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# 1,5-Bis(4-chlorophenyl)-3-phenylpentane-1,5-dione

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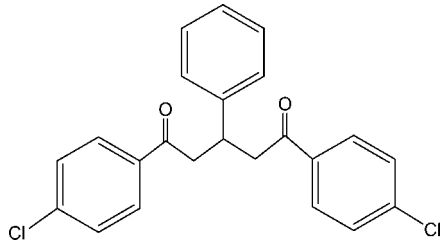
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.095; data-to-parameter ratio = 17.8.

The title compound, $C_{23}H_{18}Cl_2O_2$, is the reaction product of a Michael addition. The two chlorophenyl rings are almost perpendicular to the phenyl ring.

## Related literature

For related literature, see: Emori *et al.* (1998); Qian & Widenhoefer (2003); Sasai *et al.* (1994); Murai *et al.* (2000); Wang & Shen (1999); Wang *et al.* (2005).




## Experimental

*Crystal data*

$C_{23}H_{18}Cl_2O_2$
$M_r$ = 397.27
Monoclinic, $P2_1/c$
$a$ = 15.5591 (4) Å
$b$ = 10.7610 (3) Å
$c$ = 11.6784 (3) Å
$\beta$ = 101.616 (1)°
$V$ = 1915.28 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.35 mm$^{-1}$
$T$ = 153 (2) K
0.58 × 0.42 × 0.28 mm

*Data collection*

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.790, $T_{max}$ = 0.984
(expected range = 0.727–0.906)
18363 measured reflections
4359 independent reflections
4090 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
$S$ = 1.02
4359 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2349).

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# supplementary materials

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# 1,5-Bis(4-chlorophenyl)-3-phenylpentane-1,5-dione

**X.-X. Mo, Z.-F. Xie and F.-M. Liu**

## Comment

The Michael addition is one of the most important C—C bond forming reactions employed in organic synthesis (Qian & Widenhoefer, 2003). In recent years, the catalytic asymmetric Michael addition promoted by chiral metal complexes has been recognized as an efficient method for carbon-carbon bond formation (Emori *et al.*, 1998). The asymmetric catalyzers of Michael reaction have metal catalyzers such as $La_3$(O-t-Bu)$_9$, $Y_3$(O-t-Bu)$_8$Cl, $Y_5$(O-i-Pr)$_{13}$O (Sasai *et al.*, 1994), lithium diisopropylamide (Murai *et al.*, 2000), and non-metal catalyzers that includes MacMillan's chiral imidazolidinone (Wang *et al.*, 2005). We synthesized 1,5-bis(4-chlorophenyl)-3-phenylpentane-1,5-dione with tetrabutylammonium bromide. The two chlorophenyl rings are almost perpendicular to the central phenyl ring.

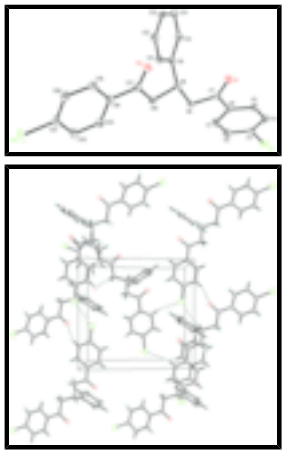
## Experimental

A mixture of 1-(4-chloro-phenyl)-3-phenyl-2-propylene-1-ketone (Wang & Shen, 1999) (1 mmol), 4-chloro-acetopnone (2 mmol) and tetrabutylammonium-bromide (0.1 mmol) was dissolved in toluene (5 mL). To this mixture was added 50% KOH (1 mL) and stirred at room temperature for 24 h. The reaction was quenched with water and extracted with ether (3 times with 10 mL). The combined organic layers were dried ($Na_2SO_4$), concentrated to furnish the crude product, which was purified by flash chromatography (yield 54%). M.p. 463 k. Analysis, found (calculated for $C_{23}H_{18}Cl_2O_2$): C 69.53 (69.55%) H 4.57 (4.53%) O 8.05 (8.11%). Crystals were grown from a mixture of ethyl acetate and petroleum ether by slow evaporation.

## Refinement

H atoms were positioned geometrically, with C—H ranging from 0.95 - 1.00Å and $U_{iso}$(H) = 1.2Ueq(C).

