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2,2-Dimethyl-3-(4-methylphenyl)-1,2-dihydroquinazolin-4(3*H*)-one

Daqing Shi,[a]* Juxian Wang,[a] Liangce Rong,[a] Xiangshan Wang[a] and Hongwen Hu[b]

[a]Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, People's Republic of China, and [b]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: dqshi@263.net

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.119
Data-to-parameter ratio = 14.3

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

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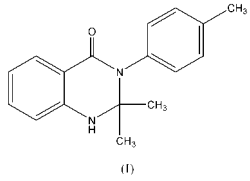
The title compound, $C_{17}H_{18}N_2O$, was synthesized by the reaction of *N*-(4-methylphenyl)-2-nitrobenzamide and acetone, induced by a low-valent titanium reagent. The dihydropyrimidine ring adopts a half-chair conformation. The molecules are connected by N—H···O hydrogen bonds, forming a linear chain along the *b* axis.

Comment

Quinazolin-4(3*H*)-one is an alkaloid (Chou *et al.*, 1948). Substituted quinazolin-4(3*H*)-ones possess a wide range of pharmacological activities, such as antibacterial (Ager *et al.*, 1977) and anticancer (Skula *et al.*, 1981). Low-valent reagents have an exceedingly high ability to promote reductive coupling of carbonyl compounds and are attracting increasing interest in organic synthesis (McMurry, 1983). We report here the crystal structure of the title compound, (I), which has been synthesized by the reaction induced by a low-valent titanium reagent.



(I)

The dihydropyrimidine ring adopts a half-chair conformation (Fig. 1 and Table 1). Atoms N1, C9, C10, C11 and N2 are coplanar (plane 1, the deviations from each atom to the plane

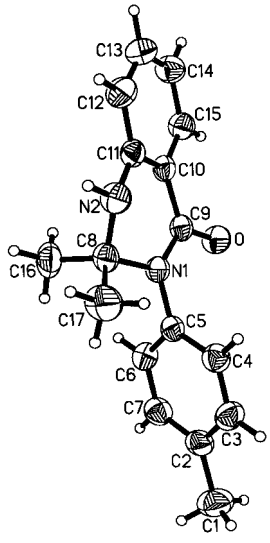


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

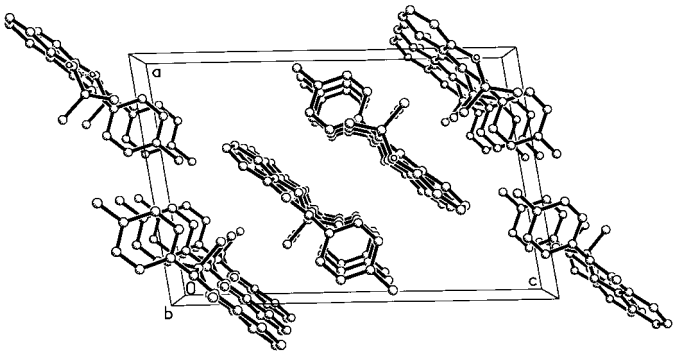


Figure 2
A molecular packing diagram of (I), viewed along the *b* axis.

are less than 0.07 Å), while C8 lies out of the plane by 0.537 (2) Å. The dihedral angle between plane 1 and the fused benzene ring C10–C15 is 1.61 (1)°. Because of the existence of conjugation, the distances N1—C9 [1.356 (2) Å] and N2—C11 [1.367 (2) Å] are significantly shorter than the typical Csp^2—N bond distance (1.426 Å; Lorente *et al.*, 1995). The molecules are linked by N—H···O hydrogen bonds, forming a linear chain along the *b* axis (Fig. 2 and Table 2).

Experimental

The title compound, (I), was prepared by the reaction of *N*-(4-methylphenyl)-2-nitrobenzamide with acetone induced by a low-valent titanium reagent ($TiCl_4$/Zn); m.p. 528–529 K. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{17}H_{18}N_2O$
M_r = 266.33
Monoclinic, $P2_1/n$
a = 11.917 (2) Å
b = 6.911 (1) Å
c = 17.821 (4) Å
β = 98.81 (1)°
V = 1450.4 (5) Å^3
Z = 4
D_x = 1.220 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 34 reflections
θ = 3.2–14.8°
μ = 0.08 mm^{-1}
T = 295 (2) K
Block, colorless
0.56 × 0.52 × 0.32 mm

Data collection

Siemens *P*4 diffractometer
ω scans
Absorption correction: none
3202 measured reflections
2706 independent reflections
1628 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.5°
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 8$
$l = -21 \rightarrow 21$
3 standard reflections
every 97 reflections
intensity decay: 2.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 0.92
2706 reflections
189 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0114 (16)

Table 1
Selected geometric parameters (Å, °).

O—C9	1.2336 (19)	N2—C8	1.449 (2)
N1—C9	1.356 (2)	C8—C17	1.509 (3)
N1—C5	1.444 (2)	C8—C16	1.516 (3)
N1—C8	1.501 (2)	C9—C10	1.468 (2)
N2—C11	1.367 (2)		
C9—N1—C5	118.7 (2)	N1—C8—C16	109.32 (15)
C9—N1—C8	122.16 (15)	O—C9—N1	121.38 (16)
C5—N1—C8	117.89 (14)	O—C9—C10	121.94 (16)
C11—N2—C8	119.65 (16)	N1—C9—C10	116.60 (15)
N2—C8—C17	106.86 (17)	N2—C11—C12	122.15 (18)
N1—C8—C17	110.75 (16)	N2—C11—C10	118.82 (17)
N2—C8—C16	111.57 (16)		
C9—N1—C5—C6	−81.4 (2)	C8—N1—C9—O	−171.53 (16)
C8—N1—C5—C6	86.1 (2)	N1—C9—C10—C15	−174.09 (16)
C11—N2—C8—N1	46.6 (2)	C8—N2—C11—C12	155.19 (18)
C5—N1—C9—O	−4.6 (2)	C8—N2—C11—C10	−28.5 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H0N···O^{i}	0.85 (2)	2.14 (2)	2.978 (2)	170.9 (19)

Symmetry code: (i) $x, 1 + y, z$.

The H atom bonded to N2 was refined isotropically. The other H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 U_{eq}(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*; software used to prepare material for publication: *SHELXTL*.

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