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2-Carboxylatopyridinium–4-nitrophenol (1/1)

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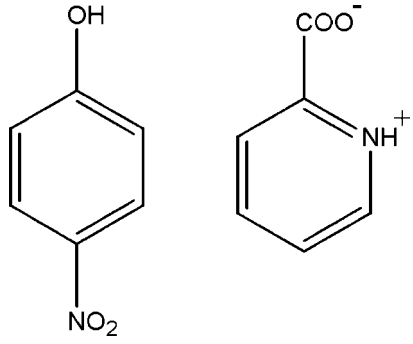
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.130; data-to-parameter ratio = 19.4.

In the title 1:1 adduct, $C_6H_5NO_3\cdot C_6H_5NO_2$, both molecules are almost planar (r.m.s. deviations for the non-H atoms = 0.027 and 0.023 Å for 4-nitrophenol and 2-carboxylatopyridinium, respectively). The pyridine molecule crystallizes as a zwitterion (nominal proton transfer from the carboxylic acid group to the N atom in the ring). In the crystal, inversion dimers of the zwitterions linked by pairs of N—H···O hydrogen bonds generate $R_2^2(10)$ loops; two 4-nitrophenol molecules link to the dimer by O—H···O hydrogen bonds, generating a four-molecule aggregate. These are linked by C—H···O interactions, forming a three-dimensional network.

Related literature

For a related structure, see: Pandi *et al.* (2012).



Experimental

Crystal data

$C_6H_5NO_3\cdot C_6H_5NO_2$
M_r = 262.22
Triclinic, $P\overline{1}$
a = 6.1743 (4) Å
b = 7.0512 (3) Å
c = 14.2222 (8) Å
α = 101.727 (3)°
β = 92.191 (2)°
γ = 104.758 (4)°
V = 583.60 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.32 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.963, T_{max} = 0.977
13952 measured reflections
3486 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 1.04
3486 reflections
180 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O5^{i}	0.84 (1)	1.77 (1)	2.5929 (15)	165 (2)
N2—H2···O4^{ii}	0.87 (1)	1.88 (1)	2.6693 (15)	151 (2)
C5—H5···O3^{iii}	0.93	2.56	3.3570 (17)	143
C9—H9···O2^{iv}	0.93	2.57	3.2009 (18)	126

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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*.

The authors thank the SAIF, IIT, Madras, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7209).

References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Pandi, P., Peramaiyan, G., Akilan, R., Chakkaravarthi, G. & Mohankumar, R. (2012). *Acta Cryst.* E**68**, o3081.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2014). E**70**, o450 [doi:10.1107/S1600536814005650]

2-Carboxylatopyridinium–4-nitrophenol (1/1)

A. Sankar, S. Ambalatharasu, G. Peramaiyan, G. Chakkaravarthi and R. Kanagadurai

1. Comment

We herin report the crystal structure of (I), (Fig. 1). The bond lengths are comparable with those in a similar structure (Pandi *et al.*, 2012).

The pyridine ring is almost planar, with the maximum deviation of 0.005 (2) Å. The carboxy group is twisted at an angle of 2.9 (1)° with the pyridine ring. The nitro group is oriented at an angle of 1.8 (1)° with the benzene ring. The crystal structure features O—H···O, N—H···O and C—H···O (Fig. 2 & Table 1) interactions to form a three dimensional network.

2. Experimental

The title material was synthesized by taking 2-carboxypyridine (1.2331 g) and p-nitrophenol (1.3911 g) in an equimolar ratio. 2-carboxypyridine was added gradually in the saturated solution of p-nitrophenol using methanol with continuous stirring for one hour and white precipitate was obtained. Then, the precipitate was dissolved using the same solvent. The prepared solution was allowed for slow evaporation at room temperature to yield colourless blocks after 10 days.

