Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Chlorophenyl)-3-(2-nitrophenyl)-propane-1,2-dione

Lin Huang,* Shuqin Li and Huisheng Li

Department of Chemistry and Biology, Xiangfan University, Xiangfan 441053, People's Republic of China
Correspondence e-mail: xfhuanglin@163.com

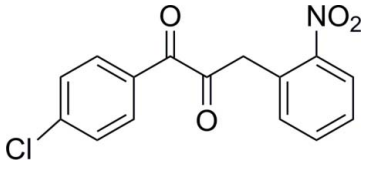
Received 10 September 2008; accepted 22 September 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 12.7.

The title compound, $C_{15}H_{10}ClNO_4$, belongs to the class of 1,2-diketones, which have important applications in both synthetic organic chemistry and supramolecular chemistry. A dihedral angle of 9.03 (1)° is found between the mean planes of the two benzene rings. C—H···O interactions help to stabilize the crystal structure.

Related literature

For the synthesis of the title compound, see: Barnes & Gist (1950). For applications of the title compound, see: Saalfrank *et al.* (1988); Schobert (1988); van Leusen & van Leusen (1977).



Experimental

Crystal data

$C_{15}H_{10}ClNO_4$
M_r = 303.69
Monoclinic, $P2_1/c$
a = 7.9995 (3) Å
b = 6.3730 (2) Å
c = 26.7750 (5) Å
β = 91.340 (2)°
V = 1364.64 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.943, T_{max} = 0.971
8762 measured reflections
2408 independent reflections
1872 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.07
2408 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3^{i}	0.93	2.53	3.279 (3)	138
C15—H15···O1	0.93	2.59	3.244 (3)	128

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Xiangfan University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2095).

References

Barnes, P. R. & Gist, L. A. (1950). *J. Am. Chem. Soc.* **72**, 2509–2510.
Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Leusen, D. van & van Leusen, A. M. (1977). *Tetrahedron Lett.* **18**, 4233–4236.
Saalfrank, R. W., Hafner, W., Markmann, J. & Bestmann, H. J. (1988). *Tetrahedron*, **44**, 5095–5100.
Schobert, R. (1988). *Angew. Chem. Int. Ed.* **27**, 855–856.
Sheldrick, G. M. (1997). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o2024 [doi:10.1107/S1600536808030559]

1-(4-Chlorophenyl)-3-(2-nitrophenyl)propane-1,2-dione

Lin Huang, Shuqin Li and Huisheng Li

S1. Comment

1,2-Diketones are important intermediates in the preparation of heterocyclic compounds in synthetic chemistry (van Leusen & van Leusen, 1977; Saalfrank *et al.*, 1988). In addition, they can also be used as ligands in supramolecular chemistry (Schobert, 1988). The molecular structure of the title compound is shown in Fig. 1. The dihedral angle of the two benzene rings is 9.03 (1)°. Molecules are mainly connected by an intermolecular C—H···O interaction.

S2. Experimental

The title compound was synthesized as previously described by Barnes & Gist (1950). Colorless crystals suitable for X-ray data collection were obtained by slow evaporation of a 5:2 ratio CH_2Cl_2:MeOH solution at 293 K.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C) (1.5U_{eq}(C) for methyl) of the parent atoms.