## Figures



### 1,5-Bis(4-chlorophenyl)-3-phenylpentane-1,5-dione

*Crystal data*

| | |
|---|---|
| $C_{23}H_{18}Cl_2O_2$ | $F_{000}$ = 824 |
| $M_r$ = 397.27 | $D_x$ = 1.378 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 17167 reflections |
| $a$ = 15.5591 (4) Å | θ = 3.1–27.5º |
| $b$ = 10.7610 (3) Å | μ = 0.35 mm$^{-1}$ |
| $c$ = 11.6784 (3) Å | $T$ = 153 (2) K |
| β = 101.6160 (10)º | Platelet, colorless |
| $V$ = 1915.28 (9) Å$^3$ | 0.58 × 0.42 × 0.28 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS SPIDER diffractometer | 4359 independent reflections |
| Radiation source: Rotating Anode | 4090 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.018 |
| $T$ = 153(2) K | $\theta_{max}$ = 27.5º |
| ω scans | $\theta_{min}$ = 3.1º |
| Absorption correction: empirical (using intensity measurements)<br>(ABSCOR; Higashi, 1995) | $h$ = −20→19 |
| $T_{min}$ = 0.790, $T_{max}$ = 0.984 | $k$ = −13→13 |
| 18363 measured reflections | $l$ = −14→15 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 1.0487P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | $(\Delta/\sigma)_{max}$ = 0.004 |
| $wR(F^2)$ = 0.096 | $\Delta\rho_{max}$ = 0.55 e Å$^{-3}$ |
| $S$ = 1.02 | $\Delta\rho_{min}$ = −0.56 e Å$^{-3}$ |
| 4359 reflections | Extinction correction: SHELXL97,<br>$Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| 245 parameters | Extinction coefficient: 0.0082 (11) |
| Primary atom site location: structure-invariant direct methods | |
| Secondary atom site location: difference Fourier map | |
| Hydrogen site location: inferred from neighbouring sites | |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.06138 (3) | 0.71183 (4) | 0.28055 (3) | 0.04330 (13) |
| Cl2 | 0.45939 (3) | −0.37752 (3) | 1.07691 (4) | 0.04019 (12) |
| O1 | 0.27113 (7) | 0.59521 (9) | 0.82643 (9) | 0.0334 (2) |
| O2 | 0.39430 (7) | 0.23645 (9) | 1.09861 (9) | 0.0302 (2) |
| C1 | 0.14266 (11) | 0.48713 (14) | 0.55234 (12) | 0.0345 (3) |
| H1A | 0.1349 | 0.4028 | 0.5719 | 0.041* |
| C2 | 0.10076 (11) | 0.53260 (15) | 0.44387 (13) | 0.0376 (3) |
| H2A | 0.0637 | 0.4802 | 0.3898 | 0.045* |
| C3 | 0.11383 (9) | 0.65468 (14) | 0.41596 (11) | 0.0290 (3) |
| C4 | 0.16723 (10) | 0.73318 (14) | 0.49289 (12) | 0.0311 (3) |
| H4A | 0.1761 | 0.8168 | 0.4719 | 0.037* |
| C5 | 0.20748 (9) | 0.68735 (13) | 0.60125 (12) | 0.0274 (3) |
| H5A | 0.2437 | 0.7407 | 0.6554 | 0.033* |
| C6 | 0.19580 (8) | 0.56417 (12) | 0.63229 (11) | 0.0228 (3) |
| C7 | 0.24130 (8) | 0.52038 (12) | 0.75086 (11) | 0.0230 (3) |
| C8 | 0.25264 (9) | 0.38214 (12) | 0.77148 (11) | 0.0255 (3) |
| H8A | 0.2932 | 0.3500 | 0.7231 | 0.031* |
| H8B | 0.1952 | 0.3410 | 0.7448 | 0.031* |
| C9 | 0.28827 (8) | 0.34624 (11) | 0.89939 (11) | 0.0214 (2) |
| H9A | 0.3416 | 0.3976 | 0.9297 | 0.026* |
| C10 | 0.22093 (8) | 0.37083 (11) | 0.97502 (11) | 0.0206 (2) |
| C11 | 0.13589 (9) | 0.32426 (13) | 0.94369 (12) | 0.0277 (3) |
| H11A | 0.1201 | 0.2751 | 0.8751 | 0.033* |
| C12 | 0.07355 (9) | 0.34871 (15) | 1.01146 (14) | 0.0333 (3) |
| H12A | 0.0159 | 0.3162 | 0.9889 | 0.040* |
| C13 | 0.09565 (9) | 0.42023 (14) | 1.11146 (13) | 0.0310 (3) |
| H13A | 0.0532 | 0.4375 | 1.1575 | 0.037* |
| C14 | 0.18007 (10) | 0.46638 (13) | 1.14393 (12) | 0.0297 (3) |
| H14A | 0.1957 | 0.5152 | 1.2128 | 0.036* |
| C15 | 0.24218 (9) | 0.44168 (12) | 1.07642 (11) | 0.0255 (3) |
| H15A | 0.3000 | 0.4736 | 1.0999 | 0.031* |
| C16 | 0.31568 (9) | 0.20906 (12) | 0.90226 (11) | 0.0239 (3) |
| H16A | 0.2621 | 0.1574 | 0.8823 | 0.029* |

