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#### Key indicators

Single-crystal X-ray study  
 $T = 291\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.039  
 $wR$  factor = 0.087  
Data-to-parameter ratio = 12.9

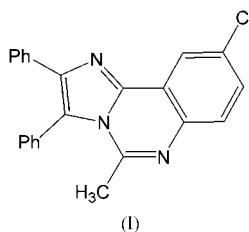
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 2-Chloro-6-methyl-8,9-diphenylimidazo-[1,2-c]quinazoline

The title compound,  $\text{C}_{23}\text{H}_{16}\text{ClN}_3$ , has been synthesized by the reaction of 4,5-diphenyl-2-(2-nitro-5-chlorophenyl)imidazole with triethyl *ortho*-acetate, induced by a low-valent titanium reagent. There are two independent molecules of similar conformation in the asymmetric unit. The dihedral angles between the pyrimidine and imidazole rings are  $2.14(2)^\circ$  and  $2.71(3)^\circ$ .

#### Comment

Quinazolines are an important class of compounds, found in many naturally occurring products (*e.g.* hinckdentine A; Blackman *et al.*, 1987; Billimoria & 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.*, 2003). We report here the crystal structure of the title compound, (I), synthesized by the reaction of 4,5-diphenyl-2-(2-nitro-5-chlorophenyl)imidazole with triethyl *ortho*-acetate, induced by a low-valent titanium reagent.



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 ring (N1/C1/C6/C7/N2/C8) and the imidazole ring (N2/C7/N3/C10/C9) is  $2.14(2)^\circ$ , and that for the other independent molecule is  $2.71(3)^\circ$ , indicating that these two rings are nearly coplanar. N1—C8 and N3—C7 [ $1.292(3)$ – $1.311(2)\text{ \AA}$ ] are double bonds, while the other C—N bond distances are in the range  $1.387(2)$ – $1.413(2)\text{ \AA}$ , corresponding to single bonds. The molecular packing is shown in Fig. 2, where the Cl and Cl' atoms are arranged alternately along the *a* axis.

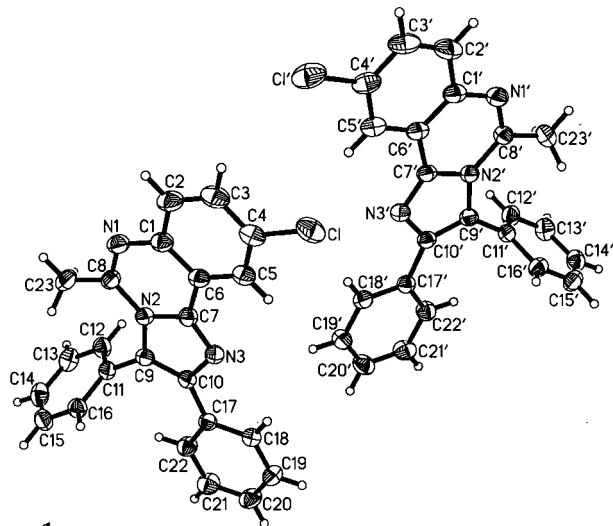
#### Experimental

The title compound, (I), was prepared by the reaction of 4,5-diphenyl-2-(2-nitro-5-chlorophenyl)imidazole with triethyl *ortho*-acetate, induced by a low-valent titanium reagent ( $\text{TiCl}_4/\text{Zn}$ ). M.p.  $452$ – $453\text{ K}$ . Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

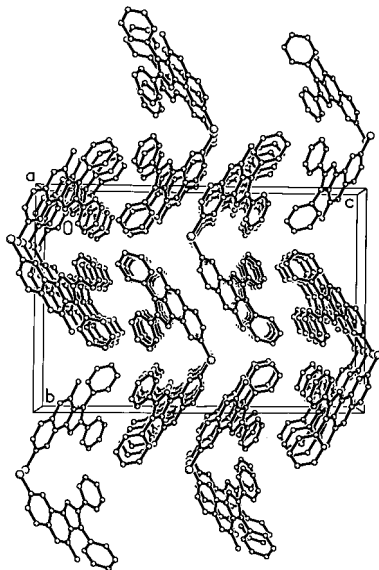
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**Figure 1**  
The molecular structure of the asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.



