

## 5,8-Bis(trimethylsilylethynyl)quinoline

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## Key indicators

Single-crystal X-ray study

T = 180 K

Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$ 

R factor = 0.083

wR factor = 0.225

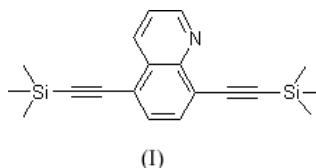
Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $\text{C}_{19}\text{H}_{23}\text{NSi}_2$ , is a TMS-protected rigid-rod di-yne. It is useful as a model compound for organometallic species of which it is a precursor and, like them, exhibits  $\pi$ -conjugation through the heteroaromatic linker unit in the backbone. The molecule is pseudo-linear, with a planar central quinoline group. Two  $\text{C}-\text{H} \cdots \text{N}$  short intermolecular contacts are found, with  $\text{C} \cdots \text{N}$  distances of 3.483 (5) and 3.671 (6)  $\text{Å}$ . An intermolecular contact between an aromatic H atom and the  $\text{C}\equiv\text{C}$  triple bond is also observed.

## Comment

In this paper, we report the structural characterization of 5,8-bis(trimethylsilylethynyl)quinoline, (I), which is a rigid-rod protected di-yne. This compound is used as a precursor of the platinum(II) di-yne species, *trans*- $[(\text{Et}_3\text{P})_2(\text{Ph})\text{Pt}-\text{C}\equiv\text{C}-R-\text{C}\equiv\text{C}-\text{Pt}(\text{Ph})(\text{Et}_3\text{P})_2]$  ( $R = \text{quinoline-5,8-diyl}$ ; Khan *et al.*, 2002), which is one of the many monomers used in the formation of rigid-rod organometallic polymers with the general formula *trans*- $[(\text{Bu}_3\text{P})_2\text{Pt}-\text{C}\equiv\text{C}-R-\text{C}\equiv\text{C}-]_\infty$  ( $R = \text{aromatic or heteroaromatic linker unit}$ ). Polymers of this type are of interest, due to the optical emission properties resulting from the extended  $\pi$ -conjugation exhibited along the backbone (Wittmann *et al.*, 1994; Beljonne *et al.*, 1996; Younus *et al.*, 1998; Chawdhury *et al.*, 1998, 1999; Wilson *et al.*, 2000, 2001, 2002). Precursors to these species, such as the title compound, are studied as models of the molecular and electronic properties and structure–property relationships in the poly-ynes.



The central ring system of the molecule (I) is planar and the backbone is pseudo-linear. The structure exhibits three intermolecular contacts of interest. Two  $\text{C}-\text{H} \cdots \text{N}$  close contacts between atoms H6 and H14c and N1 are found, where the  $\text{C6} \cdots \text{N1}$  distance is 3.483 (5)  $\text{Å}$  and the  $\text{C14} \cdots \text{N1}$  distance is 3.671 (6)  $\text{Å}$  (Table 2). Also found is an intermolecular contact between aromatic atom H2 and the triple bond  $\text{C15}\equiv\text{C16}$ . The distance between atom H2 and the centroid of C15 and C16 is 3.04  $\text{Å}$ , and the angle  $\text{C2}-\text{H2} \cdots \text{centroid}$  is  $164^\circ$ .

## Experimental

5,8-Bis(trimethylsilylethynyl)quinoline was synthesized by the following procedure. Catalytic amounts of CuI (12 mg, 0.06 mmol),

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Pd(OAc)<sub>2</sub> (12 mg, 0.048 mmol) and PPh<sub>3</sub> (36 mg, 0.13 mmol) were mixed with 5,8-diiodoquinoline (2.00 g, 5.24 mmol), trimethylsilyl-ethyne (1.28 g, 13.03 mmol) and <sup>i</sup>Pr<sub>2</sub>NH/THF (70 ml, 1:4 v/v). The crude product was filtered to eliminate the ammonium salt and the solvent mixture was removed under vacuum. The pale-brown residue was then dissolved in hexane and purified by silica column chromatography, eluting with hexane, to yield an off-white solid, the target compound in 80% yield.

