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2-Phenylimidazolium nitrate monohydrate

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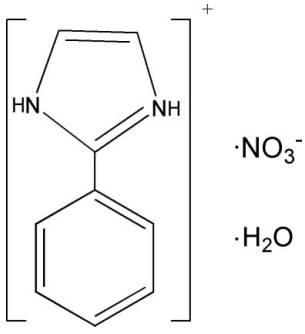
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.104; data-to-parameter ratio = 15.7.

In the title hydrated molecular salt, $C_9H_9N_2^+\cdot NO_3^-\cdot H_2O$, the dihedral angle between the aromatic rings in the cation is 11.09 (8)°. In the crystal, the components are linked into chains propagating in [101] by N—H···O and O—H···O hydrogen bonds.

Related literature

For related structures containing 2-phenylimidazole, see: Liu *et al.* (2008); Yang *et al.* (2008).



Experimental

Crystal data

$C_9H_9N_2^+\cdot NO_3^-\cdot H_2O$ M_r = 225.21
Monoclinic, $P2_1/n$
a = 8.026 (4) Å
b = 14.951 (7) Å
c = 8.895 (5) Å
β = 101.096 (5)°
V = 1047.4 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.33 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.56, T_{max} = 0.81
4388 measured reflections
2407 independent reflections
1430 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.104
S = 0.88
2407 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1W	0.86	1.92	2.753 (2)	163
N3—H3···O1^{i}	0.86	1.94	2.7809 (17)	166
O1W—HW11···O2^{ii}	0.83 (2)	2.21 (2)	2.989 (2)	155.3 (19)
O1W—HW12···O2	0.87 (2)	2.07 (2)	2.905 (2)	162.3 (19)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

We thank Yuncheng University and Jilin University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5245).

References

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supplementary materials

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2-Phenylimidazolium nitrate monohydrate

D.-C. Xia, W.-C. Li and S. Han

Comment

2-Phenylimidazole, as an important N-containing ligand with excellent coordinating abilities and fruitful aromatic systems, have been extensively used to build supramolecular architectures (Liu *et al.*, 2008; Yang *et al.*, 2008). We report here the synthesis and structure of the title compound, namely, $C_9H_{11}N_3O_4$ (I)

There are one 2-phenylimidazole cation, one nitrate anion and one water molecule in the asymmetric unit of the title compound, $C_9H_{11}N_3O_4$ (Fig. 1). In the crystal, molecules are linked into layer structures by N—H···O and O—H···O H-bonding interactions (Table 1).

Experimental

A mixture of $Cu(NO_3)_2{\cdot}2.5H_2O$ (0.5 mmol), 2-phenylimidazole (0.5 mmol), and H_2O (30 mmol) was heated in a sealed vessel at 413 K for 2 days. After the mixture was slowly cooled to room temperature, colorless blocks of (I) were obtained (23% yield).

Refinement

All H atoms on C and N atoms were positioned geometrically (C—H = 0.93 Å, N—H = 0.86Å) and refined as riding, with U_{iso}(H)=1.2U_{eq}(carrier). The water H-atoms were located in a difference map, and was refined freely.

Figures

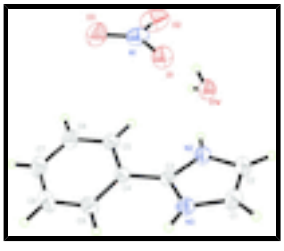

Fig. 1. The structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

2-Phenylimidazolium nitrate monohydrate

Crystal data

$C_9H_9N_2^+{\cdot}NO_3^-{\cdot}H_2O$	$F(000)$ = 472
M_r = 225.21	D_x = 1.428 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å