| | | | | |
|---|---|---|---|---|
| H16B | 0.3503 | 0.1953 | 0.8410 | 0.029* |
| C17 | 0.36896 (8) | 0.16484 (12) | 1.01783 (11) | 0.0229 (3) |
| C18 | 0.39015 (8) | 0.02895 (12) | 1.03035 (11) | 0.0225 (3) |
| C19 | 0.43314 (9) | −0.01583 (13) | 1.13895 (12) | 0.0269 (3) |
| H19A | 0.4482 | 0.0400 | 1.2029 | 0.032* |
| C20 | 0.45433 (9) | −0.14104 (13) | 1.15504 (13) | 0.0292 (3) |
| H20A | 0.4831 | −0.1714 | 1.2292 | 0.035* |
| C21 | 0.43236 (9) | −0.22036 (12) | 1.06020 (13) | 0.0278 (3) |
| C22 | 0.38999 (9) | −0.17912 (13) | 0.95109 (13) | 0.0294 (3) |
| H22A | 0.3756 | −0.2352 | 0.8873 | 0.035* |
| C23 | 0.36897 (9) | −0.05401 (13) | 0.93699 (12) | 0.0264 (3) |
| H23A | 0.3397 | −0.0243 | 0.8627 | 0.032* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0490 (2) | 0.0551 (3) | 0.02385 (18) | 0.02066 (18) | 0.00284 (15) | 0.00384 (15) |
| Cl2 | 0.0380 (2) | 0.02220 (18) | 0.0565 (3) | 0.00195 (13) | 0.00033 (17) | 0.00760 (15) |
| O1 | 0.0477 (6) | 0.0244 (5) | 0.0251 (5) | −0.0049 (4) | 0.0000 (4) | −0.0019 (4) |
| O2 | 0.0327 (5) | 0.0267 (5) | 0.0296 (5) | 0.0024 (4) | 0.0029 (4) | −0.0044 (4) |
| C1 | 0.0467 (8) | 0.0272 (7) | 0.0275 (7) | −0.0051 (6) | 0.0025 (6) | −0.0022 (5) |
| C2 | 0.0452 (8) | 0.0380 (8) | 0.0261 (7) | −0.0040 (7) | −0.0013 (6) | −0.0055 (6) |
| C3 | 0.0296 (7) | 0.0379 (7) | 0.0201 (6) | 0.0109 (6) | 0.0068 (5) | 0.0014 (5) |
| C4 | 0.0367 (7) | 0.0281 (7) | 0.0293 (7) | 0.0030 (6) | 0.0089 (6) | 0.0051 (5) |
| C5 | 0.0305 (7) | 0.0259 (7) | 0.0256 (6) | −0.0019 (5) | 0.0052 (5) | 0.0006 (5) |
| C6 | 0.0254 (6) | 0.0235 (6) | 0.0207 (6) | 0.0013 (5) | 0.0076 (5) | −0.0010 (5) |
| C7 | 0.0264 (6) | 0.0222 (6) | 0.0216 (6) | −0.0013 (5) | 0.0080 (5) | −0.0004 (5) |
| C8 | 0.0360 (7) | 0.0209 (6) | 0.0211 (6) | 0.0007 (5) | 0.0092 (5) | −0.0001 (5) |
| C9 | 0.0240 (6) | 0.0194 (6) | 0.0218 (6) | 0.0009 (4) | 0.0067 (5) | −0.0001 (4) |
| C10 | 0.0237 (6) | 0.0178 (5) | 0.0206 (5) | 0.0039 (4) | 0.0053 (5) | 0.0039 (4) |
| C11 | 0.0260 (6) | 0.0285 (7) | 0.0285 (7) | −0.0002 (5) | 0.0054 (5) | −0.0028 (5) |
| C12 | 0.0236 (6) | 0.0373 (8) | 0.0404 (8) | −0.0002 (5) | 0.0097 (6) | 0.0025 (6) |
| C13 | 0.0319 (7) | 0.0332 (7) | 0.0320 (7) | 0.0096 (6) | 0.0159 (6) | 0.0073 (6) |
| C14 | 0.0374 (7) | 0.0295 (7) | 0.0231 (6) | 0.0062 (6) | 0.0086 (5) | −0.0012 (5) |
| C15 | 0.0260 (6) | 0.0260 (6) | 0.0246 (6) | 0.0012 (5) | 0.0053 (5) | −0.0005 (5) |
| C16 | 0.0258 (6) | 0.0214 (6) | 0.0250 (6) | 0.0034 (5) | 0.0062 (5) | −0.0011 (5) |
| C17 | 0.0196 (5) | 0.0242 (6) | 0.0261 (6) | 0.0021 (5) | 0.0075 (5) | 0.0000 (5) |
| C18 | 0.0180 (5) | 0.0238 (6) | 0.0267 (6) | 0.0008 (4) | 0.0067 (5) | 0.0012 (5) |
| C19 | 0.0239 (6) | 0.0296 (7) | 0.0268 (6) | 0.0021 (5) | 0.0044 (5) | 0.0001 (5) |
| C20 | 0.0245 (6) | 0.0316 (7) | 0.0309 (7) | 0.0021 (5) | 0.0042 (5) | 0.0071 (5) |
| C21 | 0.0216 (6) | 0.0211 (6) | 0.0406 (7) | −0.0001 (5) | 0.0063 (5) | 0.0053 (5) |
| C22 | 0.0281 (6) | 0.0231 (6) | 0.0356 (7) | −0.0015 (5) | 0.0031 (6) | −0.0022 (5) |
| C23 | 0.0254 (6) | 0.0247 (6) | 0.0276 (6) | 0.0006 (5) | 0.0020 (5) | 0.0011 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C3 | 1.7393 (14) | C11—C12 | 1.3949 (19) |
| Cl2—C21 | 1.7441 (14) | C11—H11A | 0.9500 |
| O1—C7 | 1.2156 (16) | C12—C13 | 1.383 (2) |

