IUCrData

ISSN 2414-3146

7,8-Dimethyl-11*H*-indeno[1,2-*b*]quinoxalin-11-one

Lin Chen,[a,b] Jin Hu[a] and Hong-Shun Sun[a]*

[a]Targeted MRI Contrast Agents Laboratory of Jiangsu Province, Nanjing Polytechnic Institute, Nanjing 210048, People's Republic of China, and [b]School of Biology and Environment, Nanjing Polytechnic Institute, Nanjing 210048, People's Republic of China. *Correspondence e-mail: njutshs@126.com

Received 21 December 2020
Accepted 6 January 2021

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

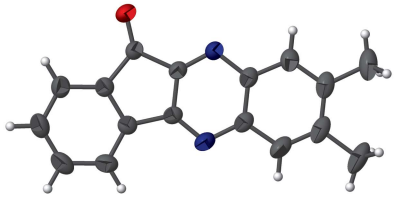
Keywords: crystal structure; indene; quinoxaline; indeno[1,2-*b*]quinoxaline.

CCDC reference: 2054191

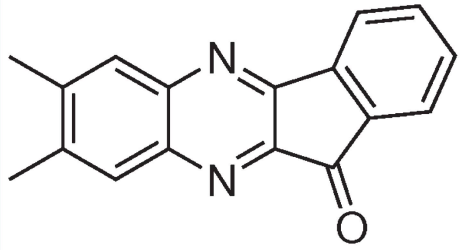
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{12}N_2O$, the mean planes of the indene ring and quinoxaline system (r.m.s. deviations = 0.0131 and 0.0082 Å) are approximately parallel to one another, making a dihedral angle of 1.2 (5)°. This means that the indeno[1,2-*b*]quinoxaline ring is almost in the same plane (r.m.s. deviation = 0.0181 Å).

3D view



Chemical scheme



Structure description

Quinoxaline based N-heteroacenes show a narrow band-gap, high thermal stability and aligned film morphology and can be applied as the hole-transport layers in quantum dot light-emitting diodes (QLEDs) (Bai *et al.*, 2015). As part of our work in this area, we now report the synthesis and crystal structure of the title indeno[1,2-*b*]quinoxaline derivative.

The molecular structure of the title compound is shown in Fig. 1. The indene ring and quinoxaline system are nearly parallel to one another [dihedral angle = 1.2 (5)°]. This means that the indeno[1,2-*b*]quinoxaline ring (N1–N2/C1–C15) is almost in the same plane (r.m.s. deviation = 0.0181 Å), which contains the two methyl groups. The packing is shown in Fig. 2.

One similar structure has been reported previously (11,11-diphenyl-11*H*-indeno[1,2-*b*]quinoxaline; Chen *et al.*, 2020). In that structure, the indeno[1,2-*b*]quinoxaline ring (r.m.s. deviations = 0.1197 Å) is twisted with respect to the two benzene ring systems by 70.0 (4) and 67.6 (3)°, respectively.

Synthesis and crystallization

A mixture of 1*H*-indene-1,2,3-trione (3.20 g, 20 mmol) and 4,5-dimethylbenzene-1,2-diamine (2.72 g, 20 mmol) in ethanol (100 ml) was heated to reflux under stirring for 5 h. 7,8-Dimethyl-11*H*-indeno[1,2-*b*]quinoxalin-11-one was obtained as a yellow powder by

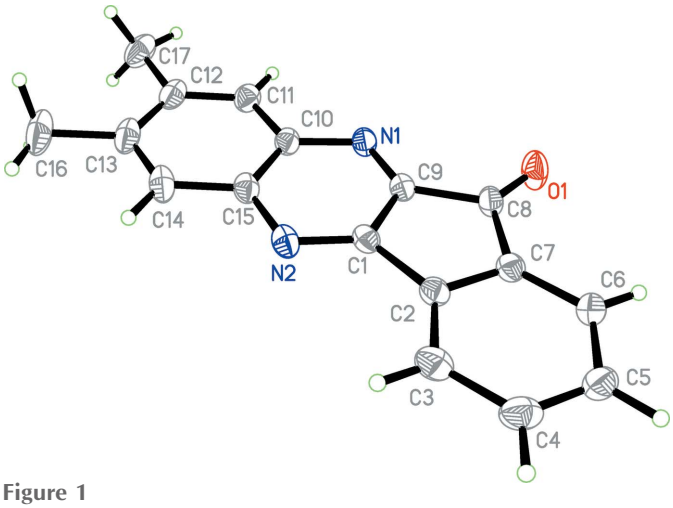


Figure 1
The molecular structure of the title molecule with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

