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(2*E*)-1-{4-[(1*E*)-Benzylideneamino]-phenyl}-3-phenylprop-2-en-1-one

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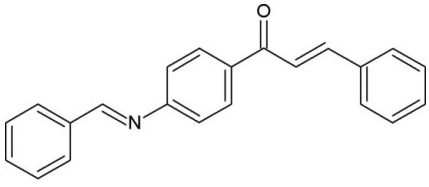
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.100; data-to-parameter ratio = 14.8.

In the title compound, $C_{22}H_{17}NO$, the dihedral angles between the central benzene ring and the two terminal phenyl rings are 48.20 (4) and 49.62 (4)°, resulting in a substantially twisted molecular conformation. Weak C—H···π interactions help to consolidate the centrosymmetric crystal packing.

Related literature

For background, see: Harrison *et al.* (2007).



Experimental

Crystal data

$C_{22}H_{17}NO$
M_r = 311.37
Monoclinic, $P2_1/c$
a = 16.8172 (15) Å
b = 5.9146 (4) Å
c = 16.6777 (15) Å
β = 93.501 (1)°
V = 1655.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.49 × 0.43 × 0.31 mm

Data collection

Bruker SMART1000 CCD diffractometer
Absorption correction: none
8346 measured reflections
3232 independent reflections
2371 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
S = 1.02
3232 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···$Cg3^{i}$	0.93	2.89	3.603 (3)	135
C12—H12···$Cg1^{ii}$	0.93	2.94	3.626 (2)	132
C15—H15···$Cg2^{iii}$	0.93	2.89	3.559 (2)	130

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y, -z+1$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ is the centroid of atoms C1–C6, $Cg2$ is the centroid of atoms C10–C15 and $Cg3$ is the centroid of atoms C17–C22.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2557).

References

Bruker (1999). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harrison, W. T. A., Kumari, V., Ravindra, H. J. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o2928.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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(2*E*)-1-{4-[(1*E*)-Benzylideneamino]phenyl}-3-phenylprop-2-en-1-one

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Comment

As part of our ongoing studies of organic nonlinear optical materials derived from substituted chalcones (Harrison *et al.*, 2007), we now report the synthesis and structure of the title compound, (I), (Fig. 1). It is centrosymmetric, therefore it does not display any second harmonic generation response.

The dihedral angle between the central (C10—C15) and terminal (C1—C6 and C17—C22) aromatic rings are 49.62 (4)° and 48.20 (4)°, respectively. The dihedral angles for the enone (C7/C8/C9/O1) fragment with respect to C1—C6 and C10—C15 are 25.47 (9)° and 24.37 (8)°, respectively. Overall, the molecule of (I) is substantially twisted.

The only possible directional interactions in (I) are weak C—H···π links (Table 1), with each of the three benzene rings accepting one such bond (Fig. 2).

Experimental

A solution of 10% aqueous NaOH (10 ml) and 30 ml me thanol was taken in a conical flask. Benzaldehyde (0.02 mol) and *p*-amino acetophenone (0.01 mol) were dissolved in 30 ml me thanol and the mixture was added to the conical flask with vigorous stirring. After stirring the solution for 90 minutes, the content were poured into a beaker containing ice cold water and allowed stand for overnight. The resulting precipitate was washed with excess of water, filtered and dried. The compound was purified by successive recrystallization from acetone. Yellow chunks of (I) were obtained by slow evaporation of an acetone solution.

Refinement

The hydrogen atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

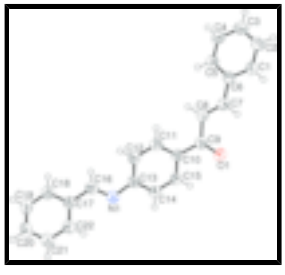


Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (H atoms are drawn as spheres of arbitrary radius).

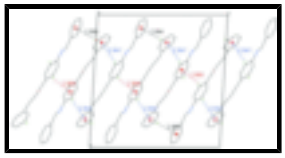


Fig. 2. Unit cell packing for (I) with hydrogen atoms not involved in C—H···π links omitted for clarity

(2E)-1-{4-[(1E)-Benzylideneamino]phenyl}-3-phenylprop-2-en-1-one

Crystal data

$C_{22}H_{17}NO$	F_{000} = 656
M_r = 311.37	D_x = 1.249 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6120 reflections
a = 16.8172 (15) Å	θ = 4.4–26.0º
b = 5.9146 (4) Å	μ = 0.08 mm^{-1}
c = 16.6777 (15) Å	T = 291 (2) K
β = 93.501 (1)º	Chunk, yellow
V = 1655.8 (2) Å^3	0.49 × 0.43 × 0.31 mm
Z = 4	

