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2-Phenylimidazolium nitrate hemihydrate

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Key indicators

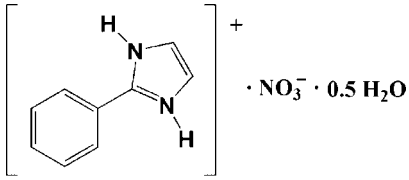
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.058
wR factor = 0.182
Data-to-parameter ratio = 15.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title compound, $C_9H_9N_2^+\cdot NO_3^-\cdot 0.5H_2O$, the 2-phenylimidazolium cation is linked to adjacent nitrate anions *via* N—H···O hydrogen bonding. The solvent water molecule is also hydrogen bonded to the nitrate anion.

Comment

As part of an investigation of the supramolecular chemistry of 2-substituted imidazoline and imidazole systems, we present here the crystal structure of the title compound, (I).



(I)

Compound (I) is composed of 2-phenylimidazolium cations, nitrate anions and solvent water molecules (Fig. 1). The bond distances and angles are normal. The nitrate anions are hydrogen bonded to the cations and water molecules (Table 1), forming a one-dimensional supramolecular structure.

Experimental

Concentrated nitric acid (16 mol l^{-1}, 0.5 ml) was added slowly to a mixture of 2-phenylimidazole (0.1445 g, 1 mmol) and methanol (15 ml) with constant stirring until all of the solids dissolved. Colorless single crystals of (I) were obtained after several days at room temperature.

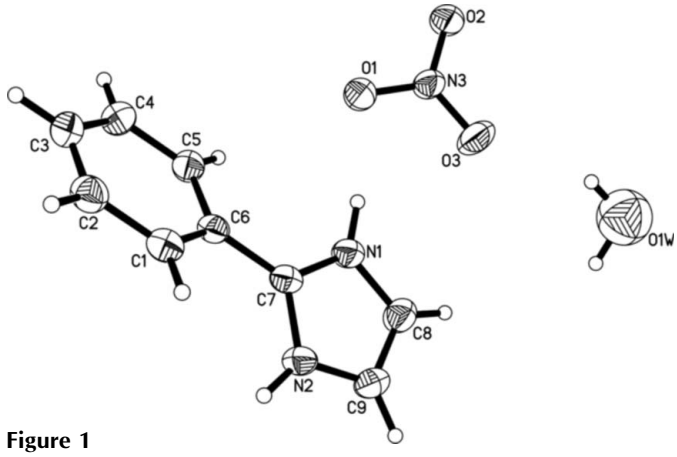


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for H atoms).

Crystal data

$C_9H_9N_2^+\cdot NO_3^-\cdot 0.5H_2O$
$M_r = 216.20$
Monoclinic, $P2_1/c$
$a = 3.7540\ (8)$ Å
$b = 20.152\ (4)$ Å
$c = 13.791\ (3)$ Å
$\beta = 95.362\ (4)^\circ$
$V = 1038.7\ (4)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 273\ (2)$ K
$0.44 \times 0.20 \times 0.08$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: none
6227 measured reflections
2447 independent reflections
1547 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.182$
$S = 1.01$
2447 reflections
154 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1	0.94 (3)	1.87 (3)	2.792 (2)	167 (2)
N2—H2N···O2^{i}	0.91 (3)	1.90 (3)	2.803 (2)	175 (3)
O1W—H1A···O3	0.917 (18)	2.11 (1)	2.868 (7)	139 (2)

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms bonded to N atoms were located in a difference Fourier map and refined isotropically. H atoms of the water molecule were located in a difference Fourier map and positional parameters were refined; the occupancy factor was fixed at 0.5 and $U_{iso}(H)$ was set at 0.12 Å^2.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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