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

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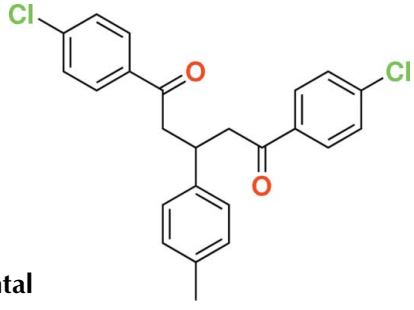
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.050; $wR$ factor = 0.146; data-to-parameter ratio = 17.0.

In the title molecule, $C_{24}H_{20}Cl_2O_2$, the central methylbenzene ring forms dihedral angles of 42.47 (10) and 34.34 (10)° with the terminal 4-chlorophenyl fragments. The dihedral angle between the chlorobenzene rings is 34.45 (11)°. A weak intramolecular C—H···O interaction generates an $S$(6) ring motif. The crystal packing exhibits weak C—H···O hydrogen bonds and C—H···$\pi$ interactions.

## Related literature

For the synthesis of 1,5-diketones, see: Yang *et al.* (2005); Hirsch & Bailey (1978). For the crystal structures of related compounds, see: Qiu *et al.* (2006); Insuasty *et al.* (2006); Jasinski *et al.* (2007); Huang *et al.* (2008); Lei & Bai (2009); Dutkiewicz *et al.* (2010); Fun *et al.* (2011). For the applications of delocalized $\pi$-systems, see: Burroughes *et al.* (1990); Smith *et al.* (2005); Li *et al.* (2004); Saricifti *et al.* (1992). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{24}H_{20}Cl_2O_2$
$M_r$ = 411.30
Monoclinic, $P2_1/c$
$a$ = 18.6794 (11) Å
$b$ = 7.5477 (4) Å
$c$ = 15.5196 (8) Å
$\beta$ = 103.622 (5)°
$V$ = 2126.5 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.32 mm$^{-1}$
$T$ = 296 K
0.51 × 0.42 × 0.37 mm

### Data collection

Agilent Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.443, $T_{max}$ = 1.000
14252 measured reflections
4341 independent reflections
3735 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.146
$S$ = 1.07
4341 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

*Cg*2 is the centroid of the C31–C36 methylbenzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4$A$···O1 | 0.97 | 2.56 | 3.130 (3) | 118 |
| C16—H16···O5$^{i}$ | 0.93 | 2.44 | 3.270 (3) | 149 |
| C55—H55···*Cg*2$^{ii}$ | 0.93 | 2.97 | 3.629 (2) | 129 |

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, y+1, z$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *DIRDIF2008* (Beurskens *et al.*, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2013* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2174).

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# supporting information

*Acta Cryst.* (2013). E**69**, o1508–o1509 [doi:10.1107/S1600536813024355]

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

**R. Chithiravel, A. Thiruvalluvar, S. Muthusubramanian and R. J. Butcher**

### S1. Comment

A simplified green chemistry approach to the Michael-addition reaction using the "Grindstone Chemistry" method for conducting exothermic reactions in the solvent-free mode has been described (Yang *et al.* 2005). We tested energy saving procedures developed in our laboratory for the preparation of 1,5-diketones starting from fragrant aldehydes and fragrant ketones in the presence of NaOH under solvent-free conditions. Using this method, we obtained the title compound, (I) (Fig. 1). The synthesis of many heterocyclic compounds (Hirsch & Bailey, 1978) form an important synthetic intermediate compounds of 1,5-Diketones. Further, compared to existing methods, the main advantages of the present procedure is fast reaction times, solvent-free, mild, simple, moderately high yields and no side product formation.

The structures of related compounds *viz*., 3-(2-Chlorophenyl)-1,5-bis(4-nitrophenyl)pentane-1,5-dione (Qiu *et al.* 2006), 1,5-Bis(4-chlorophenyl)-3- (2-chloroquinolin-3-yl)pentane-1,5-dione (Insuasty *et al.* 2006), 3-(2-Chlorophenyl)-1,5-bis-(4-chlorophenyl)pentane-1,5-dione (Jasinski *et al.* 2007), 1,5-Bis(4-chlorophenyl)-3-(2-thienyl)pentane-1,5-dione (Huang *et al.* 2008), 1,5-Bis(4-chlorophenyl)-3-[4-(dimethylamino)phenyl]pentane-1,5-dione (Lei & Bai, 2009), 3-(3-Bromo-4-methoxyphenyl)-1,5-diphenylpentane-1,5-dione (Dutkiewicz *et al.* 2010) and 1,5-Bis(thiophen-2-yl)-3-(2,4,5-trimethoxy-phenyl) pentane-1,5-dione (Fun *et al.* 2011) have been reported. Many promising applications from linear $\pi$-conjugated organic molecules and polymers have attracted considerable interest for organic light-emitting diodes, non-linear optical properties, conductivity, photocells, field effect transistors, and so on due to their delocalized $\pi$ systems (Burroughes *et al.*, 1990; Smith *et al.*, 2005; Li *et al.*, 2004; Sariciftci *et al.*, 1992). A new title compound was synthesized and the crystal structure is reported here.

