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2-Phenylimidazolium chloride monohydrate

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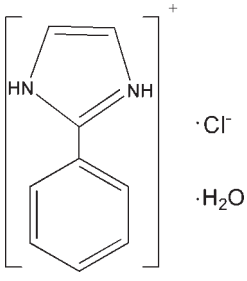
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.074; data-to-parameter ratio = 16.1.

In the title hydrated molecular salt, $C_9H_9N_2^+\cdot Cl^-\cdot H_2O$, the dihedral angle between the five- and six-membered rings in the cation is 18.00 (2)°. O—H···Cl, N—H···O and N—H···Cl hrdrogen-bonding interactions are present in the crystal structure.

Related literature

For related 2-phenylimidazolium nitrate structures, see: Zhang *et al.* (2007); Xia *et al.* (2009). For a phosphate salt of phenylimadazole, see: Xia & Yao (2010) and for a silver complex, see: Han *et al.* (2010).



Experimental

Crystal data

$C_9H_9N_2^+\cdot Cl^-\cdot H_2O$
M_r = 198.65
Triclinic, $P\overline{1}$
a = 7.2751 (10) Å
b = 8.8816 (13) Å
c = 9.3228 (10) Å
α = 105.486 (11)°
β = 106.516 (11)°
γ = 109.337 (13)°
V = 499.65 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 293 K
0.31 × 0.24 × 0.22 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.52, T_{max} = 0.78
3460 measured reflections
2030 independent reflections
1198 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.074
S = 0.81
2030 reflections
126 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1W	0.86	1.96	2.774 (2)	157
N2—H2···Cl1^{i}	0.86	2.28	3.1371 (14)	172
O1W—HW11···Cl1	0.86 (3)	2.33 (3)	3.177 (2)	174 (2)
O1W—HW12···Cl1^{ii}	0.88 (3)	2.32 (3)	3.190 (2)	176 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); 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 for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2320).

References

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supporting information

Acta Cryst. (2010). E**66**, o673 [doi:10.1107/S1600536810006136]

2-Phenylimidazolium chloride monohydrate

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S1. Comment

The 2-phenylimidazolium nitrate structure has been reported as a hemihydrate (Zhang *et al.*, 2007) and as a hydrate (Xia *et al.*, 2009). Here we report the synthesis and structure of the chloride hydrate, namely, $C_9H_{11}ClN_2O$.

The asymmetric unit of the title compound contains one 2-phenylimidazolium cation, one chloride anion and one water molecule (Fig. 1). There are O—H···Cl, N—H···O and N—H···Cl H-bonding interactions in the structure (Table I).

S2. Experimental

A mixture of 2-phenylimidazole (0.5 mmol), hydrochloric acid (0.5 mmol) and H_2O (30 mmol) was mixed. After two weeks, colorless crystals were obtained at room temperature (22% yield).