3. Refinement

H atoms for $C_{aromatic}$ were positioned geometrically and refined using riding model, with C-H = 0.93 Å and Uiso(H) = 1.2Ueq(C). H atoms bounded to N and O atoms were fixed from the fourier map and refined freely with the distance restraints: 0.82 (1)Å for O—H and 0.86 (1)Å for N—H.

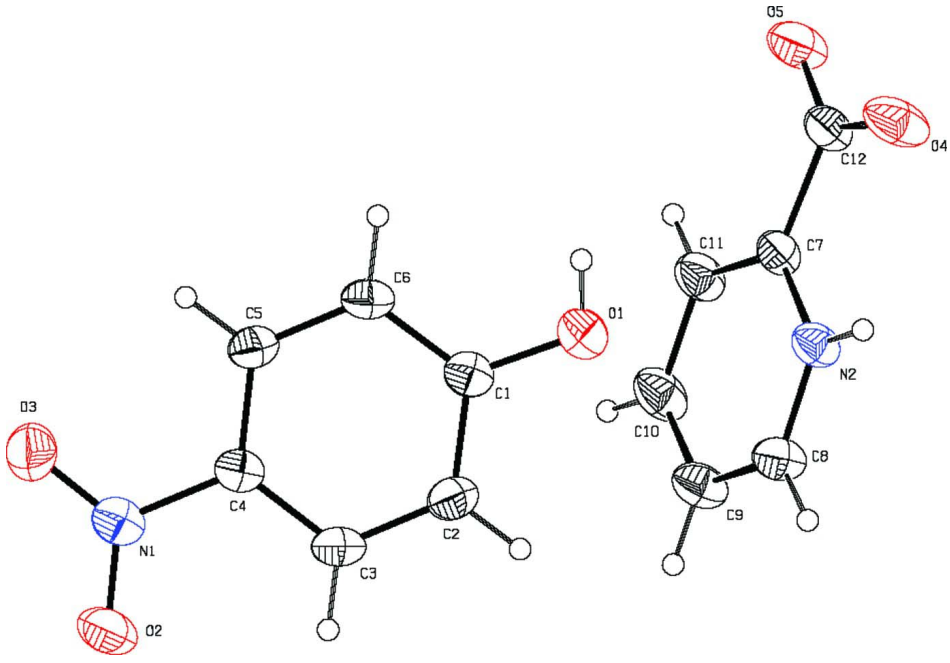


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

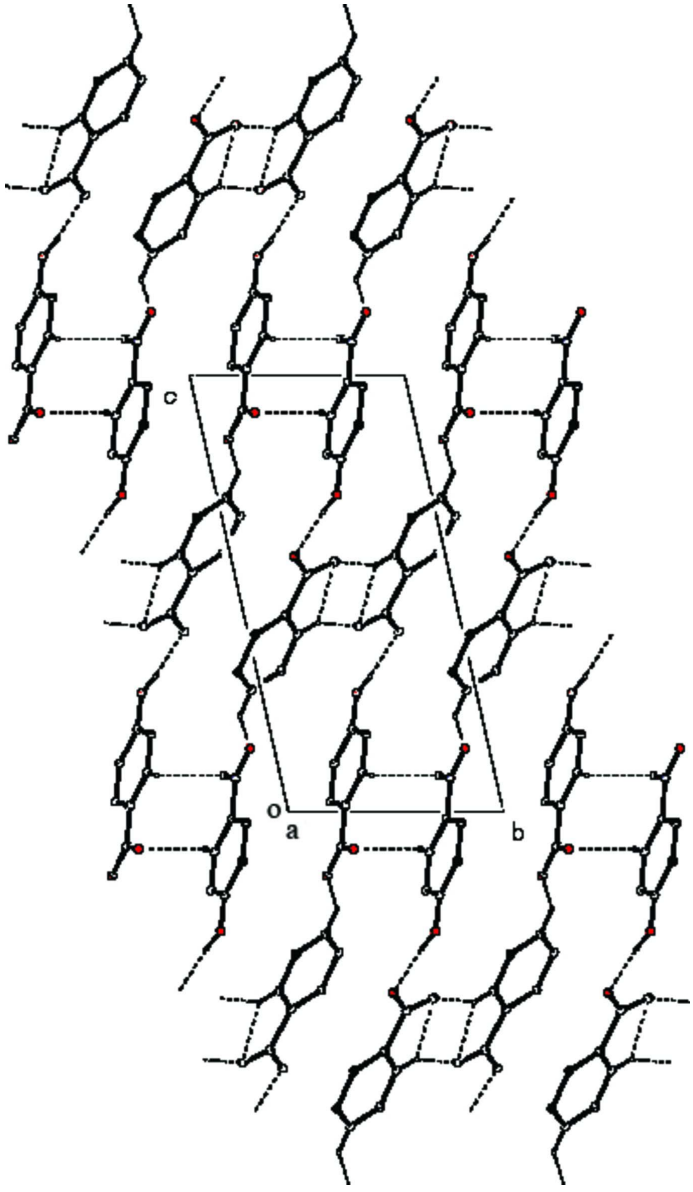


Figure 2

The packing of (I), viewed down *a* axis. Intermolecular Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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Crystal data

$C_6H_5NO_3 \cdot C_6H_5NO_2$
$M_r = 262.22$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.1743$ (4) Å
$b = 7.0512$ (3) Å
$c = 14.2222$ (8) Å
$\alpha = 101.727$ (3)°
$\beta = 92.191$ (2)°
$\gamma = 104.758$ (4)°
$V = 583.60$ (6) Å^3
$Z = 2$
$F(000) = 272$
$D_x = 1.492$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4728 reflections
$\theta = 2.9$–27.7°
$\mu = 0.12$ mm^{-1}

T = 295 K
Block, colourless

0.32 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.963, T_{max} = 0.977

