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4-Benzylpyridinium hydrogen selenate

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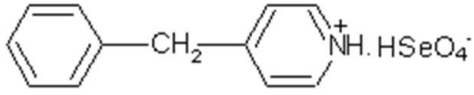
Key indicators: single-crystal X-ray study; T = 289 K; mean σ(C–C) = 0.007 Å; R factor = 0.037; wR factor = 0.087; data-to-parameter ratio = 13.6.

The structure of the title salt, $C_{12}H_{12}N^+\cdot HSeO_4^-$, consists of infinite parallel two-dimensional planes built of 4-benzylpyridinium and hydrogen selenate ions that are mutually connected by strong O—H···O and N—H···O hydrogen bonds. There are no contacts other than normal van der Waals interactions between the layers.

Related literature

For general background, see Fleck (2006); Baran *et al.* (2000). For related compounds, see: Ben Hamada & Jouini (2006); Kaabi *et al.* (2004); Ben Djemaa *et al.* (2007); Gowda *et al.* (2007).



Experimental

Crystal data

$C_{12}H_{12}N^+\cdot HSeO_4^-$
M_r = 314.19
Orthorhombic, *Pbca*
a = 27.449 (5) Å
b = 10.821 (6) Å
c = 8.830 (1) Å
V = 2623 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.87 mm^{-1}
T = 289 (2) K
0.11 × 0.09 × 0.04 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.743, T_{max} = 0.894
3179 measured reflections
2817 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
2 standard reflections
frequency: 120 min
intensity decay: 11%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
S = 0.98
2817 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 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
O3—HO3···O4^{i}	0.82	1.89	2.617 (4)	148
N—HN···O2^{ii}	0.95 (4)	1.82 (5)	2.762 (5)	168 (4)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2065).

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4-Benzylpyridinium hydrogen selenate

Wassim Maalej, Zakaria Elaoud, Tahar Mhiri, Abdelaziz Daoud and Ahmed Driss

S1. Comment

The title compound $C_6H_5CH_2C_5H_4NH^+$ $HSeO_4^-$ crystallizes in the orthorhombic space group Pbca. Correspondingly, there are eight formula units per unit cell. The crystal is built up of monohydrogenselenate anions connected by hydrogen bonds of the O—H···O type forming infinite chains $[HSeO_4]_n^{n-}$ perpendicular to the [001] directions.

These chains are themselves interconnected by means of N—H···O hydrogen bonds originating from the $[C_6H_5CH_2C_5H_4NH]^+$ cation, so as to build a three-dimensional network. The distances Se—O in the $[HSeO_4]^-$ anions range from 1.608 (3) to 1.705 (3) Å (Fig. 1). These values are comparable to reported data (Fleck, 2006). The longest Se—O(2) distance of 1.705 (3) Å, is due to the presence of the acidic hydrogen atom on the SeO_4 tetrahedron (Baran *et al.*, 2000).

The organic groups are located in the (011) planes at x = 1/4 and x = 3/4. The average values of the C—C, C—N and C═C bond lengths of 1.5165 (6) Å, 1.3305 (6) Å and 1.3753 (6) Å in the $[C_6H_5CH_2C_5H_4NH]^+$ cation are similar to those observed in related compounds (Ben Hamada & Jouini, 2006; Kaabi *et al.*, 2004; Ben Djemaa *et al.*, 2007; Gowda *et al.*, 2007). The C—C perpendicular interplanar distances range from 1.74 to 4.83 Å and the dihedral angle between two planes of rings is 67.04°, indicating the existence of strong van der Waals interactions by contacts between $[C_6H_5CH_2C_5H_4NH]^+$ cations.

All the hydrogen bonds (D—H···O, Table 1) and the van der Waals contacts give rise to a three dimensional network in the crystal structure.

S2. Experimental

Crystals of the title compound $C_6H_5CH_2C_5H_4NH^+$ $HSeO_4^-$ were prepared by slowly adding, at room temperature, an equimolecular proportion of H_2SeO_4 (1.9 cm^3) to a solution of 4-benzyl pyridine (5 cm^3). A crystalline precipitate was formed. After dissolving the precipitate by adding H_2O, the solution is allowed to slowly evaporate at room temperature for several days until the formation of pink prismatic crystals with dimensions suitable for a crystallographic study occurs.

