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(2E)-1-(2,4-Dichlorophenyl)-3-(quinolin-8-yl)prop-2-en-1-one

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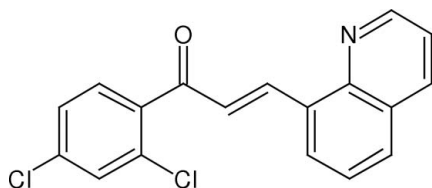
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.057; wR factor = 0.154; data-to-parameter ratio = 14.0.

The geometric parameters of the molecule of the title compound, $\text{C}_{18}\text{H}_{11}\text{Cl}_2\text{NO}$, a chalcone derivative, are in the usual ranges. The central $\text{C}=\text{C}$ double bond is *trans* configured. The dihedral angle between the two aromatic residues is 41.90 (8)°.

Related literature

For related structures, see: Yathirajan, Sarojini, Bindya *et al.* (2006); Yathirajan, Narayana *et al.* (2006); Yathirajan, Sarojini, Narayana *et al.* (2006); Yathirajan, Mayekar, Sarojini *et al.* (2007); Yathirajan, Mayekar, Narayana *et al.* (2007); Bouraiou *et al.* (2007). For related background, see: Dhar (1981); Dimmock *et al.* (1999); Fichou *et al.* (1988); Go *et al.* (2005); Goto *et al.* (1991).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{11}\text{Cl}_2\text{NO}$
 $M_r = 328.18$

Monoclinic, $P2_1/c$
 $a = 11.9121$ (16) Å

$b = 10.7112$ (10) Å
 $c = 12.7824$ (15) Å
 $\beta = 113.181$ (9)°
 $V = 1499.3$ (3) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.43$ mm⁻¹
 $T = 173$ (2) K
 $0.35 \times 0.35 \times 0.33$ mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan [MULABS (Spek, 2003; Blessing, 1995)]
 $T_{\min} = 0.863$, $T_{\max} = 0.870$

12134 measured reflections
2808 independent reflections
2328 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.062$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.154$
 $S = 1.03$
2808 reflections

200 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.50$ e Å⁻³

Data collection: X-Area (Stoe & Cie, 2001); cell refinement: X-Area; data reduction: X-Area; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

ANM thanks the University of Mysore for permission to carry out this research work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2452).

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supplementary materials

Acta Cryst. (2007). E63, o3488 [doi:10.1107/S1600536807032746]

(2E)-1-(2,4-Dichlorophenyl)-3-(quinolin-8-yl)prop-2-en-1-one

B. K. Sarojini, H. S. Yathirajan, A. N. Mayekar, B. Narayana and M. Bolte

Comment

Chalcones are one of the major classes of natural products have been recently subjects of great interest for their interesting pharmacological activities. Reviews on the bioactivities of varieties of chalcones are described. Recently, it has been noted that, among many organic compounds reported for their second harmonic generation, chalcone derivatives are known for their excellent blue light transmittance and good crystallizability. In continuation of our work on chalcones, the present paper reports the crystal structure of a newly synthesized chalcone. Geometric parameters of the title compound are in the usual ranges. The central C=C double bond is *trans* configured. The dihedral angle between the two aromatic residues is 41.90 (8)°. The C=C double bond is almost coplanar with the quinolyl residue [C2—C3—C21—C22 10.7 (4)°], but the two atoms of the carbonyl moiety are significantly twisted out of the plane of the dichlorophenyl substituent [O1—C1—C11—C12 – 53.3 (3)°]

Experimental

To a thoroughly stirred solution of 2,4-dichloroacetophenone (1.89 g, 0.01 mol) and quinoline-8-carbaldehyde (1.57 g, 0.01 mol) in 25 ml methanol, 5 ml of 40% KOH solution was added. The solution was stirred overnight and filtered. The product was crystallized from (1:1) acetone/toluene mixture (m.p.: 361–371 K). Analysis for C₁₈H₁₁Cl₂NO: Found (Calculated): C: 65.79 (65.87); H: 3.32 (3.38); N: 4.23 (4.27).

