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4-Oxo-2,4-diphenylbutanenitrile

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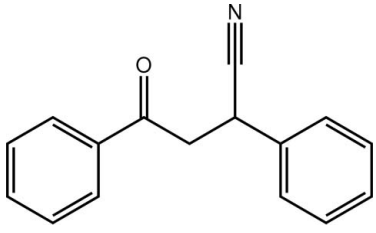
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 15.3.

The title molecule, $C_{16}H_{13}NO$, is twisted, the dihedral angle between the terminal phenyl rings being 68.40 (6)°. In the crystal, C—H···O and C—H···N interactions lead to supramolecular layers in the *bc* plane.

Related literature

For background to the synthetic applications of 2,4-diaryl-4-oxo-butanenitriles, see: Coudert *et al.* (1990, 1988); Iida *et al.* (2007). For the preparation of the title compound, see Coudert *et al.* (1990). For the structure of the methoxy derivative, see: Abdel-Aziz *et al.* (2012).



Experimental

Crystal data

$C_{16}H_{13}NO$
M_r = 235.27
Monoclinic, $P2_1/c$
a = 14.2158 (3) Å
b = 8.9244 (2) Å
c = 9.7553 (2) Å
β = 99.217 (2)°
V = 1221.65 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 100 K
0.30 × 0.30 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.752, T_{max} = 1.000
4625 measured reflections
2496 independent reflections
2187 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.02
2496 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.95	2.62	3.3669 (17)	136
C8—H8b···O1^{ii}	0.99	2.56	3.5246 (14)	163

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5469).

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S1. Comment

2,4-Diaryl-4-oxo-butanenitriles constitute an important class of difunctional intermediates for both the synthesis of biologically active heterocycles, such as pyridazine derivatives, and as a source ketone (Coudert *et al.*, 1990; Coudert *et al.*, 1988; Iida *et al.*, 2007). Herein, the crystal structure of a 2,4-diaryl-4-oxo-butanenitrile derivative, 2,4-diphenyl-4-oxo-butanenitrile (I), is described. This compound has been prepared previously (Coudert *et al.*, 1990) and the structure of the methoxy derivative is known (Abdel-Aziz *et al.*, 2012).

The molecule of (I), Fig. 1, is twisted as seen in the value of the dihedral angle between the terminal benzene rings of 68.40 (6)°. The twist occurs between the C9—C11 bond [the C8—C9—C11—C12 torsion angle is 107.79 (12)°] with the other part of the molecule being relatively planar [the C7—C8—C9—C11 torsion angle is -179.69 (9)°].

Supramolecular layers in the *bc* plane are formed in the crystal packing *via* C—H···O and C—H···N interactions, Fig. 2 and Table 1. These stack along the *a* axis with no specific intermolecular interactions between the layers, Fig. 3.

S2. Experimental

Acetone cyanohydrin (0.045 mol) and 10% aqueous sodium carbonate (0.0015 mol and 1.5 ml water) were added to solution of benzalacetophenone (0.015 mol) in ethanol (50 ml). The mixture was heated at reflux temperature for 4 h. After cooling, the product which separated out was filtered off and recrystallized from methanol.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 1.00 Å, U_{iso}(H) = 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation.

