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Molecular conformation and supramolecular aggregation in four 2,3,4,5-tetrahydro-3,4-diphenyl-benzothiazepines

Manivannan Muthukumar,[a] Kanagasabapathy Thanikasalam,[a] E. Mothi Mohamed,[a] John N. Low[b]‡ and Christopher Glidewell[c]*

[a]Department of Chemistry, Bharathidasan University, Tiruchirappalli, Tamil Nadu 620 024, India, [b]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [c]School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland
Correspondence e-mail: cg@st-andrews.ac.uk

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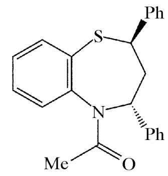
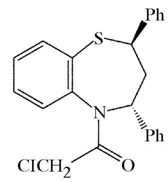
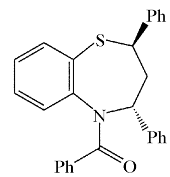
In (2*RS*,4*RS*)-1-acetyl-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine, $C_{23}H_{21}NOS$, (I), and (2*RS*,4*RS*)-1-chloroacetyl-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine, $C_{23}H_{20}ClNOS$, (II), the seven-membered rings have boat conformations, whereas in (2*RS*,4*RS*)-1-benzoyl-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine, $C_{28}H_{23}NOS$, (III), this ring has a conformation intermediate between the boat and twist-boat forms. The molecules of (I) are linked into isolated $R_2^2(16)$ dimers by two C—H···O hydrogen bonds [H···O = 2.41 and 2.47 Å, C···O = 3.268 (3) and 3.336 (3) Å, and C—H···O = 150 and 152°]. In (II), the molecules are again linked by two C—H···O hydrogen bonds [H···O = 2.42 and 2.48 Å, C···O = 3.295 (3) and 3.364 (2) Å, and C—H···O = 153 and 154°], forming chains of alternating $R_2^2(18)$ and $R_2^2(22)$ rings. Two C—H···O hydrogen bonds [H···O = 2.49 and 2.53 Å, C···O = 3.347 (2) and 3.295 (2) Å, and C—H···O = 150 and 138°] link the molecules of (III) into sheets containing alternating $R_2^2(22)$ and $R_6^4(30)$ rings. Re-examination of the published structure of (2*RS*,4*RS*)-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine shows that the molecules are linked by three C—H···π(arene) hydrogen bonds into a three-dimensional framework.

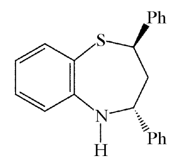
Comment

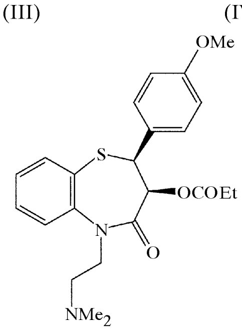
We report here the molecular and supramolecular structures of three *N*-acyl-*C*-phenylated tetrahydrobenzothiazepines, (I)–(III), and we compare these with the simpler analogue, (IV), which is unsubstituted at the N atom and whose structure has recently been reported (Laavanya *et al.*, 2002). These compounds are of interest as their molecular constitutions all bear some resemblance to that of the calcium antagonist drug diltiazem [or (2*S*,3*S*)-3-acetoxy-5-(dimethylaminoethyl)-2-(4-methoxyphenyl)-2,3-dihydro-1,5-benzothiazepine-4(5*H*)-one, (V)] and its 2*R*,3*R* enantiomer (Kojić-Prodić *et al.*, 1984).


(I)


(II)


(III)


(IV)


(V)

Each of (I)–(III) (Figs. 1–3) contains two stereogenic C atoms, C2 and C4, and hence the formation of diastereoisomers is possible. However, each of the crystalline samples examined contained a single pair of enantiomers, *R*,*R* and *S*,*S*, and for each compound the reference molecule was selected as having the *R*,*R* configuration. In this respect, the configurations of (I)–(III) are identical to that of (IV) (Laavanya *et al.*, 2002). It should, however, be noted here that the schematic view of (IV) in the original report shows the incorrect 2*S*,4*R* isomer. The interbond angles at the N atom in each of (I)–(III) sum to ~360.0°, so that no further configurational isomers are possible.

Compound (I) crystallizes with $Z' = 2$; the thiazepine rings in the two independent molecules in (I) and in the molecules of (II) and (III) all adopt similar conformations, as shown by the ring torsion angles (Table 5). Apart from the S1—C10—C11—N5 angle, there are corresponding pairs of torsion angles having similar magnitudes but opposite signs. This fact indicates conformations that, apart from the obvious differences in atom types and bond lengths, approximate in (I) and (II) to pseudo-mirror symmetry; this conformation may be best described as the boat conformation (Evans & Boeyens, 1989). The conformation of the thiazepine ring in (III) does not exhibit even approximate symmetry and it cannot be described in terms of a single primitive form (Evans & Boeyens, 1989). Instead, the conformation is intermediate between the boat and twist-boat forms. By contrast, the thia-

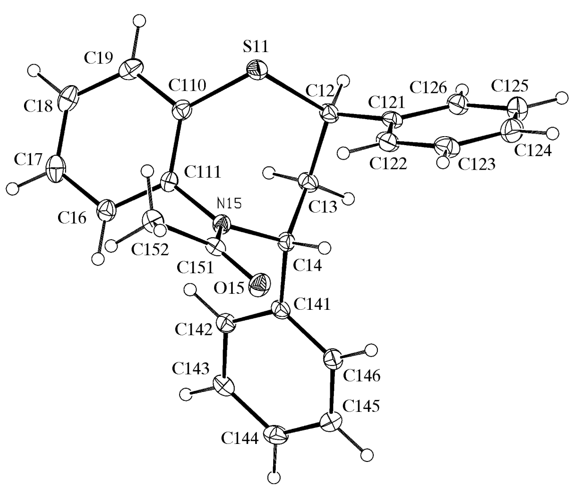
‡ Postal address: Department of Electrical Engineering and Physics, University of Dundee, Dundee DD1 4HN, Scotland.

zepine ring in (IV) exhibits approximate pseudo-twofold rotational symmetry, as the corresponding pairs of torsion angles have similar magnitudes with the same signs, although all four primitive forms contribute to the overall conformation of (IV).