Data collection

Bruker SMART1000 CCD diffractometer	2371 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.037
Monochromator: graphite	θ_{max} = 26.0º
T = 291(2) K	θ_{min} = 4.4º
ω scans	h = −20→18
Absorption correction: none	k = −7→4
8346 measured reflections	l = −20→20
3232 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.1191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.100	$(\Delta/\sigma)_{max} < 0.001$
S = 1.02	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
3232 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
218 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0044 (9)

Secondary atom site location: difference Fourier map

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}
C1	0.22678 (8)	0.2767 (2)	0.58028 (8)	0.0475 (3)
H1	0.2367	0.4183	0.6030	0.057*
C2	0.16855 (8)	0.1416 (3)	0.60961 (9)	0.0571 (4)
H2	0.1404	0.1906	0.6527	0.068*
C3	0.15194 (9)	−0.0658 (3)	0.57527 (10)	0.0635 (4)
H3	0.1123	−0.1565	0.5948	0.076*
C4	0.19421 (9)	−0.1390 (2)	0.51180 (10)	0.0586 (4)
H4	0.1825	−0.2786	0.4882	0.070*
C5	0.25364 (8)	−0.0068 (2)	0.48311 (8)	0.0494 (3)
H5	0.2823	−0.0587	0.4408	0.059*
C6	0.27113 (7)	0.2047 (2)	0.51708 (7)	0.0424 (3)
C7	0.33125 (8)	0.3563 (2)	0.48715 (8)	0.0464 (3)
H7	0.3290	0.5054	0.5046	0.056*
C8	0.38872 (8)	0.3101 (2)	0.43830 (8)	0.0466 (3)
H8	0.3969	0.1616	0.4224	0.056*
C9	0.43976 (8)	0.4922 (2)	0.40893 (8)	0.0462 (3)
C10	0.51183 (7)	0.4348 (2)	0.36626 (7)	0.0411 (3)
C11	0.55233 (8)	0.2297 (2)	0.37675 (8)	0.0450 (3)
H11	0.5319	0.1180	0.4089	0.054*
C12	0.62236 (8)	0.1911 (2)	0.33977 (8)	0.0459 (3)
H12	0.6493	0.0549	0.3481	0.055*
C13	0.65306 (7)	0.3551 (2)	0.28991 (8)	0.0426 (3)
C14	0.61208 (8)	0.5581 (2)	0.27870 (8)	0.0471 (3)
H14	0.6318	0.6685	0.2455	0.057*
C15	0.54268 (8)	0.5977 (2)	0.31622 (8)	0.0443 (3)
H15	0.5161	0.7345	0.3081	0.053*
C16	0.74793 (8)	0.1473 (2)	0.22590 (8)	0.0475 (3)
H16	0.7121	0.0275	0.2251	0.057*
C17	0.82613 (8)	0.1113 (2)	0.19330 (8)	0.0458 (3)
C18	0.84178 (9)	−0.0890 (2)	0.15418 (9)	0.0555 (4)
H18	0.8034	−0.2024	0.1509	0.067*
C19	0.91353 (10)	−0.1226 (3)	0.12000 (10)	0.0685 (5)

