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3-[4-(Dimethylamino)benzylideneamino]-2-methylquinazolin-4(3*H*)-one

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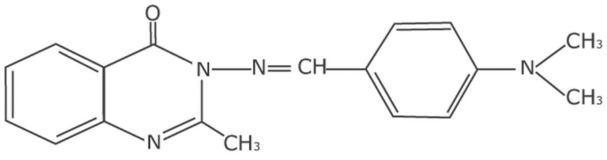
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.149; data-to-parameter ratio = 12.8.

In the title compound, $C_{18}H_{18}N_4O$, the dihedral angle between the quinazoline and benzylidene groups is 54.0 (4)°. In the crystal structure, the molecules associate into centrosymmetric dimers *via* C—H···O interactions.

Related literature

For related literature, see: Alagarsamy *et al.* (2003, 2004); El-Meligie *et al.* (2001).



Experimental

Crystal data

$C_{18}H_{18}N_4O$
M_r = 306.36
Triclinic, $P\overline{1}$
a = 7.5175 (10) Å
b = 9.3631 (13) Å
c = 12.7886 (17) Å
α = 98.198 (2)°
β = 103.259 (2)°
γ = 112.517 (2)°
V = 782.33 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
0.21 × 0.18 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: none
9011 measured reflections
3582 independent reflections
2863 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.150
S = 1.03
3582 reflections
280 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18B···O1^{i}	0.94 (2)	2.58 (3)	3.379 (2)	143.0 (19)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997), *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2537).

References

Alagarsamy, V., Murugananthan, G. & Venkateshperumal, R. (2003). *Biol. Pharm. Bull.* **26**, 1711–1714.
Alagarsamy, V., Rajesh, R., Ramaseshu, M., Vijayakumar, S., Ramaseshu, K. V. & Duraianandakumar, T. (2004). *Biol. Pharm. Bull.* **27**, 652–656.
Bruker (2001). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
El-Meligie, S., El-Ansary, A. K., Said, M. M. & Hussein, M. M. M. (2001). *Ind. J. Chem. Sect. B*, **40**, 62–69.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

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3-[4-(Dimethylamino)benzylideneamino]-2-methylquinazolin-4(3*H*)-one

P. Kumaradhas, G. Sankara Lakshmi, B. Sridhar, P. Paneer Selvam and G. Saravanan

Comment

Quinazolin related compounds exhibit multiple medicinal activities, such as analgesic (Alagarsamy *et al.*, 2004), anti-inflammatory (Alagarsamy *et al.*, 2003), and anticonvulsant (El-Meligie *et al.*, 2001) properties. As part of our studies of these systems, we now present the synthesis and structure of the title compound, (I), (Fig. 1).

In the quinazolin ring, the single bond C—N distances [C8—N2 = 1.385 (2) Å; C7—N2 = 1.398 (2) Å and C3—N1 = 1.387 (2) Å] are almost equal and longer than C14—N4 [1.364 (2) Å]. The non-ring C—N bond distances such as C17—N4 and C18—N4 are significantly, longer than the above C—N distances. These differences are attributed to the different attached groups. As expected, the bridging bond C10—C11 [1.447 (2) Å] is much longer than the C—C distances of the rings in the molecule. The torsion angles N3—N2—C8—C9 and O1—C7—N2—N3 are −7.9 (2)° and 8.3 (2)° respectively. This small angle of bond twist indicate that the bonded atoms are *cis* oriented. In the molecule, the quinazolin ring and the benzylidene group are twisted with each other and the corresponding torsion angle is −178.2 (2)° confirms that the bonds are *trans* oriented. This wide-angle twist indicates that the the groups are significantly rotated and the dihedral angle between the planes is 54.0 (4)°. A small value of the dihedral angle [2.10 (4)°] between the aromatic and quinazolin rings show they are almost coplanar. The quinazolin ring is statistically planar with a maximum deviation of 0.02 (1) Å [C8].

The molecular packing is stabilized by C—H···O hydrogen bonding interactions which result in centrosymmetric dimers (Table 1, Fig. 2).

Experimental

A mixture of 2–methyl benzo(1,3) oxazin–4–one (0.01 mole; 1.61 g) and hydrazine hydrate (0.03 mole; 1.5 g) in ethanol was refluxed for two hours, then *p*-dimethyl amino benzaldehyde (2.24 g) was added. Then the solution was poured into ice cold water. The separated solid was filtered and recrystallized from ethanol and dried in an oven. Yield 73.1%; melting point 412–414 K. Yellow needles of (I) were recrystallized from ethyl acetate solution.

Refinement

All the H atoms were positioned geometrically and their positions and U_{iso} values were freely refined.

