Crystal structure of 2-phenylimidazolium hydrogen sulfate, $[C_9H_9N_2][HSO_4]$

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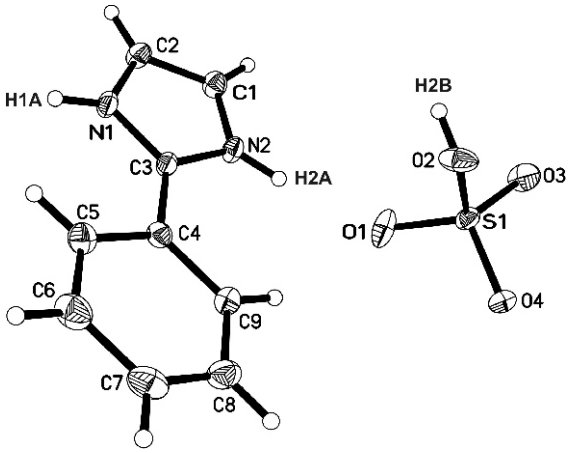

Abstract

$C_9H_{10}N_2O_4S$, triclinic, $P\bar{1}$ (no. 2), a = 4.481(5) Å, b = 9.300(5) Å, c = 13.014(5) Å, α = 93.829(5)°, β = 99.633(5)°, γ = 102.739(5)°, V = 518.5 Å^3, Z = 2, $R_{gt}(F)$ = 0.048, $wR_{ref}(F^2)$ = 0.132, T = 293 K.

Source of material

A mixture of 2-phenylimidazole (0.5 mmol) and H_2SO_4 (0.2 mL) was disolved in water (10 mL). Colorless crystals were obtained at room temperature after two weeks.

Experimental details

All H atoms bound to carbon atoms were positioned geometrically and treated as riding with d(C—H) = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C). H atoms bonded to N and O were located in difference Fourier maps and refined isotropically with distance restraints of d(O—H) = 0.82(1) Å and d(N—H) = 0.86(1) Å.

Discussion

2-Phenylimidazole is an important N-containing ligand with excellent coordinating abilities and fruitful aromatic systems. The current interest in 2-phenylimidazole or its derivative is rapidly expanding for their potential applications in medical chemistry, host-guest chemistry, ion exchange, and nonlinear optics [1].

There are one 2-phenylimidazolium cation and one hydrogen sulfate anion in the asymmetric unit of the title compound, $[(C_9H_9N_2)(HSO_4)]$. The bond lengths d(C1—C2), d(C1—N2), d(C2—N1), d(C3—N1) and d(C3—N2) are 1.339(3), 1.360(3), 1.367(3), 1.331(3) and 1.332(3) Å, respectively. The C1/C2/N1/C3/N2 ring is an imidazole group.

In the crystal, molecules are linked into layer by H-bonding interactions: d(N1–H1A···O4) = 2.963(3) Å, ∠N1–H1A···O4 = 178(3)° and d(N2–H2A···O1) = 2.736(3) Å, ∠N2–H2A···O1 = 175(3)°, d(O2–H2B···O4) = 2.637(3) Å, ∠O2–H2B···O4 = 174(3)°.

Table 1. Data collection and handling.

Crystal:	colorless sheet, size 0.12 × 0.14 × 0.21 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	3.13 cm^{-1}
Diffractometer, scan mode:	Oxford Diffraction Gemini R Ultra, ω
$2\theta_{max}$:	58.38°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3733, 2348
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1714
$N(param)_{refined}$:	158
Programs:	SHELXS-97, SHELXL-97 [2]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	0.4846	0.3285	0.0090	0.050
H(2)	2*i*	0.2593	0.0753	0.0425	0.051
H(5)	2*i*	0.9312	0.0495	0.3471	0.059
H(6)	2*i*	1.3042	0.0795	0.4962	0.073
H(7)	2*i*	1.7082	0.2895	0.5326	0.073
H(8)	2*i*	1.7354	0.4699	0.4193	0.065
H(9)	2*i*	1.3577	0.4447	0.2724	0.051
H(2A)	2*i*	0.936(5)	0.419(2)	0.140(2)	0.055(7)
H(1A)	2*i*	0.577(7)	0.028(2)	0.195(2)	0.066(8)
H(2B)	2*i*	0.777(4)	0.741(3)	0.274(2)	0.061(9)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	2*i*	0.5613(6)	0.2783(2)	0.0631(2)	0.047(1)	0.040(1)	0.038(1)	0.009(1)	0.007(1)	0.0094(9)
C(2)	2*i*	0.4376(6)	0.1397(2)	0.0812(2)	0.039(1)	0.038(1)	0.043(1)	–0.0002(9)	0.004(1)	0.002(1)
C(3)	2*i*	0.8588(5)	0.2298(2)	0.2029(2)	0.034(1)	0.0263(9)	0.038(1)	0.0043(8)	0.0114(9)	0.0026(8)
C(4)	2*i*	1.1028(5)	0.2445(2)	0.2944(2)	0.036(1)	0.035(1)	0.037(1)	0.0107(9)	0.0086(9)	0.0034(9)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(5)	2*i*	1.0912(6)	0.1350(3)	0.3620(2)	0.051(2)	0.045(1)	0.055(1)	0.013(1)	0.011(1)	0.014(1)
C(6)	2*i*	1.3148(7)	0.1525(3)	0.4506(2)	0.064(2)	0.072(2)	0.053(2)	0.027(2)	0.008(1)	0.023(1)
C(7)	2*i*	1.5565(7)	0.2781(4)	0.4724(2)	0.055(2)	0.083(2)	0.047(1)	0.029(2)	0.000(1)	0.001(1)
C(8)	2*i*	1.5716(6)	0.3860(3)	0.4051(2)	0.044(1)	0.056(2)	0.056(2)	0.007(1)	0.001(1)	–0.011(1)
C(9)	2*i*	1.3471(5)	0.3707(2)	0.3172(2)	0.042(1)	0.037(1)	0.046(1)	0.007(1)	0.006(1)	0.003(1)
O(1)	2*i*	1.1560(5)	0.6169(2)	0.1418(1)	0.089(2)	0.0317(8)	0.065(1)	–0.0065(9)	0.024(1)	0.0035(8)
O(2)	2*i*	0.9321(4)	0.7087(2)	0.2786(2)	0.037(1)	0.084(1)	0.070(1)	0.0259(9)	0.0206(9)	0.048(1)
O(3)	2*i*	1.0100(4)	0.8519(2)	0.1328(1)	0.049(1)	0.058(1)	0.065(1)	0.0061(8)	0.0024(8)	0.0345(9)
O(4)	2*i*	1.4461(3)	0.8280(2)	0.2581(1)	0.0291(8)	0.0429(9)	0.065(1)	0.0020(7)	0.0008(8)	0.0030(8)
S(1)	2*i*	1.1431(1)	0.75412(5)	0.19663(4)	0.0294(3)	0.0326(3)	0.0450(4)	–0.0004(2)	0.0037(2)	0.0129(2)
N(1)	2*i*	0.6257(4)	0.1118(2)	0.1680(2)	0.041(1)	0.0262(9)	0.046(1)	0.0018(8)	0.0062(8)	0.0092(8)
N(2)	2*i*	0.8195(4)	0.3322(2)	0.1384(1)	0.041(1)	0.0275(9)	0.0399(9)	0.0012(8)	0.0075(8)	0.0079(8)

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