Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2-Amino-2-thiazoline and its 1:1 organic salt with 2-naphthoxyacetic acid

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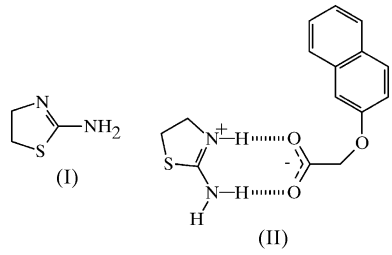
Received 15 June 2004
Accepted 25 June 2004
Online 21 August 2004

The crystal structures of 2-amino-2-thiazoline, $C_3H_6N_2S$, and 2-amino-2-thiazolinium 2-naphthoxyacetate, $C_3H_7N_2S^+\cdot C_{12}H_9O_3^-$, are reported. The structure of 2-amino-2-thiazoline consists of two unique molecules that construct a convoluted hydrogen-bonded ribbon involving $R_2^2(8)$ graph-set association *via* both N—H···N and N—H···S interactions. The organic salt structure consists of the two molecules associated *via* an $R_2^2(8)$ graph-set dimer through N—H···O interactions, with the hydrogen-bonding network propagated *via* additional N—H···O three-centre interactions from the second 2-amine H atom.

Comment

2-Amino-2-thiazoline has been reported as a potential inducer of the reverse transformation of tumour cells, with the mechanism for anticancer action depending on strong metal–ligand binding *via* the N atoms (Brugarolas & Gosálvez, 1982). Alternatively, the placement of the N atoms in this molecule also makes it suitable for association with carboxylic acids, and four subsequent crystal structures have been reported (Lynch *et al.*, 1998; Lynch, Cooper *et al.*, 1999; Lynch, Nicholls *et al.*, 1999). Such structures are part of a broader study of complexes of carboxylic acids with 2-aminothiazole derivatives that has thus far resulted in the characterization of 19 published crystal structures, with three others published recently (Lynch *et al.*, 2004). Although the structure of 2-aminothiazole was published by Caranoni & Reboul (1982), the structure of 2-amino-2-thiazoline has not been reported; the structure of this compound, (I), is reported here. 2-Naphthoxyacetic acid is used as a plant hormone to promote growth of roots on clippings and to prevent fruit from falling prematurely, although stunted growth results if it is used in excess (The Merck Index, 2001). 2-Naphthoxyacetic acid is related in structure to phenoxyacetic acid, whose chloro derivatives have been used extensively by the author for complexing with carboxylic acids (Lynch, Cooper *et al.*, 1999) and should thus have comparable structural properties. Furthermore, the Cambridge Structural Database (Allen, 2002) contains only four previously reported crystal structures containing the compound, of which two are the parent structure (Howie *et al.*, 2001), thus more structures containing 2-naphthoxyacetic acid are required. For these reasons, the structure of the 1:1 organic salt of (I) with 2-naphthoxyacetic acid is also reported here, *viz*. (II).



Compound (I) packs with two unique thiazoline molecules associated in a hydrogen-bonded $R_2^2(8)$ graph-set dimer (Etter, 1990) *via* N—H···N interactions (Fig. 1). The hydrogen-bonding network is then extended by N—H···S interactions, resulting in further $R_2^2(8)$ graph-set arrangements. Hydrogen-bonding associations for this compound are listed in Table 1. Together, these interactions create a convoluted

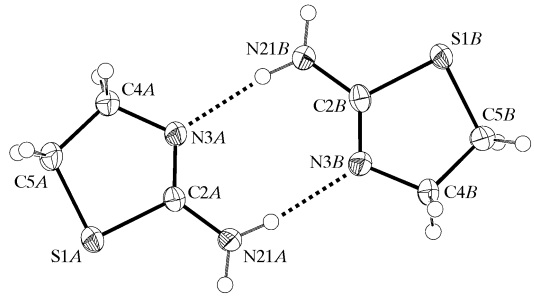


Figure 1
A view of the asymmetric unit and atom-numbering scheme of (I). Displacement ellipsoids are drawn at the 50% probability level. Broken lines indicate intramolecular hydrogen bonds.

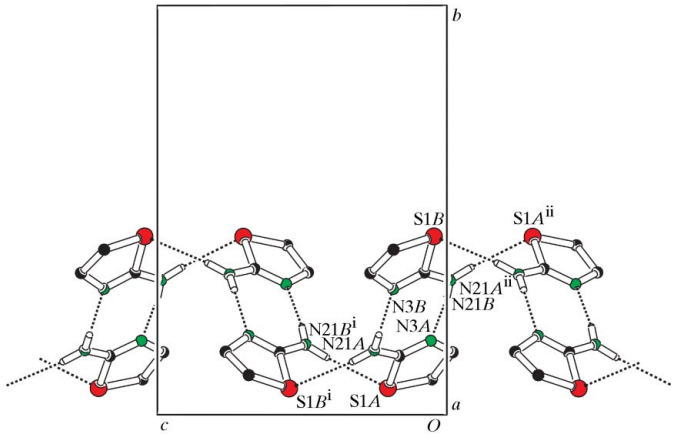


Figure 2
A packing diagram for (I). [Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.]

