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2-Chloro-*N*′-[(*E*)-(2-methoxy-1-naphthyl)-methylene]benzohydrazide

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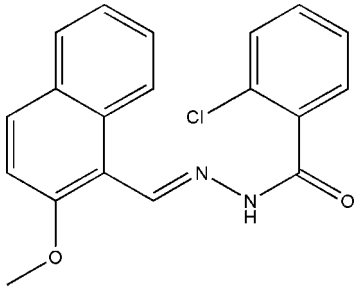
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.062; wR factor = 0.142; data-to-parameter ratio = 15.7.

In the molecule of the title Schiff base compound, $C_{19}H_{15}ClN_2O_2$, the dihedral angle between the benzene ring and naphthyl ring system is 77.1 (2)°. In the crystal structure, centrosymmetrically related molecules are linked into dimers through pairs of intermolecular N–H···O hydrogen bonds, generating rings of graph set $R_2^2(8)$.

Related literature

For related structures, see: Tang (2007, 2008). For bond-length data, see: Allen *et al.* (1987). For graph-set analysis, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{15}ClN_2O_2$
M_r = 338.78
Monoclinic, $P2_1/c$
a = 10.751 (2) Å
b = 11.405 (2) Å
c = 14.376 (3) Å
β = 107.794 (10)°
V = 1678.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 298 K
0.30 × 0.28 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.931, T_{max} = 0.938
13186 measured reflections
3473 independent reflections
1295 reflections with $I > 2\sigma(I)$
R_{int} = 0.158

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.142
S = 0.88
3473 reflections
221 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.90 (3)	1.99 (3)	2.886 (4)	172 (4)

Symmetry code: (i) $-x+1, -y+1, -z$.

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: *SHELXL97*.

Financial support from Jiaying University Research Fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2320).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tang, C.-B. (2007). *Acta Cryst.* E**63**, o4841.
Tang, C.-B. (2008). *Acta Cryst.* E**64**, o1381.

supporting information

Acta Cryst. (2009). E**65**, o1254 [doi:10.1107/S1600536809016936]

2-Chloro-*N*′-[(*E*)-(2-methoxy-1-naphthyl)methylene]benzohydrazide

Chunbao Tang

S1. Comment

Recently, the author has reported the structures of a few Schiff base compounds (Tang, 2007; Tang 2008). In a continuation of work in this area, the crystal structure of the title compound is reported herein.

In the title compound (Fig. 1), the dihedral angle between the benzene ring and the naphthyl ring system is 77.1 (2) °. The molecule adopts an E configuration about the C═N bond. All the bond lengths are within normal values (Allen *et al.*, 1987). In the crystal structure (Fig. 2), centrosymmetrically related molecules are linked into dimers through intermolecular N–H···O hydrogen bonds (Table 1), forming rings of graph set $R^2_2(8)$ (Etter *et al.*, 1990; Bernstein *et al.*, 1995).

S2. Experimental

2-Methoxy-1-naphthylaldehyde (0.1 mmol, 18.6 mg) and 2-chlorobenzohydrazide (0.1 mmol, 12.6 mg) were dissolved in a methanol solution (20 ml). The mixture was stirred at reflux for 10 min to give a clear colourless solution. Colourless block-like crystals of the compound were formed by slow evaporation of the solvent over several days.

S3. Refinement

Atom H2 was located from a difference Fourier map and refined isotropically, with U_{iso} restrained to 0.08Å^2. Other H atoms were constrained to ideal geometries, with C–H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.

