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(2*E*)-3-(Biphenyl-4-yl)-1-(quinolin-2-yl)-prop-2-en-1-one

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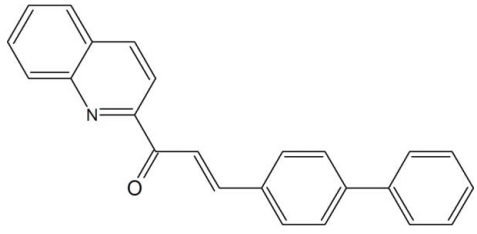
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.148; data-to-parameter ratio = 24.0.

In the title molecule, $C_{24}H_{17}NO$, the mean planes of the two aromatic rings of the biphenyl group make a dihedral angle of 45.0 (8)°. The mean plane of the quinolin-2-yl group makes angles of 18.2 (6) and 61.9 (8)° with the benzene rings closest to and farthest away from the prop-2-en-1-one group, and 7.4 (1)° with the plane of the prop-2-en-1-one group. The structure is stabilized by intermolecular C—H···O hydrogen-bond interactions.

Related literature

For related structures, see: Fischer *et al.* (2007*a*,*b*,*c*,*d*,*e*); Sarojini *et al.* (2007); Yathirajan *et al.* (2007). For related literature, see: Fichou *et al.* (1988); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{17}NO$
M_r = 335.39
Triclinic, $P\overline{1}$
a = 5.9808 (12) Å
b = 11.9617 (18) Å
c = 13.2239 (16) Å
α = 109.401 (12)°
β = 92.981 (13)°
γ = 102.967 (15)°
V = 861.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 203 K
0.57 × 0.43 × 0.19 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.922, T_{max} = 1.000
12993 measured reflections
5643 independent reflections
3561 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.148
S = 1.04
5643 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18A···O^{i}	0.94	2.51	3.3222 (13)	145

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2342).

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supplementary materials

Acta Cryst. (2007). E**63**, o3546 [**doi:10.1107/S1600536807034721**]

(2*E*)-3-(Biphenyl-4-yl)-1-(quinolin-2-yl)prop-2-en-1-one

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Comment

Chalcones have been reported to possess many useful properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities. Among several organic compounds reported for their non linear optical (NLO) property, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. We have synthesized a new chalcone, (I), and herein report the crystal structure of (I) (Fig. 1).

Intermolecular C—H···O hydrogen bond interactions occur between C18—H18A and O, and stabilize the structure as indicated in the packing diagram (Fig. 2).

Experimental

5 ml of 40% KOH solution was added to a thoroughly stirred solution of 2-acetylquinoline (1.71 g, 0.01 mol) and 4-biphenylaldehyde (1.82 g, 0.01 mol) in 25 ml me thanol. The solution was stirred overnight and filtered. The product obtained was crystallized from acetone/toluene (1:1) mixture (m.p.: 419–421 K). Analysis for $C_{24}H_{17}NO$: Found (Calculated): C 85.83 (85.94), H 5.07(5.11), N 4.12% (4.18%).

Refinement

The H atoms were included in the riding model approximation with C—H = 0.94 Å, and with U_{iso}(H) = 1.18–1.49U_{eq}(C). The maximum residual electron density peaks of 0.28 and −0.30 e Å^3, were located at 0.74 and 0.53Å from the C16 and C11 atoms, respectively.

Figures

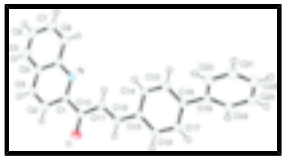

Fig. 1. Molecular structure of the title compound (I), showing atom labeling and 50% probability displacement ellipsoids.

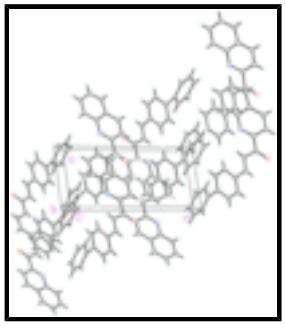

Fig. 2. Packing diagram of (I) viewed down the *b* axis. Dashed lines indicate C–H···O hydrogen bonds.

