

Crystal structure of 3-[(2-acetamidophenyl)imino]-butan-2-one

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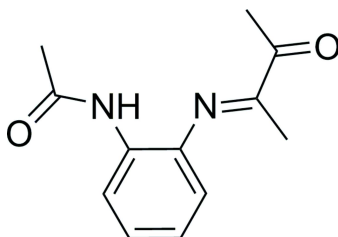
Keywords: crystal structure; iminoketone; hydrogen bonding.**CCDC reference:** 1553771**Supporting information:** this article has supporting information at journals.iucr.org/e

In the title compound, 3-[(2-acetamidophenyl)imino]butan-2-one, $C_{12}H_{14}N_2O_2$, the imine $C=N$ bond is essentially coplanar with the ketone $C=O$ bond in an *s-trans* conformation. The benzene ring is twisted away from the plane of the $C=N$ bond by $53.03(14)^\circ$. The acetamido unit is essentially coplanar with the benzene ring. In the crystal, molecules are connected into chains along the *c* axis through $C-H \cdots O$ hydrogen bonds, with two adjacent chains being hinged by $C-H \cdots O$ hydrogen bonds.

1. Chemical context

α -(Arylimino)ketone compounds, resulting from condensation between α -diketones and anilines in a 1:1 fashion, are useful bidentate ligands in transition metal coordination chemistry (Binotti *et al.*, 2004) and important synthetic intermediates toward α -diimines (Schmid *et al.*, 2002) and imine-based multidentate ligands (Schmiege *et al.*, 2007). X-ray structural studies of α -(arylimino)ketones have primarily focused on those derived from aromatic diketones such as acenaphthenequinone (Kovach *et al.*, 2011), benzil (Kovach *et al.*, 2014; Güner *et al.*, 2000), and phenanthrenequinone (Farrell *et al.*, 2017). In contrast, structural reports on α -(arylimino)ketone compounds derived from aliphatic α -diketones are rare (Azoulay *et al.*, 2009).

Our group is interested in *N,N*-diaryl α -diimine ligands that contain hydrogen-bonding units for transition-metal-catalyzed copolymerization of polar vinyl monomers with ethylene (Zhai & Jordan, 2014; Zhai *et al.*, 2017). We obtained the title compound during the attempted synthesis of an α -diimine compound containing an *ortho*-acetamido group and report its crystal structure in the present work.



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The arylimine unit exhibits an *E* conformation. The ketone carbonyl group (C2–O1) and the imine $C=N$ group (C3–N1) are almost coplanar [torsion angle O1–C2–C3–N1

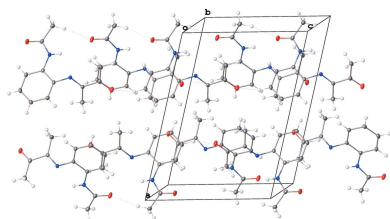


Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C8—H8···O1 ⁱ	0.95	2.54	3.3286 (14)	141
C9—H9···O2	0.95	2.24	2.8523 (15)	122
C12—H12B···O2 ⁱⁱ	0.98	2.39	3.3387 (15)	164

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

$-177.87(10)^\circ$] and *trans* with respect to the C2—C3 bond. The imine plane is twisted from the plane of the aryl ring (C5—C10) by a dihedral angle of $53.03(14)^\circ$ [defined by atoms C3/N1/C5/C6]. The acetamido group is essentially coplanar with the aryl ring [torsion angle C11—N2—C10—C9, $-0.14(18)^\circ$]. The molecular structure of **1** also features intramolecular C9—H9···O2 hydrogen bond (Table 1). This bond, in combination with conjugation between the amide group and the aryl ring, is likely responsible for the coplanarity between the acetamido and the aryl groups.

