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(3*SR*,2′*SR*)-3-(2′-Anilino-2′-phenylethyl)-phthalide

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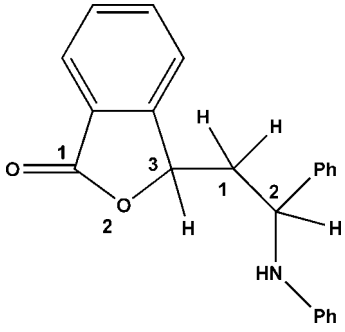
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.083; data-to-parameter ratio = 12.6.

Evolution of the major spiroadduct obtained by cycloaddition of *C,N*-diphenylnitrone with 3-methylenephthalide in Zn/3 *M* HCl media gives a rearrangement product. The reaction did not stop at the formation of an aminoalcohol but was followed by dehydration; the title compound, $C_{22}H_{19}NO_2$, was obtained after hydrogenation. It exists in the diastereoisomer *SS*/*RR* form. The packing is stabilized by weak N—H···O and C—H···O hydrogen-bond interactions.

Related literature

For related structures, see: Daran *et al.* (2006); Laghrib *et al.* (2007). For related literature, see: Goti *et al.* (1997); Jung & Vu (1996); Padwa *et al.* (1981); Roussel *et al.* (2003).



Experimental

Crystal data

$C_{22}H_{19}NO_2$
M_r = 329.38
Triclinic, $P\overline{1}$
a = 6.303 (2) Å
b = 7.774 (2) Å
c = 17.466 (5) Å
α = 88.15 (3)°
β = 88.99 (4)°
γ = 86.62 (4)°
V = 853.8 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 180 (2) K
0.28 × 0.14 × 0.06 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: none
7801 measured reflections
2852 independent reflections
1706 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.083
S = 0.81
2852 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.88	2.60	3.390 (2)	150
C3—H3···O2^{i}	1.00	2.36	3.279 (3)	152
C51—H51···O2^{ii}	0.95	2.57	3.366 (2)	141

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+1, -z$.

Data collection: *IPDS* (Stoe, 2000); cell refinement: *IPDS*; data reduction: *X-RED* (Stoe, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); 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: RK2049).

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supplementary materials

Acta Cryst. (2007). E**63**, o4333 [**doi:10.1107/S1600536807050039**]

(3*SR*,2'*SR*)-3-(2'-Anilino-2'-phenylethyl)phthalide

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Comment

We previously reported that 1,3-dipolar cycloaddition of *C*,*N*-diphenylnitrone (**1**) to 3-methylenephtalide (**2**) produced a mixture of diastereoisomers (Roussel *et al.*, 2003). The molecular structure of the major cycloadduct (**3a**) was confirmed by single-crystal X-ray diffraction (Daran *et al.*, 2006) (Fig. 1).

In a previous paper (Laghrib *et al.*, 2007), we described the evolution of isoxazolidines obtained by cycloaddition of *C*-tolyl-*N*-phenylnitrone with Tulipalin A in Zn / HCl media. The reduction of the nitrogen-oxygen bond of the heterocycle led to a functionalized γ-lactam. This reduction process has been successfully applied for the preparation of biologically active compounds (Goti *et al.*, 1997; Padwa *et al.*, 1981; Jung & Vu, 1996). We report here, on the evolution of major spiroadduct (**3a**) treated with Zn / 3*M* HCl. The reaction did not stop at the formation of aminoalcohol but was followed by dehydratation and hydrogenation to give (**4**) (Fig.2).

^{1}H and ^{13}C NMR studies of (**4**) did not provide much information on the structural behaviour of this product, therefore, we conducted single-crystal X-ray diffraction studies to get detailed information of the stereochemistry of (**4**).

The title compound (**4**) is built up from a phtalide fragment connected to a 2-*N*-phenyl-2-phenylethyl moiety (Fig. 2). The structural anlysis shows that compound (**4**) is the (*SR*/*RS*) diastereoisomer. The phtalide group is planar as expected with the largest deviation from the mean plane being 0.030 (2)Å at C41. It makes a dihedral angle of 51.37 (6)° with the *N*-phenyl group and 81.06 (6)° with the benzene ring. The benzene and the *N*-phenyl rings are nearly perpendicular with a dihedral angle of 80.01 (7)°. The occurrence of weak N–H···O and C–H···O hydrogen bonding interactions (see Table) help in stabilizing the packing.

