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1-(3-Amino-1*H*-inden-2-yl)ethanone

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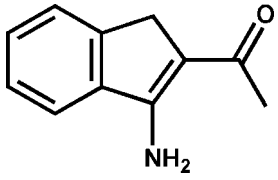
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.060; wR factor = 0.171; data-to-parameter ratio = 17.7.

The title compound, $C_{11}H_{11}NO$, was synthesized by the reaction of 2-(bromomethyl)benzonitrile and acetylacetone in the presence of KOH. In the crystal packing, molecules are linked by intermolecular N—H···O hydrogen bonds into chains running parallel to the b axis. Centrosymmetrically-related chains interact further through weak C—H···π interactions.

Related literature

For the crystal structures of related compounds, see: Choi *et al.* (1999); Fu & Zhao (2007).



Experimental

Crystal data

$C_{11}H_{11}NO$
M_r = 173.21
Monoclinic, $P2_1/c$
a = 8.1794 (4) Å
b = 10.6905 (5) Å
c = 10.5602 (6) Å
β = 93.783 (8)°
V = 921.39 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.25 × 0.16 × 0.14 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.980, T_{max} = 0.989
9369 measured reflections
2108 independent reflections
1385 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.171
S = 1.04
2108 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 is the centroid of the C7–C11/C13 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O2	0.86	2.17	2.766 (2)	126
N1—H1*B*···O2^{i}	0.86	2.09	2.924 (2)	164
C2—H2*B*···*Cg*1^{ii}	0.97	2.77	3.631 (2)	148

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+2, -z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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* and *PRPKAPPA* (Ferguson, 1999).

This work was supported by a Start-up Grant from Southeast University to ZRQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2252).

References

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Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
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supporting information

Acta Cryst. (2008). E**64**, o2239 [doi:10.1107/S1600536808033485]

1-(3-Amino-1*H*-inden-2-yl)ethanone

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S1. Comment

In recent years, the synthesis and characterization of new ligands containing amino donor groups has received considerable attention due to the potential applications in coordination chemistry (Choi *et al.*, 1999; Fu & Zhao, 2007). We report here the crystal structure of the title compound, which was obtained by the reaction of *o*-(bromomethyl)benzonitrile and acetylacetone in the presence of KOH.

In the molecule of the title compound (Fig. 1), the five-membered ring formed through the reaction is planar, and the geometric parameters are in the usual ranges. The molecular conformation is stabilized by an intramolecular N—H···O hydrogen bond (Table 1). In the crystal structure (Fig. 2), molecules are connected by intermolecular N—H···O hydrogen bonds into chains running parallel to the *b* axis (Table 1). Centrosymmetrically-related chains are further interacting through weak C—H···π interactions (Table 1).

S2. Experimental

Acetylacetone (0.5 g, 0.5 mmol) and *o*-(bromomethyl)-benzonitrile (0.98 g, 0.5 mmol) were dissolved in methanol (30 ml) in the presence of KOH (0.28 g, 0.5 mmol) and the mixture refluxed for 24 h at 393K. After cooling to room temperature, most of the solvent was removed by vacuum filtration. Colourless crystals of the title compound suitable for X-ray diffraction analysis were obtained by slow evaporation of the remaining solvent.

S3. Refinement

All H atoms were placed at calculated positions and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å, N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(C) for methyl H atoms.

