N-Phenylformamide

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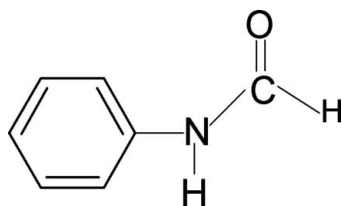Correspondence e-mail: gowdabt@yahoo.com

There are two independent molecules in the asymmetric unit of the title compound, C_7H_7NO. The conformation of the N—H bond in the structure is *syn* to the C=O bond in one of the molecules and *anti* in the other. In the crystal, molecules are packed into chains diagonally in the *ac* plane *via* N—H$\cdots$O hydrogen bonds.

Related literature

For related structures, see: Gowda *et al.* (2006); Brown (1966). For our study of the effect of ring and side chain substitutions on the crystal structures of aromatic amides, see: Gowda *et al.* (2000, 2007, 2009).

Experimental

Crystal data

C_7H_7NO	$b = 6.1737$ (6) Å
$M_r = 121.14$	$c = 14.814$ (1) Å
Monoclinic, $C2/c$	$\beta = 113.14$ (1)°
$a = 30.923$ (3) Å	$V = 2600.6$ (4) Å^3

$Z = 16$	$T = 298$ K
Mo $K\alpha$ radiation	$0.48 \times 0.44 \times 0.40$ mm
$\mu = 0.08$ mm^{-1}	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	Diffraction, 2009)
	$T_{min} = 0.966$, $T_{max} = 0.969$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford	8394 measured reflections
	2383 independent reflections
	1679 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.115$	
$S = 1.12$	$\Delta\rho_{max} = 0.11$ e Å^{-3}
2383 reflections	$\Delta\rho_{min} = -0.10$ e Å^{-3}
170 parameters	

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$N\cdots$O2^i	0.888 (16)	1.936 (16)	2.8239 (17)	178.1 (14)
N2—H2$N\cdots$O1^{ii}	0.857 (16)	2.007 (16)	2.8637 (17)	177.0 (14)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

References

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supporting information

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S1. Comment

As part of a study of the effect of ring and side chain substitutions on the crystal structures of aromatic amides (Gowda *et al.*, 2000; 2007; 2009), the structure of *N*–(phenyl)–formamide (**I**) has been determined. The asymmetric unit contains two independent molecules (Fig. 1). The conformation of the N—H bond is *syn* to the C═O bond in the side chain, in one of the molecules and is *anti* in the other, in contrast to the *anti* conformation observed in *N*–(2,6–dichlorophenyl)–formamide (Gowda *et al.*, 2000 and *N*–(phenyl)–acetamide (Brown *et al.*, 1966). The molecules in (**I**) are linked through intermolecular N—H···O hydrogen bonding (Tab. 1) and the chains formed diagonally as viewed in the *ac* plane (Fig. 2).

S2. Experimental

The purity of the commmercial sample (Aldrich Chemicals) was checked by determining its melting point and characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2006). The single crystals used in *X*–ray diffraction studies were grown in ethanol solution by slow evaporation at room temperature.

S3. Refinement

The H atoms were located in difference map and their positional parameters were refined with C—H = 0.9300 Å with $U_{iso}(H) = 1.2U_{eq}(C)$. The N–bonded H atoms refined freely.
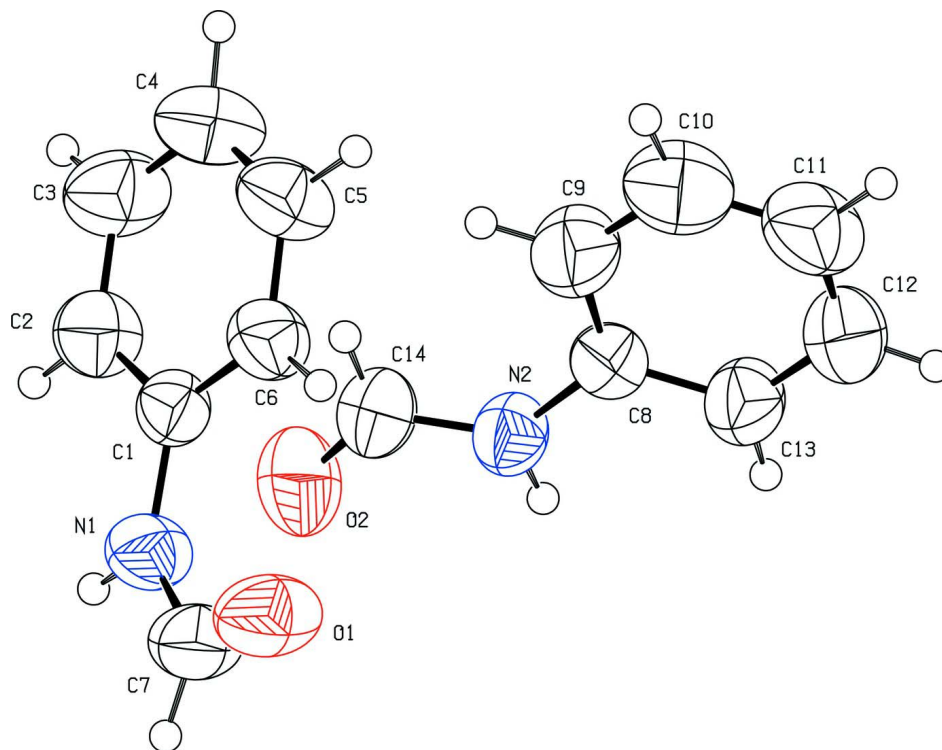
Figure 1

