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S-Benzylisothiouronium nitrate

P. Hemalatha[a] and V. Veeravazhuthi[b]*

[a]Department of Physics, PSG College of Technology, Coimbatore 641 004, TamilNadu, India, and [b]Department of Physics, PSG College of Arts and Science, Coimbatore 641 014, TamilNadu, India
Correspondence e-mail: vv_vazhuthi@rediffmail.com

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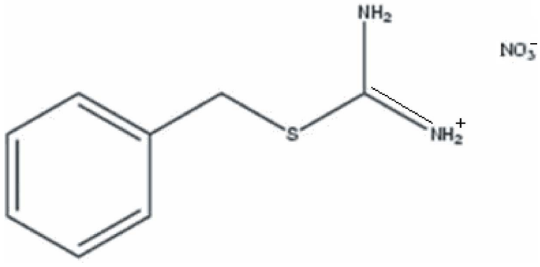
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.074; wR factor = 0.229; data-to-parameter ratio = 18.3.

In the crystal structure of the title compound, $C_8H_{11}N_2S^+\cdot NO_3^-$, cations and anions are linked by intermolecular N—H···O hydrogen bonds, forming one-dimensional chains along [110].

Related literature

For related literature, see: Barker & Powell (1998); Boyd (1989); Hemalatha *et al.* (2006); Zaccaro *et al.* (1999); Zyss *et al.* (1984).



Experimental

Crystal data

$C_8H_{11}N_2S^+\cdot NO_3^-$
M_r = 229.26
Monoclinic, $P2_1/c$
a = 5.8569 (4) Å
b = 7.5931 (5) Å
c = 23.9488 (16) Å
β = 93.304 (1)°
V = 1063.28 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 293 (2) K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
11620 measured reflections
2492 independent reflections
2282 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.229
S = 1.00
2492 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2	0.86	1.98	2.803 (4)	160
N1—H1B···O3^{i}	0.86	2.23	3.009 (4)	151
N2—H2A···O1	0.86	2.21	3.040 (5)	164
N2—H2A···O2	0.86	2.56	3.240 (4)	136
N2—H2B···O1^{ii}	0.86	2.12	2.913 (4)	152

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+1, -y+1, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2669).

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supporting information

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S-Benzylisothiouronium nitrate

P. Hemalatha and V. Veeravazhuthi

S1. Comment

Organic molecular materials have many potential applications in integrated optics, and one of the most attractive applications is diode laser frequency doublers (Boyd, 1989). In the last two decades, extensive research has shown that organic crystals can exhibit nonlinear optical [NLO] efficiencies higher than those of inorganic materials (Zyss *et al.*, 1984 & Zaccaro *et al.*, 1999). Organic nonlinear optical materials are often formed by weak Vander Waals and hydrogen bonds and hence posses high degree of delocalization. Organic materials are molecular materials that offer unique opportunities for fundamental research as well as for technological applications. The title compound (I) is potentially in the above category of materials, therefore we have undertaken its crystal structure determination.

The title molecule is shown in Fig. 1. The C—N, S—C bond lengths and C—S—C and N—C—N bond angles are comparable with the similar structure reported earlier (Barker & Powell, 1998). The bond angles for O1—N3—O3 is 128.7 (4); O1—N3—O2 is 116.7 (4); O3—N3—O2 is 114.6 (3), indicating slight deviations in the bond angle from the expected 120° in terms of the sp^2 hybridization. In the title crystal structure, $C_8H_{11}N_2S$, NO_3, cations and anions are linked by intermolecular N—H···O hydrogen bonds to form one-dimensional chains along [110] (Fig. 2).

S2. Experimental

S-benzylisothiouronium chloride (SBTC) was synthesized as reported earlier (Hemalatha *et al.*, 2006). The solutions of SBTC (5 g m) and potassium nitrate (5 g m) were prepared in water separately. These solutions were mixed together, and then stirred for 1 hr at room temperature. The precipitate was filtered off and washed with triple distilled water and the product was recrystallized from 0.2 *M* nitric acid. Single crystals were grown by slow evaporation of a solution of the title compound in water.