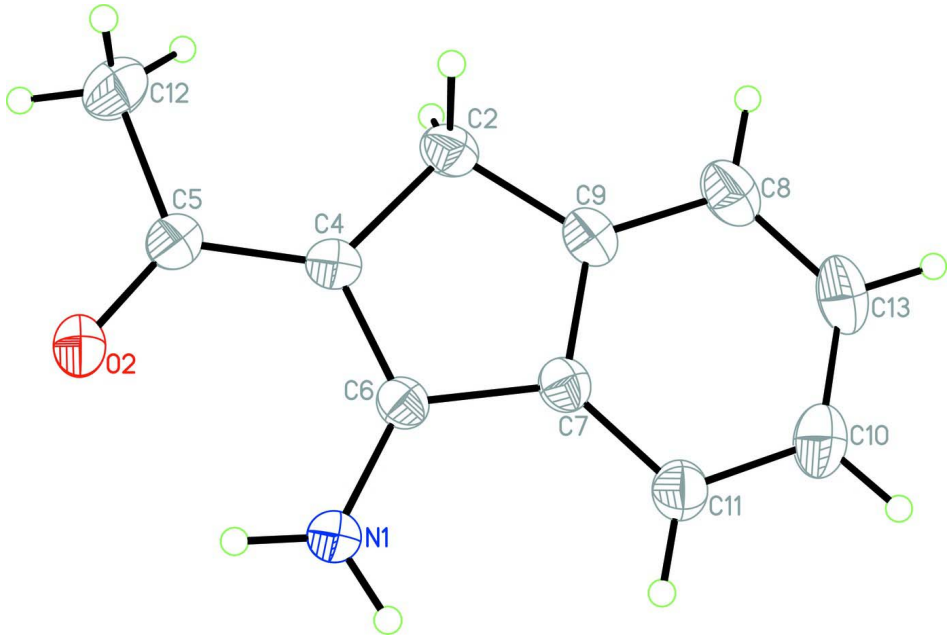

Figure 1

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

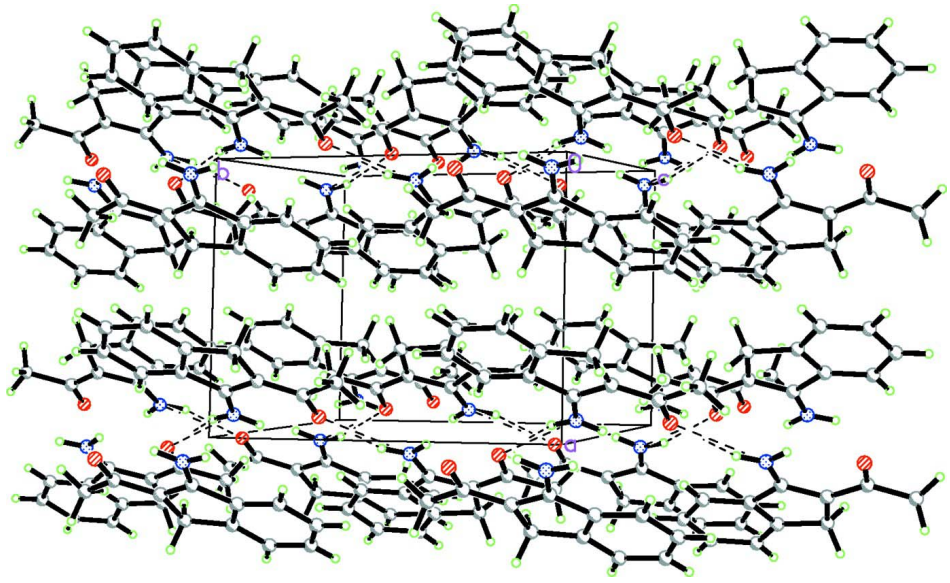

Figure 2

Packing diagram of the title compound. Intermolecular hydrogen bonds are shown as dashed lines.

1-(3-Amino-1*H*-inden-2-yl)ethanone

Crystal data

$C_{11}H_{11}NO$
M_r = 173.21
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.1794 (4) Å
b = 10.6905 (5) Å

c = 10.5602 (6) Å
β = 93.783 (8)°
V = 921.39 (8) Å^3
Z = 4
F(000) = 368
D_x = 1.249 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 4430 reflections
θ = 3.1–27.4°
μ = 0.08 mm^{-1}
T = 293 K
Block, colourless
0.25 × 0.16 × 0.14 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.980, T_{max} = 0.989

9369 measured reflections
2108 independent reflections
1385 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −10→10
k = −13→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.171
S = 1.04
2108 reflections
119 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
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 0.2011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C2	0.6932 (2)	0.90032 (19)	−0.07286 (18)	0.0447 (5)
H2A	0.7446	0.8647	−0.1448	0.054*
H2B	0.5859	0.8630	−0.0672	0.054*
C4	0.7981 (2)	0.88190 (18)	0.04815 (17)	0.0393 (5)
C5	0.8500 (2)	0.76630 (18)	0.1034 (2)	0.0434 (5)
C6	0.8406 (2)	0.99769 (18)	0.10065 (17)	0.0363 (4)
C7	0.7680 (2)	1.09672 (19)	0.01929 (18)	0.0389 (5)
C8	0.5992 (3)	1.1144 (2)	−0.1751 (2)	0.0584 (6)
H8	0.5401	1.0783	−0.2440	0.070*