In the title molecule, $C_{24}H_{20}Cl_2O_2$, (Fig. 1), the pentane-1,5-dione unit (C1—C5/O1/O5) is puckered with the torsion angles C1—C2—C3—C4 = 72.49 (19)° and C2—C3—C4—C5 = -179.02 (16)°, making the two ketone groups pointing towards opposite directions. The central methylbenzene ring forms dihedral angles of 42.47 (10) and 34.34 (10)° with the two terminal 4-chlorophenyl fragments. The dihedral angle between the two chlorobenzene rings is 34.45 (11)°. A weak intramolecular C4—H4A···O1 interaction (Table 1) which generates an S(6) ring motif (Bernstein *et al.*, 1995) helps to stabilize this conformation. The crystal packing exhibits weak intermolecular C16—H16···O5 hydrogen bonded C(9) chains (Bernstein *et al.*, 1995) and C55—H55···$\pi$ interactions involving (C31—C36) methylbenzene ring (Table 1, Fig. 2 & Fig. 3). The C—C, $C_{ar}$—$C_{ar}$, C—Cl and C=O bond lengths in (I) are within their normal ranges (Allen *et al.*, 1987).

### S2. Experimental

The title compound was synthesized according to a modified solvent-free greener approach method (Yang *et al.*, 2005). 4-Chloroacetophenone (0.5 g, 3 mmol), 1-(4-chlorophenyl)-3-(4-methylpenyl)prop-2-ene-1-one (0.8 g, 4 mmol) and commercial powdered NaOH (0.06 g, 1.5 mmol) were crushed together for 20 mt s, using a pestle and mortar. Recystallization from methanol gave colourless crystals. Yield: 1.1 g (90%).

### S3. Refinement

All H-atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 (aromatic), 0.97 (methylene group) and 0.98 Å (methine), with $U_{iso}$(H) = 1.2$U_{eq}$(C); 0.96 Å, $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl group.