| | | | |
|---|---|---|---|
| O2—C17 | 1.2204 (16) | C12—H12A | 0.9500 |
| C1—C6 | 1.3899 (19) | C13—C14 | 1.384 (2) |
| C1—C2 | 1.392 (2) | C13—H13A | 0.9500 |
| C1—H1A | 0.9500 | C14—C15 | 1.3904 (19) |
| C2—C3 | 1.378 (2) | C14—H14A | 0.9500 |
| C2—H2A | 0.9500 | C15—H15A | 0.9500 |
| C3—C4 | 1.382 (2) | C16—C17 | 1.5115 (18) |
| C4—C5 | 1.3849 (19) | C16—H16A | 0.9900 |
| C4—H4A | 0.9500 | C16—H16B | 0.9900 |
| C5—C6 | 1.3956 (18) | C17—C18 | 1.4997 (17) |
| C5—H5A | 0.9500 | C18—C19 | 1.3952 (18) |
| C6—C7 | 1.4986 (17) | C18—C23 | 1.3963 (18) |
| C7—C8 | 1.5115 (17) | C19—C20 | 1.391 (2) |
| C8—C9 | 1.5345 (17) | C19—H19A | 0.9500 |
| C8—H8A | 0.9900 | C20—C21 | 1.386 (2) |
| C8—H8B | 0.9900 | C20—H20A | 0.9500 |
| C9—C10 | 1.5232 (16) | C21—C22 | 1.384 (2) |
| C9—C16 | 1.5351 (17) | C22—C23 | 1.3875 (19) |
| C9—H9A | 1.0000 | C22—H22A | 0.9500 |
| C10—C15 | 1.3911 (18) | C23—H23A | 0.9500 |
| C10—C11 | 1.3930 (18) | | |
| C6—C1—C2 | 120.53 (14) | C13—C12—C11 | 120.07 (13) |
| C6—C1—H1A | 119.7 | C13—C12—H12A | 120.0 |
| C2—C1—H1A | 119.7 | C11—C12—H12A | 120.0 |
| C3—C2—C1 | 119.08 (14) | C12—C13—C14 | 119.47 (12) |
| C3—C2—H2A | 120.5 | C12—C13—H13A | 120.3 |
| C1—C2—H2A | 120.5 | C14—C13—H13A | 120.3 |
| C2—C3—C4 | 121.78 (13) | C13—C14—C15 | 120.38 (13) |
| C2—C3—Cl1 | 119.17 (11) | C13—C14—H14A | 119.8 |
| C4—C3—Cl1 | 119.04 (11) | C15—C14—H14A | 119.8 |
| C3—C4—C5 | 118.58 (13) | C14—C15—C10 | 120.95 (12) |
| C3—C4—H4A | 120.7 | C14—C15—H15A | 119.5 |
| C5—C4—H4A | 120.7 | C10—C15—H15A | 119.5 |
| C4—C5—C6 | 121.13 (13) | C17—C16—C9 | 114.98 (10) |
| C4—C5—H5A | 119.4 | C17—C16—H16A | 108.5 |
| C6—C5—H5A | 119.4 | C9—C16—H16A | 108.5 |
| C1—C6—C5 | 118.88 (12) | C17—C16—H16B | 108.5 |
| C1—C6—C7 | 122.65 (12) | C9—C16—H16B | 108.5 |
| C5—C6—C7 | 118.46 (12) | H16A—C16—H16B | 107.5 |
| O1—C7—C6 | 120.18 (12) | O2—C17—C18 | 120.65 (12) |
| O1—C7—C8 | 121.40 (12) | O2—C17—C16 | 121.68 (12) |
| C6—C7—C8 | 118.35 (11) | C18—C17—C16 | 117.67 (11) |
| C7—C8—C9 | 114.24 (11) | C19—C18—C23 | 118.92 (12) |
| C7—C8—H8A | 108.7 | C19—C18—C17 | 118.76 (12) |
| C9—C8—H8A | 108.7 | C23—C18—C17 | 122.32 (12) |
| C7—C8—H8B | 108.7 | C20—C19—C18 | 120.97 (13) |
| C9—C8—H8B | 108.7 | C20—C19—H19A | 119.5 |
| H8A—C8—H8B | 107.6 | C18—C19—H19A | 119.5 |
| C10—C9—C8 | 111.40 (10) | C21—C20—C19 | 118.37 (13) |

