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2-(4-Chloro-1*H*-indol-3-yl)acetonitrile

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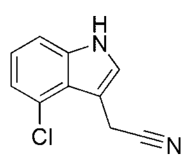
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.048; wR factor = 0.111; data-to-parameter ratio = 17.2.

The title compound, $C_{10}H_7ClN_2$, contains two approximately planar molecules, *A* and *B* (r.m.s. deviations = 0.039 and 0.064 Å, respectively) in the asymmetric unit. In the crystal, N—H···N hydrogen bonds link the molecules into *C*(7) chains of alternating *A* and *B* molecules propagating along the *a*-axis direction. The crystal used for the data collection was found to be a racemic twin.

Related literature

For a related structure, see: Ge *et al.* (2012).



Experimental

Crystal data

$C_{10}H_7ClN_2$
M_r = 190.63
Orthorhombic, $Pca2_1$
a = 7.5091 (15) Å
b = 11.041 (2) Å
c = 21.380 (4) Å
V = 1772.6 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 293 K
0.33 × 0.25 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.893, T_{max} = 0.927
17075 measured reflections
4057 independent reflections
2753 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
2 standard reflections every 150 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.111
S = 1.03
4057 reflections
236 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 1968 Friedel pairs
Flack parameter: 0.66 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···N4	0.86	2.42	3.089 (6)	135
N2—H2*A*···N3^{i}	0.86	2.21	3.058 (6)	170

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

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: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the starter fund of Southeast University for financial support to buy the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6554).

References

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supplementary materials

Acta Cryst. (2012). E**68**, o203 [**doi:10.1107/S1600536811054079**]

2-(4-Chloro-1*H*-indol-3-yl)acetonitrile

M.-L. Pan, X. Li and Y.-H. Luo

Experimental

The title compound 3-(cyanomethyl)indole-4-chlorine was purchased commercially from ChemFuture PharmaTech, Ltd (Nanjing, Jiangsu). and were used as received without further purification. Colourles prisms were obstained by slow evaporation of a methanol solution.

Refinement

Positional parameters of all H atoms were calculated geometrically and the H atoms were set to ride the C atoms and N atoms to which they are bonded, with *U*̃iso~(H)= 1.2 *U*̃iso~(C, N).C—H atoms were included with bond distances ranging from 0.93 to 0.97 Å. Amide N—H hydrogen atoms were included witha distance set to 0.86 Å.

Figures

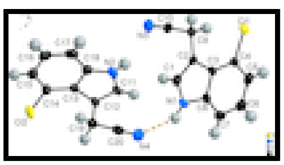

Fig. 1. The molecular structure of the title compound showing 30% displacement ellipsoids.

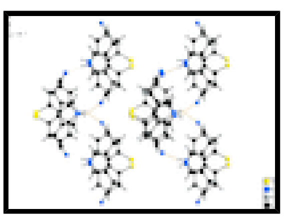

Fig. 2. Packing diagram of the title compound, showing the structure from the *a* axis. Hydrogen bonds are shown as dashed lines.

2-(4-Chloro-1*H*-indol-3-yl)acetonitrile

Crystal data

$C_{10}H_7ClN_2$	F(000) = 784
M_r = 190.63	D_x = 1.429 Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 4057 reflections
a = 7.5091 (15) Å	θ = 2.5–27.5°
b = 11.041 (2) Å	μ = 0.38 mm^{-1}
c = 21.380 (4) Å	T = 293 K
V = 1772.6 (6) Å^3	Prism, colourless
Z = 8	0.33 × 0.25 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer	2753 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.058$
graphite	$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
CCD_Profile_fitting scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$k = -14 \rightarrow 14$
$T_{min} = 0.893$, $T_{max} = 0.927$	$l = -27 \rightarrow 27$
17075 measured reflections	2 standard reflections every 150 reflections
4057 independent reflections	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.1573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
4057 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
236 parameters	Extinction correction: *SHELXL97* (Sheldrick, 2008)
1 restraint	Extinction coefficient: 0
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), **1968 Friedel pairs**
Secondary atom site location: difference Fourier map	Flack parameter: 0.66 (10)