 DOI: 10.1107/S0108270104015604

hydrogen-bonded ribbon that runs in the direction of the *ac* axis diagonal (Fig. 2). The incorporation of the S atoms into the hydrogen-bonding network is not observed in the structure of 2-aminothiazole but is seen in the structure of a related 2-aminothiazole derivative, *viz*. 2-amino-4-(4-bisphenyl)-1,3-thiazole (Lynch *et al.*, 2002). In (I), there is a single S···S close contact [3.520 (5) Å] between atom S1*B* and the symmetry-equivalent atom at $(2-x, 1-y, -z)$.

The structure of (II) comprises the organic salt of a non-planar acetate molecule and a protonated thiazoline molecule arranged in a packing mode commonly observed for these types of molecules. In contrast to its planar parent structure, the acetate chain of the naphthoxyacetate molecule in (II) adopts an anticlinical (or hooked) arrangement, as classified for phenoxyacetic acids (Smith & Kennard, 1979) and defined by the C2*B*—O11*B*—C12*B*—C13*B* torsion angle [92.8 (2)°; Fig. 3]. Packing with the thiazoline molecule has an associated effect on (2,4,5-trichlorophenoxy)acetic acid, whose structure is planar in the parent compound but hooked in the salt complex (Lynch, Cooper *et al.*, 1999). The components of (II), like those of the vast majority of adducts/organic salts comprising a 2-amino-heterocycle and a carboxylic acid molecule, associate *via* an unsymmetrical $R_2^2(8)$ graph-set dimer between the N=C—NH_2 site and the carboxylate group (Fig. 4). In general, this association is unsymmetrical in that the N3*A*···O14*B* distance, or equivalent, is (apart from a very few cases) shorter than the N21*A*···O15*B* distance, although the values listed in Table 2 indicate that the structure of (I) is one of the very few exceptions where the opposite has occurred. Another common feature of this association is the inconsistency of the C2*A*—N21*A* [1.302 (2) Å] and C2*A*—N3*A* [1.324 (2) Å] bond lengths, as previously highlighted (Lynch *et al.*, 2000). The propagation of the hydrogen-bonding network *via* the N21*A*—H22*A*···O14*B*$(x, y-1, z)$ interaction has also been observed previously for these types of systems

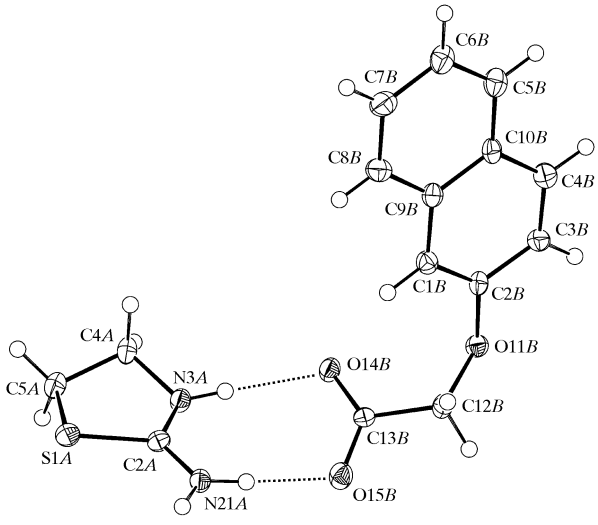


Figure 3
A view of the asymmetric unit and atom-numbering scheme of (II). Displacement ellipsoids are drawn at the 50% probability level. Broken lines indicate intramolecular hydrogen bonds.

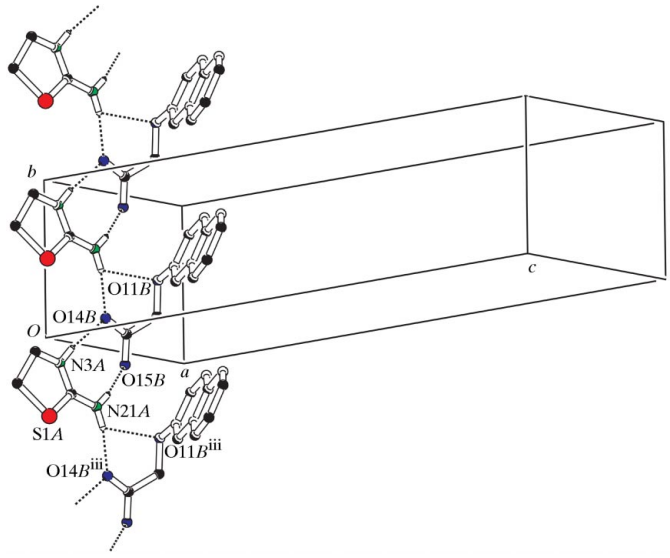


Figure 4
A packing diagram for (II). [Symmetry code: (iii) $x, y-1, z$.]