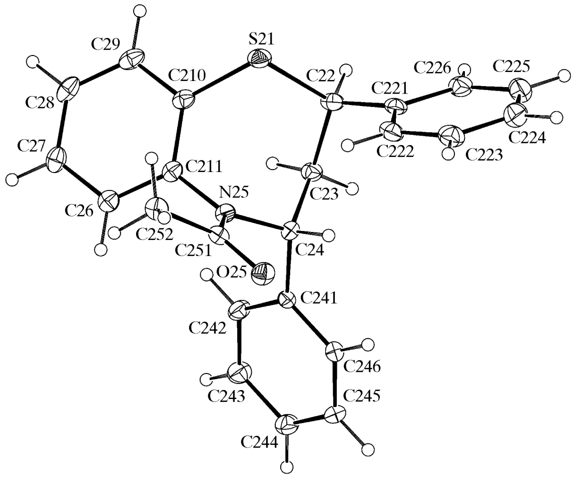
The only significant difference between the bond lengths in (I)–(III) and those in (IV) occurs for the N5—C11 bond. In (I)–(III), where atom N5 is coplanar with the thiazepine ring, this distance lies in the range 1.427 (3)–1.439 (2) Å, whereas in (IV), where the configuration involving atom N5 is pyramidal, this distance is 1.395 (3) Å. By contrast, the mean values for bonds of types $C_{aryl}—NC_2$, involving planar N atoms, and $C_{aryl}—NHC$, involving pyramidal N atoms, are 1.371 and 1.419 Å, respectively (Allen *et al.*, 1987). The remaining bond lengths in (I)–(III) show no unusual values.

The supramolecular structures of (I)–(III) all have different dimensionality. In (I), the two independent molecules are linked by a pair of C—H···O hydrogen bonds (Table 1). Atom C145 in the type 1 molecule at (x, y, z) acts as a hydrogen-bond donor to carbonyl atom O25 in the type 2 molecule at ($1 - x$, $1 - y$, $1 - z$), while atom C245 at ($1 - x$, $1 - y$, $1 - z$) in turn acts as a donor to carbonyl atom O15 at (x, y, z). In this manner, an approximately centrosymmetric $R_2^2(16)$ dimer is formed (Fig. 4). This dimeric aggregate is centred at approximately (0.75, 0.37, 0.75), and this alone precludes the possibility of any additional symmetry. While such an aggregate would normally have been selected as the asymmetric unit, in this instance the asymmetric unit was selected so that each of the independent molecules had the *R*,*R* configuration. The $R_2^2(16)$ dimer contains one *R*,*R* molecule and one *S*,*S* molecule. There are four of these dimeric units in each unit cell, but there are no direction-specific interactions between adjacent dimers.

In (II), the molecules are linked by two C—H···O hydrogen bonds (Table 2) into a chain of rings. Atom C24 in the molecule at (x, y, z) acts as a hydrogen-bond donor to carbonyl atom O5 in the molecule at ($1 - x$, $-y$, $1 - z$), so forming an $R_2^2(22)$ ring centred at ($\frac{1}{2}$, 0, $\frac{1}{2}$), while atom C44 at



(*a*)



(*b*)

Figure 1
The two independent molecules of (I), showing the atom-labelling schemes: (*a*) molecule 1 and (*b*) molecule 2. Displacement ellipsoids are drawn at the 30% probability level.

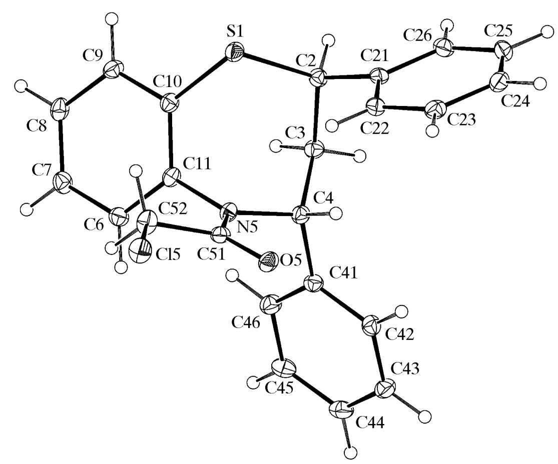


Figure 2
The molecule of (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

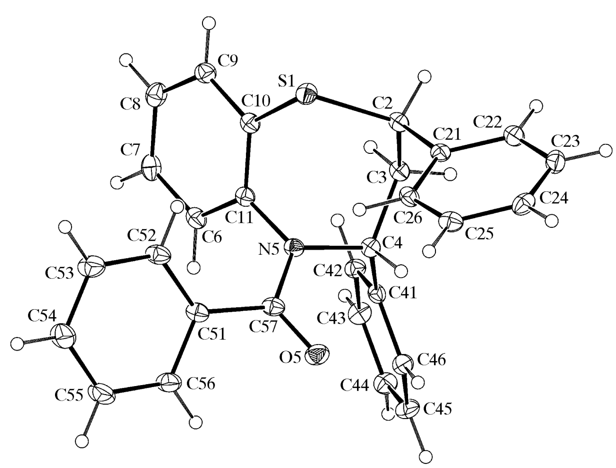


Figure 3
The molecule of (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

(x, y, z) acts as a donor to atom O5 at $(1 - x, 1 - y, 1 - z)$, thus forming an $R_2^2(18)$ ring centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Propagation of these two hydrogen bonds then generates a chain of rings along $(\frac{1}{2}, y, \frac{1}{2})$, with $R_2^2(18)$ rings centred at $(\frac{1}{2}, n + \frac{1}{2}, \frac{1}{2})$ (n = zero or integer) and $R_2^2(22)$ rings centred at $(\frac{1}{2}, n, \frac{1}{2})$ (n = zero or integer) (Fig. 5). Two chains of this type pass through each unit cell, but there are no direction-specific interactions between adjacent chains.

As in (II), the supramolecular structure of (III) is again dictated by two intermolecular C—H···O hydrogen bonds (Table 3), but now their effect is to generate a sheet structure, in contrast with the chain of rings in (II). The stronger of these two hydrogen bonds gives rise to a chain running parallel to the [010] direction. Atom C23 in the molecule at (x, y, z) acts as a hydrogen-bond donor to carbonyl atom O5 in the molecule at $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z)$, so producing a $C(10)$ chain, generated by the 2_1 screw axis along $(\frac{1}{4}, y, \frac{3}{4})$ (Fig. 6). Four of these chains pass through each unit cell; two, lying in the domain $-0.02 < x < 0.52$, are generated by screw axes at $x = \frac{1}{4}$, while the other two, lying in the domain $0.48 < x < 1.02$, are generated by screw axes at $x = \frac{3}{4}$. Within each domain, the

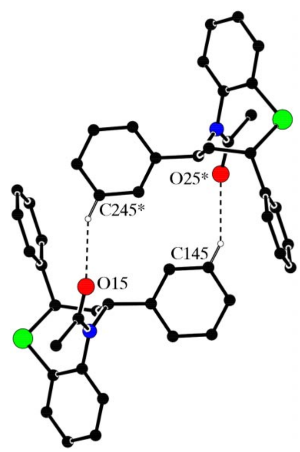


Figure 4
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded $R_2^2(16)$ dimer. For clarity, the unit-cell box and H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(1 - x, 1 - y, 1 - z)$.

