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Orthorhombic modification of (*E*)-4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-one: whole molecule disorder

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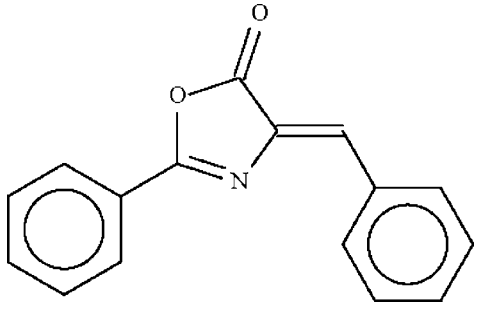
Key indicators: single-crystal X-ray study; T = 140 K; mean σ(O–C) = 0.008 Å; disorder in main residue; R factor = 0.044; wR factor = 0.125; data-to-parameter ratio = 9.0.

The title molecule, $C_{16}H_{11}NO_2$, is disordered about a pseudo-twofold rotation axis that approximately bisects the molecule along the C=O double bond. The two overlapping components are planar [r.m.s. deviation = 0.10 Å in the major 0.537 (4) component and 0.07 Å in the minor component]. The two components are aligned at 1.8 (3)°.

Related literature

For the monoclinic modification, see: Busetti *et al.* (1993).



Experimental

Crystal data

$C_{16}H_{11}NO_2$
M_r = 249.26
Orthorhombic, $P2_12_12_1$
a = 3.9320 (1) Å
b = 14.7692 (5) Å
c = 20.6690 (6) Å
V = 1200.30 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 140 K
0.45 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
8204 measured reflections
1640 independent reflections
1312 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.03
1640 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

I thank Professor Abdullah Mohamed Asiri of King Abdul Aziz University for providing the crystal for this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2490).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supplementary materials

Acta Cryst. (2009). E**65**, o1857 [**doi:10.1107/S1600536809025999**]

Orthorhombic modification of (*E*)-4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-one: whole molecule disorder

S. W. Ng

Experimental

Anhydrous sodium acetate (0.26 g, 0.0036 mol) was added to solution of benzaldehyde (1 g, 0.0036 mol) and hippuric acid (0.77 g, 0.0043 mol) in acetic anhydride (0.27 ml, 0028 mol). The mixture was heated to 353 K for 2 h. Ethanol (10 ml) was added to the cool mixture to precipitate a yellow solid. This was collected and recrystallized from aqueous acetone to give yellow crystals in 60% yield; m.p. 443 K.

Refinement

The molecule is disordered about a false 2-fold rotation axis that approximately bisects the molecule along the carbon-oxygen double bond. The aromatic rings were refined as rigid hexagons of 1.39 Å sides. The displacement factors of the primed atoms were restrained to those of the umprimed ones.

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation with U(H) fixed at 1.2U_{eq}(C).

In the absence of significant anomalous scattering effects, 1076 Friedel pairs were averaged in the final refinement.

Figures

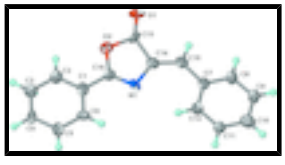

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the major, 0.537 (4), component of disordered $C_{16}H_{11}NO_2$, shown at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

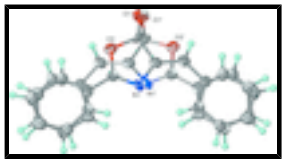

Fig. 2. Detail showing the disorder. The minor disorder component is indicated with primed atoms and dotted bonds.