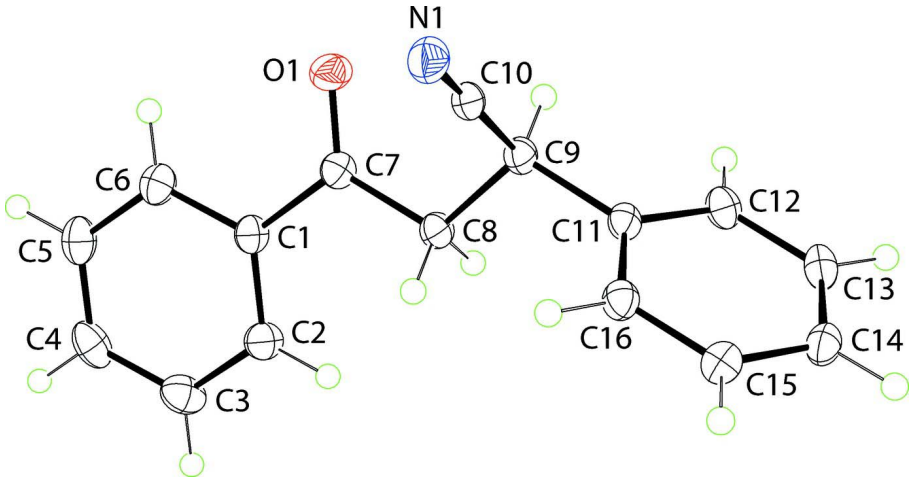

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

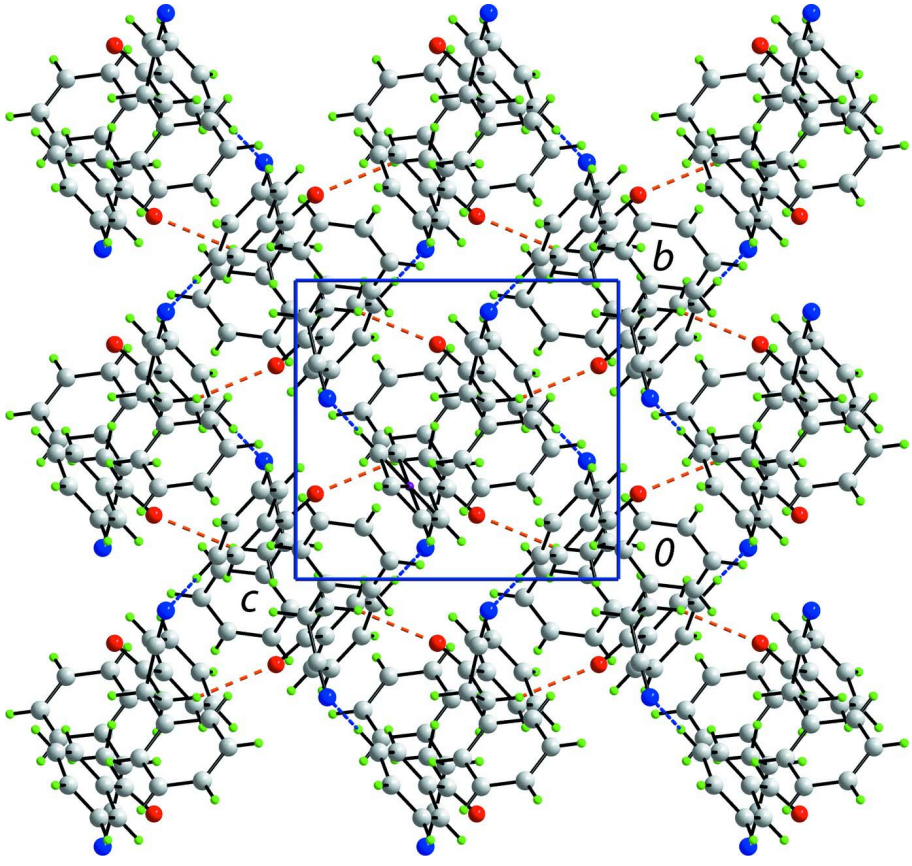

Figure 2

A view of the supramolecular in the *bc* plane in (I). The C—H···O and C—H···N interactions are shown as orange and blue dashed lines, respectively.