Hall symbol: -P 2yn	Cell parameters from 2407 reflections
a = 8.026 (4) Å	θ = 3.0–29.2°
b = 14.951 (7) Å	μ = 0.11 mm^{-1}
c = 8.895 (5) Å	T = 293 K
β = 101.096 (5)°	Block, colourless
V = 1047.4 (9) Å^3	0.33 × 0.28 × 0.22 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	2407 independent reflections
Radiation source: fine-focus sealed tube	1430 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.018
φ and ω scans	θ_{max} = 29.2°, θ_{min} = 2.7°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −10→10
T_{min} = 0.56, T_{max} = 0.81	k = −19→20
4388 measured reflections	l = −7→12

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.040	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.104	H atoms treated by a mixture of independent and constrained refinement
S = 0.88	$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2407 reflections	$(\Delta/\sigma)_{max} < 0.001$
153 parameters	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.21 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.41911 (19)	−0.16151 (10)	1.11954 (17)	0.0528 (4)
H1	0.4944	−0.1975	1.1858	0.063*
C2	0.31545 (19)	−0.18758 (10)	0.99079 (18)	0.0532 (4)
H2A	0.3044	−0.2452	0.9508	0.064*
C3	0.27630 (15)	−0.04284 (9)	1.01806 (14)	0.0382 (3)
C4	0.21609 (15)	0.04875 (9)	0.99206 (14)	0.0375 (3)
C5	0.11719 (17)	0.07305 (9)	0.85184 (15)	0.0475 (4)
H5	0.0869	0.0302	0.7756	0.057*
C6	0.0641 (2)	0.15982 (10)	0.82541 (19)	0.0591 (4)
H6	−0.0019	0.1753	0.7313	0.071*
C7	0.1073 (2)	0.22399 (10)	0.9361 (2)	0.0626 (5)
H7	0.0726	0.2829	0.9169	0.075*
C8	0.2026 (2)	0.20012 (10)	1.0760 (2)	0.0609 (4)
H8	0.2306	0.2432	1.1521	0.073*
C9	0.25738 (17)	0.11317 (9)	1.10495 (17)	0.0502 (4)
H9	0.3218	0.0979	1.1999	0.060*
N1	0.31081 (15)	0.01630 (11)	0.54668 (14)	0.0575 (4)
N2	0.22881 (14)	−0.11327 (7)	0.92928 (13)	0.0452 (3)
H2	0.1546	−0.1123	0.8455	0.054*
N3	0.39323 (14)	−0.07206 (7)	1.13512 (12)	0.0455 (3)
H3	0.4446	−0.0394	1.2093	0.055*
O1	0.39439 (12)	−0.03171 (7)	0.64925 (11)	0.0619 (3)
O2	0.20267 (15)	−0.01926 (11)	0.44597 (13)	0.0921 (5)
O1W	0.03846 (18)	−0.13296 (8)	0.63882 (14)	0.0607 (3)
O3	0.33396 (17)	0.09768 (10)	0.54776 (15)	0.0860 (4)
HW11	−0.049 (3)	−0.1037 (14)	0.606 (2)	0.090 (7)*
HW12	0.104 (2)	−0.1081 (14)	0.584 (2)	0.097 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0531 (9)	0.0454 (9)	0.0587 (10)	0.0079 (7)	0.0078 (7)	0.0124 (7)
C2	0.0587 (9)	0.0372 (8)	0.0638 (10)	0.0043 (7)	0.0121 (7)	0.0023 (7)
C3	0.0371 (7)	0.0404 (7)	0.0367 (7)	−0.0022 (6)	0.0065 (5)	0.0017 (6)
C4	0.0352 (6)	0.0388 (7)	0.0394 (7)	−0.0026 (6)	0.0094 (5)	0.0004 (6)
C5	0.0537 (8)	0.0446 (8)	0.0435 (8)	0.0045 (7)	0.0076 (6)	0.0002 (6)
C6	0.0647 (9)	0.0536 (10)	0.0584 (9)	0.0137 (8)	0.0103 (7)	0.0122 (8)
C7	0.0614 (10)	0.0393 (8)	0.0896 (13)	0.0091 (7)	0.0210 (9)	0.0066 (8)
C8	0.0573 (9)	0.0459 (9)	0.0798 (12)	−0.0053 (8)	0.0140 (8)	−0.0217 (8)
C9	0.0478 (8)	0.0504 (8)	0.0502 (9)	−0.0019 (7)	0.0037 (6)	−0.0079 (7)
N1	0.0460 (7)	0.0799 (11)	0.0466 (8)	0.0057 (7)	0.0090 (6)	0.0068 (7)
N2	0.0488 (7)	0.0375 (6)	0.0461 (7)	−0.0002 (5)	0.0013 (5)	0.0004 (5)
N3	0.0459 (6)	0.0464 (7)	0.0418 (7)	0.0006 (5)	0.0020 (5)	0.0022 (5)
O1	0.0602 (7)	0.0620 (7)	0.0550 (7)	0.0060 (5)	−0.0102 (5)	0.0027 (5)

