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

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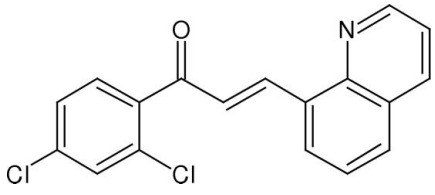
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.057; $wR$ factor = 0.154; data-to-parameter ratio = 14.0.

The geometric parameters of the molecule of the title compound, $C_{18}H_{11}Cl_2NO$, a chalcone derivative, 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)°.

## 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*

$C_{18}H_{11}Cl_2NO$
$M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.43 mm$^{-1}$
$T$ = 173 (2) K
0.35 × 0.35 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −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*.

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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). E**63**, o3488 [ **doi:10.1107/S1600536807032746** ]

# (2*E*)-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 me thanol, 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 $C_{18}H_{11}Cl_2NO$: 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 = 0.95Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

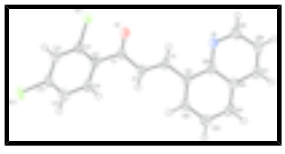


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

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

*Crystal data*

| | |
|---|---|
| $C_{18}H_{11}Cl_2NO$ | $F_{000}$ = 672 |
| $M_r$ = 328.18 | $D_x$ = 1.454 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |

| | |
|---|---|
| | λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 10809 reflections |
| $a$ = 11.9121 (16) Å | θ = 3.6–25.7º |
| $b$ = 10.7112 (10) Å | μ = 0.43 $mm^{-1}$ |
| $c$ = 12.7824 (15) Å | $T$ = 173 (2) K |
| β = 113.181 (9)º | Block, light yellow |
| $V$ = 1499.3 (3) $Å^3$ | 0.35 × 0.35 × 0.33 mm |
| $Z$ = 4 | |

*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 | $R_{int}$ = 0.062 |
| $T$ = 173(2) K | $\theta_{max}$ = 25.6º |
| ω scans | $\theta_{min}$ = 3.6º |
| Absorption correction: multi-scan [MULABS (Spek, 2003; Blessing, 1995)] | $h = -14 \rightarrow 13$ |
| $T_{min}$ = 0.863, $T_{max}$ = 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 | $w = 1/[\sigma^2(F_o^2) + (0.0986P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.154 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.03 | $\Delta\rho_{max}$ = 0.55 e $Å^{-3}$ |
| 2808 reflections | $\Delta\rho_{min}$ = −0.50 e $Å^{-3}$ |
| 200 parameters | Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.027 (4) |
| Secondary atom site location: difference Fourier map | |

*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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

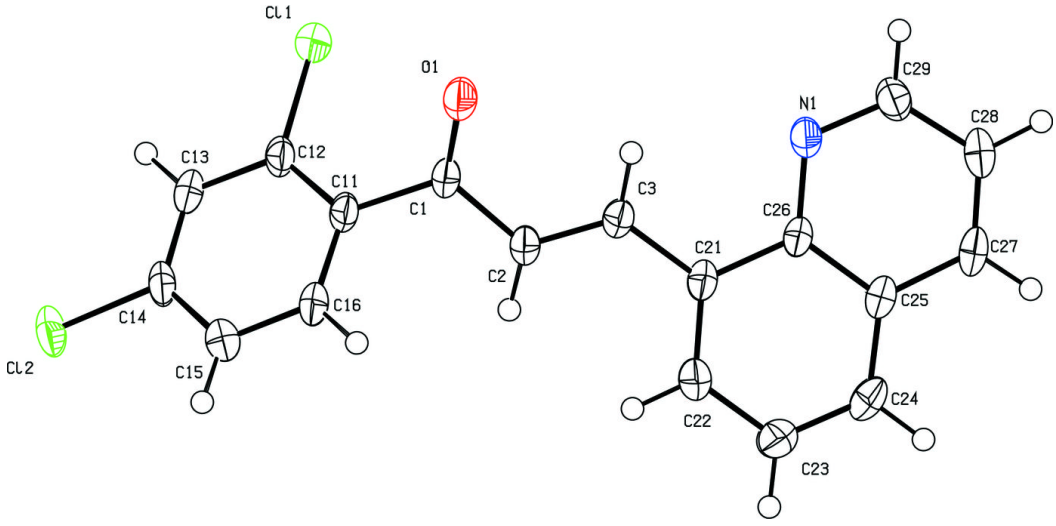
| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0284 (12) | 0.0301 (13) | 0.0377 (13) | −0.0005 (9) | 0.0217 (10) | −0.0018 (9) |
| C3 | 0.0287 (12) | 0.0293 (12) | 0.0336 (12) | −0.0022 (10) | 0.0193 (10) | 0.0008 (10) |
| C11 | 0.0287 (12) | 0.0289 (12) | 0.0334 (12) | −0.0010 (9) | 0.0215 (10) | 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) |
| Cl1—C12 | 1.740 (2) | C21—C26 | 1.444 (3) |
| Cl2—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—Cl1 | 121.32 (18) | C27—C25—C26 | 117.7 (2) |
| C13—C12—Cl1 | 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—Cl2 | 119.36 (19) | C25—C27—H27 | 120.3 |
| C13—C14—Cl2 | 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—Cl1 | 177.84 (18) | C27—C25—C26—N1 | 0.3 (3) |
| C1—C11—C12—Cl1 | 0.2 (3) | C24—C25—C26—C21 | −0.4 (3) |
| C11—C12—C13—C14 | −1.0 (3) | C27—C25—C26—C21 | 180.0 (2) |
| Cl1—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—Cl2 | 176.53 (18) | C22—C21—C26—C25 | 1.6 (3) |
| C13—C14—C15—C16 | 2.5 (4) | C3—C21—C26—C25 | −176.2 (2) |
| Cl2—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**


Cl1
O1
C29
N1
C28
C13
C12
C11
C1
C3
C26
C21
C27
C2
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C14
C16
Cl2
C15
C24
C22
C23