Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1*H*-Benzimidazol-3-ium-2-carboxylate dihydrate

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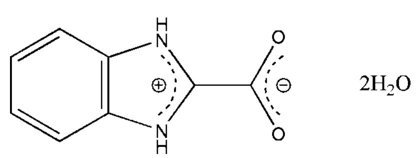
Received 29 April 2011; accepted 9 May 2011

Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.043; *wR* factor = 0.111; data-to-parameter ratio = 13.8.

The title compound, $C_8H_6N_2O_2\cdot 2H_2O$, crystallized as a zwitterion with the carboxyl group deprotonated and the imidazole group protonated. The dihedral angle between the benzimidazole ring and the pendant $-CO_2$ group is 0.62 (2)°. In the crystal, molecules are linked into a three-dimensional network by N—H···O and O—H···O hydrogen bonds.

Related literature

For the crystal structure of related zwitterionic benzimidazole-2-carboxylic acid monohydrate, see: Krawczyk *et al.* (2005). For the synthesis of the title compound, see: Thakurdesai *et al.* (2007).



Experimental

Crystal data

$C_8H_6N_2O_2\cdot 2H_2O$
M_r = 198.18
Monoclinic, $P2_1/c$
a = 6.8503 (15) Å
b = 7.3679 (17) Å
c = 18.939 (4) Å
β = 109.728 (7)°
V = 899.8 (3) Å^3
Z = 4
Mo *K*α radiation
μ = 0.12 mm^{-1}
T = 298 K
0.42 × 0.38 × 0.35 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.952, T_{max} = 0.960
4496 measured reflections
1760 independent reflections
1342 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.03
1760 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H6···O1	0.85	2.01	2.8608 (19)	174
N1—H1···O3^{i}	0.86	1.86	2.7135 (18)	170
O4—H9···O3^{i}	0.84	2.06	2.874 (2)	163
N2—H2*A*···O2^{ii}	0.86	1.87	2.6708 (18)	155
O3—H7···O4^{iii}	0.84	1.93	2.756 (2)	165
O4—H8···O1^{iv}	0.85	2.53	3.142 (2)	130

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y+1, -z+2$; (iii) $x-1, y, z$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5086).

References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Krawczyk, S., Gdaniec, M. & Saczewski, F. (2005). *Acta Cryst.* E**61**, o4185–o4187.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Thakurdesai, P. A., Wadodkar, S. G. & Chopade, C. T. (2007). *Pharmacologyonline*, **1**, 314–329.

supporting information

Acta Cryst. (2011). E**67**, o1399   [doi:10.1107/S1600536811017399]

1*H*-Benzimidazol-3-ium-2-carboxylate dihydrate

Xing-Jun Yao and Qian Yuan

S1. Comment

Recently, the crystal structure of zwitterionic compound benzimidazole-2-carboxylic acid monohydrate (I) has been reported by Krawczyk *et al.* (2005). Herewith we present the crystal structure of its dihydrate form, the title compound (II).

In (II) (Fig. 1), the bond lengths and angles are normal and comparable with those observed in (I). The equal bond lengths of C7—N1 and C7—N2 of the imidazolium fragment, and C8—O1 and C8—O2 of the carboxylate group show both N atoms of the benzimidazole group are protonated and both O atoms of the carboxylate group are deprotonated. The dihedral angle between the benzimidazole and carboxylate groupe is 0.62 (2) °. The molecule is essentially planar, the r.m.s. deviation for all non-H atoms being 0.0249 Å. An extensive three-dimensional hydrogen-bonding network (Table 1) stabilize the crystal packing.

S2. Experimental

The title compound was synthesized according to the method reported in the literature (Thakurdesai *et al.*, 2007). Colourless single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution of the compound.

S3. Refinement

H atoms bonded to the water O atom were located in an electron density and refined with O—H distances constrained to 0.84-0.85 Å. Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, and N—H = 0.86 Å. For those bound to C and N, U_{iso}(H) = 1.2U_{eq}(C, N), while for those bound to O, U_{iso}(H) = 1.5 U_{eq}(O).