3. Supramolecular features

In the crystal, C8—H8···O1ⁱⁱ [symmetry code: (ii) $x, y, z - 1$] hydrogen bonds arrange the molecules into chains along the *c* axis (Fig. 2, Table 2). Two chains in close proximity are linked by C12—H12B···O2ⁱ hydrogen bonds [symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$]. There are no other significant contacts between the chains (Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.38, update May 2017; Groom *et al.*, 2016) indicated that no other α -(arylimino)ketone compounds derived from 2,3-butanedione have been structurally characterized. Two

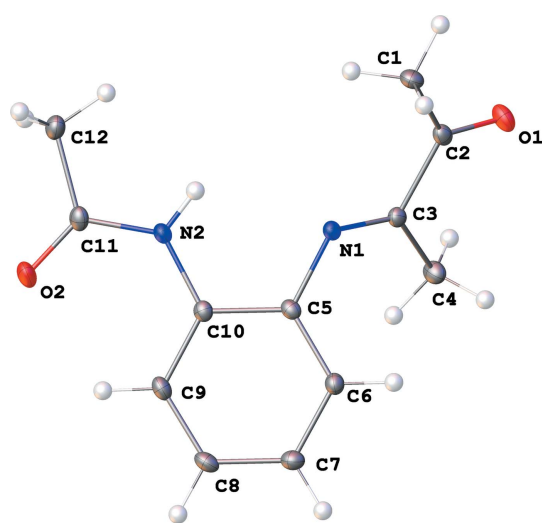


Figure 1
The molecular structure. Displacement ellipsoids are shown at the 50% probability level.

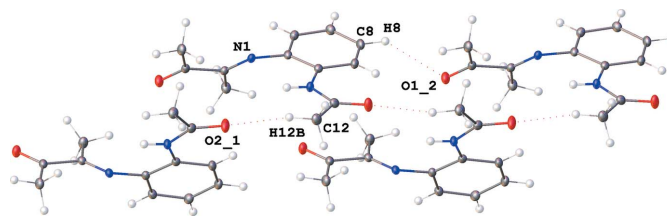


Figure 2
Chains running along the *c*-axis direction. [Symmetry codes: (−1) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (−2) $x, y, z - 1$.]

structurally similar α -(arylimino)ketones have been reported, namely 2,4-bis(2,6-diisopropylphenylimino)pentan-3-one [CCDC refcode COPLAV (Azoulay *et al.*, 2009) and its identical structure COPLAV01 (Zhang *et al.*, 2012)] and 2-(2,6-diisopropylphenylimino)-1-phenylpropan-1-one (IFADAV; Ferreira *et al.*, 2006).

5. Synthesis and crystallization

A Schlenk flask was charged with *N*-(2-aminophenyl)acetamide (Shirin *et al.*, 2002) (2.00 g, 13.3 mmol) and anhydrous MeOH (11 mL) under nitrogen. The mixture was cooled to 273 K. Butane-2,3-dione (2.30 g, 26.7 mmol) and a catalytic amount of formic acid (2–3 drops) were added to the reaction mixture, and the mixture was stirred at 273 K for 1 h. The mixture was warmed to room temperature, and the volatiles were removed under vacuum. The yellow solid residue was washed three times with diethyl ether and dried under vacuum to yield the title compound (2.04 g, 70%). This material slowly degrades under air at room temperature. Storage under vacuum or nitrogen is recommended.

¹H NMR (500 MHz, CDCl₃): δ 8.31 (*d*, $J = 8.0$, 1H), 7.64 (*br s*, 1H, *NH*), 7.24 (*t*, $J = 7.5$, 1H), 7.08 (*t*, $J = 7.5$, 1H), 6.78 (*d*, $J = 8.0$, 1H), 2.55 (*s*, 3H, CH₃), 2.17 (*s*, 3H, CH₃), 2.16 (*s*, 3H, CH₃). ¹³C{¹H NMR (126 MHz, CDCl₃): δ 199.5, 168.0, 167.1, 136.4, 131.5, 127.7, 123.6, 120.5, 119.4, 25.1, 25.0, 14.9. Single crystals were obtained from diffusion of diethyl ether into a THF solution at room temperature under nitrogen.

