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2-Chloro-*N*-methyl-*N*-phenylacetamide

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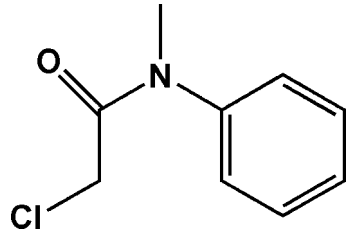
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.136; data-to-parameter ratio = 27.3.

In the title compound, $C_9H_{10}ClNO$, the non-H atoms, excluding the phenyl group, are almost coplanar (r.m.s. deviation of the non-H atoms = 0.1015 Å). The dihedral angle formed between this plane and the benzene ring is 87.07 (5)°. Weak intermolecular C—H···O interactions help to stabilize the packing.

Related literature

For the synthesis of lanthanide complexes with amide-type ligands, see: Wu *et al.* (2008). For related a structure, see: Yuan *et al.* (2010).



Experimental

Crystal data

$C_9H_{10}ClNO$
M_r = 183.63
Monoclinic, $P2_1/c$
a = 7.3391 (12) Å
b = 6.5898 (10) Å
c = 18.941 (3) Å
β = 91.192 (9)°
V = 915.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 296 K
0.26 × 0.21 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.912, T_{max} = 0.936
9758 measured reflections
3003 independent reflections
1869 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.136
S = 1.04
3003 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.58	3.4356 (19)	154

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: VM2064).

References

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Yuan, M.-S., Li, Z. & Wang, Q. (2010). *Acta Cryst.* E**66**, o2017.

supporting information

Acta Cryst. (2011). E**67**, o68 [https://doi.org/10.1107/S1600536810050427]

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S1. Comment

The luminescent properties of lanthanide complexes with amide type ligands have been investigated in our previous work (Wu *et al.*, 2008). As part of our ongoing studies of the amide type ligands, the title compound was synthesized and characterized by X-ray diffraction.

In the title compound (Fig. 1), the C—N bond lengths are shorter than those observed in a similar compound (Yuan *et al.*,2010). The non-hydrogen atoms excluding the phenyl group are almost coplanar (r.m.s. deviation of the non-hydrogen atoms being 0.1015 Å). The dihedral angle formed between this plane and the benzene ring (r.m.s. deviation 0.0021 Å) is 87.07 (5)°.

As expected, there are no classic hydrogen bonds in the structure. However, there is a weak intermolecular C2—H2···O1 hydrogen bond stabilizing the packing. An intramolecular C7—H7A···O1 hydrogen bond is also present (Table 1).

S2. Experimental

A chloroform solution containing chloroacetyl chloride (2.26 g, 0.02 mol) was added dropwise to a solution of *N*-methyl-benzenamine (2.14 g, 0.02 mol) and pyridine (2.60 g, 0.03 mol) in chloroform (20 ml) under stirring on an ice-water bath. The reaction mixture was stirred at room temperature for 3.5 h. A solid product was separated from the solution by suction filtration, purified by succesive washing with water, 0.5 mol/*L* HCl, 0.5 mol/*L* NaOH and distilled water, respectively. Colourless block crystals were obtained by slow evaporation of the ethanol solution at room temperature.

S3. Refinement

The H atoms were placed at calculated positions and refined in riding mode, with the carrier atom-H distances = 0.93 Å for aryl, 0.97 for methylene, 0.96 Å for the methyl. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for the methyl H atoms and $1.2U_{eq}$ for the remaining H atoms.

