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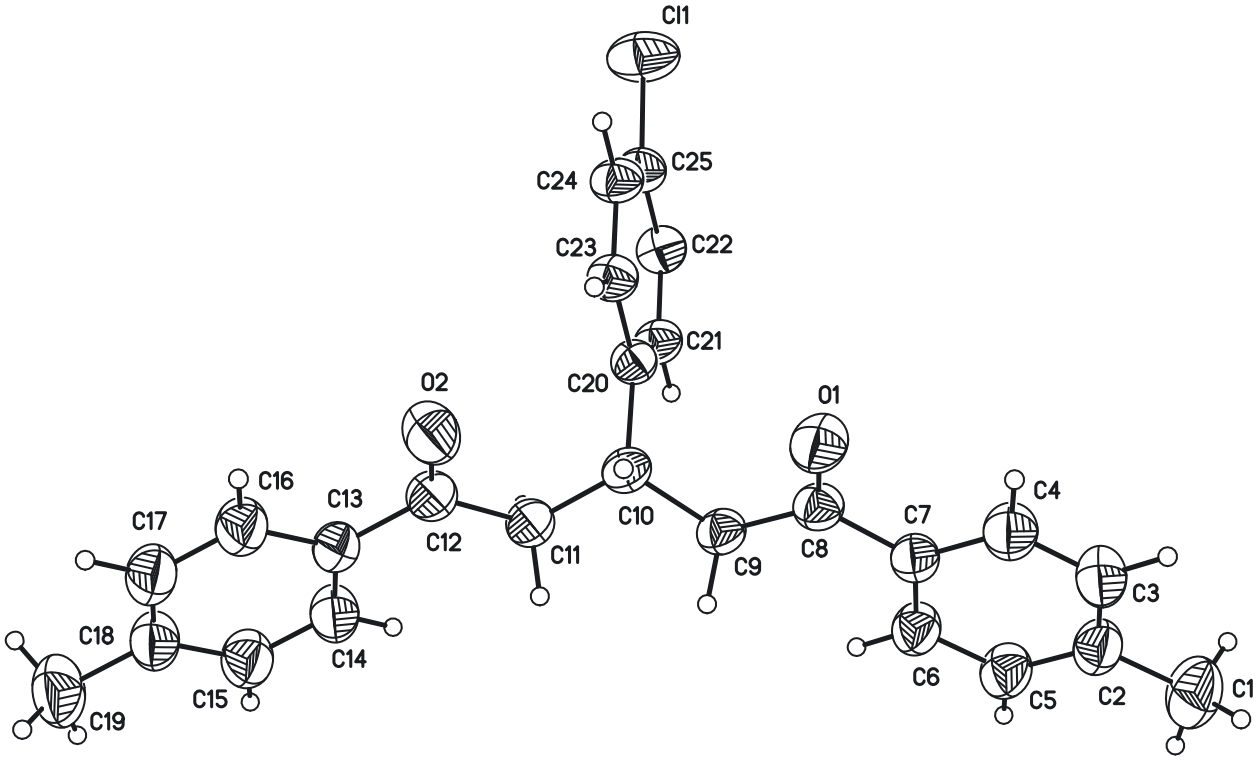
# The crystal structure of 3-(4-chlorophenyl)-1,5-di-*p*-tolylpentane-1,5-dione, $C_{25}H_{23}ClO_2$

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**Abstract**

$C_{25}H_{23}ClO_2$, orthorhombic, $P2_12_12_1$, $a$ = 5.5648(5) Å, $b$ = 17.6062(15) Å, $c$ = 21.5033(19) Å, $V$ = 2106.8(3) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0529, $wR_{ref}(F^2)$ = 0.1371, T = 298 K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colorless block |
| Size: | 0.13 × 0.12 × 0.11 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.20 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART, $\varphi$ and $\omega$-scans |
| $\theta_{max}$, completeness: | 25°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 10,728, 3700, 0.077 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 1931 |
| $N(param)_{refined}$: | 255 |
| Programs: | Bruker programs [1], SHELX [2] |