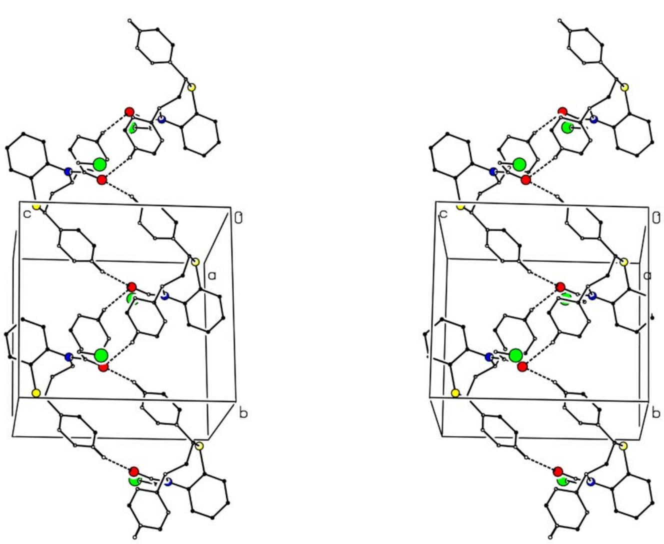


Figure 5
A stereoview of part of the crystal structure of (II), showing the formation of a chain of alternating $R_2^2(18)$ and $R_2^2(22)$ rings along [010]. For clarity, H atoms not involved in the motif shown have been omitted.

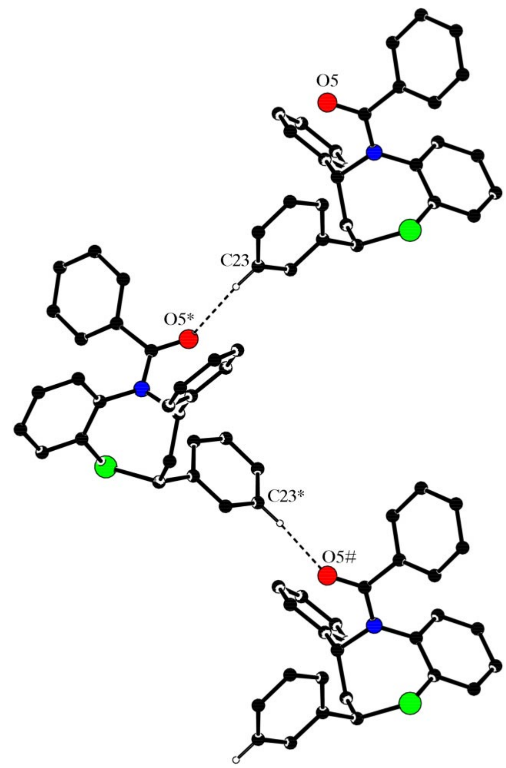


Figure 6
Part of the crystal structure of (III), showing the formation of a $C(10)$ chain along [010]. For clarity, the unit-cell box and H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z)$ and $(x, 1 + y, z)$, respectively.

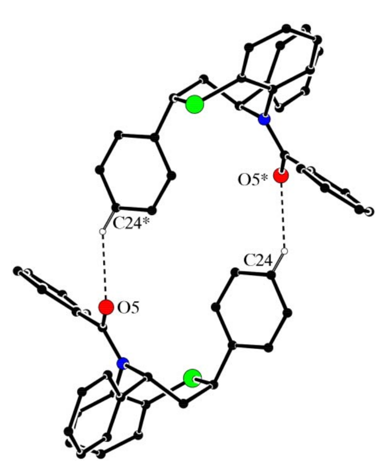


Figure 7
Part of the crystal structure of (III), showing the formation of an $R_2^2(22)$ dimer. For clarity, the unit-cell box and H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(\frac{1}{2} - x, \frac{1}{2} - y, 2 - z)$.

$C(10)$ chains are linked into sheets by the second of the C—H···O hydrogen bonds. Atom C24 in the molecule at (x, y, z), which lies in the $C(10)$ chain along ($\frac{1}{4}$, y, $\frac{3}{4}$), acts as a hydrogen-bond donor to carbonyl atom O5 in the molecule at ($\frac{1}{2} - x$, $\frac{1}{2} - y$, $2 - z$), which lies in the $C(10)$ chain along ($\frac{1}{4}$, y, $\frac{5}{4}$), so forming a centrosymmetric $R_2^2(22)$ ring centred at ($\frac{1}{4}$, $\frac{1}{4}$, 1) (Fig. 7). The combination of the $R_2^2(22)$ rings and the $C(10)$ chains generates a (100) sheet built from $R_2^2(22)$ and $R_6^4(30)$ rings alternating in a chessboard fashion (Fig. 8). Two sheets of this type pass through each unit cell, one in each domain of x as defined above, but there are no direction-specific interactions between adjacent sheets. Despite the presence of at least three independent aryl rings in each of (I)–(III), there are neither C—H···π(arene) hydrogen bonds nor aromatic π–π stacking interactions present in any of their structures.

In the light of the very different supramolecular structures adopted by (I)–(III), it seemed of interest to re-examine the supramolecular structure of (IV) using space group $P2_1/n$, with $Z' = 1$, and the atomic coordinates established by Laavanya *et al.* (2002), where the atom labelling is identical to that employed in (I)–(III). There are, in fact, three C—H···π(arene) hydrogen bonds, all with H···centroid distances of less than 3.0 Å (Table 4), which were not noted in the original report but which together link the molecules of (IV) into a continuous three-dimensional framework.

In the first of these interactions, atom C6 in the molecule at (x, y, z) acts as a hydrogen-bond donor to the C6–C11 ring in the molecule at ($\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$), so producing a [010] chain generated by the 2_1 screw axis along ($\frac{1}{4}$, y, $\frac{1}{4}$) (Fig. 9). In a similar way, atom C21 at (x, y, z) acts as a donor to the C20–C25 ring (original atom numbering) in the molecule at ($\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$), so producing a second [010] chain, this time generated by the screw axis along ($\frac{3}{4}$, y, $\frac{1}{4}$). The combination of these two chains then generates a (001) sheet in the form of a (4,4)-net (Batten & Robson, 1998), lying in the domain $-0.04 < z < 0.54$ (Fig. 10); a second sheet, related to the first by inversion, lies in the domain $0.46 < z < 1.04$.