Refinement

H atoms were found in a difference map, but they were refined using a riding model with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

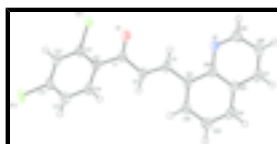


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

(2E)-1-(2,4-Dichlorophenyl)-3-quinolin-8-ylprop-2-en-1-one

Crystal data

C₁₈H₁₁Cl₂NO

$M_r = 328.18$

Monoclinic, $P2_1/c$

$F_{000} = 672$

$D_x = 1.454 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

supplementary materials

Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 11.9121 (16) \text{ \AA}$	Cell parameters from 10809 reflections
$b = 10.7112 (10) \text{ \AA}$	$\theta = 3.6\text{--}25.7^\circ$
$c = 12.7824 (15) \text{ \AA}$	$\mu = 0.43 \text{ mm}^{-1}$
$\beta = 113.181 (9)^\circ$	$T = 173 (2) \text{ K}$
$V = 1499.3 (3) \text{ \AA}^3$	Block, light yellow
$Z = 4$	$0.35 \times 0.35 \times 0.33 \text{ mm}$

Data collection

Stoe IPDS II two-circle diffractometer	2808 independent reflections
Radiation source: fine-focus sealed tube	2328 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.062$
$T = 173(2) \text{ K}$	$\theta_{\text{max}} = 25.6^\circ$
ω scans	$\theta_{\text{min}} = 3.6^\circ$
Absorption correction: multi-scan [MULABS (Spek, 2003; Blessing, 1995)]	$h = -14 \rightarrow 13$
$T_{\text{min}} = 0.863, T_{\text{max}} = 0.870$	$k = -12 \rightarrow 13$
12134 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0986P)^2]$
$wR(F^2) = 0.154$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2808 reflections	$\Delta\rho_{\text{max}} = 0.55 \text{ e \AA}^{-3}$
200 parameters	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.027 (4)

Special details

Experimental ;

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 calculat-

ing 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.67231 (18)	0.19606 (18)	0.46299 (17)	0.0292 (5)
O1	0.42301 (17)	0.13077 (16)	0.68460 (17)	0.0405 (5)
Cl1	0.14246 (5)	0.16535 (6)	0.57220 (5)	0.0364 (2)
Cl2	0.05375 (5)	0.50927 (6)	0.83447 (5)	0.0379 (3)
C1	0.4147 (2)	0.2440 (2)	0.6895 (2)	0.0286 (5)
C2	0.4905 (2)	0.3314 (2)	0.6565 (2)	0.0294 (5)
H2	0.4889	0.4178	0.6728	0.035*
C3	0.5614 (2)	0.2921 (2)	0.60420 (19)	0.0284 (5)
H3	0.5581	0.2057	0.5864	0.034*
C11	0.3234 (2)	0.3035 (2)	0.7296 (2)	0.0275 (5)
C12	0.1999 (2)	0.2740 (2)	0.68172 (19)	0.0277 (5)
C13	0.1160 (2)	0.3352 (2)	0.7146 (2)	0.0297 (6)
H13	0.0316	0.3152	0.6805	0.036*
C14	0.1587 (2)	0.4260 (2)	0.7982 (2)	0.0294 (5)
C15	0.2815 (2)	0.4551 (3)	0.8504 (2)	0.0348 (6)
H15	0.3095	0.5154	0.9096	0.042*
C16	0.3627 (2)	0.3944 (2)	0.8143 (2)	0.0337 (6)
H16	0.4469	0.4152	0.8482	0.040*
C21	0.6436 (2)	0.3695 (2)	0.57184 (19)	0.0272 (5)
C22	0.6716 (2)	0.4906 (2)	0.6084 (2)	0.0329 (6)
H22	0.6328	0.5274	0.6530	0.039*
C23	0.7559 (2)	0.5617 (2)	0.5819 (2)	0.0348 (6)
H23	0.7729	0.6453	0.6083	0.042*
C24	0.8138 (2)	0.5113 (2)	0.5181 (2)	0.0335 (6)
H24	0.8722	0.5595	0.5022	0.040*
C25	0.7873 (2)	0.3886 (2)	0.47589 (19)	0.0275 (5)
C26	0.7016 (2)	0.3163 (2)	0.50200 (18)	0.0248 (5)
C27	0.8423 (2)	0.3326 (2)	0.4070 (2)	0.0339 (6)
H27	0.8989	0.3782	0.3865	0.041*
C28	0.8130 (2)	0.2129 (3)	0.3707 (2)	0.0362 (6)
H28	0.8502	0.1733	0.3260	0.043*
C29	0.7268 (2)	0.1488 (2)	0.4003 (2)	0.0334 (6)
H29	0.7066	0.0658	0.3733	0.040*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0296 (11)	0.0304 (10)	0.0347 (10)	0.0011 (8)	0.0204 (8)	-0.0002 (8)
O1	0.0429 (11)	0.0303 (10)	0.0648 (13)	-0.0002 (8)	0.0389 (10)	-0.0012 (8)
Cl1	0.0338 (4)	0.0379 (4)	0.0442 (4)	-0.0070 (2)	0.0225 (3)	-0.0095 (3)
Cl2	0.0354 (4)	0.0447 (4)	0.0453 (4)	0.0112 (3)	0.0285 (3)	0.0025 (3)
C1	0.0253 (12)	0.0318 (13)	0.0365 (12)	-0.0014 (10)	0.0204 (10)	-0.0014 (10)