S3. Refinement

Hydrogen atoms at C_6, C_9 and O_3 were positioned geometrically, with C—H = 0.93 Å and O—H = 0.82 Å, and were refined with $U_{iso}(H) = 1.41U_{eq}$ of the corresponding parent atom. The other H atoms bound to C (cyclic and CH_2) groups, and N atoms were located from the difference Fourier map, and refined with distance restraints of [C—H = 0.90 (4)–1.00 (5) Å and $U_{iso}(H)$ = 0.06 (1)–0.10 (2) $Å^2$, (cyclic groups)], [C—H = 0.88 (6)–1.00 (4) Å and $U_{iso}(H)$ = 0.06 (1)–0.12 (2) $Å^2$, (CH_2 group)], and N—H = 0.95 (4) Å with $U_{iso}(H) = 1.14U_{eq}(N)$ for NH bond.

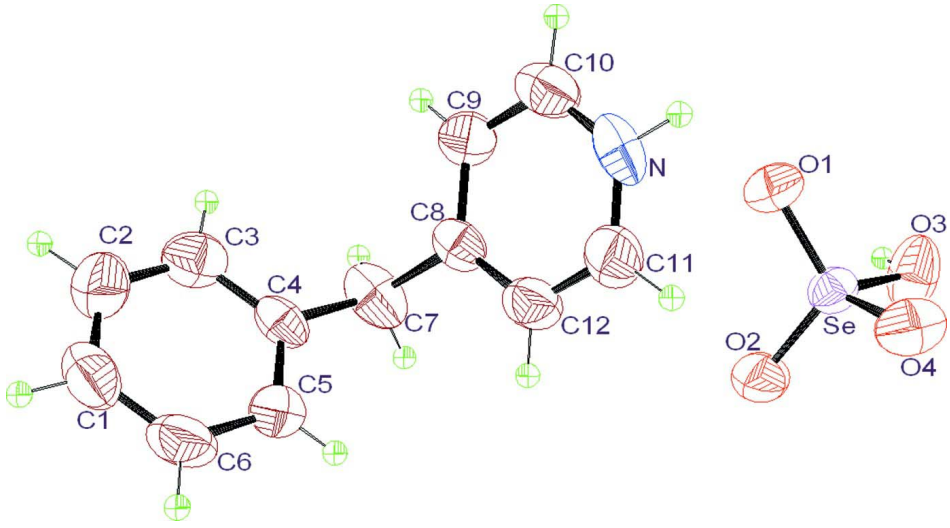

Figure 1

ORTEP drawing of $[C_6H_5CH_2C_5H_4NH]^+$ $[HSeO_4]^-$.

