Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-5-nitropyridinium hydrogen selenate

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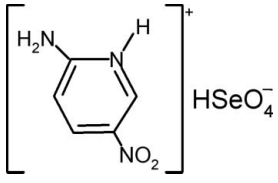
Received 8 October 2009; accepted 15 October 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.043; wR factor = 0.101; data-to-parameter ratio = 16.2.

There are two cations and two anions in the asymmetric unit of the title compound, $C_5H_6N_3O_2^+\cdot HSeO_4^-$. In the crystal, there are two independent chains of $HSeO_4^-$ anions running along the *a* axis, linked by O—H···O hydrogen bonds. Ribbons of cations linked by N—H···O hydrogen bonds run along the *b*-axis direction, and are further hydrogen bonded to the anions by N—H···O and C—H···O links, generating a three-dimensional network.

Related literature

For related structures of 2-amino-5-nitropyridinium salts, see: Pécaut *et al.* (1993*a*,*b*); Masse & Zyss (1991); Zyss *et al.* (1993); Watanabe *et al.* (1993); Pécaut & Masse (1994). For hydrogen bonds, see: Desiraju (1991); Steiner (1993, 1994). For bond lengths in related structures, see: Aakeröy *et al.* (1998). Ferraris & Ivaldi (1984).



Experimental

Crystal data

$C_5H_6N_3O_2^+\cdot HSeO_4^-$
M_r = 284.10
Orthorhombic, *Pbca*
a = 9.092 (3) Å
b = 13.416 (2) Å
c = 30.149 (4) Å
V = 3677.5 (14) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 4.10 mm^{-1}
T = 298 K
0.23 × 0.21 × 0.19 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.403, T_{max} = 0.444
8480 measured reflections
4426 independent reflections
2650 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
2 standard reflections
frequency: 120 min
intensity decay: 6%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.101
S = 0.97
4426 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O4^{i}	0.82	1.75	2.527 (5)	158
O8—H8···O7^{ii}	0.82	1.73	2.546 (5)	173
N1—H1···O3	0.86	1.95	2.773 (5)	161
N2—H2*A*···O3	0.86	2.46	3.152 (6)	138
N2—H2*B*···O6	0.86	2.15	2.943 (6)	152
N2—H2*B*···O9^{iii}	0.86	2.54	3.057 (6)	119
N4—H4···O5	0.86	2.01	2.769 (5)	146
N5—H5*A*···O5	0.86	2.27	2.958 (6)	137
N5—H5*B*···O1	0.86	2.02	2.833 (6)	157
N5—H5*B*···O11^{iv}	0.86	2.56	3.016 (6)	115
C2—H2*C*···O6	0.93	2.37	3.132 (6)	139
C8—H8*C*···O4^{v}	0.93	2.37	3.261 (6)	159
C3—H3···O7^{vi}	0.93	2.41	3.202 (6)	143
C5—H5*C*···O2^{i}	0.93	2.50	3.245 (6)	137
C5—H5*C*···O10^{vii}	0.93	2.50	3.150 (6)	128
C7—H7···O1	0.93	2.52	3.228 (6)	134
C10—H10···O5^{ii}	0.93	2.23	3.130 (6)	162

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (ii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (iii) $x-1, y, z$; (iv) $x+1, y, z$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (vi) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (vii) $-x+2, -y+1, -z+1$.

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: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Putz, 2005); 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: HB5132).

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supplementary materials

Acta Cryst. (2009). E**65**, o3009-o3010 [**doi:10.1107/S1600536809042354**]

2-Amino-5-nitropyridinium hydrogen selenate

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Comment

The 2-amino-5-nitropyridine (2 A5NP) chromophore is promising candidate for non linear optics. From this molecule, several salts having noncentrosymmetric structures were obtained: dihydrogenphosphate, dihydrogenarsenate, chloride, bromide, tartrate, and acetophosphonate of 2-amino-5-nitropyridinium (Pécaut *et al.*, 1993a,b; Masse *et al.*, 1991; Pécaut *et al.*, 1993, Zyss *et al.*, 1993; Watanabe *et al.*, 1993; Pécaut Masse, 1994). In the framework of our systematic research on nitropyridine chromophore, we report on the new compound $(C_5H_6N_3O_2)^+$, $HSeO_4^-$ synthesized from the 2-amino-5-nitropyridine and selenic acid.