S3. Refinement

All H-atoms were refined using a riding-model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic, 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 and 0.86Å for N-H with U_{iso}(H) = 1.2U_{eq}(N).

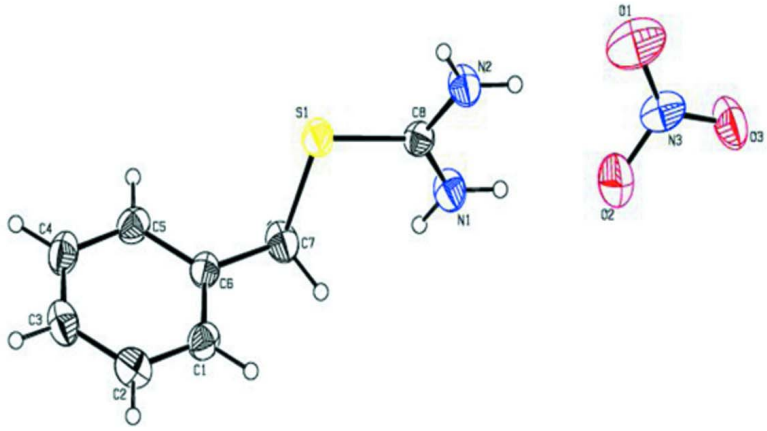

Figure 1

The molecular structure of title compound, showing 30% probability displacement ellipsoids.

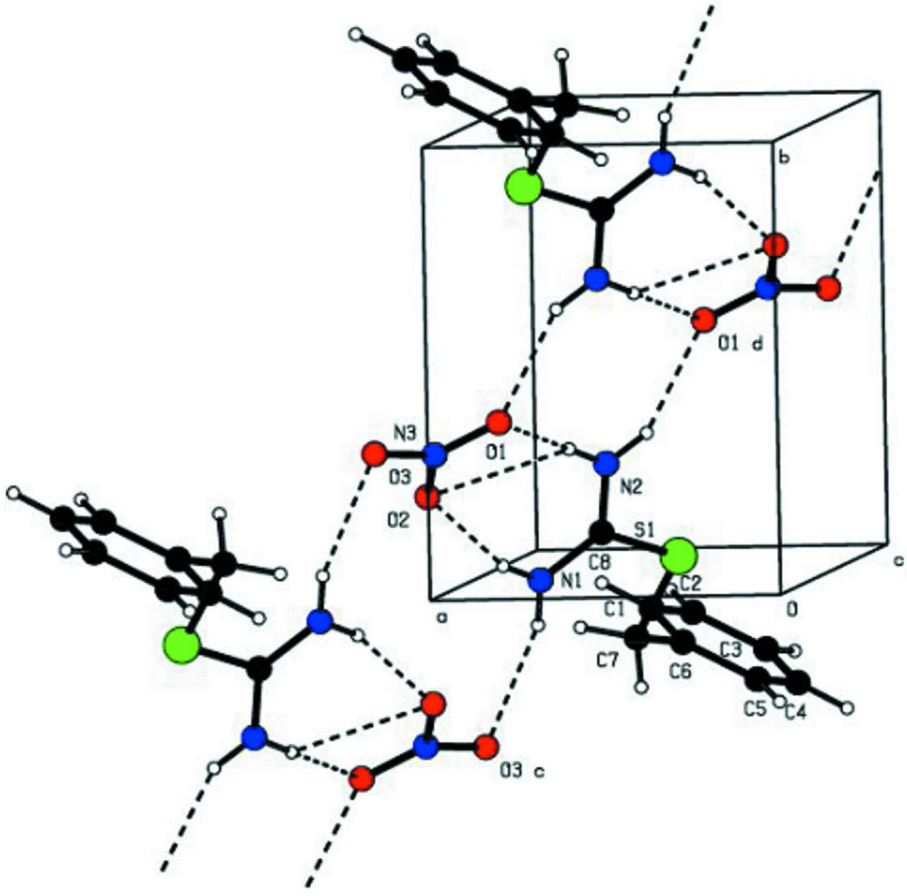

Figure 2

Part of the crystal structure of (I) showing hydrogen bonds as dashed lines.

