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# 8,9-Diphenylimidazo[1,2-*c*]quinazoline

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**Key indicators**

Single-crystal X-ray study
*T* = 291 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.042
*wR* factor = 0.094
Data-to-parameter ratio = 13.0

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



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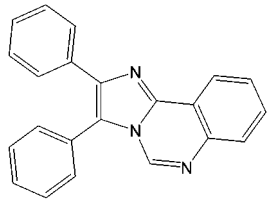
The title compound, $C_{22}H_{15}N_3$, was synthesized by the reaction of 4,5-diphenyl-2-(2-nitrophenyl)imidazole with triethyl orthoformate, induced by a low-valent titanium reagent ($TiCl_4$/Zn). There are two independent molecules of similar conformation in the asymmetric unit. X-ray analysis reveals that the imidazole ring and pyrimidine ring are essentially coplanar.

## Comment

Quinazolines are an important class of compounds found in many naturally occurring products (*e.g.* hinckdentine A; Blackman *et al.*, 1987; Billimmoria & Cava, 1994) and employed as potent cytotoxic agents (Ibrahim *et al.*, 1988; Riou *et al.*, 1991; Brana *et al.*, 1994; Helissey *et al.*, 1994). 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.*, 1993, 1997, 1998, 2003). We report here the crystal structure of 8,9-diphenylimidazo[1,2-*c*]quinazoline, (I), synthesized by the reaction of 4,5-diphenyl-2-(2-nitrophenyl)imidazole with triethyl orthoformate, induced by a low-valent titanium reagent ($TiCl_4$/Zn).




(I)

In (I), there are two independent molecules of similar conformation in the asymmetric unit (Fig. 1 and Table 1). The dihedral angle between the pyrimidine (N3/C1/C6/C7/N2/C8) and imidazole rings (N1/C7/N2/C9/C10) is 0.71 (1)°, indicating that these two rings are nearly coplanar. N1—C7 and N3—C8 [1.321 (2) and 1.283 (2) Å] are double bonds, while the other C—N bond distances are in the range 1.380 (2)–1.398 (2) Å, corresponding to single bonds. Atoms N3 and N3′ are involved in weak intermolecular C—H···N interactions (Fig. 2 and Table 2).

## Experimental

The title compound, (I), was prepared by the reaction of 4,5-diphenyl-2-(2-nitrophenyl)imidazole with triethyl orthoformate, induced by a low-valent titanium reagent ($TiCl_4$/Zn) (m.p. 466–468 K). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

*Crystal data*

| | |
|---|---|
| $C_{22}H_{15}N_3$ | $D_x$ = 1.283 Mg m$^{-3}$ |
| $M_r$ = 321.37 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/c$ | Cell parameters from 31 reflections |
| $a$ = 13.262 (2) Å | $\theta$ = 3.1–13.4° |
| $b$ = 10.814 (1) Å | $\mu$ = 0.08 mm$^{-1}$ |
| $c$ = 23.462 (4) Å | $T$ = 291 (2) K |
| $\beta$ = 98.40 (1)° | Block, colourless |
| $V$ = 3328.6 (8) Å$^3$ | 0.44 × 0.42 × 0.40 mm |
| $Z$ = 8 | |

