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Aberdeen, Scotland**Keywords:** crystal structure; isothiazoyl; oxathiazolone; conjugation; nitrile sulfide; π -stacking.**CCDC references:** 1580338; 1580337**Supporting information:** this article has
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The crystal structures of two isomers of 5-(phenylisothiazolyl)-1,3,4-oxathiazol-2-one

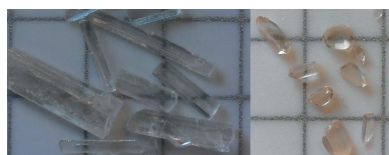
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The syntheses and crystal structures of two isomers of phenyl isothiazolyl oxathiazolone, C₁₁H₆N₂O₂S₂, are described [systematic names: 5-(3-phenylisothiazol-5-yl)-1,3,4-oxathiazol-2-one, (I), and 5-(3-phenylisothiazol-4-yl)-1,3,4-oxathiazol-2-one, (II)]. There are two almost planar (r.m.s. deviations = 0.032 and 0.063 Å) molecules of isomer (I) in the asymmetric unit, which form centrosymmetric tetramers linked by strong S···N [3.072 (2) Å] and S···O contacts [3.089 (1) Å]. The tetramers are π -stacked parallel to the *a*-axis direction. The single molecule in the asymmetric unit of isomer (II) is twisted into a non-planar conformation by steric repulsion [dihedral angles between the central isothiazolyl ring and the pendant oxathiazolone and phenyl rings are 13.27 (6) and 61.18 (7)°, respectively], which disrupts the π -conjugation between the heteroaromatic isothiazoloyl ring and the non-aromatic oxathiazolone heterocycle. In the crystal of isomer (II), the strong S···O [3.020 (1) Å] and S···C contacts [3.299 (2) Å] and the non-planar structure of the molecule lead to a form of π -stacking not observed in isomer (I) or other oxathiazolone derivatives.

1. Chemical context

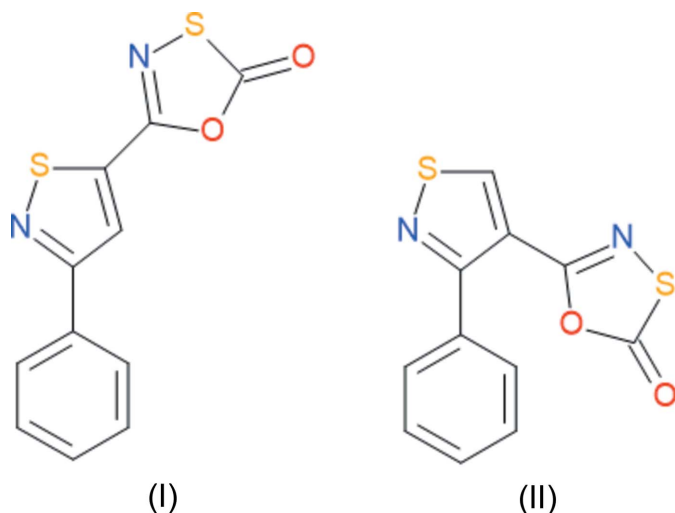
Compounds containing the isothiazolyl moiety are well known in organic and pharmacological research, with extensive reviews on the synthesis and chemistry of the ring (Abdel-Sattar & Elgazwy, 2003) and the medicinal and industrial uses of compounds containing the isothiazolyl heterocycle (Kaberdin & Potkin 2002). The solid-state structural features of isothiazole derivatives have been reviewed (Abdel-Sattar & Elgazwy, 2003). In general, the isothiazolyl ring is recognised as a heteroaromatic ring with extensive π -delocalization (incorporating the empty sulfur 3*d*-orbitals) within the ring leading to almost planar heterocycles.

Derivatives of the oxathiazolone heterocycle have been known since their first preparation fifty years ago (Muhlbauer & Weiss, 1967). The facile synthesis of the heterocycle from commercially available amides reacting with chlorocarbonyl sulfenyl chloride under a range of conditions has resulted in the publication of significant libraries of substituted oxathiazolone compounds (Senning & Rasmussen, 1973; Howe *et al.*, 1978; Lin *et al.*, 2009; Fordyce *et al.*, 2010; Russo *et al.*, 2015) leading to hundreds of known oxathiazolone derivatives. The predominant chemistry of the heterocycle has been the thermal cycloreversion to the short lived nitrile sulfide [$R-C\equiv N^{(+)}-S^{(-)}$], a propargyl allenyl 1,3-dipole, which can be



trapped by electron-deficient π bonds in reasonable yield to give families of new heterocycles (Paton, 1989), including isothiazole derivatives. As a result of the electronic properties of the short-lived nitrile sulfide intermediates, optimal conditions for cyclization require trapping reactions with electron-deficient dipolariphiles. Industrially, various derivatives of the oxathiazolone heterocycle have been reported as potential fungicides (Klaus *et al.*, 1965), pesticides (Hölzl, 2004) and as polymer additives (Crosby 1978). More recently, the medicinal properties of the oxathiazolone heterocycle have been explored as selective inhibitors for tuberculosis (Lin *et al.*, 2009), inflammatory diseases (Fan *et al.*, 2014) and as proteasome inhibitors (Russo *et al.*, 2015).

In previous structural studies on oxathiazolone compounds, the non-aromatic heterocyclic rings were found to be planar with largely localized C=N and C=O double bonds. The extent of π -delocalization within the oxathiazolone ring and to the substituent group and the effect on the structure and chemical properties have been discussed spectroscopically (Markgraf *et al.*, 2007) and structurally (Krayushkin *et al.*, 2010*a,b*). Our interest in this system was prompted by the possibility that catenated systems of isothiazolone heterocycles may have useful electronic properties as the number of π systems is increased.



