

A 2:1 cocrystal of 2,3-bis(4-bromophenyl)quinoxaline  
and 1,2-bis(4-bromophenyl)ethane-1,2-diolLiang-Ce Rong,\* Xiao-Yue Li,  
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## Key indicators

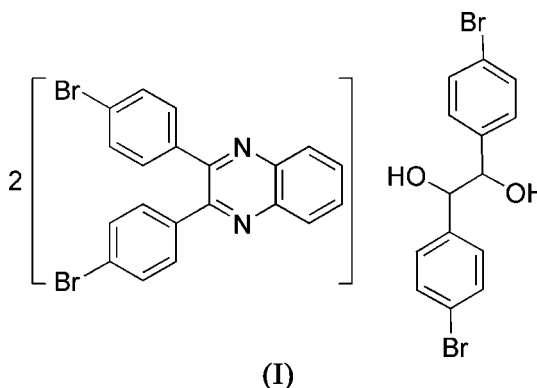
Single-crystal X-ray study  
 $T = 193\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.038  
 $wR$  factor = 0.097  
Data-to-parameter ratio = 14.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $\text{C}_{20}\text{H}_{12}\text{Br}_2\text{N}_2 \cdot 0.5\text{C}_{14}\text{H}_{12}\text{Br}_2\text{O}_2$ , was synthesized by the one-pot reaction of benzofurazan oxide and 1,2-bis(4-bromophenyl)ethane-1,2-dione induced by a low-valent titanium reagent. X-ray analysis reveals that the 1,2-bis(4-bromophenyl)ethane-1,2-diol molecule is located on an inversion centre. The molecules are linked *via*  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonds and  $\text{C}-\text{H} \cdots \pi$  interactions.

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## Comment

Quinoxaline derivatives are an important class of nitrogen-containing heterocycles and they constitute useful intermediates in organic synthesis. They have been reported for their applications in the fields of dyes (Brock *et al.*, 1999) and pharmaceuticals (Gazit *et al.*, 1996; Sehlstedt *et al.*, 1998) and have also been used as building blocks for the synthesis of organic semiconductors (Dailey *et al.*, 2001). Low-valent titanium reagents have an exceedingly high ability to promote reductive coupling of carbonyl compounds and are attracting increasing interest in organic synthesis (McMurry, 1983; Shi *et al.*, 2003). We report here the crystal structure of the title compound, (I).



The asymmetric unit of (I) contains one 2,3-bis(4-bromophenyl)quinoxaline (bbq) molecule and one half-molecule of 1,2-bis(4-bromophenyl)ethane-1,2-diol (bbe) which is located on an inversion centre (Fig. 1). Bond lengths and angles in the molecules show normal values (Table 1). The C16–C21 and C22–C27 benzene rings form dihedral angles of 38.1 (1) and 51.8 (1)°, respectively, with the mean quinoxaline plane. The C2–C7 and C2A–C7A benzene rings are parallel by symmetry.

Two bbq molecules and one bbe molecule are connected *via*  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonds to form a trimer. In addition,  $\text{C}-\text{H} \cdots \pi$  interactions involving the C2–C7 benzene ring (centroid  $C_g$ ) are observed (Table 2).

Experimental

Compound (I) was prepared by the reaction of benzofurazan oxide (2 mmol) and 1,2-bis(4-bromophenyl)ethane-1,2-dione (2 mmol) with a low-valent titanium reagent (TiCl<sub>4</sub>/Zn; 1.1 ml/1.30 g) in THF (15 ml). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

C<sub>20</sub>H<sub>12</sub>Br<sub>2</sub>N<sub>2</sub>·0.5C<sub>14</sub>H<sub>12</sub>Br<sub>2</sub>O<sub>2</sub> V = 1176.7 (3) Å<sup>3</sup>  
 M<sub>r</sub> = 626.13 Z = 2  
 Triclinic, P $\bar{1}$  D<sub>x</sub> = 1.767 Mg m<sup>-3</sup>  
 a = 7.8746 (7) Å Mo K $\alpha$  radiation  
 b = 11.9601 (9) Å  $\mu$  = 5.17 mm<sup>-1</sup>  
 c = 14.446 (2) Å T = 193 (2) K  
 $\alpha$  = 66.121 (11)° Block, yellow  
 $\beta$  = 83.931 (17)° 0.30 × 0.24 × 0.13 mm  
 $\gamma$  = 71.126 (15)°