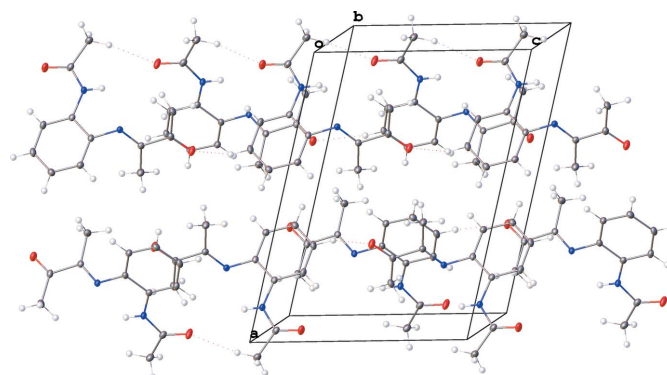


Figure 3
Crystal packing of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₁₄ N ₂ O ₂
<i>M</i> _r	218.25
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.987 (3), 7.7950 (14), 10.3135 (18)
β (°)	105.556 (4)
<i>V</i> (Å ³)	1083.3 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.24 × 0.18 × 0.12
Data collection	
Diffraction	Broker D8 Venture
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.692, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	25254, 2600, 2238
<i>R</i> _{int}	0.045
(sin θ/λ) _{max} (Å ⁻¹)	0.660
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.038, 0.103, 1.06
No. of reflections	2600
No. of parameters	152
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.38, -0.16

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015a), *SHELXL2017* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

6. Refinement

Crystal data, data collection and structural refinement details are summarized in Table 2. Carbon-bound H atoms were placed in calculated positions (C–H = 0.95–0.98 Å) and were included in the refinement in the riding-model approximation, with *U*_{iso}(H) set to 1.2–1.5*U*_{eq}(C). The hydrogen atom attached to the N2 atom was found in a difference-Fourier map and was freely refined without any restraints.

Funding information

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Crystal structure of 3-[(2-acetamidophenyl)imino]butan-2-one

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Computing details

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINTE* (Bruker, 2015); data reduction: *SAINTE* (Bruker, 2015); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

3-[(2-Acetamidophenyl)imino]butan-2-one

Crystal data

$C_{12}H_{14}N_2O_2$

$M_r = 218.25$

Monoclinic, $P2_1/c$

$a = 13.987$ (3) Å

$b = 7.7950$ (14) Å

$c = 10.3135$ (18) Å

$\beta = 105.556$ (4)°

$V = 1083.3$ (3) Å³

$Z = 4$

$F(000) = 464$

$D_x = 1.338$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9891 reflections

$\theta = 3.0$ – 28.0 °

$\mu = 0.09$ mm⁻¹

$T = 100$ K

Prism, yellow

$0.24 \times 0.18 \times 0.12$ mm

Data collection

Bruker D8 Venture
diffractometer

Radiation source: micro-focus X-ray tube,
INCOATEC ImuS

Mirrors monochromator

Detector resolution: 10.4167 pixels mm⁻¹

ω and ϕ scans

Absorption correction: multi-scan
(SADABS; Bruker, 2015)

$T_{\min} = 0.692$, $T_{\max} = 0.746$

25254 measured reflections

2600 independent reflections

2238 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 28.0$ °, $\theta_{\min} = 3.0$ °

$h = -18$ → 18

$k = -10$ → 10

$l = -13$ → 13

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.103$

$S = 1.06$

2600 reflections

152 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.4447P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.38$ e Å⁻³