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}
Cl1	0.57185 (18)	0.47362 (9)	−0.10226 (5)	0.0585 (3)
N1	0.3359 (6)	0.4908 (3)	0.1147 (2)	0.0451 (11)
H1A	0.3006	0.4743	0.1520	0.054*

N3	0.4392 (5)	0.9029 (3)	0.05314 (18)	0.0781 (11)
C1	0.3547 (5)	0.6055 (3)	0.0894 (2)	0.0470 (11)
H1B	0.3234	0.6773	0.1093	0.056*
C2	0.4252 (4)	0.5977 (3)	0.0317 (2)	0.0372 (8)
C3	0.4428 (6)	0.4720 (4)	0.0164 (2)	0.0356 (8)
C4	0.4979 (4)	0.4026 (3)	−0.03431 (17)	0.0399 (7)
C5	0.4984 (6)	0.2769 (3)	−0.0313 (2)	0.0528 (12)
H5A	0.5375	0.2322	−0.0656	0.063*
C6	0.4413 (6)	0.2172 (4)	0.0222 (3)	0.0571 (13)
H6A	0.4426	0.1330	0.0233	0.069*
C7	0.3829 (4)	0.2803 (3)	0.07360 (19)	0.0521 (9)
H7A	0.3450	0.2411	0.1097	0.062*
C8	0.3834 (5)	0.4034 (3)	0.0688 (2)	0.0412 (10)
C9	0.4689 (6)	0.7050 (3)	−0.00949 (18)	0.0454 (10)
H9A	0.5898	0.6971	−0.0249	0.055*
H9B	0.3894	0.7056	−0.0452	0.055*
C10	0.4518 (6)	0.8176 (3)	0.0240 (2)	0.0491 (10)
Cl2	0.31981 (19)	1.02214 (9)	0.39526 (5)	0.0628 (4)
N2	0.0887 (6)	1.0076 (3)	0.1779 (2)	0.0540 (13)
H2A	0.0441	1.0232	0.1417	0.065*
N4	0.1867 (6)	0.5920 (3)	0.23876 (19)	0.0798 (11)
C11	0.1204 (5)	0.8969 (4)	0.20034 (19)	0.0454 (10)
H11A	0.1048	0.8260	0.1775	0.054*
C12	0.1782 (4)	0.9000 (3)	0.26055 (19)	0.0401 (8)
C13	0.1928 (6)	1.0261 (4)	0.2749 (2)	0.0385 (9)
C14	0.2470 (4)	1.0945 (3)	0.32694 (17)	0.0442 (8)
C15	0.2436 (6)	1.2171 (3)	0.3253 (2)	0.0531 (11)
H15A	0.2807	1.2608	0.3601	0.064*
C16	0.1853 (6)	1.2786 (4)	0.2721 (3)	0.0618 (14)
H16A	0.1840	1.3628	0.2720	0.074*
C17	0.1308 (4)	1.2175 (4)	0.2208 (2)	0.0594 (10)
H17A	0.0889	1.2594	0.1861	0.071*
C18	0.1377 (5)	1.0878 (3)	0.2203 (2)	0.0422 (10)
C19	0.2208 (6)	0.7932 (3)	0.30169 (19)	0.0468 (10)
H19A	0.3417	0.8005	0.3172	0.056*
H19B	0.1410	0.7926	0.3374	0.056*
C20	0.2024 (7)	0.6794 (4)	0.2670 (3)	0.0579 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0658 (7)	0.0684 (5)	0.0413 (6)	−0.0070 (6)	0.0135 (6)	−0.0086 (8)
N1	0.050 (3)	0.056 (2)	0.029 (3)	−0.0015 (13)	0.004 (2)	0.0031 (12)
N3	0.124 (3)	0.050 (2)	0.060 (2)	−0.011 (2)	−0.015 (2)	−0.0052 (17)
C1	0.037 (2)	0.043 (2)	0.061 (3)	0.0015 (15)	0.0014 (18)	−0.013 (2)
C2	0.0324 (18)	0.0367 (19)	0.042 (2)	−0.0052 (15)	−0.0034 (17)	−0.0017 (16)
C3	0.030 (2)	0.0480 (19)	0.029 (2)	0.001 (2)	−0.0011 (15)	−0.004 (2)
C4	0.0335 (17)	0.0480 (18)	0.0383 (19)	−0.0033 (16)	0.0004 (14)	−0.0022 (15)