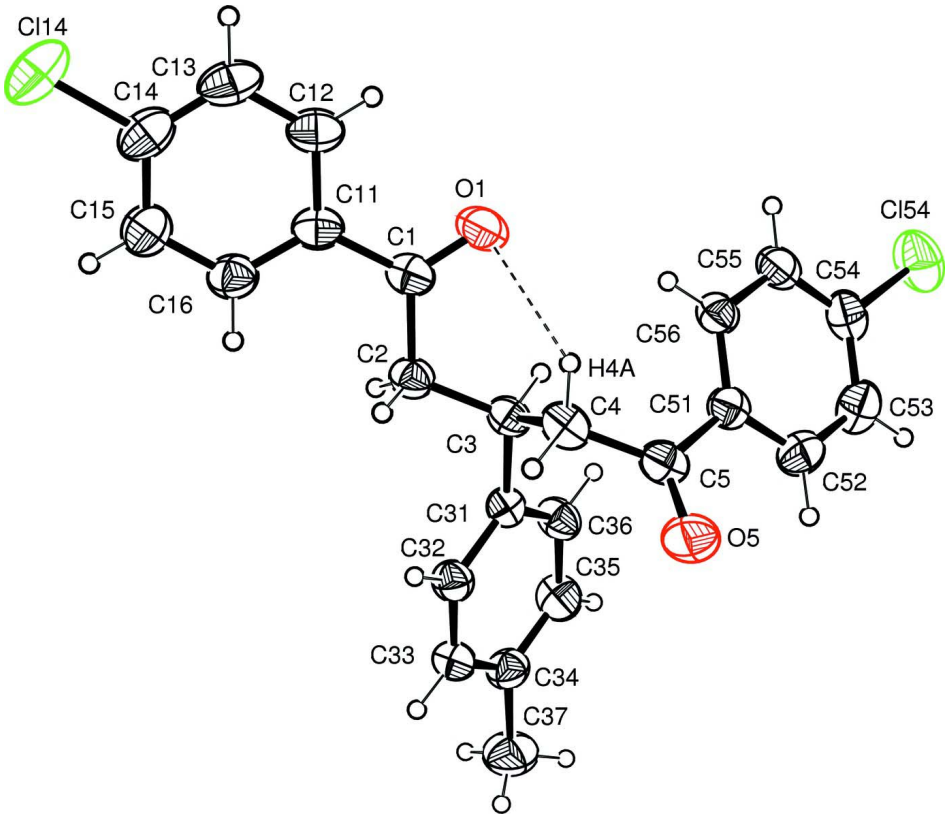


**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius. The dashed line indicates a weak C—H···O intramolecular hydrogen bond.

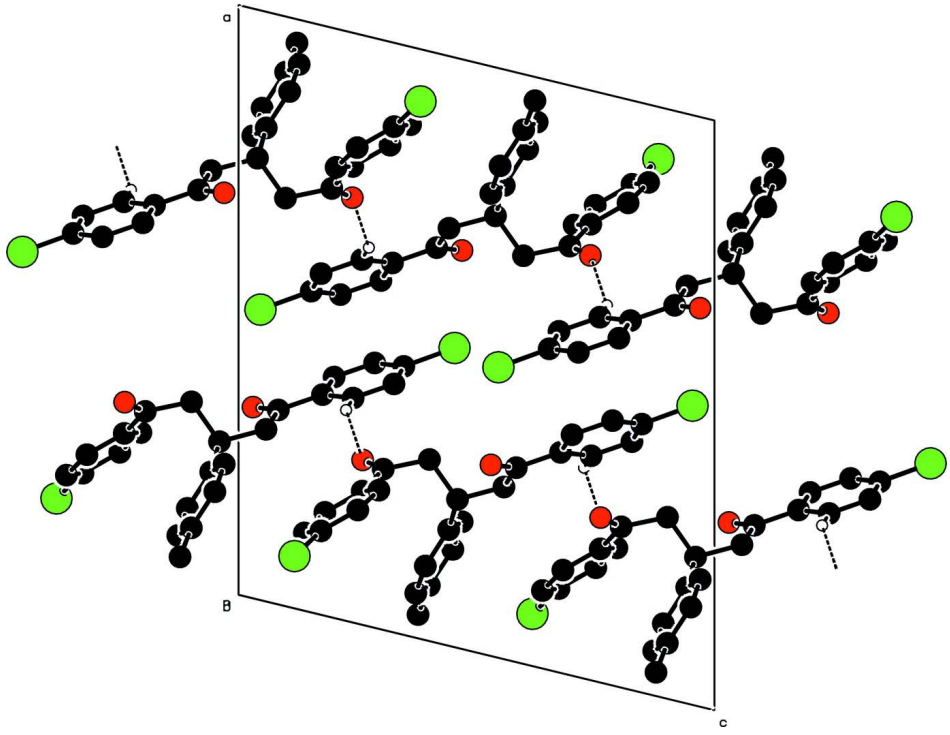


**Figure 2**

The partial packing of the title compound, viewed along the *b* axis. Dashed lines indicate hydrogen-bonded C(9) chains along the *c* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