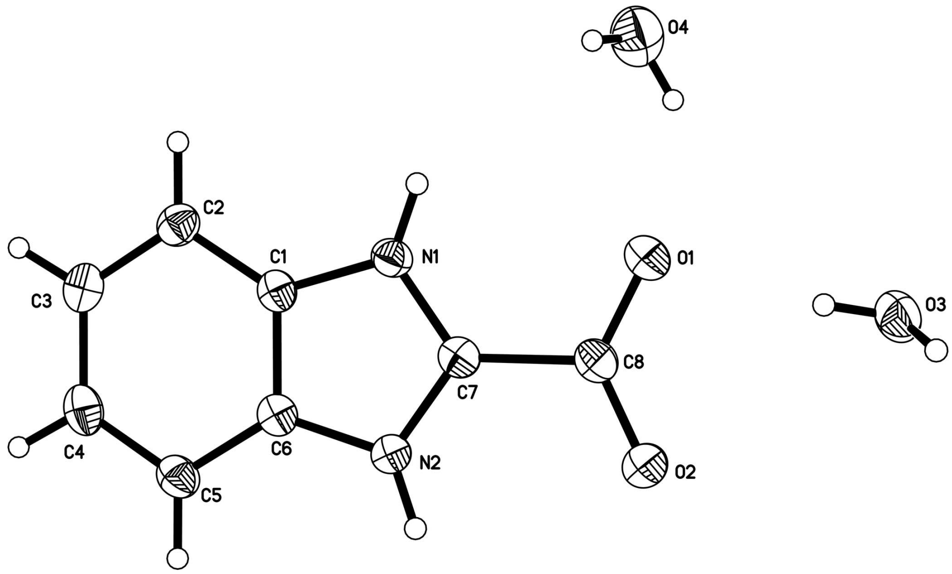


Figure 1

View of the title compound showing the atomic labeling and 30% probability displacement ellipsoids.

1*H*-Benzimidazol-3-ium-2-carboxylate dihydrate

Crystal data

$C_8H_6N_2O_2 \cdot 2H_2O$
$M_r = 198.18$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.8503$ (15) Å
$b = 7.3679$ (17) Å
$c = 18.939$ (4) Å
$\beta = 109.728$ (7)°
$V = 899.8$ (3) Å^3
$Z = 4$
$F(000) = 416$
$D_x = 1.463$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1540 reflections
$\theta = 2.3$–26.2°
$\mu = 0.12$ mm^{-1}
$T = 298$ K
Block, colorless
0.42 × 0.38 × 0.35 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.952$, $T_{max} = 0.960$
4496 measured reflections
1760 independent reflections
1342 reflections with $I > 2\sigma(I)$
$R_{int} = 0.095$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -6 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -23 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.111$
$S = 1.03$
1760 reflections
128 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

$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.0001P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.097 (8)

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	0.4666 (2)	0.4099 (2)	0.80063 (6)	0.0549 (4)
O2	0.36643 (18)	0.48692 (18)	0.89664 (6)	0.0503 (4)
N1	0.8395 (2)	0.27481 (18)	0.90210 (7)	0.0352 (4)
H1	0.8355	0.2552	0.8569	0.042*
N2	0.74817 (19)	0.35912 (18)	0.99579 (7)	0.0354 (4)
H2A	0.6754	0.4029	1.0209	0.043*
C8	0.4882 (3)	0.4223 (2)	0.86784 (9)	0.0378 (4)
C7	0.6902 (3)	0.3506 (2)	0.92144 (8)	0.0346 (4)
C1	1.0037 (2)	0.2319 (2)	0.96623 (9)	0.0338 (4)
C2	1.1954 (3)	0.1538 (2)	0.97674 (9)	0.0392 (4)
H2	1.2351	0.1172	0.9366	0.047*
C3	1.3236 (3)	0.1332 (2)	1.04979 (10)	0.0443 (5)
H3	1.4546	0.0830	1.0594	0.053*
C4	1.2623 (3)	0.1857 (3)	1.11020 (10)	0.0451 (5)
H4	1.3532	0.1678	1.1588	0.054*
C5	1.0734 (3)	0.2625 (2)	1.10005 (9)	0.0415 (5)
H5	1.0331	0.2970	1.1403	0.050*
C6	0.9443 (2)	0.2864 (2)	1.02604 (9)	0.0344 (4)
O3	0.1521 (2)	0.67445 (19)	0.73470 (6)	0.0542 (4)
H7	0.0403	0.6248	0.7338	0.081*
H6	0.2413	0.5942	0.7569	0.081*
O4	0.7592 (2)	0.5359 (2)	0.70601 (8)	0.0747 (5)
H8	0.6747	0.5904	0.7228	0.112*
H9	0.7617	0.4321	0.7248	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0504 (8)	0.0778 (10)	0.0330 (7)	0.0132 (7)	0.0096 (6)	−0.0016 (6)
O2	0.0422 (7)	0.0669 (9)	0.0417 (8)	0.0109 (7)	0.0138 (6)	−0.0024 (6)