(Lynch, Nicholls *et al.*, 1999), although the additional interaction with atom O11*B* is not common amongst complexes of 2-aminothiazole derivatives and phenoxyacetic acids (Lynch, Cooper *et al.*, 1999).

The structure of (II) is actually the eighth known complex of a carboxylic acid with (I), with three others currently unpublished (Lynch *et al.*, 2004). Elucidation of the structure of (I) is important because, as highlighted above, when collecting data on the inconsistencies in the bond distances across the N=C—NH_2 site for any type of complexed 2-amino-heterocyclic compound, it is important to compare bond distances against those of the parent structure. For example, compare the C2*A*—N21*A* and C2*A*—N3*A* distances listed above with those for (I), *viz*. 1.348 (5)/1.267 (5) and 1.351 (5)/1.276 (5) Å for molecules *A* and *B*, respectively. The mean respective distances for the seven complex structures are 1.305 (5) and 1.314 (5) Å. Also of interest is the N3—C2—N21 (or equivalent) angle, which decreases upon association with a carboxylic acid. Compare, for (I), values of 124.8 (3) and 125.8 (3)° with that of 124.53 (17)° in (II) [the mean angle over the eight structures is 124.0 (5)°]. In one or two instances where N1*A* is a quaternary N atom, it might be suitable to suggest that the N1*A*—C2*A* double bond has moved to C2*A*—N21*A*, but this simple 'pushing of the double bond around' does not fit a significant portion of the available data. It is the intention of the author to publish such findings in a dedicated paper, but not without each of the parent structures and a supportive list of different complexes, which the structures in this paper add to.

Experimental

Crystals of (I) were grown from an ethanol solution. For (II), equimolar amounts of (I) and 2-naphthoxyacetic acid were refluxed in ethanol for 20 min. Crystals of (II) were grown by slow evaporation of the reaction solution.

Compound (I)

Crystal data

$C_3H_6N_2S$	D_x = 1.481 Mg m^{-3}
M_r = 102.17	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 8580 reflections
a = 5.8980 (5) Å	θ = 2.9–27.5°
b = 14.8324 (12) Å	μ = 0.53 mm^{-1}
c = 10.7092 (8) Å	T = 120 (2) K
β = 101.974 (4)°	Prism, yellow
V = 916.47 (13) Å^3	0.20 × 0.20 × 0.10 mm
Z = 8	

Data collection

Nonius KappaCCD area-detector diffractometer	2101 independent reflections
φ and ω scans	1149 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	R_{int} = 0.112
T_{min} = 0.826, T_{max} = 0.948	θ_{max} = 27.5°
10 396 measured reflections	$h = -7 \rightarrow 7$
	$k = -19 \rightarrow 19$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.061	$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.160	$(\Delta/\sigma)_{max} < 0.001$
S = 1.02	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
2101 reflections	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
109 parameters	

Table 1
Hydrogen-bonding geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
N21A—H21A···N3B	0.88	2.09	2.950 (5)	164
N21A—H22A···S1B^{i}	0.88	2.75	3.575 (3)	156
N21B—H21B···N3A	0.88	2.04	2.916 (5)	171
N21B—H22B···S1A^{ii}	0.88	2.70	3.526 (3)	156

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

Compound (II)

Crystal data

$C_3H_7N_2S^+\cdot C_{12}H_9O_3^-$	D_x = 1.441 Mg m^{-3}
M_r = 304.36	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4067 reflections
a = 8.3669 (2) Å	θ = 2.9–27.5°
b = 6.3707 (1) Å	μ = 0.24 mm^{-1}
c = 26.3457 (6) Å	T = 120 (2) K
β = 92.1992 (9)°	Plate, colourless
V = 1403.27 (5) Å^3	0.32 × 0.10 × 0.04 mm
Z = 4	

Data collection

Nonius KappaCCD area-detector diffractometer	3183 independent reflections
φ and ω scans	2546 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	R_{int} = 0.091
T_{min} = 0.710, T_{max} = 0.990	θ_{max} = 27.4°
15 534 measured reflections	$h = -10 \rightarrow 10$
	$k = -7 \rightarrow 8$
	$l = -34 \rightarrow 34$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.8055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.121	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
3183 reflections	
194 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 2
Hydrogen-bonding geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N21A—H21A···O15B	0.88	1.88	2.754 (2)	171
N21A—H22A···O14B^{iii}	0.88	1.93	2.787 (2)	166
N21A—H22A···O11B^{iii}	0.88	2.56	2.965 (2)	109
N3A—H3A···O14B	0.87 (2)	2.01 (2)	2.871 (2)	170 (2)

Symmetry code: (iii) $x, y-1, z$.