2. Structural commentary

There are two independent molecules in the asymmetric unit of (I) (Fig. 1). In general, the two molecules are not significantly different with the exception of the C—S bonds in the oxathiazolone rings. In one of the molecules, the C1—S1 distance [1.762 (2) Å] is longer than the same bond in the second molecule, C12—S3 [1.746 (2) Å]. The difference may arise from the nature of the intermolecular contacts to the sulfur atoms, with a strong pair of co-planar S \cdots N contacts [3.086 (2) Å] in the first molecule but only one S \cdots N contact [3.072 (2) Å] in the second molecule (which is also twisted out of the plane of the molecule). These differences are due to the position of the independent molecules in the tetramer that will be described below. For the purposes of further structural

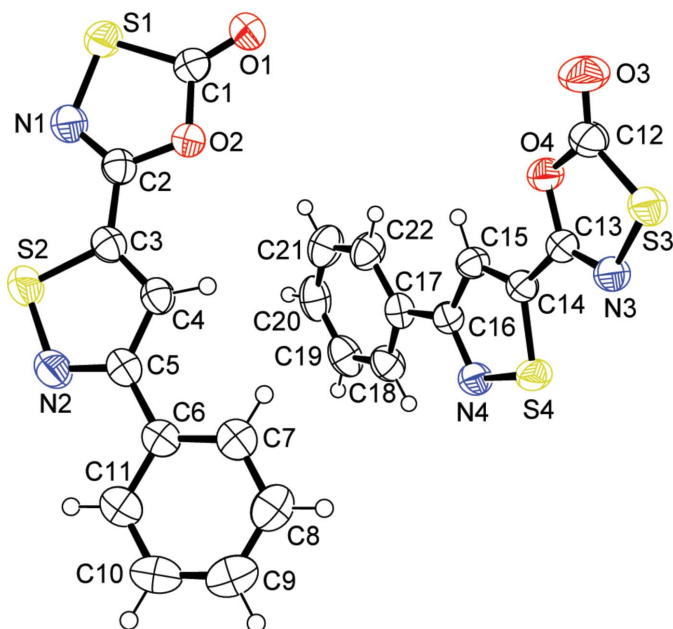


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

analysis, we will restrict our discussion to the first molecule in the asymmetric unit. The asymmetric unit of (II) is shown in Fig. 2.

The bond distances and angles within the terminal phenyl rings in compounds (I) and (II) are not significantly different from the those reported for related compounds (Schriver & Zaworotko, 1995; Krayushkin *et al.*, 2010*a,b*). The sum of the endocyclic bond angles in the isothiazole moieties for both (I) and (II) (540.0°) is consistent with planar (ideal sum = 540°) π -delocalized five-membered rings, as expected. The bond lengths of the endocyclic bonds in the isothiazolyl moieties in (I) and (II) are not significantly ($\delta > 3\sigma$) different from the

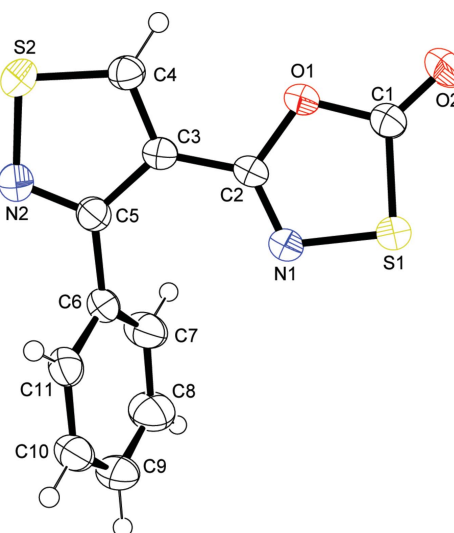


Figure 2
The molecular structure of (II), showing 50% probability displacement ellipsoids.

statistical averages from previous structural studies (Bridson *et al.*, 1994, 1995). While the C=N bonds in the isothiazolyl rings of (I) [1.327 (3) Å] and (II) [1.321 (2) Å] and the C=C bonds in (I) [1.361 (3) Å] and (II) [1.374 (2) Å] are mostly longer than the statistical averages for C=N [1.308 ± 0.016 Å] and C=C bonds [1.369 ± 0.002 Å], the differences are not sufficient to warrant an assessment of their cause or their effect on the structure.

The bond distances and angles within the oxathiazolone rings in compounds (I) and (II) are not significantly different ($\delta \geq 3\sigma$) from the statistical averages for published crystal structures (Schriver & Zaworotko, 1995; Bridson *et al.* 1994, 1995; Vorontsova *et al.*, 1996; McMillan *et al.*, 2006; Krayushkin *et al.*, 2010*a,b*; Nason *et al.*, 2017). The sum of the endocyclic bond angles in the oxathiazolone rings for both (I) and (II) (540.0°) is consistent with planar rings (ideal sum = 540°). The S–N bonds in the oxathiazolone rings of (I) [1.685 (2) Å] and (II) [1.682 (1) Å], the C_{sub}–O bonds in (I) [1.364 (2) Å] and (II) [1.375 (1) Å] and the inter-ring Csp²–Csp² bonds in (I) [1.449 (3) Å] and (II) [1.451 (2) Å] are all consistently shorter than the statistical averages for S–N [1.696 ± 0.022 Å], C_{sub}–O [1.392 ± 0.030 Å] and C=C bonds [1.461 ± 0.025 Å]. These differences, however, are not sufficient to warrant an assessment of their cause or their effect on the structure.

The three rings in the molecules of (I) are nearly co-planar, with the dihedral angles between central isothiazolyl ring and

the pendant oxathiazolone and phenyl rings being 3.06 (11) and 1.10 (12) $^\circ$, respectively, for the S1 molecule and 2.62 (9) and 6.84 (10) $^\circ$, respectively, for the S3 molecule. Overall r.m.s. deviations for the S1 and S3 molecules are 0.032 and 0.063 Å, respectively. In contrast to the near planarity of both asymmetric molecules of (I), the single molecule of (II) features significant twists between the central isothiazolyl ring and the pendant oxathiazolone and phenyl rings [dihedral angles of 13.27 (6) and 61.18 (7) $^\circ$, respectively], which may be ascribed to steric crowding. It has been argued, based on spectroscopic and structural evidence, that π -delocalization extends between the rings of oxathiazolone heterocycles attached to aromatic rings, resulting in observable differences (Schriver & Zaworotko, 1995; Krayushkin *et al.*, 2010*a,b*; Markgraf *et al.*, 2007). In this work it can be seen that nearly identical molecules result, even when torsion angles are present that would effectively disrupt any π conjugation between the rings, suggesting that the presence or absence of inter-ring π delocalization does not have a significant effect on the structure of the molecules.

