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2,3-Diphenylquinoxaline

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In the title compound, $C_{20}H_{14}N_2$, the presence of adjacent phenyl rings causes an out-of-plane twist in the quinoxaline system of approximately 12°.

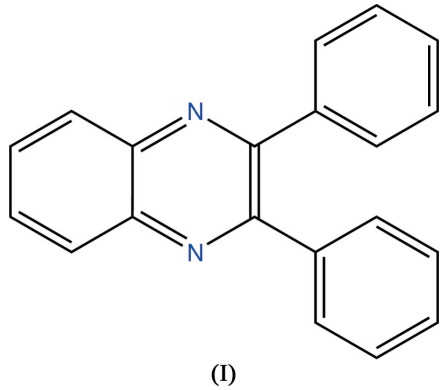
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.112
Data-to-parameter ratio = 17.1

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

Comment

Compounds containing a quinoxaline group are of considerable interest due to the potential use of their metal complexes as molecular devices and DNA probes (Holmlin & Barton, 1995; Balzani, Campagna *et al.*, 1998; Balzani, Gomez-Loez & Stoddart, 1998; Du & Zhao, 2003).



(I)

In (I), the quinoxaline unit makes a dihedral angle of 37.1 (1)° with the C11–C16 phenyl ring and 53.3 (1)° with the C17–C22 phenyl ring. The presence of the two adjacent phenyl rings causes an out-of-plane twist in the quinoxaline system [C17—C2—C3—C11 = 12.0 (2)°].

Experimental

Benzil (0.50 mg, 2,38 mmol), 1,2-diaminobenzene (0.26 mg, 2.40 mmol), molecular sieves (1 g) and manganese oxide (0.10 mg) as a catalyst were heated in a glass vial using domestic microwave oven. After 1 min the vial was cooled to room temperature and the solution was filtered. The product was recrystallized from ethanol to give (I) (yield 0.570 mg, 76.49%).

Crystal data

$C_{20}H_{14}N_2$
M_r = 282.33
Monoclinic, $P2_1/n$
a = 6.0306 (2) Å
b = 10.9269 (5) Å
c = 22.5309 (8) Å
β = 95.005 (3)°
V = 1479.03 (10) Å^3
Z = 4
D_x = 1.268 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 (2) K
Prism, light yellow
0.5 × 0.45 × 0.3 mm

Data collection

Oxford Diffraction CrysAlisCCD diffractometer
ω-2θ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.93, T_{max} = 0.98
16180 measured reflections
3413 independent reflections
2773 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 1.13
3413 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0092 (16)

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.3228 (18)	C3—N4	1.3213 (19)
N1—C6	1.3678 (19)	N4—C5	1.3683 (19)
C3—C2—C17	123.34 (13)	C2—C3—C11	122.99 (12)

All H atoms were positioned geometrically (C—H = 0.95 Å) refined as riding on their parent atoms, with U_{iso}(H)= 1.2U_{eq}(parent).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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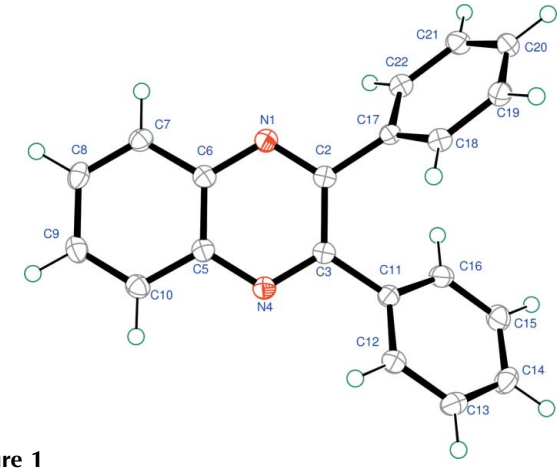

Figure 1
The molecular structure, with displacement ellipsoids drawn at the 50% probability level.

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