All H atoms, except for the H atom on the N^+ ion in (II), were included in the refinement at calculated positions in the riding-model approximation, with N—H distances of 0.88 Å, and C—H distances of 0.95 (aromatic H atoms) and 0.99 Å (CH_2 H atoms). The U_{iso}(H) values were set at 1.25U_{eq} of the carrier atom. The H atom on the N^+ ion was located in a difference synthesis and both the positional and displacement parameters were refined. A high R_{int} value for (I) was the result of weak high-angle data.

For both compounds, data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*, *SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLUTON*94 (Spek, 1994) and *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

The authors thank the EPSRC National Crystallography Service (Southampton, England).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1737). Services for accessing these data are described at the back of the journal.

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supporting information

Acta Cryst. (2004). C**60**, o677–o679 [doi:10.1107/S0108270104015604]

2-Amino-2-thiazoline and its 1:1 organic salt with 2-naphthoxyacetic acid

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Computing details

For both compounds, data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*, *SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLUTON94* (Spek, 1994) and *PLATON97* (Spek, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

(I) 2-Amino-2-thiazoline

Crystal data

$C_3H_6N_2S$
$M_r = 102.17$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.8980\ (5)$ Å
$b = 14.8324\ (12)$ Å
$c = 10.7092\ (8)$ Å
$\beta = 101.974\ (4)°$
$V = 916.47\ (13)$ Å^3
$Z = 8$
$F(000) = 432$
$D_x = 1.481$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8580 reflections
$\theta = 2.9–27.5°$
$\mu = 0.53$ mm^{-1}
$T = 120$ K
Prism, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.826$, $T_{max} = 0.948$
10396 measured reflections
2101 independent reflections
1149 reflections with $I > 2\sigma(I)$
$R_{int} = 0.112$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -7\rightarrow7$
$k = -19\rightarrow19$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.160$
$S = 1.02$
2101 reflections
109 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

$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	−0.02730 (17)	0.06496 (7)	0.20321 (9)	0.0269 (3)
C2A	0.1754 (6)	0.1438 (2)	0.1644 (4)	0.0219 (8)
N21A	0.3725 (6)	0.1576 (2)	0.2517 (3)	0.0295 (8)
H21A	0.4788	0.1946	0.2348	0.037*
H22A	0.3949	0.1296	0.3257	0.037*
N3A	0.1270 (5)	0.1808 (2)	0.0554 (3)	0.0263 (8)
C4A	−0.0968 (7)	0.1525 (3)	−0.0198 (4)	0.0271 (9)
H41A	−0.1959	0.2062	−0.0434	0.034*
H42A	−0.0732	0.1238	−0.0996	0.034*
C5A	−0.2206 (7)	0.0864 (3)	0.0520 (4)	0.0309 (10)
H51A	−0.3679	0.1127	0.0655	0.039*
H52A	−0.2554	0.0297	0.0031	0.039*
S1B	0.77862 (17)	0.43581 (7)	0.04456 (9)	0.0246 (3)
C2B	0.5938 (6)	0.3476 (2)	0.0781 (4)	0.0228 (8)
N21B	0.4037 (5)	0.3289 (2)	−0.0124 (3)	0.0289 (8)
H21B	0.3088	0.2856	0.0002	0.036*
H22B	0.3747	0.3599	−0.0840	0.036*
N3B	0.6540 (5)	0.3076 (2)	0.1853 (3)	0.0260 (8)
C4B	0.8603 (6)	0.3461 (3)	0.2639 (4)	0.0270 (9)
H41B	0.9621	0.2972	0.3062	0.034*
H42B	0.8163	0.3841	0.3311	0.034*
C5B	0.9918 (7)	0.4032 (3)	0.1840 (4)	0.0306 (10)
H51B	1.1178	0.3678	0.1592	0.038*
H52B	1.0599	0.4571	0.2322	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0240 (6)	0.0311 (6)	0.0266 (6)	−0.0060 (4)	0.0077 (4)	0.0016 (4)
C2A	0.020 (2)	0.0226 (19)	0.024 (2)	−0.0013 (15)	0.0066 (17)	−0.0004 (16)
N21A	0.0234 (18)	0.0421 (19)	0.0225 (18)	−0.0074 (16)	0.0039 (14)	0.0078 (15)
N3A	0.0228 (18)	0.0346 (18)	0.0217 (18)	−0.0079 (14)	0.0049 (14)	0.0011 (15)
C4A	0.024 (2)	0.031 (2)	0.026 (2)	−0.0034 (17)	0.0041 (17)	0.0014 (18)
C5A	0.020 (2)	0.043 (3)	0.030 (2)	−0.0073 (18)	0.0067 (19)	0.0003 (19)
S1B	0.0229 (6)	0.0269 (5)	0.0253 (6)	0.0042 (4)	0.0079 (4)	−0.0014 (4)
C2B	0.019 (2)	0.0241 (19)	0.028 (2)	0.0016 (16)	0.0109 (17)	0.0035 (17)
N21B	0.0272 (19)	0.0346 (18)	0.0232 (18)	0.0097 (14)	0.0014 (15)	−0.0031 (15)
N3B	0.0213 (18)	0.0331 (18)	0.0229 (18)	0.0037 (14)	0.0034 (15)	−0.0018 (14)
C4B	0.020 (2)	0.032 (2)	0.028 (2)	0.0064 (17)	0.0043 (17)	−0.0013 (18)
C5B	0.024 (2)	0.040 (2)	0.027 (2)	0.0027 (18)	0.0037 (18)	−0.0074 (19)