(*E*)-4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-one

Crystal data

$C_{16}H_{11}NO_2$	F_{000} = 520
M_r = 249.26	D_x = 1.379 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 1737 reflections

a = 3.9320 (1) Å	θ = 2.5–25.8º
b = 14.7692 (5) Å	μ = 0.09 mm^{-1}
c = 20.6690 (6) Å	T = 140 K
V = 1200.30 (6) Å^3	Prism, yellow
Z = 4	0.45 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer	1312 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.036
Monochromator: graphite	θ_{max} = 27.5º
T = 140 K	θ_{min} = 1.7º
ω scans	h = −5→4
Absorption correction: None	k = −19→19
8204 measured reflections	l = −25→26
1640 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.1226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.125	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.03	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
1640 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
182 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: nd
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	−0.109 (5)	0.373 (3)	0.2237 (16)	0.031 (2)	0.537 (4)
O2	0.1605 (8)	0.2739 (2)	0.28782 (13)	0.0282 (5)	0.537 (4)
N1	0.432 (3)	0.3613 (3)	0.3629 (6)	0.0229 (10)	0.537 (4)
C1	0.4568 (11)	0.19591 (18)	0.37320 (16)	0.0256 (7)	0.537 (4)
C2	0.3888 (11)	0.1143 (2)	0.34231 (13)	0.0280 (10)	0.537 (4)
H2	0.2715	0.1139	0.3021	0.034*	0.537 (4)
C3	0.4924 (12)	0.03323 (18)	0.37021 (15)	0.0304 (9)	0.537 (4)
H3	0.4460	−0.0225	0.3491	0.037*	0.537 (4)
C4	0.6641 (13)	0.03378 (19)	0.42900 (16)	0.0236 (10)	0.537 (4)
H4	0.7349	−0.0216	0.4481	0.028*	0.537 (4)
C5	0.7321 (13)	0.1154 (2)	0.45989 (15)	0.0285 (11)	0.537 (4)
H5	0.8494	0.1158	0.5001	0.034*	0.537 (4)