3. Supramolecular features

In all previous reports on the solid-state structures of compounds containing the oxathiazolone heterocycle, the intermolecular interactions have been ignored or described as insignificant, with the exception of the recent observation of

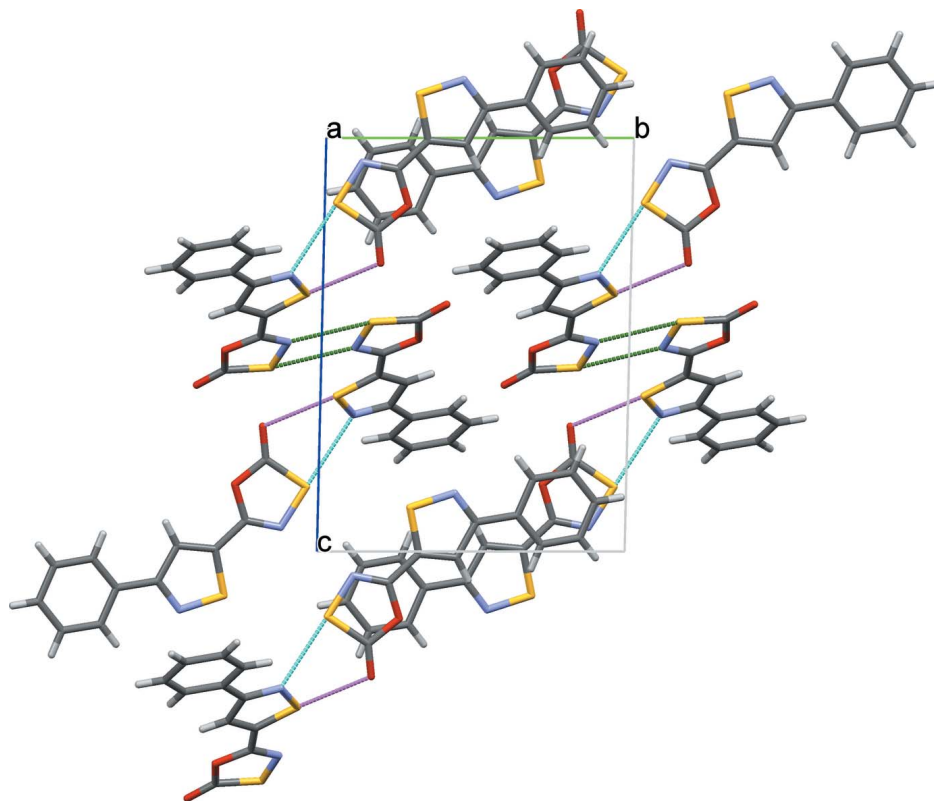


Figure 3

A packing diagram of (I) showing π – π stacking parallel to the *a*-axis direction (top). Co-planar paired head-to-head molecules [green lines, S \cdots N distance of 3.086 (2) Å] and paired molecules separated by out-of-plane contacts [blue lines, S \cdots N distance of 3.072 (2) Å], violet lines S \cdots O distance of 3.089 (1) Å].

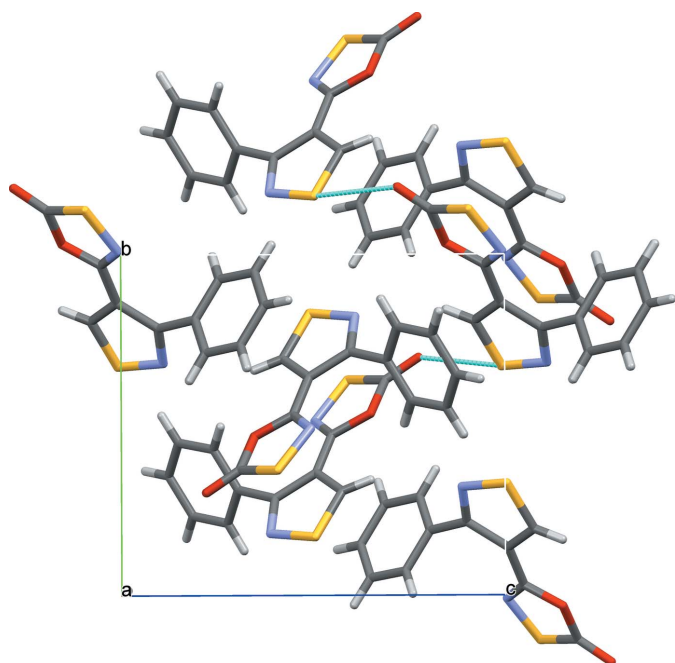


Figure 4
A packing diagram of (II) within the unit cell showing molecular pairs linked by S \cdots O contacts of 3.020 (1) Å.

π -stacking in the styryl derivative (Nason *et al.*, 2017). The strongest intermolecular contacts in (I) are S3 \cdots N3 [3.086 (2) Å], S1 \cdots N4 [3.072 (2) Å] and S4 \cdots O1 [3.089 (1) Å] (Fig. 3). The S3 \cdots N3 contacts assist in the formation of a coplanar pair of identical molecules within the asymmetric unit. The other molecules in the asymmetric unit are connected *via* the S1 \cdots N4 [3.072 (2) Å] and S4 \cdots O1 [3.089 (1) Å] contacts. Taken together, the contacts between two pairs of identical molecules in the asymmetric unit form a centrosymmetric tetramer that in turn form π -stacks parallel to the *a* axis. The intermolecular contacts between sulfur and nitrogen and oxygen have been observed in another oxathiazolone ring that also resulted in π -stacking of the planar molecules (Nason *et al.*, 2017).