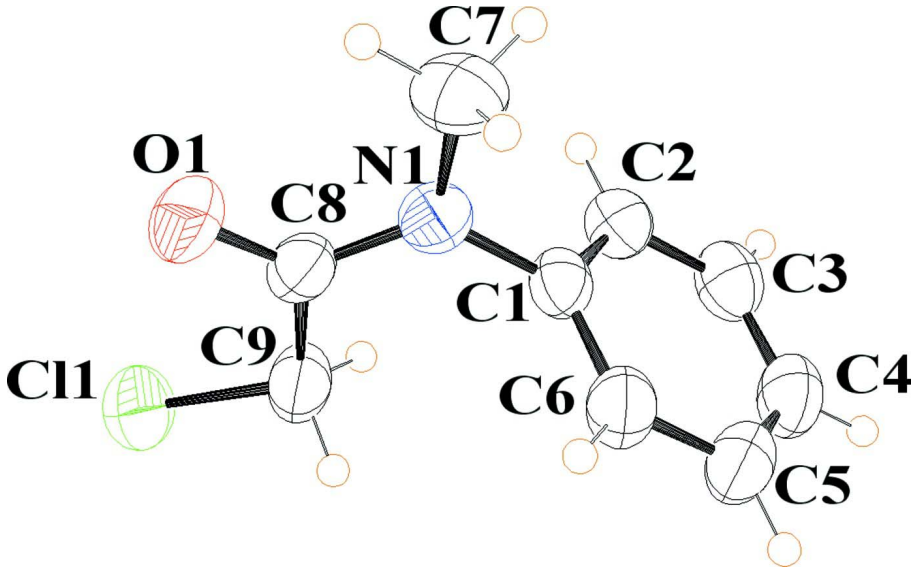

Figure 1

The molecular structure shown with 50% probability displacement ellipsoids.

2-Chloro-*N*-methyl-*N*-phenylacetamide

Crystal data

$C_9H_{10}ClNO$
$M_r = 183.63$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3391$ (12) Å
$b = 6.5898$ (10) Å
$c = 18.941$ (3) Å
$\beta = 91.192$ (9)°
$V = 915.9$ (2) Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3217 reflections
$\theta = 2.8$–25.4°
$\mu = 0.37$ mm^{-1}
$T = 296$ K
Block, colourless
0.26 × 0.21 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.912$, $T_{max} = 0.936$
9758 measured reflections
3003 independent reflections
1869 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 31.5°$, $\theta_{min} = 2.2°$
$h = -10\rightarrow9$
$k = -9\rightarrow9$
$l = -26\rightarrow27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.136$
$S = 1.04$
3003 reflections
110 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

$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.0768P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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}
Cl1	0.13525 (7)	0.14663 (8)	0.40483 (2)	0.07202 (19)
N1	0.29635 (16)	0.47779 (19)	0.56727 (6)	0.0477 (3)
C1	0.2909 (2)	0.3393 (2)	0.62581 (7)	0.0435 (3)
C8	0.22967 (19)	0.4317 (2)	0.50259 (7)	0.0457 (3)
C2	0.4463 (2)	0.2337 (2)	0.64621 (7)	0.0494 (3)
H2	0.5533	0.2483	0.6212	0.059*
C6	0.1317 (2)	0.3191 (3)	0.66275 (8)	0.0542 (4)
H6	0.0279	0.3909	0.6489	0.065*
O1	0.21932 (15)	0.55459 (18)	0.45449 (6)	0.0632 (3)
C4	0.2821 (2)	0.0864 (3)	0.74123 (8)	0.0605 (4)
H4	0.2794	0.0017	0.7805	0.073*
C9	0.1674 (2)	0.2147 (3)	0.49372 (7)	0.0566 (4)
H9A	0.0539	0.1962	0.5182	0.068*
H9B	0.2575	0.1252	0.5154	0.068*
C3	0.4407 (2)	0.1065 (3)	0.70395 (8)	0.0574 (4)
H3	0.5442	0.0341	0.7178	0.069*
C5	0.1284 (2)	0.1911 (3)	0.72052 (8)	0.0620 (4)
H5	0.0214	0.1758	0.7455	0.074*
C7	0.3571 (3)	0.6832 (3)	0.58295 (10)	0.0643 (4)
H7A	0.3770	0.7546	0.5396	0.096*
H7B	0.4686	0.6784	0.6103	0.096*
H7C	0.2656	0.7523	0.6093	0.096*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0829 (3)	0.0883 (4)	0.0447 (2)	−0.0124 (2)	−0.0002 (2)	−0.00826 (18)
N1	0.0533 (7)	0.0396 (7)	0.0501 (6)	−0.0039 (5)	−0.0009 (5)	0.0047 (5)
C1	0.0526 (8)	0.0397 (7)	0.0379 (6)	−0.0028 (6)	−0.0028 (5)	−0.0021 (5)
C8	0.0450 (7)	0.0475 (8)	0.0446 (7)	0.0003 (6)	0.0043 (5)	0.0089 (5)
C2	0.0499 (8)	0.0490 (9)	0.0494 (7)	−0.0004 (7)	−0.0012 (6)	−0.0011 (6)
C6	0.0542 (9)	0.0634 (10)	0.0449 (7)	0.0054 (7)	0.0002 (6)	0.0026 (6)