C5	0.050 (2)	0.037 (2)	0.072 (3)	0.0072 (18)	−0.005 (2)	−0.018 (2)
C6	0.050 (2)	0.047 (2)	0.074 (3)	−0.001 (2)	−0.008 (2)	0.005 (2)
C7	0.049 (2)	0.057 (2)	0.051 (2)	−0.0046 (16)	−0.0075 (17)	0.014 (2)
C8	0.042 (2)	0.046 (2)	0.036 (2)	0.0043 (15)	−0.0130 (18)	−0.0005 (16)
C9	0.051 (2)	0.045 (2)	0.040 (2)	−0.0052 (17)	−0.0022 (19)	−0.0067 (16)
C10	0.064 (3)	0.036 (2)	0.047 (2)	−0.0061 (19)	−0.0045 (19)	−0.0002 (19)
Cl2	0.0702 (8)	0.0734 (6)	0.0447 (7)	0.0137 (6)	−0.0164 (6)	−0.0136 (9)
N2	0.056 (3)	0.071 (3)	0.035 (3)	0.0072 (15)	−0.009 (3)	0.0068 (14)
N4	0.122 (3)	0.043 (2)	0.074 (3)	−0.005 (2)	0.009 (2)	−0.0032 (18)
C11	0.050 (2)	0.056 (2)	0.030 (2)	0.0035 (18)	0.0019 (16)	0.0035 (17)
C12	0.0360 (19)	0.054 (2)	0.031 (2)	0.0018 (17)	0.0026 (17)	−0.0042 (17)
C13	0.033 (2)	0.0450 (18)	0.038 (2)	0.003 (2)	0.0077 (16)	0.000 (2)
C14	0.0391 (19)	0.0499 (19)	0.044 (2)	0.0003 (17)	0.0050 (16)	−0.0071 (17)
C15	0.048 (2)	0.053 (2)	0.058 (3)	−0.001 (2)	0.006 (2)	−0.007 (2)
C16	0.066 (3)	0.033 (2)	0.087 (4)	−0.001 (2)	0.022 (3)	0.002 (2)
C17	0.051 (2)	0.061 (2)	0.066 (3)	0.0055 (19)	0.008 (2)	0.023 (2)
C18	0.032 (2)	0.041 (2)	0.053 (3)	0.0096 (15)	0.002 (2)	0.0007 (18)
C19	0.049 (2)	0.045 (2)	0.046 (3)	0.0065 (17)	0.0035 (19)	0.0020 (17)
C20	0.075 (3)	0.052 (2)	0.046 (3)	0.003 (2)	0.009 (2)	0.008 (2)

Geometric parameters (Å, °)