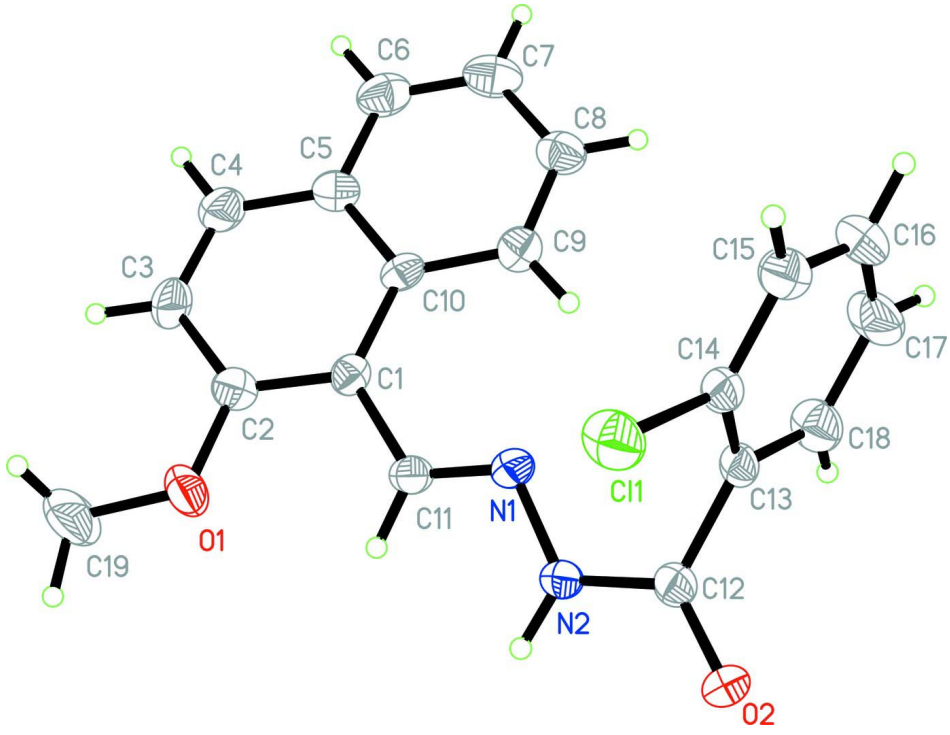


Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

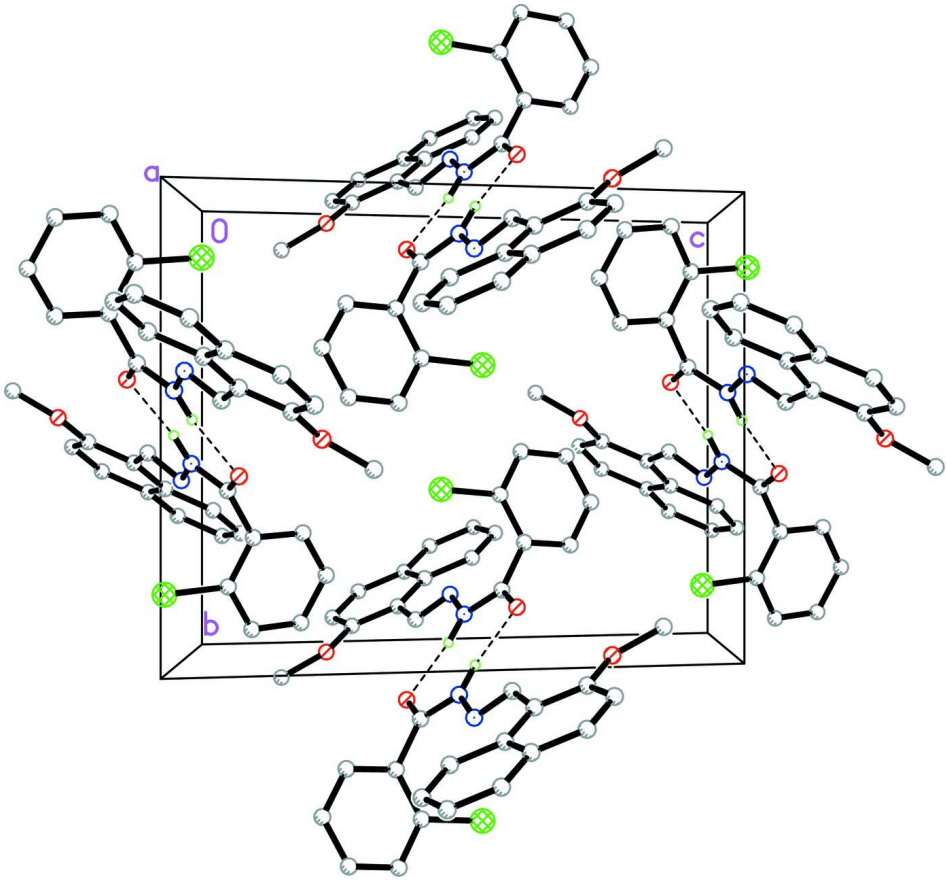


Figure 2

Packing diagram of the title compound viewed along the *a* axis. Intermolecular hydrogen bonds are drawn as dashed lines. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity.

2-chloro-N′-[(E)-(2-methoxy-1-naphthyl)methylene]benzohydrazide

Crystal data

$C_{19}H_{15}ClN_2O_2$
$M_r = 338.78$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.751\ (2)$ Å
$b = 11.405\ (2)$ Å
$c = 14.376\ (3)$ Å
$\beta = 107.794\ (10)°$
$V = 1678.4\ (6)$ Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.341$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 394 reflections
$\theta = 2.3–24.5°$
$\mu = 0.24$ mm^{-1}
$T = 298$ K
Block, colourless
0.30 × 0.28 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.931$, $T_{max} = 0.938$
13186 measured reflections
3473 independent reflections
1295 reflections with $I > 2\sigma(I)$

R_{int} = 0.158
θ_{max} = 26.5°, θ_{min} = 2.0°
h = −13→12
k = −14→14
