002 (6)	0.0006 (7)
C6	0.0207 (8)	0.0227 (9)	0.0146 (7)	0.0004 (7)	0.0014 (6)	0.0019 (7)
C7	0.0200 (8)	0.0221 (9)	0.0138 (7)	0.0002 (7)	0.0007 (6)	0.0016 (7)
C8	0.0227 (9)	0.0233 (9)	0.0151 (8)	−0.0009 (7)	0.0005 (6)	0.0016 (7)
C9	0.0258 (9)	0.0246 (10)	0.0181 (8)	0.0028 (8)	0.0001 (7)	−0.0033 (7)
C10	0.0219 (9)	0.0235 (9)	0.0167 (8)	0.0015 (7)	0.0018 (6)	0.0022 (7)
C11	0.0250 (9)	0.0284 (10)	0.0180 (8)	0.0005 (8)	−0.0025 (7)	−0.0035 (7)
C12	0.0244 (9)	0.0333 (11)	0.0216 (9)	0.0006 (8)	−0.0053 (7)	0.0005 (8)
C13	0.0245 (9)	0.0382 (12)	0.0247 (9)	−0.0057 (8)	−0.0022 (7)	−0.0022 (9)
C14	0.0232 (9)	0.0289 (10)	0.0226 (9)	0.0054 (8)	−0.0005 (7)	−0.0004 (8)

Geometric parameters (Å, º)

N1—C7	1.367 (2)	C5—H5	0.9500
N1—C6	1.404 (2)	C8—C9	1.384 (3)
N1—H1N	0.8800	C8—C11	1.481 (2)
N2—C7	1.341 (2)	C9—C10	1.392 (3)
N2—C8	1.343 (2)	C9—H9	0.9500
N3—C10	1.337 (2)	C10—C14	1.498 (3)
N3—C7	1.355 (2)	C11—C13	1.507 (3)
C1—C2	1.387 (3)	C11—C12	1.514 (3)

C1—C6	1.400 (2)	C11—H11	1.0000
C1—H1	0.9500	C12—C13	1.488 (3)
C2—C3	1.388 (3)	C12—H12A	0.9900
C2—H2	0.9500	C12—H12B	0.9900
C3—C4	1.392 (3)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
C4—C5	1.383 (3)	C14—H14A	0.9800
C4—H4	0.9500	C14—H14B	0.9800
C5—C6	1.402 (3)	C14—H14C	0.9800

C7—N1—C6	130.97 (15)	C8—C9—H9	121.0
C7—N1—H1N	114.5	C10—C9—H9	121.0
C6—N1—H1N	114.5	N3—C10—C9	121.56 (17)
C7—N2—C8	116.06 (16)	N3—C10—C14	117.93 (16)
C10—N3—C7	116.01 (16)	C9—C10—C14	120.50 (17)
C2—C1—C6	119.45 (18)	C8—C11—C13	119.78 (16)
C2—C1—H1	120.3	C8—C11—C12	119.22 (18)
C6—C1—H1	120.3	C13—C11—C12	58.99 (14)
C1—C2—C3	121.81 (18)	C8—C11—H11	115.7
C1—C2—H2	119.1	C13—C11—H11	115.7
C3—C2—H2	119.1	C12—C11—H11	115.7
C2—C3—C4	118.62 (18)	C13—C12—C11	60.26 (14)
C2—C3—H3	120.7	C13—C12—H12A	117.7
C4—C3—H3	120.7	C11—C12—H12A	117.7
C5—C4—C3	120.47 (18)	C13—C12—H12B	117.7
C5—C4—H4	119.8	C11—C12—H12B	117.7
C3—C4—H4	119.8	H12A—C12—H12B	114.9
C4—C5—C6	120.82 (17)	C12—C13—C11	60.74 (14)
C4—C5—H5	119.6	C12—C13—H13A	117.7
C6—C5—H5	119.6	C11—C13—H13A	117.7
C1—C6—C5	118.84 (17)	C12—C13—H13B	117.7
C1—C6—N1	125.02 (17)	C11—C13—H13B	117.7
C5—C6—N1	116.12 (16)	H13A—C13—H13B	114.8
N2—C7—N3	126.65 (17)	C10—C14—H14A	109.5
N2—C7—N1	119.35 (16)	C10—C14—H14B	109.5
N3—C7—N1	114.00 (16)	H14A—C14—H14B	109.5
N2—C8—C9	121.73 (17)	C10—C14—H14C	109.5
N2—C8—C11	117.43 (17)	H14A—C14—H14C	109.5
C9—C8—C11	120.82 (17)	H14B—C14—H14C	109.5
C8—C9—C10	117.96 (18)		

C6—C1—C2—C3	−0.5 (3)	C6—N1—C7—N3	172.68 (17)
C1—C2—C3—C4	0.5 (3)	C7—N2—C8—C9	1.2 (3)
C2—C3—C4—C5	−0.2 (3)	C7—N2—C8—C11	179.58 (16)
C3—C4—C5—C6	−0.1 (3)	N2—C8—C9—C10	0.0 (3)
C2—C1—C6—C5	0.2 (3)	C11—C8—C9—C10	−178.32 (18)
C2—C1—C6—N1	−178.05 (18)	C7—N3—C10—C9	1.0 (3)
C4—C5—C6—C1	0.1 (3)	C7—N3—C10—C14	−179.81 (17)

C4—C5—C6—N1	178.52 (17)	C8—C9—C10—N3	−1.2 (3)
C7—N1—C6—C1	−8.8 (3)	C8—C9—C10—C14	179.64 (18)
C7—N1—C6—C5	172.85 (18)	N2—C8—C11—C13	35.3 (3)
C8—N2—C7—N3	−1.5 (3)	C9—C8—C11—C13	−146.3 (2)
C8—N2—C7—N1	179.34 (16)	N2—C8—C11—C12	−33.6 (3)
C10—N3—C7—N2	0.4 (3)	C9—C8—C11—C12	144.84 (19)
C10—N3—C7—N1	179.63 (16)	C8—C11—C12—C13	109.1 (2)
C6—N1—C7—N2	−8.0 (3)	C8—C11—C13—C12	−108.2 (2)