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Salicylaldehyde–4-(dimethylamino)-pyridine (1/1)

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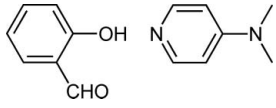
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.163; data-to-parameter ratio = 17.5.

In the title compound, $C_7H_{10}N_2\cdot C_7H_6O_2$, the components are linked by an O—H···N hydrogen bond. The mean planes of two molecules form a dihedral angle of 78.68 (5)°. The crystal packing exhibits weak non-classical C—H···O contacts.

Related literature

For background to hydrogen bonding in crystal engineering, see: Bosch (2010); Desiraju (1989); Lehn (1995). For related structures, see: Bosch (2010); Vembu *et al.* (2003); Lo & Ng (2009).



Experimental

Crystal data

$C_7H_{10}N_2\cdot C_7H_6O_2$
M_r = 244.29
Triclinic, $P\overline{1}$
a = 7.540 (3) Å
b = 8.473 (3) Å
c = 10.413 (4) Å
α = 85.370 (11)°
β = 77.371 (10)°
γ = 87.203 (10)°
V = 646.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.4 × 0.4 × 0.38 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.967, T_{max} = 0.968
4199 measured reflections
2913 independent reflections
1882 reflections with $I > 2\sigma(I)$
R_{int} = 0.02

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.163
S = 1.01
2913 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N1	0.82	1.82	2.637 (2)	174
C9—H9···O1^{i}	0.93	2.69	3.456 (3)	140
C5—H5···O1^{ii}	0.93	2.7	3.583 (3)	158

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2756).

References

Bosch, E. (2010). *Cryst. Growth Des.* **10**, 3808–3813.
Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. (1989). *Crystal Engineering: The Design of Organic Solids.* Amsterdam: Elsevier.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lehn, J. M. (1995). *Supramolecular Chemistry.* New York: VCH.
Lo, K. M. & Ng, S. W. (2009). *Acta Cryst.* E**65**, m958–m959.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Vembu, N., Nallu, M., Garrison, J. & Youngs, W. J. (2003). *Acta Cryst.* E**59**, o913–o916.

supporting information

Acta Cryst. (2010). E**66**, o2423 [https://doi.org/10.1107/S1600536810034185]

Salicylaldehyde–4-(dimethylamino)pyridine (1/1)

Chuttree Phurat, Thapong Teerawatananond and Nongnuj Muangsin

S1. Comment

Hydrogen bonding is the most important and the essential tool for both crystal engineering and supramolecular chemistry (Bosch, 2010; Desiraju, 1989 & Lehn, 1995). The non-classical C—H···N hydrogen bonds in pyridine and pyrimidine derivatives have remarkable potentials and patterns (Bosch, 2010; Desiraju, 1989; Lehn, 1995; Lo & Ng, 2009 & Vembu *et al.*, 2003;). In order to investigate the hydrogen bonding patterns of 4-(dimethylamino)pyridine, the co-crystals with various derivatives of benzaldehyde were prepared.

We report here the structure of the title co-crystal compound (Fig.1), formed from salicylaldehyde and 4-(dimethylamino)pyridine. The asymmetric unit contains one molecule of salicylaldehyde and one molecule of 4-(dimethylamino)-pyridine linked by O—H···N hydrogen bond (Table 1). The mean planes of two molecules form a dihedral angle of 78.68 (5)°. The crystal packing exhibits weak non-classical C—H···O contacts (Table 1).

S2. Experimental

The title cocrystal was crystallized by slow evaporation from the refluxed mixture of an equimolar solution of salicyl-aldehyde and 4-(dimethylamino)pyridine in a solution of methanol.

S3. Refinement

All H-atoms were geometrically positioned and refined using a riding model, with C—H = 0.93 Å (aromatic), 0.98 Å (CH_3) and O–H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq} (C) for aromatic and 1.5U_{eq} for O and C_{methyl}.