The asymmetric unit of the title compound (I) that contains two 2-amino-5-nitropyridinium cations and two hydrogen selenate anions, is shown in Fig. 1. The connection between theses independent components generate a three-dimensional supramolecular network which is stabilized by hydrogen bonds, Van Der Waals and electrostatic interactions. In fact, The two hydrogen selenate anions are connected through strong hydrogen bonds characterized by relatively short distances, from 1.73 to 1.75 A% (Table 1), to form two independent robust chains extending along a direction (Fig. 2). Both cations are arranged in ribbons and anchored onto both adjacent anionic chains *via* N—H···O and C—H···O hydrogen bonds. The C—H···O bonds have already been evidenced by several authors in molecular crystals; (Desiraju *et al.*, 1991; Steiner *et al.*, 1993 and 1994). With regards to the organic subnetwork, each 2 A5NP cation is hydrogen bonded to symmetry-equivalent 2 A5NP cation by rather long N—H···O and C—H···O bonds (with distances N2—H2B···O9 (x - 1, y, z) = 2.54A% and C5—H5C···O10 (-x + 2, -y + 1, -z + 1) = 2.50 A%) as to form ribbons running along the b axis. In the selenate chains, it is noteworthy that the O···O distances involved in hydrogen bonds (2.527 (5) to 2.546 (5) A%) are of the same order of magnitude as the O···O distances in $HSeO_4$ (2.41 to 2.56A%); this should allow us to consider the $(HSeO_4^-)_n$ subnetwork as a polyanion. The geometrical features of $HSeO_4$ entities, show that the Se—O bonds are significantly shorter [1.592 (4) to 1.623 (3) A% than the Se—OH bonds [1.690 (4) to 1.696 (4)A%], which is in accordance with the data relative to the protonated oxoanions as reported by (Ferraris *et al.*, 1984) Bond lengths and angles of the organic cations can be regarded as normal and are comparable with values of other 2-amino-5-nitropyridinium compounds. The organic ring atoms of both independent cations are essentially planar (the deviations from least-square planes are 0.001 and 0.002 Å). The angles between the plane of the NO_2 group and the pyridinium rings are 4.9 (3) and 5.8 (4)°. This distortion is evident because the oxygen atoms of the NO_2 group are the seat of various types of inter-and intramolecular hydrogen bonds. Moreover, the C—NH_2 (1.312 (6) and 1.315 (6)Å) and C—NO_2 (1.459 (6) and 1.466 (6) Å) distances in the 2 A5NP cations are respectively shortened and lengthened with respect to the C—NH_2 (1.337 (4) Å) and C—NO_2 (1.429 (4) Å) observed in the 2-amino-5-nitropyridine molecular crystal (Aakeröy, *et al.*, 1998). All the 2-amino-5-nitropyridinium cations hosted in various organic or inorganic matrices show the same changes in C—NH_2 and C—NO_2 distances, revealing a weak increase of π bond character in C—NH_2 and a decrease in C—NO_2.

Experimental

The starting materials, 2-amino-5-nitropyridine (2-A5NP) and selenic acid (Aldrich, 40 wt% in H_2O, 99.95%) were used as supplied. 5 mmol of selenic acid was added to a hot solution (20 ml of water and 5 ml of ethanol) of 2-A5NP (5 mmol). The mixture was cooled and slowly evaporated at room temperature for several days until it resulted in yellow prisms of (I).

Figures

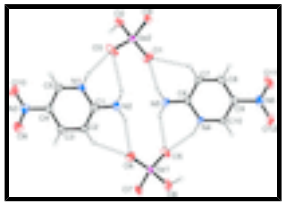

Fig. 1. A view of (I) with displacement ellipsoids drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are represented as dashed lines.

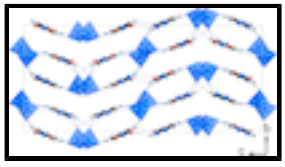

Fig. 2. Projection of (I) along the *a* axis.