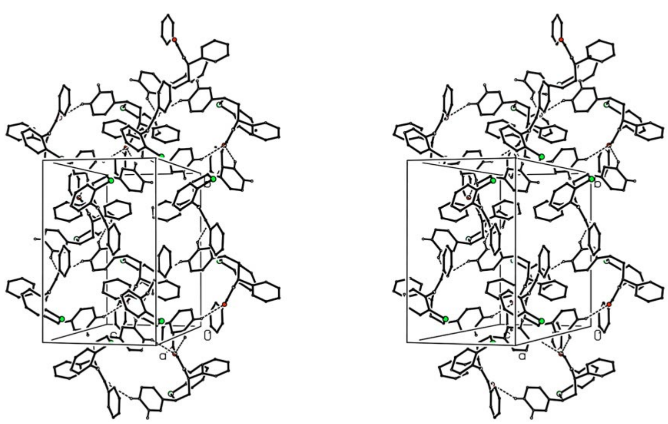


Figure 8
A stereoview of part of the crystal structure of (III), showing the formation of a (100) sheet built from alternating $R_2^2(22)$ and $R_6^4(30)$ rings. For clarity, H atoms not involved in the motif shown have been omitted.

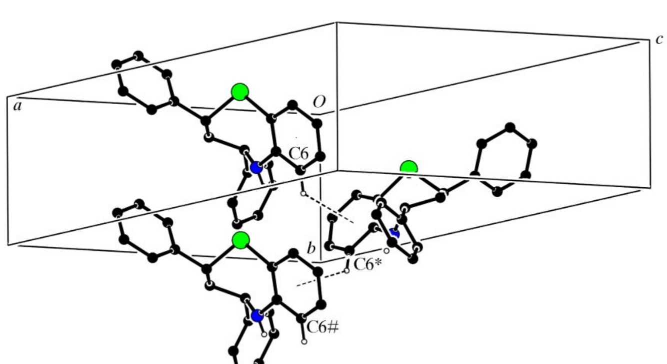


Figure 9
Part of the crystal structure of (IV) (Laavanya *et al.*, 2002), showing the formation of a C—H···π(arene) chain along ($\frac{1}{4}$, y, $\frac{1}{4}$). For clarity, H atoms bonded to C atoms but not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions ($\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$) and ($x$, $1 + y$, z), respectively.

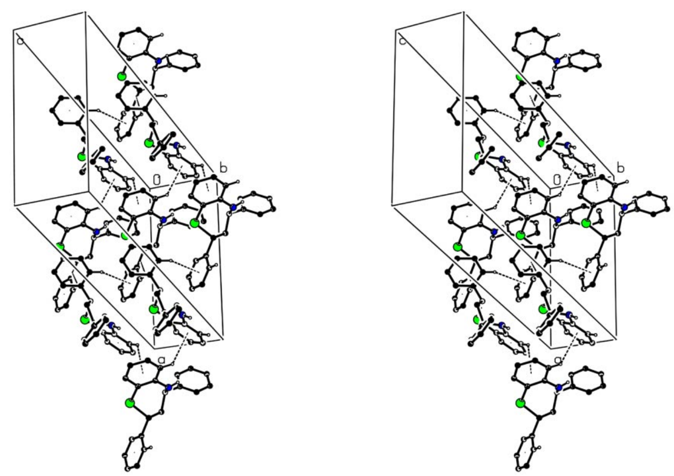


Figure 10
A stereoview of part of the crystal structure of (IV), showing the formation of a (001) sheet. For clarity, H atoms not involved in the motif shown have been omitted.

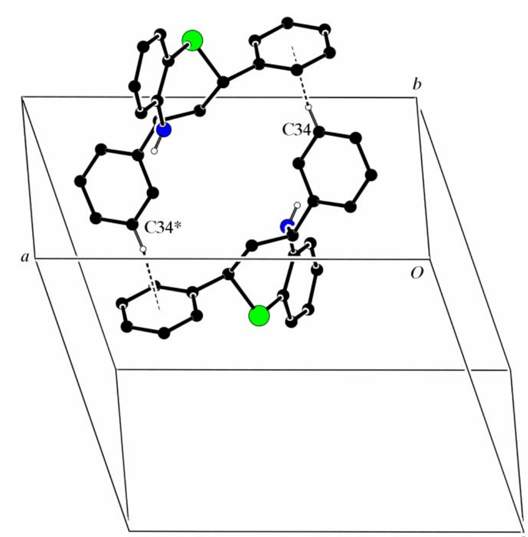


Figure 11
Part of the crystal structure of (IV), showing the formation of the centrosymmetric motif that links the (001) sheets. For clarity, H atoms bonded to C atoms but not involved in the motif shown have been omitted. The atom marked with an asterisk (*) is at the symmetry position ($1 - x$, $1 - y$, $-z$).

The third C—H···π(arene) hydrogen bond links adjacent (001) sheets; atom C34 in the molecule at (x, y, z), which lies in the domain $-0.04 < z < 0.54$, acts as a hydrogen-bond donor to ring C20–C25 in the molecule at $(1 - x, 1 - y, -z)$, which lies in the domain $-0.54 < z < 0.04$. The resulting centrosymmetric motif (Fig. 11) thus serves to link sheets in different domains and in this manner to link all of the (001) sheets into a single framework.

It is also timely to re-evaluate the intermolecular N—H···S interaction in (IV). This interaction was originally discounted (Laavanya *et al.*, 2002) as insignificant on the grounds that the shortest intermolecular N···S distance (Table 4) is in excess of the 3.3 Å sum of the van der Waals radii (Bondi, 1964). However, an analysis (Allen *et al.*, 1997) of hydrogen bonds having two-coordinate S as the acceptor, using data retrieved from the Cambridge Structural Database (Allen, 2002), indicated mean H···S, N···S and N—H···S parameters in such bonds where S is bonded to two C atoms of 2.74 (2) Å, 3.58 (3) Å and 145 (3)° respectively. Accordingly, if the N—H···S contact in (IV) is not considered to be a significant intermolecular interaction, it is more soundly rejected on the grounds of the long H···S distance and the small N—H···S angle than on the grounds of the N···S distance.

In summary, we have shown that the very closely related series of compounds (I)–(IV) exhibit supramolecular aggregation in zero, one, two and three dimensions, respectively, and that while in (I)–(III) the aggregation depends solely on C—H···O hydrogen bonds, in (IV) it depends solely on C—H···π(arene) hydrogen bonds. The occurrence of such differences resulting from very modest changes in molecular constitution undoubtedly presents a considerable challenge for computational methods that seek to predict, whether from first principles or otherwise, the crystal structures of simple molecular compounds (Lommerse *et al.*, 2000; Motherwell *et al.*, 2002).

Experimental

Compounds (I)–(III) were prepared by acylation of (IV) (Laavanya *et al.*, 2002) with acetic anhydride, chloroacetyl chloride and benzoyl chloride, respectively, in the presence of triethylamine in dry benzene under reflux conditions. Analyses found for (I): C 77.0, H 6.1, N 3.7%; $C_{23}H_{21}NOS$ requires: C 76.8, H 5.9, N 3.9%; found for (II): C 70.2, H 5.0, N 3.6%; $C_{23}H_{20}ClNOS$ requires: C 70.1, H 5.1, N 3.6%; found for (III): C 79.5, H 5.6, N 3.3%; $C_{28}H_{23}NOS$ requires: C 79.8, H 5.5, N 3.3%. Crystals of (I)–(III) suitable for single-crystal X-ray diffraction were grown from solutions in ethanol; m.p.: (I) 401–404 K, (II) 393–397 K, and (III) 445–449 K.