S-Benzylisothiouronium nitrate

Crystal data

$C_8H_{11}N_2S^+·NO_3^-$
M_r = 229.26
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 5.8569 (4) Å
b = 7.5931 (5) Å
c = 23.9488 (16) Å
β = 93.304 (1)°
V = 1063.28 (12) Å^3
Z = 4
$F(000)$ = 480
D_x = 1.432 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1296 reflections
θ = 1.7–28.0°
μ = 0.30 mm^{-1}
T = 293 K
Needle, colorless
0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEXCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
11620 measured reflections
2492 independent reflections
2282 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 28.0°, θ_{min} = 1.7°
h = −7→7
k = −10→9
l = −31→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.229
S = 1.00
2492 reflections
136 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1605P)^2 + 0.7215P]$, where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-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}
C1	0.4484 (5)	−0.0528 (3)	0.25594 (13)	0.0508 (6)
H1	0.5878	0.0053	0.2547	0.061*
C2	0.3462 (6)	−0.0682 (4)	0.30628 (13)	0.0593 (7)
H2	0.4173	−0.0216	0.3387	0.071*

C3	0.1385 (6)	−0.1527 (4)	0.30829 (13)	0.0604 (7)
H3	0.0683	−0.1617	0.3420	0.072*
C4	0.0359 (5)	−0.2230 (4)	0.26081 (14)	0.0582 (7)
H4	−0.1030	−0.2815	0.2626	0.070*
C5	0.1357 (4)	−0.2085 (3)	0.21013 (12)	0.0498 (6)
H5	0.0632	−0.2555	0.1779	0.060*
C6	0.3459 (4)	−0.1230 (3)	0.20739 (11)	0.0429 (5)
C7	0.4602 (5)	−0.1054 (4)	0.15294 (12)	0.0552 (7)
H7A	0.4431	−0.2135	0.1316	0.066*
H7B	0.6222	−0.0821	0.1600	0.066*
C8	0.5290 (4)	0.1362 (3)	0.06841 (10)	0.0436 (5)
N1	0.7023 (4)	0.0351 (3)	0.05812 (10)	0.0574 (6)
H1A	0.8017	0.0699	0.0355	0.069*
H1B	0.7168	−0.0662	0.0740	0.069*
N2	0.5046 (4)	0.2908 (3)	0.04458 (10)	0.0563 (6)
H2A	0.6031	0.3268	0.0219	0.068*
H2B	0.3900	0.3563	0.0516	0.068*
N3	0.9654 (5)	0.3266 (4)	−0.04824 (12)	0.0660 (7)
O1	0.7787 (6)	0.3965 (5)	−0.05407 (17)	0.1137 (13)
O2	1.0010 (6)	0.2296 (5)	−0.00529 (14)	0.0993 (10)
O3	1.1270 (5)	0.3341 (4)	−0.07925 (11)	0.0832 (8)
S1	0.32436 (11)	0.07656 (10)	0.11423 (3)	0.0538 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0463 (13)	0.0418 (12)	0.0640 (15)	−0.0041 (10)	0.0002 (11)	0.0033 (11)
C2	0.0728 (19)	0.0505 (15)	0.0540 (15)	−0.0015 (13)	−0.0025 (13)	−0.0016 (11)
C3	0.0714 (19)	0.0498 (15)	0.0619 (16)	0.0045 (13)	0.0204 (14)	0.0105 (12)
C4	0.0469 (14)	0.0474 (14)	0.0814 (19)	−0.0040 (10)	0.0136 (13)	0.0093 (13)
C5	0.0441 (12)	0.0435 (12)	0.0613 (14)	−0.0011 (10)	−0.0015 (11)	−0.0005 (11)
C6	0.0398 (11)	0.0346 (10)	0.0547 (13)	0.0050 (8)	0.0067 (9)	0.0049 (9)
C7	0.0588 (16)	0.0471 (13)	0.0612 (15)	0.0176 (11)	0.0168 (12)	0.0101 (11)
C8	0.0415 (12)	0.0452 (12)	0.0444 (11)	0.0058 (9)	0.0048 (9)	−0.0018 (9)
N1	0.0560 (14)	0.0561 (13)	0.0625 (13)	0.0195 (11)	0.0231 (11)	0.0085 (11)
N2	0.0581 (14)	0.0493 (12)	0.0632 (13)	0.0138 (10)	0.0174 (11)	0.0117 (10)
N3	0.0584 (14)	0.0686 (16)	0.0700 (16)	0.0209 (12)	−0.0037 (12)	−0.0270 (13)
O1	0.089 (2)	0.104 (2)	0.146 (3)	0.0491 (18)	−0.008 (2)	−0.031 (2)
O2	0.0851 (19)	0.126 (3)	0.0893 (18)	−0.0035 (19)	0.0280 (15)	0.0245 (19)
O3	0.0965 (19)	0.0875 (18)	0.0691 (14)	0.0096 (15)	0.0337 (13)	0.0199 (13)
S1	0.0424 (4)	0.0579 (5)	0.0624 (5)	0.0142 (2)	0.0143 (3)	0.0142 (3)

