organic compounds

Bis(4-nitrophenyl) succinate

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The title compound, $C_{16}H_{12}N_2O_8$, was prepared by the reaction of succinyl dichloride with 4-nitrophenol. The molecule is centrosymmetric and the two benzene rings are coplanar.

Related literature

For a related structure, see: Zhu *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).
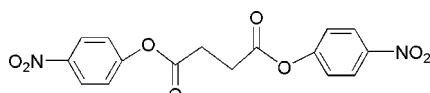
Experimental

Crystal data

$C_{16}H_{12}N_2O_8$

$M_r = 360.28$

Monoclinic, $C2/c$
$a = 13.539\ (13)$ Å
$b = 9.049\ (9)$ Å
$c = 14.662\ (14)$ Å
$\beta = 116.609\ (15)°$
$V = 1606\ (3)$ Å^3

$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 294\ (2)$ K
$0.20 \times 0.18 \times 0.14$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.976$, $T_{max} = 0.983$

3797 measured reflections
1415 independent reflections
698 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.196$
$S = 1.01$
1415 reflections

118 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

References

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Sheldrick, G. M. (1996). *SADABS*. Version 2.03. University of Göttingen, Germany.
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supplementary materials

Bis(4-nitrophenyl) succinate

H.-T. Du, H.-J. Du, M. Lu and L.-L. Sun

Comment

As part of our ongoing studies, we synthesized the title compound, (I), and report herein its synthesis and crystal structure.

In the molecule of (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It is centrosymmetric. Ring A (C1—C6) is, of course, planar and the two symmetry related phenyl rings are coplanar. However in the similar structure, 1,4-Bis(3-pyridylaminomethyl)benzene (Zhu *et al.*, 2007), the dihedral angle between the pyridyl ring and the central benzene ring is 63.6 (2)°.

Experimental

For the preparation of the title compound, a solution of the appropriate succinyl dichloride (10 mmol) in pyridine (0.5 ml) was added to a solution of 4-nitro-phenol (20 mmol) in dry acetonitrile (30 ml) and the mixture was heated under reflux for 5–6 h. The moisture was excluded by using a calcium chloride guard tube on the reflux condenser. On cooling, the precipitates were collected, dried and recrystallized from chloroform-acetonitrile to give the title compond. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetone solution.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures
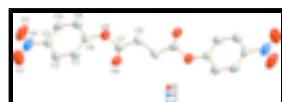
Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are omitted for clarity.

Bis(4-nitrophenyl) succinate

Crystal data

$C_{16}H_{12}N_2O_8$	$F_{000} = 744$
$M_r = 360.28$	$D_x = 1.490$ Mg m^{-3}
Monoclinic, *C2/c*	Melting point: 445 K
Hall symbol: -C 2yc	Mo *Kα* radiation $λ = 0.71073$ Å
a = 13.539 (13) Å	Cell parameters from 851 reflections
b = 9.049 (9) Å	θ = 3.1–26.3°

$c = 14.662\ (14)$ Å

$\beta = 116.609\ (15)°$

$V = 1606\ (3)$ Å^3

$Z = 4$

$\mu = 0.12$ mm^{-1}

$T = 294\ (2)$ K

Prism, colorless

$0.20 \times 0.18 \times 0.14$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	1415 independent reflections
Radiation source: fine-focus sealed tube	698 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.057$
$T = 294(2)$ K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16 \rightarrow 14$
$T_{min} = 0.976$, $T_{max} = 0.983$	$k = -6 \rightarrow 10$
3797 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.062$	H-atom parameters constrained
$wR(F^2) = 0.196$	$w = 1/[\sigma^2(F_o^2) + (0.0987P)^2 + 0.291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
1415 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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$^2 > 2$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	$U_{iso}*/U_{eq}$
O1	−0.0763 (4)	−0.1228 (5)	0.3236 (4)	0.1213 (16)