Geometric parameters (Å, º)

S1A—C2A	1.782 (4)	S1B—C2B	1.786 (4)
S1A—C5A	1.805 (4)	S1B—C5B	1.807 (4)
C2A—N3A	1.267 (5)	C2B—N3B	1.276 (5)
C2A—N21A	1.348 (5)	C2B—N21B	1.351 (5)
N21A—H21A	0.88	N21B—H21B	0.88
N21A—H22A	0.88	N21B—H22B	0.88
N3A—C4A	1.458 (5)	N3B—C4B	1.446 (5)
C4A—C5A	1.522 (5)	C4B—C5B	1.525 (5)
C4A—H41A	0.99	C4B—H41B	0.99
C4A—H42A	0.99	C4B—H42B	0.99
C5A—H51A	0.99	C5B—H51B	0.99
C5A—H52A	0.99	C5B—H52B	0.99
C2A—S1A—C5A	90.24 (18)	C2B—S1B—C5B	89.24 (18)
N3A—C2A—N21A	124.8 (3)	N3B—C2B—N21B	125.8 (3)
N3A—C2A—S1A	117.7 (3)	N3B—C2B—S1B	117.1 (3)
N21A—C2A—S1A	117.5 (3)	N21B—C2B—S1B	117.2 (3)
C2A—N21A—H21A	120.0	C2B—N21B—H21B	120.0
C2A—N21A—H22A	120.0	C2B—N21B—H22B	120.0
H21A—N21A—H22A	120.0	H21B—N21B—H22B	120.0
C2A—N3A—C4A	112.9 (3)	C2B—N3B—C4B	112.5 (3)
N3A—C4A—C5A	112.4 (3)	N3B—C4B—C5B	110.9 (3)
N3A—C4A—H41A	109.1	N3B—C4B—H41B	109.5
C5A—C4A—H41A	109.1	C5B—C4B—H41B	109.5
N3A—C4A—H42A	109.1	N3B—C4B—H42B	109.5
C5A—C4A—H42A	109.1	C5B—C4B—H42B	109.5
H41A—C4A—H42A	107.9	H41B—C4B—H42B	108.0
C4A—C5A—S1A	106.7 (3)	C4B—C5B—S1B	105.3 (3)
C4A—C5A—H51A	110.4	C4B—C5B—H51B	110.7
S1A—C5A—H51A	110.4	S1B—C5B—H51B	110.7
C4A—C5A—H52A	110.4	C4B—C5B—H52B	110.7
S1A—C5A—H52A	110.4	S1B—C5B—H52B	110.7
H51A—C5A—H52A	108.6	H51B—C5B—H52B	108.8
C5A—S1A—C2A—N3A	−2.7 (3)	C5B—S1B—C2B—N3B	9.6 (3)
C5A—S1A—C2A—N21A	179.3 (3)	C5B—S1B—C2B—N21B	−170.0 (3)
N21A—C2A—N3A—C4A	179.2 (4)	N21B—C2B—N3B—C4B	−177.2 (4)
S1A—C2A—N3A—C4A	1.4 (4)	S1B—C2B—N3B—C4B	3.3 (4)
C2A—N3A—C4A—C5A	1.0 (5)	C2B—N3B—C4B—C5B	−17.9 (5)
N3A—C4A—C5A—S1A	−2.8 (4)	N3B—C4B—C5B—S1B	23.4 (4)
C2A—S1A—C5A—C4A	2.9 (3)	C2B—S1B—C5B—C4B	−17.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21*A*—H21*A*···N3*B*	0.88	2.09	2.950 (5)	164