**Figure 2**  
The crystal structure of (I) projected along the *a* axis.

#### Crystal data

$C_{23}H_{16}ClN_3$   
 $M_r = 369.84$   
Monoclinic,  $P2_1/c$   
 $a = 7.789$  (1) Å  
 $b = 17.777$  (2) Å  
 $c = 26.040$  (3) Å  
 $\beta = 94.70$  (1)°  
 $V = 3593.7$  (9) Å<sup>3</sup>  
 $Z = 8$

#### Data collection

Siemens P4 diffractometer  
 $\omega$  scans  
Absorption correction:  $\psi$  scan  
(XSCANS; Siemens, 1994)  
 $T_{\min} = 0.882$ ,  $T_{\max} = 0.926$   
7325 measured reflections  
6330 independent reflections  
3063 reflections with  $I > 2\sigma(I)$

$D_x = 1.367$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 35 reflections  
 $\theta = 2.9$ – $14.9^\circ$   
 $\mu = 0.23$  mm<sup>-1</sup>  
 $T = 291$  (2) K  
Block, colourless  
 $0.54 \times 0.48 \times 0.34$  mm

$R_{\text{int}} = 0.011$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = 0 \rightarrow 9$   
 $k = 0 \rightarrow 21$   
 $l = -30 \rightarrow 30$   
3 standard reflections  
every 97 reflections  
intensity decay: 1.9%

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.087$   
 $S = 0.80$   
6330 reflections  
490 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.23$  e Å<sup>-3</sup>  
Extinction correction: *SHELXTL*  
Extinction coefficient: 0.0035 (2)

**Table 1**

Selected geometric parameters (Å, °).

N1—C8	1.292 (3)	N1'—C8'	1.290 (3)
N1—C1	1.391 (3)	N1'—C1'	1.388 (3)
N2—C7	1.394 (2)	N2'—C7'	1.390 (2)
N2—C8	1.409 (3)	N2'—C8'	1.404 (3)
N2—C9	1.413 (2)	N2'—C9'	1.408 (3)
N3—C7	1.311 (2)	N3'—C7'	1.307 (2)
N3—C10	1.387 (2)	N3'—C10'	1.383 (2)
C6—C7	1.429 (3)	C6'—C7'	1.435 (3)
C8—C23	1.485 (3)	C8'—C23'	1.487 (3)
C9—C10	1.374 (3)	C9'—C10'	1.382 (3)
C8—N1—C1	120.0 (2)	N3—C7—N2	112.1 (2)
C7—N2—C8	120.07 (19)	N3—C7—C6	128.9 (2)
C7—N2—C9	105.96 (17)	N2—C7—C6	119.0 (2)
C8—N2—C9	133.89 (19)	N1—C8—N2	121.7 (2)
C7—N3—C10	105.64 (18)	N2—C9—C11	124.60 (19)
N1—C1—C6	122.8 (2)	C9—C10—N3	111.4 (2)
N1—C1—C2	118.5 (2)	C8—N1—C1—C2	-179.4 (2)
C8—N1—C1—C2	-179.4 (2)	C9—N2—C8—N1	177.1 (2)
C5—C6—C7—N3	1.4 (4)	C7—N3—C10—C17	179.11 (18)
C1—N1—C8—N2	-0.6 (3)	N2—C9—C11—C12	75.3 (3)
C1—N1—C8—C23	-179.95 (19)	C9—C10—C17—C18	-178.0 (2)

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  $U_{\text{iso}}(\text{H})$  values were set equal to  $1.2U_{\text{eq}}(\text{C})$ .

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*.

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