O2	−0.1973 (3)	−0.0053 (4)	0.1964 (3)	0.1081 (14)
O3	0.0744 (2)	0.5257 (3)	0.4503 (2)	0.0595 (9)
O4	0.2214 (2)	0.4987 (3)	0.4210 (2)	0.0615 (9)
N1	−0.1159 (4)	−0.0091 (5)	0.2796 (4)	0.0771 (12)
C1	0.0807 (3)	0.2616 (4)	0.4553 (3)	0.0543 (11)
H1	0.1474	0.2637	0.5144	0.065*
C2	0.0313 (3)	0.1298 (4)	0.4138 (3)	0.0530 (11)
H2	0.0635	0.0408	0.4444	0.064*
C3	−0.0665 (3)	0.1317 (4)	0.3262 (3)	0.0505 (10)
C4	−0.1169 (3)	0.2599 (5)	0.2803 (3)	0.0553 (11)
H4	−0.1838	0.2582	0.2215	0.066*
C5	−0.0677 (3)	0.3909 (5)	0.3219 (3)	0.0523 (11)
H5	−0.1003	0.4800	0.2919	0.063*
C6	0.0305 (3)	0.3890 (4)	0.4087 (3)	0.0458 (10)
C7	0.1701 (3)	0.5718 (4)	0.4517 (3)	0.0426 (9)
C8	0.1953 (3)	0.7226 (4)	0.4931 (3)	0.0526 (11)
H8A	0.1934	0.7249	0.5585	0.063*
H8B	0.1383	0.7889	0.4474	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.116 (4)	0.071 (3)	0.144 (4)	−0.024 (2)	0.030 (3)	−0.024 (3)
O2	0.072 (3)	0.140 (4)	0.092 (3)	−0.050 (2)	0.019 (2)	−0.041 (2)
O3	0.0515 (18)	0.0563 (18)	0.078 (2)	−0.0078 (14)	0.0353 (16)	−0.0143 (14)
O4	0.0440 (17)	0.0658 (19)	0.072 (2)	−0.0064 (14)	0.0239 (16)	−0.0237 (14)
N1	0.054 (3)	0.091 (4)	0.084 (3)	−0.028 (3)	0.029 (3)	−0.025 (3)
C1	0.039 (2)	0.062 (3)	0.047 (3)	0.002 (2)	0.006 (2)	−0.004 (2)
C2	0.043 (2)	0.056 (3)	0.055 (3)	0.000 (2)	0.017 (2)	0.000 (2)
C3	0.035 (2)	0.065 (3)	0.054 (3)	−0.014 (2)	0.022 (2)	−0.013 (2)
C4	0.029 (2)	0.082 (3)	0.046 (2)	−0.003 (2)	0.0089 (19)	−0.001 (2)
C5	0.040 (2)	0.064 (3)	0.052 (3)	0.006 (2)	0.020 (2)	0.009 (2)
C6	0.036 (2)	0.051 (2)	0.052 (2)	−0.0056 (19)	0.022 (2)	−0.0077 (19)
C7	0.031 (2)	0.054 (2)	0.033 (2)	0.0016 (18)	0.0053 (17)	0.0022 (17)
C8	0.047 (2)	0.043 (2)	0.065 (3)	−0.0007 (18)	0.023 (2)	−0.0063 (19)

Geometric parameters (Å, °)

O1—N1	1.206 (5)	C2—H2	0.9300
O2—N1	1.224 (5)	C3—C4	1.362 (5)
O3—C7	1.352 (4)	C4—C5	1.362 (5)
O3—C6	1.389 (4)	C4—H4	0.9300
O4—C7	1.186 (4)	C5—C6	1.368 (5)
N1—C3	1.458 (5)	C5—H5	0.9300
C1—C6	1.357 (5)	C7—C8	1.470 (5)
C1—C2	1.369 (5)	C8—C8^i	1.488 (7)
C1—H1	0.9300	C8—H8A	0.9700
C2—C3	1.371 (6)	C8—H8B	0.9700

C7—O3—C6	120.1 (3)	C4—C5—C6	118.8 (4)
O1—N1—O2	122.9 (5)	C4—C5—H5	120.6
O1—N1—C3	119.6 (5)	C6—C5—H5	120.6
O2—N1—C3	117.5 (5)	C1—C6—C5	122.5 (4)
C6—C1—C2	118.7 (4)	C1—C6—O3	121.1 (4)
C6—C1—H1	120.6	C5—C6—O3	116.3 (4)
C2—C1—H1	120.6	O4—C7—O3	122.9 (3)
C1—C2—C3	118.7 (4)	O4—C7—C8	127.4 (3)
C1—C2—H2	120.6	O3—C7—C8	109.7 (3)
C3—C2—H2	120.6	C7—C8—C8^i	113.5 (4)
C4—C3—C2	122.2 (4)	C7—C8—H8A	108.9
C4—C3—N1	119.3 (4)	C8^i—C8—H8A	108.9
C2—C3—N1	118.4 (4)	C7—C8—H8B	108.9
C3—C4—C5	118.9 (4)	C8^i—C8—H8B	108.9
C3—C4—H4	120.5	H8A—C8—H8B	107.7
C5—C4—H4	120.5		
C6—C1—C2—C3	0.6 (5)	C2—C1—C6—C5	0.1 (5)
C1—C2—C3—C4	−1.2 (6)	C2—C1—C6—O3	177.0 (3)
C1—C2—C3—N1	177.1 (3)	C4—C5—C6—C1	−0.2 (5)
O1—N1—C3—C4	−174.5 (4)	C4—C5—C6—O3	−177.3 (3)
O2—N1—C3—C4	5.2 (6)	C7—O3—C6—C1	69.0 (4)
O1—N1—C3—C2	7.1 (6)	C7—O3—C6—C5	−113.9 (4)
O2—N1—C3—C2	−173.1 (4)	C6—O3—C7—O4	−1.9 (5)
C2—C3—C4—C5	1.0 (5)	C6—O3—C7—C8	176.4 (3)
N1—C3—C4—C5	−177.2 (3)	O4—C7—C8—C8^i	−7.3 (7)
C3—C4—C5—C6	−0.3 (5)	O3—C7—C8—C8^i	174.5 (4)

Symmetry codes: (i) $-x+1/2, -y+3/2, -z+1$.

Fig. 1