H19	0.9230	−0.2566	0.0930	0.082*
C20	0.97104 (10)	0.0432 (3)	0.12605 (11)	0.0746 (5)
H20	1.0193	0.0222	0.1026	0.090*
C21	0.95689 (10)	0.2413 (3)	0.16705 (12)	0.0755 (5)
H21	0.9962	0.3517	0.1722	0.091*
C22	0.88512 (9)	0.2756 (3)	0.20010 (10)	0.0602 (4)
H22	0.8759	0.4096	0.2272	0.072*
N1	0.72731 (6)	0.33426 (19)	0.25502 (7)	0.0490 (3)
O1	0.42194 (6)	0.69165 (17)	0.41848 (7)	0.0684 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0461 (7)	0.0471 (8)	0.0494 (8)	0.0043 (6)	0.0043 (6)	−0.0034 (6)
C2	0.0505 (8)	0.0672 (10)	0.0551 (9)	0.0042 (7)	0.0156 (7)	0.0037 (7)
C3	0.0541 (9)	0.0618 (10)	0.0758 (11)	−0.0096 (8)	0.0123 (8)	0.0118 (9)
C4	0.0620 (9)	0.0446 (8)	0.0690 (10)	−0.0073 (7)	0.0034 (8)	0.0008 (7)
C5	0.0527 (8)	0.0459 (8)	0.0500 (8)	0.0028 (7)	0.0076 (6)	−0.0016 (6)
C6	0.0392 (7)	0.0424 (7)	0.0454 (7)	0.0028 (6)	0.0017 (6)	0.0031 (6)
C7	0.0466 (7)	0.0427 (7)	0.0502 (8)	0.0010 (6)	0.0046 (6)	−0.0017 (6)
C8	0.0466 (7)	0.0427 (7)	0.0513 (8)	0.0013 (6)	0.0089 (6)	−0.0018 (6)
C9	0.0465 (7)	0.0449 (8)	0.0474 (8)	0.0008 (6)	0.0050 (6)	−0.0024 (6)
C10	0.0414 (7)	0.0408 (7)	0.0410 (7)	−0.0032 (6)	0.0023 (5)	−0.0020 (6)
C11	0.0487 (8)	0.0405 (7)	0.0462 (7)	−0.0020 (6)	0.0065 (6)	0.0047 (6)
C12	0.0462 (7)	0.0406 (7)	0.0509 (8)	0.0031 (6)	0.0030 (6)	0.0039 (6)
C13	0.0370 (7)	0.0443 (7)	0.0465 (7)	−0.0050 (6)	0.0023 (5)	−0.0031 (6)
C14	0.0487 (8)	0.0410 (7)	0.0521 (8)	−0.0051 (6)	0.0072 (6)	0.0055 (6)
C15	0.0455 (7)	0.0374 (7)	0.0501 (7)	0.0006 (6)	0.0030 (6)	0.0017 (6)
C16	0.0442 (7)	0.0487 (8)	0.0497 (8)	−0.0066 (6)	0.0035 (6)	0.0001 (6)
C17	0.0447 (7)	0.0463 (8)	0.0464 (7)	0.0011 (6)	0.0040 (6)	0.0027 (6)
C18	0.0571 (9)	0.0499 (8)	0.0594 (9)	0.0000 (7)	0.0031 (7)	−0.0041 (7)
C19	0.0715 (11)	0.0599 (10)	0.0750 (11)	0.0164 (9)	0.0113 (9)	−0.0103 (8)
C20	0.0528 (9)	0.0749 (12)	0.0985 (13)	0.0134 (9)	0.0239 (9)	0.0007 (10)
C21	0.0494 (9)	0.0637 (10)	0.1154 (15)	−0.0027 (8)	0.0208 (9)	−0.0049 (10)
C22	0.0500 (8)	0.0501 (8)	0.0815 (11)	−0.0006 (7)	0.0126 (7)	−0.0076 (8)
N1	0.0421 (6)	0.0480 (7)	0.0576 (7)	−0.0015 (5)	0.0081 (5)	−0.0009 (6)
O1	0.0734 (7)	0.0434 (6)	0.0920 (8)	0.0057 (5)	0.0340 (6)	−0.0004 (5)

Geometric parameters (Å, °)

C1—C2	1.3764 (19)	C12—C13	1.3969 (18)
C1—C6	1.3945 (18)	C12—H12	0.9300
C1—H1	0.9300	C13—C14	1.3917 (18)
C2—C3	1.375 (2)	C13—N1	1.4148 (16)
C2—H2	0.9300	C14—C15	1.3776 (18)
C3—C4	1.380 (2)	C14—H14	0.9300
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.3774 (19)	C16—N1	1.2648 (17)
C4—H4	0.9300	C16—C17	1.4688 (18)