Geometric parameters (Å, º)

C1—C2	1.381 (4)	C7—H7A	0.9700
C1—C6	1.384 (4)	C7—H7B	0.9700
C1—H1	0.9300	C8—N1	1.307 (3)
C2—C3	1.379 (5)	C8—N2	1.309 (3)

C2—H2	0.9300	C8—S1	1.731 (3)
C3—C4	1.364 (5)	N1—H1A	0.8600
C3—H3	0.9300	N1—H1B	0.8600
C4—C5	1.382 (4)	N2—H2A	0.8600
C4—H4	0.9300	N2—H2B	0.8600
C5—C6	1.396 (3)	N3—O1	1.217 (4)
C5—H5	0.9300	N3—O3	1.237 (4)
C6—C7	1.506 (4)	N3—O2	1.273 (4)
C7—S1	1.821 (3)		

C2—C1—C6	120.8 (3)	C6—C7—H7A	110.2
C2—C1—H1	119.6	S1—C7—H7A	110.2
C6—C1—H1	119.6	C6—C7—H7B	110.2
C1—C2—C3	119.8 (3)	S1—C7—H7B	110.2
C1—C2—H2	120.1	H7A—C7—H7B	108.5
C3—C2—H2	120.1	N1—C8—N2	120.7 (2)
C4—C3—C2	120.0 (3)	N1—C8—S1	122.6 (2)
C4—C3—H3	120.0	N2—C8—S1	116.66 (19)
C2—C3—H3	120.0	C8—N1—H1A	120.0
C3—C4—C5	120.8 (3)	C8—N1—H1B	120.0
C3—C4—H4	119.6	H1A—N1—H1B	120.0
C5—C4—H4	119.6	C8—N2—H2A	120.0
C4—C5—C6	119.8 (3)	C8—N2—H2B	120.0
C4—C5—H5	120.1	H2A—N2—H2B	120.0
C6—C5—H5	120.1	O1—N3—O3	128.7 (4)
C1—C6—C5	118.7 (2)	O1—N3—O2	116.7 (4)
C1—C6—C7	120.0 (2)	O3—N3—O2	114.6 (3)
C5—C6—C7	121.3 (3)	C8—S1—C7	102.89 (12)
C6—C7—S1	107.78 (17)		

C6—C1—C2—C3	−0.7 (4)	C4—C5—C6—C7	179.7 (2)
C1—C2—C3—C4	0.9 (5)	C1—C6—C7—S1	−99.7 (3)
C2—C3—C4—C5	−1.0 (5)	C5—C6—C7—S1	79.9 (3)
C3—C4—C5—C6	0.9 (4)	N1—C8—S1—C7	15.6 (3)
C2—C1—C6—C5	0.6 (4)	N2—C8—S1—C7	−163.5 (2)
C2—C1—C6—C7	−179.8 (2)	C6—C7—S1—C8	158.3 (2)
C4—C5—C6—C1	−0.7 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2	0.86	1.98	2.803 (4)	160
N1—H1*B*···O3^{i}	0.86	2.23	3.009 (4)	151
N2—H2*A*···O1	0.86	2.21	3.040 (5)	164
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Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+1, −*y*+1, −*z*.