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3-Isopropyl-2-morpholinobenzofuro-[3,2-*d*]pyrimidin-4(3*H*)-one

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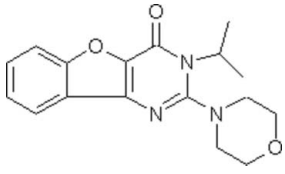
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.132; data-to-parameter ratio = 14.7.

In the title compound, $C_{17}H_{19}N_3O_3$, the three fused rings of the benzofuro[3,2-*d*]pyrimidine system are almost coplanar. The morpholine ring exhibits a distorted chair conformation. Intramolecular C—H···O and C—H···N hydrogen bonds stabilize the molecular structure. The packing of the molecules is mainly governed by a π–π interaction between benzofuro[3,2-*d*]pyrimidine units; the interplanar separation is *ca* 3.7 Å.

Related literature

Related preparation and biological activity were described by Hayakawa *et al.* (2007) and Aly (2005). For related literature, see: Ding *et al.* (2004); Janiak (2000). For crystal structures of other fused pyrimidinone derivatives, see: Hu *et al.* (2005, 2006, 2007).



Experimental

Crystal data

$C_{17}H_{19}N_3O_3$
M_r = 313.35
Monoclinic, $P2_1/c$
a = 14.6943 (8) Å
b = 8.7163 (6) Å
c = 12.8126 (10) Å
β = 107.656 (1)°
V = 1563.73 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.973, T_{max} = 0.982
10348 measured reflections
3056 independent reflections
2351 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.132
S = 1.02
3056 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17*C*···O2	0.96	2.44	3.015 (2)	118
C16—H16*A*···O2	0.96	2.33	2.916 (2)	119
C15—H15···N1	0.98	2.24	2.776 (2)	113

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2240).

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supplementary materials

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3-Isopropyl-2-morpholinobenzofuro[3,2-*d*]pyrimidin-4(3*H*)-one

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Comment

Pyrimidine derivatives are attracting increasing attention in the synthetic chemistry community because of the important role played by such systems in many natural products, antibiotics and drugs (Hayakawa *et al.*, 2007; Aly, 2005). In recent years, we have been engaged in the preparation of derivatives of heterocycles using the aza-Wittig reaction (Ding *et al.*, 2004). Some X-ray crystal structures of fused pyrimidinone derivatives have been reported (Hu *et al.*, 2005, 2006, 2007). In this paper, we present X-ray crystallographic analysis of the compound, (I), which may be used as a new precursor for obtaining bioactive molecules.

In the molecule, the bond lengths and angles are unexceptional. All ring atoms in the benzofuro[3,2-*d*]pyrimidine system are essentially coplanar (Fig. 1). The morpholino ring shows a distorted chair conformation [φ = 203 (2)° and θ = 5.75 (2)°, puckering amplitude = 0.574 (2) Å]. Intramolecular C—H···O and C—H···N hydrogen bonds stabilize the conformation of the molecule (Table 1). Further stability of the crystal structure is provided by offset π–π stacking interactions (Janiak, 2000) involving the fused benzofuro[3,2-*d*]pyrimidine system (Fig. 2). The interplanar distance is 3.355 (1)–3.376 (1) Å, with distances of 3.497 (1)–3.584 (1) Å between adjacent ring centroids (symmetry code relating the adjacent ring: $1 - x$, $1 - y$, $1 - z$).

Experimental

To a solution of the ethyl 3-[(isopropylimino)methyleneamino]benzofuran-2-carboxylate (3 mmol) in dichloromethane (5 ml) was added morpholine (3 mmol). After stirring the reaction mixture for 4 h, the solvent was removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 4 h at room temperature. The solution was concentrated under reduced pressure and purification was accomplished by column chromatography on silica gel to give the title compound in a yield of 84%. Crystals suitable for single-crystal X-ray diffraction were obtained by vapour diffusion a mixed solvent of ethanol and dichloromethane (1:1 *v*/*v*) at room temperature.

Refinement

All H-atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

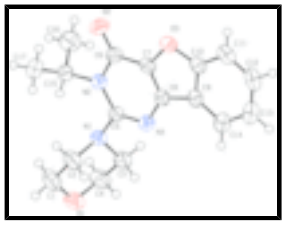

Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

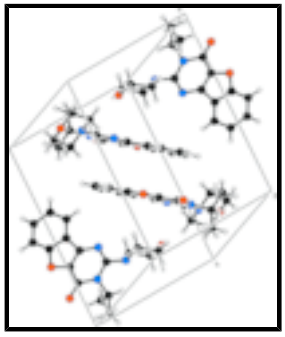

Fig. 2. A packing diagram of the title compound, showing the π–π stacking interactions.