C6	0.6284 (12)	0.19646 (18)	0.43199 (17)	0.0246 (9)	0.537 (4)
H6	0.6749	0.2522	0.4531	0.029*	0.537 (4)
C7	0.4345 (10)	0.5780 (2)	0.35423 (15)	0.0225 (7)	0.537 (4)
C8	0.4110 (11)	0.6682 (2)	0.33534 (13)	0.0264 (9)	0.537 (4)
H8	0.3029	0.6835	0.2957	0.032*	0.537 (4)
C9	0.5458 (14)	0.73583 (17)	0.37442 (17)	0.0291 (9)	0.537 (4)
H9	0.5297	0.7974	0.3615	0.035*	0.537 (4)
C10	0.7040 (15)	0.7134 (2)	0.43239 (17)	0.0333 (13)	0.537 (4)
H10	0.7960	0.7597	0.4591	0.040*	0.537 (4)
C11	0.7274 (14)	0.6233 (3)	0.45127 (17)	0.0255 (10)	0.537 (4)
H11	0.8356	0.6080	0.4909	0.031*	0.537 (4)
C12	0.5927 (12)	0.55561 (18)	0.41219 (18)	0.0270 (10)	0.537 (4)
H12	0.6088	0.4940	0.4251	0.032*	0.537 (4)
C13	0.081 (5)	0.3626 (7)	0.2675 (10)	0.0237 (18)	0.537 (4)
C14	0.2749 (12)	0.4188 (3)	0.31640 (18)	0.0247 (5)	0.537 (4)
C15	0.2789 (12)	0.5102 (3)	0.31202 (19)	0.0255 (6)	0.537 (4)
H15	0.1616	0.5341	0.2757	0.031*	0.537 (4)
C16	0.3550 (11)	0.2805 (3)	0.34289 (17)	0.0234 (6)	0.537 (4)
O1'	−0.037 (6)	0.376 (3)	0.2199 (18)	0.031 (2)	0.463
O2'	0.1691 (10)	0.4755 (2)	0.28423 (15)	0.0282 (5)	0.463
N1'	0.421 (4)	0.3896 (4)	0.3594 (7)	0.0229 (10)	0.463
C1'	0.4779 (13)	0.5543 (2)	0.36785 (19)	0.0256 (7)	0.463
C2'	0.4019 (13)	0.6351 (3)	0.33667 (16)	0.0280 (10)	0.463
H2'	0.2789	0.6345	0.2971	0.034*	0.463 (4)
C3'	0.5060 (16)	0.7170 (2)	0.3634 (2)	0.0304 (9)	0.463
H3'	0.4540	0.7723	0.3420	0.037*	0.463 (4)
C4'	0.6860 (18)	0.7179 (2)	0.4212 (2)	0.0236 (10)	0.463
H4'	0.7571	0.7738	0.4395	0.028*	0.463 (4)
C5'	0.7620 (17)	0.6370 (3)	0.4524 (2)	0.0285 (11)	0.463
H5'	0.8850	0.6377	0.4920	0.034*	0.463 (4)
C6'	0.6580 (15)	0.5552 (2)	0.4257 (2)	0.0246 (9)	0.463
H6'	0.7099	0.4999	0.4470	0.029*	0.463 (4)
C7'	0.4147 (13)	0.1731 (2)	0.35940 (18)	0.0225 (7)	0.463
C8'	0.3876 (14)	0.0824 (3)	0.34221 (15)	0.0264 (9)	0.463
H8'	0.2839	0.0660	0.3024	0.032*	0.463 (4)
C9'	0.5123 (17)	0.0157 (2)	0.38330 (19)	0.0291 (9)	0.463
H9'	0.4938	−0.0463	0.3716	0.035*	0.463 (4)
C10'	0.6641 (17)	0.0397 (3)	0.44157 (19)	0.0333 (13)	0.463
H10B	0.7493	−0.0059	0.4696	0.040*	0.463 (4)
C11'	0.6911 (16)	0.1304 (3)	0.45875 (19)	0.0255 (10)	0.463
H11B	0.7948	0.1468	0.4986	0.031*	0.463 (4)
C12'	0.5664 (15)	0.1971 (2)	0.4177 (2)	0.0270 (10)	0.463
H12B	0.5849	0.2591	0.4294	0.032*	0.463 (4)
C13'	0.112 (6)	0.3856 (9)	0.2697 (12)	0.0237 (18)	0.463
C14'	0.2695 (14)	0.3313 (3)	0.3171 (2)	0.0247 (5)	0.463
C15'	0.2625 (14)	0.2393 (3)	0.3151 (2)	0.0255 (6)	0.463
H15B	0.1408	0.2141	0.2797	0.031*	0.463 (4)
C16'	0.3654 (13)	0.4697 (3)	0.3398 (2)	0.0234 (6)	0.463