Experimental

Spiroadduct (**3a**) was synthesized by the procedure described in (Roussel *et al.*, 2003). Synthesis of (**4**): to a solution of spiroheterocycle (**3a**) (0.64 mmol) in the minimum volume of acetone (3 ml) was added activated zinc dust (61.18 mmol). To the resulting suspension was slowly added 3*M* HCl (52.5 ml). The mixture was then stirred for 2 h at room temperature. The zinc was filtered off and rinsed with 3 *M* HCl and $CHCl_3$. To this mixture, while vigorously stirring, solid K_2CO_3 was slowly added until pH = 7. After stirring for two additional hours, the organic layer was separated, dried with Na_2SO_4, filtered and concentrated to give the product as a solid, which was recrystallized from CH_2Cl_2.

Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C–H = 0.95Å (aromatic), 0.99Å (methylene), 1.00Å (methine) and N–H = 0.88 Å with U_{iso}(H) = 1.2U_{eq}(C or N).

Figures

Fig. 1. The scheme of formation the major cycloadduct (**3a**), which confirmed by single-crystal X-ray diffraction (Daran *et al.*, 2006).

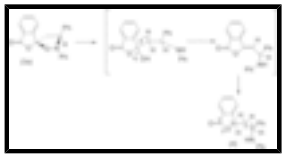


Fig. 2. The scheme of formation the title compound (**4**).

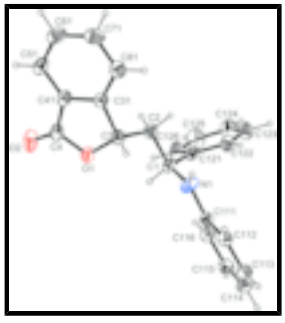


Fig. 3. Molecular view of the title compound with the atom-labelling scheme. Displacements ellipsoids are shown at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

(3SR,2'S*R*)-3-(2'-Anilino-2'-phenylethyl)phtalide

Crystal data

$C_{22}H_{19}NO_2$	$Z = 2$
$M_r = 329.38$	$F_{000} = 348$
Triclinic, $P\overline{1}$	$D_x = 1.281$ Mg m^{-3}
$a = 6.303$ (2) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 7.774$ (2) Å	Cell parameters from 1428 reflections
$c = 17.466$ (5) Å	$\theta = 2.2$–26.2º
$\alpha = 88.15$ (3)º	$\mu = 0.08$ mm^{-1}
$\beta = 88.99$ (4)º	$T = 180$ (2) K
$\gamma = 86.62$ (4)º	Plate, colourless
$V = 853.8$ (4) Å^3	0.28 × 0.14 × 0.06 mm

Data collection

Stoe IPDS diffractometer	1706 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.064$
Monochromator: Graphite	$\theta_{max} = 25.0$º
$T = 180(2)$ K	$\theta_{min} = 2.3$º
φ scans	$h = -7 \rightarrow 7$
Absorption correction: none	$k = -9 \rightarrow 9$
7801 measured reflections	$l = -20 \rightarrow 20$
2852 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.81$	$(\Delta/\sigma)_{max} = 0.001$
2852 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data were collected on a Stoe Imaging Plate Diffraction System (*IPDS*). The crystal-to-detector distance was 70 mm. 167 frames (3 min per frame) were obtained with 0 < φ < 250.5° and with the crystals rotated through 1.5° in φ. Coverage of the unique set was over 93.5% complete to at least 26.08°. Crystal decay was monitored by measuring 200 reflections per frame. The Stoe *IPDS* because of the fixed phi spindle does not allow easy access to the cusp of data along the mount axis which explains why the _diffrn_measured_fraction_theta_full is low, 0.94. This is an instrumentation-based restriction, which the authors have little control over.