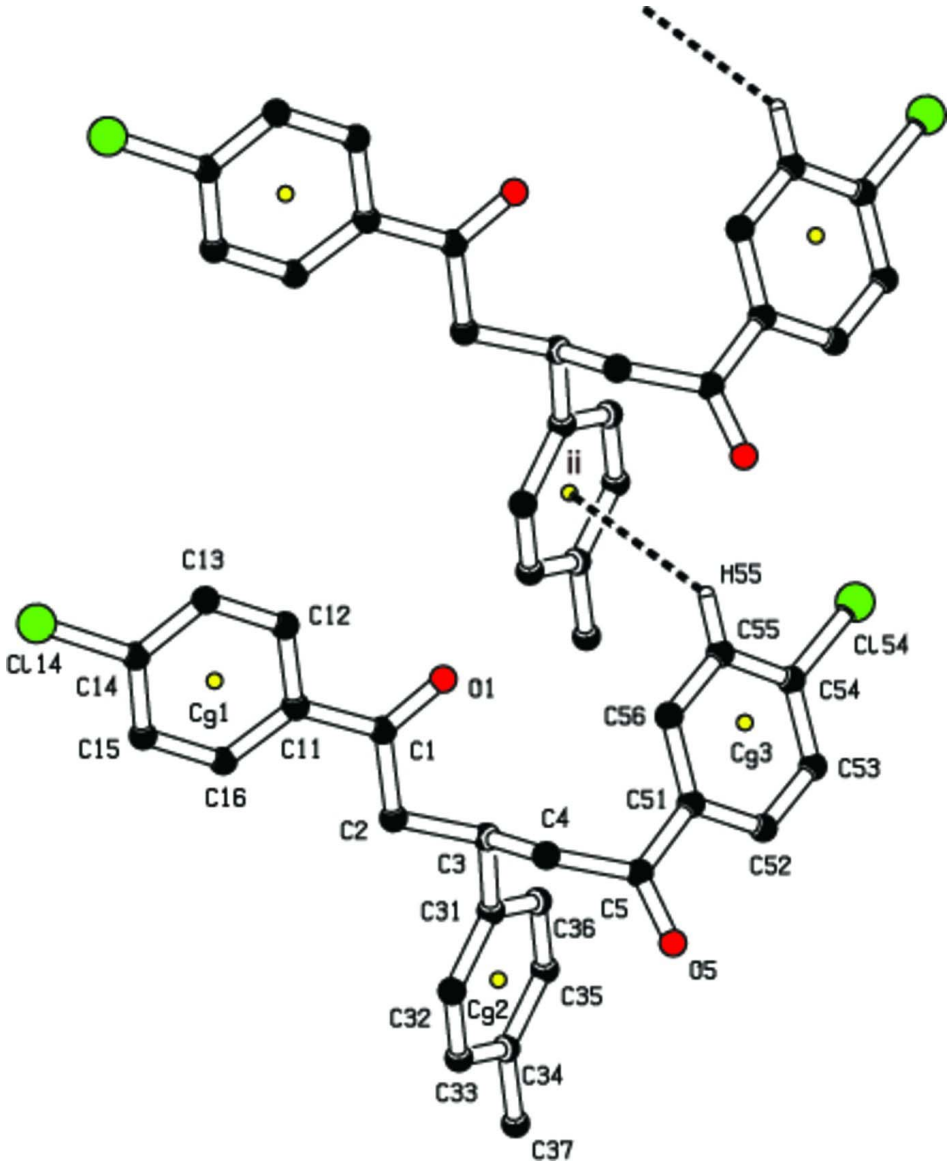


**Figure 3**

Crystal structure of the title compound, showing the formation of a C—H···$\pi$ interaction. Symmetry code (ii): $x$, $y$ + 1, $z$.

**1,5-Bis(4-chlorophenyl)-3-(4-methylphenyl)pentane-1,5-dione**

*Crystal data*

$C_{24}H_{20}Cl_2O_2$
$M_r$ = 411.30
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 18.6794 (11) Å
$b$ = 7.5477 (4) Å
$c$ = 15.5196 (8) Å
$\beta$ = 103.622 (5)°
$V$ = 2126.5 (2) Å$^3$
$Z$ = 4

$F(000)$ = 856
$D_x$ = 1.285 Mg m$^{-3}$
Melting point: 327(2) K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5569 reflections
$\theta$ = 3.3–75.4°
$\mu$ = 0.32 mm$^{-1}$
$T$ = 296 K
Prism, colourless
0.51 × 0.42 × 0.37 mm

*Data collection*

Agilent Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.443, $T_{max}$ = 1.000
14252 measured reflections
4341 independent reflections
3735 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 26.5°, $\theta_{min}$ = 2.2°
$h$ = −23→21
$k$ = −9→8
$l$ = −19→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.146
$S$ = 1.07
4341 reflections
255 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 0.5487P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$
Extinction correction: *SHELXL2013* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0227 (17)