13952 measured reflections
3486 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 30.4°, θ_{min} = 2.9°
h = −8→8
k = −10→9
l = −17→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 1.04
3486 reflections
180 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.0686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.3865 (2)	0.38442 (18)	0.19001 (9)	0.0451 (3)
C2	0.2381 (2)	0.2646 (2)	0.11160 (10)	0.0498 (3)
H2A	0.0853	0.2230	0.1187	0.060*
C3	0.3152 (2)	0.20783 (19)	0.02422 (9)	0.0474 (3)
H3	0.2155	0.1288	−0.0281	0.057*
C4	0.5424 (2)	0.26918 (17)	0.01464 (9)	0.0414 (3)
C5	0.6929 (2)	0.38640 (18)	0.09160 (9)	0.0459 (3)
H5	0.8455	0.4274	0.0840	0.055*
C6	0.6153 (2)	0.44171 (18)	0.17923 (9)	0.0474 (3)
H6	0.7161	0.5179	0.2317	0.057*
C7	0.1820 (2)	0.19479 (19)	0.45093 (8)	0.0429 (3)
C8	−0.1051 (2)	0.1161 (2)	0.32506 (10)	0.0512 (3)
H8	−0.2284	0.1462	0.2981	0.061*
C9	−0.0352 (3)	−0.0443 (2)	0.27958 (10)	0.0550 (3)
H9	−0.1090	−0.1236	0.2211	0.066*
C10	0.1445 (3)	−0.0868 (2)	0.32101 (10)	0.0589 (4)
H10	0.1930	−0.1968	0.2912	0.071*
C11	0.2543 (3)	0.0336 (2)	0.40725 (9)	0.0529 (3)