2-Amino-5-nitropyridinium hydrogen selenate

Crystal data

$C_5H_6N_3O_2^+ \cdot HO_4Se^-$	F_{000} = 2240
M_r = 284.10	D_x = 2.052 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 9.092 (3) Å	θ = 9–11°
b = 13.416 (2) Å	μ = 4.10 mm^{-1}
c = 30.149 (4) Å	*T* = 298 K
V = 3677.5 (14) Å^3	Prism, yellow
Z = 16	0.23 × 0.21 × 0.19 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	R_{int} = 0.075
Monochromator: graphite	θ_{max} = 28.0°
T = 298 K	θ_{min} = 2.6°
Non–profiled ω scans	*h* = −10→11
Absorption correction: multi-scan (Blessing, 1995)	*k* = 0→17
T_{min} = 0.403, T_{max} = 0.444	*l* = 0→39
8480 measured reflections	2 standard reflections
4426 independent reflections	every 120 min

2650 reflections with $I > 2\sigma(I)$

intensity decay: 6%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.101$

$S = 0.97$

4426 reflections

273 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.59$ e Å^{-3}

$\Delta\rho_{min} = -0.59$ e Å^{-3}

Extinction correction: none

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}
Se1	0.36683 (5)	0.57372 (4)	0.271792 (15)	0.02983 (13)
Se2	0.41005 (5)	0.29253 (4)	0.487699 (15)	0.03145 (13)
O1	0.3545 (5)	0.2664 (4)	0.43901 (12)	0.0799 (15)
O2	0.5188 (4)	0.1974 (3)	0.50425 (14)	0.0553 (11)
H2	0.5936	0.1963	0.4890	0.083*
O3	0.5015 (5)	0.3935 (3)	0.49155 (15)	0.0644 (12)
O4	0.2793 (4)	0.2887 (3)	0.52431 (10)	0.0452 (9)
O5	0.2967 (4)	0.4638 (3)	0.27541 (12)	0.0459 (9)
O6	0.4460 (4)	0.6107 (3)	0.31613 (11)	0.0476 (10)
O7	0.4741 (4)	0.5824 (3)	0.22931 (11)	0.0554 (11)
O8	0.2301 (4)	0.6563 (3)	0.26121 (17)	0.0647 (13)
H8	0.1503	0.6299	0.2659	0.097*
O9	1.1750 (4)	0.5569 (3)	0.38425 (14)	0.0651 (13)
O10	1.1601 (4)	0.5021 (3)	0.45094 (14)	0.0589 (11)
O11	−0.3916 (4)	0.2918 (3)	0.36698 (16)	0.0712 (14)
O12	−0.3715 (4)	0.3419 (4)	0.29945 (16)	0.0713 (13)
N1	0.7158 (4)	0.4848 (3)	0.44020 (13)	0.0345 (9)