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	0.6495 (3)	0.8355 (2)	0.27286 (9)	0.0254 (4)
H1	0.5358	0.9230	0.2560	0.030*
C2	0.6137 (3)	0.6640 (2)	0.23486 (9)	0.0272 (4)
H2A	0.7379	0.5834	0.2456	0.033*
H2B	0.4879	0.6140	0.2596	0.033*
C3	0.5806 (3)	0.6733 (2)	0.14912 (9)	0.0247 (4)
H3	0.7025	0.7274	0.1223	0.030*
C4	0.2424 (3)	0.6721 (3)	0.09876 (9)	0.0289 (5)
C31	0.5482 (3)	0.4991 (2)	0.11756 (9)	0.0239 (4)
C41	0.3477 (3)	0.5016 (2)	0.08731 (9)	0.0248 (4)
C51	0.2692 (3)	0.3550 (3)	0.05605 (9)	0.0321 (5)

H51	0.1308	0.3573	0.0352	0.039*
C61	0.4010 (4)	0.2075 (3)	0.05679 (10)	0.0387 (5)
H61	0.3534	0.1060	0.0354	0.046*
C71	0.6024 (4)	0.2038 (3)	0.08808 (10)	0.0392 (5)
H71	0.6887	0.0994	0.0886	0.047*
C81	0.6799 (3)	0.3501 (3)	0.11865 (9)	0.0322 (5)
H81	0.8181	0.3479	0.1395	0.039*
C111	0.9257 (3)	1.0536 (2)	0.26694 (9)	0.0241 (4)
C112	1.1168 (3)	1.1053 (2)	0.23592 (9)	0.0273 (4)
H112	1.1921	1.0348	0.1999	0.033*
C113	1.1997 (3)	1.2580 (3)	0.25650 (10)	0.0310 (5)
H113	1.3323	1.2898	0.2355	0.037*
C114	1.0895 (3)	1.3644 (2)	0.30772 (10)	0.0321 (5)
H114	1.1458	1.4692	0.3220	0.039*
C115	0.8979 (3)	1.3164 (2)	0.33753 (9)	0.0303 (5)
H115	0.8216	1.3893	0.3724	0.036*
C116	0.8137 (3)	1.1633 (2)	0.31757 (9)	0.0274 (4)
H116	0.6801	1.1329	0.3383	0.033*
C121	0.6298 (3)	0.8057 (2)	0.35941 (9)	0.0265 (4)
C122	0.8025 (3)	0.7506 (2)	0.40326 (9)	0.0321 (5)
H122	0.9399	0.7382	0.3802	0.039*
C123	0.7758 (4)	0.7132 (3)	0.48085 (10)	0.0406 (5)
H123	0.8948	0.6733	0.5105	0.049*
C124	0.5789 (4)	0.7336 (3)	0.51517 (11)	0.0451 (6)
H124	0.5615	0.7079	0.5684	0.054*
C125	0.4071 (4)	0.7910 (3)	0.47233 (11)	0.0486 (6)
H125	0.2707	0.8059	0.4960	0.058*
C126	0.4324 (3)	0.8273 (3)	0.39477 (10)	0.0385 (5)
H126	0.3128	0.8674	0.3655	0.046*
N1	0.8532 (2)	0.8946 (2)	0.24813 (8)	0.0309 (4)
H1A	0.9361	0.8266	0.2197	0.037*
O1	0.38175 (19)	0.77239 (16)	0.13285 (6)	0.0298 (3)
O2	0.0643 (2)	0.72846 (19)	0.08469 (7)	0.0448 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0253 (10)	0.0290 (11)	0.0227 (9)	−0.0062 (9)	−0.0024 (7)	−0.0033 (8)
C2	0.0311 (11)	0.0294 (11)	0.0216 (8)	−0.0062 (9)	−0.0027 (7)	−0.0021 (8)
C3	0.0195 (10)	0.0293 (11)	0.0253 (9)	−0.0010 (9)	−0.0016 (7)	0.0001 (8)
C4	0.0252 (11)	0.0414 (13)	0.0204 (9)	−0.0025 (10)	−0.0013 (8)	−0.0063 (8)
C31	0.0259 (10)	0.0278 (11)	0.0183 (8)	−0.0038 (9)	0.0020 (7)	−0.0031 (7)
C41	0.0262 (10)	0.0316 (11)	0.0174 (8)	−0.0065 (9)	0.0027 (7)	−0.0048 (8)
C51	0.0339 (11)	0.0409 (13)	0.0231 (9)	−0.0140 (11)	0.0011 (8)	−0.0058 (9)
C61	0.0602 (15)	0.0329 (13)	0.0246 (10)	−0.0137 (12)	0.0026 (9)	−0.0080 (9)
C71	0.0592 (15)	0.0280 (12)	0.0299 (10)	0.0027 (11)	0.0035 (10)	−0.0049 (9)
C81	0.0341 (12)	0.0355 (12)	0.0265 (10)	0.0010 (10)	0.0000 (8)	−0.0019 (8)
C111	0.0251 (10)	0.0264 (11)	0.0209 (9)	−0.0028 (9)	−0.0030 (7)	0.0003 (8)

