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7-Nitro-2-phenyl-4*H*-3,1-benzoxazin-4-one

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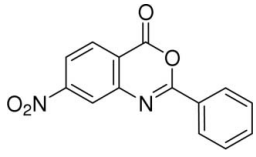
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.171; data-to-parameter ratio = 11.7.

The title compound, $C_{14}H_8N_2O_4$, was synthesized by reacting *p*-nitroanthranilic acid and benzoyl chloride at ambient temperature. The structure is stabilized by an intramolecular C—H···O hydrogen bond and an intermolecular C—H···O hydrogen bond. Additionally, weak π–π stacking interactions [centroid–centroid distance 3.6 (17) Å] between adjacent molecules further stabilize the crystal structure and form parallel layers along the *b* axis.

Related literature

For related literature, see: Allen *et al.* (1987); Bain & Smalley (1968); Bernstein *et al.* (1995); Bouillant *et al.* (1983); Colson *et al.* (2005); El-Din (2000); Fenton *et al.* (1989); Francis *et al.* (2000); Gutschow *et al.* (1998); Hamprecht *et al.* (2004); Hauteville *et al.* (1988); Hodson *et al.* (2000); Johnson & Pattison (1986); Kakuta *et al.* (2001); Krantz *et al.* (1990); Mayama *et al.* (1981); Pavlidis & Perry (1994); Ponchet *et al.* (1984); Shalaby *et al.* (2000); Ulrich (1991); Uejima *et al.* (1993).



Experimental

Crystal data

$C_{14}H_8N_2O_4$
M_r = 268.22
Monoclinic, $P2_1/c$
a = 7.6403 (14) Å
b = 7.4693 (13) Å
c = 22.047 (4) Å
β = 105.595 (6)°
V = 1211.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.45 × 0.42 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.952, T_{max} = 0.990
5798 measured reflections
2109 independent reflections
1821 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.171
S = 1.00
2109 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O1^{i}	0.93	2.56	3.301 (3)	137
C14—H14A···O2	0.93	2.41	2.738 (3)	100

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2096).

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supplementary materials

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7-Nitro-2-phenyl-4*H*-3,1-benzoxazin-4-one

Z. A. Khan, K. M. Khan and S. Anjum

Comment

Recent work by the medicinal chemists had led to a number of drugs related uses being found for this class of heterocyclic compound. Fenton *et al.* have described plasma lipid altering characteristics of a series of 2-substituted-4*H*-3,1-benzoxazin-4-one as high density lipoprotein elevators for the treatment of patients suffering from hyperlipoproteinemia and associated diseases (Fenton *et al.*, 1989). 2-Substituted-4*H*-3,1-benzoxazin-4-one base has been utilized as potent inhibitors of human leukocyte elastase (Krantz *et al.*, 1990) and serine proteases (Gutschow *et al.*, 1998). The National Cancer Institute, Washington, USA has also shown interest in 1-[3-(7-chloro-4-oxo-3,1-benzoxazin-4-yl) phenyl] methyl pyridinium chloride (NSC-341, 964) (Johnson & Pattison, 1986), evaluating its anti-neoplastic activity. Initial studies on 2-substituted-4*H*-3,1-benzoxazin-4-one showed good cytotoxic activity (Pavlidis & Perry, 1994) and herbicidal properties (Hamprecht *et al.*, 2004). A variety of biological activities were associated with 2-Substituted-4*H*-3,1-benzoxazin-4-ones for example anti-fungal, antibacterial (Bouillant *et al.*, 1983; Ponchet *et al.*, 1984; Mayama *et al.*, 1981; Hauteville *et al.*, 1988; El-Din, 2000; Shalaby *et al.*, 2000) and anti-elastase properties (Colson *et al.*, 2005). They can be used for the treatment of obesity (Hodson *et al.*, 2000) and also found to be novel specific puromycin-sensitive aminopeptidase inhibitors (Kakuta *et al.*, 2001).