filtering after cooling, yield 82%. Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

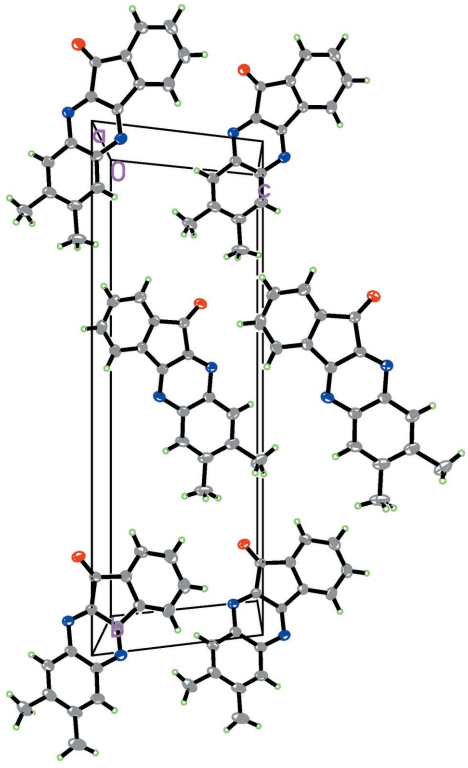


Figure 2
A packing diagram of the title compound.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{12}N_2O$
M_r	260.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	282
a, b, c (Å)	7.4548 (9), 22.976 (3), 8.3149 (10)
β (°)	115.866 (3)
V (Å^3)	1281.5 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.45 × 0.3 × 0.22
Data collection	
Diffractometer	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.606, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10114, 3134, 2437
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.153, 1.05
No. of reflections	3134
No. of parameters	183
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.23

Computer programs: *SMART* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

The authors thank the Center of Testing and Analysis, Nanjing University, for support.

Funding information

Funding for this research was provided by: Natural Science Foundation of Jiangsu Province (grant No. BK20181486); Natural Science Foundation of the Jiangsu Higher Education Institutions (grant No. 17KJB320001); Training program of Students innovation and entrepreneurship in Jiangsu Province (grant No. 202012920001Y); Qing Lan Project of Jiangsu Province.

References

Bai, L., Yang, X., Ang, C. Y., Nguyen, K. T., Ding, T., Bose, P., Gao, Q., Mandal, A. K., Sun, X. W., Demir, H. V. & Zhao, Y. (2015). *Nanoscale.* **7**, 11531–11535.
Bruker (2014). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, L., Hu, J., Wu, L.-L. & Sun, H.-S. (2020). *IUCrData*, **5**, x201213.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2021). **6**, x210018 [https://doi.org/10.1107/S2414314621000183]

7,8-Dimethyl-11*H*-indeno[1,2-*b*]quinoxalin-11-one

Lin Chen, Jin Hu and Hong-Shun Sun

7,8-Dimethyl-11*H*-indeno[1,2-*b*]quinoxalin-11-one

Crystal data

$C_{17}H_{12}N_2O$
M_r = 260.29
Monoclinic, $P2_1/n$
a = 7.4548 (9) Å
b = 22.976 (3) Å
c = 8.3149 (10) Å
β = 115.866 (3)°
V = 1281.5 (3) Å^3
Z = 4
$F(000)$ = 544
D_x = 1.349 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5967 reflections
θ = 2.7–28.4°
μ = 0.09 mm^{-1}
T = 282 K
Block, colorless
0.45 × 0.3 × 0.22 mm