supplementary materials

C2	0.0284 (12)	0.0301 (13)	0.0377 (13)	-0.0005 (9)	0.0217 (10)	-0.0018 (9)
C3	0.0287 (12)	0.0293 (12)	0.0336 (12)	-0.0022 (10)	0.0193 (10)	0.0008 (10)
C11	0.0287 (12)	0.0289 (12)	0.0334 (12)	-0.0010 (9)	0.0215 (10)	0.0020 (9)
C12	0.0297 (12)	0.0297 (12)	0.0321 (12)	0.0005 (10)	0.0212 (10)	0.0024 (10)
C13	0.0241 (12)	0.0366 (14)	0.0347 (12)	-0.0004 (9)	0.0184 (10)	0.0044 (10)
C14	0.0297 (12)	0.0330 (13)	0.0358 (12)	0.0067 (10)	0.0239 (10)	0.0052 (10)
C15	0.0349 (13)	0.0382 (14)	0.0383 (13)	-0.0011 (11)	0.0219 (11)	-0.0058 (11)
C16	0.0271 (12)	0.0411 (15)	0.0421 (14)	-0.0036 (10)	0.0234 (11)	-0.0049 (11)
C21	0.0258 (12)	0.0321 (13)	0.0292 (12)	-0.0004 (9)	0.0168 (10)	0.0023 (9)
C22	0.0355 (13)	0.0352 (14)	0.0366 (13)	-0.0014 (10)	0.0235 (11)	-0.0024 (10)
C23	0.0379 (13)	0.0321 (13)	0.0374 (13)	-0.0070 (11)	0.0179 (11)	-0.0021 (10)
C24	0.0307 (13)	0.0384 (14)	0.0341 (12)	-0.0080 (10)	0.0159 (10)	0.0068 (10)
C25	0.0222 (11)	0.0346 (13)	0.0293 (11)	-0.0004 (9)	0.0140 (9)	0.0047 (9)
C26	0.0219 (11)	0.0292 (12)	0.0277 (11)	0.0012 (9)	0.0144 (9)	0.0043 (9)
C27	0.0274 (12)	0.0475 (16)	0.0349 (13)	-0.0001 (10)	0.0210 (10)	0.0053 (11)
C28	0.0341 (14)	0.0466 (16)	0.0374 (13)	0.0051 (11)	0.0244 (11)	0.0016 (11)
C29	0.0377 (14)	0.0333 (13)	0.0365 (13)	0.0045 (10)	0.0224 (11)	-0.0007 (10)

Geometric parameters (Å, °)

N1—C29	1.315 (3)	C15—H15	0.9500
N1—C26	1.375 (3)	C16—H16	0.9500
O1—C1	1.221 (3)	C21—C22	1.375 (4)
C11—C12	1.740 (2)	C21—C26	1.444 (3)
C12—C14	1.741 (2)	C22—C23	1.404 (3)
C1—C2	1.472 (3)	C22—H22	0.9500
C1—C11	1.515 (3)	C23—C24	1.368 (4)
C2—C3	1.335 (3)	C23—H23	0.9500
C2—H2	0.9500	C24—C25	1.409 (3)
C3—C21	1.462 (3)	C24—H24	0.9500
C3—H3	0.9500	C25—C27	1.420 (3)
C11—C12	1.389 (3)	C25—C26	1.423 (3)
C11—C16	1.393 (4)	C27—C28	1.361 (4)
C12—C13	1.391 (3)	C27—H27	0.9500
C13—C14	1.385 (3)	C28—C29	1.405 (4)
C13—H13	0.9500	C28—H28	0.9500
C14—C15	1.383 (4)	C29—H29	0.9500
C15—C16	1.386 (4)		
C29—N1—C26	117.8 (2)	C22—C21—C26	118.1 (2)
O1—C1—C2	123.1 (2)	C22—C21—C3	122.7 (2)
O1—C1—C11	121.2 (2)	C26—C21—C3	119.2 (2)
C2—C1—C11	115.6 (2)	C21—C22—C23	122.1 (2)
C3—C2—C1	121.5 (2)	C21—C22—H22	119.0
C3—C2—H2	119.3	C23—C22—H22	119.0
C1—C2—H2	119.3	C24—C23—C22	120.4 (2)
C2—C3—C21	126.0 (2)	C24—C23—H23	119.8
C2—C3—H3	117.0	C22—C23—H23	119.8
C21—C3—H3	117.0	C23—C24—C25	120.5 (2)
C12—C11—C16	118.4 (2)	C23—C24—H24	119.8

