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4-Hydroxybenzoic acid–1*H*-imidazole (1/1)

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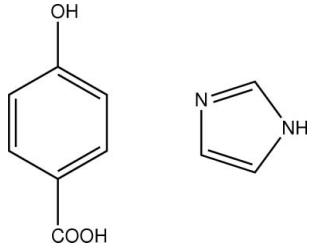
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.066; wR factor = 0.213; data-to-parameter ratio = 13.7.

In the title 1:1 adduct, $C_7H_6O_3\cdot C_3H_4N_2$, the crystal packing features π–π stacking interactions [centroid–centroid distances = 3.799 (2) and 3.753 (1) Å] as well as N—H···(O,O) (O,O) O—H···O and C—H···O hydrogen bonds.

Related literature

For related structures, see: Li *et al.* (2005); Wan *et al.* (2005). For the synthesis, see: Wang *et al.* (2006). For bond-length data, see Allen *et al.* (1987).



Experimental

Crystal data

$C_7H_6O_3\cdot C_3H_4N_2$
M_r = 206.20
Monoclinic, $P2_1/n$
a = 9.601 (2) Å
b = 10.530 (2) Å
c = 10.586 (2) Å
β = 113.759 (3)°
V = 979.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.47 × 0.29 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.955, T_{max} = 0.987
5200 measured reflections
1858 independent reflections
1583 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.213
S = 1.11
1858 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	2.53	3.057 (3)	121
N1—H1···O2	0.86	1.82	2.678 (3)	177
O3—H3···O1^{i}	0.82	1.83	2.635 (3)	166
C8—H8···O1^{ii}	0.93	1.89	2.748 (3)	153

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2768).

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4-Hydroxybenzoic acid–1*H*-imidazole (1/1)

Wei Wang, Bang-Wei Liu, Jing Liu and Rui Ren

S1. Comment

Imidazole compounds have received considerable attention in the literature. We have reported the structure of 3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one, (II) (Li *et al.*, 2005). In order to obtain comprehensive structural information of imidazole compounds and in our ongoing search for new imidazole compounds, the title compound, (I), was prepared hydrothermally and we report its structure here.

A view of the molecule of the title compound, (I), is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The bonds in the imidazole and hydroxybenzoate systems show intermediate character between single and double bonds, indicating a highly π-conjugated delocalization. The crystal structure is stabilized by π–π interactions involving the imidazole and hydroxybenzoate rings: *Cg*1···*Cg*1 (-*x*, 2 - *y*, 1 - *z*) = 3.799 Å and *Cg*1···*Cg*2 (-*x*, 1 - *y*, 1 - *z*) = 3.753 Å, where *Cg*1 and *Cg*2 denote the centroids of the N1/N2/C7—C9 imidazole and C1—C6 benzene rings, respectively. In the crystal packing, molecules are linked into three-dimension network by C—H···O and O—H···O intermolecular hydrogen bonds (Table 1).

S2. Experimental

The title compound was prepared according to the literature method of Wang *et al.* (2006). It was hydrothermally prepared from a reaction mixture of $CdCl_2.2.5H_2O$, 4-hydroxybenzoic acid, 1*H*-imidazole, and distilled water (10 ml) in a molar ratio of 1:2:6:555. The mixture was stirred for 20 min at room temperature and then crystallized in a Teflon-lined stainless steel autoclave with a 23 ml capacity at 433 K for five days. After cooling, single crystals of (I) suitable for X-ray measurements were obtained.

S3. Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å, O—H = 0.82 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2 U_{eq}(C,N) or 1.5 U_{eq}(O) for hydroxy H atoms.