The strongest intermolecular contacts in (II) are S2 \cdots O2 [3.020 (1) Å], S1 \cdots C10 [3.299 (2) Å] and C4 \cdots O2

[3.100 (2) Å] (Fig. 4). The C4 \cdots O2 contact, while significantly shorter than the sum of van der Waals radii for the atoms, is to some extent, the result of the adjacent stronger S2 \cdots O2 contact. The geometry of the molecule (II) reduces the opportunity for the formation of π -stacks but it is observed that the centroid of the terminal phenyl ring is 3.632 (2) Å above and parallel to the nearly planar portion of an adjacent molecule formed by the two heterocyclic rings (Fig. 4).

3.1. Database survey

A search of the Cambridge Structural Database (Version 5.38; Groom *et al.*, 2016) revealed that eleven crystal structures of oxathiazolone derivatives in peer-reviewed journals have been reported previously (Bridson *et al.*, 1994, 1995; Schriver & Zaworotko, 1995; Vorontsova *et al.*, 1996; McMillan *et al.*, 2006; Krayushkin *et al.*, 2010*a,b*; Nason *et al.*, 2017), which have been partially reviewed (McMillan *et al.*, 2006 and Krayushkin *et al.*, 2010*a,b*). An additional five X-ray oxathiazolone crystal structures have been reported in these (Demas, 1982; Zhu, 1997). There are also two published gas-phase electron-diffraction structures of oxathiazolone derivatives (Bak *et al.*, 1978, 1982). The structures fall into two groups: those that feature a Csp²–Csp³ bond between the heterocycle and the saturated organic substituent and those that feature a Csp²–Csp² bond between the heterocycle and the unsaturated organic substituent (either a phenyl group, heterocyclic ring or alkenyl moiety).

4. Synthesis and crystallization

Compound (I) was prepared following a local variation of literature methods (Howe *et al.*, 1978). 3-Phenylisothiazole-4-carbonamide (Zhu, 1997) (2.90 g, 14.2 mmol) was placed in 50 ml of toluene under nitrogen and chlorocarbonyl sulfonyl chloride (4.20 g, 32.0 mmol, approximately 2 \times molar excess) was added dropwise to the stirred solution. The resulting mixture was heated (363–373 K) under nitrogen for 1.5 h and allowed to evaporate to a solid residue. The evaporate was recrystallized from toluene solution to give colourless needle-shaped crystals (Fig. 5) (3.20 g, 12.2 mmol, 86%). Elemental



Figure 5
A photograph of crystals of (I) (5 \times 5 mm background grid).



Figure 6
A photograph of crystals of (II) (5 \times 5 mm background grid).

Table 1
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{11}H_6N_2O_2S_2$	$C_{11}H_6N_2O_2S_2$
M_r	262.30	262.30
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$
Temperature (K)	296	296
a, b, c (Å)	7.2739 (7), 11.2713 (11), 14.6909 (15)	9.7202 (6), 9.9723 (6), 11.2165 (7)
α, β, γ (°)	87.562 (1), 78.341 (1), 71.624 (1)	90, 90.399 (1), 90
V (Å ³)	1119.16 (19)	1087.22 (12)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	0.46	0.48
Crystal size (mm)	0.49 × 0.25 × 0.14	0.48 × 0.43 × 0.37
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2008)	Multi-scan (SADABS; Bruker, 2008)
T_{\min} , T_{\max}	0.804, 0.936	0.719, 0.837
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7476, 3862, 3485	8041, 2362, 2228
R_{int}	0.015	0.017
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.595	0.639
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.106, 1.04	0.030, 0.083, 1.02
No. of reflections	3862	2362
No. of parameters	308	155
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.33, -0.23	0.37, -0.28

Computer programs: APEX2 and SAINT (Bruker, 2008), SHELXS97 (Sheldrick, 2008) and SHELXL2014 (Sheldrick, 2015).

analysis: calculated % (Found %): 50.35 (50.2); H 2.3 (2.4); N 10.7 (10.7). IR (KBr): 3100 (*w*), 1812 (*w*), 1749 (*s*), 1735 (*s*), 1598 (*s*), 1182 (*m*), 1088 (*m*), 1014 (*w*), 959 (*s*), 884 (*ms*), 834 (*ms*), 765 (*s*), 734 (*s*), 692 (*ms*). ¹H NMR (400 MHz, CDCl₃, δ p.p.m.): 9.28 (5, 1H), 7.61 (*m*, 2H), 7.46 (*m*, 3H). ¹³C NMR (100 MHz, CDCl₃, δ p.p.m.): 172.7, 167.0, 154.1, 152.1, 134.0, 129.6, 129.0, 128.2, 123.3. MS (EI): $C_{11}H_6N_2O_2S_2$ requires (M^+), 262.301, found m/e (%), assign.): 262 (22, M^+), 218 (2, $M-\text{CO}_2$), 188 (78, $M-\text{CONS}$), 186 (100, $C_6H_5[\text{CCCNS})\text{CN}$), 160 (1 3, $M-\text{COCONS}$), 135 (26, $C_6H_5\text{CNS}$), 103 (13, $C_6H_5\text{CN}$), 77 (29, C_6H_5). UV-visible spectroscopy (hexane) λ_{max} (log ϵ): 275–230 nm (4.11), 197 nm (4.72).

Compound (II) prepared following a local variation of literature methods (Howe *et al.*, 1978). 3-Phenylisothiazole-5-carbonamide (Zhu, 1997) (4.08 g, 20.0 mmol) was placed in 50 ml of toluene under nitrogen and chlorocarbonyl sulfonyl chloride (6.50 g, 50.0 mmol, approximately 2.5 × molar excess) was added dropwise to the stirred solution. The resulting mixture was heated (363–373 K) under nitrogen for 8.5 h and allowed to evaporate to a solid residue (6.093 g). The evaporate was recrystallized from toluene solution to give colourless block-shaped crystals (Fig. 6) (4.20 g, 20.6 mmol, 83%), Elemental analysis: calculated % (found%) 50.35 (50.0); H 2.3 (2.35); N 10.7 (10.5). IR (KBr): 3097 (*w*), 3066 (*w*), 3032 (*w*), 1813 (*ms*), 1759 (*s*), 1738 (*s*), 1600 (*ms*), 1590 (*ms*), 1517 (*s*), 1496 (*s*), 1055 (*ms*), 973 (*s*), 902 (*s*), 776 (*s*), 695 (*s*) cm⁻¹. ¹H NMR (400 MHz, CDCl₃, δ p.p.m.): 7.425–7.487 (*m*, 3H), 7.906–7.937 (*m*, 2H), 7.976 (5, 1H). ¹³C