Figures

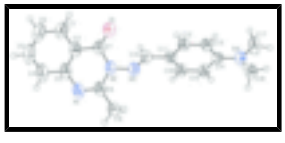

Fig. 1. View of the molecular structure of (I). The displacement ellipsoids are drawn at 50% probability level and H atoms are drawn as spheres of arbitrary radius.

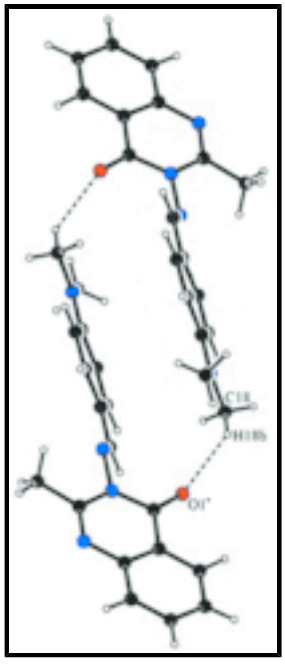

Fig. 2. A centrosymmetric dimer of (I), linked by C—H···O interactions. Atom marked with an asterisk (*) are at the symmetry position (−*x*, −*y*, 1 − *z*).

3-[4-(Dimethylamino)benzylideneamino]-2-methylquinazolin-4(3*H*)-one

Crystal data

$C_{18}H_{18}N_4O$	$Z = 2$
$M_r = 306.36$	$F_{000} = 324$
Triclinic, $P\overline{1}$	$D_x = 1.301$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.5175$ (10) Å	Cell parameters from 50 reflections
$b = 9.3631$ (13) Å	$\theta = 1.7$–28.0º
$c = 12.7886$ (17) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 98.198$ (2)º	$T = 296$ (2) K
$\beta = 103.259$ (2)º	Block, yellow
$\gamma = 112.517$ (2)º	0.21 × 0.18 × 0.10 mm
$V = 782.33$ (18) Å^3	

Data collection

Bruker APEXII CCD diffractometer	$R_{int} = 0.021$
ω scans	$\theta_{max} = 28.0$º
Absorption correction: none	$\theta_{min} = 1.7$º
9011 measured reflections	$h = -9 \rightarrow 9$
3582 independent reflections	$k = -12 \rightarrow 12$
2863 reflections with $I > 2\sigma(I)$	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	All H-atom parameters refined
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0824P)^2 + 0.0881P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.150$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
3582 reflections	Extinction correction: none
280 parameters	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0239 (3)	0.7144 (2)	0.16094 (15)	0.0761 (5)
C2	0.1029 (2)	0.63717 (16)	0.16193 (11)	0.0590 (4)
C3	0.2288 (3)	0.66170 (16)	0.09561 (11)	0.0628 (4)
C4	0.2239 (4)	0.7645 (2)	0.02596 (14)	0.0830 (5)
C5	0.0992 (4)	0.8384 (2)	0.02555 (17)	0.0969 (7)
C6	−0.0240 (4)	0.8146 (2)	0.09299 (16)	0.0937 (7)
C7	0.0971 (2)	0.52499 (16)	0.23043 (11)	0.0574 (3)
C8	0.3481 (2)	0.48483 (17)	0.15228 (11)	0.0584 (3)
C9	0.4731 (3)	0.3951 (3)	0.14777 (16)	0.0759 (5)
C10	0.25148 (19)	0.35813 (15)	0.37531 (11)	0.0494 (3)
C11	0.25379 (18)	0.23922 (15)	0.43582 (10)	0.0468 (3)
C12	0.2940 (2)	0.27515 (16)	0.55046 (11)	0.0513 (3)
C13	0.3045 (2)	0.16600 (17)	0.61039 (11)	0.0536 (3)
C14	0.27102 (18)	0.01191 (15)	0.55708 (10)	0.0482 (3)
C15	0.2322 (2)	−0.02347 (16)	0.44130 (11)	0.0539 (3)
C16	0.2239 (2)	0.08687 (16)	0.38322 (11)	0.0532 (3)
C17	0.3175 (4)	−0.0651 (3)	0.73240 (15)	0.0841 (6)
C18	0.2354 (3)	−0.25892 (19)	0.55635 (16)	0.0678 (4)
N1	0.3542 (2)	0.58551 (16)	0.09249 (10)	0.0669 (4)
N2	0.22998 (18)	0.45569 (13)	0.22242 (9)	0.0528 (3)
N3	0.22249 (19)	0.32720 (13)	0.27105 (9)	0.0566 (3)
N4	0.27461 (19)	−0.10011 (14)	0.61397 (10)	0.0593 (3)
O1	−0.01214 (18)	0.49096 (15)	0.28877 (10)	0.0773 (4)
H1	−0.117 (3)	0.691 (3)	0.2099 (18)	0.104 (7)*
H4	0.315 (3)	0.783 (2)	−0.0153 (17)	0.085 (6)*