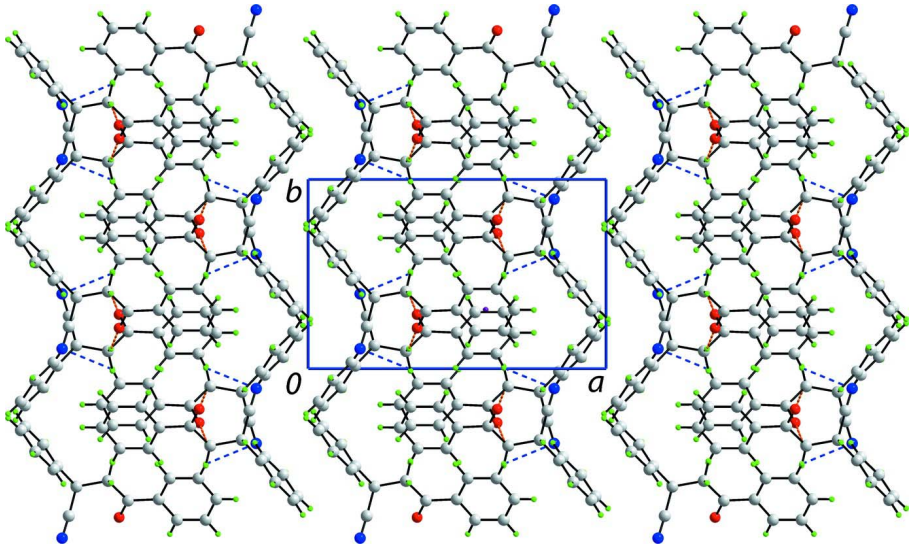

Figure 3

A view in projection down the *c* axis of the unit-cell contents for (I). The C—H···O and C—H···N interactions are shown as orange and blue dashed lines, respectively.