C12—C11—C1	122.2 (2)	C25—C24—H24	119.8
C16—C11—C1	119.4 (2)	C24—C25—C27	122.9 (2)
C11—C12—C13	121.4 (2)	C24—C25—C26	119.4 (2)
C11—C12—C11	121.32 (18)	C27—C25—C26	117.7 (2)
C13—C12—C11	117.16 (18)	N1—C26—C25	121.8 (2)
C14—C13—C12	118.4 (2)	N1—C26—C21	118.7 (2)
C14—C13—H13	120.8	C25—C26—C21	119.5 (2)
C12—C13—H13	120.8	C28—C27—C25	119.3 (2)
C15—C14—C13	121.8 (2)	C28—C27—H27	120.3
C15—C14—C12	119.36 (19)	C25—C27—H27	120.3
C13—C14—C12	118.79 (18)	C27—C28—C29	119.0 (2)
C14—C15—C16	118.6 (2)	C27—C28—H28	120.5
C14—C15—H15	120.7	C29—C28—H28	120.5
C16—C15—H15	120.7	N1—C29—C28	124.4 (2)
C15—C16—C11	121.4 (2)	N1—C29—H29	117.8
C15—C16—H16	119.3	C28—C29—H29	117.8
C11—C16—H16	119.3		
O1—C1—C2—C3	9.5 (4)	C26—C21—C22—C23	-1.3 (4)
C11—C1—C2—C3	-170.0 (2)	C3—C21—C22—C23	176.4 (2)
C1—C2—C3—C21	-177.4 (2)	C21—C22—C23—C24	-0.3 (4)
O1—C1—C11—C12	-53.3 (3)	C22—C23—C24—C25	1.6 (4)
C2—C1—C11—C12	126.2 (2)	C23—C24—C25—C27	178.4 (2)
O1—C1—C11—C16	129.1 (3)	C23—C24—C25—C26	-1.3 (3)
C2—C1—C11—C16	-51.4 (3)	C29—N1—C26—C25	0.2 (3)
C16—C11—C12—C13	1.7 (3)	C29—N1—C26—C21	-179.4 (2)
C1—C11—C12—C13	-175.9 (2)	C24—C25—C26—N1	180.0 (2)
C16—C11—C12—C11	177.84 (18)	C27—C25—C26—N1	0.3 (3)
C1—C11—C12—C11	0.2 (3)	C24—C25—C26—C21	-0.4 (3)
C11—C12—C13—C14	-1.0 (3)	C27—C25—C26—C21	180.0 (2)
C11—C12—C13—C14	-177.24 (18)	C22—C21—C26—N1	-178.7 (2)
C12—C13—C14—C15	-1.2 (3)	C3—C21—C26—N1	3.5 (3)
C12—C13—C14—C12	176.53 (18)	C22—C21—C26—C25	1.6 (3)
C13—C14—C15—C16	2.5 (4)	C3—C21—C26—C25	-176.2 (2)
C12—C14—C15—C16	-175.2 (2)	C24—C25—C27—C28	179.2 (2)
C14—C15—C16—C11	-1.7 (4)	C26—C25—C27—C28	-1.1 (4)
C12—C11—C16—C15	-0.4 (4)	C25—C27—C28—C29	1.4 (4)
C1—C11—C16—C15	177.3 (2)	C26—N1—C29—C28	0.1 (4)
C2—C3—C21—C22	10.7 (4)	C27—C28—C29—N1	-0.9 (4)
C2—C3—C21—C26	-171.6 (2)		

Fig. 1