N21*A*—H22*A*···S1*B*^{i}	0.88	2.75	3.575 (3)	156
N21*B*—H21*B*···N3*A*	0.88	2.04	2.916 (5)	171
N21*B*—H22*B*···S1*A*^{ii}	0.88	2.70	3.526 (3)	156

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

(II) 2-Amino-2-thiazolium 2-naphthoxyacetate

Crystal data

$C_3H_7N_2S^+\cdot C_{12}H_9O_3^-$
$M_r = 304.36$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.3669$ (2) Å
$b = 6.3707$ (1) Å
$c = 26.3457$ (6) Å
$\beta = 92.1992$ (9)°
$V = 1403.27$ (5) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.441$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4067 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.24$ mm^{-1}
$T = 120$ K
Plate, colourless
0.32 × 0.10 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.710$, $T_{max} = 0.990$
15534 measured reflections
3183 independent reflections
2546 reflections with $I > 2\sigma(I)$
$R_{int} = 0.091$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.1°$
$h = -10\rightarrow10$
$k = -7\rightarrow8$
$l = -34\rightarrow34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.121$
$S = 1.02$
3183 reflections
194 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.8055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	−0.19892 (6)	−0.56175 (8)	0.06199 (19)	0.02416 (16)
C2A	−0.0340 (2)	−0.3943 (3)	0.06063 (7)	0.0173 (4)
N21A	0.11091 (18)	−0.4589 (3)	0.07144 (6)	0.0198 (4)
H21A	0.1913	−0.3698	0.0712	0.025*
H22A	0.1285	−0.5917	0.0790	0.025*
N3A	−0.07266 (19)	−0.1983 (3)	0.04883 (6)	0.0188 (3)
H3A	−0.005 (3)	−0.097 (4)	0.0543 (8)	0.023 (6)*

C4A	−0.2446 (2)	−0.1539 (3)	0.04747 (7)	0.0218 (4)
H41A	−0.2715	−0.0441	0.0220	0.027*
H42A	−0.2781	−0.1050	0.0811	0.027*
C5A	−0.3271 (2)	−0.3597 (3)	0.03314 (8)	0.0228 (4)
H51A	−0.3356	−0.3768	−0.0042	0.029*
H52A	−0.4356	−0.3655	0.0468	0.029*
C1B	0.2758 (2)	0.3025 (3)	0.19187 (7)	0.0194 (4)
H1B	0.2442	0.1666	0.1805	0.024*
C2B	0.3684 (2)	0.4257 (3)	0.16244 (7)	0.0177 (4)
C3B	0.4200 (2)	0.6263 (3)	0.17909 (7)	0.0206 (4)
H3B	0.4866	0.7082	0.1584	0.026*
C4B	0.3745 (2)	0.7029 (3)	0.22471 (7)	0.0215 (4)
H4B	0.4095	0.8381	0.2355	0.027*
C5B	0.2202 (2)	0.6600 (3)	0.30307 (7)	0.0241 (4)
H5B	0.2536	0.7948	0.3147	0.030*
C6B	0.1201 (2)	0.5432 (3)	0.33145 (7)	0.0258 (5)
H6B	0.0818	0.5985	0.3622	0.032*
C7B	0.0730 (2)	0.3398 (3)	0.31514 (7)	0.0274 (5)
H7B	0.0042	0.2588	0.3353	0.034*
C8B	0.1256 (2)	0.2589 (3)	0.27081 (7)	0.0234 (4)
H8B	0.0945	0.1213	0.2607	0.029*
C9B	0.2266 (2)	0.3787 (3)	0.23966 (7)	0.0201 (4)
C10B	0.2751 (2)	0.5823 (3)	0.25623 (7)	0.0199 (4)
O11B	0.41670 (15)	0.3708 (2)	0.11458 (5)	0.0190 (3)
C12B	0.4426 (2)	0.1542 (3)	0.10439 (8)	0.0209 (4)
H12B	0.4765	0.0852	0.1367	0.026*
H13B	0.5329	0.1433	0.0813	0.026*
C13B	0.3018 (2)	0.0295 (3)	0.08086 (7)	0.0177 (4)
O14B	0.16423 (15)	0.1099 (2)	0.07750 (5)	0.0199 (3)
O15B	0.34007 (16)	−0.15009 (2)	0.06632 (5)	0.0239 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0187 (3)	0.0224 (3)	0.0313 (3)	0.00326 (18)	−0.00004 (19)	−0.0037 (2)
C2A	0.0178 (9)	0.0186 (10)	0.0157 (8)	0.0009 (7)	0.0024 (7)	0.0017 (7)
N21A	0.0162 (8)	0.0173 (9)	0.0259 (8)	−0.0007 (6)	−0.0005 (6)	−0.0011 (6)
N3A	0.0152 (8)	0.0182 (9)	0.0229 (8)	−0.0009 (7)	−0.0005 (6)	0.0009 (7)
C4A	0.0170 (9)	0.0251 (11)	0.0231 (10)	−0.0058 (8)	−0.0003 (7)	0.0008 (8)
C5A	0.0165 (9)	0.0267 (11)	0.0253 (10)	−0.0024 (8)	0.0003 (7)	0.0004 (8)
C1B	0.0177 (9)	0.0178 (10)	0.0225 (10)	0.0003 (7)	−0.0019 (7)	−0.0003 (7)
C2B	0.0149 (9)	0.0197 (10)	0.0185 (9)	−0.0031 (7)	−0.0014 (7)	0.0001 (7)
C3B	0.0183 (9)	0.0208 (10)	0.0226 (10)	0.0012 (7)	−0.0001 (7)	−0.0036 (8)
C4B	0.0213 (9)	0.0187 (10)	0.0241 (10)	0.0010 (8)	−0.0026 (7)	0.0015 (8)
C5B	0.0213 (10)	0.0300 (12)	0.0207 (10)	−0.0030 (8)	−0.0047 (8)	0.0022 (8)
C6B	0.0224 (10)	0.0369 (13)	0.0179 (10)	−0.0050 (8)	−0.0019 (8)	0.0009 (8)
C7B	0.0214 (10)	0.0394 (13)	0.0213 (10)	0.0020 (9)	−0.0005 (8)	−0.0064 (9)
C8B	0.0218 (10)	0.0263 (11)	0.0218 (10)	0.0042 (8)	−0.0034 (7)	−0.0044 (8)