Data collection

Bruker SMART CCD 6000 area detector diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
Detector resolution: 5.6 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.606, T_{max} = 0.746
10114 measured reflections
3134 independent reflections
2437 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.4°, θ_{min} = 3.1°
h = −9→9
k = −30→30
l = −11→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.153
S = 1.05
3134 reflections
183 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.7679P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.1899 (2)	0.67104 (6)	0.38760 (19)	0.0613 (4)
N1	0.1135 (2)	0.54175 (6)	0.3195 (2)	0.0400 (4)
N2	0.3665 (2)	0.48258 (6)	0.6458 (2)	0.0417 (4)
C1	0.3614 (2)	0.53906 (7)	0.6270 (2)	0.0348 (4)
C2	0.4780 (2)	0.58312 (7)	0.7599 (2)	0.0366 (4)
C3	0.6183 (3)	0.57743 (9)	0.9349 (3)	0.0483 (5)
H3	0.6505	0.5411	0.9892	0.058*
C4	0.7104 (3)	0.62748 (10)	1.0279 (3)	0.0542 (5)
H4	0.8068	0.6244	1.1455	0.065*
C5	0.6616 (3)	0.68157 (9)	0.9493 (3)	0.0517 (5)
H5	0.7257	0.7144	1.0146	0.062*
C6	0.5187 (3)	0.68793 (8)	0.7744 (3)	0.0463 (5)
H6	0.4851	0.7245	0.7217	0.056*
C7	0.4275 (3)	0.63822 (8)	0.6807 (2)	0.0381 (4)
C8	0.2716 (3)	0.63268 (7)	0.4928 (2)	0.0400 (4)
C9	0.2358 (2)	0.56799 (7)	0.4648 (2)	0.0362 (4)
C10	0.1132 (3)	0.48201 (7)	0.3342 (2)	0.0381 (4)
C11	−0.0140 (3)	0.44895 (8)	0.1861 (3)	0.0448 (4)
H11	−0.0943	0.4680	0.0802	0.054*
C12	−0.0229 (3)	0.38935 (8)	0.1933 (3)	0.0490 (5)
C13	0.1007 (3)	0.36040 (8)	0.3545 (3)	0.0528 (5)
C14	0.2283 (3)	0.39190 (8)	0.4996 (3)	0.0500 (5)
H14	0.3106	0.3723	0.6037	0.060*
C15	0.2382 (3)	0.45313 (7)	0.4951 (2)	0.0389 (4)
C16	0.0931 (4)	0.29501 (9)	0.3674 (4)	0.0773 (8)
H16A	0.1901	0.2825	0.4830	0.116*
H16B	0.1219	0.2775	0.2765	0.116*
H16C	−0.0375	0.2834	0.3511	0.116*
C17	−0.1623 (4)	0.35635 (10)	0.0302 (4)	0.0665 (7)
H17A	−0.2286	0.3831	−0.0665	0.100*
H17B	−0.2595	0.3362	0.0560	0.100*
H17C	−0.0878	0.3287	−0.0030	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0802 (11)	0.0335 (7)	0.0499 (8)	0.0066 (7)	0.0095 (7)	0.0056 (6)
N1	0.0444 (8)	0.0322 (7)	0.0406 (8)	0.0024 (6)	0.0159 (7)	0.0001 (6)
N2	0.0491 (9)	0.0341 (7)	0.0459 (9)	0.0071 (6)	0.0245 (7)	0.0067 (6)
C1	0.0365 (8)	0.0343 (8)	0.0375 (9)	0.0055 (6)	0.0197 (7)	0.0032 (7)
C2	0.0345 (8)	0.0395 (9)	0.0381 (9)	0.0041 (7)	0.0179 (7)	−0.0004 (7)
C3	0.0451 (10)	0.0541 (11)	0.0408 (10)	0.0099 (8)	0.0143 (8)	0.0063 (8)
C4	0.0406 (10)	0.0733 (14)	0.0405 (10)	0.0042 (9)	0.0102 (8)	−0.0085 (10)
C5	0.0409 (10)	0.0557 (12)	0.0533 (12)	−0.0030 (8)	0.0157 (9)	−0.0163 (9)
C6	0.0435 (10)	0.0409 (10)	0.0517 (11)	0.0003 (8)	0.0182 (9)	−0.0077 (8)