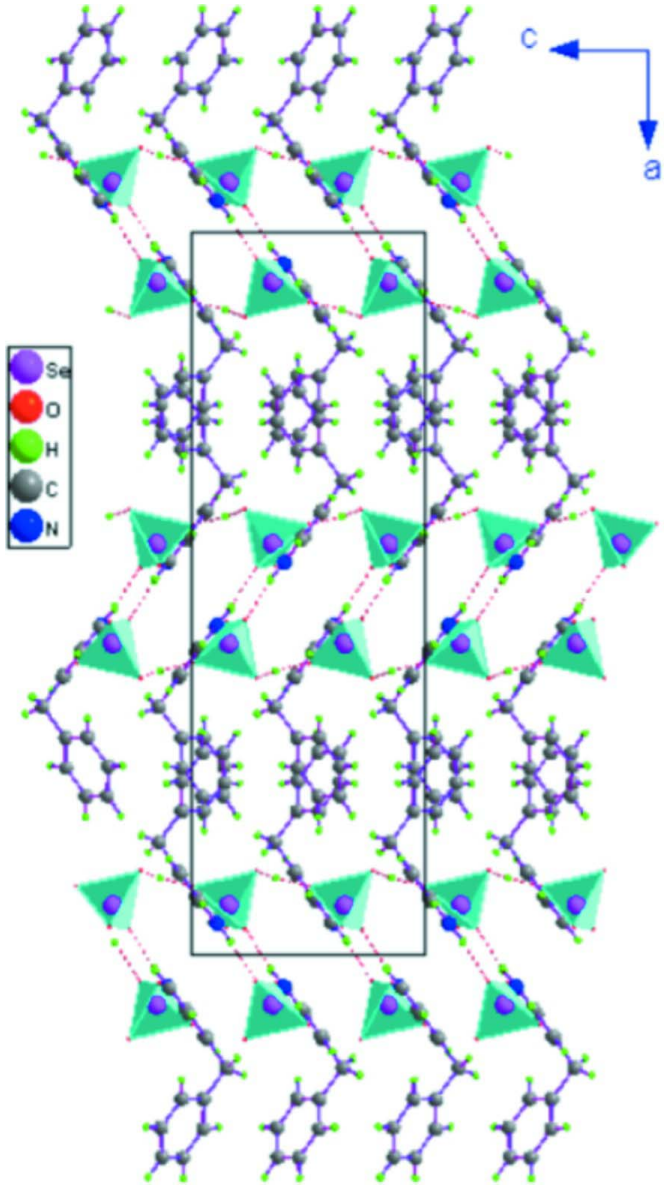

Figure 2

Projection along the *b* axis of the crystal structure of $[C_6H_5CH_2C_5H_4NH]^+$ $[HSeO_4]^-$.

4-Benzylpyridinium hydrogen selenate

Crystal data

$C_{12}H_{12}N^+ \cdot HSeO_4^-$
$M_r = 314.19$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 27.449$ (5) Å
$b = 10.821$ (6) Å
$c = 8.830$ (1) Å
$V = 2623$ (2) Å^3
$Z = 8$
$F(000) = 1264$
$D_x = 1.592$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 14$–16°
$\mu = 2.87$ mm^{-1}
$T = 289$ K
Prism, pink
0.11 × 0.09 × 0.04 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Non–profiled $\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.743, T_{max} = 0.894
3179 measured reflections

2817 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.0°, θ_{min} = 2.4°
h = 0→35
k = 0→13
l = −2→11
2 standard reflections every 120 min
intensity decay: 11%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
S = 0.98
2817 reflections
207 parameters
0 restraints

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (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}
Se	0.568598 (14)	0.68653 (3)	0.34450 (4)	0.04502 (15)
O1	0.53870 (10)	0.8139 (2)	0.3574 (4)	0.0652 (8)
O2	0.53625 (10)	0.5754 (2)	0.2732 (4)	0.0685 (9)
O3	0.61665 (10)	0.7080 (3)	0.2250 (4)	0.0779 (10)
HO3	0.6065	0.7281	0.1411	0.11 (2)*
O4	0.59571 (11)	0.6441 (3)	0.4996 (3)	0.0644 (8)
C1	0.22067 (18)	0.5917 (5)	0.6315 (6)	0.0675 (14)
C2	0.21967 (19)	0.6932 (5)	0.5412 (7)	0.0746 (15)
C3	0.25920 (19)	0.7237 (5)	0.4540 (6)	0.0624 (13)
C4	0.30049 (14)	0.6492 (4)	0.4530 (4)	0.0460 (10)
C5	0.30108 (17)	0.5471 (4)	0.5468 (6)	0.0564 (12)
C6	0.26129 (17)	0.5184 (4)	0.6359 (6)	0.0681 (14)
HC6	0.2621	0.4494	0.6988	0.061 (13)*
C7	0.3437 (2)	0.6798 (6)	0.3529 (6)	0.0683 (14)
C8	0.38461 (14)	0.7417 (4)	0.4400 (4)	0.0462 (10)
C9	0.38853 (17)	0.8693 (4)	0.4482 (5)	0.0538 (11)