4-Oxo-2,4-diphenylbutanenitrile

Crystal data

$C_{16}H_{13}NO$
$M_r = 235.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.2158\ (3)$ Å
$b = 8.9244\ (2)$ Å
$c = 9.7553\ (2)$ Å
$\beta = 99.217\ (2)°$
$V = 1221.65\ (5)$ Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.279$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 2233 reflections
$\theta = 3.2–76.0°$
$\mu = 0.63$ mm^{-1}
$T = 100$ K
Prism, colourless
0.30 × 0.30 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.752$, $T_{max} = 1.000$
4625 measured reflections
2496 independent reflections
2187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 76.2°$, $\theta_{min} = 3.2°$
$h = -17\rightarrow17$
$k = -11\rightarrow6$
$l = -11\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 1.02$
2496 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.3439P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.36576 (6)	0.21438 (10)	0.43914 (9)	0.0285 (2)
N1	0.17432 (7)	0.10500 (12)	0.59790 (12)	0.0279 (2)
C1	0.49902 (8)	0.30995 (13)	0.59134 (12)	0.0208 (2)
C2	0.53560 (8)	0.42071 (14)	0.68608 (12)	0.0247 (3)
H2	0.4947	0.4960	0.7124	0.030*
C3	0.63208 (9)	0.42086 (16)	0.74205 (13)	0.0298 (3)
H3	0.6570	0.4966	0.8062	0.036*
C4	0.69199 (8)	0.31074 (16)	0.70442 (13)	0.0299 (3)
H4	0.7575	0.3102	0.7441	0.036*
C5	0.65640 (9)	0.20143 (15)	0.60905 (14)	0.0297 (3)
H5	0.6976	0.1268	0.5826	0.036*
C6	0.56030 (9)	0.20125 (14)	0.55228 (13)	0.0252 (3)
H6	0.5361	0.1267	0.4865	0.030*
C7	0.39562 (8)	0.30324 (13)	0.53106 (12)	0.0205 (2)
C8	0.32829 (7)	0.40714 (13)	0.59087 (12)	0.0201 (2)
H8	0.3436	0.5120	0.5698	0.024*
H8B	0.3386	0.3957	0.6931	0.024*
C9	0.22257 (7)	0.37701 (13)	0.53382 (12)	0.0198 (2)
H9	0.2119	0.3901	0.4307	0.024*
C10	0.19687 (8)	0.22196 (13)	0.56679 (12)	0.0211 (2)
C11	0.15783 (7)	0.48444 (12)	0.59617 (12)	0.0187 (2)
C12	0.11047 (8)	0.59901 (13)	0.51696 (12)	0.0218 (2)
H12	0.1195	0.6126	0.4233	0.026*
C13	0.04974 (8)	0.69400 (13)	0.57491 (13)	0.0232 (3)
H13	0.0177	0.7726	0.5207	0.028*
C14	0.03583 (8)	0.67459 (13)	0.71113 (13)	0.0224 (2)
H14	−0.0067	0.7384	0.7496	0.027*
C15	0.08427 (8)	0.56136 (13)	0.79140 (12)	0.0234 (2)
H15	0.0755	0.5483	0.8852	0.028*
C16	0.14544 (8)	0.46762 (12)	0.73418 (12)	0.0211 (2)
H16	0.1792	0.3913	0.7895	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0216 (4)	0.0328 (5)	0.0314 (5)	−0.0005 (4)	0.0048 (3)	−0.0109 (4)
N1	0.0227 (5)	0.0233 (5)	0.0370 (6)	0.0003 (4)	0.0031 (4)	−0.0017 (4)
C1	0.0179 (5)	0.0224 (5)	0.0228 (5)	0.0004 (4)	0.0057 (4)	0.0020 (4)
C2	0.0196 (5)	0.0287 (6)	0.0265 (6)	−0.0012 (5)	0.0058 (4)	−0.0036 (5)
C3	0.0223 (6)	0.0390 (7)	0.0281 (6)	−0.0062 (5)	0.0038 (5)	−0.0029 (6)
C4	0.0165 (5)	0.0441 (8)	0.0290 (6)	−0.0001 (5)	0.0032 (5)	0.0087 (6)
C5	0.0217 (6)	0.0319 (7)	0.0365 (7)	0.0067 (5)	0.0081 (5)	0.0053 (5)
C6	0.0233 (6)	0.0239 (6)	0.0294 (6)	0.0020 (5)	0.0071 (5)	0.0007 (5)
C7	0.0187 (5)	0.0212 (5)	0.0223 (5)	−0.0007 (4)	0.0052 (4)	0.0003 (4)
C8	0.0155 (5)	0.0214 (5)	0.0233 (5)	−0.0004 (4)	0.0032 (4)	−0.0014 (4)
C9	0.0163 (5)	0.0210 (5)	0.0222 (5)	0.0011 (4)	0.0030 (4)	−0.0002 (4)
C10	0.0145 (5)	0.0231 (6)	0.0250 (5)	0.0026 (4)	0.0012 (4)	−0.0036 (5)
C11	0.0136 (5)	0.0177 (5)	0.0248 (5)	−0.0015 (4)	0.0029 (4)	−0.0007 (4)
C12	0.0171 (5)	0.0243 (6)	0.0241 (6)	−0.0001 (4)	0.0042 (4)	0.0043 (5)
C13	0.0167 (5)	0.0208 (5)	0.0317 (6)	0.0019 (4)	0.0023 (4)	0.0047 (5)
C14	0.0175 (5)	0.0193 (5)	0.0308 (6)	0.0011 (4)	0.0054 (4)	−0.0021 (5)
C15	0.0239 (6)	0.0220 (5)	0.0250 (6)	0.0006 (5)	0.0060 (4)	−0.0002 (5)
C16	0.0207 (5)	0.0180 (5)	0.0243 (6)	0.0007 (4)	0.0027 (4)	0.0012 (4)

Geometric parameters (Å, º)