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.017 (7)	0.048 (3)	0.029 (3)	−0.004 (7)	−0.006 (5)	0.000 (2)
O2	0.0293 (11)	0.0299 (10)	0.0255 (10)	−0.0017 (12)	−0.0039 (9)	−0.0011 (10)
N1	0.0248 (13)	0.021 (3)	0.0229 (14)	0.007 (4)	0.0002 (11)	0.006 (3)
C1	0.0230 (17)	0.0248 (14)	0.0290 (17)	0.0008 (17)	0.0078 (14)	−0.0006 (12)
C2	0.0316 (18)	0.027 (3)	0.0250 (15)	−0.001 (3)	0.0010 (12)	−0.0002 (14)
C3	0.032 (2)	0.0311 (17)	0.0284 (16)	0.001 (2)	0.0008 (15)	0.0019 (14)
C4	0.027 (3)	0.0140 (17)	0.0296 (17)	−0.004 (2)	0.0084 (16)	0.0016 (13)
C5	0.030 (2)	0.0227 (18)	0.033 (3)	0.0016 (19)	0.0003 (19)	−0.0007 (14)
C6	0.0154 (19)	0.0302 (19)	0.0281 (17)	0.0010 (17)	−0.0032 (15)	−0.0020 (14)
C7	0.0216 (16)	0.0235 (15)	0.0224 (13)	0.0007 (17)	0.0047 (12)	−0.0011 (12)
C8	0.0321 (19)	0.022 (2)	0.0253 (16)	0.000 (2)	0.0020 (14)	0.0007 (14)
C9	0.035 (2)	0.0214 (13)	0.0310 (17)	−0.0025 (18)	0.0019 (16)	0.0021 (12)
C10	0.030 (3)	0.042 (3)	0.0281 (18)	0.007 (3)	−0.0007 (18)	−0.0018 (17)
C11	0.0223 (19)	0.0247 (17)	0.030 (2)	0.000 (2)	−0.0010 (17)	0.0008 (15)
C12	0.027 (2)	0.0239 (18)	0.030 (2)	0.0014 (18)	−0.0006 (17)	−0.0007 (14)
C13	0.022 (4)	0.024 (6)	0.0252 (15)	−0.009 (5)	−0.002 (2)	−0.007 (5)
C14	0.0217 (13)	0.0305 (13)	0.0217 (12)	0.0035 (16)	0.0004 (11)	−0.0006 (14)
C15	0.0237 (15)	0.0306 (14)	0.0221 (13)	0.0036 (16)	0.0002 (12)	0.0011 (15)
C16	0.0222 (14)	0.0279 (14)	0.0202 (12)	−0.0010 (17)	0.0009 (11)	−0.0006 (15)
O1'	0.017 (7)	0.048 (3)	0.029 (3)	−0.004 (7)	−0.006 (5)	0.000 (2)
O2'	0.0293 (11)	0.0299 (10)	0.0255 (10)	−0.0017 (12)	−0.0039 (9)	−0.0011 (10)
N1'	0.0248 (13)	0.021 (3)	0.0229 (14)	0.007 (4)	0.0002 (11)	0.006 (3)
C1'	0.0230 (17)	0.0248 (14)	0.0290 (17)	0.0008 (17)	0.0078 (14)	−0.0006 (12)
C2'	0.0316 (18)	0.027 (3)	0.0250 (15)	−0.001 (3)	0.0010 (12)	−0.0002 (14)
C3'	0.032 (2)	0.0311 (17)	0.0284 (16)	0.001 (2)	0.0008 (15)	0.0019 (14)
C4'	0.027 (3)	0.0140 (17)	0.0296 (17)	−0.004 (2)	0.0084 (16)	0.0016 (13)
C5'	0.030 (2)	0.0227 (18)	0.033 (3)	0.0016 (19)	0.0003 (19)	−0.0007 (14)
C6'	0.0154 (19)	0.0302 (19)	0.0281 (17)	0.0010 (17)	−0.0032 (15)	−0.0020 (14)
C7'	0.0216 (16)	0.0235 (15)	0.0224 (13)	0.0007 (17)	0.0047 (12)	−0.0011 (12)
C8'	0.0321 (19)	0.022 (2)	0.0253 (16)	0.000 (2)	0.0020 (14)	0.0007 (14)
C9'	0.035 (2)	0.0214 (13)	0.0310 (17)	−0.0025 (18)	0.0019 (16)	0.0021 (12)
C10'	0.030 (3)	0.042 (3)	0.0281 (18)	0.007 (3)	−0.0007 (18)	−0.0018 (17)
C11'	0.0223 (19)	0.0247 (17)	0.030 (2)	0.000 (2)	−0.0010 (17)	0.0008 (15)
C12'	0.027 (2)	0.0239 (18)	0.030 (2)	0.0014 (18)	−0.0006 (17)	−0.0007 (14)
C13'	0.022 (4)	0.024 (6)	0.0252 (15)	−0.009 (5)	−0.002 (2)	−0.007 (5)
C14'	0.0217 (13)	0.0305 (13)	0.0217 (12)	0.0035 (16)	0.0004 (11)	−0.0006 (14)
C15'	0.0237 (15)	0.0306 (14)	0.0221 (13)	0.0036 (16)	0.0002 (12)	0.0011 (15)
C16'	0.0222 (14)	0.0279 (14)	0.0202 (12)	−0.0010 (17)	0.0009 (11)	−0.0006 (15)