S3. Refinement

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

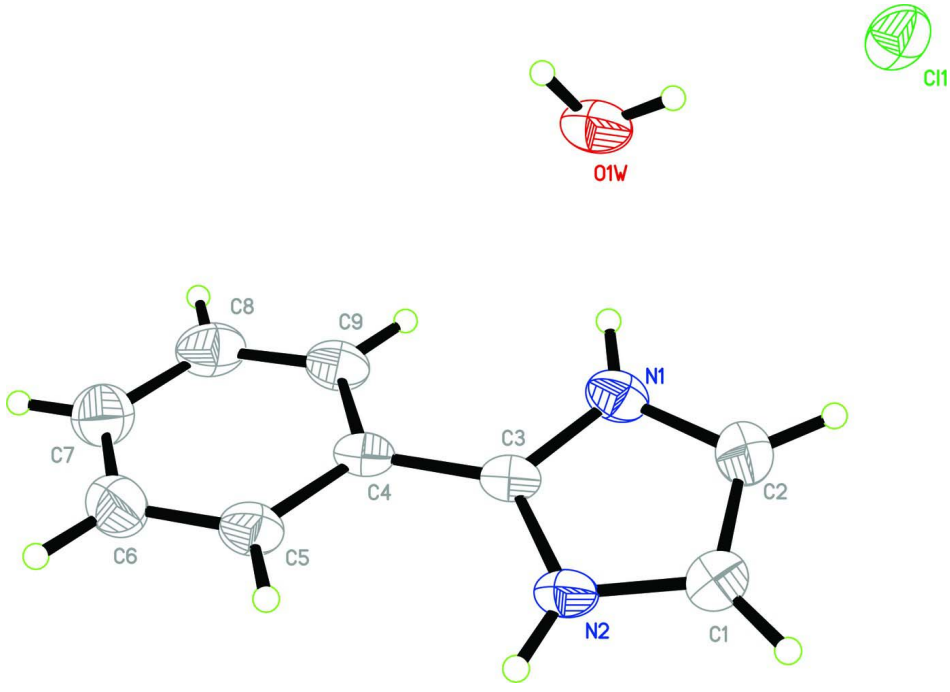

Figure 1

The structure of the title compound showing the atomic numbering scheme and displacement ellipsoids at the 30% probability level.

2-Phenylimidazolium chloride monohydrate

Crystal data

$C_9H_9N_2^+·Cl^-·H_2O$
M_r = 198.65
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.2751 (10) Å
b = 8.8816 (13) Å
c = 9.3228 (10) Å
α = 105.486 (11)°
β = 106.516 (11)°
γ = 109.337 (13)°
V = 499.65 (15) Å^3

Z = 2
$F(000)$ = 208
D_x = 1.320 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2030 reflections
θ = 2.5–26.4°
μ = 0.34 mm^{-1}
T = 293 K
Block, colorless
0.31 × 0.24 × 0.22 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.52, T_{max} = 0.78

3460 measured reflections
2030 independent reflections
1198 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.4°, θ_{min} = 2.5°
h = −6→9
k = −10→11
l = −11→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.074
S = 0.81
2030 reflections
126 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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.

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	0.4640 (3)	0.2399 (2)	0.3466 (2)	0.0617 (5)
H1A	0.5140	0.2530	0.4549	0.074*

C2	0.4744 (3)	0.3668 (2)	0.2929 (2)	0.0653 (6)
H2A	0.5322	0.4849	0.3570	0.078*
C3	0.3188 (3)	0.1197 (2)	0.0774 (2)	0.0437 (4)
C4	0.2201 (3)	−0.0061 (2)	−0.0909 (2)	0.0441 (4)
C5	0.1124 (3)	−0.1827 (2)	−0.1299 (2)	0.0548 (5)
H5	0.1007	−0.2215	−0.0482	0.066*
C6	0.0231 (3)	−0.3006 (2)	−0.2889 (2)	0.0665 (6)
H6	−0.0509	−0.4186	−0.3146	0.080*
C7	0.0428 (3)	−0.2445 (3)	−0.4101 (3)	0.0693 (6)
H7	−0.0167	−0.3247	−0.5174	0.083*
C8	0.1500 (3)	−0.0708 (3)	−0.3728 (2)	0.0661 (6)
H8	0.1634	−0.0336	−0.4551	0.079*
C9	0.2382 (3)	0.0496 (2)	−0.2145 (2)	0.0550 (5)
H9	0.3095	0.1676	−0.1903	0.066*
N1	0.3844 (2)	0.29054 (16)	0.12684 (18)	0.0543 (4)
H1	0.3719	0.3448	0.0635	0.065*
N2	0.3658 (2)	0.08756 (17)	0.21156 (17)	0.0504 (4)
H2	0.3385	−0.0138	0.2129	0.060*
O1W	0.2454 (3)	0.4594 (2)	−0.0598 (3)	0.0680 (4)
HW11	0.249 (4)	0.538 (3)	0.019 (3)	0.114 (11)*
HW12	0.107 (5)	0.407 (3)	−0.117 (3)	0.122 (11)*
Cl1	0.26211 (8)	0.73220 (5)	0.25005 (5)	0.0634 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0669 (14)	0.0637 (12)	0.0518 (12)	0.0312 (10)	0.0177 (10)	0.0234 (10)
C2	0.0746 (14)	0.0527 (11)	0.0572 (14)	0.0266 (10)	0.0189 (11)	0.0164 (9)
C3	0.0437 (10)	0.0496 (10)	0.0537 (11)	0.0267 (8)	0.0245 (8)	0.0305 (8)
C4	0.0444 (10)	0.0503 (10)	0.0551 (11)	0.0291 (8)	0.0245 (9)	0.0311 (8)
C5	0.0648 (13)	0.0558 (11)	0.0580 (12)	0.0308 (10)	0.0284 (10)	0.0340 (9)
C6	0.0788 (15)	0.0552 (11)	0.0645 (14)	0.0289 (10)	0.0271 (11)	0.0255 (10)
C7	0.0787 (15)	0.0748 (14)	0.0579 (13)	0.0407 (12)	0.0277 (11)	0.0229 (10)
C8	0.0818 (15)	0.0869 (14)	0.0602 (14)	0.0500 (12)	0.0389 (11)	0.0459 (11)
C9	0.0628 (12)	0.0587 (11)	0.0663 (13)	0.0335 (10)	0.0350 (10)	0.0397 (10)
N1	0.0650 (10)	0.0474 (9)	0.0635 (11)	0.0286 (7)	0.0295 (8)	0.0324 (7)
N2	0.0566 (10)	0.0501 (8)	0.0560 (10)	0.0293 (7)	0.0218 (8)	0.0316 (7)
O1W	0.0656 (12)	0.0655 (9)	0.0919 (12)	0.0366 (8)	0.0345 (9)	0.0460 (9)
Cl1	0.0715 (3)	0.0529 (3)	0.0548 (3)	0.0174 (2)	0.0143 (2)	0.0311 (2)