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl14 | 0.50733 (5) | 0.76817 (14) | 0.95387 (6) | 0.1283 (4) |
| Cl54 | 0.08862 (5) | 1.03187 (11) | 0.11762 (5) | 0.1154 (3) |
| O1 | 0.32422 (10) | 0.76750 (19) | 0.53035 (12) | 0.0873 (6) |
| O5 | 0.27979 (11) | 0.3043 (2) | 0.26076 (12) | 0.0939 (7) |
| C1 | 0.32982 (10) | 0.6468 (3) | 0.58359 (14) | 0.0638 (6) |
| C2 | 0.29189 (10) | 0.4711 (2) | 0.55773 (13) | 0.0621 (6) |
| C3 | 0.25188 (9) | 0.4591 (2) | 0.46011 (12) | 0.0555 (5) |
| C4 | 0.30797 (10) | 0.4435 (3) | 0.40126 (13) | 0.0647 (6) |
| C5 | 0.27264 (11) | 0.4342 (3) | 0.30405 (14) | 0.0644 (6) |
| C11 | 0.37394 (9) | 0.6711 (3) | 0.67653 (14) | 0.0626 (6) |
| C12 | 0.40855 (12) | 0.8328 (3) | 0.70082 (17) | 0.0809 (8) |
| C13 | 0.44906 (13) | 0.8624 (4) | 0.7860 (2) | 0.0933 (10) |
| C14 | 0.45523 (12) | 0.7294 (4) | 0.84725 (17) | 0.0838 (9) |
| C15 | 0.42146 (13) | 0.5692 (3) | 0.82660 (16) | 0.0813 (8) |
| C16 | 0.38072 (11) | 0.5404 (3) | 0.74081 (14) | 0.0705 (7) |
| C31 | 0.19689 (9) | 0.3081 (2) | 0.44168 (11) | 0.0525 (5) |
| C32 | 0.21576 (10) | 0.1365 (2) | 0.46994 (12) | 0.0596 (5) |
| C33 | 0.16507 (11) | 0.0008 (3) | 0.45037 (13) | 0.0649 (6) |
| C34 | 0.09424 (12) | 0.0296 (3) | 0.40097 (13) | 0.0676 (6) |
| C35 | 0.07564 (11) | 0.1993 (3) | 0.37249 (15) | 0.0754 (7) |