H11	0.3772	0.0051	0.4356	0.063*
C12	0.2879 (2)	0.3378 (2)	0.54544 (9)	0.0477 (3)
N1	0.6252 (2)	0.21159 (16)	−0.07787 (8)	0.0501 (3)
N2	0.00405 (19)	0.22997 (16)	0.40848 (7)	0.0452 (3)
O1	0.29906 (19)	0.44091 (17)	0.27221 (8)	0.0619 (3)
O2	0.4895 (2)	0.11237 (18)	−0.14600 (7)	0.0689 (3)
O3	0.82814 (19)	0.26305 (17)	−0.08431 (8)	0.0714 (3)
O4	0.2047 (2)	0.47818 (17)	0.57395 (7)	0.0701 (3)
O5	0.44519 (18)	0.29715 (16)	0.58610 (7)	0.0666 (3)
H2	−0.039 (3)	0.3351 (18)	0.4342 (11)	0.066 (5)*
H1	0.400 (3)	0.524 (2)	0.3119 (12)	0.085 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0519 (7)	0.0382 (6)	0.0449 (6)	0.0139 (5)	−0.0003 (5)	0.0071 (5)
C2	0.0394 (6)	0.0514 (7)	0.0550 (7)	0.0101 (5)	−0.0036 (5)	0.0075 (6)
C3	0.0460 (7)	0.0433 (6)	0.0476 (7)	0.0104 (5)	−0.0116 (5)	0.0030 (5)
C4	0.0478 (7)	0.0346 (6)	0.0427 (6)	0.0150 (5)	−0.0034 (5)	0.0066 (5)
C5	0.0404 (6)	0.0410 (6)	0.0525 (7)	0.0091 (5)	−0.0041 (5)	0.0054 (5)
C6	0.0476 (7)	0.0409 (6)	0.0469 (6)	0.0078 (5)	−0.0091 (5)	0.0019 (5)
C7	0.0500 (7)	0.0472 (7)	0.0334 (5)	0.0184 (5)	0.0041 (5)	0.0067 (5)
C8	0.0550 (8)	0.0496 (7)	0.0459 (7)	0.0160 (6)	−0.0074 (6)	0.0034 (5)
C9	0.0678 (9)	0.0471 (7)	0.0443 (7)	0.0161 (6)	−0.0051 (6)	−0.0021 (5)
C10	0.0792 (10)	0.0547 (8)	0.0458 (7)	0.0334 (7)	0.0042 (7)	−0.0016 (6)
C11	0.0617 (8)	0.0616 (8)	0.0412 (6)	0.0335 (7)	0.0005 (6)	0.0039 (6)
C12	0.0572 (8)	0.0530 (7)	0.0350 (5)	0.0238 (6)	0.0008 (5)	0.0034 (5)
N1	0.0602 (7)	0.0435 (6)	0.0477 (6)	0.0192 (5)	−0.0009 (5)	0.0071 (5)
N2	0.0544 (6)	0.0435 (6)	0.0386 (5)	0.0206 (5)	−0.0001 (4)	0.0024 (4)
O1	0.0611 (7)	0.0658 (7)	0.0513 (6)	0.0141 (5)	0.0066 (5)	−0.0004 (5)
O2	0.0762 (7)	0.0787 (7)	0.0460 (6)	0.0263 (6)	−0.0106 (5)	−0.0033 (5)
O3	0.0627 (7)	0.0734 (7)	0.0691 (7)	0.0119 (6)	0.0161 (5)	0.0013 (6)
O4	0.0938 (8)	0.0667 (7)	0.0520 (6)	0.0483 (6)	−0.0173 (5)	−0.0117 (5)
O5	0.0763 (7)	0.0785 (7)	0.0471 (5)	0.0448 (6)	−0.0138 (5)	−0.0082 (5)

Geometric parameters (Å, º)