#### Crystal data

C <sub>19</sub> H <sub>23</sub> NSi <sub>2</sub>	$D_x = 1.091 \text{ Mg m}^{-3}$
$M_r = 321.56$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4490 reflections
$a = 15.334 (2) \text{ \AA}$	$\theta = 3.8\text{--}25.2^\circ$
$b = 10.604 (2) \text{ \AA}$	$\mu = 0.18 \text{ mm}^{-1}$
$c = 12.465 (2) \text{ \AA}$	$T = 180 (2) \text{ K}$
$\beta = 104.96 (1)^\circ$	Block, colourless
$V = 1958.1 (5) \text{ \AA}^3$	$0.30 \times 0.30 \times 0.25 \text{ mm}$
$Z = 4$	

#### Data collection

Rigaku R-Axis IIC diffractometer	$R_{\text{int}} = 0.067$
$\varphi$ scans	$\theta_{\text{max}} = 25.2^\circ$
Absorption correction: none	$h = -18 \rightarrow 17$
5136 measured reflections	$k = -12 \rightarrow 0$
3166 independent reflections	$l = 0 \rightarrow 14$
2003 reflections with $I > 2\sigma(I)$	

#### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.1197P)^2]$
$wR(F^2) = 0.225$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3166 reflections	$\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
205 parameters	$\Delta\rho_{\text{min}} = -0.36 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Si1—C11	1.832 (4)	C5—C6	1.382 (5)
Si2—C16	1.835 (4)	C5—C10	1.446 (5)
N1—C1	1.313 (5)	C6—C7	1.401 (5)
N1—C9	1.372 (5)	C7—C8	1.364 (5)
C1—C2	1.404 (5)	C8—C9	1.429 (5)
C2—C3	1.362 (5)	C8—C15	1.443 (5)
C3—C4	1.410 (5)	C10—C11	1.207 (5)
C4—C5	1.419 (5)	C15—C16	1.207 (5)
C4—C9	1.432 (5)		
C11—C10—C5	174.3 (4)	C16—C15—C8	176.1 (4)
C10—C11—Si1	172.8 (4)	C15—C16—Si2	176.8 (4)
C2—C3—C4—C5	−178.6 (4)	C1—N1—C9—C8	−179.8 (4)
C3—C4—C5—C6	178.5 (4)	C7—C8—C9—N1	−178.6 (4)

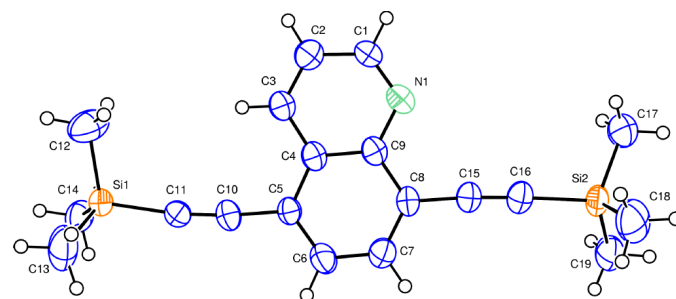
**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
C6—H6 $\cdots$ N1 <sup>i</sup>	0.95	2.69	3.483 (5)	141
C14—H14C $\cdots$ N1 <sup>ii</sup>	0.98	2.80	3.671 (6)	149

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

Aromatic and methyl H atoms were constrained as riding atoms, fixed to the parent atoms with distances of 0.95 and 0.98  $\text{\AA}$ , respec-



**Figure 1**

The molecular structure of 5,8-bis(trimethylsilylethynyl)quinoline, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

tively. The isotropic displacement parameters were fixed at  $1.2U_{\text{eq}}(\text{C})$  for aromatic and  $1.5U_{\text{eq}}(\text{C})$  for methyl H atoms.

Data collection: *R-Axis IIC Control Software* (Rigaku/MS, 1997); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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