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(*E*,*E*)-*N*′-{4-[(2-Benzoylhydrazin-1-ylidene)methyl]benzylidene}benzohydrazide

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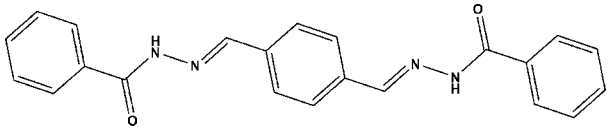
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.078; data-to-parameter ratio = 11.7.

In the title compound, $C_{22}H_{18}N_4O_2$, the molecules lie across an inversion centre. The dihedral angle between the mean planes of the central and terminal benzene rings is 66.03 (2)°. The molecule displays *trans* and *anti* conformations about the C=N and N—N bonds, respectively. In the crystal, N—H···O hydrogen bonds, with the O atoms of C=O groups acting as acceptors, link the molecules into a chain along [101].

Related literature

For historical background to aroylhydrazones, see: Savanini *et al.* (2002). For related structures, see: Bikas *et al.* (2012, 2010*a*,*b*); Hosseini Monfared *et al.* (2010*a*). For catalytic applications of aroylhydrazones, see: Hosseini Monfared *et al.* (2010*b*).



Experimental

Crystal data

$C_{22}H_{18}N_4O_2$
M_r = 370.40
Monoclinic, $C2/c$
a = 30.569 (3) Å
b = 5.1845 (3) Å
c = 12.5191 (11) Å
β = 112.408 (7)°
V = 1834.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.42 × 0.22 × 0.08 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.976, T_{max} = 0.992
13265 measured reflections
1905 independent reflections
965 reflections with $I > 2\sigma(I)$
R_{int} = 0.105

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.078
S = 0.94
1905 reflections
163 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.87 (2)	2.19 (2)	3.056 (3)	171 (2)

Symmetry code: (i) $x, y-1, z$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2059).

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supporting information

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(*E*,*E*)-*N*′-{4-[(2-Benzoylhydrazin-1-ylidene)methyl]benzylidene}benzohydrazide

Ramin Karimian, Hassan Hosseini-Monfared, Rahman Bikas, N. Burcu Arslan, Canan Kazak and Ahmet Koroglu

S1. Comment

The design, synthesis, and characterization of metal complexes with Schiff-base ligands play a vital role in the coordination chemistry of transition metals. Hydrazones are a special group of compounds in the Schiff base family that are characterized by the presence of *RR*′C=N–N=C(O)*R*″ which two inter-linked nitrogen atoms (–N—N–) separate them from imines, oximes, *etc*. Hydrazone ligands derived from the condensation of acid hydrazides (R–CO–NH–NH_2) with aromatic carbonyl compounds are important O, N-donor ligands. As biologically active compounds, hydrazones find application in the treatment of diseases such as tuberculosis, leprosy and mental disorder and also as anti-tumor agents. Hydrazone Schiff bases also have wide spread applications in fields such as coordination chemistry, bioinorganic chemistry , magnetics, electronics, nonlinear optics and fluorescent materials. Aroylhydrazone complexes also seem to be good candidates for catalytic oxidation studies because of their resistance to oxidation (Hosseini Monfared *et al.*, 2010*b*). As part of our studies on the synthesis and characterization of hydrazone derivatives (Bikas *et al.*, 2012, 2010*a,b*), we report here the crystal structure of (*N′,N″E,N′,N″E*)-*N′,N″*-(1,4-phenylenebis(methan-1-yl-1-ylidene))dibenzohydrazide. The molecules of $C_{22}H_{18}N_4O_2$, lie across inversion centres and the asymmetric unit contains a half molecule (Fig. 1). The terminal benzene rings are parallel to each other and the distance of two planes which embrace these rings is 3.168 Å apart. The dihedral angle between the mean planes of the central and two terminal benzene rings is 66.03 (2)°. The molecule displays a *trans* configuration with respect to the C=N and N—N bonds. The packing diagram of the title compound is shown in Fig. 2. There are two strong intermolecular N—H···O hydrogen bonds in which the O atoms of the carbonyl groups (–C=O) act as hydrogen acceptors for the hydrogen of N—H and a one-dimensional chain is formed by these hydrogen bonds (Fig. 3).

S2. Experimental

For preparing the title compound a methanol (10 ml) solution of benzhydrazide (3 mmol) was added drop-wise to a methanol solution (10 ml) of terephthalaldehyde (1.5 mmol), and the mixture was refluxed for 4 h. The solution was then evaporated on a steam bath to 5 cm^3 and cooled to room temperature. The white precipitates of the title compound were separated and filtered off, washed with 3 ml of cooled methanol and then dried in air. Colorless crystals were obtained from its methanol solution by thermal gradient method. Yield: 93%. IR (cm^{-1}): 3253 (s, broad, N—H), 1654 (*vs*, C=O), 1607 (*s*, C=N), 1546 (*vs*), 1507 (*m*), 1361 (*s*), 1284 (*vs*), 1146 (*s*), 1069 (*s*), 969 (*m*), 915 (*m*), 846 (*m*), 723 (*s*), 692 (*s*), 661 (*s*), 569 (*w*), 538 (*w*), 423 (*w*).