(2E)-3-(Biphenyl-4-yl)-1-(quinolin-2-yl)prop-2-en-1-one

Crystal data

$C_{24}H_{17}NO$	$Z = 2$
$M_r = 335.39$	$F_{000} = 352$
Triclinic, $P\overline{1}$	$D_x = 1.293$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.9808$ (12) Å	Cell parameters from 5911 reflections
$b = 11.9617$ (18) Å	$\theta = 4.6$–32.4°
$c = 13.2239$ (16) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 109.401$ (12)°	$T = 203$ K
$\beta = 92.981$ (13)°	Plate, colourless
$\gamma = 102.967$ (15)°	0.57 × 0.43 × 0.19 mm
$V = 861.3$ (3) Å^3	

Data collection

Oxford Diffraction Gemini R diffractometer	5643 independent reflections
Radiation source: fine-focus sealed tube	3561 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 203$ K	$\theta_{max} = 32.5^\circ$
φ and ω scans	$\theta_{min} = 4.6^\circ$
Absorption correction: multi-scan (DENZO/SCALEPACK; Otwinowski & Minor, 1997)	$h = -8 \rightarrow 7$
$T_{min} = 0.922$, $T_{max} = 1.000$	$k = -17 \rightarrow 17$
12993 measured reflections	$l = -19 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0888P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
5643 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.30$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O	−0.19597 (14)	0.61552 (7)	0.49028 (7)	0.0421 (2)
N	0.24910 (15)	0.59911 (7)	0.32703 (7)	0.0276 (2)
C1	0.14418 (18)	0.64559 (9)	0.41063 (8)	0.0258 (2)
C2	0.2344 (2)	0.76334 (9)	0.49132 (9)	0.0325 (2)
H2A	0.1537	0.7920	0.5497	0.039*
C3	0.4399 (2)	0.83407 (10)	0.48259 (9)	0.0353 (3)
H3A	0.5034	0.9119	0.5357	0.042*
C4	0.55752 (19)	0.79045 (9)	0.39372 (9)	0.0315 (2)
C5	0.7716 (2)	0.85790 (11)	0.37748 (11)	0.0417 (3)
H5A	0.8394	0.9377	0.4265	0.050*
C6	0.8798 (2)	0.80849 (12)	0.29189 (11)	0.0440 (3)
H6A	1.0218	0.8543	0.2825	0.053*
C7	0.7806 (2)	0.68917 (11)	0.21717 (10)	0.0399 (3)
H7A	0.8573	0.6558	0.1586	0.048*
C8	0.5735 (2)	0.62167 (11)	0.22940 (9)	0.0345 (3)
H8A	0.5086	0.5424	0.1789	0.041*
C9	0.45601 (18)	0.67022 (9)	0.31745 (8)	0.0279 (2)
C10	−0.08621 (19)	0.56987 (9)	0.41909 (8)	0.0279 (2)
C11	−0.17124 (19)	0.44328 (9)	0.34193 (8)	0.0283 (2)
H11A	−0.0762	0.4093	0.2923	0.034*
C12	−0.38345 (18)	0.37616 (9)	0.34197 (8)	0.0272 (2)
H12A	−0.4748	0.4151	0.3908	0.033*
C13	−0.48699 (17)	0.24784 (9)	0.27318 (8)	0.0245 (2)
C14	−0.36185 (18)	0.17609 (9)	0.20453 (9)	0.0305 (2)
H14A	−0.2070	0.2110	0.2001	0.037*
C15	−0.46337 (18)	0.05480 (9)	0.14335 (9)	0.0307 (2)
H15A	−0.3751	0.0082	0.0987	0.037*
C16	−0.69470 (17)	−0.00094 (8)	0.14600 (8)	0.0248 (2)
C17	−0.82021 (18)	0.07111 (9)	0.21369 (8)	0.0276 (2)
H17A	−0.9764	0.0368	0.2165	0.033*
C18	−0.71725 (18)	0.19243 (9)	0.27675 (8)	0.0288 (2)
H18A	−0.8041	0.2385	0.3229	0.035*
C19	−0.79925 (18)	−0.13074 (9)	0.07668 (8)	0.0258 (2)