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.142
S = 0.88
3473 reflections
221 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.58262 (12)	0.13770 (9)	0.03814 (8)	0.0647 (4)
N2	0.6442 (3)	0.4212 (3)	−0.0046 (2)	0.0427 (8)
O1	0.9807 (3)	0.5231 (3)	0.2634 (2)	0.0675 (9)
N1	0.7735 (3)	0.3824 (3)	0.0222 (2)	0.0435 (9)
C1	0.9913 (4)	0.4199 (3)	0.1258 (3)	0.0386 (10)
O2	0.4392 (3)	0.3960 (2)	−0.10180 (18)	0.0516 (8)
C10	1.0644 (4)	0.3584 (3)	0.0738 (3)	0.0397 (10)
C12	0.5539 (4)	0.3633 (3)	−0.0752 (3)	0.0416 (10)
C13	0.5987 (3)	0.2590 (3)	−0.1185 (3)	0.0379 (10)
C2	1.0565 (4)	0.4677 (3)	0.2165 (3)	0.0474 (11)
C11	0.8515 (4)	0.4435 (3)	0.0891 (3)	0.0413 (10)
H11	0.8179	0.5057	0.1158	0.050*
C5	1.2017 (4)	0.3485 (3)	0.1163 (3)	0.0493 (11)
C14	0.6132 (3)	0.1509 (4)	−0.0725 (3)	0.0417 (10)
C6	1.2771 (4)	0.2898 (4)	0.0656 (4)	0.0627 (13)
H6	1.3670	0.2834	0.0940	0.075*
C9	1.0092 (4)	0.3089 (3)	−0.0203 (3)	0.0480 (11)
H9	0.9197	0.3150	−0.0509	0.058*
C3	1.1932 (4)	0.4552 (4)	0.2586 (3)	0.0581 (12)
H3	1.2352	0.4869	0.3198	0.070*
C8	1.0851 (4)	0.2527 (3)	−0.0668 (3)	0.0547 (12)