C5—C6	1.3974 (19)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.3859 (19)
C6—C7	1.4618 (18)	C17—C22	1.3881 (19)
C7—C8	1.3299 (18)	C18—C19	1.380 (2)
C7—H7	0.9300	C18—H18	0.9300
C8—C9	1.4794 (18)	C19—C20	1.377 (2)
C8—H8	0.9300	C19—H19	0.9300
C9—O1	1.2296 (16)	C20—C21	1.385 (2)
C9—C10	1.4820 (18)	C20—H20	0.9300
C10—C15	1.3952 (17)	C21—C22	1.372 (2)
C10—C11	1.3972 (17)	C21—H21	0.9300
C11—C12	1.3813 (18)	C22—H22	0.9300
C11—H11	0.9300		
C2—C1—C6	121.10 (13)	C11—C12—H12	119.8
C2—C1—H1	119.4	C13—C12—H12	119.8
C6—C1—H1	119.4	C14—C13—C12	118.76 (12)
C3—C2—C1	120.03 (14)	C14—C13—N1	117.53 (12)
C3—C2—H2	120.0	C12—C13—N1	123.50 (12)
C1—C2—H2	120.0	C15—C14—C13	120.79 (12)
C2—C3—C4	119.88 (14)	C15—C14—H14	119.6
C2—C3—H3	120.1	C13—C14—H14	119.6
C4—C3—H3	120.1	C14—C15—C10	120.71 (12)
C5—C4—C3	120.45 (14)	C14—C15—H15	119.6
C5—C4—H4	119.8	C10—C15—H15	119.6
C3—C4—H4	119.8	N1—C16—C17	122.78 (12)
C4—C5—C6	120.44 (13)	N1—C16—H16	118.6
C4—C5—H5	119.8	C17—C16—H16	118.6
C6—C5—H5	119.8	C18—C17—C22	118.79 (13)
C1—C6—C5	118.07 (12)	C18—C17—C16	119.88 (13)
C1—C6—C7	118.95 (12)	C22—C17—C16	121.33 (13)
C5—C6—C7	122.93 (12)	C19—C18—C17	120.89 (14)
C8—C7—C6	128.81 (13)	C19—C18—H18	119.6
C8—C7—H7	115.6	C17—C18—H18	119.6
C6—C7—H7	115.6	C20—C19—C18	119.70 (15)
C7—C8—C9	120.74 (12)	C20—C19—H19	120.1
C7—C8—H8	119.6	C18—C19—H19	120.1
C9—C8—H8	119.6	C19—C20—C21	119.85 (15)
O1—C9—C8	120.31 (12)	C19—C20—H20	120.1
O1—C9—C10	119.66 (12)	C21—C20—H20	120.1
C8—C9—C10	120.02 (11)	C22—C21—C20	120.35 (16)
C15—C10—C11	118.57 (12)	C22—C21—H21	119.8
C15—C10—C9	118.29 (12)	C20—C21—H21	119.8
C11—C10—C9	123.07 (12)	C21—C22—C17	120.38 (15)
C12—C11—C10	120.66 (12)	C21—C22—H22	119.8
C12—C11—H11	119.7	C17—C22—H22	119.8
C10—C11—H11	119.7	C16—N1—C13	120.24 (12)
C11—C12—C13	120.48 (12)		
C6—C1—C2—C3	−1.6 (2)	C11—C12—C13—C14	0.41 (18)

C1—C2—C3—C4	0.5 (2)	C11—C12—C13—N1	175.06 (12)
C2—C3—C4—C5	0.7 (2)	C12—C13—C14—C15	0.27 (19)
C3—C4—C5—C6	−1.0 (2)	N1—C13—C14—C15	−174.70 (11)
C2—C1—C6—C5	1.35 (19)	C13—C14—C15—C10	−0.09 (19)
C2—C1—C6—C7	178.86 (12)	C11—C10—C15—C14	−0.75 (18)
C4—C5—C6—C1	−0.06 (19)	C9—C10—C15—C14	176.29 (11)
C4—C5—C6—C7	−177.47 (12)	N1—C16—C17—C18	−172.78 (13)
C1—C6—C7—C8	167.12 (13)	N1—C16—C17—C22	6.6 (2)
C5—C6—C7—C8	−15.5 (2)	C22—C17—C18—C19	−2.3 (2)
C6—C7—C8—C9	174.54 (12)	C16—C17—C18—C19	177.14 (13)
C7—C8—C9—O1	−11.7 (2)	C17—C18—C19—C20	1.2 (2)
C7—C8—C9—C10	169.53 (12)	C18—C19—C20—C21	0.7 (3)
O1—C9—C10—C15	−20.47 (18)	C19—C20—C21—C22	−1.5 (3)
C8—C9—C10—C15	158.27 (12)	C20—C21—C22—C17	0.5 (3)
O1—C9—C10—C11	156.43 (13)	C18—C17—C22—C21	1.4 (2)
C8—C9—C10—C11	−24.84 (18)	C16—C17—C22—C21	−177.99 (14)
C15—C10—C11—C12	1.43 (18)	C17—C16—N1—C13	−176.22 (11)
C9—C10—C11—C12	−175.46 (11)	C14—C13—N1—C16	−143.44 (13)
C10—C11—C12—C13	−1.27 (19)	C12—C13—N1—C16	41.85 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···Cg3^{i}	0.93	2.89	3.603 (3)	135
C12—H12···Cg1^{ii}	0.93	2.94	3.626 (2)	132
C15—H15···Cg2^{iii}	0.93	2.89	3.559 (2)	130