Compound (I)

Crystal data

$C_{23}H_{21}NOS$
$M_r = 359.48$
Monoclinic, $P2_1/c$
$a = 20.3579$ (4) Å
$b = 8.3014$ (1) Å
$c = 22.2513$ (4) Å
$\beta = 93.865$ (1)°
$V = 3751.90$ (11) Å^3
$Z = 8$
$D_x = 1.273$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8274 reflections
$\theta = 3.0$–27.1°
$\mu = 0.18$ mm^{-1}
$T = 120$ (2) K
Plate, colourless
0.20 × 0.04 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
$T_{min} = 0.954$, $T_{max} = 0.994$
51 290 measured reflections
8274 independent reflections
4659 reflections with $I > 2\sigma(I)$
$R_{int} = 0.109$
$\theta_{max} = 27.1°$
$h = -25 \rightarrow 26$
$k = -10 \rightarrow 9$
$l = -26 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.125$
$S = 1.00$
8274 reflections
471 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.0549P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C145—H145···O25[i]	0.95	2.47	3.336 (3)	152
C245—H245···O15[i]	0.95	2.41	3.268 (3)	150

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C24—H24···O5[ii]	0.95	2.42	3.295 (3)	153
C44—H44···O5[i]	0.95	2.48	3.364 (2)	154

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

Compound (II)

Crystal data

$C_{23}H_{20}ClNOS$
$M_r = 393.92$
Monoclinic, $P2_1/n$
$a = 12.6348$ (4) Å
$b = 11.9337$ (5) Å
$c = 12.7904$ (5) Å
$\beta = 92.549$ (2)°
$V = 1926.63$ (13) Å^3
$Z = 4$
$D_x = 1.358$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4418 reflections
$\theta = 3.2$–27.5°
$\mu = 0.32$ mm^{-1}
$T = 120$ (2) K
Plate, colourless
0.28 × 0.24 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
$T_{min} = 0.926$, $T_{max} = 0.987$
26 344 measured reflections
4418 independent reflections
2950 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$
$\theta_{max} = 27.5°$
$h = -16 \rightarrow 16$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.098$
$S = 1.00$
4418 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Table 3
Hydrogen-bonding geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O5^{iii}	0.95	2.49	3.347 (2)	150
C24—H24···O5^{iv}	0.95	2.53	3.295 (2)	138

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

Table 4
Hydrogen bonds and short intermolecular contact parameters (Å, °) for (IV).

Original atom numbering (Laavanya *et al.*, 2002). *Cg*1 and *Cg*2 are the centroids of the C6–C11 and C20–C25 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···$Cg1^{v}$	0.98	2.82	3.521 (3)	129
C21—H21···$Cg2^{vi}$	0.94	2.99	3.746 (3)	139
C34—H34···$Cg2^{vii}$	0.91	2.98	3.669 (4)	133
N5—H5···S1^{viii}	0.82 (2)	3.05 (2)	3.490 (3)	116 (2)

Symmetry codes: (v) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (vi) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (vii) $1-x, 1-y, -z$; (viii) $x, 1+y, z$.

Compound (III)

Crystal data

$C_{28}H_{23}NOS$
$M_r = 421.53$
Monoclinic, $C2/c$
$a = 30.1891$ (8) Å
$b = 14.8005$ (3) Å
$c = 9.7965$ (3) Å
$\beta = 102.2570$ (16)°
$V = 4277.43$ (19) Å^3
$Z = 8$
$D_x = 1.309$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4894 reflections
$\theta = 3.0$–27.5°
$\mu = 0.17$ mm^{-1}
$T = 120$ (2) K
Block, colourless
0.36 × 0.26 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
$T_{min} = 0.937$, $T_{max} = 0.973$
21 732 measured reflections
4894 independent reflections
3535 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 27.5°$
$h = -39 \rightarrow 35$
$k = -19 \rightarrow 18$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.109$
$S = 1.03$
4894 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 1.1026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

For (I) and (II), space groups $P2_1/c$ and $P2_1/n$, respectively, were uniquely assigned from the systematic absences. For (III), the systematic absences permitted Cc and $C2/c$ as possible space groups; $C2/c$ was selected and confirmed by successful structure analysis. All H atoms were located from difference maps and subsequently treated as riding atoms, with C—H distances of 0.95 (aromatic), 0.99 (CH_2) and 1.00 Å (aliphatic CH). Examination of the refined structure of (I) for possible additional symmetry using *ADDSYM* in *PLATON* (Spek, 2003) showed that none could be detected.

For all compounds, data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

Table 5
Selected torsion angles (°) for (I)–(IV).

Torsion angle	(I)		(II)	(III)	(IV)
	Mol. 1	Mol. 2			
x	1	2	nil	nil	nil
Sx1—Cx10—Cx11—Xx5	−7.2 (3)	−6.3 (2)	−2.6 (2)	−8.6 (2)	0.7 (3)
Cx11—Cx10—Sx1—Cx2	64.1 (2)	63.2 (2)	62.6 (2)	60.3 (2)	32.2 (2)
Cx10—Cx11—Xx5—Cx4	−71.8 (3)	−72.0 (3)	−74.3 (2)	−75.1 (2)	38.4 (3)
Sx1—Cx2—Cx3—Cx4	−64.6 (2)	−64.5 (2)	−63.4 (2)	−70.7 (2)	45.9 (3)
Xx5—Cx4—Cx3—Cx2	64.1 (2)	64.2 (2)	66.3 (2)	58.1 (2)	45.3 (3)
Cx10—Sx1—Cx2—Cx3	−18.1 (2)	−18.4 (2)	−20.8 (2)	−9.0 (2)	−83.4 (2)
Cx11—Xx5—Cx4—Cx3	33.1 (3)	32.9 (3)	30.4 (2)	42.3 (2)	−96.3 (3)

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants that have provided computing facilities for this work.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FA1057). Services for accessing these data are described at the back of the journal.