Data collection

Rigaku Mercury diffractometer 11766 measured reflections  
 $\omega$  scans 4295 independent reflections  
 Absorption correction: multi-scan 3425 reflections with I > 2 $\sigma$ (I)  
 (Jacobson, 1998) R<sub>int</sub> = 0.037  
 T<sub>min</sub> = 0.306, T<sub>max</sub> = 0.553  $\theta_{max}$  = 25.3°  
 (expected range = 0.283–0.511)

Refinement

Refinement on F<sup>2</sup> H-atom parameters constrained  
 R[F<sup>2</sup> > 2 $\sigma$ (F<sup>2</sup>)] = 0.038 w = 1/[ $\sigma^2(F_o^2) + (0.0531P)^2$ ]  
 wR(F<sup>2</sup>) = 0.097 where P = (F<sub>o</sub><sup>2</sup> + 2F<sub>c</sub><sup>2</sup>)/3  
 S = 1.03 ( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 4295 reflections  $\Delta\rho_{max}$  = 1.04 e Å<sup>-3</sup>  
 300 parameters  $\Delta\rho_{min}$  = -0.65 e Å<sup>-3</sup>

Table 1 Selected geometric parameters (Å, °).

Br1—C5	1.904 (3)	N1—C8	1.373 (4)
Br2—C19	1.900 (4)	N2—C10	1.319 (4)
Br3—C25	1.899 (3)	N2—C9	1.372 (4)
N1—C11	1.318 (4)		
C11—N1—C8	118.6 (3)	N2—C10—C16	115.5 (3)
C10—N2—C9	118.6 (3)	C11—C10—C16	123.5 (3)
O1—C1—C2	112.4 (3)	N1—C11—C22	115.6 (3)
O1—C1—C1 <sup>i</sup>	108.3 (4)	C10—C11—C22	123.5 (3)
C2—C1—C1 <sup>i</sup>	111.1 (3)		

Symmetry code: (i) -x + 2, -y, -z.

Table 2 Hydrogen-bond geometry (Å, °).

C<sub>g</sub> is the centroid of the C2–C7 benzene ring.

D—H...A	D—H	H...A	D...A	D—H...A
O1—H1...N1 <sup>ii</sup>	0.84	2.05	2.882 (4)	168
C12—H12...C <sub>g</sub> <sup>iii</sup>	0.95	2.84	3.666 (4)	146

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

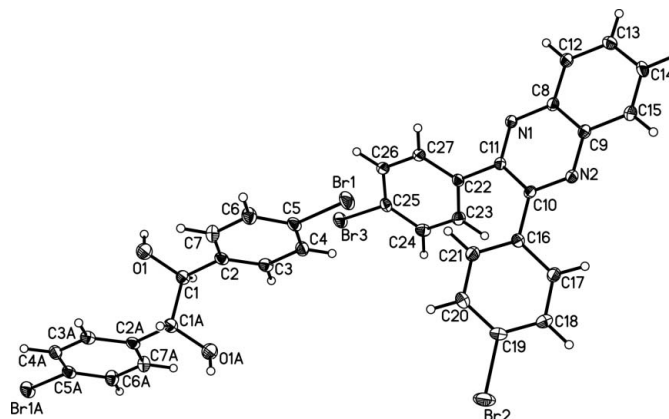


Figure 1 The structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. Atoms labelled with the suffix A are generated by the symmetry operation (2 - x, -y, -z).

H atoms were positioned geometrically and treated as riding, with an O—H distance of 0.84 Å and C—H distances in the range 0.95–1.00 Å, and with U<sub>iso</sub>(H) = 1.5U<sub>eq</sub>(C) for methyl H atoms and 1.2U<sub>eq</sub>(C) for others. The highest peak is located 0.56 Å from atom H1A.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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