C20	−0.6782 (2)	−0.22039 (9)	0.06761 (9)	0.0330 (2)
H20A	−0.5313	−0.1987	0.1082	0.040*
C21	−0.7720 (2)	−0.34030 (10)	−0.00032 (10)	0.0381 (3)
H21A	−0.6892	−0.3995	−0.0047	0.046*
C22	−0.9867 (2)	−0.37409 (10)	−0.06192 (9)	0.0368 (3)
H22A	−1.0477	−0.4553	−0.1095	0.044*
C23	−1.1119 (2)	−0.28698 (10)	−0.05302 (9)	0.0344 (2)
H23A	−1.2593	−0.3095	−0.0933	0.041*
C24	−1.01799 (19)	−0.16680 (9)	0.01560 (9)	0.0304 (2)
H24A	−1.1032	−0.1083	0.0212	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.0385 (5)	0.0370 (4)	0.0374 (5)	0.0026 (4)	0.0143 (4)	−0.0006 (4)
N	0.0268 (5)	0.0251 (4)	0.0284 (4)	0.0029 (4)	0.0031 (3)	0.0090 (3)
C1	0.0279 (5)	0.0221 (5)	0.0249 (5)	0.0036 (4)	0.0000 (4)	0.0077 (4)
C2	0.0395 (6)	0.0263 (5)	0.0265 (5)	0.0051 (5)	0.0028 (4)	0.0050 (4)
C3	0.0388 (6)	0.0238 (5)	0.0345 (6)	−0.0006 (5)	−0.0040 (5)	0.0059 (4)
C4	0.0299 (6)	0.0278 (5)	0.0349 (6)	0.0022 (4)	−0.0028 (4)	0.0132 (4)
C5	0.0358 (7)	0.0335 (6)	0.0503 (7)	−0.0036 (5)	−0.0038 (5)	0.0172 (5)
C6	0.0304 (6)	0.0491 (7)	0.0580 (8)	0.0000 (5)	0.0037 (6)	0.0328 (6)
C7	0.0344 (6)	0.0506 (7)	0.0440 (7)	0.0121 (5)	0.0113 (5)	0.0269 (6)
C8	0.0342 (6)	0.0367 (6)	0.0339 (6)	0.0085 (5)	0.0056 (5)	0.0143 (5)
C9	0.0265 (5)	0.0272 (5)	0.0302 (5)	0.0030 (4)	0.0008 (4)	0.0134 (4)
C10	0.0294 (5)	0.0258 (5)	0.0259 (5)	0.0042 (4)	0.0039 (4)	0.0074 (4)
C11	0.0309 (6)	0.0249 (5)	0.0259 (5)	0.0049 (4)	0.0064 (4)	0.0060 (4)
C12	0.0286 (5)	0.0256 (5)	0.0246 (5)	0.0056 (4)	0.0050 (4)	0.0061 (4)
C13	0.0238 (5)	0.0241 (4)	0.0251 (5)	0.0057 (4)	0.0039 (4)	0.0081 (4)
C14	0.0223 (5)	0.0297 (5)	0.0345 (6)	0.0037 (4)	0.0070 (4)	0.0062 (4)
C15	0.0253 (5)	0.0281 (5)	0.0349 (5)	0.0080 (4)	0.0102 (4)	0.0048 (4)
C16	0.0247 (5)	0.0221 (4)	0.0266 (5)	0.0047 (4)	0.0048 (4)	0.0082 (4)
C17	0.0222 (5)	0.0262 (5)	0.0311 (5)	0.0040 (4)	0.0069 (4)	0.0069 (4)
C18	0.0261 (5)	0.0278 (5)	0.0300 (5)	0.0085 (4)	0.0085 (4)	0.0051 (4)
C19	0.0251 (5)	0.0240 (5)	0.0270 (5)	0.0046 (4)	0.0063 (4)	0.0079 (4)
C20	0.0295 (6)	0.0280 (5)	0.0402 (6)	0.0076 (4)	0.0029 (5)	0.0104 (5)
C21	0.0422 (7)	0.0265 (5)	0.0442 (7)	0.0107 (5)	0.0092 (5)	0.0088 (5)
C22	0.0457 (7)	0.0244 (5)	0.0325 (6)	0.0013 (5)	0.0065 (5)	0.0049 (4)
C23	0.0317 (6)	0.0328 (5)	0.0321 (6)	−0.0004 (5)	0.0012 (4)	0.0093 (4)
C24	0.0293 (6)	0.0285 (5)	0.0328 (5)	0.0073 (4)	0.0052 (4)	0.0100 (4)

Geometric parameters (Å, °)

O—C10	1.2243 (13)	C12—H12A	0.9400
N—C1	1.3211 (13)	C13—C18	1.3985 (14)
N—C9	1.3735 (13)	C13—C14	1.4008 (14)
C1—C2	1.4192 (14)	C14—C15	1.3791 (15)
C1—C10	1.5016 (15)	C14—H14A	0.9400
C2—C3	1.3612 (16)	C15—C16	1.4024 (14)