N1	0.0398 (8)	0.0360 (8)	0.0295 (7)	0.0008 (6)	0.0114 (6)	−0.0015 (6)
N2	0.0344 (8)	0.0386 (9)	0.0340 (8)	0.0029 (6)	0.0126 (6)	−0.0001 (6)
C8	0.0391 (10)	0.0389 (10)	0.0336 (9)	−0.0026 (8)	0.0099 (7)	−0.0008 (7)
C7	0.0379 (9)	0.0324 (9)	0.0334 (9)	−0.0022 (7)	0.0118 (7)	−0.0006 (7)
C1	0.0357 (9)	0.0299 (9)	0.0341 (9)	−0.0029 (7)	0.0097 (7)	0.0013 (7)
C2	0.0407 (10)	0.0342 (9)	0.0446 (10)	−0.0003 (8)	0.0169 (8)	−0.0006 (7)
C3	0.0390 (10)	0.0387 (11)	0.0523 (11)	0.0026 (8)	0.0114 (8)	0.0028 (8)
C4	0.0430 (11)	0.0422 (11)	0.0411 (10)	−0.0019 (8)	0.0025 (8)	0.0042 (8)
C5	0.0471 (11)	0.0415 (10)	0.0338 (9)	−0.0015 (8)	0.0110 (7)	−0.0009 (7)
C6	0.0354 (9)	0.0314 (9)	0.0350 (9)	−0.0036 (7)	0.0101 (7)	−0.0001 (7)
O3	0.0540 (8)	0.0618 (9)	0.0446 (8)	0.0048 (7)	0.0137 (6)	0.0122 (6)
O4	0.0629 (10)	0.0848 (12)	0.0758 (11)	−0.0023 (8)	0.0225 (8)	0.0131 (8)

Geometric parameters (Å, º)

O1—C8	1.234 (2)	C2—H2	0.9300
O2—C8	1.236 (2)	C3—C4	1.400 (3)
N1—C7	1.321 (2)	C3—H3	0.9300
N1—C1	1.385 (2)	C4—C5	1.366 (2)
N1—H1	0.8600	C4—H4	0.9300
N2—C7	1.3291 (18)	C5—C6	1.393 (2)
N2—C6	1.379 (2)	C5—H5	0.9300
N2—H2A	0.8601	O3—H7	0.8435
C8—C7	1.508 (2)	O3—H6	0.8525
C1—C2	1.385 (2)	O4—H8	0.8496
C1—C6	1.386 (2)	O4—H9	0.8415
C2—C3	1.374 (2)		
C7—N1—C1	109.21 (13)	C3—C2—H2	121.8
C7—N1—H1	125.4	C1—C2—H2	121.8
C1—N1—H1	125.4	C2—C3—C4	121.77 (17)
C7—N2—C6	108.83 (13)	C2—C3—H3	119.1
C7—N2—H2A	125.6	C4—C3—H3	119.1
C6—N2—H2A	125.5	C5—C4—C3	122.08 (16)
O1—C8—O2	128.31 (16)	C5—C4—H4	119.0
O1—C8—C7	115.57 (15)	C3—C4—H4	119.0
O2—C8—C7	116.11 (14)	C4—C5—C6	116.33 (16)
N1—C7—N2	109.33 (13)	C4—C5—H5	121.8
N1—C7—C8	125.56 (14)	C6—C5—H5	121.8
N2—C7—C8	125.09 (14)	N2—C6—C1	106.67 (13)
N1—C1—C2	132.13 (15)	N2—C6—C5	131.73 (15)
N1—C1—C6	105.95 (14)	C1—C6—C5	121.59 (15)
C2—C1—C6	121.92 (15)	H7—O3—H6	101.8
C3—C2—C1	116.30 (16)	H8—O4—H9	100.9
C1—N1—C7—N2	−0.27 (19)	C1—C2—C3—C4	1.0 (3)
C1—N1—C7—C8	177.85 (15)	C2—C3—C4—C5	−0.9 (3)
C6—N2—C7—N1	0.32 (18)	C3—C4—C5—C6	−0.1 (3)

C6—N2—C7—C8	−177.81 (16)	C7—N2—C6—C1	−0.25 (17)
O1—C8—C7—N1	−1.3 (3)	C7—N2—C6—C5	−179.71 (17)
O2—C8—C7—N1	179.22 (16)	N1—C1—C6—N2	0.09 (17)
O1—C8—C7—N2	176.57 (16)	C2—C1—C6—N2	179.40 (15)
O2—C8—C7—N2	−2.9 (3)	N1—C1—C6—C5	179.61 (15)
C7—N1—C1—C2	−179.11 (17)	C2—C1—C6—C5	−1.1 (2)
C7—N1—C1—C6	0.11 (18)	C4—C5—C6—N2	−179.49 (17)
N1—C1—C2—C3	179.09 (17)	C4—C5—C6—C1	1.1 (2)
C6—C1—C2—C3	0.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H6···O1	0.85	2.01	2.8608 (19)	174
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Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, *y*+1/2, −*z*+3/2.