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

Fig. 1

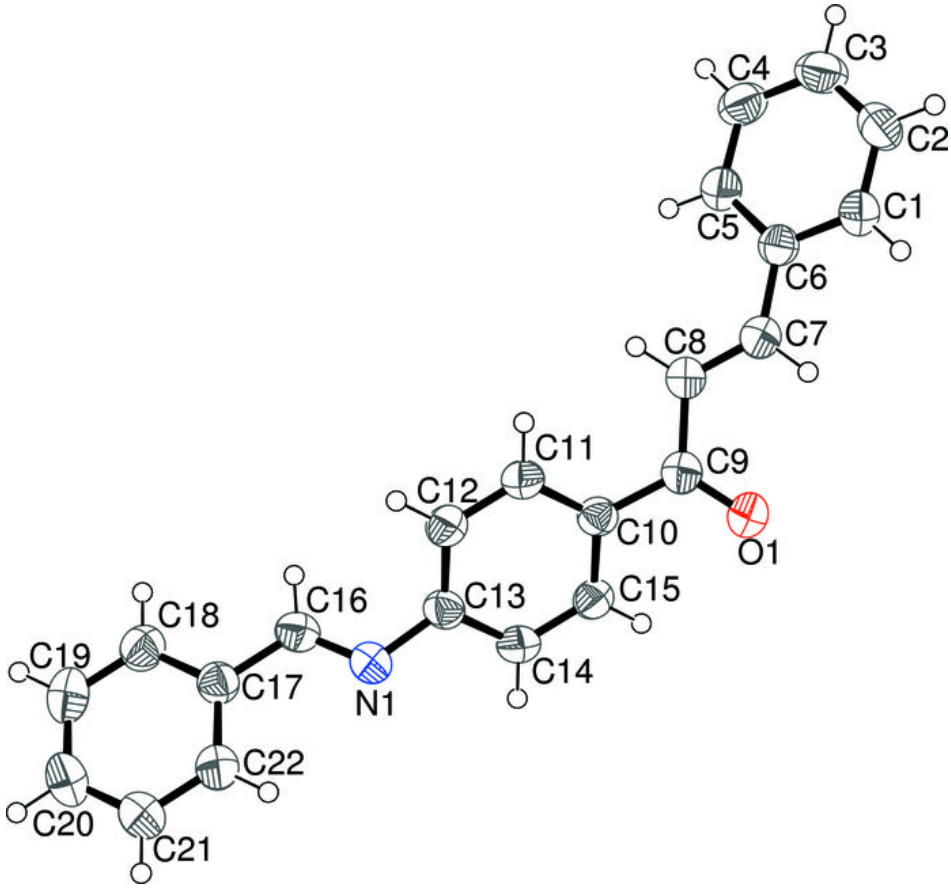
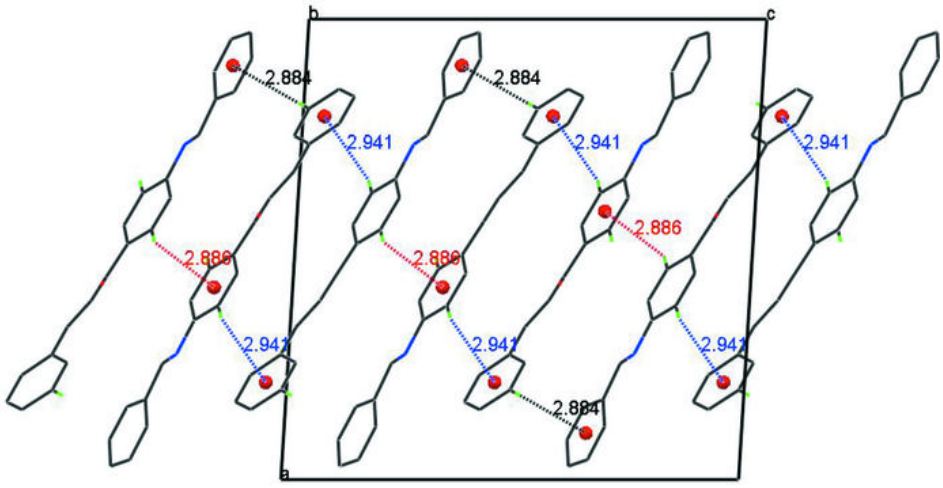

C3
C4
C2
C1
C5
C6
C7
C8
C9
C11
C12
C10
O1
C15
C13
C16
C18
C19
C17
N1
C14
C22
C20
C21

Fig. 2


b
c
a
2.884
2.884
2.941
2.941
2.941
2.886
2.886
2.886
2.941
2.941
2.941
2.884