HC9	0.3662	0.9193	0.3977	0.046 (11)*
C10	0.42554 (19)	0.9215 (5)	0.5313 (6)	0.0630 (13)
C11	0.45454 (18)	0.7264 (5)	0.5991 (6)	0.0631 (13)
C12	0.41870 (17)	0.6719 (5)	0.5168 (6)	0.0580 (12)
N	0.45683 (14)	0.8484 (4)	0.6053 (5)	0.0621 (11)
HC1	0.1926 (15)	0.573 (4)	0.690 (5)	0.077 (15)*
HC2	0.1914 (18)	0.742 (5)	0.540 (6)	0.102 (18)*
HC3	0.2621 (16)	0.795 (4)	0.388 (5)	0.082 (16)*
HC5	0.3276 (13)	0.498 (4)	0.547 (4)	0.058 (13)*
H1C7	0.334 (2)	0.729 (6)	0.280 (7)	0.12 (2)*
H2C7	0.3573 (13)	0.602 (4)	0.309 (4)	0.062 (14)*
HC10	0.4295 (16)	1.006 (4)	0.543 (5)	0.090 (17)*
HC11	0.4786 (18)	0.680 (4)	0.661 (6)	0.104 (19)*
HC12	0.4167 (16)	0.587 (5)	0.503 (5)	0.087 (16)*
HN	0.4820 (15)	0.885 (4)	0.664 (5)	0.071 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se	0.0483 (2)	0.0418 (2)	0.0450 (2)	0.00559 (19)	0.0005 (2)	−0.0042 (2)
O1	0.0665 (18)	0.0466 (16)	0.082 (2)	0.0135 (15)	−0.0004 (18)	−0.0093 (17)
O2	0.0725 (19)	0.0479 (17)	0.085 (2)	0.0001 (16)	−0.0203 (18)	−0.0108 (17)
O3	0.0505 (17)	0.120 (3)	0.063 (2)	0.0120 (19)	0.0084 (16)	0.027 (2)
O4	0.093 (2)	0.0568 (17)	0.0429 (16)	0.0089 (17)	−0.0115 (16)	−0.0017 (15)
C1	0.057 (3)	0.070 (3)	0.075 (4)	−0.022 (3)	0.012 (3)	−0.016 (3)
C2	0.054 (3)	0.075 (4)	0.095 (4)	0.005 (3)	−0.007 (3)	−0.004 (4)
C3	0.075 (3)	0.055 (3)	0.057 (3)	−0.002 (3)	−0.013 (3)	0.008 (2)
C4	0.053 (3)	0.048 (2)	0.037 (2)	−0.019 (2)	0.001 (2)	−0.0074 (19)
C5	0.055 (3)	0.046 (3)	0.068 (3)	−0.001 (2)	0.007 (3)	0.001 (2)
C6	0.084 (4)	0.045 (3)	0.076 (4)	−0.013 (2)	0.016 (3)	0.013 (3)
C7	0.077 (3)	0.081 (4)	0.047 (3)	−0.028 (3)	0.010 (3)	−0.014 (3)
C8	0.053 (2)	0.050 (2)	0.036 (2)	−0.012 (2)	0.011 (2)	0.002 (2)
C9	0.060 (3)	0.051 (2)	0.050 (3)	−0.001 (2)	0.002 (2)	0.014 (2)
C10	0.072 (3)	0.051 (3)	0.066 (3)	−0.016 (3)	0.014 (3)	−0.006 (3)
C11	0.055 (3)	0.064 (3)	0.071 (3)	−0.006 (3)	0.008 (3)	0.020 (3)
C12	0.062 (3)	0.047 (3)	0.066 (3)	−0.009 (2)	0.011 (2)	0.005 (3)
N	0.045 (2)	0.082 (3)	0.059 (3)	−0.025 (2)	0.0041 (19)	0.000 (2)

Geometric parameters (Å, º)