| | | | |
|---|---|---|---|
| C10—C9—C16 | 112.02 (10) | C21—C20—H20A | 120.8 |
| C8—C9—C16 | 107.92 (10) | C19—C20—H20A | 120.8 |
| C10—C9—H9A | 108.5 | C22—C21—C20 | 122.23 (13) |
| C8—C9—H9A | 108.5 | C22—C21—Cl2 | 118.24 (11) |
| C16—C9—H9A | 108.5 | C20—C21—Cl2 | 119.52 (11) |
| C15—C10—C11 | 118.11 (12) | C21—C22—C23 | 118.52 (13) |
| C15—C10—C9 | 121.02 (11) | C21—C22—H22A | 120.7 |
| C11—C10—C9 | 120.87 (11) | C23—C22—H22A | 120.7 |
| C10—C11—C12 | 121.02 (13) | C22—C23—C18 | 120.98 (12) |
| C10—C11—H11A | 119.5 | C22—C23—H23A | 119.5 |
| C12—C11—H11A | 119.5 | C18—C23—H23A | 119.5 |
| C6—C1—C2—C3 | 1.1 (2) | C10—C11—C12—C13 | 0.0 (2) |
| C1—C2—C3—C4 | −0.2 (2) | C11—C12—C13—C14 | −0.5 (2) |
| C1—C2—C3—Cl1 | −179.88 (12) | C12—C13—C14—C15 | 0.3 (2) |
| C2—C3—C4—C5 | −0.8 (2) | C13—C14—C15—C10 | 0.3 (2) |
| Cl1—C3—C4—C5 | 178.91 (10) | C11—C10—C15—C14 | −0.65 (19) |
| C3—C4—C5—C6 | 0.9 (2) | C9—C10—C15—C14 | 178.53 (12) |
| C2—C1—C6—C5 | −1.0 (2) | C10—C9—C16—C17 | −68.81 (14) |
| C2—C1—C6—C7 | 179.07 (13) | C8—C9—C16—C17 | 168.21 (11) |
| C4—C5—C6—C1 | 0.0 (2) | C9—C16—C17—O2 | −6.14 (17) |
| C4—C5—C6—C7 | 179.93 (12) | C9—C16—C17—C18 | 173.98 (10) |
| C1—C6—C7—O1 | −164.12 (14) | O2—C17—C18—C19 | 5.18 (18) |
| C5—C6—C7—O1 | 15.91 (18) | C16—C17—C18—C19 | −174.94 (11) |
| C1—C6—C7—C8 | 18.73 (19) | O2—C17—C18—C23 | −174.32 (12) |
| C5—C6—C7—C8 | −161.24 (12) | C16—C17—C18—C23 | 5.55 (17) |
| O1—C7—C8—C9 | 10.93 (18) | C23—C18—C19—C20 | −0.41 (19) |
| C6—C7—C8—C9 | −171.95 (11) | C17—C18—C19—C20 | −179.93 (12) |
| C7—C8—C9—C10 | 69.29 (14) | C18—C19—C20—C21 | 0.5 (2) |
| C7—C8—C9—C16 | −167.34 (11) | C19—C20—C21—C22 | −0.3 (2) |
| C8—C9—C10—C15 | −126.99 (12) | C19—C20—C21—Cl2 | 179.10 (10) |
| C16—C9—C10—C15 | 112.02 (13) | C20—C21—C22—C23 | 0.0 (2) |
| C8—C9—C10—C11 | 52.17 (15) | Cl2—C21—C22—C23 | −179.46 (10) |
| C16—C9—C10—C11 | −68.83 (15) | C21—C22—C23—C18 | 0.2 (2) |
| C15—C10—C11—C12 | 0.5 (2) | C19—C18—C23—C22 | 0.04 (19) |
| C9—C10—C11—C12 | −178.68 (12) | C17—C18—C23—C22 | 179.55 (12) |