Molecular structure of (**I**), showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as a small spheres of arbitrary radii.
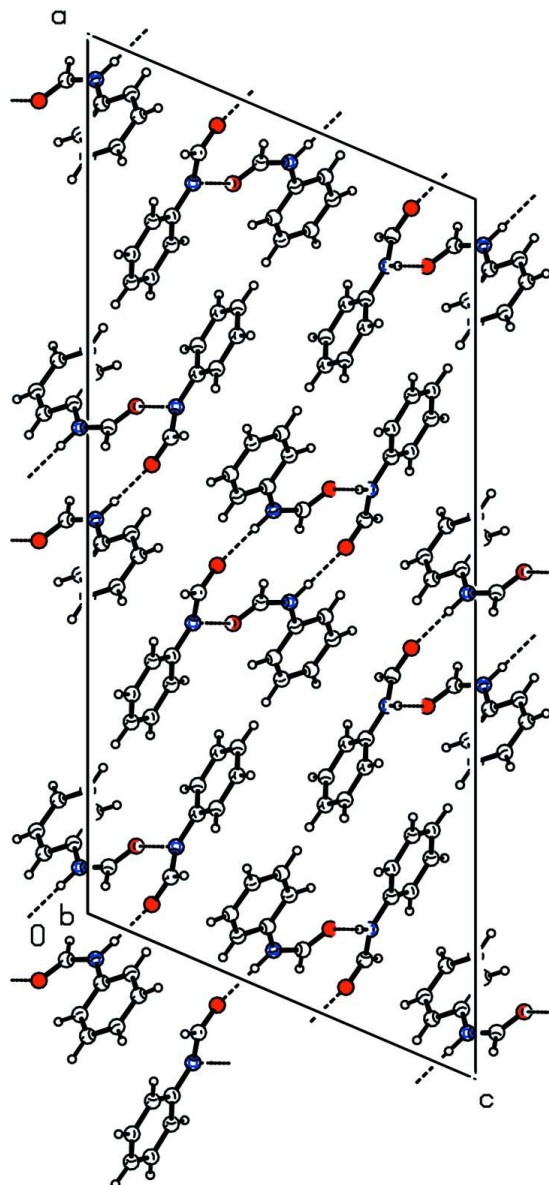
Figure 2

Molecular packing of (**I**) with hydrogen bonding shown as dashed lines.

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Crystal data

C_7H_7NO
$M_r = 121.14$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 30.923$ (3) Å
$b = 6.1737$ (6) Å
$c = 14.814$ (1) Å
$\beta = 113.14$ (1)°
$V = 2600.6$ (4) Å^3
$Z = 16$

$F(000) = 1024$
$D_x = 1.238$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2475 reflections
$\theta = 2.7–28.2°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Needle, colourless
$0.48 \times 0.44 \times 0.40$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	8394 measured reflections
	2383 independent reflections
Radiation source: Fine–focus sealed tube	1679 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.016$
ω and φ scans	$\theta_{max} = 25.4°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$h = -37 \rightarrow 36$
	$k = -7 \rightarrow 7$
$T_{min} = 0.966$, $T_{max} = 0.969$	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.115$	
$S = 1.12$	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2]$
2383 reflections	where $P = (F_o^2 + 2F_c^2)/3$
170 parameters	$(\Delta/\sigma)_{max} < 0.001$
0 restraints	$\Delta\rho_{max} = 0.11$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.10$ e Å^{-3}
	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0028 (7)