C7	0.0371 (9)	0.0388 (9)	0.0399 (9)	0.0026 (7)	0.0181 (8)	−0.0024 (7)
C8	0.0463 (10)	0.0313 (8)	0.0395 (9)	0.0029 (7)	0.0161 (8)	−0.0019 (7)
C9	0.0386 (8)	0.0317 (8)	0.0389 (9)	0.0030 (6)	0.0175 (7)	0.0015 (7)
C10	0.0419 (9)	0.0337 (8)	0.0457 (10)	−0.0001 (7)	0.0257 (8)	−0.0023 (7)
C11	0.0485 (10)	0.0413 (10)	0.0499 (11)	−0.0045 (8)	0.0264 (9)	−0.0078 (8)
C12	0.0565 (11)	0.0417 (10)	0.0663 (13)	−0.0115 (8)	0.0429 (11)	−0.0148 (9)
C13	0.0715 (13)	0.0330 (9)	0.0784 (15)	−0.0068 (9)	0.0554 (12)	−0.0073 (9)
C14	0.0690 (13)	0.0325 (9)	0.0617 (12)	0.0054 (8)	0.0408 (11)	0.0060 (8)
C15	0.0467 (9)	0.0320 (8)	0.0488 (10)	0.0026 (7)	0.0308 (8)	0.0015 (7)
C16	0.114 (2)	0.0324 (10)	0.112 (2)	−0.0109 (12)	0.0750 (19)	−0.0078 (12)
C17	0.0766 (15)	0.0572 (13)	0.0820 (17)	−0.0262 (11)	0.0497 (14)	−0.0305 (12)

Geometric parameters (Å, º)

O1—C8	1.203 (2)	C8—C9	1.510 (2)
N1—C9	1.301 (2)	C10—C11	1.405 (2)
N1—C10	1.378 (2)	C10—C15	1.418 (3)
N2—C1	1.306 (2)	C11—H11	0.9300
N2—C15	1.377 (2)	C11—C12	1.374 (3)
C1—C2	1.471 (2)	C12—C13	1.418 (3)
C1—C9	1.427 (2)	C12—C17	1.505 (3)
C2—C3	1.378 (3)	C13—C14	1.372 (3)
C2—C7	1.401 (2)	C13—C16	1.509 (3)
C3—H3	0.9300	C14—H14	0.9300
C3—C4	1.389 (3)	C14—C15	1.410 (2)
C4—H4	0.9300	C16—H16A	0.9600
C4—C5	1.377 (3)	C16—H16B	0.9600
C5—H5	0.9300	C16—H16C	0.9600
C5—C6	1.385 (3)	C17—H17A	0.9600
C6—H6	0.9300	C17—H17B	0.9600
C6—C7	1.382 (2)	C17—H17C	0.9600
C7—C8	1.491 (2)		
C9—N1—C10	114.01 (15)	N1—C10—C15	121.59 (16)
C1—N2—C15	114.02 (15)	C11—C10—C15	119.23 (16)
N2—C1—C2	128.14 (16)	C10—C11—H11	119.1
N2—C1—C9	123.29 (16)	C12—C11—C10	121.88 (19)
C9—C1—C2	108.57 (14)	C12—C11—H11	119.1
C3—C2—C1	130.93 (17)	C11—C12—C13	118.99 (18)
C3—C2—C7	120.44 (17)	C11—C12—C17	119.4 (2)
C7—C2—C1	108.62 (15)	C13—C12—C17	121.62 (19)
C2—C3—H3	120.9	C12—C13—C16	120.3 (2)
C2—C3—C4	118.18 (19)	C14—C13—C12	119.94 (17)
C4—C3—H3	120.9	C14—C13—C16	119.7 (2)
C3—C4—H4	119.4	C13—C14—H14	119.1
C5—C4—C3	121.26 (19)	C13—C14—C15	121.82 (19)
C5—C4—H4	119.4	C15—C14—H14	119.1
C4—C5—H5	119.5	N2—C15—C10	122.55 (15)