Geometric parameters (Å, °)

O1—C13	1.18 (4)	O1'—C13'	1.19 (5)
O2—C16	1.375 (5)	O2'—C13'	1.378 (13)
O2—C13	1.412 (15)	O2'—C16'	1.386 (6)
N1—C16	1.300 (9)	N1'—C16'	1.270 (8)

N1—C14	1.424 (9)	N1'—C14'	1.365 (14)
C1—C2	1.3900	C1'—C2'	1.3900
C1—C6	1.3900	C1'—C6'	1.3900
C1—C16	1.453 (4)	C1'—C16'	1.446 (6)
C2—C3	1.3900	C2'—C3'	1.3900
C2—H2	0.9500	C2'—H2'	0.9500
C3—C4	1.3900	C3'—C4'	1.3900
C3—H3	0.9500	C3'—H3'	0.9500
C4—C5	1.3900	C4'—C5'	1.3900
C4—H4	0.9500	C4'—H4'	0.9500
C5—C6	1.3900	C5'—C6'	1.3900
C5—H5	0.9500	C5'—H5'	0.9500
C6—H6	0.9500	C6'—H6'	0.9500
C7—C8	1.3900	C7'—C8'	1.3900
C7—C12	1.3900	C7'—C12'	1.3900
C7—C15	1.463 (5)	C7'—C15'	1.467 (6)
C8—C9	1.3900	C8'—C9'	1.3900
C8—H8	0.9500	C8'—H8'	0.9500
C9—C10	1.3900	C9'—C10'	1.3900
C9—H9	0.9500	C9'—H9'	0.9500
C10—C11	1.3900	C10'—C11'	1.3900
C10—H10	0.9500	C10'—H10B	0.9500
C11—C12	1.3900	C11'—C12'	1.3900
C11—H11	0.9500	C11'—H11B	0.9500
C12—H12	0.9500	C12'—H12B	0.9500
C13—C14	1.515 (15)	C13'—C14'	1.41 (2)
C14—C15	1.352 (5)	C14'—C15'	1.359 (6)
C15—H15	0.9500	C15'—H15B	0.9500
C16—O2—C13	107.7 (8)	C13'—O2'—C16'	102.2 (11)
C16—N1—C14	103.4 (8)	C16'—N1'—C14'	107.9 (10)
C2—C1—C6	120.0	C2'—C1'—C6'	120.0
C2—C1—C16	119.6 (3)	C2'—C1'—C16'	119.4 (3)
C6—C1—C16	120.4 (3)	C6'—C1'—C16'	120.6 (3)
C3—C2—C1	120.0	C3'—C2'—C1'	120.0
C3—C2—H2	120.0	C3'—C2'—H2'	120.0
C1—C2—H2	120.0	C1'—C2'—H2'	120.0
C2—C3—C4	120.0	C2'—C3'—C4'	120.0
C2—C3—H3	120.0	C2'—C3'—H3'	120.0
C4—C3—H3	120.0	C4'—C3'—H3'	120.0
C5—C4—C3	120.0	C5'—C4'—C3'	120.0
C5—C4—H4	120.0	C5'—C4'—H4'	120.0
C3—C4—H4	120.0	C3'—C4'—H4'	120.0
C6—C5—C4	120.0	C4'—C5'—C6'	120.0
C6—C5—H5	120.0	C4'—C5'—H5'	120.0
C4—C5—H5	120.0	C6'—C5'—H5'	120.0
C5—C6—C1	120.0	C5'—C6'—C1'	120.0
C5—C6—H6	120.0	C5'—C6'—H6'	120.0
C1—C6—H6	120.0	C1'—C6'—H6'	120.0
C8—C7—C12	120.0	C8'—C7'—C12'	120.0