NMR (100MHz, CDCl₃, δ p.p.m.): 171.5, 167.9, 150.7, 150.5, 133.4, 129.9, 128.9, 126.8, 122.5. MS (EI): $C_{11}H_6N_2O_2S_2$ requires (M^+), 262.301, found m/e (%), assign.): 262 (52, M^+), 218 (3, $M-\text{CO}_2$), 188 (100, $M-\text{CONS}$), 160 (9, $M-\text{COCONS}$), 135 (2, $M-\text{HC}-\text{CCOCONS}$). UV-visible spectroscopy (hexane) λ_{max} (log ϵ): 283 nm (4.25), 248 nm (4.36), 203 nm (94.49).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were positioned geometrically ($C-H = 0.93$ Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

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supporting information

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The crystal structures of two isomers of 5-(phenylisothiazolyl)-1,3,4-oxathiazol-2-one

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Computing details

For both structures, data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

5-(3-Phenylisothiazol-5-yl)-1,3,4-oxathiazol-2-one (I)

Crystal data

$C_{11}H_6N_2O_2S_2$
 $M_r = 262.30$
 Triclinic, $P\bar{1}$
 $a = 7.2739$ (7) Å
 $b = 11.2713$ (11) Å
 $c = 14.6909$ (15) Å
 $\alpha = 87.562$ (1)°
 $\beta = 78.341$ (1)°
 $\gamma = 71.624$ (1)°
 $V = 1119.16$ (19) Å³

$Z = 4$
 $F(000) = 536$
 $D_x = 1.557$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 5699 reflections
 $\theta = 2.4$ – 28.6 °
 $\mu = 0.46$ mm⁻¹
 $T = 296$ K
 Needle, colourless
 $0.49 \times 0.25 \times 0.14$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2008)
 $T_{\min} = 0.804$, $T_{\max} = 0.936$
 7476 measured reflections

3862 independent reflections
 3485 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\text{max}} = 25.0$ °, $\theta_{\text{min}} = 1.9$ °
 $h = -5 \rightarrow 8$
 $k = -13 \rightarrow 13$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.106$
 $S = 1.04$
 3862 reflections
 308 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.2729P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³

$$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL2014
(Sheldrick, 2015),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.031 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.85294 (8)	0.03895 (4)	0.15683 (4)	0.05223 (17)
O1	0.8238 (2)	0.18576 (13)	0.30252 (9)	0.0593 (4)
N1	0.8263 (3)	0.12000 (15)	0.05875 (12)	0.0510 (4)
C1	0.8229 (3)	0.17293 (17)	0.22295 (13)	0.0446 (4)
S2	0.77918 (10)	0.29901 (5)	-0.10629 (4)	0.05823 (18)
O2	0.7971 (2)	0.27252 (11)	0.16249 (8)	0.0443 (3)
N2	0.7537 (3)	0.44255 (17)	-0.14107 (11)	0.0541 (4)
C2	0.8016 (3)	0.23440 (17)	0.07498 (12)	0.0415 (4)
S3	0.59888 (8)	0.83750 (5)	0.55508 (4)	0.05152 (17)
O3	0.6679 (3)	0.59670 (16)	0.59752 (14)	0.0797 (5)
N3	0.4193 (2)	0.89051 (14)	0.49359 (11)	0.0454 (4)
C3	0.7806 (3)	0.33109 (18)	0.00604 (12)	0.0415 (4)
S4	0.09624 (8)	0.94818 (4)	0.37616 (4)	0.05119 (17)
O4	0.4345 (2)	0.68529 (12)	0.51338 (9)	0.0472 (3)
N4	-0.0487 (3)	0.89146 (15)	0.33086 (11)	0.0479 (4)
C4	0.7628 (3)	0.45417 (17)	0.01441 (12)	0.0419 (4)
H4B	0.7607	0.4931	0.0693	0.050*
C5	0.7479 (3)	0.51552 (18)	-0.07130 (12)	0.0410 (4)
C6	0.7266 (3)	0.64887 (18)	-0.08776 (13)	0.0425 (4)
C7	0.7228 (3)	0.72818 (19)	-0.01704 (14)	0.0503 (5)
H7A	0.7348	0.6969	0.0418	0.060*
C8	0.7015 (3)	0.8528 (2)	-0.03326 (18)	0.0604 (6)
H8A	0.6980	0.9050	0.0149	0.073*
C9	0.6854 (3)	0.9007 (2)	-0.12035 (19)	0.0652 (6)
H9A	0.6719	0.9847	-0.1312	0.078*
C10	0.6895 (4)	0.8231 (2)	-0.19106 (17)	0.0658 (6)
H10A	0.6784	0.8551	-0.2498	0.079*
C11	0.7101 (3)	0.6982 (2)	-0.17573 (15)	0.0553 (5)
H11A	0.7129	0.6467	-0.2242	0.066*
C12	0.5796 (3)	0.68671 (19)	0.56116 (15)	0.0526 (5)
C13	0.3557 (3)	0.80060 (16)	0.47969 (12)	0.0396 (4)
C14	0.2024 (3)	0.81178 (16)	0.42756 (12)	0.0399 (4)
C15	0.1224 (3)	0.72317 (17)	0.40912 (12)	0.0411 (4)
H15A	0.1576	0.6415	0.4299	0.049*
C16	-0.0219 (3)	0.77277 (16)	0.35387 (12)	0.0400 (4)