| | | | | |
|---|---|---|---|---|
| C36 | 0.12561 (10) | 0.3367 (3) | 0.39251 (14) | 0.0668 (6) |
| C37 | 0.04025 (16) | −0.1219 (4) | 0.3772 (2) | 0.1036 (10) |
| C51 | 0.22673 (10) | 0.5860 (2) | 0.25994 (12) | 0.0591 (6) |
| C52 | 0.17530 (13) | 0.5558 (3) | 0.18151 (14) | 0.0766 (8) |
| C53 | 0.13217 (14) | 0.6916 (4) | 0.13849 (15) | 0.0844 (9) |
| C54 | 0.14217 (13) | 0.8596 (3) | 0.17322 (14) | 0.0739 (7) |
| C55 | 0.19288 (12) | 0.8948 (3) | 0.25063 (14) | 0.0701 (7) |
| C56 | 0.23502 (11) | 0.7562 (2) | 0.29495 (13) | 0.0619 (6) |
| H2A | 0.25663 | 0.45128 | 0.59369 | 0.0745* |
| H2B | 0.32834 | 0.37735 | 0.57095 | 0.0745* |
| H3 | 0.22450 | 0.56978 | 0.44428 | 0.0666* |
| H4A | 0.34075 | 0.54492 | 0.41221 | 0.0776* |
| H4B | 0.33758 | 0.33800 | 0.41830 | 0.0776* |
| H12 | 0.40425 | 0.92255 | 0.65885 | 0.0970* |
| H13 | 0.47188 | 0.97108 | 0.80159 | 0.1118* |
| H15 | 0.42573 | 0.48107 | 0.86937 | 0.0975* |
| H16 | 0.35758 | 0.43174 | 0.72612 | 0.0846* |
| H32 | 0.26327 | 0.11248 | 0.50255 | 0.0714* |
| H33 | 0.17890 | −0.11285 | 0.47092 | 0.0778* |
| H35 | 0.02834 | 0.22220 | 0.33896 | 0.0905* |
| H36 | 0.11120 | 0.45041 | 0.37267 | 0.0802* |
| H37A | 0.01457 | −0.13765 | 0.42342 | 0.1553* |
| H37B | 0.06642 | −0.22851 | 0.37049 | 0.1553* |
| H37C | 0.00548 | −0.09558 | 0.32250 | 0.1553* |
| H52 | 0.16976 | 0.44229 | 0.15749 | 0.0920* |
| H53 | 0.09667 | 0.66994 | 0.08653 | 0.1012* |
| H55 | 0.19902 | 1.00942 | 0.27314 | 0.0842* |
| H56 | 0.26892 | 0.77754 | 0.34828 | 0.0742* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl14 | 0.1032 (5) | 0.1647 (9) | 0.1004 (5) | −0.0240 (5) | −0.0091 (4) | −0.0387 (5) |
| Cl54 | 0.1193 (6) | 0.1104 (6) | 0.1139 (6) | 0.0419 (4) | 0.0225 (4) | 0.0407 (4) |
| O1 | 0.0932 (11) | 0.0590 (8) | 0.0993 (11) | −0.0099 (8) | 0.0019 (9) | 0.0133 (8) |
| O5 | 0.1211 (14) | 0.0656 (9) | 0.1022 (12) | 0.0217 (9) | 0.0405 (11) | −0.0103 (8) |
| C1 | 0.0529 (9) | 0.0552 (10) | 0.0820 (12) | 0.0002 (8) | 0.0131 (8) | 0.0033 (9) |
| C2 | 0.0566 (10) | 0.0565 (10) | 0.0712 (11) | −0.0045 (8) | 0.0112 (8) | 0.0022 (8) |
| C3 | 0.0497 (8) | 0.0505 (9) | 0.0668 (10) | 0.0040 (7) | 0.0150 (7) | 0.0062 (7) |
| C4 | 0.0532 (9) | 0.0616 (10) | 0.0823 (12) | 0.0055 (8) | 0.0222 (9) | 0.0091 (9) |
| C5 | 0.0671 (11) | 0.0552 (10) | 0.0787 (12) | 0.0025 (8) | 0.0326 (9) | 0.0011 (9) |
| C11 | 0.0463 (9) | 0.0605 (10) | 0.0822 (12) | −0.0050 (8) | 0.0174 (8) | −0.0064 (9) |
| C12 | 0.0711 (13) | 0.0719 (13) | 0.1003 (16) | −0.0206 (10) | 0.0214 (11) | −0.0078 (12) |
| C13 | 0.0734 (14) | 0.0910 (17) | 0.115 (2) | −0.0313 (13) | 0.0215 (13) | −0.0300 (15) |
| C14 | 0.0568 (11) | 0.1059 (18) | 0.0862 (15) | −0.0097 (11) | 0.0121 (10) | −0.0243 (14) |
| C15 | 0.0712 (13) | 0.0886 (15) | 0.0796 (14) | −0.0029 (11) | 0.0088 (10) | −0.0025 (12) |
| C16 | 0.0611 (11) | 0.0675 (12) | 0.0801 (13) | −0.0088 (9) | 0.0109 (9) | −0.0048 (10) |
| C31 | 0.0515 (8) | 0.0530 (9) | 0.0538 (9) | 0.0018 (7) | 0.0142 (7) | 0.0021 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C32 | 0.0578 (9) | 0.0564 (9) | 0.0618 (10) | 0.0035 (8) | 0.0088 (7) | 0.0024 (8) |
| C33 | 0.0763 (12) | 0.0512 (9) | 0.0673 (11) | −0.0017 (8) | 0.0174 (9) | 0.0012 (8) |
| C34 | 0.0693 (11) | 0.0680 (11) | 0.0656 (11) | −0.0139 (9) | 0.0161 (9) | −0.0065 (9) |
| C35 | 0.0532 (10) | 0.0831 (14) | 0.0836 (14) | −0.0055 (10) | 0.0034 (9) | 0.0072 (11) |
| C36 | 0.0554 (10) | 0.0615 (10) | 0.0802 (12) | 0.0041 (8) | 0.0094 (9) | 0.0126 (9) |
| C37 | 0.0965 (18) | 0.0865 (16) | 0.120 (2) | −0.0326 (15) | 0.0096 (15) | −0.0107 (15) |
| C51 | 0.0632 (10) | 0.0577 (10) | 0.0627 (10) | 0.0011 (8) | 0.0274 (8) | 0.0007 (8) |
| C52 | 0.0894 (15) | 0.0721 (13) | 0.0706 (12) | 0.0036 (11) | 0.0232 (11) | −0.0134 (10) |
| C53 | 0.0842 (15) | 0.1014 (17) | 0.0645 (12) | 0.0120 (13) | 0.0116 (10) | −0.0041 (12) |
| C54 | 0.0799 (13) | 0.0783 (13) | 0.0691 (12) | 0.0179 (11) | 0.0291 (10) | 0.0167 (10) |
| C55 | 0.0856 (13) | 0.0558 (10) | 0.0752 (12) | 0.0018 (9) | 0.0313 (10) | 0.0071 (9) |
| C56 | 0.0692 (11) | 0.0561 (10) | 0.0632 (10) | −0.0044 (8) | 0.0214 (8) | 0.0026 (8) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Cl14—C14 | 1.736 (3) | C51—C56 | 1.389 (2) |
| Cl54—C54 | 1.741 (2) | C52—C53 | 1.376 (4) |
| O1—C1 | 1.218 (3) | C53—C54 | 1.373 (4) |
| O5—C5 | 1.214 (3) | C54—C55 | 1.369 (3) |
| C1—C2 | 1.513 (3) | C55—C56 | 1.390 (3) |
| C1—C11 | 1.495 (3) | C2—H2A | 0.9700 |
| C2—C3 | 1.526 (3) | C2—H2B | 0.9700 |
| C3—C4 | 1.548 (3) | C3—H3 | 0.9800 |
| C3—C31 | 1.516 (2) | C4—H4A | 0.9700 |
| C4—C5 | 1.499 (3) | C4—H4B | 0.9700 |
| C5—C51 | 1.497 (3) | C12—H12 | 0.9300 |
| C11—C12 | 1.391 (3) | C13—H13 | 0.9300 |
| C11—C16 | 1.387 (3) | C15—H15 | 0.9300 |
| C12—C13 | 1.378 (4) | C16—H16 | 0.9300 |
| C13—C14 | 1.369 (4) | C32—H32 | 0.9300 |
| C14—C15 | 1.367 (4) | C33—H33 | 0.9300 |
| C15—C16 | 1.386 (3) | C35—H35 | 0.9300 |
| C31—C32 | 1.386 (2) | C36—H36 | 0.9300 |
| C31—C36 | 1.387 (3) | C37—H37A | 0.9600 |
| C32—C33 | 1.379 (3) | C37—H37B | 0.9600 |
| C33—C34 | 1.381 (3) | C37—H37C | 0.9600 |
| C34—C35 | 1.373 (3) | C52—H52 | 0.9300 |
| C34—C37 | 1.512 (4) | C53—H53 | 0.9300 |
| C35—C36 | 1.381 (3) | C55—H55 | 0.9300 |
| C51—C52 | 1.381 (3) | C56—H56 | 0.9300 |
| | | | |
| O1—C1—C2 | 121.06 (19) | C1—C2—H2B | 109.00 |
| O1—C1—C11 | 120.2 (2) | C3—C2—H2A | 109.00 |
| C2—C1—C11 | 118.76 (18) | C3—C2—H2B | 109.00 |
| C1—C2—C3 | 113.88 (15) | H2A—C2—H2B | 108.00 |
| C2—C3—C4 | 110.43 (15) | C2—C3—H3 | 108.00 |
| C2—C3—C31 | 112.56 (14) | C4—C3—H3 | 108.00 |
| C4—C3—C31 | 110.75 (14) | C31—C3—H3 | 108.00 |