H1	0.6641	0.4587	0.4611	0.041*
N2	0.5007 (4)	0.5204 (3)	0.40355 (15)	0.0420 (11)
H2A	0.4529	0.4972	0.4259	0.050*
H2B	0.4539	0.5430	0.3809	0.050*
N3	1.1047 (5)	0.5295 (3)	0.41618 (15)	0.0419 (11)
N4	0.0710 (4)	0.3519 (3)	0.31176 (13)	0.0358 (10)
H4	0.1237	0.3769	0.2909	0.043*
N5	0.2842 (4)	0.3237 (3)	0.35110 (14)	0.0436 (11)
H5A	0.3340	0.3483	0.3294	0.052*
H5B	0.3288	0.3025	0.3744	0.052*
N6	−0.3196 (5)	0.3149 (3)	0.33474 (19)	0.0468 (12)
C1	0.6453 (5)	0.5211 (3)	0.40398 (16)	0.0327 (11)
C2	0.7316 (5)	0.5571 (3)	0.36909 (14)	0.0309 (11)
H2C	0.6864	0.5780	0.3430	0.037*
C3	0.8802 (5)	0.5620 (3)	0.37265 (15)	0.0328 (11)
H3	0.9374	0.5874	0.3497	0.039*
C4	0.9448 (5)	0.5275 (4)	0.41192 (16)	0.0311 (11)
C5	0.8634 (5)	0.4879 (4)	0.44491 (16)	0.0342 (11)
H5C	0.9080	0.4632	0.4704	0.041*
C6	0.1403 (5)	0.3185 (3)	0.34854 (15)	0.0305 (10)
C9	−0.1590 (5)	0.3146 (3)	0.33920 (17)	0.0330 (11)
C8	−0.0953 (5)	0.2830 (3)	0.37952 (16)	0.0341 (11)
H8C	−0.1541	0.2621	0.4030	0.041*
C7	0.0523 (5)	0.2838 (3)	0.38333 (15)	0.0312 (11)
H7	0.0960	0.2611	0.4093	0.037*
C10	−0.0746 (5)	0.3482 (4)	0.30600 (16)	0.0356 (11)
H10	−0.1167	0.3687	0.2794	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0236 (2)	0.0403 (3)	0.0256 (2)	−0.0052 (2)	0.00113 (19)	−0.0015 (2)
Se2	0.0267 (2)	0.0409 (3)	0.0268 (2)	−0.0001 (2)	0.00137 (19)	0.0081 (2)
O1	0.061 (3)	0.148 (5)	0.030 (2)	0.001 (3)	−0.006 (2)	−0.004 (3)
O2	0.035 (2)	0.051 (2)	0.080 (3)	0.0063 (18)	0.0125 (19)	0.029 (2)
O3	0.070 (3)	0.039 (2)	0.084 (3)	−0.015 (2)	0.034 (2)	0.000 (2)
O4	0.0268 (19)	0.076 (3)	0.0327 (19)	−0.0044 (18)	0.0055 (14)	0.0082 (19)
O5	0.045 (2)	0.038 (2)	0.054 (2)	−0.0077 (17)	0.0136 (18)	−0.0064 (18)
O6	0.052 (2)	0.061 (3)	0.0296 (19)	−0.007 (2)	−0.0080 (17)	−0.0101 (18)
O7	0.035 (2)	0.100 (3)	0.0312 (19)	−0.023 (2)	0.0111 (16)	−0.006 (2)
O8	0.029 (2)	0.049 (2)	0.117 (4)	−0.0035 (18)	−0.009 (2)	0.025 (2)
O9	0.033 (2)	0.105 (4)	0.058 (3)	−0.007 (2)	0.012 (2)	0.002 (3)
O10	0.039 (2)	0.075 (3)	0.062 (3)	0.008 (2)	−0.015 (2)	0.004 (2)
O11	0.033 (2)	0.086 (4)	0.094 (4)	−0.004 (2)	0.025 (2)	0.012 (3)
O12	0.031 (2)	0.093 (4)	0.091 (4)	0.002 (2)	−0.016 (2)	0.016 (3)
N1	0.031 (2)	0.041 (2)	0.032 (2)	−0.0018 (19)	0.0058 (17)	0.0056 (19)
N2	0.025 (2)	0.057 (3)	0.044 (3)	−0.003 (2)	0.0021 (18)	0.007 (2)
N3	0.033 (3)	0.046 (3)	0.047 (3)	0.004 (2)	0.001 (2)	−0.007 (2)

N4	0.028 (2)	0.050 (3)	0.029 (2)	−0.0023 (19)	−0.0010 (17)	0.0121 (19)
N5	0.031 (2)	0.059 (3)	0.040 (2)	−0.005 (2)	−0.0055 (18)	0.008 (2)
N6	0.030 (2)	0.032 (3)	0.079 (4)	0.0035 (19)	−0.003 (3)	0.000 (2)
C1	0.038 (3)	0.024 (2)	0.036 (3)	0.001 (2)	0.000 (2)	−0.004 (2)
C2	0.030 (3)	0.039 (3)	0.024 (2)	0.002 (2)	0.000 (2)	0.002 (2)
C3	0.034 (3)	0.031 (3)	0.033 (3)	0.001 (2)	0.007 (2)	0.001 (2)
C4	0.027 (3)	0.034 (3)	0.033 (3)	0.001 (2)	0.000 (2)	−0.006 (2)
C5	0.035 (3)	0.035 (3)	0.032 (3)	0.002 (2)	−0.008 (2)	−0.001 (2)
C6	0.028 (2)	0.030 (3)	0.034 (3)	−0.001 (2)	−0.006 (2)	−0.003 (2)
C9	0.027 (3)	0.027 (3)	0.046 (3)	−0.001 (2)	0.000 (2)	−0.004 (2)
C8	0.039 (3)	0.030 (3)	0.033 (3)	0.000 (2)	0.012 (2)	−0.004 (2)
C7	0.037 (3)	0.032 (3)	0.024 (2)	0.002 (2)	−0.004 (2)	0.001 (2)
C10	0.033 (3)	0.041 (3)	0.034 (3)	−0.002 (2)	−0.010 (2)	0.010 (2)

Geometric parameters (Å, °)