C112	0.0268 (11)	0.0296 (11)	0.0255 (9)	−0.0019 (9)	0.0015 (8)	−0.0006 (8)
C113	0.0272 (11)	0.0326 (12)	0.0332 (10)	−0.0053 (10)	0.0012 (8)	0.0037 (9)
C114	0.0409 (13)	0.0266 (11)	0.0298 (10)	−0.0089 (10)	−0.0034 (9)	−0.0008 (8)
C115	0.0387 (12)	0.0277 (12)	0.0246 (9)	−0.0012 (10)	−0.0003 (8)	−0.0033 (8)
C116	0.0269 (11)	0.0308 (11)	0.0249 (9)	−0.0039 (9)	0.0030 (7)	−0.0038 (8)
C121	0.0311 (11)	0.0263 (11)	0.0230 (9)	−0.0064 (9)	−0.0006 (8)	−0.0064 (8)
C122	0.0328 (12)	0.0361 (12)	0.0279 (10)	−0.0021 (10)	−0.0027 (8)	−0.0066 (9)
C123	0.0480 (14)	0.0443 (14)	0.0295 (10)	−0.0001 (12)	−0.0105 (9)	−0.0018 (9)
C124	0.0549 (15)	0.0545 (15)	0.0257 (10)	−0.0036 (13)	0.0025 (10)	0.0005 (10)
C125	0.0404 (13)	0.0701 (17)	0.0346 (11)	−0.0037 (13)	0.0123 (10)	0.0017 (11)
C126	0.0268 (11)	0.0565 (15)	0.0322 (11)	−0.0037 (11)	0.0001 (8)	0.0018 (10)
N1	0.0305 (9)	0.0307 (10)	0.0328 (8)	−0.0095 (8)	0.0096 (7)	−0.0128 (7)
O1	0.0283 (7)	0.0317 (8)	0.0298 (7)	0.0007 (6)	−0.0061 (5)	−0.0077 (6)
O2	0.0276 (8)	0.0636 (11)	0.0433 (8)	0.0077 (8)	−0.0087 (6)	−0.0151 (7)

Geometric parameters (Å, °)

C1—N1	1.443 (2)	C111—N1	1.393 (2)
C1—C121	1.526 (2)	C111—C116	1.401 (2)
C1—C2	1.539 (2)	C112—C113	1.385 (3)
C1—H1	1.0000	C112—H112	0.9500
C2—C3	1.514 (2)	C113—C114	1.388 (2)
C2—H2A	0.9900	C113—H113	0.9500
C2—H2B	0.9900	C114—C115	1.374 (3)
C3—O1	1.459 (2)	C114—H114	0.9500
C3—C31	1.505 (2)	C115—C116	1.389 (3)
C3—H3	1.0000	C115—H115	0.9500
C4—O2	1.207 (2)	C116—H116	0.9500
C4—O1	1.365 (2)	C121—C122	1.381 (3)
C4—C41	1.465 (3)	C121—C126	1.383 (3)
C31—C41	1.377 (2)	C122—C123	1.386 (3)
C31—C81	1.385 (3)	C122—H122	0.9500
C41—C51	1.399 (3)	C123—C124	1.372 (3)
C51—C61	1.376 (3)	C123—H123	0.9500
C51—H51	0.9500	C124—C125	1.371 (3)
C61—C71	1.389 (3)	C124—H124	0.9500
C61—H61	0.9500	C125—C126	1.383 (3)
C71—C81	1.389 (3)	C125—H125	0.9500
C71—H71	0.9500	C126—H126	0.9500
C81—H81	0.9500	N1—H1A	0.8800
C111—C112	1.388 (3)		
N1—C1—C121	113.53 (14)	C112—C111—C116	118.24 (16)
N1—C1—C2	109.13 (14)	N1—C111—C116	122.22 (16)
C121—C1—C2	107.81 (16)	C113—C112—C111	121.20 (16)
N1—C1—H1	108.8	C113—C112—H112	119.4
C121—C1—H1	108.8	C111—C112—H112	119.4
C2—C1—H1	108.8	C112—C113—C114	120.14 (18)
C3—C2—C1	116.27 (15)	C112—C113—H113	119.9
C3—C2—H2A	108.2	C114—C113—H113	119.9