*Data collection*

| | |
|---|---|
| Siemens $P4$ diffractometer | $\theta_{max}$ = 25.0° |
| $\omega$ scans | $h = 0 \rightarrow 15$ |
| Absorption correction: none | $k = 0 \rightarrow 12$ |
| 6709 measured reflections | $l = -27 \rightarrow 27$ |
| 5856 independent reflections | 3 standard reflections |
| 2804 reflections with $I > 2\sigma(I)$ | every 97 reflections |
| $R_{int}$ = 0.015 | intensity decay: 1.5% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0408P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.042 | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2)$ = 0.094 | $\Delta\rho_{max}$ = 0.17 e Å$^{-3}$ |
| $S$ = 0.80 | $\Delta\rho_{min}$ = −0.14 e Å$^{-3}$ |
| 5856 reflections | Extinction correction: *SHELXTL* |
| 452 parameters | Extinction coefficient: 0.0034 (2) |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N1—C7 | 1.321 (2) | N1′—C7′ | 1.320 (2) |
| N1—C10 | 1.391 (2) | N1′—C10′ | 1.394 (2) |
| N2—C7 | 1.380 (2) | N2′—C8′ | 1.384 (2) |
| N2—C8 | 1.383 (2) | N2′—C7′ | 1.387 (2) |
| N2—C9 | 1.398 (2) | N2′—C9′ | 1.394 (2) |
| N3—C8 | 1.283 (2) | N3′—C8′ | 1.283 (2) |
| N3—C1 | 1.392 (2) | N3′—C1′ | 1.398 (3) |
| C6—C7 | 1.428 (3) | C6′—C7′ | 1.433 (3) |
| C9—C10 | 1.375 (3) | C9′—C10′ | 1.371 (2) |
| | | | |
| C7—N1—C10 | 105.23 (16) | N1—C7—C6 | 130.98 (19) |
| C7—N2—C8 | 121.24 (19) | N2—C7—C6 | 117.55 (18) |
| C7—N2—C9 | 107.41 (16) | N3—C8—N2 | 123.3 (2) |
| C8—N2—C9 | 131.32 (18) | C10—C9—N2 | 104.49 (16) |
| C8—N3—C1 | 118.26 (18) | N2—C9—C17 | 121.50 (18) |
| N3—C1—C2 | 118.4 (2) | C9—C10—N1 | 111.38 (17) |
| N3—C1—C6 | 122.7 (2) | N1—C10—C11 | 119.13 (18) |
| N1—C7—N2 | 111.46 (18) | | |
| C8—N3—C1—C2 | −178.7 (2) | C8—N2—C7—N1 | 179.63 (18) |
| C8—N3—C1—C6 | 0.4 (3) | C9—N2—C7—N1 | 1.3 (2) |
| N3—C1—C2—C3 | 179.4 (2) | C9—N2—C7—C6 | −178.07 (18) |
| N3—C1—C6—C5 | −178.2 (2) | C5—C6—C7—N1 | −1.3 (4) |
| N3—C1—C6—C7 | 1.4 (3) | C1—C6—C7—N1 | 179.1 (2) |
| C10—N1—C7—N2 | −0.6 (2) | C5—C6—C7—N2 | 177.9 (2) |
| C10—N1—C7—C6 | 178.7 (2) | C9—N2—C8—N3 | 179.5 (2) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8···N3′ | 0.93 | 2.59 | 3.267 (3) | 130 |
| C8′—H8′···N3 | 0.93 | 2.63 | 3.280 (3) | 128 |

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.97 Å; the $U_{iso}$(H) values were set equal to1.2$U_{eq}$(C).

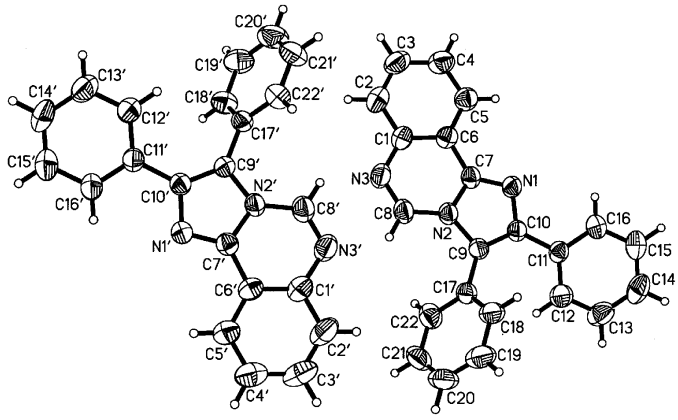



**Figure 1**
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

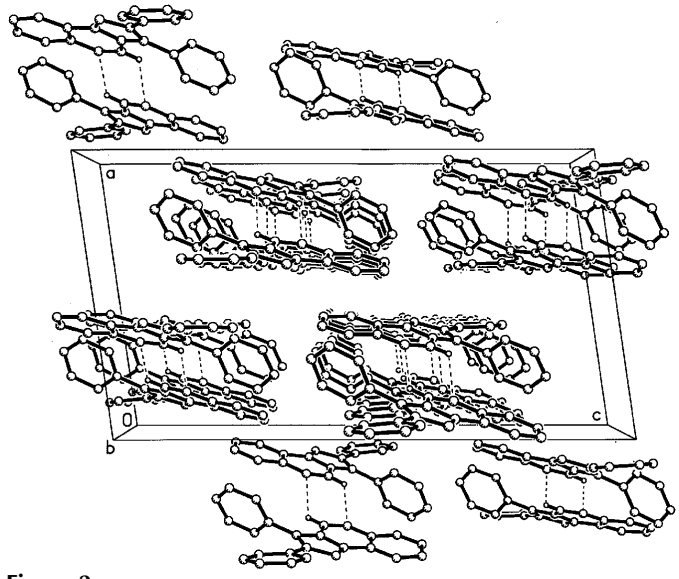



**Figure 2**
The molecular packing in the crystal structure of (I).

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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