The 2-aryl-substituted-4*H*-3,1-benzoxazin-4-ones act as novel active substances for the cardiovascular system. They exhibit relaxing effect on smooth musculature in particular and markedly increase coronary flow through langendroff hearts (Ulrich, 1991). The promising therapeutic potential of this class of compounds prompted us to synthesize and biologically screen series of structural variants of 2-substituted-4*H*-3,1-benzoxazin-4-one. The title compound (I), is expected to possess some interesting biological activities; however present paper describes the X-ray diffraction studies that would be very help for us in molecular modeling and future drug design.

The title compound (I), was synthesized by employing (Scheme-1) Bain & Smalley methodology (Bain & Smalley, 1968); the reaction of *p*-nitroanthranilic acid with benzoylchloride in excess of pyridine gave title compound (I) in 90% yield.

All bond lengths in the title compound (I) show normal values (Allen *et al.*, 1987). The title compound (I) is nearly planar with slight deviation [4.31 (13)°] of benzene ring from the mean plane of bezoxazine moiety. The one intramolecular C—H···O hydrogen bond generates the S(5) graph set motif, while one intermolecular C—H···O hydrogen bond keeps the molecules in parallel layers along *ac* plane in head to head fashion by two fold inversion axis (Bernstein *et al.*, 1995). The additional π—π stacking interactions between adjacent molecules further stabilize the crystal structure along *b* axis. The centroid–centroid distances between the rings are $Cg1$–$Cg3^{ii}$ = 3.5757 (17) Å [symmetry code ii: 2 − *x*, −*y*, −*z*], where *Cg*1 and *Cg*3 are the centroids of the rings C1/O2/C2/N1/C8/C7 and C9/C10/C11/C12/C13/C14, respectively.

Experimental

To a solution of *p*-nitroanthranilic acid (1.1 g, 6.04 mmol) in pyridine (25 ml) was added benzoylchloride (1.69 g, 12.08 mmol). The mixture was shaken for 5 min and placed at room temperature for a further 25 min., with occasional shaking.

The reaction mixture was stirred into cold water (200 ml) and the precipitate was filtered off. The residue was washed free of pyridine with cold water (3x 60 ml) and dried. The title compound (I) was crystallized from ethanol in 90% yield (1.46 g).

Refinement

All the rest of atoms were placed in calculated positions with a C—H distances in 0.93 Å and U_{iso}(H) values were constrained to be $1.5U_{eq}$(C) of all the carrier atoms.

Figures

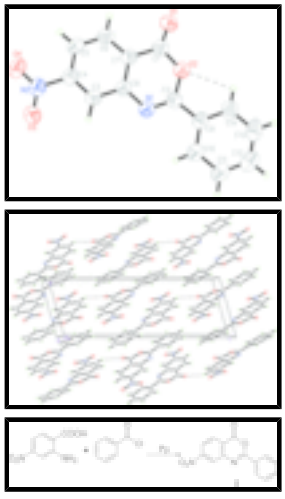


Fig. 1 The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. A dashed line indicates the intramolecular hydrogen bonds.
Fig. 2 The crystal packing of (I), viewed down the *b* axis.

7-Nitro-2-phenyl-4*H*-3,1-benzoxazin-4-one

Crystal data

$C_{14}H_8N_2O_4$	F_{000} = 552
M_r = 268.22	D_x = 1.470 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 430 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.6403 (14) Å	Cell parameters from 3298 reflections
b = 7.4693 (13) Å	θ = 2.8–27.8º
c = 22.047 (4) Å	μ = 0.11 mm^{-1}
β = 105.595 (6)º	T = 293 (2) K
V = 1211.9 (4) Å^3	Plate, yellow
Z = 4	0.45 × 0.42 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2109 independent reflections
Radiation source: fine-focus sealed tube	1821 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019

Detector resolution: 8.33 pixels mm^{-1}

T = 293(2) K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.952, T_{max} = 0.990

5798 measured reflections

θ_{max} = 25.0º

θ_{min} = 2.8º

h = −9→7

k = −8→8

l = −26→24

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.057

$wR(F^2)$ = 0.171

S = 1.00

2109 reflections

181 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0828P)^2 + 0.9147P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.18 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.29 e $Å^{-3}$

