

Sang Ho Nam,^a Byeong Kwon Park,^a Cheal Kim^{a*} and Youngmee Kim^{b*}

^aDepartment of Fine Chemistry, Seoul National University of Technology, Seoul 139-743, South Korea, and ^bDivision of Nano Sciences, Ewha Women's University, Seoul 120-750, South Korea

Correspondence e-mail: chealkim@sunt.ac.kr, ymeekim@ewha.ac.kr

Key indicators

Single-crystal X-ray study
 $T = 170$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.035
 wR factor = 0.076
 Data-to-parameter ratio = 13.7

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

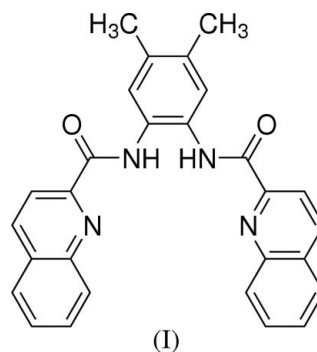
4,5-Dimethyl-1,2-bis(quinoline-2-carboxamido)-benzene

The molecule of the title compound [systematic name: *N,N'*-(4,5-dimethyl-*o*-phenylene)bis(quinoline-2-carboxamide), $\text{H}_2\text{Me}_2\text{bpq}$], $\text{C}_{28}\text{H}_{22}\text{N}_4\text{O}_2$, is twisted, with a dihedral angle of $54.48(3)^\circ$ between the two quinoline ring systems. Weak C—H···O hydrogen-bonding interactions generate a two-dimensional network.

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Comment

Non-heme biomimetic iron complexes have been extensively studied due to their ability to mimic some functional properties of non-heme iron monooxygenases (Costas *et al.*, 2004; Belda & Moberg, 2005). Although a number of iron complexes have been synthesized to carry out biomimetic olefin epoxidation and alkane hydroxylation using oxygen-donating reagents such as hydrogen peroxide, *tert*-butyl hydroperoxide, *m*-chloroperbenzoic acid and iodosylbenzene (Rohde *et al.*, 2003; Foster & Caradonna, 2003), only a few catalytic systems allow the selective oxidation of olefin and alkane to the corresponding products (Chen *et al.*, 2002). Therefore, in order to develop further the functional models for mononuclear non-heme iron oxygenases, we synthesized and crystallized a new N_4 -type tetradentate ligand, namely 4,5-dimethyl-1,2-bis(quinoline-2-carboxamido)benzene ($\text{H}_2\text{Me}_2\text{bpq}$), (I).



The asymmetric unit of (I) contains a whole molecule. The benzene ring is nearly coplanar with one of the quinoline ring systems (atoms N1/C1–C9), having a dihedral angle of $6.99(8)^\circ$. Due to steric hindrance, the two quinoline ring systems are twisted with respect to each other by a dihedral angle of $54.48(3)^\circ$ (Fig. 1). There are weak intramolecular C—H···O hydrogen-bond interactions (Table 1). Weak intermolecular C—H···O interactions, as described by Janaik & Scharmann (2003), are also present (Table 1). These weak hydrogen-bonding interactions generate a two-dimensional network (Fig. 2).

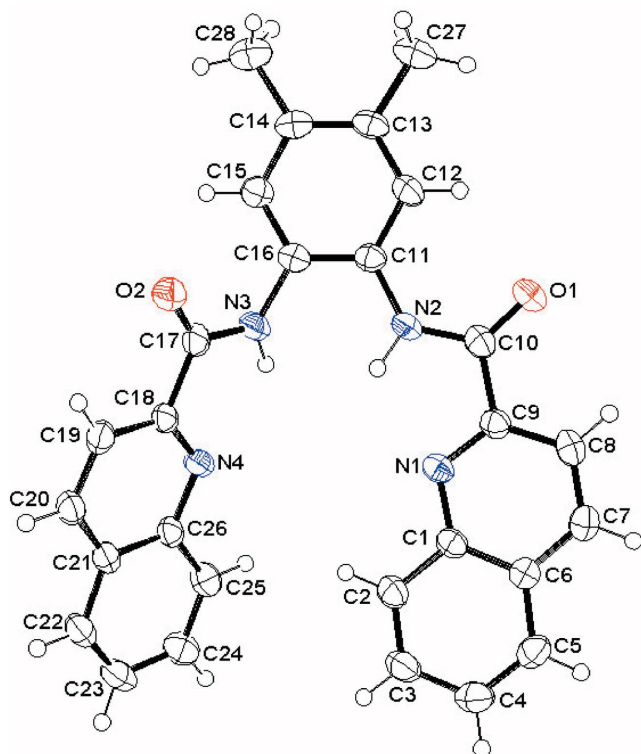


Figure 1
A molecular view of $\text{H}_2\text{Me}_2\text{bpq}$ with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