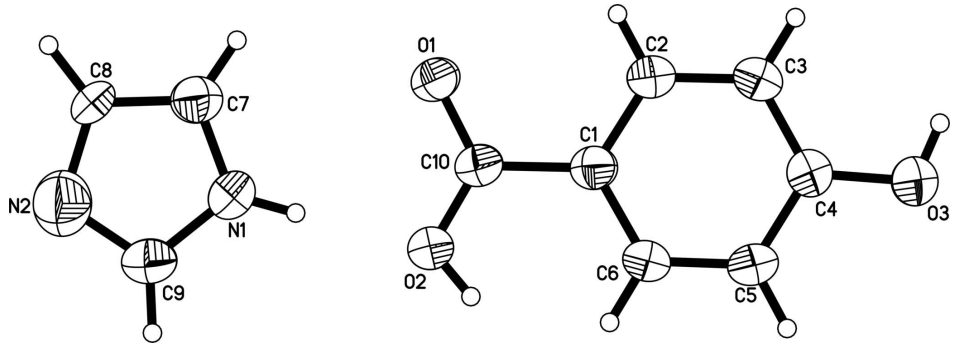

Figure 1

The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

4-Hydroxybenzoic acid–1*H*-imidazole (1/1)

Crystal data

$C_7H_6O_3·C_3H_4N_2$
M_r = 206.20
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 9.601 (2) Å
b = 10.530 (2) Å
c = 10.586 (2) Å
β = 113.759 (3)°
V = 979.6 (4) Å^3
Z = 4
$F(000)$ = 440
D_x = 1.398 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2125 reflections
θ = 2.9–25.6°
μ = 0.11 mm^{-1}
T = 293 K
Block, colourless
0.47 × 0.29 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.955, T_{max} = 0.987
5200 measured reflections
1858 independent reflections
1583 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.7°, θ_{min} = 2.4°
h = −10→11
k = −12→12
l = −12→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.213
S = 1.11
1858 reflections
136 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1212P)^2 + 0.6043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 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}
O1	−0.0067 (2)	0.60204 (17)	0.30887 (18)	0.0406 (5)
O2	0.1226 (2)	0.62774 (19)	0.53341 (19)	0.0494 (6)
H2	0.1995	0.5993	0.5951	0.080*
C1	0.2147 (3)	0.4753 (2)	0.4208 (2)	0.0376 (6)
N1	−0.0869 (3)	0.8121 (2)	0.4675 (2)	0.0444 (6)
H1	−0.0212	0.7516	0.4899	0.080*
C10	0.1036 (3)	0.5752 (2)	0.4219 (3)	0.0361 (6)
O3	0.5211 (3)	0.1947 (2)	0.4273 (2)	0.0614 (7)
H3	0.5014	0.1663	0.3499	0.080*
C2	0.2031 (3)	0.4185 (3)	0.2978 (3)	0.0421 (7)
H2A	0.1256	0.4433	0.2149	0.080*
C8	−0.2648 (3)	0.9398 (2)	0.3478 (3)	0.0364 (6)
H8	−0.3401	0.9793	0.2727	0.080*
C7	−0.1811 (3)	0.8415 (3)	0.3413 (3)	0.0461 (7)
H7	−0.1880	0.8005	0.2611	0.080*
C4	0.4199 (3)	0.2872 (3)	0.4201 (3)	0.0438 (7)
C6	0.3317 (3)	0.4363 (3)	0.5424 (3)	0.0478 (7)
H6	0.3420	0.4738	0.6253	0.080*
C3	0.3048 (3)	0.3260 (3)	0.2973 (3)	0.0449 (7)
H3A	0.2960	0.2896	0.2143	0.080*
C5	0.4330 (4)	0.3435 (3)	0.5433 (3)	0.0545 (8)
H5	0.5102	0.3183	0.6262	0.080*
N2	−0.2226 (4)	0.9731 (3)	0.4821 (3)	0.0715 (9)
C9	−0.1105 (4)	0.8937 (3)	0.5572 (3)	0.0519 (8)
H9	−0.0586	0.8941	0.6528	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0403 (10)	0.0418 (10)	0.0347 (10)	0.0012 (7)	0.0099 (8)	0.0032 (7)
O2	0.0488 (11)	0.0549 (12)	0.0346 (10)	0.0151 (9)	0.0065 (8)	−0.0054 (8)
C1	0.0384 (13)	0.0386 (13)	0.0336 (13)	−0.0009 (10)	0.0121 (11)	−0.0003 (10)
N1	0.0458 (12)	0.0424 (12)	0.0412 (13)	0.0075 (10)	0.0137 (10)	0.0059 (10)
C10	0.0366 (13)	0.0371 (13)	0.0319 (13)	−0.0023 (10)	0.0108 (10)	0.0022 (9)
O3	0.0610 (13)	0.0710 (15)	0.0436 (12)	0.0277 (11)	0.0122 (10)	−0.0073 (10)
C2	0.0438 (14)	0.0463 (14)	0.0319 (13)	0.0046 (11)	0.0109 (11)	0.0005 (10)