C9B	0.0150 (9)	0.0241 (10)	0.0208 (9)	−0.0002 (7)	−0.0040 (7)	−0.0028 (8)
C10B	0.0163 (9)	0.0216 (10)	0.0214 (9)	−0.0031 (7)	−0.0039 (7)	−0.0008 (8)
O11B	0.0194 (7)	0.0172 (7)	0.0206 (7)	−0.0004 (5)	0.0032 (5)	0.0014 (5)
C12B	0.0163 (9)	0.0188 (10)	0.0277 (10)	−0.0017 (7)	0.0019 (7)	0.0023 (8)
C13B	0.0175 (9)	0.0190 (10)	0.0167 (9)	−0.0012 (7)	0.0042 (7)	−0.0029 (7)
O14B	0.0152 (6)	0.0200 (7)	0.0245 (7)	−0.0006 (5)	0.0001 (5)	0.0008 (5)
O15B	0.0221 (7)	0.0189 (8)	0.0309 (8)	−0.0016 (5)	0.0018 (6)	0.0038 (6)

Geometric parameters (Å, º)

S1A—C2A	1.7455 (19)	C3B—H3B	0.95
S1A—C5A	1.823 (2)	C4B—C10B	1.423 (3)
C2A—N21A	1.302 (2)	C4B—H4B	0.95
C2A—N3A	1.324 (2)	C5B—C6B	1.365 (3)
N21A—H21A	0.88	C5B—C10B	1.422 (3)
N21A—H22A	0.88	C5B—H5B	0.95
N3A—C4A	1.465 (2)	C6B—C7B	1.417 (3)
N3A—H3A	0.87 (2)	C6B—H6B	0.95
C4A—C5A	1.523 (3)	C7B—C8B	1.365 (3)
C4A—H41A	0.99	C7B—H7B	0.95
C4A—H42A	0.99	C8B—C9B	1.422 (3)
C5A—H51A	0.99	C8B—H8B	0.95
C5A—H52A	0.99	C9B—C10B	1.423 (3)
C1B—C2B	1.365 (3)	O11B—C12B	1.424 (2)
C1B—C9B	1.425 (3)	C12B—C13B	1.532 (3)
C1B—H1B	0.95	C12B—H12B	0.99
C2B—O11B	1.384 (2)	C12B—H13B	0.99
C2B—C3B	1.413 (3)	C13B—O15B	1.252 (2)
C3B—C4B	1.365 (3)	C13B—O14B	1.260 (2)
C2A—S1A—C5A	90.73 (9)	C3B—C4B—C10B	120.65 (18)
N21A—C2A—N3A	124.53 (17)	C3B—C4B—H4B	119.7
N21A—C2A—S1A	122.19 (15)	C10B—C4B—H4B	119.7
N3A—C2A—S1A	113.27 (14)	C6B—C5B—C10B	120.7 (2)
C2A—N21A—H21A	120.0	C6B—C5B—H5B	119.6
C2A—N21A—H22A	120.0	C10B—C5B—H5B	119.6
H21A—N21A—H22A	120.0	C5B—C6B—C7B	120.13 (19)
C2A—N3A—C4A	114.77 (16)	C5B—C6B—H6B	119.9
C2A—N3A—H3A	120.5 (15)	C7B—C6B—H6B	119.9
C4A—N3A—H3A	120.0 (15)	C8B—C7B—C6B	120.66 (19)
N3A—C4A—C5A	105.96 (15)	C8B—C7B—H7B	119.7
N3A—C4A—H41A	110.5	C6B—C7B—H7B	119.7
C5A—C4A—H41A	110.5	C7B—C8B—C9B	120.64 (19)
N3A—C4A—H42A	110.5	C7B—C8B—H8B	119.7
C5A—C4A—H42A	110.5	C9B—C8B—H8B	119.7
H41A—C4A—H42A	108.7	C8B—C9B—C10B	118.74 (18)
C4A—C5A—S1A	104.53 (12)	C8B—C9B—C1B	121.69 (18)
C4A—C5A—H51A	110.8	C10B—C9B—C1B	119.54 (17)