Se1—O6	1.597 (3)	N4—C10	1.337 (6)
Se1—O5	1.610 (3)	N4—C6	1.352 (6)
Se1—O7	1.614 (3)	N4—H4	0.8600
Se1—O8	1.696 (4)	N5—C6	1.312 (6)
Se2—O1	1.592 (4)	N5—H5A	0.8600
Se2—O3	1.594 (4)	N5—H5B	0.8600
Se2—O4	1.623 (3)	N6—C9	1.466 (6)
Se2—O2	1.690 (4)	C1—C2	1.398 (6)
O2—H2	0.8200	C2—C3	1.357 (6)
O8—H8	0.8200	C2—H2C	0.9300
O9—N3	1.213 (5)	C3—C4	1.400 (6)
O10—N3	1.220 (5)	C3—H3	0.9300
O11—N6	1.213 (6)	C4—C5	1.349 (7)
O12—N6	1.219 (6)	C5—H5C	0.9300
N1—C5	1.350 (6)	C6—C7	1.399 (6)
N1—C1	1.356 (6)	C9—C10	1.339 (7)
N1—H1	0.8600	C9—C8	1.412 (7)
N2—C1	1.315 (6)	C8—C7	1.347 (6)
N2—H2A	0.8600	C8—H8C	0.9300
N2—H2B	0.8600	C7—H7	0.9300
N3—C4	1.459 (6)	C10—H10	0.9300
O6—Se1—O5	113.95 (19)	O12—N6—C9	117.8 (5)
O6—Se1—O7	111.69 (19)	N2—C1—N1	118.5 (5)
O5—Se1—O7	111.02 (19)	N2—C1—C2	123.8 (5)
O6—Se1—O8	106.5 (2)	N1—C1—C2	117.7 (5)
O5—Se1—O8	108.74 (19)	C3—C2—C1	121.1 (5)
O7—Se1—O8	104.3 (2)	C3—C2—H2C	119.5
O1—Se2—O3	114.9 (3)	C1—C2—H2C	119.5
O1—Se2—O4	112.8 (2)	C2—C3—C4	117.9 (4)
O3—Se2—O4	111.1 (2)	C2—C3—H3	121.0
O1—Se2—O2	107.0 (3)	C4—C3—H3	121.0
O3—Se2—O2	108.3 (2)	C5—C4—C3	121.5 (4)
O4—Se2—O2	101.76 (18)	C5—C4—N3	119.3 (4)

Se2—O2—H2	109.5	C3—C4—N3	119.1 (4)
Se1—O8—H8	109.5	C4—C5—N1	118.7 (4)
C5—N1—C1	122.9 (4)	C4—C5—H5C	120.6
C5—N1—H1	118.6	N1—C5—H5C	120.6
C1—N1—H1	118.6	N5—C6—N4	119.7 (4)
C1—N2—H2A	120.0	N5—C6—C7	123.0 (4)
C1—N2—H2B	120.0	N4—C6—C7	117.3 (4)
H2A—N2—H2B	120.0	C10—C9—C8	120.7 (4)
O9—N3—O10	123.7 (5)	C10—C9—N6	120.0 (5)
O9—N3—C4	117.4 (4)	C8—C9—N6	119.2 (5)
O10—N3—C4	118.8 (4)	C7—C8—C9	118.7 (4)
C10—N4—C6	123.8 (4)	C7—C8—H8C	120.7
C10—N4—H4	118.1	C9—C8—H8C	120.7
C6—N4—H4	118.1	C8—C7—C6	120.6 (4)
C6—N5—H5A	120.0	C8—C7—H7	119.7
C6—N5—H5B	120.0	C6—C7—H7	119.7
H5A—N5—H5B	120.0	N4—C10—C9	118.9 (4)
O11—N6—O12	124.5 (5)	N4—C10—H10	120.6
O11—N6—C9	117.6 (5)	C9—C10—H10	120.6
C5—N1—C1—N2	−175.8 (4)	C10—N4—C6—N5	179.0 (5)
C5—N1—C1—C2	4.3 (7)	C10—N4—C6—C7	−4.0 (7)
N2—C1—C2—C3	175.6 (5)	O11—N6—C9—C10	−173.8 (5)
N1—C1—C2—C3	−4.5 (7)	O12—N6—C9—C10	3.5 (7)
C1—C2—C3—C4	1.6 (7)	O11—N6—C9—C8	3.1 (7)
C2—C3—C4—C5	1.8 (7)	O12—N6—C9—C8	−179.5 (5)
C2—C3—C4—N3	178.4 (4)	C10—C9—C8—C7	−2.5 (7)
O9—N3—C4—C5	173.2 (5)	N6—C9—C8—C7	−179.5 (4)
O10—N3—C4—C5	−5.4 (7)	C9—C8—C7—C6	2.2 (7)
O9—N3—C4—C3	−3.4 (7)	N5—C6—C7—C8	177.8 (5)
O10—N3—C4—C3	177.9 (5)	N4—C6—C7—C8	0.9 (7)
C3—C4—C5—N1	−2.2 (7)	C6—N4—C10—C9	3.7 (8)
N3—C4—C5—N1	−178.8 (4)	C8—C9—C10—N4	−0.3 (8)
C1—N1—C5—C4	−1.0 (7)	N6—C9—C10—N4	176.6 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4^{i}	0.82	1.75	2.527 (5)	158
O8—H8···O7^{ii}	0.82	1.73	2.546 (5)	173
N1—H1···O3	0.86	1.95	2.773 (5)	161
N2—H2A···O3	0.86	2.46	3.152 (6)	138
N2—H2B···O6	0.86	2.15	2.943 (6)	152
N2—H2B···O9^{iii}	0.86	2.54	3.057 (6)	119
N4—H4···O5	0.86	2.01	2.769 (5)	146
N5—H5A···O5	0.86	2.27	2.958 (6)	137
N5—H5B···O1	0.86	2.02	2.833 (6)	157
N5—H5B···O11^{iv}	0.86	2.56	3.016 (6)	115
C2—H2C···O6	0.93	2.37	3.132 (6)	139