C17	-0.1434 (3)	0.70474 (18)	0.32326 (12)	0.0430 (4)
C18	-0.2967 (3)	0.7675 (2)	0.27896 (14)	0.0523 (5)
H18A	-0.3229	0.8525	0.2681	0.063*
C19	-0.4109 (3)	0.7038 (2)	0.25083 (15)	0.0595 (6)
H19A	-0.5127	0.7462	0.2207	0.071*
C20	-0.3750 (3)	0.5778 (2)	0.26715 (16)	0.0622 (6)
H20A	-0.4528	0.5355	0.2485	0.075*
C21	-0.2239 (4)	0.5153 (2)	0.31101 (18)	0.0665 (6)
H21A	-0.1988	0.4303	0.3219	0.080*
C22	-0.1083 (3)	0.5782 (2)	0.33915 (16)	0.0551 (5)
H22A	-0.0063	0.5351	0.3690	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0666 (4)	0.0408 (3)	0.0557 (3)	-0.0208 (2)	-0.0206 (2)	0.0026 (2)
O1	0.0852 (11)	0.0496 (8)	0.0412 (8)	-0.0173 (7)	-0.0144 (7)	0.0018 (6)
N1	0.0606 (11)	0.0476 (9)	0.0501 (9)	-0.0188 (8)	-0.0199 (8)	-0.0004 (7)
C1	0.0459 (10)	0.0403 (9)	0.0471 (11)	-0.0130 (8)	-0.0093 (8)	0.0029 (8)
S2	0.0818 (4)	0.0563 (3)	0.0435 (3)	-0.0271 (3)	-0.0187 (3)	-0.0022 (2)
O2	0.0543 (8)	0.0386 (7)	0.0404 (7)	-0.0131 (6)	-0.0127 (6)	0.0008 (5)
N2	0.0673 (11)	0.0586 (10)	0.0407 (9)	-0.0234 (9)	-0.0148 (8)	0.0033 (7)
C2	0.0387 (9)	0.0452 (10)	0.0420 (9)	-0.0133 (8)	-0.0108 (7)	-0.0007 (7)
S3	0.0545 (3)	0.0546 (3)	0.0554 (3)	-0.0224 (2)	-0.0255 (2)	0.0045 (2)
O3	0.0906 (13)	0.0567 (10)	0.1022 (14)	-0.0145 (9)	-0.0602 (11)	0.0188 (9)
N3	0.0500 (9)	0.0432 (8)	0.0505 (9)	-0.0191 (7)	-0.0202 (7)	0.0050 (7)
C3	0.0358 (9)	0.0496 (10)	0.0399 (9)	-0.0125 (8)	-0.0105 (7)	0.0008 (7)
S4	0.0666 (3)	0.0398 (3)	0.0594 (3)	-0.0221 (2)	-0.0330 (3)	0.0094 (2)
O4	0.0534 (8)	0.0396 (7)	0.0538 (8)	-0.0150 (6)	-0.0225 (6)	0.0052 (6)
N4	0.0575 (10)	0.0443 (9)	0.0500 (9)	-0.0191 (7)	-0.0244 (7)	0.0048 (7)
C4	0.0408 (10)	0.0469 (10)	0.0387 (9)	-0.0130 (8)	-0.0099 (7)	-0.0016 (7)
C5	0.0322 (9)	0.0530 (10)	0.0381 (9)	-0.0136 (7)	-0.0070 (7)	-0.0002 (8)
C6	0.0329 (9)	0.0512 (10)	0.0434 (9)	-0.0129 (7)	-0.0084 (7)	0.0039 (8)
C7	0.0424 (10)	0.0569 (12)	0.0515 (11)	-0.0151 (9)	-0.0098 (8)	0.0013 (9)
C8	0.0518 (12)	0.0536 (12)	0.0756 (15)	-0.0155 (10)	-0.0120 (11)	-0.0060 (10)
C9	0.0525 (13)	0.0535 (12)	0.0885 (17)	-0.0163 (10)	-0.0142 (11)	0.0128 (12)
C10	0.0649 (15)	0.0684 (14)	0.0657 (14)	-0.0224 (11)	-0.0186 (11)	0.0252 (12)
C11	0.0554 (12)	0.0638 (13)	0.0487 (11)	-0.0201 (10)	-0.0139 (9)	0.0073 (9)
C12	0.0551 (12)	0.0499 (11)	0.0563 (12)	-0.0133 (9)	-0.0248 (9)	0.0056 (9)
C13	0.0423 (10)	0.0378 (9)	0.0394 (9)	-0.0129 (7)	-0.0094 (7)	0.0012 (7)
C14	0.0419 (10)	0.0391 (9)	0.0399 (9)	-0.0125 (7)	-0.0115 (7)	0.0016 (7)
C15	0.0418 (10)	0.0377 (9)	0.0456 (10)	-0.0134 (7)	-0.0119 (8)	0.0033 (7)
C16	0.0411 (10)	0.0416 (9)	0.0380 (9)	-0.0139 (7)	-0.0081 (7)	0.0002 (7)
C17	0.0419 (10)	0.0496 (10)	0.0391 (9)	-0.0179 (8)	-0.0046 (7)	-0.0051 (7)
C18	0.0532 (12)	0.0622 (12)	0.0491 (11)	-0.0252 (10)	-0.0164 (9)	0.0030 (9)
C19	0.0531 (12)	0.0857 (16)	0.0502 (11)	-0.0313 (11)	-0.0171 (9)	-0.0032 (11)
C20	0.0600 (14)	0.0822 (16)	0.0566 (12)	-0.0385 (12)	-0.0090 (10)	-0.0175 (11)
C21	0.0719 (16)	0.0575 (13)	0.0790 (16)	-0.0310 (11)	-0.0153 (12)	-0.0107 (11)

C22 0.0540 (12) 0.0494 (11) 0.0671 (13) -0.0195 (9) -0.0170 (10) -0.0051 (9)

Geometric parameters (Å, °)