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.6749 (3)	0.2424 (3)	−0.15791 (9)	0.0724 (6)
O2	0.7645 (3)	0.1864 (2)	−0.05594 (8)	0.0574 (5)
O3	0.3710 (3)	−0.6371 (3)	−0.09118 (9)	0.0771 (7)
O4	0.2699 (3)	−0.6007 (3)	−0.19100 (10)	0.0854 (7)
N1	0.7048 (3)	−0.0810 (3)	−0.01017 (9)	0.0538 (6)
N2	0.3523 (3)	−0.5488 (3)	−0.13872 (11)	0.0608 (6)
C1	0.6737 (4)	0.1380 (4)	−0.11668 (12)	0.0546 (6)
C2	0.7748 (3)	0.0731 (3)	−0.00586 (11)	0.0482 (6)
C3	0.5316 (4)	−0.3121 (3)	−0.07507 (11)	0.0520 (6)
H3A	0.5450	−0.3848	−0.0399	0.062*
C4	0.4358 (3)	−0.3700 (3)	−0.13323 (11)	0.0502 (6)

C5	0.4115 (3)	−0.2681 (4)	−0.18714 (11)	0.0533 (6)
H5A	0.3444	−0.3114	−0.2260	0.064*
C6	0.4892 (4)	−0.1012 (4)	−0.18178 (11)	0.0551 (6)
H6A	0.4760	−0.0306	−0.2175	0.066*
C7	0.5873 (3)	−0.0367 (3)	−0.12344 (11)	0.0484 (6)
C8	0.6090 (3)	−0.1414 (3)	−0.06941 (11)	0.0467 (6)
C9	0.8768 (3)	0.1498 (3)	0.05463 (12)	0.0510 (6)
C10	0.9067 (3)	0.0449 (4)	0.10843 (12)	0.0573 (7)
H10A	0.8632	−0.0719	0.1058	0.069*
C11	1.0012 (4)	0.1145 (4)	0.16582 (13)	0.0664 (8)
H11A	1.0204	0.0443	0.2019	0.080*
C12	1.0670 (4)	0.2860 (5)	0.17032 (15)	0.0708 (9)
H12A	1.1314	0.3313	0.2092	0.085*
C13	1.0377 (4)	0.3911 (5)	0.11741 (16)	0.0761 (9)
H13A	1.0820	0.5077	0.1206	0.091*
C14	0.9423 (4)	0.3238 (4)	0.05931 (14)	0.0672 (8)
H14A	0.9223	0.3952	0.0235	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0975 (16)	0.0616 (12)	0.0559 (11)	−0.0156 (11)	0.0169 (10)	0.0115 (10)
O2	0.0667 (11)	0.0534 (10)	0.0503 (10)	−0.0101 (8)	0.0125 (8)	0.0019 (8)
O3	0.1085 (17)	0.0565 (12)	0.0608 (12)	−0.0212 (11)	0.0135 (11)	0.0014 (10)
O4	0.1070 (17)	0.0685 (13)	0.0624 (13)	−0.0169 (12)	−0.0087 (12)	−0.0156 (11)
N1	0.0614 (13)	0.0562 (13)	0.0416 (11)	−0.0105 (10)	0.0099 (9)	−0.0005 (9)
N2	0.0667 (14)	0.0547 (13)	0.0549 (13)	−0.0045 (11)	0.0061 (11)	−0.0067 (11)
C1	0.0587 (15)	0.0574 (15)	0.0476 (14)	−0.0031 (12)	0.0139 (11)	0.0038 (12)
C2	0.0473 (13)	0.0520 (14)	0.0471 (13)	−0.0032 (11)	0.0156 (10)	−0.0011 (11)
C3	0.0598 (15)	0.0523 (14)	0.0426 (13)	−0.0010 (12)	0.0114 (11)	0.0039 (11)
C4	0.0496 (13)	0.0523 (14)	0.0484 (13)	−0.0008 (11)	0.0128 (11)	−0.0041 (11)
C5	0.0534 (14)	0.0639 (16)	0.0402 (13)	0.0013 (12)	0.0086 (10)	−0.0046 (11)
C6	0.0607 (15)	0.0613 (16)	0.0420 (13)	−0.0005 (12)	0.0119 (11)	0.0060 (11)
C7	0.0485 (13)	0.0535 (14)	0.0443 (13)	0.0012 (11)	0.0143 (10)	0.0028 (10)
C8	0.0489 (13)	0.0491 (13)	0.0412 (12)	−0.0010 (10)	0.0107 (10)	−0.0017 (10)
C9	0.0457 (13)	0.0567 (15)	0.0511 (14)	−0.0060 (11)	0.0139 (11)	−0.0091 (11)
C10	0.0541 (14)	0.0628 (16)	0.0527 (14)	−0.0010 (12)	0.0106 (12)	−0.0053 (12)
C11	0.0620 (17)	0.077 (2)	0.0539 (16)	−0.0014 (15)	0.0058 (13)	−0.0085 (14)
C12	0.0580 (17)	0.091 (2)	0.0608 (18)	−0.0057 (15)	0.0107 (13)	−0.0198 (16)
C13	0.0690 (19)	0.0730 (19)	0.088 (2)	−0.0243 (16)	0.0233 (16)	−0.0246 (18)
C14	0.0728 (18)	0.0660 (18)	0.0656 (17)	−0.0172 (15)	0.0236 (14)	−0.0066 (14)