Geometric parameters (Å, º)

C1—C2	1.339 (2)	C6—C7	1.375 (3)
C1—N2	1.366 (2)	C6—H6	0.9300
C1—H1A	0.9300	C7—C8	1.368 (3)
C2—N1	1.362 (2)	C7—H7	0.9300
C2—H2A	0.9300	C8—C9	1.378 (3)
C3—N1	1.3282 (19)	C8—H8	0.9300

C3—N2	1.332 (2)	C9—H9	0.9300
C3—C4	1.455 (2)	N1—H1	0.8600
C4—C5	1.388 (2)	N2—H2	0.8600
C4—C9	1.392 (2)	O1W—HW11	0.86 (3)
C5—C6	1.374 (3)	O1W—HW12	0.88 (3)
C5—H5	0.9300		

C2—C1—N2	106.67 (17)	C7—C6—H6	119.9
C2—C1—H1A	126.7	C8—C7—C6	120.01 (19)
N2—C1—H1A	126.7	C8—C7—H7	120.0
C1—C2—N1	107.20 (16)	C6—C7—H7	120.0
C1—C2—H2A	126.4	C7—C8—C9	120.68 (17)
N1—C2—H2A	126.4	C7—C8—H8	119.7
N1—C3—N2	106.63 (14)	C9—C8—H8	119.7
N1—C3—C4	126.29 (15)	C8—C9—C4	119.67 (16)
N2—C3—C4	127.06 (15)	C8—C9—H9	120.2
C5—C4—C9	119.14 (16)	C4—C9—H9	120.2
C5—C4—C3	120.82 (15)	C3—N1—C2	109.75 (14)
C9—C4—C3	120.01 (15)	C3—N1—H1	125.1
C6—C5—C4	120.30 (16)	C2—N1—H1	125.1
C6—C5—H5	119.8	C3—N2—C1	109.74 (14)
C4—C5—H5	119.8	C3—N2—H2	125.1
C5—C6—C7	120.18 (18)	C1—N2—H2	125.1
C5—C6—H6	119.9	HW11—O1W—HW12	97 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1*W*	0.86	1.96	2.774 (2)	157
N2—H2···Cl1^{i}	0.86	2.28	3.1371 (14)	172
O1*W*—H*W*11···Cl1	0.86 (3)	2.33 (3)	3.177 (2)	174 (2)
O1*W*—H*W*12···Cl1^{ii}	0.88 (3)	2.32 (3)	3.190 (2)	176 (2)

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