C4—C5—C6	121.09 (19)	N2—C15—C14	119.32 (17)
C6—C5—H5	119.5	C14—C15—C10	118.13 (17)
C5—C6—H6	121.0	C13—C16—H16A	109.5
C7—C6—C5	117.92 (18)	C13—C16—H16B	109.5
C7—C6—H6	121.0	C13—C16—H16C	109.5
C2—C7—C8	110.02 (15)	H16A—C16—H16B	109.5
C6—C7—C2	121.10 (17)	H16A—C16—H16C	109.5
C6—C7—C8	128.89 (17)	H16B—C16—H16C	109.5
O1—C8—C7	127.95 (16)	C12—C17—H17A	109.5
O1—C8—C9	127.57 (17)	C12—C17—H17B	109.5
C7—C8—C9	104.47 (14)	C12—C17—H17C	109.5
N1—C9—C1	124.53 (15)	H17A—C17—H17B	109.5
N1—C9—C8	127.17 (15)	H17A—C17—H17C	109.5
C1—C9—C8	108.30 (14)	H17B—C17—H17C	109.5
N1—C10—C11	119.18 (16)		

O1—C8—C9—N1	2.1 (3)	C6—C7—C8—C9	178.41 (18)
O1—C8—C9—C1	−178.2 (2)	C7—C2—C3—C4	−1.4 (3)
N1—C10—C11—C12	−179.08 (17)	C7—C8—C9—N1	−179.01 (17)
N1—C10—C15—N2	0.1 (3)	C7—C8—C9—C1	0.66 (18)
N1—C10—C15—C14	179.67 (16)	C9—N1—C10—C11	179.60 (16)
N2—C1—C2—C3	−0.6 (3)	C9—N1—C10—C15	−0.4 (2)
N2—C1—C2—C7	178.74 (17)	C9—C1—C2—C3	179.88 (18)
N2—C1—C9—N1	0.2 (3)	C9—C1—C2—C7	−0.79 (19)
N2—C1—C9—C8	−179.51 (16)	C10—N1—C9—C1	0.3 (2)
C1—N2—C15—C10	0.3 (2)	C10—N1—C9—C8	179.93 (16)
C1—N2—C15—C14	−179.21 (16)	C10—C11—C12—C13	−0.4 (3)
C1—C2—C3—C4	177.84 (18)	C10—C11—C12—C17	179.93 (17)
C1—C2—C7—C6	−178.38 (16)	C11—C10—C15—N2	−179.92 (16)
C1—C2—C7—C8	1.22 (19)	C11—C10—C15—C14	−0.4 (2)
C2—C1—C9—N1	179.72 (16)	C11—C12—C13—C14	−0.7 (3)
C2—C1—C9—C8	0.04 (18)	C11—C12—C13—C16	179.44 (19)
C2—C3—C4—C5	0.9 (3)	C12—C13—C14—C15	1.3 (3)
C2—C7—C8—O1	177.7 (2)	C13—C14—C15—N2	178.80 (17)
C2—C7—C8—C9	−1.16 (19)	C13—C14—C15—C10	−0.8 (3)
C3—C2—C7—C6	1.0 (3)	C15—N2—C1—C2	−179.95 (15)
C3—C2—C7—C8	−179.36 (16)	C15—N2—C1—C9	−0.5 (2)
C3—C4—C5—C6	0.0 (3)	C15—C10—C11—C12	1.0 (3)
C4—C5—C6—C7	−0.5 (3)	C16—C13—C14—C15	−178.83 (19)
C5—C6—C7—C2	−0.1 (3)	C17—C12—C13—C14	178.92 (18)
C5—C6—C7—C8	−179.59 (18)	C17—C12—C13—C16	−0.9 (3)
C6—C7—C8—O1	−2.7 (3)		