Special details

Experimental. Absorption correction: CrysAlis RED (Oxford Diffraction, 2009); empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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	0.09999 (4)	0.21410 (18)	0.62537 (8)	0.0921 (4)
N1	0.04841 (4)	0.34831 (19)	0.47961 (9)	0.0694 (4)
H1N	0.0202 (6)	0.322 (2)	0.4332 (11)	0.083*
C1	0.07229 (4)	0.5289 (2)	0.46365 (9)	0.0561 (3)
C2	0.04734 (5)	0.6657 (3)	0.38753 (10)	0.0727 (4)
H2	0.0159	0.6367	0.3491	0.087*
C3	0.06857 (6)	0.8441 (3)	0.36825 (12)	0.0893 (5)
H3	0.0515	0.9351	0.3164	0.107*
C4	0.11462 (6)	0.8895 (3)	0.42461 (12)	0.0890 (5)
H4	0.1289	1.0119	0.4119	0.107*
C5	0.13948 (6)	0.7535 (3)	0.49972 (12)	0.0828 (5)
H5	0.1709	0.7834	0.5378	0.099*
C6	0.11890 (5)	0.5734 (2)	0.51989 (11)	0.0687 (4)

H6	0.1363	0.4818	0.5712	0.082*
C7	0.06296 (6)	0.2094 (2)	0.55435 (12)	0.0792 (5)
H7	0.0426	0.0966	0.5518	0.095*
O2	0.04140 (4)	0.2563 (2)	0.16582 (9)	0.0996 (4)
N2	0.11861 (4)	0.1904 (2)	0.22825 (8)	0.0628 (3)
H2N	0.1131 (5)	0.067 (3)	0.1994 (10)	0.075*
C8	0.16640 (5)	0.2389 (2)	0.28235 (9)	0.0565 (3)
C9	0.18179 (6)	0.4299 (3)	0.33258 (13)	0.0862 (5)
H9	0.1603	0.5369	0.3309	0.103*
C10	0.22921 (7)	0.4618 (3)	0.38543 (14)	0.1024 (6)
H10	0.2394	0.5901	0.4202	0.123*
C11	0.26131 (6)	0.3093 (3)	0.38760 (14)	0.0963 (6)
H11	0.2932	0.3324	0.4235	0.116*
C12	0.24605 (6)	0.1230 (3)	0.33668 (13)	0.0919 (5)
H12	0.2678	0.0184	0.3371	0.110*
C13	0.19895 (5)	0.0867 (2)	0.28451 (11)	0.0750 (4)
H13	0.1891	−0.0425	0.2503	0.090*
C14	0.08175 (6)	0.3109 (3)	0.21441 (12)	0.0771 (4)
H14	0.0867	0.4471	0.2436	0.093*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0813 (8)	0.0791 (7)	0.0881 (8)	−0.0120 (6)	0.0032 (6)	0.0215 (5)
N1	0.0527 (7)	0.0658 (8)	0.0743 (8)	−0.0096 (6)	0.0082 (6)	0.0067 (6)
C1	0.0522 (8)	0.0564 (8)	0.0570 (7)	−0.0001 (6)	0.0186 (6)	−0.0032 (6)
C2	0.0644 (9)	0.0780 (10)	0.0644 (9)	−0.0023 (7)	0.0131 (7)	0.0049 (7)
C3	0.1006 (14)	0.0823 (11)	0.0750 (10)	−0.0058 (10)	0.0236 (9)	0.0207 (9)
C4	0.0993 (14)	0.0849 (12)	0.0826 (11)	−0.0263 (10)	0.0355 (10)	0.0063 (9)
C5	0.0682 (10)	0.0902 (12)	0.0847 (11)	−0.0210 (9)	0.0242 (8)	0.0026 (9)
C6	0.0555 (8)	0.0699 (9)	0.0742 (9)	−0.0033 (7)	0.0184 (7)	0.0063 (7)
C7	0.0714 (10)	0.0648 (9)	0.0897 (11)	−0.0116 (8)	0.0189 (9)	0.0098 (8)
O2	0.0556 (7)	0.1164 (10)	0.1092 (9)	0.0152 (6)	0.0132 (6)	0.0123 (7)
N2	0.0567 (7)	0.0615 (7)	0.0645 (7)	0.0048 (6)	0.0175 (6)	−0.0040 (5)
C8	0.0557 (8)	0.0602 (8)	0.0522 (7)	−0.0013 (6)	0.0197 (6)	0.0026 (6)
C9	0.0790 (12)	0.0746 (10)	0.1005 (12)	−0.0037 (8)	0.0303 (9)	−0.0202 (9)
C10	0.0939 (14)	0.0939 (13)	0.1047 (13)	−0.0311 (11)	0.0233 (11)	−0.0271 (10)
C11	0.0647 (11)	0.1055 (15)	0.0999 (13)	−0.0158 (11)	0.0122 (9)	0.0068 (11)
C12	0.0601 (10)	0.0924 (12)	0.1119 (13)	0.0070 (9)	0.0218 (9)	0.0067 (10)
C13	0.0618 (9)	0.0680 (9)	0.0873 (10)	0.0029 (7)	0.0209 (8)	−0.0064 (7)
C14	0.0667 (11)	0.0739 (10)	0.0865 (11)	0.0132 (8)	0.0256 (9)	0.0104 (8)