H5	0.097 (4)	0.905 (3)	−0.023 (2)	0.119 (7)*
H6	−0.120 (4)	0.861 (3)	0.0914 (19)	0.110 (7)*
H9A	0.385 (4)	0.279 (3)	0.1317 (19)	0.114 (7)*
H9B	0.575 (3)	0.424 (2)	0.2179 (19)	0.097 (6)*
H9C	0.532 (3)	0.415 (2)	0.0904 (17)	0.089 (6)*
H10	0.279 (2)	0.4627 (18)	0.4204 (12)	0.057 (4)*
H12	0.313 (2)	0.378 (2)	0.5871 (13)	0.063 (4)*
H13	0.333 (2)	0.1965 (19)	0.6874 (15)	0.072 (5)*
H15	0.211 (2)	−0.125 (2)	0.4051 (13)	0.068 (4)*
H16	0.196 (2)	0.0572 (19)	0.3046 (14)	0.070 (4)*
H17A	0.243 (4)	−0.015 (3)	0.757 (2)	0.135 (10)*
H17B	0.455 (4)	0.021 (3)	0.766 (2)	0.126 (8)*
H17C	0.314 (4)	−0.156 (3)	0.757 (2)	0.118 (7)*
H18A	0.097 (3)	−0.314 (2)	0.4942 (16)	0.088 (5)*
H18B	0.236 (4)	−0.319 (3)	0.6088 (19)	0.116 (7)*
H18C	0.336 (3)	−0.255 (2)	0.5189 (16)	0.093 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0992 (12)	0.0659 (9)	0.0662 (9)	0.0470 (9)	0.0123 (9)	0.0144 (7)
C2	0.0747 (9)	0.0475 (7)	0.0453 (7)	0.0256 (6)	0.0048 (6)	0.0090 (5)
C3	0.0849 (10)	0.0481 (7)	0.0441 (7)	0.0242 (7)	0.0071 (6)	0.0122 (5)
C4	0.1266 (16)	0.0663 (10)	0.0574 (9)	0.0415 (11)	0.0240 (10)	0.0282 (8)
C5	0.158 (2)	0.0683 (11)	0.0683 (11)	0.0602 (13)	0.0138 (12)	0.0297 (9)
C6	0.1408 (19)	0.0795 (12)	0.0722 (11)	0.0703 (13)	0.0122 (12)	0.0210 (9)
C7	0.0660 (8)	0.0531 (7)	0.0513 (7)	0.0270 (6)	0.0121 (6)	0.0145 (6)
C8	0.0695 (8)	0.0597 (8)	0.0453 (7)	0.0268 (7)	0.0162 (6)	0.0168 (6)
C9	0.0916 (12)	0.0981 (14)	0.0661 (10)	0.0562 (11)	0.0376 (10)	0.0384 (10)
C10	0.0482 (7)	0.0472 (6)	0.0506 (7)	0.0196 (5)	0.0122 (5)	0.0143 (5)
C11	0.0436 (6)	0.0477 (6)	0.0490 (6)	0.0191 (5)	0.0128 (5)	0.0156 (5)
C12	0.0546 (7)	0.0479 (7)	0.0504 (7)	0.0222 (6)	0.0152 (5)	0.0111 (5)
C13	0.0584 (7)	0.0575 (7)	0.0439 (7)	0.0243 (6)	0.0145 (5)	0.0143 (5)
C14	0.0422 (6)	0.0523 (7)	0.0537 (7)	0.0211 (5)	0.0160 (5)	0.0202 (5)
C15	0.0621 (8)	0.0482 (7)	0.0547 (7)	0.0262 (6)	0.0193 (6)	0.0139 (6)
C16	0.0614 (8)	0.0533 (7)	0.0451 (7)	0.0248 (6)	0.0158 (6)	0.0140 (5)
C17	0.1134 (16)	0.0731 (11)	0.0595 (9)	0.0356 (12)	0.0155 (10)	0.0306 (8)
C18	0.0755 (10)	0.0576 (8)	0.0822 (11)	0.0337 (8)	0.0294 (9)	0.0308 (8)
N1	0.0867 (9)	0.0676 (7)	0.0515 (7)	0.0335 (7)	0.0240 (6)	0.0259 (6)
N2	0.0647 (7)	0.0482 (6)	0.0464 (6)	0.0245 (5)	0.0152 (5)	0.0176 (4)
N3	0.0719 (7)	0.0502 (6)	0.0534 (6)	0.0290 (5)	0.0197 (5)	0.0218 (5)
N4	0.0667 (7)	0.0593 (7)	0.0600 (7)	0.0306 (6)	0.0209 (5)	0.0269 (5)
O1	0.0864 (8)	0.0928 (8)	0.0825 (8)	0.0533 (7)	0.0408 (6)	0.0441 (6)