## Source of materials

In a typical experiment, 4-chlorobenzaldehyde (0.5 mmol), 4-methylacetophenone (1 mmol) and commercial powdered NaOH (1 mmol) were crushed together for 60 min. After the reaction was completed, the mixture was washed by hot water and recystallized from methanol, the colourless crystals were achieved, yield: 81%.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 1.2006 (7) | 0.0135 (2) | 0.33311 (17) | 0.0952 (12) |
| O2 | 1.0145 (9) | 0.0085 (2) | 0.11194 (17) | 0.1138 (14) |
| Cl1 | 0.7099 (3) | −0.31333 (8) | 0.25143 (9) | 0.1188 (7) |
| C1 | 0.9177 (14) | 0.1757 (4) | 0.5917 (3) | 0.131 (2) |
| H1A | 0.875125 | 0.135156 | 0.619460 | 0.197* |
| H1B | 0.792941 | 0.213345 | 0.591814 | 0.197* |
| H1C | 1.065782 | 0.198344 | 0.605179 | 0.197* |
| C2 | 0.9482 (13) | 0.1446 (3) | 0.5267 (3) | 0.0880 (16) |
| C3 | 1.1334 (12) | 0.0989 (3) | 0.5114 (3) | 0.0978 (16) |
| H3 | 1.248065 | 0.087287 | 0.541413 | 0.117* |
| C4 | 1.1570 (12) | 0.0693 (3) | 0.4531 (3) | 0.0924 (15) |
| H4 | 1.287364 | 0.038084 | 0.444201 | 0.111* |
| C5 | 0.7814 (12) | 0.1598 (3) | 0.4825 (3) | 0.0926 (15) |
| H5 | 0.650418 | 0.190386 | 0.492231 | 0.111* |
| C6 | 0.8031 (10) | 0.1306 (3) | 0.4229 (2) | 0.0831 (14) |
| H6 | 0.687548 | 0.142178 | 0.393114 | 0.100* |
| C7 | 0.9929 (10) | 0.0847 (3) | 0.4072 (2) | 0.0703 (12) |
| C8 | 1.0245 (10) | 0.0508 (3) | 0.3449 (2) | 0.0690 (12) |
| C9 | 0.8354 (9) | 0.0637 (3) | 0.2968 (2) | 0.0687 (12) |
| H9A | 0.822426 | 0.117790 | 0.288945 | 0.082* |
| H9B | 0.682109 | 0.046527 | 0.313087 | 0.082* |
| C10 | 0.8845 (9) | 0.0228 (2) | 0.2351 (2) | 0.0658 (12) |
| H10 | 1.054317 | 0.030387 | 0.224701 | 0.079* |
| C11 | 0.7336 (10) | 0.0584 (3) | 0.1830 (2) | 0.0732 (13) |
| H11A | 0.572474 | 0.037491 | 0.184778 | 0.088* |
| H11B | 0.721611 | 0.112629 | 0.190217 | 0.088* |
| C12 | 0.8334 (11) | 0.0455 (3) | 0.1189 (2) | 0.0776 (13) |
| C13 | 0.7105 (10) | 0.0809 (3) | 0.0653 (2) | 0.0755 (13) |
| C14 | 0.5094 (12) | 0.1237 (3) | 0.0701 (3) | 0.0929 (15) |
| H14 | 0.437999 | 0.130434 | 0.108793 | 0.111* |
| C15 | 0.4096 (12) | 0.1572 (3) | 0.0188 (3) | 0.1040 (17) |
| H15 | 0.272539 | 0.186788 | 0.023594 | 0.125* |
| C16 | 0.8138 (12) | 0.0726 (3) | 0.0068 (3) | 0.0957 (15) |
| H16 | 0.953902 | 0.044343 | 0.002119 | 0.115* |
| C17 | 0.7090 (13) | 0.1060 (3) | −0.0441 (3) | 0.1007 (17) |
| H17 | 0.779074 | 0.099580 | −0.083047 | 0.121* |
| C18 | 0.5050 (13) | 0.1484 (3) | −0.0392 (3) | 0.0953 (16) |
| C19 | 0.3939 (14) | 0.1853 (4) | −0.0957 (3) | 0.136 (3) |
| H19A | 0.260560 | 0.216257 | −0.083141 | 0.204* |
| H19B | 0.338794 | 0.146651 | −0.123848 | 0.204* |
| H19C | 0.511707 | 0.216317 | −0.116167 | 0.204* |
| C20 | 0.8414 (8) | −0.0616 (2) | 0.2409 (2) | 0.0606 (11) |
| C21 | 0.6331 (9) | −0.0915 (3) | 0.2670 (2) | 0.0690 (12) |
| H21 | 0.515975 | −0.058841 | 0.282371 | 0.083* |
| C22 | 0.5985 (9) | −0.1682 (3) | 0.2704 (2) | 0.0728 (13) |
| H22 | 0.458318 | −0.186939 | 0.288246 | 0.087* |
| C23 | 1.0093 (9) | −0.1127 (2) | 0.2188 (2) | 0.0665 (12) |
| H23 | 1.150957 | −0.094801 | 0.201076 | 0.080* |
| C24 | 0.9695 (9) | −0.1900 (3) | 0.2226 (2) | 0.0703 (13) |
| H24 | 1.084460 | −0.223609 | 0.207572 | 0.084* |
| C25 | 0.7641 (9) | −0.2172 (2) | 0.2483 (2) | 0.0677 (12) |