Geometric parameters (Å, º)

O1—C7	1.2132 (17)	O2—C14	1.2178 (18)
N1—C7	1.3314 (19)	N2—C14	1.3082 (19)
N1—C1	1.4076 (17)	N2—C8	1.4089 (17)
N1—H1N	0.888 (16)	N2—H2N	0.857 (16)

C1—C2	1.3771 (19)	C8—C13	1.3684 (19)
C1—C6	1.3797 (18)	C8—C9	1.375 (2)
C2—C3	1.369 (2)	C9—C10	1.378 (2)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.367 (2)	C10—C11	1.359 (3)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.365 (2)	C11—C12	1.354 (3)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.371 (2)	C12—C13	1.373 (2)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—H7	0.9300	C14—H14	0.9300
C7—N1—C1	128.45 (13)	C14—N2—C8	128.51 (14)
C7—N1—H1N	115.8 (10)	C14—N2—H2N	115.9 (10)
C1—N1—H1N	115.7 (10)	C8—N2—H2N	115.6 (10)
C2—C1—C6	119.24 (13)	C13—C8—C9	118.76 (14)
C2—C1—N1	117.46 (12)	C13—C8—N2	117.69 (12)
C6—C1—N1	123.29 (12)	C9—C8—N2	123.55 (13)
C3—C2—C1	120.27 (14)	C8—C9—C10	119.64 (16)
C3—C2—H2	119.9	C8—C9—H9	120.2
C1—C2—H2	119.9	C10—C9—H9	120.2
C4—C3—C2	120.51 (15)	C11—C10—C9	121.22 (17)
C4—C3—H3	119.7	C11—C10—H10	119.4
C2—C3—H3	119.7	C9—C10—H10	119.4
C5—C4—C3	119.30 (15)	C12—C11—C10	118.93 (17)
C5—C4—H4	120.4	C12—C11—H11	120.5
C3—C4—H4	120.4	C10—C11—H11	120.5
C4—C5—C6	121.06 (15)	C11—C12—C13	120.85 (17)
C4—C5—H5	119.5	C11—C12—H12	119.6
C6—C5—H5	119.5	C13—C12—H12	119.6
C5—C6—C1	119.62 (14)	C8—C13—C12	120.59 (15)
C5—C6—H6	120.2	C8—C13—H13	119.7
C1—C6—H6	120.2	C12—C13—H13	119.7
O1—C7—N1	126.94 (14)	O2—C14—N2	124.22 (16)
O1—C7—H7	116.5	O2—C14—H14	117.9
N1—C7—H7	116.5	N2—C14—H14	117.9
C7—N1—C1—C2	−171.26 (15)	C14—N2—C8—C13	−178.73 (14)
C7—N1—C1—C6	9.0 (2)	C14—N2—C8—C9	1.3 (2)
C6—C1—C2—C3	−0.2 (2)	C13—C8—C9—C10	−1.4 (2)
N1—C1—C2—C3	180.00 (14)	N2—C8—C9—C10	178.58 (15)
C1—C2—C3—C4	−0.5 (3)	C8—C9—C10—C11	1.1 (3)
C2—C3—C4—C5	0.8 (3)	C9—C10—C11—C12	0.0 (3)
C3—C4—C5—C6	−0.5 (3)	C10—C11—C12—C13	−0.8 (3)
C4—C5—C6—C1	−0.2 (2)	C9—C8—C13—C12	0.7 (2)
C2—C1—C6—C5	0.5 (2)	N2—C8—C13—C12	−179.34 (13)
N1—C1—C6—C5	−179.70 (14)	C11—C12—C13—C8	0.4 (3)

C1—N1—C7—O1	1.5 (3)	C8—N2—C14—O2	179.62 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2[i]	0.888 (16)	1.936 (16)	2.8239 (17)	178.1 (14)
N2—H2*N*···O1[ii]	0.857 (16)	2.007 (16)	2.8637 (17)	177.0 (14)

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