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Molecular conformation and supramolecular aggregation in four 2,3,4,5-tetrahydro-3,4-diphenylbenzothiazepines

Manivannan Muthukumar, Kanagasabapathy Thanikasalam, E. Mothi Mohamed, John N. Low and Christopher Glidewell

Computing details

For all compounds, data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO*–SMN (Otwinowski & Minor, 1997); data reduction: *DENZO*–SMN; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

(I) (2RS,4RS)-*N*-Acetyl-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine

Crystal data

$C_{23}H_{21}NOS$
M_r = 359.48
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 20.3579 (4) Å
b = 8.3014 (1) Å
c = 22.2513 (4) Å
β = 93.865 (1)°
V = 3751.90 (11) Å^3
Z = 8
$F(000)$ = 1520
D_x = 1.273 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8274 reflections
θ = 3.0–27.1°
μ = 0.18 mm^{-1}
T = 120 K
Plate, colourless
0.20 × 0.04 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.954, T_{max} = 0.994
51290 measured reflections
8274 independent reflections
4659 reflections with $I > 2\sigma(I)$
R_{int} = 0.109
θ_{max} = 27.1°, θ_{min} = 3.0°
$h = -25 \rightarrow 26$
$k = -10 \rightarrow 9$
$l = -26 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.125
S = 1.00
8274 reflections
471 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

$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.0549P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S11	0.55232 (3)	−0.07017 (7)	0.57493 (3)	0.03099 (16)
O15	0.67431 (8)	0.02049 (19)	0.75018 (7)	0.0325 (4)
N15	0.68042 (9)	−0.0501 (2)	0.65265 (8)	0.0225 (4)
C12	0.58165 (11)	0.1376 (3)	0.56443 (10)	0.0254 (5)
C13	0.65673 (11)	0.1552 (3)	0.57227 (10)	0.0255 (5)
C14	0.68905 (11)	0.1205 (2)	0.63497 (9)	0.0220 (5)
C16	0.73112 (12)	−0.2785 (3)	0.60441 (10)	0.0270 (5)
C17	0.72932 (13)	−0.3975 (3)	0.56066 (11)	0.0329 (6)
C18	0.67562 (13)	−0.4102 (3)	0.51975 (10)	0.0328 (6)
C19	0.62276 (13)	−0.3058 (3)	0.52263 (10)	0.0313 (6)
C110	0.62335 (11)	−0.1872 (2)	0.56696 (10)	0.0250 (5)
C111	0.67867 (11)	−0.1736 (2)	0.60785 (9)	0.0221 (5)
C121	0.54498 (11)	0.2516 (3)	0.60390 (10)	0.0262 (5)
C122	0.53382 (12)	0.2194 (3)	0.66392 (11)	0.0325 (6)
C123	0.50062 (12)	0.3283 (3)	0.69761 (11)	0.0362 (6)
C124	0.47750 (13)	0.4716 (3)	0.67236 (12)	0.0411 (7)
C125	0.48880 (13)	0.5060 (3)	0.61306 (12)	0.0400 (6)
C126	0.52254 (12)	0.3968 (3)	0.57951 (11)	0.0316 (6)
C141	0.76039 (11)	0.1735 (3)	0.63839 (9)	0.0231 (5)
C142	0.80901 (11)	0.0895 (3)	0.61025 (10)	0.0251 (5)
C143	0.87325 (11)	0.1438 (3)	0.61409 (10)	0.0277 (5)
C144	0.89028 (12)	0.2833 (3)	0.64524 (10)	0.0315 (6)
C145	0.84242 (12)	0.3692 (3)	0.67280 (11)	0.0325 (6)
C146	0.77795 (12)	0.3143 (3)	0.66906 (10)	0.0277 (5)
C151	0.67074 (11)	−0.0851 (3)	0.71171 (10)	0.0249 (5)
C152	0.65498 (12)	−0.2565 (3)	0.72614 (10)	0.0293 (5)
S21	0.05595 (3)	0.18797 (7)	0.07576 (3)	0.03175 (16)
O25	0.17490 (8)	0.28513 (19)	0.25344 (7)	0.0326 (4)
N25	0.18202 (9)	0.2128 (2)	0.15618 (8)	0.0233 (4)
C22	0.08467 (11)	0.3966 (3)	0.06528 (10)	0.0285 (5)
C23	0.15942 (11)	0.4159 (3)	0.07507 (10)	0.0258 (5)
C24	0.19022 (11)	0.3833 (2)	0.13820 (9)	0.0234 (5)
C26	0.23402 (12)	−0.0194 (3)	0.11198 (10)	0.0275 (5)
C27	0.23264 (13)	−0.1442 (3)	0.07002 (10)	0.0316 (6)
C28	0.18027 (13)	−0.1585 (3)	0.02737 (10)	0.0336 (6)
C29	0.12798 (13)	−0.0516 (3)	0.02691 (10)	0.0316 (6)
C210	0.12758 (12)	0.0702 (3)	0.06994 (10)	0.0265 (5)
C211	0.18183 (12)	0.0882 (3)	0.11200 (9)	0.0249 (5)
C221	0.04604 (11)	0.5107 (3)	0.10293 (10)	0.0285 (5)

C222	0.03703 (12)	0.4833 (3)	0.16379 (11)	0.0330 (6)
C223	0.00275 (12)	0.5934 (3)	0.19640 (12)	0.0399 (6)
C224	−0.02376 (13)	0.7306 (3)	0.16882 (13)	0.0448 (7)
C225	−0.01514 (13)	0.7585 (3)	0.10878 (13)	0.0443 (7)
C226	0.01995 (12)	0.6496 (3)	0.07629 (12)	0.0353 (6)
C241	0.26101 (11)	0.4412 (2)	0.14320 (9)	0.0218 (5)
C242	0.30873 (12)	0.3744 (3)	0.10869 (10)	0.0306 (6)
C243	0.37224 (12)	0.4348 (3)	0.11246 (11)	0.0352 (6)
C244	0.38912 (12)	0.5630 (3)	0.14960 (11)	0.0327 (6)
C245	0.34213 (12)	0.6318 (3)	0.18363 (10)	0.0307 (5)
C246	0.27833 (11)	0.5706 (2)	0.17998 (10)	0.0257 (5)
C251	0.17183 (11)	0.1786 (3)	0.21500 (10)	0.0246 (5)
C252	0.15496 (13)	0.0075 (3)	0.23008 (10)	0.0307 (6)
H12	0.5686	0.1674	0.5218	0.030*
H192	0.5493	0.1213	0.6818	0.039*
H123	0.4936	0.3047	0.7385	0.043*
H124	0.4541	0.5456	0.6955	0.049*
H125	0.4734	0.6043	0.5954	0.048*
H126	0.5305	0.4219	0.5390	0.038*
H13A	0.6764	0.0820	0.5433	0.031*
H13B	0.6682	0.2667	0.5611	0.031*
H14	0.6660	0.1882	0.6642	0.026*
H142	0.7979	−0.0059	0.5883	0.030*
H143	0.9061	0.0847	0.5951	0.033*
H144	0.9346	0.3200	0.6477	0.038*
H145	0.8537	0.4654	0.6942	0.039*
H146	0.7452	0.3742	0.6878	0.033*
H15A	0.6384	−0.2622	0.7664	0.044*
H15B	0.6949	−0.3222	0.7251	0.044*
H15C	0.6214	−0.2974	0.6964	0.044*
H16	0.7685	−0.2689	0.6321	0.032*
H17	0.7651	−0.4704	0.5589	0.040*
H18	0.6748	−0.4909	0.4894	0.039*
H19	0.5860	−0.3152	0.4942	0.038*
H22	0.0729	0.4248	0.0222	0.034*
H222	0.0545	0.3888	0.1829	0.040*
H223	−0.0026	0.5748	0.2379	0.048*
H224	−0.0478	0.8052	0.1912	0.054*
H225	−0.0332	0.8524	0.0897	0.053*
H226	0.0262	0.6705	0.0351	0.042*
H23A	0.1802	0.3427	0.0468	0.031*
H23B	0.1708	0.5274	0.0639	0.031*
H24	0.1657	0.4503	0.1666	0.028*
H242	0.2976	0.2870	0.0824	0.037*
H243	0.4045	0.3872	0.0892	0.042*
H244	0.4328	0.6040	0.1518	0.039*
H245	0.3533	0.7204	0.2094	0.037*
H246	0.2461	0.6187	0.2032	0.031*