C1—C2—H2A	108.2	C115—C114—C113	119.20 (18)
C3—C2—H2B	108.2	C115—C114—H114	120.4
C1—C2—H2B	108.2	C113—C114—H114	120.4
H2A—C2—H2B	107.4	C114—C115—C116	121.14 (17)
O1—C3—C31	103.91 (14)	C114—C115—H115	119.4
O1—C3—C2	109.13 (13)	C116—C115—H115	119.4
C31—C3—C2	112.10 (15)	C115—C116—C111	120.04 (17)
O1—C3—H3	110.5	C115—C116—H116	120.0
C31—C3—H3	110.5	C111—C116—H116	120.0
C2—C3—H3	110.5	C122—C121—C126	118.79 (17)
O2—C4—O1	120.36 (17)	C122—C121—C1	121.80 (16)
O2—C4—C41	131.13 (18)	C126—C121—C1	119.35 (16)
O1—C4—C41	108.50 (15)	C121—C122—C123	120.20 (19)
C41—C31—C81	121.00 (17)	C121—C122—H122	119.9
C41—C31—C3	108.59 (15)	C123—C122—H122	119.9
C81—C31—C3	130.33 (16)	C124—C123—C122	120.47 (19)
C31—C41—C51	121.69 (18)	C124—C123—H123	119.8
C31—C41—C4	108.45 (15)	C122—C123—H123	119.8
C51—C41—C4	129.77 (17)	C125—C124—C123	119.72 (19)
C61—C51—C41	117.12 (18)	C125—C124—H124	120.1
C61—C51—H51	121.4	C123—C124—H124	120.1
C41—C51—H51	121.4	C124—C125—C126	120.1 (2)
C51—C61—C71	121.41 (18)	C124—C125—H125	120.0
C51—C61—H61	119.3	C126—C125—H125	120.0
C71—C61—H61	119.3	C125—C126—C121	120.71 (19)
C61—C71—C81	121.17 (19)	C125—C126—H126	119.6
C61—C71—H71	119.4	C121—C126—H126	119.6
C81—C71—H71	119.4	C111—N1—C1	123.48 (14)
C31—C81—C71	117.60 (18)	C111—N1—H1A	118.3
C31—C81—H81	121.2	C1—N1—H1A	118.3
C71—C81—H81	121.2	C4—O1—C3	110.49 (13)
C112—C111—N1	119.53 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.88	2.60	3.390 (2)	150
C3—H3···O2^{i}	1.00	2.36	3.279 (3)	152
C51—H51···O2^{ii}	0.95	2.57	3.366 (2)	141