3-Isopropyl-2-morpholinobenzofuro[3,2-*d*]pyrimidin-4(3*H*)-one

Crystal data

$C_{17}H_{19}N_3O_3$	F_{000} = 664
M_r = 313.35	D_x = 1.331 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3120 reflections
a = 14.6943 (8) Å	θ = 2.8–25.0º
b = 8.7163 (6) Å	μ = 0.09 mm^{-1}
c = 12.8126 (10) Å	T = 295 (2) K
β = 107.656 (1)º	Block, colourless
V = 1563.73 (18) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3056 independent reflections
Radiation source: fine-focus sealed tube	2351 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 295(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −17→18
T_{min} = 0.973, T_{max} = 0.982	k = −10→10
10348 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.132$	$w = 1/[\sigma^2(F_o^2) + (0.0749P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
3056 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.16216 (18)	0.5943 (2)	−0.03191 (15)	0.0677 (6)
H1A	0.1847	0.5485	−0.0885	0.081*
H1B	0.0999	0.5510	−0.0382	0.081*
C2	0.22977 (15)	0.5537 (2)	0.07802 (14)	0.0536 (5)
H2A	0.2315	0.4433	0.0878	0.064*
H2B	0.2937	0.5884	0.0829	0.064*
C3	0.19492 (14)	0.7938 (2)	0.14628 (14)	0.0486 (5)
H3A	0.2579	0.8315	0.1500	0.058*
H3B	0.1743	0.8448	0.2026	0.058*
C4	0.12570 (15)	0.8262 (2)	0.03509 (15)	0.0557 (5)
H4A	0.0627	0.7906	0.0333	0.067*
H4B	0.1220	0.9362	0.0228	0.067*
C5	0.24703 (11)	0.58098 (18)	0.27059 (13)	0.0346 (4)
C6	0.25432 (11)	0.39190 (18)	0.41491 (13)	0.0380 (4)
C7	0.33065 (11)	0.48739 (18)	0.47503 (13)	0.0367 (4)
C8	0.35964 (11)	0.61393 (18)	0.43272 (13)	0.0352 (4)
C9	0.43885 (11)	0.67559 (18)	0.51855 (13)	0.0388 (4)
C10	0.44830 (11)	0.57894 (19)	0.60791 (13)	0.0392 (4)