Cl1—C4	1.742 (4)	Cl2—C14	1.752 (4)
N1—C1	1.385 (5)	N2—C18	1.319 (6)
N1—C8	1.421 (6)	N2—C11	1.335 (5)
N1—H1A	0.8600	N2—H2A	0.8601
N3—C10	1.132 (5)	N4—C20	1.144 (6)
C1—C2	1.346 (5)	C11—C12	1.359 (5)
C1—H1B	0.9300	C11—H11A	0.9300
C2—C3	1.432 (4)	C12—C13	1.430 (5)
C2—C9	1.511 (5)	C12—C19	1.506 (5)
C3—C4	1.391 (5)	C13—C14	1.405 (6)
C3—C8	1.424 (6)	C13—C18	1.413 (6)
C4—C5	1.390 (5)	C14—C15	1.354 (5)
C5—C6	1.388 (7)	C15—C16	1.395 (7)
C5—H5A	0.9300	C15—H15A	0.9300
C6—C7	1.373 (7)	C16—C17	1.351 (7)
C6—H6A	0.9300	C16—H16A	0.9300
C7—C8	1.364 (5)	C17—C18	1.434 (6)
C7—H7A	0.9300	C17—H17A	0.9300
C9—C10	1.441 (5)	C19—C20	1.466 (6)
C9—H9A	0.9700	C19—H19A	0.9700
C9—H9B	0.9700	C19—H19B	0.9700
C1—N1—C8	109.0 (4)	C18—N2—C11	108.5 (5)
C1—N1—H1A	125.9	C18—N2—H2A	126.4
C8—N1—H1A	125.1	C11—N2—H2A	125.2
C2—C1—N1	109.9 (4)	N2—C11—C12	112.0 (4)
C2—C1—H1B	125.1	N2—C11—H11A	124.0
N1—C1—H1B	125.1	C12—C11—H11A	124.0

C1—C2—C3	107.9 (3)	C11—C12—C13	104.6 (4)
C1—C2—C9	124.7 (3)	C11—C12—C19	127.0 (3)
C3—C2—C9	127.4 (4)	C13—C12—C19	128.4 (4)
C4—C3—C8	114.4 (3)	C14—C13—C18	118.7 (4)
C4—C3—C2	137.6 (4)	C14—C13—C12	135.7 (4)
C8—C3—C2	107.9 (4)	C18—C13—C12	105.6 (4)
C3—C4—C5	121.0 (3)	C15—C14—C13	120.7 (4)
C3—C4—Cl1	119.8 (3)	C15—C14—Cl2	118.9 (3)
C5—C4—Cl1	119.2 (3)	C13—C14—Cl2	120.4 (3)
C6—C5—C4	120.7 (4)	C14—C15—C16	120.9 (4)
C6—C5—H5A	119.6	C14—C15—H15A	119.5
C4—C5—H5A	119.6	C16—C15—H15A	119.5
C7—C6—C5	121.2 (4)	C17—C16—C15	120.9 (4)
C7—C6—H6A	119.4	C17—C16—H16A	119.5
C5—C6—H6A	119.4	C15—C16—H16A	119.5
C6—C7—C8	116.4 (4)	C16—C17—C18	119.6 (4)
C6—C7—H7A	121.8	C16—C17—H17A	120.2
C8—C7—H7A	121.8	C18—C17—H17A	120.2
C7—C8—C3	126.2 (4)	N2—C18—C13	109.1 (4)
C7—C8—N1	128.6 (4)	N2—C18—C17	131.7 (4)
C3—C8—N1	105.1 (3)	C13—C18—C17	119.0 (4)
C10—C9—C2	111.5 (3)	C20—C19—C12	110.8 (4)
C10—C9—H9A	109.3	C20—C19—H19A	109.5
C2—C9—H9A	109.3	C12—C19—H19A	109.5
C10—C9—H9B	109.3	C20—C19—H19B	109.5
C2—C9—H9B	109.3	C12—C19—H19B	109.5
H9A—C9—H9B	108.0	H19A—C19—H19B	108.1
N3—C10—C9	176.5 (5)	N4—C20—C19	178.4 (5)