H25A	0.1946	−0.0595	0.2297	0.046*
H25B	0.1215	−0.0333	0.2002	0.046*
H25C	0.1379	0.0037	0.2702	0.046*
H26	0.2706	−0.0079	0.1405	0.033*
H27	0.2678	−0.2196	0.0707	0.038*
H28	0.1802	−0.2422	−0.0018	0.040*
H29	0.0924	−0.0614	−0.0028	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S11	0.0231 (3)	0.0268 (3)	0.0426 (4)	−0.0020 (2)	−0.0014 (3)	0.0020 (3)
C12	0.0223 (13)	0.0234 (11)	0.0300 (12)	0.0000 (9)	−0.0015 (10)	0.0066 (10)
C121	0.0158 (12)	0.0278 (12)	0.0343 (13)	−0.0013 (10)	−0.0029 (10)	0.0012 (10)
C122	0.0243 (14)	0.0346 (13)	0.0376 (14)	−0.0003 (10)	−0.0043 (11)	0.0049 (11)
C123	0.0250 (14)	0.0475 (15)	0.0360 (13)	0.0012 (12)	0.0013 (11)	−0.0034 (12)
C124	0.0328 (15)	0.0380 (15)	0.0527 (17)	0.0034 (12)	0.0038 (13)	−0.0135 (13)
C125	0.0374 (16)	0.0276 (13)	0.0543 (17)	0.0035 (11)	−0.0022 (13)	0.0006 (12)
C126	0.0269 (14)	0.0293 (13)	0.0382 (13)	−0.0009 (11)	−0.0022 (11)	0.0034 (11)
C13	0.0231 (13)	0.0260 (12)	0.0273 (12)	0.0005 (10)	−0.0001 (10)	0.0066 (10)
C14	0.0218 (12)	0.0185 (10)	0.0256 (11)	0.0007 (9)	0.0021 (9)	0.0018 (9)
C141	0.0223 (12)	0.0236 (11)	0.0230 (11)	0.0020 (10)	−0.0010 (9)	0.0044 (9)
C142	0.0255 (13)	0.0252 (11)	0.0243 (11)	0.0011 (10)	0.0000 (10)	0.0006 (9)
C143	0.0220 (13)	0.0334 (13)	0.0278 (12)	0.0049 (10)	0.0020 (10)	0.0036 (10)
C144	0.0220 (13)	0.0366 (13)	0.0353 (13)	−0.0053 (11)	−0.0020 (11)	0.0050 (11)
C145	0.0308 (14)	0.0288 (13)	0.0371 (13)	−0.0037 (11)	−0.0029 (11)	−0.0037 (11)
C146	0.0264 (13)	0.0246 (11)	0.0319 (12)	0.0020 (10)	0.0010 (10)	0.0019 (10)
N15	0.0260 (11)	0.0202 (9)	0.0212 (9)	0.0009 (8)	0.0006 (8)	0.0014 (8)
C151	0.0184 (12)	0.0296 (12)	0.0263 (12)	0.0027 (10)	−0.0011 (10)	0.0017 (10)
O15	0.0413 (11)	0.0301 (9)	0.0262 (8)	0.0008 (8)	0.0024 (8)	−0.0046 (7)
C152	0.0314 (14)	0.0303 (12)	0.0267 (12)	0.0011 (11)	0.0050 (10)	0.0054 (10)
C16	0.0321 (14)	0.0232 (11)	0.0259 (12)	0.0009 (10)	0.0022 (10)	0.0025 (10)
C17	0.0385 (15)	0.0261 (12)	0.0356 (13)	0.0040 (11)	0.0131 (12)	0.0050 (11)
C18	0.0491 (17)	0.0257 (12)	0.0248 (12)	−0.0025 (11)	0.0117 (12)	−0.0038 (10)
C19	0.0406 (15)	0.0303 (13)	0.0225 (12)	−0.0090 (11)	−0.0009 (11)	0.0022 (10)
C110	0.0275 (13)	0.0221 (11)	0.0256 (11)	−0.0028 (10)	0.0022 (10)	0.0018 (10)
C111	0.0260 (13)	0.0196 (11)	0.0211 (11)	0.0003 (9)	0.0042 (9)	−0.0002 (9)
S21	0.0263 (4)	0.0311 (3)	0.0371 (3)	−0.0078 (3)	−0.0034 (3)	0.0034 (3)
C22	0.0251 (13)	0.0311 (13)	0.0282 (12)	−0.0068 (10)	−0.0059 (10)	0.0057 (10)
C221	0.0187 (12)	0.0302 (12)	0.0356 (13)	−0.0056 (10)	−0.0067 (10)	0.0053 (11)
C222	0.0222 (13)	0.0386 (14)	0.0376 (14)	−0.0001 (11)	−0.0037 (11)	0.0047 (11)
C223	0.0266 (15)	0.0479 (16)	0.0448 (15)	−0.0004 (12)	−0.0002 (12)	−0.0025 (13)
C224	0.0344 (16)	0.0391 (15)	0.0606 (19)	0.0019 (12)	0.0011 (14)	−0.0092 (14)
C225	0.0345 (16)	0.0327 (14)	0.0642 (19)	0.0006 (12)	−0.0072 (14)	0.0072 (14)
C226	0.0314 (15)	0.0313 (13)	0.0419 (14)	−0.0083 (11)	−0.0057 (12)	0.0077 (12)
C23	0.0235 (13)	0.0259 (12)	0.0276 (12)	−0.0042 (10)	−0.0005 (10)	0.0037 (10)
C24	0.0251 (13)	0.0198 (11)	0.0253 (11)	−0.0014 (9)	0.0008 (10)	−0.0019 (9)
C241	0.0207 (12)	0.0205 (11)	0.0237 (11)	0.0007 (9)	−0.0021 (9)	0.0018 (9)