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| C3—C4—C5 | 113.49 (16) | C3—C4—H4A | 109.00 |
| O5—C5—C4 | 121.0 (2) | C3—C4—H4B | 109.00 |
| O5—C5—C51 | 119.42 (19) | C5—C4—H4A | 109.00 |
| C4—C5—C51 | 119.57 (18) | C5—C4—H4B | 109.00 |
| C1—C11—C12 | 119.0 (2) | H4A—C4—H4B | 108.00 |
| C1—C11—C16 | 122.9 (2) | C11—C12—H12 | 119.00 |
| C12—C11—C16 | 118.1 (2) | C13—C12—H12 | 119.00 |
| C11—C12—C13 | 121.2 (2) | C12—C13—H13 | 120.00 |
| C12—C13—C14 | 119.0 (3) | C14—C13—H13 | 121.00 |
| Cl14—C14—C13 | 118.4 (2) | C14—C15—H15 | 121.00 |
| Cl14—C14—C15 | 119.8 (2) | C16—C15—H15 | 121.00 |
| C13—C14—C15 | 121.8 (2) | C11—C16—H16 | 119.00 |
| C14—C15—C16 | 118.9 (2) | C15—C16—H16 | 119.00 |
| C11—C16—C15 | 121.0 (2) | C31—C32—H32 | 120.00 |
| C3—C31—C32 | 122.17 (15) | C33—C32—H32 | 120.00 |
| C3—C31—C36 | 120.46 (15) | C32—C33—H33 | 119.00 |
| C32—C31—C36 | 117.34 (17) | C34—C33—H33 | 119.00 |
| C31—C32—C33 | 120.93 (18) | C34—C35—H35 | 119.00 |
| C32—C33—C34 | 121.6 (2) | C36—C35—H35 | 119.00 |
| C33—C34—C35 | 117.5 (2) | C31—C36—H36 | 119.00 |
| C33—C34—C37 | 120.9 (2) | C35—C36—H36 | 119.00 |
| C35—C34—C37 | 121.6 (2) | C34—C37—H37A | 109.00 |
| C34—C35—C36 | 121.5 (2) | C34—C37—H37B | 109.00 |
| C31—C36—C35 | 121.2 (2) | C34—C37—H37C | 109.00 |
| C5—C51—C52 | 118.80 (17) | H37A—C37—H37B | 110.00 |
| C5—C51—C56 | 122.00 (17) | H37A—C37—H37C | 109.00 |
| C52—C51—C56 | 119.20 (17) | H37B—C37—H37C | 109.00 |
| C51—C52—C53 | 120.8 (2) | C51—C52—H52 | 120.00 |
| C52—C53—C54 | 119.2 (2) | C53—C52—H52 | 120.00 |
| Cl54—C54—C53 | 119.08 (18) | C52—C53—H53 | 120.00 |
| Cl54—C54—C55 | 119.21 (18) | C54—C53—H53 | 120.00 |
| C53—C54—C55 | 121.7 (2) | C54—C55—H55 | 121.00 |
| C54—C55—C56 | 118.8 (2) | C56—C55—H55 | 121.00 |
| C51—C56—C55 | 120.30 (18) | C51—C56—H56 | 120.00 |
| C1—C2—H2A | 109.00 | C55—C56—H56 | 120.00 |