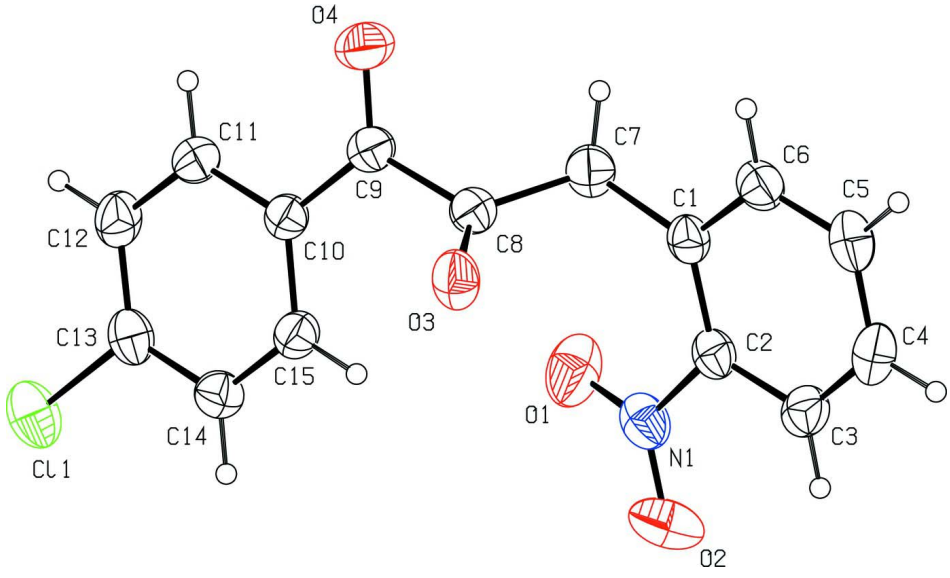


Figure 1

View of the title molecule showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of arbitrary radius.

1-(4-Chlorophenyl)-3-(2-nitrophenyl)propane-1,2-dione

Crystal data

$C_{15}H_{10}ClNO_4$
$M_r = 303.69$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.9995$ (3) Å
$b = 6.3730$ (2) Å
$c = 26.7750$ (5) Å
$\beta = 91.340$ (2)°
$V = 1364.64$ (7) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.478$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2433 reflections
$\theta = 2.6$–$23.4°$
$\mu = 0.30$ mm^{-1}
$T = 298$ K
Block, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{min} = 0.943$, $T_{max} = 0.971$
8762 measured reflections
2408 independent reflections
1872 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 7$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.133$
$S = 1.07$
2408 reflections
190 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.2924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4590 (2)	0.5187 (3)	0.67527 (7)	0.0496 (5)
C2	0.4028 (3)	0.7133 (3)	0.65828 (7)	0.0498 (5)
C3	0.2727 (3)	0.8197 (4)	0.68005 (9)	0.0606 (6)
H3	0.2382	0.9492	0.6676	0.073*
C4	0.1952 (3)	0.7326 (5)	0.72019 (9)	0.0675 (7)
H4	0.1075	0.8028	0.7351	0.081*
C5	0.2471 (3)	0.5421 (4)	0.73831 (9)	0.0669 (7)
H5	0.1947	0.4829	0.7656	0.080*
C6	0.3771 (3)	0.4379 (4)	0.71616 (8)	0.0588 (6)
H6	0.4111	0.3089	0.7291	0.071*
C7	0.6000 (3)	0.3935 (4)	0.65391 (9)	0.0602 (6)
H7A	0.6018	0.2561	0.6695	0.072*
H7B	0.5777	0.3735	0.6185	0.072*