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

Fig. 1

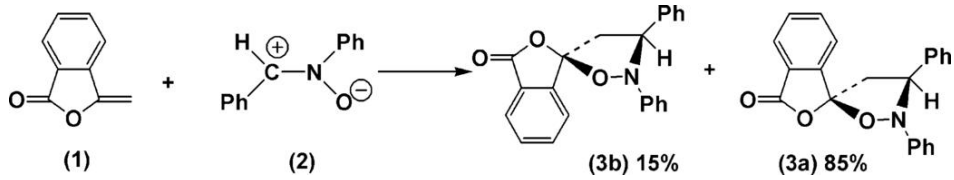


Fig. 2

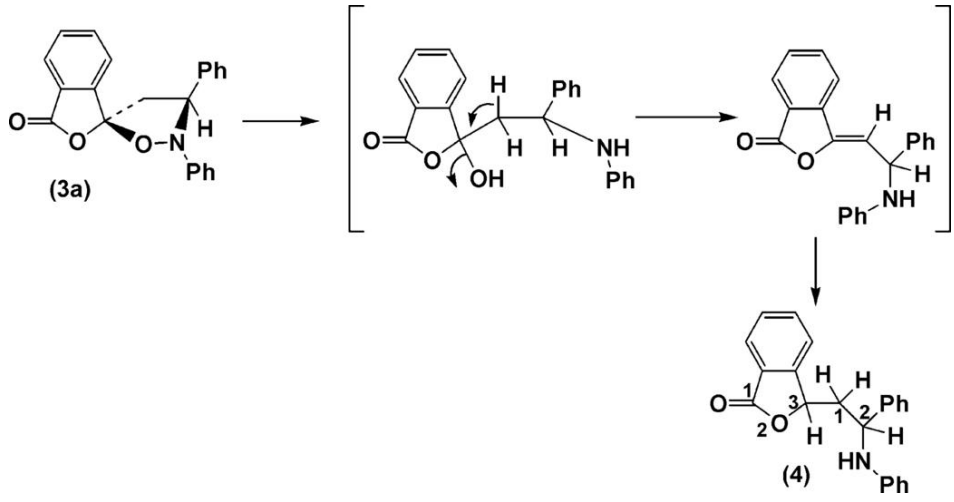
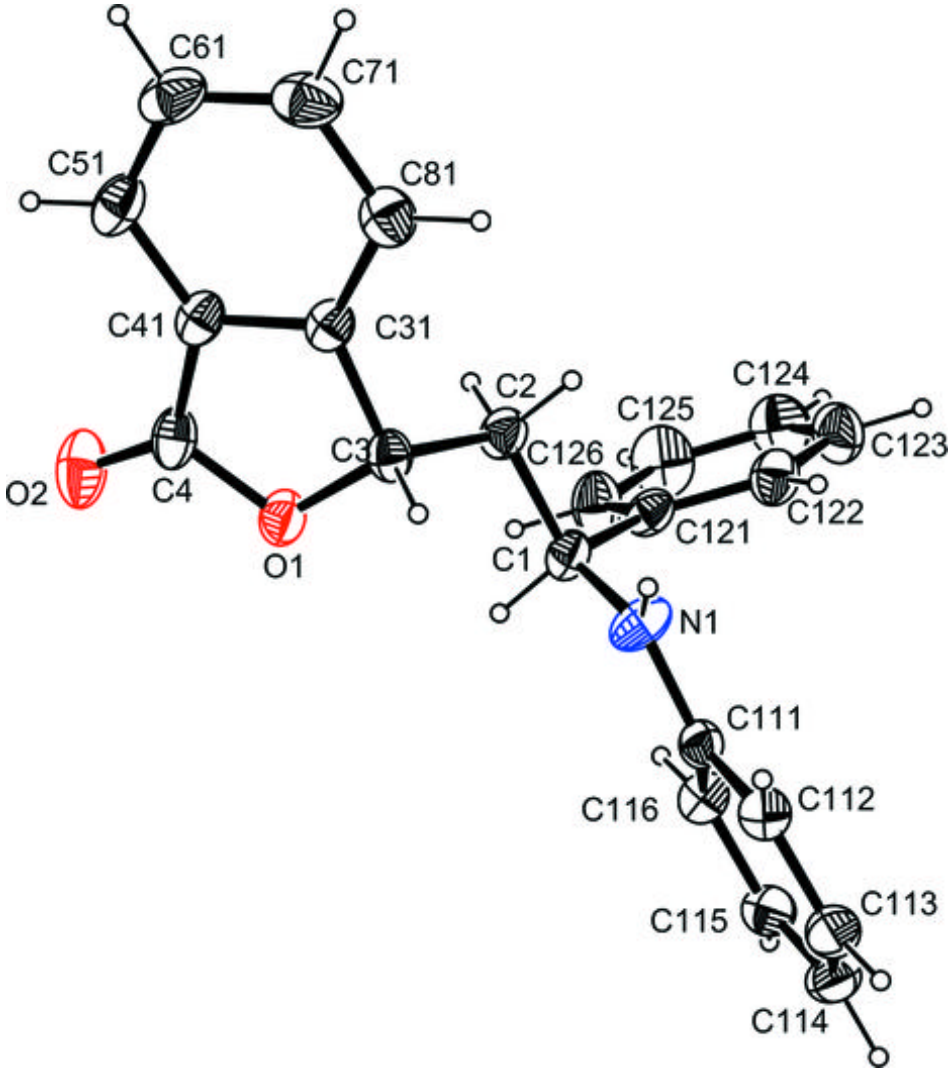


Fig. 3


C61
C71
C51
C81
C41
C31
C2
C124
C125
C123
C3
C126
O2
C4
C122
C121
O1
C1
N1
C111
C116
C112
C115
C113
C114