C8—C7—C15	117.4 (3)	C8'—C7'—C15'	116.8 (4)
C12—C7—C15	122.5 (3)	C12'—C7'—C15'	123.1 (4)
C9—C8—C7	120.0	C7'—C8'—C9'	120.0
C9—C8—H8	120.0	C7'—C8'—H8'	120.0
C7—C8—H8	120.0	C9'—C8'—H8'	120.0
C8—C9—C10	120.0	C8'—C9'—C10'	120.0
C8—C9—H9	120.0	C8'—C9'—H9'	120.0
C10—C9—H9	120.0	C10'—C9'—H9'	120.0
C11—C10—C9	120.0	C11'—C10'—C9'	120.0
C11—C10—H10	120.0	C11'—C10'—H10B	120.0
C9—C10—H10	120.0	C9'—C10'—H10B	120.0
C10—C11—C12	120.0	C10'—C11'—C12'	120.0
C10—C11—H11	120.0	C10'—C11'—H11B	120.0
C12—C11—H11	120.0	C12'—C11'—H11B	120.0
C11—C12—C7	120.0	C11'—C12'—C7'	120.0
C11—C12—H12	120.0	C11'—C12'—H12B	120.0
C7—C12—H12	120.0	C7'—C12'—H12B	120.0
O1—C13—O2	119 (2)	O1'—C13'—O2'	113 (3)
O1—C13—C14	140 (2)	O1'—C13'—C14'	138 (3)
O2—C13—C14	101.4 (13)	O2'—C13'—C14'	109.0 (15)
C15—C14—N1	129.4 (5)	C15'—C14'—N1'	131.3 (6)
C15—C14—C13	120.5 (7)	C15'—C14'—C13'	122.6 (7)
N1—C14—C13	110.1 (8)	N1'—C14'—C13'	106.1 (7)
C14—C15—C7	130.4 (4)	C14'—C15'—C7'	129.7 (5)
C14—C15—H15	114.8	C14'—C15'—H15B	115.2
C7—C15—H15	114.8	C7'—C15'—H15B	115.2
N1—C16—O2	117.3 (6)	N1'—C16'—O2'	114.7 (8)
N1—C16—C1	126.0 (6)	N1'—C16'—C1'	128.5 (8)
O2—C16—C1	116.7 (4)	O2'—C16'—C1'	116.7 (4)
C6—C1—C2—C3	0.0	C6'—C1'—C2'—C3'	0.0
C16—C1—C2—C3	178.5 (4)	C16'—C1'—C2'—C3'	179.5 (5)
C1—C2—C3—C4	0.0	C1'—C2'—C3'—C4'	0.0
C2—C3—C4—C5	0.0	C2'—C3'—C4'—C5'	0.0
C3—C4—C5—C6	0.0	C3'—C4'—C5'—C6'	0.0
C4—C5—C6—C1	0.0	C4'—C5'—C6'—C1'	0.0
C2—C1—C6—C5	0.0	C2'—C1'—C6'—C5'	0.0
C16—C1—C6—C5	−178.5 (4)	C16'—C1'—C6'—C5'	−179.5 (5)
C12—C7—C8—C9	0.0	C12'—C7'—C8'—C9'	0.0
C15—C7—C8—C9	178.2 (4)	C15'—C7'—C8'—C9'	−177.1 (5)
C7—C8—C9—C10	0.0	C7'—C8'—C9'—C10'	0.0
C8—C9—C10—C11	0.0	C8'—C9'—C10'—C11'	0.0
C9—C10—C11—C12	0.0	C9'—C10'—C11'—C12'	0.0
C10—C11—C12—C7	0.0	C10'—C11'—C12'—C7'	0.0
C8—C7—C12—C11	0.0	C8'—C7'—C12'—C11'	0.0
C15—C7—C12—C11	−178.1 (4)	C15'—C7'—C12'—C11'	176.9 (5)
C16—O2—C13—O1	−173.9 (18)	C16'—O2'—C13'—O1'	−175 (2)
C16—O2—C13—C14	3.3 (13)	C16'—O2'—C13'—C14'	1.1 (18)
C16—N1—C14—C15	−178.0 (5)	C16'—N1'—C14'—C15'	177.7 (7)
C16—N1—C14—C13	2.4 (13)	C16'—N1'—C14'—C13'	−0.4 (16)