C2—H2A	0.9400	C15—H15A	0.9400
C3—C4	1.4113 (17)	C16—C17	1.3983 (14)
C3—H3A	0.9400	C16—C19	1.4836 (14)
C4—C5	1.4200 (16)	C17—C18	1.3865 (14)
C4—C9	1.4265 (15)	C17—H17A	0.9400
C5—C6	1.3613 (19)	C18—H18A	0.9400
C5—H5A	0.9400	C19—C24	1.3983 (15)
C6—C7	1.4098 (18)	C19—C20	1.4003 (14)
C6—H6A	0.9400	C20—C21	1.3819 (15)
C7—C8	1.3676 (16)	C20—H20A	0.9400
C7—H7A	0.9400	C21—C22	1.3842 (17)
C8—C9	1.4165 (15)	C21—H21A	0.9400
C8—H8A	0.9400	C22—C23	1.3918 (17)
C10—C11	1.4719 (14)	C22—H22A	0.9400
C11—C12	1.3410 (14)	C23—C24	1.3869 (15)
C11—H11A	0.9400	C23—H23A	0.9400
C12—C13	1.4677 (14)	C24—H24A	0.9400
C1—N—C9	117.67 (9)	C18—C13—C14	117.74 (9)
N—C1—C2	123.87 (10)	C18—C13—C12	119.83 (9)
N—C1—C10	117.76 (9)	C14—C13—C12	122.41 (9)
C2—C1—C10	118.36 (9)	C15—C14—C13	120.71 (10)
C3—C2—C1	118.77 (10)	C15—C14—H14A	119.6
C3—C2—H2A	120.6	C13—C14—H14A	119.6
C1—C2—H2A	120.6	C14—C15—C16	121.78 (9)
C2—C3—C4	119.95 (10)	C14—C15—H15A	119.1
C2—C3—H3A	120.0	C16—C15—H15A	119.1
C4—C3—H3A	120.0	C17—C16—C15	117.47 (9)
C3—C4—C5	123.93 (10)	C17—C16—C19	122.43 (9)
C3—C4—C9	117.45 (10)	C15—C16—C19	120.08 (9)
C5—C4—C9	118.61 (11)	C18—C17—C16	120.84 (9)
C6—C5—C4	120.86 (11)	C18—C17—H17A	119.6
C6—C5—H5A	119.6	C16—C17—H17A	119.6
C4—C5—H5A	119.6	C17—C18—C13	121.44 (9)
C5—C6—C7	120.50 (11)	C17—C18—H18A	119.3
C5—C6—H6A	119.8	C13—C18—H18A	119.3
C7—C6—H6A	119.8	C24—C19—C20	117.87 (9)
C8—C7—C6	120.43 (11)	C24—C19—C16	121.22 (9)
C8—C7—H7A	119.8	C20—C19—C16	120.88 (9)
C6—C7—H7A	119.8	C21—C20—C19	120.80 (10)
C7—C8—C9	120.60 (11)	C21—C20—H20A	119.6
C7—C8—H8A	119.7	C19—C20—H20A	119.6
C9—C8—H8A	119.7	C20—C21—C22	120.66 (10)
N—C9—C8	118.72 (10)	C20—C21—H21A	119.7
N—C9—C4	122.27 (10)	C22—C21—H21A	119.7
C8—C9—C4	119.01 (10)	C21—C22—C23	119.56 (10)
O—C10—C11	122.40 (10)	C21—C22—H22A	120.2
O—C10—C1	118.77 (9)	C23—C22—H22A	120.2
C11—C10—C1	118.83 (9)	C24—C23—C22	119.70 (11)
C12—C11—C10	120.39 (9)	C24—C23—H23A	120.2