$\Delta\rho_{\min} = -0.16$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.25794 (6)	-0.00837 (12)	0.18433 (9)	0.0135 (2)
N2	0.13175 (7)	0.12269 (12)	-0.04210 (9)	0.0152 (2)
H2	0.1258 (11)	0.1242 (19)	0.0383 (16)	0.025 (4)*
O1	0.34355 (6)	0.09306 (11)	0.52268 (8)	0.0226 (2)
O2	0.05883 (7)	0.20570 (12)	-0.25772 (8)	0.0254 (2)
C1	0.19297 (8)	-0.05200 (15)	0.41627 (11)	0.0186 (2)
H1A	0.199647	-0.175214	0.401962	0.028*
H1B	0.139946	-0.004880	0.342575	0.028*
H1C	0.176645	-0.033654	0.501886	0.028*
C2	0.28862 (8)	0.03613 (14)	0.41993 (10)	0.0154 (2)
C3	0.31963 (8)	0.04845 (13)	0.29018 (10)	0.0137 (2)
C4	0.41926 (8)	0.12803 (15)	0.30273 (11)	0.0190 (2)
H4A	0.471461	0.045455	0.343678	0.029*
H4B	0.426448	0.230613	0.359472	0.029*
H4C	0.425014	0.160061	0.213243	0.029*
C5	0.28445 (8)	-0.02162 (14)	0.06164 (10)	0.0136 (2)
C6	0.36956 (8)	-0.10852 (14)	0.05394 (11)	0.0155 (2)
H6	0.413667	-0.152562	0.133672	0.019*
C7	0.39089 (8)	-0.13174 (15)	-0.06887 (11)	0.0173 (2)
H7	0.448663	-0.192741	-0.073564	0.021*
C8	0.32711 (8)	-0.06509 (15)	-0.18428 (11)	0.0181 (2)
H8	0.342227	-0.078164	-0.268210	0.022*
C9	0.24121 (8)	0.02072 (15)	-0.17894 (11)	0.0169 (2)
H9	0.198150	0.066045	-0.258987	0.020*
C10	0.21796 (8)	0.04058 (13)	-0.05641 (10)	0.0137 (2)
C11	0.05744 (8)	0.19599 (14)	-0.13980 (11)	0.0169 (2)
C12	-0.02681 (8)	0.26801 (16)	-0.09199 (11)	0.0197 (2)
H12A	-0.036247	0.389215	-0.117457	0.030*
H12B	-0.011413	0.257572	0.006139	0.030*
H12C	-0.087703	0.204217	-0.133482	0.030*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0143 (4)	0.0147 (4)	0.0114 (4)	0.0018 (3)	0.0033 (3)	0.0017 (3)
N2	0.0165 (4)	0.0185 (5)	0.0103 (4)	0.0018 (4)	0.0031 (3)	0.0008 (3)
O1	0.0279 (5)	0.0259 (5)	0.0124 (4)	-0.0038 (3)	0.0025 (3)	-0.0016 (3)
O2	0.0289 (5)	0.0336 (5)	0.0115 (4)	0.0096 (4)	0.0016 (3)	0.0008 (3)
C1	0.0201 (5)	0.0226 (6)	0.0155 (5)	0.0006 (4)	0.0087 (4)	0.0004 (4)

C2	0.0190 (5)	0.0144 (5)	0.0126 (5)	0.0030 (4)	0.0039 (4)	0.0013 (4)
C3	0.0143 (5)	0.0135 (5)	0.0129 (5)	0.0014 (4)	0.0032 (4)	0.0016 (4)
C4	0.0169 (5)	0.0237 (6)	0.0162 (5)	-0.0045 (4)	0.0039 (4)	-0.0019 (4)
C5	0.0150 (5)	0.0141 (5)	0.0119 (5)	-0.0030 (4)	0.0040 (4)	-0.0003 (4)
C6	0.0148 (5)	0.0174 (5)	0.0136 (5)	-0.0001 (4)	0.0026 (4)	0.0016 (4)
C7	0.0167 (5)	0.0192 (5)	0.0178 (5)	-0.0006 (4)	0.0075 (4)	-0.0014 (4)
C8	0.0226 (6)	0.0202 (6)	0.0136 (5)	-0.0028 (4)	0.0086 (4)	-0.0016 (4)
C9	0.0207 (5)	0.0179 (5)	0.0110 (5)	-0.0012 (4)	0.0027 (4)	0.0009 (4)
C10	0.0142 (5)	0.0132 (5)	0.0129 (5)	-0.0018 (4)	0.0023 (4)	-0.0007 (4)
C11	0.0178 (5)	0.0162 (5)	0.0142 (5)	0.0000 (4)	-0.0002 (4)	-0.0014 (4)
C12	0.0172 (5)	0.0232 (6)	0.0165 (5)	0.0030 (4)	0.0006 (4)	-0.0003 (4)

Geometric parameters (Å, °)