O2	0.0663 (7)	0.1416 (14)	0.0571 (8)	−0.0208 (8)	−0.0163 (6)	0.0107 (8)
O1W	0.0608 (7)	0.0538 (7)	0.0612 (8)	−0.0042 (6)	−0.0041 (6)	−0.0026 (5)
O3	0.1057 (11)	0.0655 (9)	0.0903 (10)	0.0136 (7)	0.0277 (8)	0.0200 (7)

Geometric parameters (Å, °)

C1—C2	1.337 (2)	C6—H6	0.9300
C1—N3	1.3646 (19)	C7—C8	1.376 (2)
C1—H1	0.9300	C7—H7	0.9300
C2—N2	1.3678 (18)	C8—C9	1.380 (2)
C2—H2A	0.9300	C8—H8	0.9300
C3—N2	1.3274 (17)	C9—H9	0.9300
C3—N3	1.3340 (17)	N1—O3	1.2305 (19)
C3—C4	1.4556 (19)	N1—O2	1.2406 (17)
C4—C9	1.3849 (19)	N1—O1	1.2498 (16)
C4—C5	1.3917 (19)	N2—H2	0.8600
C5—C6	1.372 (2)	N3—H3	0.8600
C5—H5	0.9300	O1W—HW11	0.83 (2)
C6—C7	1.371 (2)	O1W—HW12	0.87 (2)
C2—C1—N3	106.90 (12)	C6—C7—H7	120.4
C2—C1—H1	126.5	C8—C7—H7	120.4
N3—C1—H1	126.5	C7—C8—C9	120.96 (14)
C1—C2—N2	106.88 (13)	C7—C8—H8	119.5
C1—C2—H2A	126.6	C9—C8—H8	119.5
N2—C2—H2A	126.6	C8—C9—C4	119.77 (14)
N2—C3—N3	106.43 (12)	C8—C9—H9	120.1
N2—C3—C4	127.10 (12)	C4—C9—H9	120.1
N3—C3—C4	126.46 (12)	O3—N1—O2	120.86 (15)
C9—C4—C5	118.94 (13)	O3—N1—O1	120.21 (14)
C9—C4—C3	120.88 (12)	O2—N1—O1	118.92 (17)
C5—C4—C3	120.18 (12)	C3—N2—C2	109.92 (11)
C6—C5—C4	120.35 (13)	C3—N2—H2	125.0
C6—C5—H5	119.8	C2—N2—H2	125.0
C4—C5—H5	119.8	C3—N3—C1	109.86 (12)
C7—C6—C5	120.78 (15)	C3—N3—H3	125.1
C7—C6—H6	119.6	C1—N3—H3	125.1
C5—C6—H6	119.6	HW11—O1W—HW12	98.1 (18)
C6—C7—C8	119.18 (14)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1W	0.86	1.92	2.753 (2)	163
N3—H3···O1^{i}	0.86	1.94	2.7809 (17)	166
O1W—HW11···O2^{ii}	0.83 (2)	2.21 (2)	2.989 (2)	155.3 (19)
O1W—HW12···O2	0.87 (2)	2.07 (2)	2.905 (2)	162.3 (19)

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

Fig. 1