H8	1.0462	0.2203	−0.1282	0.066*
C15	0.6539 (4)	0.0537 (4)	−0.1128 (3)	0.0568 (12)
H15	0.6640	−0.0183	−0.0810	0.068*
C7	1.2201 (5)	0.2428 (4)	−0.0240 (4)	0.0675 (14)
H7	1.2705	0.2042	−0.0567	0.081*
C18	0.6229 (4)	0.2670 (4)	−0.2066 (3)	0.0590 (13)
H18	0.6119	0.3385	−0.2392	0.071*
C4	1.2617 (4)	0.3971 (4)	0.2094 (3)	0.0604 (13)
H4	1.3514	0.3886	0.2375	0.072*
C16	0.6793 (4)	0.0650 (4)	−0.2006 (3)	0.0675 (14)
H16	0.7074	0.0004	−0.2281	0.081*
C17	0.6633 (5)	0.1709 (5)	−0.2476 (3)	0.0726 (15)
H17	0.6798	0.1779	−0.3072	0.087*
C19	1.0386 (5)	0.5842 (4)	0.3518 (4)	0.1002 (19)
H19A	1.0830	0.5296	0.4017	0.150*
H19B	0.9720	0.6240	0.3714	0.150*
H19C	1.1001	0.6404	0.3423	0.150*
H2	0.620 (4)	0.483 (2)	0.025 (3)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0873 (9)	0.0637 (8)	0.0513 (7)	0.0114 (7)	0.0332 (6)	0.0104 (6)
N2	0.035 (2)	0.045 (2)	0.047 (2)	0.0046 (19)	0.0109 (17)	−0.0093 (18)
O1	0.061 (2)	0.085 (2)	0.0540 (19)	0.0004 (18)	0.0137 (17)	−0.0316 (18)
N1	0.032 (2)	0.048 (2)	0.048 (2)	0.0042 (17)	0.0085 (18)	−0.0042 (18)
C1	0.036 (3)	0.035 (2)	0.041 (3)	−0.003 (2)	0.007 (2)	0.001 (2)
O2	0.0356 (18)	0.0600 (19)	0.0539 (18)	0.0118 (15)	0.0059 (15)	−0.0056 (15)
C10	0.030 (2)	0.045 (3)	0.045 (3)	0.005 (2)	0.012 (2)	0.009 (2)
C12	0.041 (3)	0.048 (3)	0.037 (2)	0.001 (2)	0.015 (2)	−0.003 (2)
C13	0.036 (3)	0.052 (3)	0.028 (2)	0.000 (2)	0.013 (2)	−0.003 (2)
C2	0.046 (3)	0.045 (3)	0.053 (3)	0.000 (2)	0.018 (2)	−0.003 (2)
C11	0.040 (3)	0.040 (3)	0.044 (3)	0.006 (2)	0.014 (2)	0.001 (2)
C5	0.049 (3)	0.043 (3)	0.058 (3)	0.003 (2)	0.020 (3)	0.003 (2)
C14	0.039 (3)	0.052 (3)	0.034 (2)	0.003 (2)	0.012 (2)	−0.004 (2)
C6	0.044 (3)	0.058 (3)	0.084 (4)	0.003 (3)	0.017 (3)	0.003 (3)
C9	0.044 (3)	0.052 (3)	0.048 (3)	−0.002 (2)	0.015 (2)	0.003 (2)
C3	0.045 (3)	0.064 (3)	0.052 (3)	−0.007 (2)	−0.004 (2)	−0.011 (3)
C8	0.064 (4)	0.051 (3)	0.055 (3)	0.008 (2)	0.027 (3)	0.004 (2)
C15	0.063 (3)	0.053 (3)	0.053 (3)	0.007 (2)	0.016 (2)	−0.001 (3)
C7	0.059 (4)	0.064 (3)	0.091 (4)	0.010 (3)	0.040 (3)	0.000 (3)
C18	0.077 (4)	0.058 (3)	0.046 (3)	0.005 (3)	0.024 (3)	0.005 (2)
C4	0.045 (3)	0.061 (3)	0.066 (3)	0.004 (2)	0.003 (3)	−0.009 (3)
C16	0.073 (3)	0.069 (4)	0.062 (3)	0.012 (3)	0.022 (3)	−0.022 (3)
C17	0.097 (4)	0.081 (4)	0.051 (3)	0.015 (3)	0.038 (3)	−0.009 (3)
C19	0.091 (4)	0.105 (4)	0.097 (4)	0.004 (3)	0.018 (3)	−0.064 (4)