O1—C13—C14—C15	−7(3)	O1'—C13'—C14'—C15'	−4(4)
O2—C13—C14—C15	176.8 (7)	O2'—C13'—C14'—C15'	−178.8 (9)
O1—C13—C14—N1	173 (3)	O1'—C13'—C14'—N1'	175 (3)
O2—C13—C14—N1	−3.6 (15)	O2'—C13'—C14'—N1'	−1(2)
N1—C14—C15—C7	−2.2 (10)	N1'—C14'—C15'—C7'	1.2 (13)
C13—C14—C15—C7	177.3 (10)	C13'—C14'—C15'—C7'	179.0 (13)
C8—C7—C15—C14	176.7 (4)	C8'—C7'—C15'—C14'	−175.1 (5)
C12—C7—C15—C14	−5.2 (6)	C12'—C7'—C15'—C14'	7.9 (8)
C14—N1—C16—O2	−0.2 (11)	C14'—N1'—C16'—O2'	1.2 (14)
C14—N1—C16—C1	179.5 (5)	C14'—N1'—C16'—C1'	−179.1 (6)
C13—O2—C16—N1	−2.2 (12)	C13'—O2'—C16'—N1'	−1.4 (15)
C13—O2—C16—C1	178.1 (10)	C13'—O2'—C16'—C1'	178.8 (12)
C2—C1—C16—N1	−172.6 (8)	C2'—C1'—C16'—N1'	176.8 (10)
C6—C1—C16—N1	5.9 (9)	C6'—C1'—C16'—N1'	−3.7 (11)
C2—C1—C16—O2	7.1 (5)	C2'—C1'—C16'—O2'	−3.5 (6)
C6—C1—C16—O2	−174.4 (3)	C6'—C1'—C16'—O2'	176.0 (4)

Fig. 1

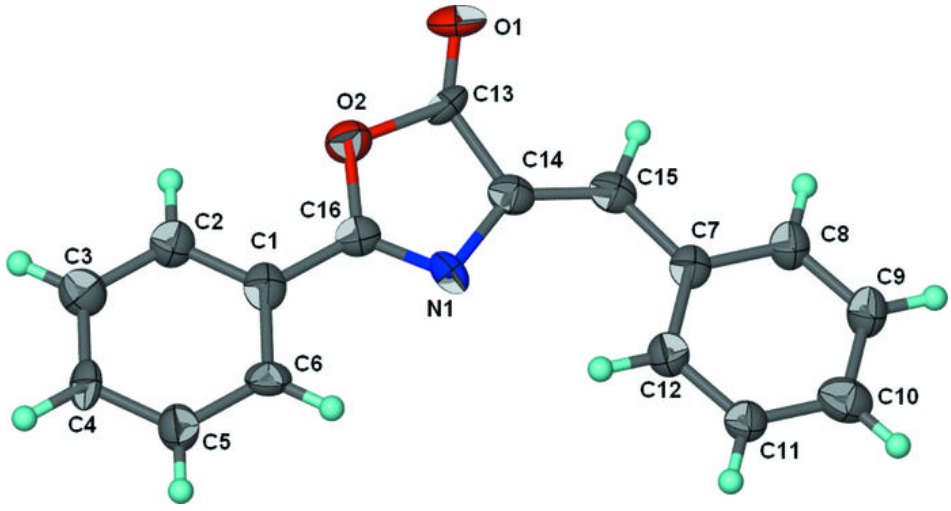

Fig. 2