Geometric parameters (Å, °)

O1—C1	1.199 (3)	C5—H5A	0.9300
O2—C2	1.376 (3)	C6—C7	1.389 (3)
O2—C1	1.380 (3)	C6—H6A	0.9300
O3—N2	1.214 (3)	C7—C8	1.397 (3)
O4—N2	1.218 (3)	C9—C14	1.386 (4)

N1—C2	1.262 (3)	C9—C10	1.389 (4)
N1—C8	1.390 (3)	C10—C11	1.379 (4)
N2—C4	1.471 (3)	C10—H10A	0.9300
C1—C7	1.452 (4)	C11—C12	1.370 (5)
C2—C9	1.468 (3)	C11—H11A	0.9300
C3—C4	1.365 (3)	C12—C13	1.374 (5)
C3—C8	1.397 (3)	C12—H12A	0.9300
C3—H3A	0.9300	C13—C14	1.387 (4)
C4—C5	1.381 (3)	C13—H13A	0.9300
C5—C6	1.372 (4)	C14—H14A	0.9300
C2—O2—C1	121.5 (2)	C6—C7—C1	121.6 (2)
C2—N1—C8	118.2 (2)	C8—C7—C1	118.0 (2)
O3—N2—O4	123.7 (2)	N1—C8—C3	118.9 (2)
O3—N2—C4	118.3 (2)	N1—C8—C7	122.1 (2)
O4—N2—C4	118.0 (2)	C3—C8—C7	119.0 (2)
O1—C1—O2	117.5 (2)	C14—C9—C10	119.5 (2)
O1—C1—C7	127.0 (2)	C14—C9—C2	121.8 (2)
O2—C1—C7	115.5 (2)	C10—C9—C2	118.7 (2)
N1—C2—O2	124.7 (2)	C11—C10—C9	119.8 (3)
N1—C2—C9	122.4 (2)	C11—C10—H10A	120.1
O2—C2—C9	113.0 (2)	C9—C10—H10A	120.1
C4—C3—C8	118.7 (2)	C12—C11—C10	120.7 (3)
C4—C3—H3A	120.6	C12—C11—H11A	119.7
C8—C3—H3A	120.6	C10—C11—H11A	119.7
C3—C4—C5	123.2 (2)	C11—C12—C13	120.0 (3)
C3—C4—N2	118.4 (2)	C11—C12—H12A	120.0
C5—C4—N2	118.3 (2)	C13—C12—H12A	120.0
C6—C5—C4	118.1 (2)	C12—C13—C14	120.2 (3)
C6—C5—H5A	120.9	C12—C13—H13A	119.9
C4—C5—H5A	120.9	C14—C13—H13A	119.9
C5—C6—C7	120.5 (2)	C9—C14—C13	119.9 (3)
C5—C6—H6A	119.7	C9—C14—H14A	120.1
C7—C6—H6A	119.7	C13—C14—H14A	120.1
C6—C7—C8	120.4 (2)		
C2—O2—C1—O1	−178.1 (2)	C2—N1—C8—C3	179.6 (2)
C2—O2—C1—C7	1.5 (3)	C2—N1—C8—C7	−0.5 (4)
C8—N1—C2—O2	−0.5 (4)	C4—C3—C8—N1	179.3 (2)
C8—N1—C2—C9	179.3 (2)	C4—C3—C8—C7	−0.6 (4)
C1—O2—C2—N1	0.0 (4)	C6—C7—C8—N1	−179.4 (2)
C1—O2—C2—C9	−179.9 (2)	C1—C7—C8—N1	2.0 (4)
C8—C3—C4—C5	0.1 (4)	C6—C7—C8—C3	0.5 (4)
C8—C3—C4—N2	−179.1 (2)	C1—C7—C8—C3	−178.1 (2)
O3—N2—C4—C3	0.5 (4)	N1—C2—C9—C14	−175.5 (3)
O4—N2—C4—C3	−178.7 (2)	O2—C2—C9—C14	4.3 (4)
O3—N2—C4—C5	−178.7 (2)	N1—C2—C9—C10	4.0 (4)
O4—N2—C4—C5	2.1 (4)	O2—C2—C9—C10	−176.1 (2)
C3—C4—C5—C6	0.7 (4)	C14—C9—C10—C11	−0.1 (4)
N2—C4—C5—C6	179.8 (2)	C2—C9—C10—C11	−179.6 (2)