N1—C3	1.2756 (14)	C4—H4C	0.9800
N1—C5	1.4147 (13)	C5—C6	1.3904 (15)
N2—H2	0.855 (15)	C5—C10	1.4053 (15)
N2—C10	1.4074 (14)	C6—H6	0.9500
N2—C11	1.3640 (14)	C6—C7	1.3888 (15)
O1—C2	1.2138 (13)	C7—H7	0.9500
O2—C11	1.2239 (14)	C7—C8	1.3831 (16)
C1—H1A	0.9800	C8—H8	0.9500
C1—H1B	0.9800	C8—C9	1.3890 (16)
C1—H1C	0.9800	C9—H9	0.9500
C1—C2	1.4954 (15)	C9—C10	1.3955 (15)
C2—C3	1.5164 (14)	C11—C12	1.5029 (16)
C3—C4	1.4990 (15)	C12—H12A	0.9800
C4—H4A	0.9800	C12—H12B	0.9800
C4—H4B	0.9800	C12—H12C	0.9800
C3—N1—C5	120.76 (9)	C5—C6—H6	119.6
C10—N2—H2	114.6 (10)	C7—C6—C5	120.81 (10)
C11—N2—H2	117.2 (10)	C7—C6—H6	119.6
C11—N2—C10	128.14 (9)	C6—C7—H7	120.4
H1A—C1—H1B	109.5	C8—C7—C6	119.29 (10)
H1A—C1—H1C	109.5	C8—C7—H7	120.4
H1B—C1—H1C	109.5	C7—C8—H8	119.6
C2—C1—H1A	109.5	C7—C8—C9	120.79 (10)
C2—C1—H1B	109.5	C9—C8—H8	119.6
C2—C1—H1C	109.5	C8—C9—H9	119.9
O1—C2—C1	122.86 (10)	C8—C9—C10	120.23 (10)
O1—C2—C3	118.91 (10)	C10—C9—H9	119.9
C1—C2—C3	118.20 (9)	C5—C10—N2	116.91 (9)
N1—C3—C2	116.44 (9)	C9—C10—N2	124.04 (10)
N1—C3—C4	128.13 (10)	C9—C10—C5	119.04 (10)
C4—C3—C2	115.42 (9)	N2—C11—C12	115.04 (10)
C3—C4—H4A	109.5	O2—C11—N2	123.23 (11)
C3—C4—H4B	109.5	O2—C11—C12	121.72 (10)

C3—C4—H4C	109.5	C11—C12—H12A	109.5
H4A—C4—H4B	109.5	C11—C12—H12B	109.5
H4A—C4—H4C	109.5	C11—C12—H12C	109.5
H4B—C4—H4C	109.5	H12A—C12—H12B	109.5
C6—C5—N1	121.37 (9)	H12A—C12—H12C	109.5
C6—C5—C10	119.77 (10)	H12B—C12—H12C	109.5
C10—C5—N1	118.58 (9)		
N1—C5—C6—C7	175.13 (10)	C6—C5—C10—N2	178.09 (9)
N1—C5—C10—N2	4.11 (14)	C6—C5—C10—C9	-2.98 (16)
N1—C5—C10—C9	-176.95 (9)	C6—C7—C8—C9	-1.56 (17)
O1—C2—C3—N1	-177.87 (10)	C7—C8—C9—C10	-0.13 (17)
O1—C2—C3—C4	1.57 (15)	C8—C9—C10—N2	-178.76 (10)
C1—C2—C3—N1	4.39 (14)	C8—C9—C10—C5	2.40 (16)
C1—C2—C3—C4	-176.18 (9)	C10—N2—C11—O2	-3.18 (18)
C3—N1—C5—C6	53.03 (15)	C10—N2—C11—C12	177.87 (10)
C3—N1—C5—C10	-133.09 (11)	C10—C5—C6—C7	1.33 (16)
C5—N1—C3—C2	-172.41 (9)	C11—N2—C10—C5	178.73 (10)
C5—N1—C3—C4	8.23 (17)	C11—N2—C10—C9	-0.15 (18)
C5—C6—C7—C8	0.95 (17)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H8...O1 ⁱ	0.95	2.54	3.3286 (14)	141
C9—H9...O2	0.95	2.24	2.8523 (15)	122
C12—H12B...O2 ⁱⁱ	0.98	2.39	3.3387 (15)	164

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