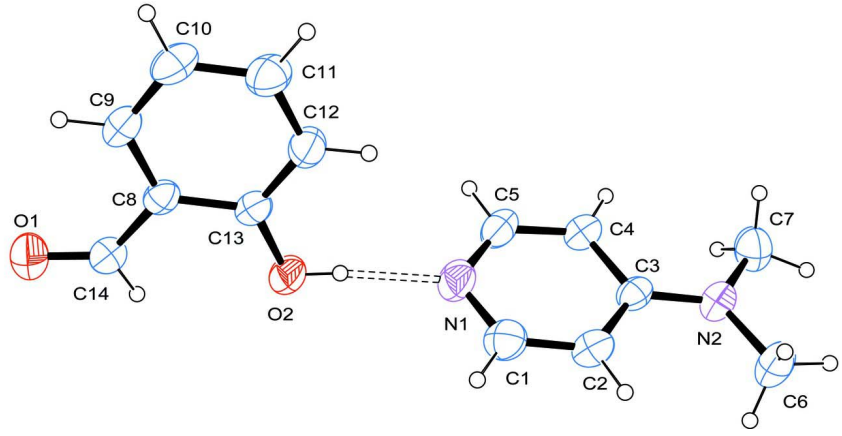

Figure 1

The content of asymmetric unit of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bond is shown as a dashed line.

2-Hydroxybenzaldehyde–4-(dimethylamino)pyridine (1/1)