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| O1—C1—C2—C3 | 3.7 (3) | C12—C13—C14—Cl14 | 179.28 (19) |
| C11—C1—C2—C3 | −177.04 (16) | C12—C13—C14—C15 | −1.0 (4) |
| O1—C1—C11—C12 | −0.3 (3) | Cl14—C14—C15—C16 | −179.36 (18) |
| O1—C1—C11—C16 | 178.2 (2) | C13—C14—C15—C16 | 0.9 (4) |
| C2—C1—C11—C12 | −179.59 (18) | C14—C15—C16—C11 | −0.1 (3) |
| C2—C1—C11—C16 | −1.1 (3) | C3—C31—C32—C33 | −178.41 (17) |
| C1—C2—C3—C4 | 72.49 (19) | C36—C31—C32—C33 | −0.6 (3) |
| C1—C2—C3—C31 | −163.18 (15) | C3—C31—C36—C35 | 177.69 (18) |
| C2—C3—C4—C5 | −179.02 (16) | C32—C31—C36—C35 | −0.1 (3) |
| C31—C3—C4—C5 | 55.6 (2) | C31—C32—C33—C34 | 1.0 (3) |
| C2—C3—C31—C32 | −51.0 (2) | C32—C33—C34—C35 | −0.6 (3) |
| C2—C3—C31—C36 | 131.25 (18) | C32—C33—C34—C37 | 177.7 (2) |

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| C4—C3—C31—C32 | 73.1 (2) | C33—C34—C35—C36 | −0.2 (3) |
| C4—C3—C31—C36 | −104.60 (19) | C37—C34—C35—C36 | −178.4 (2) |
| C3—C4—C5—O5 | −117.3 (2) | C34—C35—C36—C31 | 0.5 (3) |
| C3—C4—C5—C51 | 61.6 (2) | C5—C51—C52—C53 | −179.7 (2) |
| O5—C5—C51—C52 | 20.8 (3) | C56—C51—C52—C53 | −0.5 (3) |
| O5—C5—C51—C56 | −158.4 (2) | C5—C51—C56—C55 | 178.05 (19) |
| C4—C5—C51—C52 | −158.1 (2) | C52—C51—C56—C55 | −1.1 (3) |
| C4—C5—C51—C56 | 22.7 (3) | C51—C52—C53—C54 | 1.8 (4) |
| C1—C11—C12—C13 | 179.2 (2) | C52—C53—C54—Cl54 | 178.90 (19) |
| C16—C11—C12—C13 | 0.6 (3) | C52—C53—C54—C55 | −1.4 (4) |
| C1—C11—C16—C15 | −179.2 (2) | Cl54—C54—C55—C56 | 179.52 (17) |
| C12—C11—C16—C15 | −0.7 (3) | C53—C54—C55—C56 | −0.1 (4) |
| C11—C12—C13—C14 | 0.2 (4) | C54—C55—C56—C51 | 1.4 (3) |

*Hydrogen-bond geometry (Å, º)*

Cg2 is the centroid of the (C31-C36) methylbenzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4*A*···O1 | 0.97 | 2.56 | 3.130 (3) | 118 |
| C16—H16···O5$^{i}$ | 0.93 | 2.44 | 3.270 (3) | 149 |
| C55—H55···*Cg*2$^{ii}$ | 0.93 | 2.97 | 3.629 (2) | 129 |

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