C8	0.0331 (12)	0.0372 (12)	0.0323 (12)	0.0079 (10)	0.0065 (10)	0.0097 (10)
C7	0.0475 (15)	0.0476 (15)	0.0386 (14)	0.0003 (12)	0.0125 (12)	−0.0002 (12)
C4	0.0435 (14)	0.0466 (15)	0.0398 (14)	0.0068 (11)	0.0154 (12)	−0.0027 (11)
C6	0.0517 (16)	0.0551 (16)	0.0305 (13)	0.0116 (13)	0.0101 (12)	−0.0063 (11)
C3	0.0498 (15)	0.0503 (15)	0.0327 (13)	0.0049 (12)	0.0146 (12)	−0.0052 (11)
C5	0.0527 (16)	0.0673 (19)	0.0316 (14)	0.0177 (14)	0.0048 (12)	−0.0024 (13)
N2	0.075 (2)	0.0681 (19)	0.075 (2)	0.0103 (15)	0.0332 (17)	0.0024 (15)
C9	0.0572 (17)	0.0594 (18)	0.0343 (15)	0.0063 (14)	0.0137 (13)	0.0022 (12)

Geometric parameters (Å, º)

O1—C10	1.269 (3)	C8—C7	1.330 (4)
O2—C10	1.249 (3)	C8—N2	1.358 (4)
O2—H2	0.8200	C8—H8	0.9300
C1—C6	1.387 (4)	C7—H7	0.9300
C1—C2	1.396 (4)	C4—C3	1.386 (4)
C1—C10	1.502 (4)	C4—C5	1.391 (4)
N1—C7	1.313 (4)	C6—C5	1.376 (4)
N1—C9	1.367 (4)	C6—H6	0.9300
N1—H1	0.8600	C3—H3A	0.9300
O3—C4	1.357 (3)	C5—H5	0.9300
O3—H3	0.8200	N2—C9	1.341 (4)
C2—C3	1.381 (4)	C9—H9	0.9300
C2—H2A	0.9300		
C10—O2—H2	109.5	N1—C7—H7	125.9
C6—C1—C2	118.0 (2)	C8—C7—H7	125.9
C6—C1—C10	120.8 (2)	O3—C4—C3	123.1 (2)
C2—C1—C10	121.2 (2)	O3—C4—C5	117.4 (2)
C7—N1—C9	108.7 (2)	C3—C4—C5	119.4 (2)
C7—N1—H1	125.7	C5—C6—C1	121.5 (2)
C9—N1—H1	125.7	C5—C6—H6	119.3
O2—C10—O1	122.8 (2)	C1—C6—H6	119.3
O2—C10—C1	118.9 (2)	C2—C3—C4	120.1 (2)
O1—C10—C1	118.3 (2)	C2—C3—H3A	119.9
C4—O3—H3	109.5	C4—C3—H3A	119.9
C3—C2—C1	121.0 (2)	C6—C5—C4	119.9 (3)
C3—C2—H2A	119.5	C6—C5—H5	120.0
C1—C2—H2A	119.5	C4—C5—H5	120.0
C7—C8—N2	108.9 (2)	C9—N2—C8	106.8 (3)
C7—C8—H8	125.6	N2—C9—N1	107.3 (3)
N2—C8—H8	125.6	N2—C9—H9	126.3
N1—C7—C8	108.2 (2)	N1—C9—H9	126.3

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	2.527	3.057 (3)	120.73

N1—H1···O2	0.86	1.818	2.678 (3)	177.32
O3—H3···O1^{i}	0.82	1.831	2.635 (3)	166.35
C8—H8···O1^{ii}	0.93	1.886	2.748 (3)	153.18

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