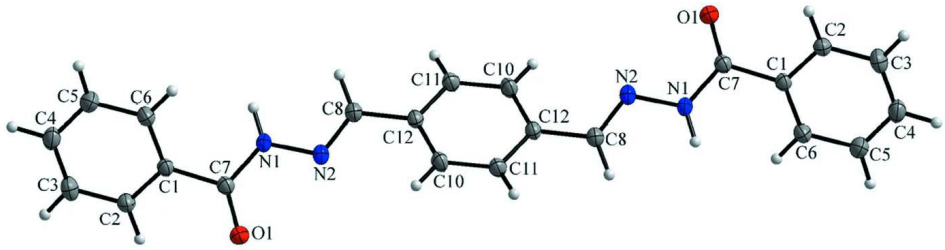

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

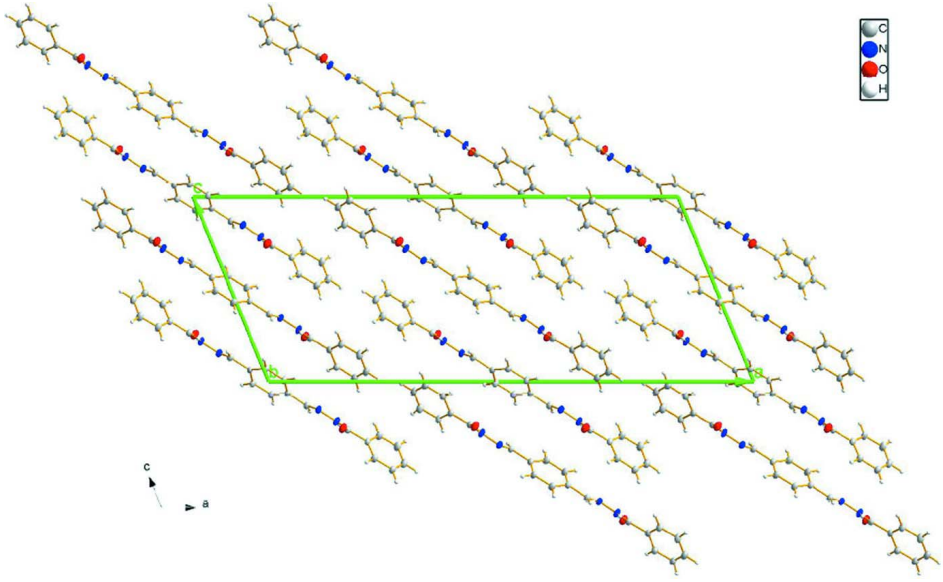

Figure 2

The packing diagram of the title compound.

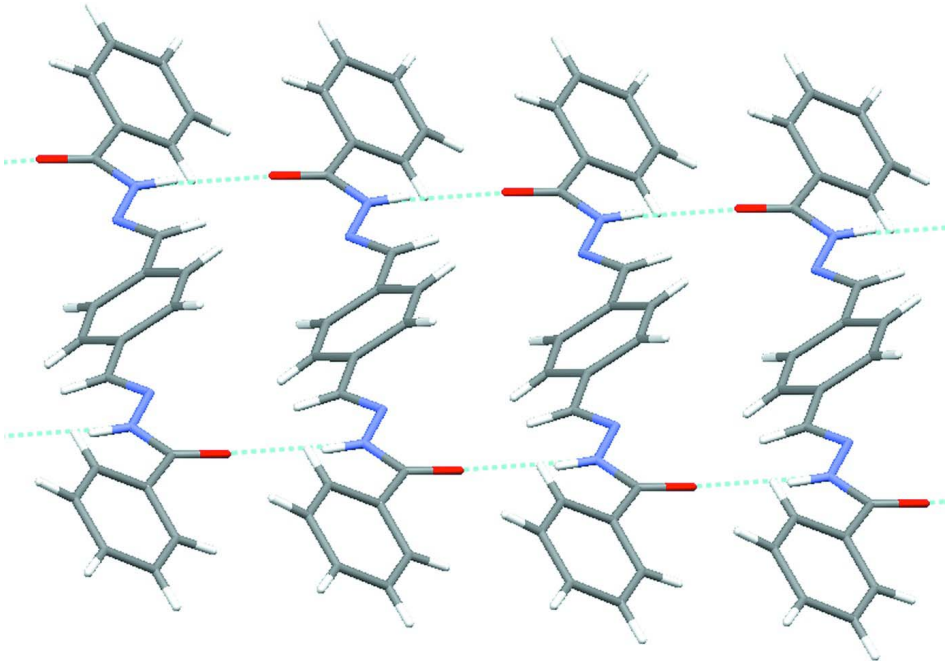

Figure 3

Hydrogen bonding in the title compound. The blue dashed lines indicate intermolecular N–H···O hydrogen bonds.