C4—C5—C6—C7	−0.8 (4)	C9—C10—C11—C12	−0.4 (4)
C5—C6—C7—C8	0.3 (4)	C10—C11—C12—C13	0.6 (5)
C5—C6—C7—C1	178.8 (2)	C11—C12—C13—C14	−0.3 (5)
O1—C1—C7—C6	−1.4 (4)	C10—C9—C14—C13	0.4 (4)
O2—C1—C7—C6	179.0 (2)	C2—C9—C14—C13	179.9 (3)
O1—C1—C7—C8	177.2 (3)	C12—C13—C14—C9	−0.2 (5)
O2—C1—C7—C8	−2.4 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···O1^{i}	0.93	2.56	3.301 (3)	137
C14—H14A···O2	0.93	2.41	2.738 (3)	100

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*−1/2.

Fig. 1

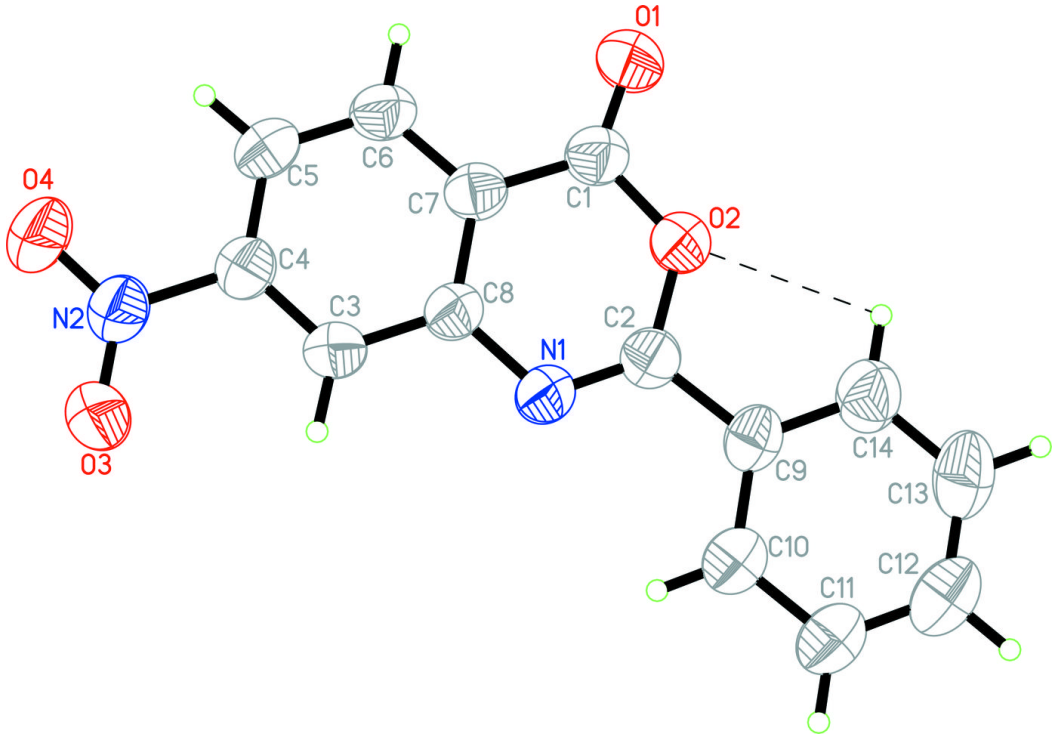


Fig. 2

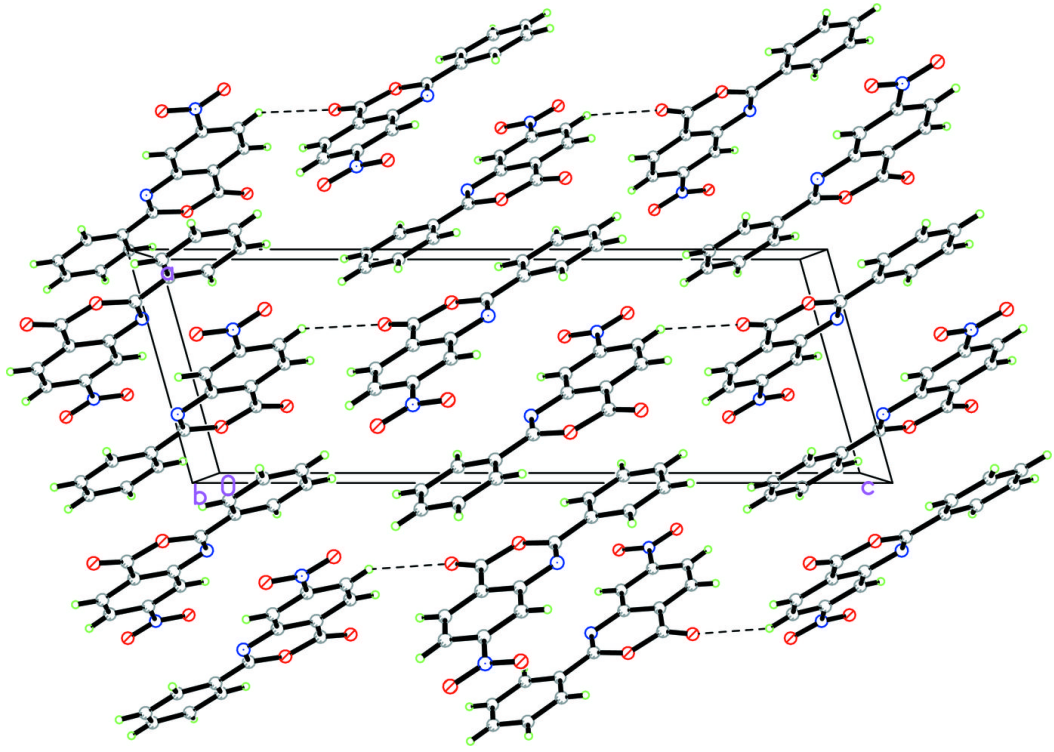
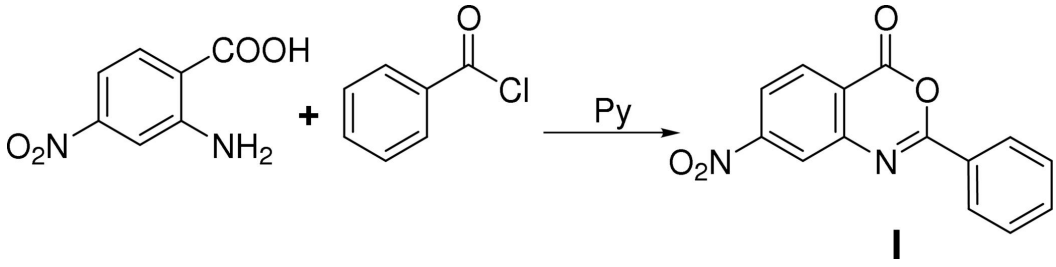


Fig. 3



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