**Fig. 1**

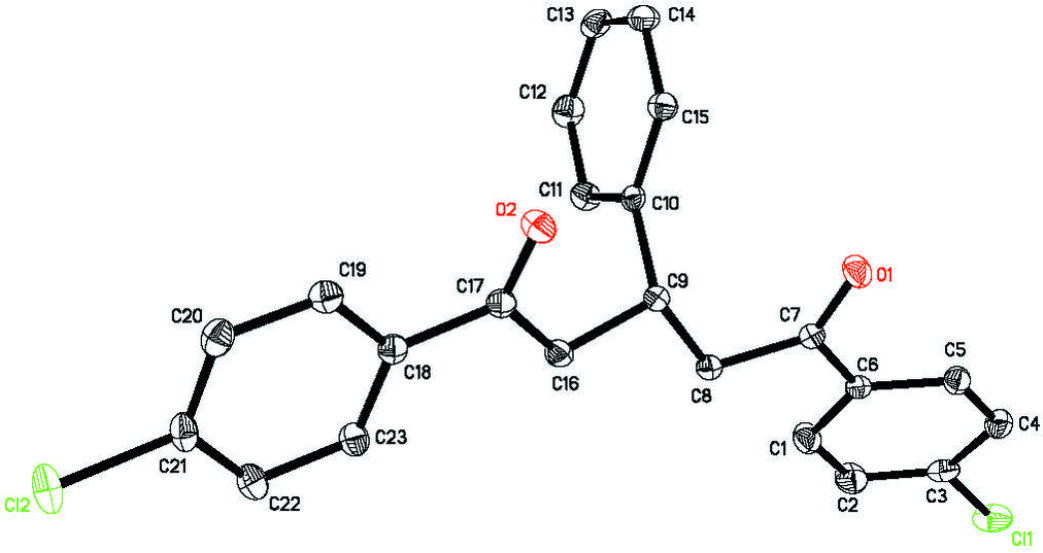

C13
C14
C12
C15
C11
C10
O2
C19
C17
C9
O1
C20
C7
C18
C16
C8
C6
C5
C4
C1
C23
C21
C2
C3
Cl2
C22
Cl1

**Fig. 2**