Crystal data

$C_7H_{10}N_2{\cdot}C_7H_6O_2$
$M_r = 244.29$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.540$ (3) Å
$b = 8.473$ (3) Å
$c = 10.413$ (4) Å
$\alpha = 85.370$ (11)°
$\beta = 77.371$ (10)°
$\gamma = 87.203$ (10)°
$V = 646.7$ (4) Å^3
$Z = 2$
$F(000) = 260$
$D_x = 1.255$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1563 reflections
$\theta = 2.8$–$27.8°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Prism, yellow
0.4 × 0.4 × 0.38 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: Mo Kα
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.967$, $T_{max} = 0.968$
4199 measured reflections
2913 independent reflections
1882 reflections with $I > 2\sigma(I)$
$R_{int} = 0.02$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.8°$
$h = -10 \rightarrow 9$
$k = -5 \rightarrow 11$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.163$
$S = 1.01$
2913 reflections
166 parameters
0 restraints
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0815P)^2 + 0.0644P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8429 (3)	0.2372 (2)	0.5097 (2)	0.0720 (5)
H1	0.868	0.1401	0.5513	0.086*
C2	0.7810 (3)	0.3587 (2)	0.58701 (17)	0.0638 (5)
H2	0.7635	0.3422	0.6782	0.077*
C3	0.7433 (2)	0.5084 (2)	0.52993 (15)	0.0521 (4)
C4	0.7680 (2)	0.5182 (2)	0.39168 (16)	0.0604 (4)
H4	0.7426	0.6132	0.3469	0.072*
C5	0.8288 (3)	0.3893 (3)	0.32350 (18)	0.0693 (5)
H5	0.8428	0.4003	0.2323	0.083*
C6	0.6562 (3)	0.6217 (3)	0.74452 (19)	0.0879 (7)
H6A	0.5548	0.5552	0.7795	0.132*
H6B	0.6298	0.725	0.777	0.132*
H6C	0.7624	0.5762	0.7717	0.132*
C7	0.6590 (3)	0.7888 (3)	0.5390 (2)	0.0798 (6)
H7A	0.7616	0.8131	0.4686	0.12*
H7B	0.6445	0.8672	0.6024	0.12*
H7C	0.5513	0.7885	0.5041	0.12*
C8	0.9510 (2)	−0.18638 (19)	0.10290 (14)	0.0500 (4)
C9	0.8248 (3)	−0.2663 (2)	0.05460 (16)	0.0603 (5)
H9	0.8641	−0.3511	0.0029	0.072*
C10	0.6437 (3)	−0.2223 (3)	0.08184 (19)	0.0724 (5)
H10	0.5604	−0.2764	0.0493	0.087*
C11	0.5875 (3)	−0.0964 (3)	0.1584 (2)	0.0754 (6)
H11	0.4652	−0.065	0.1763	0.09*
C12	0.7082 (2)	−0.0158 (2)	0.20895 (18)	0.0654 (5)
H12	0.6669	0.0687	0.2605	0.078*
C13	0.8914 (2)	−0.06070 (19)	0.18288 (14)	0.0515 (4)
C14	1.1435 (3)	−0.2309 (2)	0.06846 (17)	0.0631 (5)
H14	1.2235	−0.1669	0.0951	0.076*
N1	0.8703 (2)	0.2475 (2)	0.37777 (17)	0.0724 (5)
N2	0.6887 (2)	0.63491 (19)	0.60206 (13)	0.0636 (4)
O1	1.2084 (2)	−0.34318 (19)	0.00855 (16)	0.0891 (5)
O2	1.01269 (17)	0.01257 (16)	0.23295 (13)	0.0670 (4)
H2A	0.961	0.0844	0.2765	0.101*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0818 (13)	0.0592 (12)	0.0816 (13)	−0.0101 (9)	−0.0299 (10)	−0.0061 (9)
C2	0.0763 (12)	0.0654 (12)	0.0532 (9)	−0.0126 (9)	−0.0203 (8)	−0.0007 (8)
C3	0.0488 (8)	0.0622 (11)	0.0477 (8)	−0.0119 (7)	−0.0121 (7)	−0.0073 (7)
C4	0.0678 (10)	0.0654 (11)	0.0503 (9)	−0.0068 (8)	−0.0163 (8)	−0.0055 (8)
C5	0.0764 (12)	0.0813 (15)	0.0542 (10)	−0.0080 (10)	−0.0162 (9)	−0.0188 (9)
C6	0.1038 (16)	0.1054 (19)	0.0546 (11)	0.0003 (13)	−0.0119 (10)	−0.0232 (11)
C7	0.0877 (14)	0.0677 (14)	0.0813 (13)	0.0053 (10)	−0.0114 (11)	−0.0126 (10)
C8	0.0633 (10)	0.0484 (9)	0.0393 (7)	−0.0072 (7)	−0.0137 (7)	0.0023 (6)
C9	0.0776 (12)	0.0578 (11)	0.0483 (9)	−0.0128 (8)	−0.0154 (8)	−0.0085 (7)
C10	0.0688 (12)	0.0883 (15)	0.0667 (11)	−0.0241 (10)	−0.0209 (9)	−0.0136 (10)
C11	0.0588 (11)	0.0952 (16)	0.0755 (12)	−0.0095 (10)	−0.0163 (9)	−0.0173 (11)
C12	0.0636 (11)	0.0681 (12)	0.0668 (11)	−0.0022 (9)	−0.0141 (8)	−0.0187 (9)
C13	0.0615 (10)	0.0502 (9)	0.0455 (8)	−0.0089 (7)	−0.0170 (7)	−0.0008 (7)
C14	0.0698 (11)	0.0637 (12)	0.0600 (10)	−0.0001 (9)	−0.0218 (8)	−0.0105 (8)
N1	0.0745 (10)	0.0704 (12)	0.0794 (11)	−0.0065 (8)	−0.0232 (8)	−0.0264 (8)
N2	0.0734 (9)	0.0667 (10)	0.0507 (8)	−0.0049 (7)	−0.0103 (7)	−0.0114 (7)
O1	0.0889 (10)	0.0822 (11)	0.1002 (11)	0.0161 (8)	−0.0239 (8)	−0.0325 (8)
O2	0.0665 (8)	0.0665 (9)	0.0756 (8)	−0.0047 (6)	−0.0244 (6)	−0.0235 (6)

Geometric parameters (Å, º)