C9	0.6815 (2)	1.0401 (2)	−0.08348 (18)	0.0439 (5)
C10	0.6928 (3)	1.2986 (3)	−0.0592 (2)	0.0629 (7)
H10	0.6952	1.3853	−0.0521	0.076*
C11	0.7750 (3)	1.2260 (2)	0.0329 (2)	0.0490 (6)
H11	0.8332	1.2626	0.1019	0.059*
C12	0.7998 (3)	0.6463 (2)	0.0355 (3)	0.0667 (7)
H12A	0.8792	0.5824	0.0570	0.100*
H12B	0.7939	0.6602	−0.0545	0.100*
H12C	0.6945	0.6204	0.0608	0.100*
C13	0.6070 (3)	1.2432 (2)	−0.1617 (2)	0.0664 (7)
H13	0.5533	1.2936	−0.2231	0.080*
N1	0.9314 (2)	1.01839 (16)	0.20784 (15)	0.0490 (5)
H1A	0.9702	0.9564	0.2522	0.059*
H1B	0.9512	1.0938	0.2328	0.059*
O2	0.93402 (18)	0.75969 (13)	0.20655 (14)	0.0527 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0439 (11)	0.0511 (13)	0.0384 (11)	0.0004 (9)	−0.0018 (8)	−0.0056 (9)
C4	0.0376 (10)	0.0419 (11)	0.0383 (10)	−0.0022 (8)	0.0014 (8)	−0.0035 (8)
C5	0.0434 (11)	0.0401 (12)	0.0470 (12)	−0.0014 (9)	0.0046 (9)	−0.0010 (8)
C6	0.0332 (9)	0.0403 (11)	0.0354 (10)	−0.0004 (8)	0.0023 (7)	0.0010 (8)
C7	0.0346 (9)	0.0424 (11)	0.0399 (11)	0.0010 (8)	0.0036 (8)	0.0024 (8)
C8	0.0553 (13)	0.0740 (18)	0.0446 (13)	0.0109 (12)	−0.0053 (10)	0.0031 (11)
C9	0.0392 (10)	0.0544 (14)	0.0380 (11)	0.0049 (9)	0.0023 (8)	0.0025 (9)
C10	0.0714 (16)	0.0487 (13)	0.0685 (17)	0.0096 (12)	0.0037 (13)	0.0164 (12)
C11	0.0484 (12)	0.0456 (14)	0.0526 (12)	0.0016 (10)	0.0007 (9)	0.0042 (10)
C12	0.0854 (18)	0.0415 (13)	0.0719 (16)	−0.0014 (12)	−0.0041 (13)	−0.0100 (11)
C13	0.0691 (16)	0.0700 (17)	0.0593 (15)	0.0214 (13)	−0.0016 (12)	0.0218 (12)
N1	0.0605 (11)	0.0381 (9)	0.0461 (10)	−0.0026 (8)	−0.0137 (8)	0.0000 (7)
O2	0.0660 (10)	0.0415 (8)	0.0493 (9)	0.0033 (7)	−0.0075 (7)	0.0062 (6)

Geometric parameters (Å, º)

C2—C9	1.501 (3)	C8—C9	1.391 (3)
C2—C4	1.505 (3)	C8—H8	0.9300
C2—H2A	0.9700	C10—C11	1.383 (3)
C2—H2B	0.9700	C10—C13	1.384 (3)
C4—C6	1.391 (3)	C10—H10	0.9300
C4—C5	1.420 (3)	C11—H11	0.9300
C5—O2	1.251 (2)	C12—H12A	0.9600
C5—C12	1.513 (3)	C12—H12B	0.9600
C6—N1	1.331 (2)	C12—H12C	0.9600
C6—C7	1.464 (3)	C13—H13	0.9300
C7—C11	1.391 (3)	N1—H1A	0.8600
C7—C9	1.394 (3)	N1—H1B	0.8600
C8—C13	1.385 (4)		

C9—C2—C4	102.92 (15)	C8—C9—C7	119.4 (2)
C9—C2—H2A	111.2	C8—C9—C2	130.2 (2)
C4—C2—H2A	111.2	C7—C9—C2	110.33 (17)
C9—C2—H2B	111.2	C11—C10—C13	120.5 (3)
C4—C2—H2B	111.2	C11—C10—H10	119.7
H2A—C2—H2B	109.1	C13—C10—H10	119.7
C6—C4—C5	123.41 (18)	C10—C11—C7	118.1 (2)
C6—C4—C2	109.61 (17)	C10—C11—H11	121.0
C5—C4—C2	126.98 (18)	C7—C11—H11	121.0
O2—C5—C4	122.65 (18)	C5—C12—H12A	109.5
O2—C5—C12	118.77 (19)	C5—C12—H12B	109.5
C4—C5—C12	118.6 (2)	H12A—C12—H12B	109.5
N1—C6—C4	126.71 (18)	C5—C12—H12C	109.5
N1—C6—C7	124.11 (17)	H12A—C12—H12C	109.5
C4—C6—C7	109.18 (16)	H12B—C12—H12C	109.5
C11—C7—C9	121.81 (19)	C10—C13—C8	121.5 (2)
C11—C7—C6	130.23 (19)	C10—C13—H13	119.2
C9—C7—C6	107.96 (18)	C8—C13—H13	119.2
C13—C8—C9	118.7 (2)	C6—N1—H1A	120.0
C13—C8—H8	120.7	C6—N1—H1B	120.0
C9—C8—H8	120.7	H1A—N1—H1B	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2	0.86	2.17	2.766 (2)	126
N1—H1*B*···O2^{i}	0.86	2.09	2.924 (2)	164
C2—H2*B*···*Cg*1^{ii}	0.97	2.77	3.631 (2)	148

Symmetry codes: (i) −*x*+2, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+2, −*z*.