

Submitted to *Acta Cryst. C*

1,4-Bis(8-quinolyloxymethyl)benzene

Peter J. Steel^a and Muna R.A. Al-Mandhary^b

^aDepartment of Chemistry, University of Canterbury, Christchurch, New Zealand, and ^bCollege of Science, Sultan Qaboos University, Al-Khod 123, Sultanate of Oman

Correspondence email: peter.steel@canterbury.ac.nz

Abstract

The two quinoline rings of the title compound are differently inclined to the plane of the central benzene ring. The intermolecular packing involves C—H \cdots N and π - π stacking interactions.

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 (1), 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 1 was carried out, the results of which are reported herein.

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 rings are inclined to the plane of the central aromatic ring at angles of 47.3 (2) and 106.8 (2)°, respectively. Also, the oxygen atoms are differently displaced from the plane of the central ring, as reflected in the torsional angles C2—C1—C11—O1 = 143.5 (2) and C3—C4—C21—O2 = 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) lies in the crystal packing interactions, which contain weak C—H \cdots N (Amoore *et al.*, 2003) and π - π stacking interactions (Hunter *et al.*, 2001; Jennings *et al.*, 2001; Meyer *et al.*, 2003). Specifically, adjacent molecules are weakly linked by C—H \cdots N interactions between the quinoline rings, as defined by the following intermolecular contacts: N11—H24 = 2.42 (3) Å and N21—H14 = 2.59 (3) Å. The strongest π - π interactions are between the central aromatic rings of adjacent molecules, whose mean-planes and centroids are separated by approximately 3.49 Å 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 solution.

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART* (Bruker, 1997); 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* (Bruker, 1997).

Figures

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

1,4-Bis(8-quinolyloxymethyl)benzene

Crystal data

$C_{26}H_{20}N_2O_2$	$V = 1983.1 (8) \text{ \AA}^3$
$M_r = 392.44$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$
$a = 11.969 (3) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 14.326 (3) \text{ \AA}$	$T = 168 (2) \text{ K}$
$c = 12.622 (3) \text{ \AA}$	$0.54 \times 0.40 \times 0.35 \text{ mm}$
$\beta = 113.604 (3)^\circ$	

Data collection

CCD area detector diffractometer	3060 independent reflections
Absorption correction: multi-scan SADABS (Sheldrick, 2002)	2403 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.751$, $T_{\max} = 0.971$	$R_{\text{int}} = 0.043$
10845 measured reflections	$\theta_{\max} = 24.0^\circ$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$	271 parameters
$wR(F^2) = 0.107$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.03$	$\Delta\rho_{\max} = 0.59 \text{ e \AA}^{-3}$
3060 reflections	$\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$

Acknowledgements

We thank the Royal Society of New Zealand Marsden Fund for financial support, and Drs Lyall Hanton and Juliet Gerrard for useful discussions, mingled with expert advice.

References

- Al-Mandhary, M. R. A. & Steel, P. J. (2002). *Aust. J. Chem.* **55**, 705–708.
- Al-Mandhary, M. R. A. & Steel, P. J. (2004a). *Eur. J. Inorg. Chem.* pp. 329–334.
- Al-Mandhary, M. R. A. & Steel, P. J. (2004b). *Polyhedron* submitted.
- Amoore, J. J. M., Hanton, L. R. & Spicer, M. D. (2003). *Dalton Trans.* pp. 1056–1058, and references therein.
- Bruker (1997). *SMART, SAINT and SHELXTL*. Area Detector Control and Integration Software. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Desiraju, G. R. (2002). *Acc. Chem. Res.* **35**, 565–573 and references therein.
- Hunter, C. A., Lawson, K. R., Perkins, J. & Urch, C. J. (2001). *J. Chem. Soc., Perkin Trans.* pp. 651–669.
- Jennings, W. B., Farrell, B. M. & Malone, J. F. (2001). *Acc. Chem. Res.* **34**, 885–894.
- Meyer, E. A., Castellano, R. K. & Diederich, F. (2003). *Angew. Chem. Int. Ed.* **42**, 1210–1250.
- Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
- Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Tummler, B., Maass, G., Vogtle, F., Sieger, H., Heimann, U. & Weber, E. (1979). *J. Am. Chem. Soc.* **101**, 2588–2598.