C8	0.7691 (3)	0.4913 (3)	0.66072 (7)	0.0504 (5)
C9	0.9136 (3)	0.3769 (4)	0.63586 (8)	0.0539 (5)
C10	1.0144 (2)	0.4879 (3)	0.59876 (7)	0.0471 (5)
C11	1.1423 (3)	0.3809 (4)	0.57538 (8)	0.0568 (6)
H11	1.1665	0.2433	0.5846	0.068*
C12	1.2338 (3)	0.4757 (4)	0.53865 (8)	0.0631 (6)
H12	1.3183	0.4029	0.5228	0.076*
C13	1.1976 (3)	0.6808 (4)	0.52582 (8)	0.0571 (6)
C14	1.0729 (3)	0.7893 (4)	0.54892 (8)	0.0572 (6)
H14	1.0505	0.9278	0.5401	0.069*
C15	0.9814 (3)	0.6933 (3)	0.58507 (8)	0.0536 (5)
H15	0.8965	0.7669	0.6005	0.064*
Cl1	1.31213 (9)	0.80635 (13)	0.48046 (2)	0.0813 (3)
N1	0.4783 (3)	0.8163 (4)	0.61492 (7)	0.0653 (6)
O1	0.5769 (2)	0.7162 (4)	0.58971 (7)	0.0969 (7)
O2	0.4318 (3)	0.9934 (3)	0.60410 (8)	0.0994 (7)
O3	0.79710 (19)	0.6406 (3)	0.68656 (6)	0.0693 (5)
O4	0.9394 (2)	0.1971 (3)	0.64872 (8)	0.0855 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0428 (11)	0.0539 (13)	0.0520 (11)	−0.0072 (9)	−0.0024 (9)	−0.0057 (10)
C2	0.0441 (11)	0.0588 (14)	0.0463 (11)	−0.0084 (10)	−0.0063 (9)	−0.0001 (10)
C3	0.0509 (13)	0.0614 (15)	0.0687 (15)	0.0020 (11)	−0.0109 (11)	−0.0052 (11)
C4	0.0447 (13)	0.0881 (19)	0.0697 (15)	0.0040 (12)	0.0022 (11)	−0.0143 (14)
C5	0.0516 (14)	0.0881 (19)	0.0614 (14)	−0.0112 (13)	0.0082 (11)	0.0013 (13)
C6	0.0538 (13)	0.0602 (14)	0.0623 (13)	−0.0091 (11)	−0.0032 (10)	0.0065 (11)
C7	0.0574 (14)	0.0606 (14)	0.0627 (13)	−0.0031 (11)	0.0040 (10)	−0.0117 (11)
C8	0.0533 (13)	0.0521 (13)	0.0461 (11)	0.0014 (10)	0.0050 (9)	0.0032 (10)
C9	0.0544 (13)	0.0497 (13)	0.0579 (12)	0.0040 (10)	0.0038 (10)	0.0016 (10)
C10	0.0448 (11)	0.0478 (12)	0.0485 (11)	0.0002 (9)	−0.0008 (9)	−0.0050 (9)
C11	0.0542 (13)	0.0491 (13)	0.0676 (14)	0.0044 (10)	0.0066 (10)	−0.0056 (10)
C12	0.0537 (14)	0.0705 (17)	0.0655 (14)	0.0015 (12)	0.0141 (11)	−0.0154 (12)
C13	0.0509 (13)	0.0724 (17)	0.0479 (12)	−0.0099 (11)	0.0004 (10)	−0.0030 (10)
C14	0.0580 (13)	0.0548 (13)	0.0589 (13)	−0.0014 (11)	0.0016 (10)	0.0049 (10)
C15	0.0492 (12)	0.0549 (14)	0.0568 (12)	0.0055 (10)	0.0047 (9)	0.0001 (10)
Cl1	0.0776 (5)	0.1050 (6)	0.0619 (4)	−0.0200 (4)	0.0179 (3)	0.0070 (3)
N1	0.0593 (12)	0.0772 (16)	0.0588 (12)	−0.0135 (11)	−0.0082 (10)	0.0125 (11)
O1	0.0753 (13)	0.143 (2)	0.0732 (13)	0.0231 (13)	0.0198 (10)	0.0355 (12)
O2	0.140 (2)	0.0620 (13)	0.0966 (14)	−0.0183 (13)	0.0092 (13)	0.0166 (11)
O3	0.0546 (9)	0.0763 (11)	0.0774 (11)	−0.0077 (8)	0.0083 (8)	−0.0257 (9)
O4	0.0905 (14)	0.0608 (12)	0.1068 (14)	0.0187 (10)	0.0394 (11)	0.0232 (10)

Geometric parameters (Å, º)

C1—C6	1.388 (3)	C8—C9	1.532 (3)
C1—C2	1.392 (3)	C9—O4	1.213 (3)

C1—C7	1.505 (3)	C9—C10	1.475 (3)
C2—C3	1.382 (3)	C10—C15	1.383 (3)
C2—N1	1.475 (3)	C10—C11	1.390 (3)
C3—C4	1.371 (3)	C11—C12	1.379 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.368 (4)	C12—C13	1.380 (3)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.380 (3)	C13—C14	1.373 (3)
C5—H5	0.9300	C13—Cl1	1.734 (2)
C6—H6	0.9300	C14—C15	1.371 (3)
C7—C8	1.497 (3)	C14—H14	0.9300
C7—H7A	0.9700	C15—H15	0.9300
C7—H7B	0.9700	N1—O2	1.221 (3)
C8—O3	1.195 (3)	N1—O1	1.229 (3)