S1—N1	1.6845 (17)	C7—C8	1.380 (3)
S1—C1	1.7616 (19)	C7—H7A	0.9300
O1—C1	1.185 (2)	C8—C9	1.380 (3)
N1—C2	1.271 (2)	C8—H8A	0.9300
C1—O2	1.391 (2)	C9—C10	1.376 (4)
S2—N2	1.6406 (18)	C9—H9A	0.9300
S2—C3	1.7071 (18)	C10—C11	1.382 (3)
O2—C2	1.364 (2)	C10—H10A	0.9300
N2—C5	1.327 (2)	C11—H11A	0.9300
C2—C3	1.449 (3)	C13—C14	1.447 (3)
S3—N3	1.6790 (16)	C14—C15	1.365 (3)
S3—C12	1.746 (2)	C15—C16	1.417 (3)
O3—C12	1.187 (3)	C15—H15A	0.9300
N3—C13	1.278 (2)	C16—C17	1.479 (3)
C3—C4	1.361 (3)	C17—C22	1.386 (3)
S4—N4	1.6457 (17)	C17—C18	1.387 (3)
S4—C14	1.7084 (18)	C18—C19	1.384 (3)
O4—C13	1.361 (2)	C18—H18A	0.9300
O4—C12	1.385 (2)	C19—C20	1.380 (4)
N4—C16	1.329 (2)	C19—H19A	0.9300
C4—C5	1.417 (3)	C20—C21	1.371 (4)
C4—H4B	0.9300	C20—H20A	0.9300
C5—C6	1.476 (3)	C21—C22	1.386 (3)
C6—C7	1.390 (3)	C21—H21A	0.9300
C6—C11	1.398 (3)	C22—H22A	0.9300
N1—S1—C1	93.13 (8)	C9—C10—H10A	119.6
C2—N1—S1	109.43 (14)	C11—C10—H10A	119.6
O1—C1—O2	122.21 (17)	C10—C11—C6	120.3 (2)
O1—C1—S1	131.23 (16)	C10—C11—H11A	119.9
O2—C1—S1	106.56 (13)	C6—C11—H11A	119.9
N2—S2—C3	94.78 (9)	O3—C12—O4	122.3 (2)
C2—O2—C1	111.28 (14)	O3—C12—S3	130.15 (18)
C5—N2—S2	110.54 (13)	O4—C12—S3	107.58 (13)
N1—C2—O2	119.58 (17)	N3—C13—O4	120.27 (17)
N1—C2—C3	124.86 (17)	N3—C13—C14	123.90 (17)
O2—C2—C3	115.55 (16)	O4—C13—C14	115.82 (16)
N3—S3—C12	93.31 (9)	C15—C14—C13	128.92 (17)
C13—N3—S3	108.63 (13)	C15—C14—S4	109.41 (14)
C4—C3—C2	129.89 (17)	C13—C14—S4	121.66 (14)
C4—C3—S2	108.82 (14)	C14—C15—C16	110.62 (16)
C2—C3—S2	121.28 (14)	C14—C15—H15A	124.7
N4—S4—C14	94.50 (9)	C16—C15—H15A	124.7
C13—O4—C12	110.20 (15)	N4—C16—C15	115.12 (16)

C16—N4—S4	110.35 (13)	N4—C16—C17	119.36 (16)
C3—C4—C5	111.36 (16)	C15—C16—C17	125.51 (16)
C3—C4—H4B	124.3	C22—C17—C18	118.80 (18)
C5—C4—H4B	124.3	C22—C17—C16	120.93 (18)
N2—C5—C4	114.50 (17)	C18—C17—C16	120.26 (17)
N2—C5—C6	119.40 (16)	C19—C18—C17	120.2 (2)
C4—C5—C6	126.10 (16)	C19—C18—H18A	119.9
C7—C6—C11	118.40 (19)	C17—C18—H18A	119.9
C7—C6—C5	121.30 (17)	C20—C19—C18	120.6 (2)
C11—C6—C5	120.29 (18)	C20—C19—H19A	119.7
C8—C7—C6	120.7 (2)	C18—C19—H19A	119.7
C8—C7—H7A	119.7	C21—C20—C19	119.5 (2)
C6—C7—H7A	119.7	C21—C20—H20A	120.2
C7—C8—C9	120.5 (2)	C19—C20—H20A	120.2
C7—C8—H8A	119.7	C20—C21—C22	120.3 (2)
C9—C8—H8A	119.7	C20—C21—H21A	119.8
C10—C9—C8	119.4 (2)	C22—C21—H21A	119.8
C10—C9—H9A	120.3	C17—C22—C21	120.6 (2)
C8—C9—H9A	120.3	C17—C22—H22A	119.7
C9—C10—C11	120.7 (2)	C21—C22—H22A	119.7

5-(3-Phenylisothiazol-4-yl)-1,3,4-oxathiazol-2-one (II)

Crystal data

C₁₁H₆N₂O₂S₂
M_r = 262.30
 Monoclinic, *P*2₁/*c*
a = 9.7202 (6) Å
b = 9.9723 (6) Å
c = 11.2165 (7) Å
 β = 90.399 (1)°
V = 1087.22 (12) Å³
Z = 4

F(000) = 536
D_x = 1.602 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 6714 reflections
 θ = 2.7–28.3°
 μ = 0.48 mm⁻¹
T = 296 K
 Block, colorless
 0.48 × 0.43 × 0.37 mm

Data collection

Bruker APEXII CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2008)
T_{min} = 0.719, *T_{max}* = 0.837
 8041 measured reflections

2362 independent reflections
 2228 reflections with *I* > 2σ(*I*)
R_{int} = 0.017
 θ_{\max} = 27.0°, θ_{\min} = 2.9°
h = -12→12
k = -12→9
l = -14→14

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.030
wR(*F*²) = 0.083
S = 1.02
 2362 reflections
 155 parameters
 0 restraints

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.4061P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.37 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$

Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.018 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S2	0.45224 (4)	0.17168 (4)	0.50567 (3)	0.04262 (13)
S1	0.88687 (4)	0.63218 (4)	0.59213 (4)	0.04650 (14)
O1	0.65815 (9)	0.53305 (10)	0.65111 (8)	0.0330 (2)
C1	0.74809 (14)	0.63165 (15)	0.69017 (12)	0.0365 (3)
C3	0.62185 (13)	0.35992 (13)	0.50912 (11)	0.0288 (3)
O2	0.72696 (12)	0.69783 (14)	0.77664 (11)	0.0542 (3)
C2	0.70630 (13)	0.47087 (13)	0.55025 (10)	0.0288 (3)
N2	0.55493 (14)	0.18187 (13)	0.38899 (11)	0.0427 (3)
N1	0.82008 (12)	0.51010 (13)	0.50596 (10)	0.0395 (3)
C4	0.51836 (13)	0.30589 (14)	0.57667 (12)	0.0330 (3)
H4	0.4894	0.3384	0.6501	0.040*
C5	0.63936 (13)	0.28477 (14)	0.40146 (11)	0.0325 (3)
C6	0.74116 (14)	0.31005 (14)	0.30578 (11)	0.0337 (3)
C11	0.83741 (15)	0.21201 (15)	0.27851 (13)	0.0386 (3)
H11A	0.8384	0.1317	0.3206	0.046*
C7	0.73957 (18)	0.42883 (17)	0.24153 (14)	0.0472 (4)
H7A	0.6757	0.4951	0.2595	0.057*
C10	0.93225 (15)	0.23383 (18)	0.18830 (14)	0.0465 (4)
H10A	0.9976	0.1687	0.1710	0.056*
C9	0.92952 (19)	0.3518 (2)	0.12467 (15)	0.0530 (4)
H9A	0.9927	0.3662	0.0641	0.064*
C8	0.8330 (2)	0.4488 (2)	0.15076 (15)	0.0560 (4)
H8A	0.8307	0.5280	0.1070	0.067*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S2	0.0448 (2)	0.0372 (2)	0.0460 (2)	-0.01130 (15)	0.00795 (16)	-0.00051 (15)
S1	0.0414 (2)	0.0518 (3)	0.0465 (2)	-0.01591 (16)	0.01521 (16)	-0.01786 (17)
O1	0.0314 (4)	0.0366 (5)	0.0311 (4)	-0.0004 (4)	0.0070 (3)	-0.0061 (4)
C1	0.0343 (6)	0.0385 (7)	0.0368 (7)	0.0007 (5)	0.0045 (5)	-0.0079 (6)
C3	0.0290 (6)	0.0297 (6)	0.0277 (6)	0.0022 (5)	0.0018 (4)	0.0015 (5)
O2	0.0487 (6)	0.0632 (7)	0.0508 (6)	-0.0034 (5)	0.0123 (5)	-0.0286 (6)
C2	0.0309 (6)	0.0307 (6)	0.0248 (5)	0.0034 (5)	0.0032 (4)	-0.0011 (5)
N2	0.0485 (7)	0.0387 (7)	0.0409 (6)	-0.0091 (5)	0.0072 (5)	-0.0070 (5)

N1	0.0380 (6)	0.0447 (7)	0.0359 (6)	-0.0089 (5)	0.0103 (5)	-0.0122 (5)
C4	0.0341 (6)	0.0325 (6)	0.0325 (6)	0.0005 (5)	0.0038 (5)	0.0025 (5)
C5	0.0345 (6)	0.0321 (6)	0.0310 (6)	0.0003 (5)	0.0017 (5)	-0.0014 (5)
C6	0.0359 (7)	0.0375 (7)	0.0277 (6)	-0.0039 (5)	0.0018 (5)	-0.0069 (5)
C11	0.0390 (7)	0.0394 (7)	0.0375 (7)	-0.0018 (6)	-0.0013 (5)	-0.0091 (6)
C7	0.0556 (9)	0.0439 (9)	0.0422 (8)	0.0062 (7)	0.0132 (7)	0.0012 (7)
C10	0.0381 (7)	0.0568 (10)	0.0448 (8)	-0.0001 (7)	0.0056 (6)	-0.0179 (7)
C9	0.0525 (9)	0.0679 (11)	0.0389 (8)	-0.0095 (8)	0.0164 (7)	-0.0097 (8)
C8	0.0709 (11)	0.0543 (10)	0.0432 (8)	-0.0021 (8)	0.0166 (8)	0.0065 (7)

Geometric parameters (Å, °)

S2—N2	1.6546 (13)	C5—C6	1.4864 (18)
S2—C4	1.6827 (14)	C6—C7	1.386 (2)
S1—N1	1.6820 (12)	C6—C11	1.389 (2)
S1—C1	1.7463 (14)	C11—C10	1.391 (2)
O1—C2	1.3750 (14)	C11—H11A	0.9300
O1—C1	1.3849 (17)	C7—C8	1.383 (2)
C1—O2	1.1921 (17)	C7—H7A	0.9300
C3—C4	1.3737 (18)	C10—C9	1.376 (3)
C3—C5	1.4324 (17)	C10—H10A	0.9300
C3—C2	1.4511 (18)	C9—C8	1.380 (3)
C2—N1	1.2770 (17)	C9—H9A	0.9300
N2—C5	1.3208 (18)	C8—H8A	0.9300
C4—H4	0.9300		
N2—S2—C4	95.45 (6)	C3—C5—C6	127.12 (12)
N1—S1—C1	93.61 (6)	C7—C6—C11	119.48 (13)
C2—O1—C1	111.27 (10)	C7—C6—C5	121.01 (13)
O2—C1—O1	122.58 (13)	C11—C6—C5	119.50 (13)
O2—C1—S1	130.46 (12)	C6—C11—C10	120.07 (15)
O1—C1—S1	106.96 (9)	C6—C11—H11A	120.0
C4—C3—C5	110.58 (12)	C10—C11—H11A	120.0
C4—C3—C2	122.58 (12)	C8—C7—C6	120.03 (15)
C5—C3—C2	126.64 (11)	C8—C7—H7A	120.0
N1—C2—O1	118.86 (12)	C6—C7—H7A	120.0
N1—C2—C3	126.82 (12)	C9—C10—C11	120.04 (15)
O1—C2—C3	114.23 (11)	C9—C10—H10A	120.0
C5—N2—S2	109.98 (10)	C11—C10—H10A	120.0
C2—N1—S1	109.27 (9)	C10—C9—C8	119.98 (15)
C3—C4—S2	109.25 (10)	C10—C9—H9A	120.0
C3—C4—H4	125.4	C8—C9—H9A	120.0
S2—C4—H4	125.4	C9—C8—C7	120.40 (17)
N2—C5—C3	114.74 (12)	C9—C8—H8A	119.8
N2—C5—C6	118.14 (12)	C7—C8—H8A	119.8