C8—N1—C1—C2	−4.9 (5)	C18—N2—C11—C12	5.0 (6)
N1—C1—C2—C3	3.9 (5)	N2—C11—C12—C13	−3.6 (5)
N1—C1—C2—C9	−178.4 (4)	N2—C11—C12—C19	177.7 (4)
C1—C2—C3—C4	177.3 (5)	C11—C12—C13—C14	−178.4 (5)
C9—C2—C3—C4	−0.2 (8)	C19—C12—C13—C14	0.3 (8)
C1—C2—C3—C8	−1.5 (4)	C11—C12—C13—C18	0.9 (4)
C9—C2—C3—C8	−179.1 (4)	C19—C12—C13—C18	179.6 (4)
C8—C3—C4—C5	−2.0 (5)	C18—C13—C14—C15	1.2 (6)
C2—C3—C4—C5	179.2 (5)	C12—C13—C14—C15	−179.6 (5)
C8—C3—C4—Cl1	179.3 (3)	C18—C13—C14—Cl2	−179.0 (3)
C2—C3—C4—Cl1	0.5 (7)	C12—C13—C14—Cl2	0.3 (7)
C3—C4—C5—C6	1.0 (6)	C13—C14—C15—C16	0.4 (6)
Cl1—C4—C5—C6	179.7 (4)	Cl2—C14—C15—C16	−179.5 (4)
C4—C5—C6—C7	0.0 (7)	C14—C15—C16—C17	0.0 (7)
C5—C6—C7—C8	0.4 (6)	C15—C16—C17—C18	−1.8 (7)
C6—C7—C8—C3	−1.7 (6)	C11—N2—C18—C13	−4.2 (6)
C6—C7—C8—N1	−177.9 (4)	C11—N2—C18—C17	−179.0 (4)
C4—C3—C8—C7	2.5 (6)	C14—C13—C18—N2	−178.5 (4)
C2—C3—C8—C7	−178.3 (4)	C12—C13—C18—N2	2.0 (5)
C4—C3—C8—N1	179.4 (4)	C14—C13—C18—C17	−3.0 (6)
C2—C3—C8—N1	−1.4 (4)	C12—C13—C18—C17	177.5 (3)

C1—N1—C8—C7	−179.4 (4)	C16—C17—C18—N2	177.7 (5)
C1—N1—C8—C3	3.8 (5)	C16—C17—C18—C13	3.4 (6)
C1—C2—C9—C10	8.9 (6)	C11—C12—C19—C20	3.4 (6)
C3—C2—C9—C10	−173.9 (4)	C13—C12—C19—C20	−174.9 (4)
C2—C9—C10—N3	21 (9)	C12—C19—C20—N4	−3(20)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N4	0.86	2.42	3.089 (6)	135
N2—H2A···N3^{i}	0.86	2.21	3.058 (6)	170

Symmetry codes: (i) x−1/2, −y+2, z.

Fig. 1

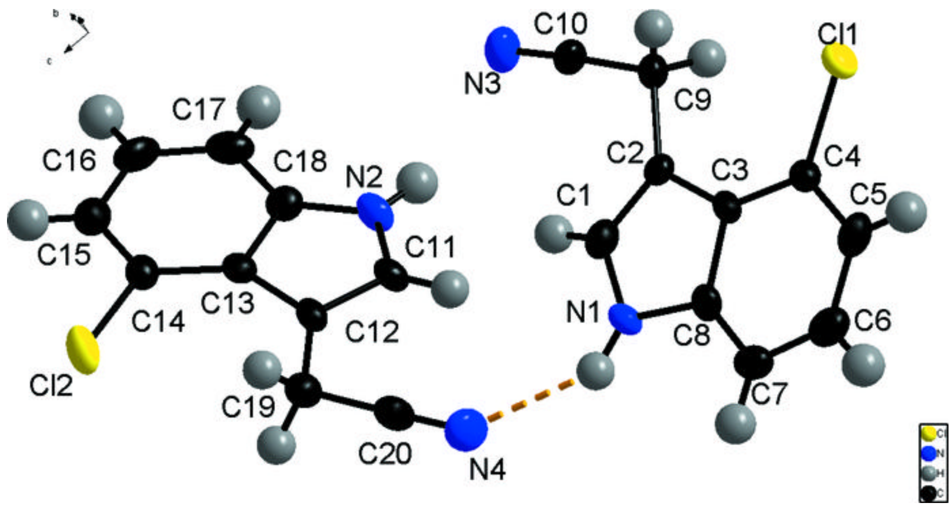
C10
N3
C9
Cl1
C17
C16
C18
N2
C2
C3
C4
C1
C5
C15
C11
C13
C14
N1
C8
C6
C12
Cl2
C19
C7
C20
N4

Fig. 2