(*E*,*E*)-*N*′-{4-[(2-Benzoylhydrazin-1- ylidene)methyl]benzylidene}benzohydrazide

Crystal data

$C_{22}H_{18}N_4O_2$
$M_r = 370.40$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 30.569\ (3)$ Å
$b = 5.1845\ (3)$ Å
$c = 12.5191\ (11)$ Å
$\beta = 112.408\ (7)°$
$V = 1834.3\ (3)$ Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.341$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8004 reflections
$\theta = 1.4–27.5°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Prism, colorless
0.42 × 0.22 × 0.08 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.976$, $T_{max} = 0.992$
13265 measured reflections
1905 independent reflections
965 reflections with $I > 2\sigma(I)$
$R_{int} = 0.105$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.4°$
$h = -38\rightarrow38$
$k = -6\rightarrow6$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.078$
$S = 0.94$
1905 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.84753 (7)	0.1985 (4)	0.32678 (19)	0.0454 (6)
C2	0.84744 (9)	0.3457 (5)	0.4191 (2)	0.0562 (7)
C3	0.81956 (9)	0.2794 (6)	0.4790 (2)	0.0658 (8)
C4	0.79059 (10)	0.0693 (6)	0.4454 (3)	0.0695 (8)
C5	0.78956 (10)	−0.0782 (5)	0.3532 (3)	0.0711 (8)
C6	0.81817 (8)	−0.0140 (5)	0.2948 (2)	0.0582 (7)
C7	0.87799 (7)	0.2804 (4)	0.26408 (19)	0.0475 (6)
C8	0.94196 (8)	−0.0556 (5)	0.1321 (2)	0.0502 (6)
C10	0.96656 (9)	0.1846 (5)	−0.0081 (2)	0.0558 (7)
C11	1.00525 (9)	−0.2099 (5)	0.0707 (2)	0.0553 (7)
C12	0.97114 (7)	−0.0250 (4)	0.06315 (18)	0.0458 (6)
N1	0.89465 (7)	0.0866 (4)	0.21865 (17)	0.0543 (6)
N2	0.92141 (7)	0.1407 (3)	0.15428 (16)	0.0516 (5)
O1	0.88701 (6)	0.5082 (3)	0.25515 (14)	0.0650 (5)
H1	0.8912 (7)	−0.074 (4)	0.2351 (18)	0.055 (7)*
H2	0.9404 (6)	−0.232 (4)	0.1624 (16)	0.052 (6)*
H3	0.8174 (7)	−0.118 (4)	0.2312 (19)	0.058 (7)*
H4	0.9424 (8)	0.305 (4)	−0.0167 (18)	0.065 (7)*
H5	1.0094 (7)	−0.343 (4)	0.1209 (18)	0.056 (7)*
H6	0.8219 (8)	0.387 (4)	0.546 (2)	0.078 (8)*
H7	0.8670 (7)	0.499 (4)	0.4386 (17)	0.068 (7)*
H8	0.7688 (9)	−0.228 (5)	0.324 (2)	0.101 (10)*
H9	0.7717 (9)	0.017 (5)	0.489 (2)	0.096 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0450 (14)	0.0457 (13)	0.0519 (16)	0.0066 (11)	0.0255 (13)	0.0039 (12)
C2	0.0568 (16)	0.0572 (16)	0.0627 (18)	−0.0026 (13)	0.0319 (15)	−0.0062 (13)
C3	0.0676 (17)	0.0798 (19)	0.0621 (19)	0.0055 (16)	0.0385 (17)	−0.0027 (16)
C4	0.0691 (19)	0.0738 (19)	0.084 (2)	0.0066 (15)	0.0495 (18)	0.0112 (17)
C5	0.0715 (19)	0.0601 (17)	0.099 (2)	−0.0068 (15)	0.0518 (19)	−0.0044 (17)
C6	0.0618 (15)	0.0521 (14)	0.0735 (19)	−0.0023 (13)	0.0401 (15)	−0.0111 (15)
C7	0.0477 (13)	0.0479 (14)	0.0513 (16)	0.0053 (12)	0.0239 (12)	0.0012 (12)
C8	0.0532 (15)	0.0486 (16)	0.0569 (16)	0.0007 (12)	0.0301 (13)	−0.0008 (12)
C10	0.0580 (16)	0.0553 (15)	0.0662 (18)	0.0137 (13)	0.0375 (15)	0.0052 (13)
C11	0.0655 (16)	0.0507 (14)	0.0605 (18)	0.0083 (13)	0.0362 (15)	0.0045 (13)
C12	0.0454 (14)	0.0483 (13)	0.0504 (15)	−0.0004 (12)	0.0259 (12)	−0.0059 (12)
N1	0.0648 (14)	0.0476 (12)	0.0704 (15)	0.0036 (11)	0.0481 (13)	0.0054 (11)
N2	0.0531 (12)	0.0537 (12)	0.0599 (13)	0.0006 (9)	0.0349 (11)	−0.0002 (10)
O1	0.0857 (12)	0.0445 (9)	0.0850 (13)	−0.0003 (9)	0.0552 (10)	0.0020 (9)