O1—C7	1.2212 (14)	C8—H8	0.9900
N1—C10	1.1470 (16)	C8—H8B	0.9900
C1—C2	1.3956 (17)	C9—C10	1.4796 (16)
C1—C6	1.3970 (16)	C9—C11	1.5217 (14)
C1—C7	1.4944 (15)	C9—H9	1.0000
C2—C3	1.3926 (17)	C11—C12	1.3889 (16)
C2—H2	0.9500	C11—C16	1.3936 (16)
C3—C4	1.3879 (19)	C12—C13	1.3929 (16)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.386 (2)	C13—C14	1.3853 (17)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.3894 (17)	C14—C15	1.3914 (16)
C5—H5	0.9500	C14—H14	0.9500
C6—H6	0.9500	C15—C16	1.3868 (16)
C7—C8	1.5151 (15)	C15—H15	0.9500
C8—C9	1.5403 (14)	C16—H16	0.9500
C2—C1—C6	119.34 (11)	H8—C8—H8B	107.7
C2—C1—C7	121.85 (10)	C10—C9—C11	108.43 (9)
C6—C1—C7	118.81 (11)	C10—C9—C8	110.20 (9)
C3—C2—C1	119.96 (11)	C11—C9—C8	111.29 (9)
C3—C2—H2	120.0	C10—C9—H9	109.0
C1—C2—H2	120.0	C11—C9—H9	109.0
C4—C3—C2	120.21 (12)	C8—C9—H9	109.0

C4—C3—H3	119.9	N1—C10—C9	176.20 (12)
C2—C3—H3	119.9	C12—C11—C16	119.46 (10)
C3—C4—C5	120.15 (11)	C12—C11—C9	120.78 (10)
C3—C4—H4	119.9	C16—C11—C9	119.76 (10)
C5—C4—H4	119.9	C11—C12—C13	119.93 (11)
C4—C5—C6	119.88 (12)	C11—C12—H12	120.0
C4—C5—H5	120.1	C13—C12—H12	120.0
C6—C5—H5	120.1	C14—C13—C12	120.41 (11)
C5—C6—C1	120.44 (12)	C14—C13—H13	119.8
C5—C6—H6	119.8	C12—C13—H13	119.8
C1—C6—H6	119.8	C13—C14—C15	119.79 (11)
O1—C7—C1	121.29 (10)	C13—C14—H14	120.1
O1—C7—C8	120.89 (10)	C15—C14—H14	120.1
C1—C7—C8	117.79 (10)	C16—C15—C14	119.82 (11)
C7—C8—C9	113.21 (9)	C16—C15—H15	120.1
C7—C8—H8	108.9	C14—C15—H15	120.1
C9—C8—H8	108.9	C15—C16—C11	120.55 (10)
C7—C8—H8B	108.9	C15—C16—H16	119.7
C9—C8—H8B	108.9	C11—C16—H16	119.7
C6—C1—C2—C3	−0.85 (18)	C7—C8—C9—C10	59.99 (12)
C7—C1—C2—C3	178.58 (11)	C7—C8—C9—C11	−179.69 (9)
C1—C2—C3—C4	−0.31 (19)	C10—C9—C11—C12	−130.84 (11)
C2—C3—C4—C5	1.11 (19)	C8—C9—C11—C12	107.79 (12)
C3—C4—C5—C6	−0.74 (19)	C10—C9—C11—C16	48.89 (13)
C4—C5—C6—C1	−0.44 (19)	C8—C9—C11—C16	−72.47 (13)
C2—C1—C6—C5	1.23 (18)	C16—C11—C12—C13	−1.27 (16)
C7—C1—C6—C5	−178.23 (11)	C9—C11—C12—C13	178.47 (10)
C2—C1—C7—O1	173.35 (11)	C11—C12—C13—C14	−0.31 (17)
C6—C1—C7—O1	−7.21 (17)	C12—C13—C14—C15	1.28 (17)
C2—C1—C7—C8	−8.53 (16)	C13—C14—C15—C16	−0.67 (17)
C6—C1—C7—C8	170.91 (10)	C14—C15—C16—C11	−0.91 (17)
O1—C7—C8—C9	5.29 (15)	C12—C11—C16—C15	1.88 (17)
C1—C7—C8—C9	−172.83 (9)	C9—C11—C16—C15	−177.85 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N1^{i}	0.95	2.62	3.3669 (17)	136
C8—H8b···O1^{ii}	0.99	2.56	3.5246 (14)	163

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