# Experimental details

All hydrogen atomic positions were taken from a difference Fourier map. Hydrogen atoms were assigned with common isotropic displacement factors $U_{iso}$(H) = 1.2 times $U_{eq}$(C, phenyl ring and methylene carbon) and $U_{iso}$(H) = 1.5 times $U_{eq}$(C, methyl). All the H atoms were refined as riding on their parent atom.

# Comment

Aromatic 1,5-dione derivatives are one class of important building blocks for preparing organic functional materials [3]. Traditionally, the production process of 1,5-dione derivatives was prepared by the condensation reaction of aromatic aldehydes or chalcone derivatives with aromatic ketones using the NaO-/t-Bu, NaOH, NaOH-$K_2CO_3$ and metallic sodium as the base catalysts, respectively. Subsequently, a series of 1,5-dione derivatives has been reported and their related structures have been studied in detail, for instance, 1,5-bis(4-chlorophenyl)-3-(2-chloroquinolin-3-yl) pentane-1,5-dione [4], 1,5-bis(4-chlorophenyl)-3-(2-thienyl) pentane-1,5-dione [5], 3-(2-chlorophenyl)-1,5-bis-(4-chlorophenyl) pentane-1,5-dione [6], 3-(2-chlorophenyl)-1,5-bis (4-nitrophenyl)pentane-1,5-dione [7], 4-(1,5-bis(2-hydroxyphenyl)-1,5-dioxopentan-3-yl)benzonitrile [8], 1,3,5-triphenylpentane-1,5-dione [9], 1,5-(4-dichlorophenyl)-3-(2, 5-dimethoxy-phenyl)pentane-1,5-dione [10], 3-phenyl-1, 5-di-p-tolylpentane-1,5-dione [11], 3-(3-chlorophenyl)-1, 5-bis(4-nitrophenyl)-pentane-1,5-dione [12], 1-(4-chlorophenyl)-3,5-diphenylpentane-1,5-dione [13], 3-(2-chlorophenyl)-1, 5-bis(4-chloro-phenyl)pentane-1,5-dione [14], 1,5-bis(4-chlorophenyl)-3-(4-methyl-phenyl)pentane-1,5-dione [15], 1,5-bis(4-methoxyphenyl)-3-phenylpentane-1,5-dione [16], 1,5-bis(4-bromophenyl)-3-phenyl-pentane-1, 5-dione [17], 1,5-bis(4-chlorophenyl)-3-phenyl-pentane-1, 5-dione [18], 1,5-bis(4-bromophenyl) 3-(3-nitrophenyl)-pentane-1,5-dione [19], and so on. However, to date, the structure of 3-(4-chlorophenyl)-1,5-di-p-tolylpentane-1,5-dione has not been reported.

In the title molecule, the central chlorobenzene ring and the two *p*-methylphenyl rings forms the dihedral angles of 88.366(2)° and 68.539(2)°, respectively, which reveals that two *p*-methylphenyl rings are almost perpendicular to the central chlorophenyl ring. The dihedral angle between the two *p*-methyl phenyl rings is 24.657(2)° [20, 21]. Additionally, the supermolecular structure of the title compound is

stabilized by the weak C–H···O intramolecular hydrogen-bonding interactions.

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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