Geometric parameters (Å, º)

Cl1—C14	1.726 (4)	C6—C7	1.356 (6)
N2—C12	1.344 (5)	C6—H6	0.9300
N2—N1	1.395 (4)	C9—C8	1.362 (5)
N2—H2	0.90 (3)	C9—H9	0.9300
O1—C2	1.361 (4)	C3—C4	1.342 (5)
O1—C19	1.416 (4)	C3—H3	0.9300
N1—C11	1.273 (4)	C8—C7	1.398 (6)
C1—C2	1.390 (5)	C8—H8	0.9300
C1—C10	1.424 (5)	C15—C16	1.377 (5)
C1—C11	1.458 (5)	C15—H15	0.9300
O2—C12	1.232 (4)	C7—H7	0.9300
C10—C9	1.418 (5)	C18—C17	1.375 (5)
C10—C5	1.419 (5)	C18—H18	0.9300
C12—C13	1.490 (5)	C4—H4	0.9300
C13—C18	1.371 (5)	C16—C17	1.369 (6)
C13—C14	1.385 (5)	C16—H16	0.9300
C2—C3	1.415 (5)	C17—H17	0.9300
C11—H11	0.9300	C19—H19A	0.9600
C5—C4	1.409 (5)	C19—H19B	0.9600
C5—C6	1.413 (5)	C19—H19C	0.9600
C14—C15	1.382 (5)		
C12—N2—N1	118.8 (3)	C8—C9—H9	119.5
C12—N2—H2	119 (3)	C10—C9—H9	119.5
N1—N2—H2	122 (3)	C4—C3—C2	119.3 (4)
C2—O1—C19	120.5 (3)	C4—C3—H3	120.3
C11—N1—N2	114.0 (3)	C2—C3—H3	120.3
C2—C1—C10	119.0 (4)	C9—C8—C7	121.3 (4)
C2—C1—C11	115.8 (4)	C9—C8—H8	119.4
C10—C1—C11	125.1 (4)	C7—C8—H8	119.4
C9—C10—C5	117.1 (4)	C16—C15—C14	119.1 (4)
C9—C10—C1	124.0 (4)	C16—C15—H15	120.4
C5—C10—C1	118.8 (4)	C14—C15—H15	120.4
O2—C12—N2	120.6 (4)	C6—C7—C8	119.6 (4)
O2—C12—C13	122.2 (4)	C6—C7—H7	120.2
N2—C12—C13	117.2 (4)	C8—C7—H7	120.2
C18—C13—C14	118.4 (4)	C13—C18—C17	121.1 (4)
C18—C13—C12	120.7 (4)	C13—C18—H18	119.5
C14—C13—C12	120.9 (3)	C17—C18—H18	119.5
O1—C2—C1	116.1 (4)	C3—C4—C5	122.0 (4)
O1—C2—C3	122.4 (4)	C3—C4—H4	119.0
C1—C2—C3	121.4 (4)	C5—C4—H4	119.0
N1—C11—C1	122.7 (4)	C17—C16—C15	120.3 (4)
N1—C11—H11	118.6	C17—C16—H16	119.8
C1—C11—H11	118.6	C15—C16—H16	119.8
C4—C5—C6	120.5 (4)	C16—C17—C18	120.0 (4)

C4—C5—C10	119.4 (4)	C16—C17—H17	120.0
C6—C5—C10	120.1 (4)	C18—C17—H17	120.0
C15—C14—C13	121.1 (4)	O1—C19—H19A	109.5
C15—C14—Cl1	119.3 (3)	O1—C19—H19B	109.5
C13—C14—Cl1	119.5 (3)	H19A—C19—H19B	109.5
C7—C6—C5	120.9 (4)	O1—C19—H19C	109.5
C7—C6—H6	119.6	H19A—C19—H19C	109.5
C5—C6—H6	119.6	H19B—C19—H19C	109.5
C8—C9—C10	121.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.90 (3)	1.99 (3)	2.886 (4)	172 (4)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.