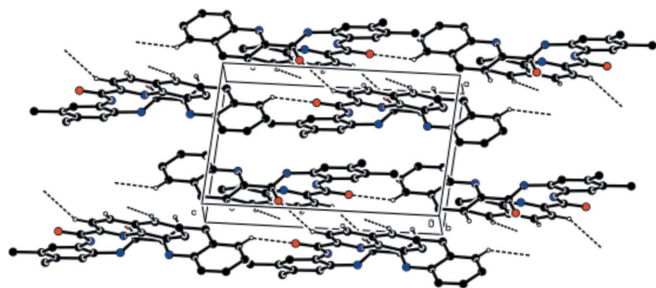


Figure 2
Packing view showing the $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions (dashed lines) leading to a two-dimensional network. H atoms not involved in intermolecular interactions have been omitted for clarity.

Experimental

For the preparation of the title compound, a slightly modified version of the method of Kim *et al.* (2005) was used. To a stirred solution of quinaldic acid (1.73 g, 10 mmol) in pyridine (10 ml), a solution of 4,5-dimethyl-1,2-phenylenediamine (0.68 g, 5 mmol) in pyridine (5 ml) was added dropwise. The solution was stirred for 15 min and triphenyl phosphite (2.62 ml, 10 mmol) was slowly added. The reaction mixture was warmed up to 393 K and the mixture stirred for 4 h. The volume of the solution was then reduced to 2 ml and it was kept in air. A pale-yellow precipitate formed and was filtered off. Crystallization from an aqueous solution afforded a pale-yellow powder, which was washed with ethanol. Pale-yellow crystals were obtained by slow evaporation of a dichloromethane–methanol solution (1:1) at room temperature.

Crystal data

$\text{C}_{28}\text{H}_{22}\text{N}_4\text{O}_2$
 $M_r = 446.50$
 Triclinic, $P\bar{1}$
 $a = 7.7346$ (10) Å
 $b = 11.9127$ (17) Å
 $c = 13.0732$ (18) Å
 $\alpha = 105.682$ (2)°
 $\beta = 92.228$ (3)°
 $\gamma = 106.699$ (2)°
 $V = 1101.9$ (3) Å³

$Z = 2$
 $D_x = 1.346$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 975 reflections
 $\theta = 2.8\text{--}24.1$ °
 $\mu = 0.09$ mm⁻¹
 $T = 170$ (2) K
 Block, pale yellow
 $0.25 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: none
 6147 measured reflections
 4222 independent reflections

1789 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$
 $\theta_{\text{max}} = 26.0$ °
 $h = -9 \rightarrow 8$
 $k = -14 \rightarrow 14$
 $l = -16 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.076$
 $S = 0.96$
 4222 reflections
 309 parameters
 H-atom parameters constrained

$w = [\exp(5(\sin\theta/\lambda)^2)] / [\sigma^2(F_o^2) + (0.0127P)^2]$
 where $P = 0.33333F_o^2 + 0.66667F_c^2$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N}2-\text{H}2\cdots\text{N}1$	0.88	2.16	2.625 (2)	112
$\text{N}3-\text{H}3\cdots\text{N}4$	0.88	2.28	2.682 (2)	108
$\text{C}12-\text{H}12\cdots\text{O}1$	0.95	2.31	2.928 (2)	122
$\text{C}22-\text{H}22\cdots\text{O}1^{\text{i}}$	0.95	2.39	3.064 (2)	128
$\text{C}5-\text{H}5\cdots\text{O}2^{\text{ii}}$	0.95	2.47	3.364 (2)	157
$\text{C}8-\text{H}8\cdots\text{O}2^{\text{iii}}$	0.95	2.54	3.389 (2)	149

Symmetry codes: (i) $x, y, z + 1$; (ii) $x, y + 1, z$; (iii) $-x, -y + 1, -z + 1$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $\text{C}-\text{H} = 0.95$ (aromatic) or 0.98 Å (CH_3) and $\text{N}-\text{H} = 0.88$ Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{ar}}, \text{N})$ or $1.5U_{\text{eq}}(\text{C}_{\text{Me}})$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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