C11	0.51631 (13)	0.5987 (2)	0.70796 (14)	0.0489 (5)
H11	0.5211	0.5327	0.7664	0.059*
C12	0.57683 (13)	0.7216 (2)	0.71648 (16)	0.0544 (5)
H12	0.6232	0.7403	0.7830	0.065*
C13	0.57051 (13)	0.8188 (2)	0.62820 (17)	0.0554 (5)
H13	0.6134	0.8997	0.6368	0.066*
C14	0.50233 (13)	0.7976 (2)	0.52880 (16)	0.0478 (5)
H14	0.4986	0.8626	0.4701	0.057*
C15	0.12556 (12)	0.3688 (2)	0.23733 (14)	0.0427 (4)
H15	0.1030	0.4273	0.1690	0.051*
C16	0.04567 (13)	0.3724 (3)	0.28998 (17)	0.0638 (6)
H16A	0.0637	0.3120	0.3557	0.096*
H16B	−0.0116	0.3312	0.2399	0.096*
H16C	0.0345	0.4764	0.3076	0.096*
C17	0.14822 (15)	0.2078 (2)	0.20649 (17)	0.0598 (5)
H17A	0.1975	0.2129	0.1716	0.090*
H17B	0.0918	0.1630	0.1571	0.090*
H17C	0.1696	0.1459	0.2713	0.090*
N1	0.19776 (9)	0.62709 (15)	0.16330 (11)	0.0378 (3)
N2	0.21314 (9)	0.44906 (14)	0.30752 (10)	0.0355 (3)
N3	0.31837 (9)	0.66373 (15)	0.32785 (11)	0.0369 (3)
O1	0.15263 (10)	0.75437 (16)	−0.04967 (10)	0.0588 (4)
O2	0.22487 (9)	0.27625 (14)	0.44809 (10)	0.0539 (4)
O3	0.38168 (8)	0.46168 (14)	0.58250 (9)	0.0431 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.1010 (17)	0.0613 (13)	0.0350 (11)	0.0039 (12)	0.0117 (11)	−0.0025 (10)
C2	0.0752 (13)	0.0481 (11)	0.0393 (11)	0.0116 (9)	0.0200 (10)	−0.0001 (8)
C3	0.0659 (12)	0.0399 (10)	0.0391 (10)	0.0046 (8)	0.0146 (9)	0.0044 (8)
C4	0.0674 (13)	0.0540 (11)	0.0440 (11)	0.0124 (9)	0.0141 (10)	0.0119 (9)
C5	0.0393 (9)	0.0324 (8)	0.0332 (9)	0.0022 (7)	0.0126 (7)	0.0010 (7)
C6	0.0428 (9)	0.0354 (9)	0.0371 (9)	0.0008 (7)	0.0141 (8)	0.0033 (7)
C7	0.0419 (9)	0.0385 (9)	0.0291 (9)	0.0040 (7)	0.0097 (7)	0.0032 (7)
C8	0.0374 (8)	0.0330 (8)	0.0345 (9)	0.0033 (7)	0.0102 (7)	−0.0011 (7)
C9	0.0419 (9)	0.0350 (9)	0.0388 (10)	0.0045 (7)	0.0110 (8)	−0.0058 (7)
C10	0.0407 (9)	0.0417 (9)	0.0358 (9)	0.0055 (7)	0.0124 (8)	−0.0043 (7)
C11	0.0499 (10)	0.0587 (12)	0.0363 (10)	0.0064 (9)	0.0105 (8)	−0.0050 (9)
C12	0.0487 (11)	0.0624 (13)	0.0439 (11)	0.0080 (9)	0.0017 (9)	−0.0188 (10)
C13	0.0490 (11)	0.0461 (11)	0.0650 (14)	−0.0027 (8)	0.0081 (10)	−0.0155 (10)
C14	0.0472 (10)	0.0409 (10)	0.0522 (12)	0.0001 (8)	0.0104 (9)	−0.0052 (8)
C15	0.0439 (10)	0.0461 (10)	0.0343 (9)	−0.0095 (7)	0.0062 (8)	0.0005 (8)
C16	0.0426 (11)	0.0864 (15)	0.0617 (13)	−0.0057 (10)	0.0150 (10)	−0.0009 (12)
C17	0.0696 (13)	0.0501 (11)	0.0589 (13)	−0.0179 (10)	0.0181 (11)	−0.0119 (10)
N1	0.0454 (8)	0.0365 (8)	0.0308 (7)	−0.0003 (6)	0.0107 (6)	0.0026 (6)
N2	0.0386 (7)	0.0332 (7)	0.0347 (8)	−0.0017 (6)	0.0112 (6)	0.0009 (6)
N3	0.0404 (8)	0.0348 (7)	0.0349 (8)	−0.0021 (6)	0.0105 (6)	0.0019 (6)

O1	0.0795 (9)	0.0604 (9)	0.0360 (7)	0.0025 (7)	0.0170 (7)	0.0114 (6)
O2	0.0622 (8)	0.0488 (7)	0.0486 (8)	−0.0137 (6)	0.0135 (7)	0.0134 (6)
O3	0.0480 (7)	0.0470 (7)	0.0316 (7)	−0.0015 (5)	0.0079 (5)	0.0041 (5)

Geometric parameters (Å, °)