Se—O1	1.608 (3)	C6—HC6	0.93
Se—O2	1.622 (3)	C7—C8	1.518 (6)
Se—O4	1.625 (3)	C7—H1C7	0.88 (6)
Se—O3	1.705 (3)	C7—H2C7	1.00 (4)
O3—HO3	0.82	C8—C12	1.381 (6)
C1—C2	1.358 (7)	C8—C9	1.387 (6)
C1—C6	1.369 (7)	C9—C10	1.375 (6)
C1—HC1	0.95 (4)	C9—HC9	0.93

C2—C3	1.371 (7)	C10—N	1.338 (6)
C2—HC2	0.94 (5)	C10—HC10	0.93 (5)
C3—C4	1.391 (6)	C11—N	1.323 (6)
C3—HC3	0.97 (4)	C11—C12	1.358 (7)
C4—C5	1.381 (6)	C11—HC11	1.00 (5)
C4—C7	1.515 (6)	C12—HC12	0.93 (5)
C5—C6	1.382 (6)	N—HN	0.95 (4)
C5—HC5	0.90 (4)		

O1—Se—O2	112.56 (15)	C4—C7—C8	112.4 (4)
O1—Se—O4	114.59 (15)	C4—C7—H1C7	109 (4)
O2—Se—O4	111.61 (15)	C8—C7—H1C7	109 (4)
O1—Se—O3	108.78 (16)	C4—C7—H2C7	109 (2)
O2—Se—O3	106.51 (16)	C8—C7—H2C7	107 (2)
O4—Se—O3	101.89 (16)	H1C7—C7—H2C7	110 (5)
Se—O3—HO3	109.5	C12—C8—C9	117.8 (4)
C2—C1—C6	120.1 (5)	C12—C8—C7	120.6 (4)
C2—C1—HC1	118 (3)	C9—C8—C7	121.5 (5)
C6—C1—HC1	122 (3)	C10—C9—C8	119.6 (4)
C1—C2—C3	120.6 (5)	C10—C9—HC9	120.2
C1—C2—HC2	119 (3)	C8—C9—HC9	120.2
C3—C2—HC2	121 (3)	N—C10—C9	119.5 (4)
C2—C3—C4	120.6 (5)	N—C10—HC10	117 (3)
C2—C3—HC3	126 (3)	C9—C10—HC10	123 (3)
C4—C3—HC3	113 (3)	N—C11—C12	119.3 (5)
C5—C4—C3	118.0 (4)	N—C11—HC11	117 (3)
C5—C4—C7	121.0 (4)	C12—C11—HC11	124 (3)
C3—C4—C7	121.0 (5)	C11—C12—C8	121.1 (5)
C4—C5—C6	120.8 (4)	C11—C12—HC12	123 (3)
C4—C5—HC5	119 (3)	C8—C12—HC12	116 (3)
C6—C5—HC5	121 (3)	C11—N—C10	122.6 (5)
C1—C6—C5	119.8 (5)	C11—N—HN	118 (3)
C1—C6—HC6	120.1	C10—N—HN	119 (3)
C5—C6—HC6	120.1		

C6—C1—C2—C3	−0.2 (8)	C4—C7—C8—C12	85.0 (6)
C1—C2—C3—C4	2.0 (8)	C4—C7—C8—C9	−93.6 (6)
C2—C3—C4—C5	−2.6 (7)	C12—C8—C9—C10	−0.1 (6)
C2—C3—C4—C7	177.9 (4)	C7—C8—C9—C10	178.5 (4)
C3—C4—C5—C6	1.6 (7)	C8—C9—C10—N	−1.1 (6)
C7—C4—C5—C6	−178.9 (4)	N—C11—C12—C8	−0.2 (7)
C2—C1—C6—C5	−0.8 (8)	C9—C8—C12—C11	0.8 (6)
C4—C5—C6—C1	0.0 (7)	C7—C8—C12—C11	−177.8 (4)
C5—C4—C7—C8	−78.7 (6)	C12—C11—N—C10	−1.1 (7)
C3—C4—C7—C8	100.8 (6)	C9—C10—N—C11	1.8 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H*O*3···O4^{i}	0.82	1.89	2.617 (4)	148
N—H*N*···O2^{ii}	0.95 (4)	1.82 (5)	2.762 (5)	168 (4)

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*+1/2.