C1—N1	1.340 (3)	C7—H7B	0.96
C1—C2	1.359 (3)	C7—H7C	0.96
C1—H1	0.93	C8—C9	1.394 (2)
C2—C3	1.400 (3)	C8—C13	1.401 (2)
C2—H2	0.93	C8—C14	1.455 (3)
C3—N2	1.355 (2)	C9—C10	1.372 (3)
C3—C4	1.407 (2)	C9—H9	0.93
C4—C5	1.357 (3)	C10—C11	1.378 (3)
C4—H4	0.93	C10—H10	0.93
C5—N1	1.339 (3)	C11—C12	1.378 (3)
C5—H5	0.93	C11—H11	0.93
C6—N2	1.446 (2)	C12—C13	1.389 (3)
C6—H6A	0.96	C12—H12	0.93
C6—H6B	0.96	C13—O2	1.3452 (18)
C6—H6C	0.96	C14—O1	1.205 (2)
C7—N2	1.442 (3)	C14—H14	0.93
C7—H7A	0.96	O2—H2A	0.82
N1—C1—C2	124.69 (19)	C9—C8—C13	119.44 (16)
N1—C1—H1	117.7	C9—C8—C14	120.36 (16)
C2—C1—H1	117.7	C13—C8—C14	120.19 (14)
C1—C2—C3	120.29 (17)	C10—C9—C8	121.25 (17)
C1—C2—H2	119.9	C10—C9—H9	119.4
C3—C2—H2	119.9	C8—C9—H9	119.4

N2—C3—C2	122.62 (15)	C9—C10—C11	118.68 (17)
N2—C3—C4	122.36 (16)	C9—C10—H10	120.7
C2—C3—C4	115.02 (16)	C11—C10—H10	120.7
C5—C4—C3	120.10 (18)	C10—C11—C12	121.63 (19)
C5—C4—H4	120	C10—C11—H11	119.2
C3—C4—H4	120	C12—C11—H11	119.2
N1—C5—C4	124.86 (17)	C11—C12—C13	119.98 (18)
N1—C5—H5	117.6	C11—C12—H12	120
C4—C5—H5	117.6	C13—C12—H12	120
N2—C6—H6A	109.5	O2—C13—C12	121.78 (16)
N2—C6—H6B	109.5	O2—C13—C8	119.24 (15)
H6A—C6—H6B	109.5	C12—C13—C8	118.99 (15)
N2—C6—H6C	109.5	O1—C14—C8	125.87 (17)
H6A—C6—H6C	109.5	O1—C14—H14	117.1
H6B—C6—H6C	109.5	C8—C14—H14	117.1
N2—C7—H7A	109.5	C5—N1—C1	114.99 (16)
N2—C7—H7B	109.5	C3—N2—C7	120.92 (15)
H7A—C7—H7B	109.5	C3—N2—C6	121.81 (17)
N2—C7—H7C	109.5	C7—N2—C6	117.26 (16)
H7A—C7—H7C	109.5	C13—O2—H2A	109.5
H7B—C7—H7C	109.5		

N1—C1—C2—C3	−1.0 (3)	C9—C8—C13—O2	177.74 (14)
C1—C2—C3—N2	−177.17 (16)	C14—C8—C13—O2	−3.5 (2)
C1—C2—C3—C4	2.3 (2)	C9—C8—C13—C12	−1.9 (2)
N2—C3—C4—C5	177.77 (16)	C14—C8—C13—C12	176.90 (16)
C2—C3—C4—C5	−1.7 (2)	C9—C8—C14—O1	−6.8 (3)
C3—C4—C5—N1	−0.3 (3)	C13—C8—C14—O1	174.44 (18)
C13—C8—C9—C10	1.3 (2)	C4—C5—N1—C1	1.7 (3)
C14—C8—C9—C10	−177.51 (16)	C2—C1—N1—C5	−1.1 (3)
C8—C9—C10—C11	0.1 (3)	C2—C3—N2—C7	177.21 (17)
C9—C10—C11—C12	−0.8 (3)	C4—C3—N2—C7	−2.2 (3)
C10—C11—C12—C13	0.2 (3)	C2—C3—N2—C6	−3.3 (3)
C11—C12—C13—O2	−178.43 (16)	C4—C3—N2—C6	177.28 (17)
C11—C12—C13—C8	1.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N1	0.82	1.82	2.637 (2)	174
C9—H9···O1^{i}	0.93	2.69	3.456 (3)	140
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