C1—O1	1.414 (2)	C8—C9	1.441 (2)
C1—C2	1.499 (3)	C9—C14	1.394 (2)
C1—H1A	0.9700	C9—C10	1.394 (2)
C1—H1B	0.9700	C10—C11	1.376 (2)
C2—N1	1.461 (2)	C10—O3	1.384 (2)
C2—H2A	0.9700	C11—C12	1.375 (3)
C2—H2B	0.9700	C11—H11	0.9300
C3—N1	1.468 (2)	C12—C13	1.394 (3)
C3—C4	1.505 (2)	C12—H12	0.9300
C3—H3A	0.9700	C13—C14	1.373 (3)
C3—H3B	0.9700	C13—H13	0.9300
C4—O1	1.410 (2)	C14—H14	0.9300
C4—H4A	0.9700	C15—N2	1.5007 (19)
C4—H4B	0.9700	C15—C16	1.521 (3)
C5—N3	1.300 (2)	C15—C17	1.522 (3)
C5—N2	1.392 (2)	C15—H15	0.9800
C5—N1	1.404 (2)	C16—H16A	0.9600
C6—O2	1.2230 (19)	C16—H16B	0.9600
C6—N2	1.415 (2)	C16—H16C	0.9600
C6—C7	1.421 (2)	C17—H17A	0.9600
C7—C8	1.353 (2)	C17—H17B	0.9600
C7—O3	1.3719 (18)	C17—H17C	0.9600
C8—N3	1.3664 (19)		
O1—C1—C2	112.91 (16)	O3—C10—C9	111.46 (14)
O1—C1—H1A	109.0	C12—C11—C10	116.14 (18)
C2—C1—H1A	109.0	C12—C11—H11	121.9
O1—C1—H1B	109.0	C10—C11—H11	121.9
C2—C1—H1B	109.0	C11—C12—C13	121.79 (18)
H1A—C1—H1B	107.8	C11—C12—H12	119.1
N1—C2—C1	109.10 (16)	C13—C12—H12	119.1
N1—C2—H2A	109.9	C14—C13—C12	121.41 (18)
C1—C2—H2A	109.9	C14—C13—H13	119.3
N1—C2—H2B	109.9	C12—C13—H13	119.3
C1—C2—H2B	109.9	C13—C14—C9	117.98 (18)
H2A—C2—H2B	108.3	C13—C14—H14	121.0
N1—C3—C4	107.88 (14)	C9—C14—H14	121.0
N1—C3—H3A	110.1	N2—C15—C16	111.19 (14)
C4—C3—H3A	110.1	N2—C15—C17	111.71 (14)
N1—C3—H3B	110.1	C16—C15—C17	113.16 (16)
C4—C3—H3B	110.1	N2—C15—H15	106.8
H3A—C3—H3B	108.4	C16—C15—H15	106.8
O1—C4—C3	112.25 (15)	C17—C15—H15	106.8
O1—C4—H4A	109.2	C15—C16—H16A	109.5

C3—C4—H4A	109.2	C15—C16—H16B	109.5
O1—C4—H4B	109.2	H16A—C16—H16B	109.5
C3—C4—H4B	109.2	C15—C16—H16C	109.5
H4A—C4—H4B	107.9	H16A—C16—H16C	109.5
N3—C5—N2	125.23 (14)	H16B—C16—H16C	109.5
N3—C5—N1	118.79 (14)	C15—C17—H17A	109.5
N2—C5—N1	115.97 (13)	C15—C17—H17B	109.5
O2—C6—N2	122.42 (14)	H17A—C17—H17B	109.5
O2—C6—C7	126.76 (15)	C15—C17—H17C	109.5
N2—C6—C7	110.81 (14)	H17A—C17—H17C	109.5
C8—C7—O3	113.12 (14)	H17B—C17—H17C	109.5
C8—C7—C6	123.54 (15)	C5—N1—C2	114.79 (13)
O3—C7—C6	123.34 (14)	C5—N1—C3	114.31 (13)
C7—C8—N3	123.58 (14)	C2—N1—C3	108.86 (14)
C7—C8—C9	106.12 (14)	C5—N2—C6	121.99 (13)
N3—C8—C9	130.30 (15)	C5—N2—C15	120.77 (13)
C14—C9—C10	119.10 (16)	C6—N2—C15	117.04 (13)
C14—C9—C8	135.96 (16)	C5—N3—C8	114.83 (14)
C10—C9—C8	104.93 (15)	C4—O1—C1	110.59 (15)
C11—C10—O3	124.98 (16)	C7—O3—C10	104.34 (12)
C11—C10—C9	123.56 (17)		
O1—C1—C2—N1	56.7 (2)	N2—C5—N1—C3	147.50 (15)
N1—C3—C4—O1	−59.8 (2)	C1—C2—N1—C5	171.39 (15)
O2—C6—C7—C8	179.81 (16)	C1—C2—N1—C3	−59.0 (2)
N2—C6—C7—C8	−1.0 (2)	C4—C3—N1—C5	−169.89 (14)
O2—C6—C7—O3	−1.1 (3)	C4—C3—N1—C2	60.28 (19)
N2—C6—C7—O3	178.09 (13)	N3—C5—N2—C6	0.6 (2)
O3—C7—C8—N3	−178.91 (13)	N1—C5—N2—C6	−178.25 (13)
C6—C7—C8—N3	0.3 (3)	N3—C5—N2—C15	175.37 (15)
O3—C7—C8—C9	1.80 (18)	N1—C5—N2—C15	−3.4 (2)
C6—C7—C8—C9	−179.00 (15)	O2—C6—N2—C5	179.85 (15)
C7—C8—C9—C14	177.12 (19)	C7—C6—N2—C5	0.6 (2)
N3—C8—C9—C14	−2.1 (3)	O2—C6—N2—C15	4.9 (2)
C7—C8—C9—C10	−1.57 (17)	C7—C6—N2—C15	−174.36 (13)
N3—C8—C9—C10	179.21 (16)	C16—C15—N2—C5	−116.10 (17)
C14—C9—C10—C11	1.4 (2)	C17—C15—N2—C5	116.43 (16)
C8—C9—C10—C11	−179.65 (15)	C16—C15—N2—C6	58.96 (19)
C14—C9—C10—O3	−178.08 (14)	C17—C15—N2—C6	−68.51 (18)
C8—C9—C10—O3	0.88 (17)	N2—C5—N3—C8	−1.3 (2)
O3—C10—C11—C12	179.25 (15)	N1—C5—N3—C8	177.44 (13)
C9—C10—C11—C12	−0.2 (2)	C7—C8—N3—C5	0.9 (2)
C10—C11—C12—C13	−1.1 (3)	C9—C8—N3—C5	−179.98 (15)
C11—C12—C13—C14	1.1 (3)	C3—C4—O1—C1	56.7 (2)
C12—C13—C14—C9	0.2 (3)	C2—C1—O1—C4	−55.0 (2)
C10—C9—C14—C13	−1.4 (2)	C8—C7—O3—C10	−1.25 (17)
C8—C9—C14—C13	−179.94 (17)	C6—C7—O3—C10	179.55 (15)
N3—C5—N1—C2	95.44 (18)	C11—C10—O3—C7	−179.31 (15)
N2—C5—N1—C2	−85.67 (18)	C9—C10—O3—C7	0.16 (17)
N3—C5—N1—C3	−31.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17C···O2	0.96	2.44	3.015 (2)	118
C16—H16A···O2	0.96	2.33	2.916 (2)	119
C15—H15···N1	0.98	2.24	2.776 (2)	113