C8—H8C···O4^{v}	0.93	2.37	3.261 (6)	159
C3—H3···O7^{vi}	0.93	2.41	3.202 (6)	143
C5—H5C···O2^{i}	0.93	2.50	3.245 (6)	137
C5—H5C···O10^{vii}	0.93	2.50	3.150 (6)	128
C7—H7···O1	0.93	2.52	3.228 (6)	134
C10—H10···O5^{ii}	0.93	2.23	3.130 (6)	162

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1; (ii) *x*−1/2, *y*, −*z*+1/2; (iii) *x*−1, *y*, *z*; (iv) *x*+1, *y*, *z*; (v) *x*−1/2, −*y*+1/2, −*z*+1; (vi) *x*+1/2, *y*, −*z*+1/2; (vii) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

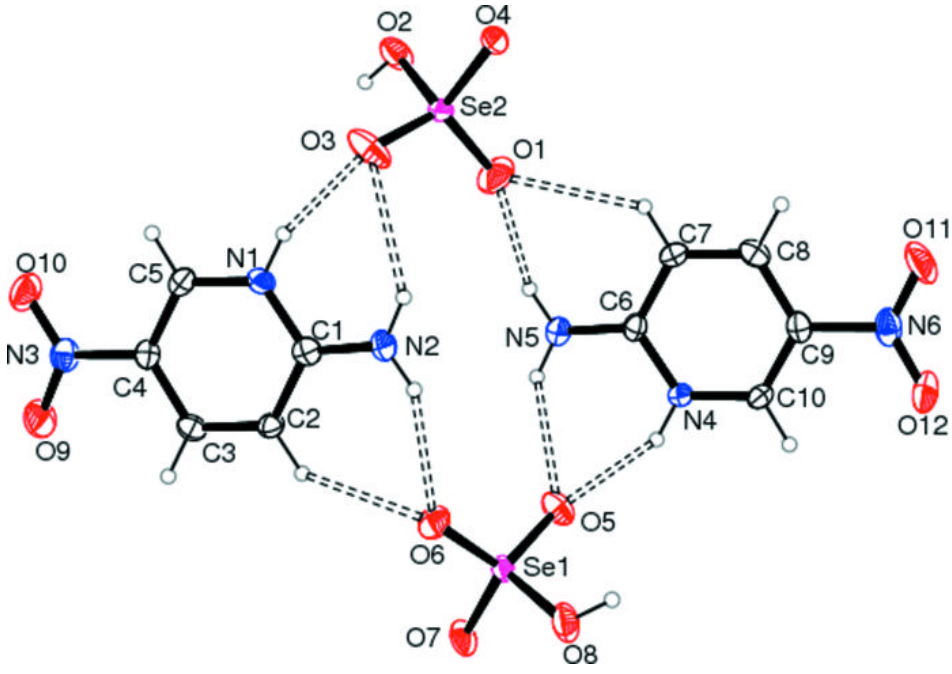
O2
O4
Se2
O3
O1
C7
C8
O11
O10
C5
N1
C6
N5
N6
C1
N2
C9
N3
C4
C10
N4
O12
C2
O9
C3
O5
O6
Se1
O7
O8

Fig. 2