Geometric parameters (Å, °)

C1—C6	1.367 (3)	C10—H10	0.982 (15)
C1—C2	1.399 (2)	C11—C12	1.3900 (18)
C1—H1	1.03 (2)	C11—C16	1.3963 (18)

C2—C3	1.387 (2)	C12—C13	1.3768 (18)
C2—C7	1.4552 (19)	C12—H12	0.950 (16)
C3—N1	1.387 (2)	C13—C14	1.4044 (19)
C3—C4	1.406 (2)	C13—H13	0.934 (17)
C4—C5	1.362 (3)	C14—N4	1.3641 (16)
C4—H4	0.939 (19)	C14—C15	1.4054 (19)
C5—C6	1.384 (3)	C15—C16	1.3673 (18)
C5—H5	0.95 (2)	C15—H15	0.931 (16)
C6—H6	0.97 (2)	C16—H16	0.955 (17)
C7—O1	1.2171 (18)	C17—N4	1.435 (2)
C7—N2	1.3976 (19)	C17—H17A	0.94 (3)
C8—N1	1.2899 (17)	C17—H17B	0.98 (3)
C8—N2	1.3848 (18)	C17—H17C	0.94 (3)
C8—C9	1.486 (2)	C18—N4	1.447 (2)
C9—H9A	1.00 (2)	C18—H18A	1.03 (2)
C9—H9B	0.96 (2)	C18—H18B	0.94 (2)
C9—H9C	0.95 (2)	C18—H18C	0.98 (2)
C10—N3	1.2718 (17)	N2—N3	1.4194 (14)
C10—C11	1.4467 (17)		
C6—C1—C2	119.2 (2)	C13—C12—C11	121.83 (12)
C6—C1—H1	122.1 (12)	C13—C12—H12	120.1 (9)
C2—C1—H1	118.6 (12)	C11—C12—H12	118.0 (9)
C3—C2—C1	120.97 (14)	C12—C13—C14	120.87 (12)
C3—C2—C7	119.54 (13)	C12—C13—H13	118.4 (10)
C1—C2—C7	119.46 (15)	C14—C13—H13	120.7 (10)
N1—C3—C2	122.88 (12)	N4—C14—C13	122.11 (12)
N1—C3—C4	118.69 (16)	N4—C14—C15	120.78 (12)
C2—C3—C4	118.40 (16)	C13—C14—C15	117.12 (11)
C5—C4—C3	120.0 (2)	C16—C15—C14	121.21 (12)
C5—C4—H4	123.4 (12)	C16—C15—H15	120.8 (10)
C3—C4—H4	116.5 (12)	C14—C15—H15	118.0 (10)
C4—C5—C6	121.16 (17)	C15—C16—C11	121.76 (12)
C4—C5—H5	118.5 (15)	C15—C16—H16	118.2 (10)
C6—C5—H5	120.4 (15)	C11—C16—H16	120.1 (10)
C1—C6—C5	120.2 (2)	N4—C17—H17A	112.6 (17)
C1—C6—H6	116.6 (14)	N4—C17—H17B	107.8 (15)
C5—C6—H6	123.0 (14)	H17A—C17—H17B	100 (2)
O1—C7—N2	121.87 (12)	N4—C17—H17C	109.6 (15)
O1—C7—C2	124.86 (14)	H17A—C17—H17C	117 (2)
N2—C7—C2	113.27 (13)	H17B—C17—H17C	108 (2)
N1—C8—N2	123.02 (13)	N4—C18—H18A	111.7 (10)
N1—C8—C9	119.66 (14)	N4—C18—H18B	107.7 (14)
N2—C8—C9	117.33 (13)	H18A—C18—H18B	109.7 (18)
C8—C9—H9A	109.1 (14)	N4—C18—H18C	111.0 (12)
C8—C9—H9B	111.3 (12)	H18A—C18—H18C	105.4 (16)
H9A—C9—H9B	107.1 (18)	H18B—C18—H18C	111.3 (18)
C8—C9—H9C	108.8 (12)	C8—N1—C3	117.79 (13)
H9A—C9—H9C	109.7 (18)	C8—N2—C7	123.41 (11)
H9B—C9—H9C	110.8 (18)	C8—N2—N3	115.22 (11)