C6—C1—C2	115.7 (2)	C7—C8—C9	115.99 (19)
C6—C1—C7	118.3 (2)	O4—C9—C10	123.5 (2)
C2—C1—C7	126.0 (2)	O4—C9—C8	116.8 (2)
C3—C2—C1	122.7 (2)	C10—C9—C8	119.63 (19)
C3—C2—N1	116.1 (2)	C15—C10—C11	118.9 (2)
C1—C2—N1	121.2 (2)	C15—C10—C9	121.91 (19)
C4—C3—C2	119.4 (2)	C11—C10—C9	119.2 (2)
C4—C3—H3	120.3	C12—C11—C10	120.9 (2)
C2—C3—H3	120.3	C12—C11—H11	119.5
C5—C4—C3	119.9 (2)	C10—C11—H11	119.5
C5—C4—H4	120.1	C11—C12—C13	118.7 (2)
C3—C4—H4	120.1	C11—C12—H12	120.6
C4—C5—C6	120.0 (2)	C13—C12—H12	120.6
C4—C5—H5	120.0	C14—C13—C12	121.0 (2)
C6—C5—H5	120.0	C14—C13—Cl1	119.0 (2)
C5—C6—C1	122.3 (2)	C12—C13—Cl1	119.99 (18)
C5—C6—H6	118.8	C15—C14—C13	119.9 (2)
C1—C6—H6	118.8	C15—C14—H14	120.0
C8—C7—C1	114.60 (19)	C13—C14—H14	120.0
C8—C7—H7A	108.6	C14—C15—C10	120.5 (2)
C1—C7—H7A	108.6	C14—C15—H15	119.7
C8—C7—H7B	108.6	C10—C15—H15	119.7
C1—C7—H7B	108.6	O2—N1—O1	123.0 (2)
H7A—C7—H7B	107.6	O2—N1—C2	118.0 (2)
O3—C8—C7	123.96 (19)	O1—N1—C2	118.8 (2)
O3—C8—C9	119.84 (19)		

C6—C1—C2—C3	−0.7 (3)	O4—C9—C10—C15	−179.9 (2)
C7—C1—C2—C3	−179.6 (2)	C8—C9—C10—C15	−0.7 (3)
C6—C1—C2—N1	−179.61 (18)	O4—C9—C10—C11	2.6 (3)
C7—C1—C2—N1	1.4 (3)	C8—C9—C10—C11	−178.20 (19)
C1—C2—C3—C4	0.3 (3)	C15—C10—C11—C12	−0.9 (3)
N1—C2—C3—C4	179.30 (19)	C9—C10—C11—C12	176.7 (2)

C2—C3—C4—C5	0.1 (3)	C10—C11—C12—C13	0.8 (3)
C3—C4—C5—C6	−0.1 (4)	C11—C12—C13—C14	−0.1 (3)
C4—C5—C6—C1	−0.3 (4)	C11—C12—C13—Cl1	179.04 (17)
C2—C1—C6—C5	0.7 (3)	C12—C13—C14—C15	−0.5 (3)
C7—C1—C6—C5	179.7 (2)	Cl1—C13—C14—C15	−179.67 (17)
C6—C1—C7—C8	−112.2 (2)	C13—C14—C15—C10	0.4 (3)
C2—C1—C7—C8	66.7 (3)	C11—C10—C15—C14	0.2 (3)
C1—C7—C8—O3	9.9 (3)	C9—C10—C15—C14	−177.2 (2)
C1—C7—C8—C9	−175.36 (19)	C3—C2—N1—O2	6.2 (3)
O3—C8—C9—O4	115.7 (3)	C1—C2—N1—O2	−174.8 (2)
C7—C8—C9—O4	−59.3 (3)	C3—C2—N1—O1	−169.5 (2)
O3—C8—C9—C10	−63.5 (3)	C1—C2—N1—O1	9.5 (3)
C7—C8—C9—C10	121.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O3^{i}	0.93	2.53	3.279 (3)	138
C15—H15···O1	0.93	2.59	3.244 (3)	128

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+3/2.