S1A—C5A—H51A	110.8	C5B—C10B—C9B	119.08 (18)
C4A—C5A—H52A	110.8	C5B—C10B—C4B	122.26 (18)
S1A—C5A—H52A	110.8	C9B—C10B—C4B	118.65 (17)
H51A—C5A—H52A	108.9	C2B—O11B—C12B	117.93 (14)
C2B—C1B—C9B	119.71 (18)	O11B—C12B—C13B	117.32 (15)
C2B—C1B—H1B	120.1	O11B—C12B—H12B	108.0
C9B—C1B—H1B	120.1	C13B—C12B—H12B	108.0
C1B—C2B—O11B	124.35 (17)	O11B—C12B—H13B	108.0
C1B—C2B—C3B	121.10 (17)	C13B—C12B—H13B	108.0
O11B—C2B—C3B	114.53 (16)	H12B—C12B—H13B	107.2
C4B—C3B—C2B	120.32 (18)	O15B—C13B—O14B	126.43 (17)
C4B—C3B—H3B	119.8	O15B—C13B—C12B	113.33 (15)
C2B—C3B—H3B	119.8	O14B—C13B—C12B	120.24 (16)

C5A—S1A—C2A—N21A	−171.09 (16)	C7B—C8B—C9B—C1B	−176.41 (17)
C5A—S1A—C2A—N3A	10.36 (15)	C2B—C1B—C9B—C8B	177.84 (17)
N21A—C2A—N3A—C4A	−169.07 (17)	C2B—C1B—C9B—C10B	−0.2 (3)
S1A—C2A—N3A—C4A	9.4 (2)	C6B—C5B—C10B—C9B	−1.2 (3)
C2A—N3A—C4A—C5A	−28.8 (2)	C6B—C5B—C10B—C4B	177.48 (17)
N3A—C4A—C5A—S1A	33.38 (17)	C8B—C9B—C10B—C5B	−0.5 (3)
C2A—S1A—C5A—C4A	−25.22 (14)	C1B—C9B—C10B—C5B	177.55 (16)
C9B—C1B—C2B—O11B	−177.00 (16)	C8B—C9B—C10B—C4B	−179.21 (17)
C9B—C1B—C2B—C3B	1.5 (3)	C1B—C9B—C10B—C4B	−1.1 (3)
C1B—C2B—C3B—C4B	−1.5 (3)	C3B—C4B—C10B—C5B	−177.51 (17)
O11B—C2B—C3B—C4B	177.12 (16)	C3B—C4B—C10B—C9B	1.1 (3)
C2B—C3B—C4B—C10B	0.2 (3)	C1B—C2B—O11B—C12B	−31.7 (2)
C10B—C5B—C6B—C7B	1.8 (3)	C3B—C2B—O11B—C12B	149.67 (16)
C5B—C6B—C7B—C8B	−0.6 (3)	C2B—O11B—C12B—C13B	92.8 (2)
C6B—C7B—C8B—C9B	−1.1 (3)	O11B—C12B—C13B—O15B	170.22 (16)
C7B—C8B—C9B—C10B	1.6 (3)	O11B—C12B—C13B—O14B	−9.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21*A*—H21*A*···O15*B*	0.88	1.88	2.754 (2)	171
N21*A*—H22*A*···O14*B*^{i}	0.88	1.93	2.787 (2)	166
N21*A*—H22*A*···O11*B*^{i}	0.88	2.56	2.965 (2)	109
N3*A*—H3*A*···O14*B*	0.87 (2)	2.01 (2)	2.871 (2)	170 (2)

Symmetry code: (i) *x*, *y*−1, *z*.