Geometric parameters (Å, º)

C1—C6	1.381 (3)	C7—N1	1.346 (3)
C1—C2	1.386 (3)	C8—N2	1.281 (3)
C1—C7	1.490 (3)	C8—C12	1.467 (3)
C2—C3	1.377 (3)	C8—H2	1.00 (2)
C2—H7	0.97 (2)	C10—C11^{i}	1.375 (3)
C3—C4	1.365 (4)	C10—C12	1.379 (3)
C3—H6	0.99 (2)	C10—H4	0.94 (2)
C4—C5	1.374 (3)	C11—C10^{i}	1.375 (3)
C4—H9	0.98 (3)	C11—C12	1.392 (3)
C5—C6	1.378 (3)	C11—H5	0.91 (2)
C5—H8	0.98 (3)	N1—N2	1.378 (2)
C6—H3	0.95 (2)	N1—H1	0.87 (2)
C7—O1	1.228 (2)		
C6—C1—C2	118.3 (2)	O1—C7—C1	121.95 (19)
C6—C1—C7	122.8 (2)	N1—C7—C1	115.0 (2)
C2—C1—C7	118.9 (2)	N2—C8—C12	120.0 (2)
C3—C2—C1	121.0 (3)	N2—C8—H2	123.2 (11)
C3—C2—H7	121.3 (13)	C12—C8—H2	116.7 (11)
C1—C2—H7	117.7 (13)	C11^{i}—C10—C12	120.8 (2)
C4—C3—C2	119.6 (3)	C11^{i}—C10—H4	120.5 (13)
C4—C3—H6	122.6 (14)	C12—C10—H4	118.5 (13)
C2—C3—H6	117.8 (14)	C10^{i}—C11—C12	120.8 (2)
C3—C4—C5	120.5 (3)	C10^{i}—C11—H5	120.9 (13)
C3—C4—H9	120.0 (15)	C12—C11—H5	118.2 (13)
C5—C4—H9	119.4 (15)	C10—C12—C11	118.4 (2)
C4—C5—C6	119.7 (3)	C10—C12—C8	122.1 (2)
C4—C5—H8	124.0 (17)	C11—C12—C8	119.5 (2)

C6—C5—H8	116.3 (17)	C7—N1—N2	120.0 (2)
C5—C6—C1	120.8 (3)	C7—N1—H1	120.9 (14)
C5—C6—H3	119.3 (13)	N2—N1—H1	118.9 (14)
C1—C6—H3	119.9 (13)	C8—N2—N1	114.51 (19)
O1—C7—N1	123.0 (2)		

C6—C1—C2—C3	1.3 (4)	C2—C1—C7—N1	149.0 (2)
C7—C1—C2—C3	179.4 (2)	C11^{i}—C10—C12—C11	0.4 (4)
C1—C2—C3—C4	−1.7 (4)	C11^{i}—C10—C12—C8	179.2 (2)
C2—C3—C4—C5	0.9 (4)	C10^{i}—C11—C12—C10	−0.4 (4)
C3—C4—C5—C6	0.3 (4)	C10^{i}—C11—C12—C8	−179.3 (2)
C4—C5—C6—C1	−0.7 (4)	N2—C8—C12—C10	−20.1 (3)
C2—C1—C6—C5	−0.1 (4)	N2—C8—C12—C11	158.7 (2)
C7—C1—C6—C5	−178.1 (2)	O1—C7—N1—N2	−3.0 (3)
C6—C1—C7—O1	147.0 (2)	C1—C7—N1—N2	177.04 (19)
C2—C1—C7—O1	−30.9 (3)	C12—C8—N2—N1	179.3 (2)
C6—C1—C7—N1	−33.0 (3)	C7—N1—N2—C8	168.7 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{ii}	0.87 (2)	2.19 (2)	3.056 (3)	171 (2)

Symmetry code: (ii) *x*, *y*−1, *z*.