C1—O1	1.3363 (16)	C8—N2	1.3349 (16)
C1—C6	1.3902 (19)	C8—C9	1.3626 (19)
C1—C2	1.3934 (18)	C8—H8	0.9300
C2—C3	1.3679 (19)	C9—C10	1.364 (2)
C2—H2A	0.9300	C9—H9	0.9300
C3—C4	1.3796 (18)	C10—C11	1.3801 (19)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.3813 (17)	C11—H11	0.9300
C4—N1	1.4482 (17)	C12—O4	1.2325 (16)
C5—C6	1.3705 (19)	C12—O5	1.2356 (15)
C5—H5	0.9300	N1—O2	1.2222 (15)
C6—H6	0.9300	N1—O3	1.2252 (15)
C7—N2	1.3352 (16)	N2—H2	0.866 (9)

C7—C11	1.3676 (18)	O1—H1	0.838 (9)
C7—C12	1.5156 (17)		
O1—C1—C6	123.25 (12)	N2—C8—H8	120.1
O1—C1—C2	117.49 (12)	C9—C8—H8	120.1
C6—C1—C2	119.25 (12)	C8—C9—C10	119.09 (13)
C3—C2—C1	120.57 (12)	C8—C9—H9	120.5
C3—C2—H2A	119.7	C10—C9—H9	120.5
C1—C2—H2A	119.7	C9—C10—C11	119.88 (13)
C2—C3—C4	119.23 (12)	C9—C10—H10	120.1
C2—C3—H3	120.4	C11—C10—H10	120.1
C4—C3—H3	120.4	C7—C11—C10	119.84 (13)
C3—C4—C5	121.20 (12)	C7—C11—H11	120.1
C3—C4—N1	119.62 (11)	C10—C11—H11	120.1
C5—C4—N1	119.18 (12)	O4—C12—O5	127.49 (12)
C6—C5—C4	119.40 (12)	O4—C12—C7	116.64 (11)
C6—C5—H5	120.3	O5—C12—C7	115.84 (11)
C4—C5—H5	120.3	O2—N1—O3	122.83 (12)
C5—C6—C1	120.31 (12)	O2—N1—C4	118.51 (12)
C5—C6—H6	119.8	O3—N1—C4	118.65 (11)
C1—C6—H6	119.8	C8—N2—C7	123.02 (11)
N2—C7—C11	118.38 (11)	C8—N2—H2	117.9 (11)
N2—C7—C12	116.75 (11)	C7—N2—H2	119.0 (11)
C11—C7—C12	124.87 (12)	C1—O1—H1	109.5 (14)
N2—C8—C9	119.78 (13)		
O1—C1—C2—C3	177.46 (13)	C12—C7—C11—C10	179.96 (13)
C6—C1—C2—C3	−1.60 (19)	C9—C10—C11—C7	0.2 (2)
C1—C2—C3—C4	0.5 (2)	N2—C7—C12—O4	−1.96 (19)
C2—C3—C4—C5	0.09 (19)	C11—C7—C12—O4	178.60 (14)
C2—C3—C4—N1	−179.33 (11)	N2—C7—C12—O5	176.51 (12)
C3—C4—C5—C6	0.42 (19)	C11—C7—C12—O5	−2.9 (2)
N1—C4—C5—C6	179.84 (11)	C3—C4—N1—O2	1.36 (18)
C4—C5—C6—C1	−1.53 (19)	C5—C4—N1—O2	−178.07 (11)
O1—C1—C6—C5	−176.89 (12)	C3—C4—N1—O3	−178.10 (12)
C2—C1—C6—C5	2.11 (19)	C5—C4—N1—O3	2.47 (18)
N2—C8—C9—C10	0.7 (2)	C9—C8—N2—C7	0.0 (2)
C8—C9—C10—C11	−0.8 (2)	C11—C7—N2—C8	−0.6 (2)
N2—C7—C11—C10	0.5 (2)	C12—C7—N2—C8	179.91 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5^{i}	0.84 (1)	1.77 (1)	2.5929 (15)	165 (2)
N2—H2···O4^{ii}	0.87 (1)	1.88 (1)	2.6693 (15)	151 (2)
C5—H5···O3^{iii}	0.93	2.56	3.3570 (17)	143
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