N3—C10—C11	120.72 (12)	C7—N2—N3	120.37 (11)
N3—C10—H10	123.6 (8)	C10—N3—N2	115.05 (11)
C11—C10—H10	115.6 (8)	C14—N4—C17	121.49 (13)
C12—C11—C16	117.20 (11)	C14—N4—C18	120.79 (13)
C12—C11—C10	120.75 (12)	C17—N4—C18	117.72 (14)
C16—C11—C10	122.01 (11)		
C6—C1—C2—C3	0.4 (2)	C13—C14—C15—C16	−1.1 (2)
C6—C1—C2—C7	−177.34 (15)	C14—C15—C16—C11	0.1 (2)
C1—C2—C3—N1	−178.80 (13)	C12—C11—C16—C15	0.5 (2)
C7—C2—C3—N1	−1.1 (2)	C10—C11—C16—C15	178.05 (12)
C1—C2—C3—C4	−0.9 (2)	N2—C8—N1—C3	−3.0 (2)
C7—C2—C3—C4	176.80 (13)	C9—C8—N1—C3	177.34 (15)
N1—C3—C4—C5	178.65 (16)	C2—C3—N1—C8	1.7 (2)
C2—C3—C4—C5	0.7 (3)	C4—C3—N1—C8	−176.17 (14)
C3—C4—C5—C6	0.1 (3)	N1—C8—N2—C7	3.9 (2)
C2—C1—C6—C5	0.4 (3)	C9—C8—N2—C7	−176.45 (15)
C4—C5—C6—C1	−0.7 (3)	N1—C8—N2—N3	172.45 (12)
C3—C2—C7—O1	−177.59 (14)	C9—C8—N2—N3	−7.92 (19)
C1—C2—C7—O1	0.1 (2)	O1—C7—N2—C8	176.29 (13)
C3—C2—C7—N2	1.63 (18)	C2—C7—N2—C8	−2.96 (19)
C1—C2—C7—N2	179.36 (13)	O1—C7—N2—N3	8.3 (2)
N3—C10—C11—C12	177.24 (12)	C2—C7—N2—N3	−170.92 (11)
N3—C10—C11—C16	−0.3 (2)	C11—C10—N3—N2	−178.16 (10)
C16—C11—C12—C13	0.07 (19)	C8—N2—N3—C10	132.15 (13)
C10—C11—C12—C13	−177.54 (11)	C7—N2—N3—C10	−58.94 (16)
C11—C12—C13—C14	−1.2 (2)	C13—C14—N4—C17	−1.4 (2)
C12—C13—C14—N4	−178.04 (11)	C15—C14—N4—C17	178.90 (16)
C12—C13—C14—C15	1.67 (19)	C13—C14—N4—C18	178.72 (13)
N4—C14—C15—C16	178.58 (12)	C15—C14—N4—C18	−1.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18B···O1^{i}	0.94 (2)	2.58 (3)	3.379 (2)	143.0 (19)

Symmetry codes: (i) −*x*, −*y*, −*z*+1.

Fig. 1

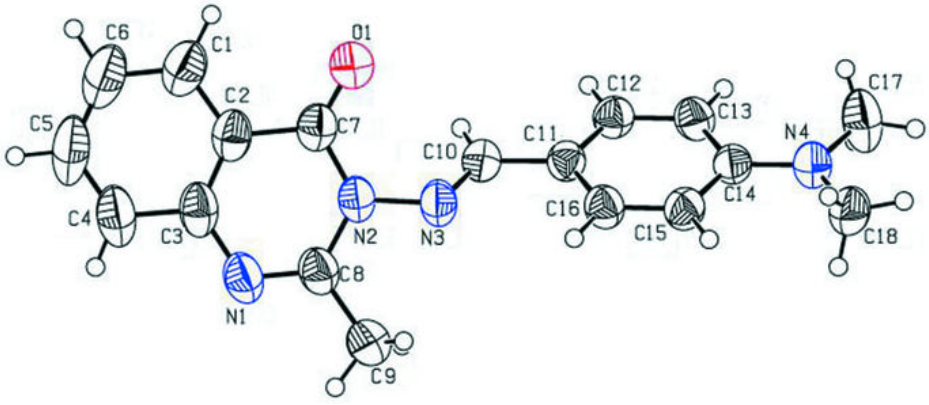
C6
C1
O1
C2
C5
C7
C12
C13
C17
C10
C11
N4
C4
C3
N2
N3
C16
C14
C15
C18
C8
N1
C9

Fig. 2