Fig. 1

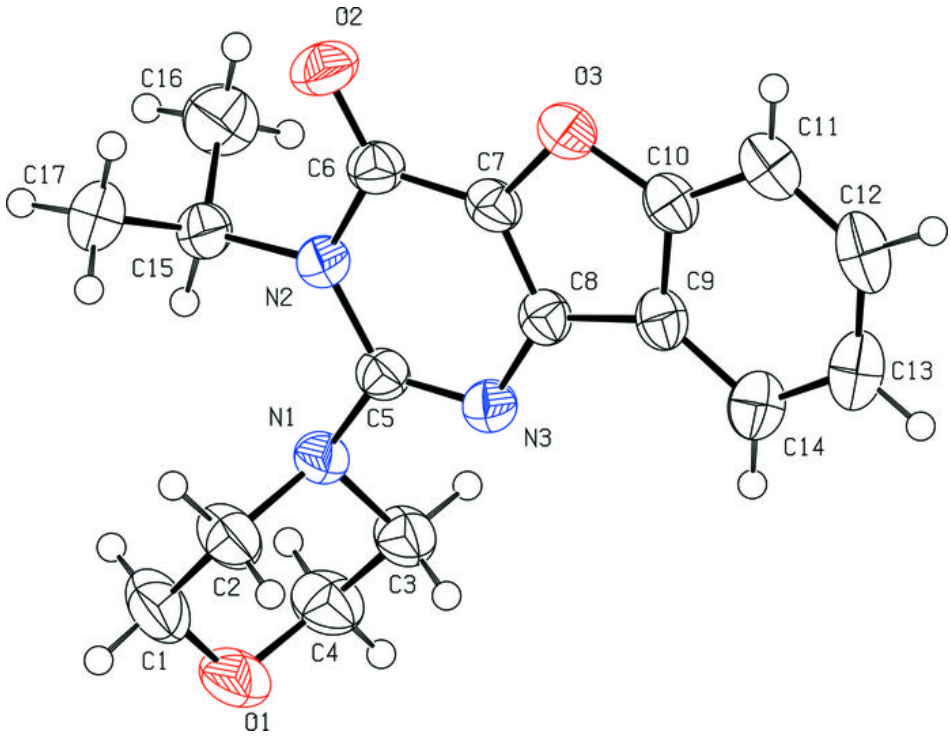
O2
C16
O3
C11
C6
C7
C10
C17
C12
C15
N2
C8
C9
C13
N1
C5
N3
C14
C2
C3
C1
C4
O1

Fig. 2