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Key indicators

Single-crystal X-ray study
 $T = 168$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.041
 wR factor = 0.107
Data-to-parameter ratio = 11.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

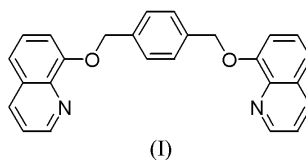
1,4-Bis(8-quinolyloxymethyl)benzene

The two quinoline ring systems of the title compound, $\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}_2$, are differently inclined to the plane of the central benzene ring. The intermolecular packing involves $\text{C}-\text{H}\cdots\text{N}$ and $\pi-\pi$ stacking interactions.

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Comment

We have recently embarked on a study of a diverse series of bridging heterocyclic ligands that comprise 8-quinolyloxy units separated by various spacer groups (Al-Mandhary & Steel, 2002). As part of this work, we prepared all three isomers of the ligands with xylylene spacers and showed that both the *ortho*- and *meta*-isomers readily formed transition metal complexes with interesting molecular structures (Al-Mandhary & Steel, 2004a). In contrast, the *para*-isomer, 1,4-bis(8-quinolyloxymethyl)benzene, (I), proved singularly resistant to the formation and isolation of any metal complexes. This raised some doubt as to the integrity of the ligand itself and, thus, a single crystal X-ray structure determination of (I) was carried out, the results of which are reported here.



The structure crystallizes in the monoclinic space group $P2_1/n$ with a full molecule in the asymmetric unit. The potential for higher crystallographic symmetry is precluded by the very different orientations of the two quinolyloxymethyl substituents; the mean planes of the two quinoline ring systems are inclined to the plane of the central aromatic ring at angles of 47.3 (2) and 73.2 (2)°, respectively. Also, the O atoms are differently displaced from the plane of the central ring, as reflected in the torsion angles $\text{C}2-\text{C}1-\text{C}11-\text{O}1 = 143.5$ (2) and $\text{C}3-\text{C}4-\text{C}21-\text{O}2 = 109.0$ (2)°. Similar variations were observed in the structure of a durene-derived tetrasubstituted analogue (Al-Mandhary & Steel, 2004b). The reason for these differences most probably (Desiraju, 2002, and references therein) lies in the crystal-packing interactions, which contain weak $\text{C}-\text{H}\cdots\text{N}$ (Amoore *et al.*, 2003, and reference therein) and $\pi-\pi$ stacking interactions (Hunter *et al.*, 2001; Jennings *et al.*, 2001; Meyer *et al.*, 2003). Specifically, adjacent molecules are weakly linked by $\text{C}-\text{H}\cdots\text{N}$ interactions between the quinoline ring systems, as defined by the following intermolecular contacts: $\text{N}11\cdots\text{H}24 = 2.42$ Å and $\text{N}21\cdots\text{H}14 = 2.59$ Å. The strongest $\pi-\pi$ interactions are between the central aromatic rings of adjacent molecules, whose mean planes and

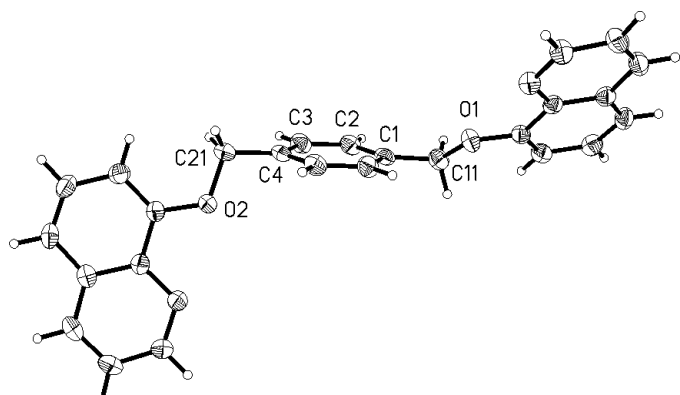


Figure 1
Perspective view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as small circles of arbitrary radii.

centroids are separated by approximately 3.49 and 3.79 Å, respectively.

Experimental

The title compound was prepared from 1,4-bis(bromomethyl)-benzene and 8-hydroxyquinoline by a literature procedure (Tummler *et al.*, 1979). Crystals suitable for X-ray analysis were formed by slow evaporation of a solution of the ligand in CH₂Cl₂/MeOH.

Crystal data

C₂₆H₂₀N₂O₂
M_r = 392.44
 Monoclinic, *P*₂₁/*n*
a = 11.969 (3) Å
b = 14.326 (3) Å
c = 12.622 (3) Å
 β = 113.604 (3)°
V = 1983.1 (8) Å³
Z = 4

D_x = 1.314 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 5016 reflections
 θ = 2.3–26.2°
 μ = 0.08 mm⁻¹
T = 168 (2) K
 Block, white
 0.54 × 0.40 × 0.35 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
T_{min} = 0.751, *T_{max}* = 0.971
 10845 measured reflections

3060 independent reflections
 2403 reflections with *I* > 2σ(*I*)
R_{int} = 0.043
 θ_{max} = 24.0°
h = -13 → 13
k = -16 → 16
l = -14 → 7

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.041
wR (*F*²) = 0.107
S = 1.03
 3060 reflections
 271 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.382P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.006$$

$$\Delta\rho_{\text{max}} = 0.59 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$$

H atoms were placed in calculated positions (C–H = 0.95–0.99 Å) and refined as riding, with *U_{iso}* = 1.2*U_{eq}* of the parent atom.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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