O1	0.0722 (7)	0.0610 (7)	0.0563 (6)	−0.0022 (6)	−0.0001 (5)	0.0232 (5)
C4	0.0796 (11)	0.0583 (10)	0.0436 (8)	−0.0018 (8)	−0.0030 (7)	0.0096 (6)
C9	0.0768 (10)	0.0539 (9)	0.0389 (7)	−0.0095 (8)	−0.0006 (7)	0.0029 (6)
C3	0.0646 (10)	0.0537 (9)	0.0533 (8)	0.0065 (8)	−0.0121 (7)	0.0034 (7)
C5	0.0650 (10)	0.0755 (12)	0.0459 (8)	−0.0011 (9)	0.0085 (7)	0.0070 (7)
C7	0.0686 (11)	0.0438 (9)	0.0803 (11)	−0.0076 (7)	−0.0038 (9)	0.0011 (8)

Geometric parameters (Å, º)

Cl1—C9	1.7537 (15)	C6—H6	0.9300
N1—C8	1.3446 (18)	C4—C5	1.373 (3)
N1—C1	1.4372 (17)	C4—C3	1.381 (2)
N1—C7	1.454 (2)	C4—H4	0.9300
C1—C6	1.380 (2)	C9—H9A	0.9700
C1—C2	1.384 (2)	C9—H9B	0.9700
C8—O1	1.2203 (16)	C3—H3	0.9300
C8—C9	1.509 (2)	C5—H5	0.9300
C2—C3	1.379 (2)	C7—H7A	0.9600
C2—H2	0.9300	C7—H7B	0.9600
C6—C5	1.382 (2)	C7—H7C	0.9600
C8—N1—C1	122.95 (12)	C8—C9—Cl1	112.56 (10)
C8—N1—C7	120.05 (13)	C8—C9—H9A	109.1
C1—N1—C7	116.56 (12)	Cl1—C9—H9A	109.1
C6—C1—C2	120.72 (13)	C8—C9—H9B	109.1
C6—C1—N1	119.34 (13)	Cl1—C9—H9B	109.1
C2—C1—N1	119.90 (13)	H9A—C9—H9B	107.8
O1—C8—N1	123.09 (14)	C2—C3—C4	120.20 (15)
O1—C8—C9	122.12 (13)	C2—C3—H3	119.9
N1—C8—C9	114.78 (12)	C4—C3—H3	119.9
C3—C2—C1	119.30 (14)	C4—C5—C6	120.32 (15)
C3—C2—H2	120.4	C4—C5—H5	119.8
C1—C2—H2	120.4	C6—C5—H5	119.8
C1—C6—C5	119.29 (15)	N1—C7—H7A	109.5
C1—C6—H6	120.4	N1—C7—H7B	109.5
C5—C6—H6	120.4	H7A—C7—H7B	109.5
C5—C4—C3	120.16 (15)	N1—C7—H7C	109.5
C5—C4—H4	119.9	H7A—C7—H7C	109.5
C3—C4—H4	119.9	H7B—C7—H7C	109.5
C8—N1—C1—C6	−80.39 (18)	N1—C1—C2—C3	177.81 (13)
C7—N1—C1—C6	91.92 (17)	C2—C1—C6—C5	−0.3 (2)
C8—N1—C1—C2	102.04 (17)	N1—C1—C6—C5	−177.81 (14)
C7—N1—C1—C2	−85.65 (17)	O1—C8—C9—Cl1	14.8 (2)
C1—N1—C8—O1	173.27 (13)	N1—C8—C9—Cl1	−165.31 (11)
C7—N1—C8—O1	1.2 (2)	C1—C2—C3—C4	−0.5 (2)
C1—N1—C8—C9	−6.6 (2)	C5—C4—C3—C2	0.8 (3)
C7—N1—C8—C9	−178.63 (14)	C3—C4—C5—C6	−0.8 (3)

C6—C1—C2—C3	0.3 (2)	C1—C6—C5—C4	0.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O1	0.96	2.37	2.749 (2)	103
C2—H2···O1^{i}	0.93	2.58	3.4356 (19)	154

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