C12—C11—H11A	119.8	C22—C23—H23A	120.2
C10—C11—H11A	119.8	C23—C24—C19	121.39 (10)
C11—C12—C13	126.36 (9)	C23—C24—H24A	119.3
C11—C12—H12A	116.8	C19—C24—H24A	119.3
C13—C12—H12A	116.8		
C9—N—C1—C2	−0.94 (15)	C10—C11—C12—C13	−177.31 (9)
C9—N—C1—C10	177.83 (8)	C11—C12—C13—C18	−175.30 (10)
N—C1—C2—C3	0.65 (16)	C11—C12—C13—C14	6.16 (16)
C10—C1—C2—C3	−178.11 (9)	C18—C13—C14—C15	−0.39 (15)
C1—C2—C3—C4	0.80 (16)	C12—C13—C14—C15	178.18 (10)
C2—C3—C4—C5	179.59 (10)	C13—C14—C15—C16	0.90 (16)
C2—C3—C4—C9	−1.80 (15)	C14—C15—C16—C17	−0.21 (15)
C3—C4—C5—C6	177.65 (11)	C14—C15—C16—C19	178.34 (9)
C9—C4—C5—C6	−0.95 (16)	C15—C16—C17—C18	−0.98 (14)
C4—C5—C6—C7	0.30 (18)	C19—C16—C17—C18	−179.49 (9)
C5—C6—C7—C8	0.33 (17)	C16—C17—C18—C13	1.51 (16)
C6—C7—C8—C9	−0.28 (16)	C14—C13—C18—C17	−0.80 (15)
C1—N—C9—C8	179.06 (9)	C12—C13—C18—C17	−179.40 (9)
C1—N—C9—C4	−0.18 (14)	C17—C16—C19—C24	44.88 (14)
C7—C8—C9—N	−179.65 (9)	C15—C16—C19—C24	−133.59 (10)
C7—C8—C9—C4	−0.38 (15)	C17—C16—C19—C20	−137.29 (11)
C3—C4—C9—N	1.53 (15)	C15—C16—C19—C20	44.24 (14)
C5—C4—C9—N	−179.78 (9)	C24—C19—C20—C21	0.50 (15)
C3—C4—C9—C8	−177.71 (9)	C16—C19—C20—C21	−177.40 (10)
C5—C4—C9—C8	0.98 (15)	C19—C20—C21—C22	0.79 (17)
N—C1—C10—O	−173.47 (9)	C20—C21—C22—C23	−1.76 (18)
C2—C1—C10—O	5.37 (15)	C21—C22—C23—C24	1.41 (17)
N—C1—C10—C11	6.87 (14)	C22—C23—C24—C19	−0.11 (16)
C2—C1—C10—C11	−174.29 (9)	C20—C19—C24—C23	−0.84 (15)
O—C10—C11—C12	5.32 (16)	C16—C19—C24—C23	177.06 (9)
C1—C10—C11—C12	−175.04 (9)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18A···O^{i}	0.94	2.51	3.3222 (13)	145

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

Fig. 1

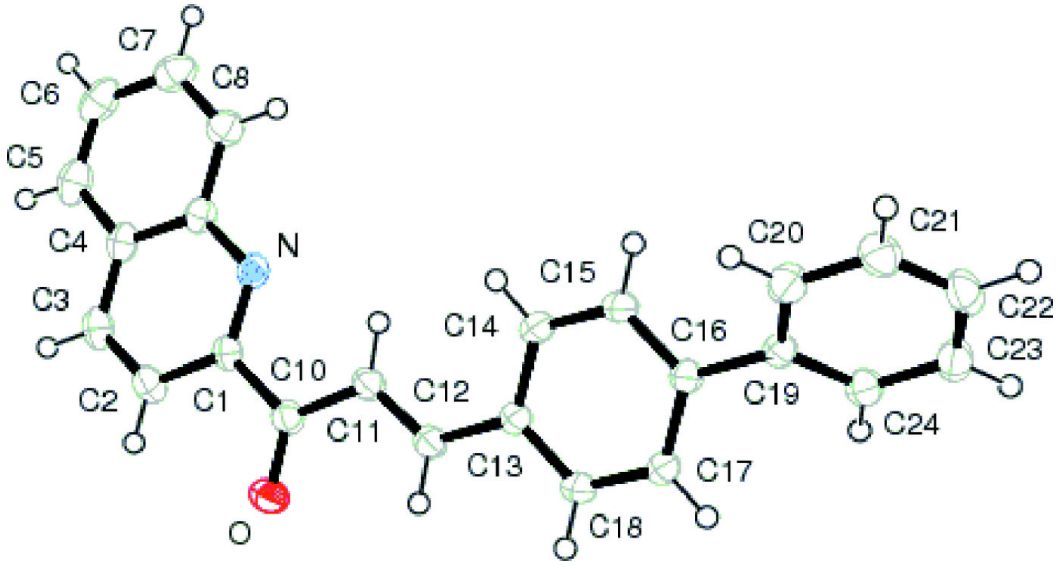
C7
C8
C6
C5
C4
N
C3
C2
C1
C10
C11
C12
C13
C14
C15
C16
C17
C18
C19
C20
C21
C22
C23
C24
O

Fig. 2