C242	0.0295 (14)	0.0301 (12)	0.0323 (13)	−0.0035 (11)	0.0019 (11)	−0.0108 (11)
C243	0.0256 (14)	0.0396 (14)	0.0410 (14)	−0.0016 (11)	0.0062 (11)	−0.0100 (12)
C244	0.0264 (14)	0.0337 (13)	0.0378 (13)	−0.0044 (11)	0.0009 (11)	−0.0031 (11)
C245	0.0295 (14)	0.0271 (12)	0.0343 (13)	−0.0039 (10)	−0.0065 (11)	−0.0060 (10)
C246	0.0256 (13)	0.0232 (11)	0.0280 (12)	0.0029 (10)	−0.0002 (10)	−0.0001 (10)
N25	0.0254 (11)	0.0232 (9)	0.0213 (9)	−0.0030 (8)	0.0004 (8)	0.0011 (8)
C251	0.0205 (12)	0.0300 (12)	0.0231 (11)	0.0023 (10)	0.0003 (9)	0.0014 (10)
O25	0.0383 (10)	0.0354 (9)	0.0240 (8)	0.0002 (8)	0.0018 (7)	−0.0033 (7)
C252	0.0332 (14)	0.0332 (13)	0.0260 (12)	−0.0018 (11)	0.0039 (11)	0.0051 (10)
C26	0.0316 (14)	0.0257 (12)	0.0256 (12)	−0.0033 (10)	0.0042 (10)	0.0038 (10)
C27	0.0437 (16)	0.0228 (12)	0.0291 (12)	−0.0005 (11)	0.0082 (11)	0.0028 (10)
C28	0.0525 (17)	0.0228 (12)	0.0261 (12)	−0.0102 (12)	0.0077 (12)	−0.0017 (10)
C29	0.0409 (16)	0.0296 (13)	0.0242 (12)	−0.0146 (11)	0.0003 (11)	0.0026 (10)
C210	0.0294 (14)	0.0252 (12)	0.0248 (11)	−0.0087 (10)	0.0010 (10)	0.0040 (10)
C211	0.0303 (13)	0.0228 (11)	0.0218 (11)	−0.0043 (10)	0.0033 (10)	0.0025 (9)

Geometric parameters (Å, º)

S11—C110	1.761 (2)	S21—C210	1.768 (2)
S11—C12	1.845 (2)	S21—C22	1.848 (2)
C12—C121	1.521 (3)	C22—C221	1.518 (3)
C12—C13	1.534 (3)	C22—C23	1.531 (3)
C12—H12	1.00	C22—H22	1.00
C121—C126	1.386 (3)	C221—C226	1.386 (3)
C121—C122	1.396 (3)	C221—C222	1.398 (3)
C122—C123	1.380 (3)	C222—C223	1.384 (3)
C122—H192	0.95	C222—H222	0.95
C123—C124	1.385 (4)	C223—C224	1.386 (4)
C123—H123	0.95	C223—H223	0.95
C124—C125	1.384 (4)	C224—C225	1.379 (4)
C124—H124	0.95	C224—H224	0.95
C125—C126	1.386 (3)	C225—C226	1.385 (4)
C125—H125	0.95	C225—H225	0.95
C126—H126	0.95	C226—H226	0.95
C13—C14	1.529 (3)	C23—C24	1.523 (3)
C13—H13A	0.99	C23—H23A	0.99
C13—H13B	0.99	C23—H23B	0.99
C14—N15	1.483 (3)	C24—N25	1.483 (3)
C14—C141	1.515 (3)	C24—C241	1.516 (3)
C14—H14	1.00	C24—H24	1.00
C141—C146	1.388 (3)	C241—C246	1.382 (3)
C141—C142	1.393 (3)	C241—C242	1.393 (3)
C142—C143	1.380 (3)	C242—C243	1.384 (3)
C142—H142	0.95	C242—H242	0.95
C143—C144	1.382 (3)	C243—C244	1.377 (3)
C143—H143	0.95	C243—H243	0.95
C144—C145	1.384 (3)	C244—C245	1.383 (3)
C144—H144	0.95	C244—H244	0.95

C145—C146	1.386 (3)	C245—C246	1.392 (3)
C145—H145	0.95	C245—H245	0.95
C146—H146	0.95	C246—H246	0.95
N15—C151	1.373 (3)	N25—C251	1.368 (3)
N15—C111	1.429 (3)	N25—C211	1.427 (3)
C151—O15	1.224 (3)	C251—O25	1.229 (3)
C151—C152	1.498 (3)	C251—C252	1.505 (3)
C152—H15A	0.98	C252—H25A	0.98
C152—H15B	0.98	C252—H25B	0.98
C152—H15C	0.98	C252—H25C	0.98
C16—C111	1.384 (3)	C26—C211	1.388 (3)
C16—C17	1.386 (3)	C26—C27	1.394 (3)
C16—H16	0.95	C26—H26	0.95
C17—C18	1.379 (4)	C27—C28	1.384 (3)
C17—H17	0.95	C27—H27	0.95
C18—C19	1.386 (3)	C28—C29	1.385 (4)
C18—H18	0.95	C28—H28	0.95
C19—C110	1.393 (3)	C29—C210	1.393 (3)
C19—H19	0.95	C29—H29	0.95
C110—C111	1.404 (3)	C210—C211	1.407 (3)

C110—S11—C12	103.17 (10)	C210—S21—C22	103.86 (10)
C121—C12—C13	113.52 (18)	C221—C22—C23	113.77 (18)
C121—C12—S11	109.46 (15)	C221—C22—S21	109.57 (15)
C13—C12—S11	113.79 (15)	C23—C22—S21	113.57 (16)
C121—C12—H12	106.5	C221—C22—H22	106.5
C13—C12—H12	106.5	C23—C22—H22	106.5
S11—C12—H12	106.5	S21—C22—H22	106.5
C126—C121—C122	118.1 (2)	C226—C221—C222	118.5 (2)
C126—C121—C12	118.5 (2)	C226—C221—C22	118.7 (2)
C122—C121—C12	123.4 (2)	C222—C221—C22	122.7 (2)
C123—C122—C121	120.8 (2)	C223—C222—C221	120.3 (2)
C123—C122—H192	119.6	C223—C222—H222	119.9
C121—C122—H192	119.6	C221—C222—H222	119.9
C122—C123—C124	120.5 (2)	C222—C223—C224	120.4 (3)
C122—C123—H123	119.7	C222—C223—H223	119.8
C124—C123—H123	119.7	C224—C223—H223	119.8
C125—C124—C123	119.4 (2)	C225—C224—C223	119.7 (3)
C125—C124—H124	120.3	C225—C224—H224	120.1
C123—C124—H124	120.3	C223—C224—H224	120.1
C124—C125—C126	119.9 (2)	C224—C225—C226	120.0 (2)
C124—C125—H125	120.0	C224—C225—H225	120.0
C126—C125—H125	120.0	C226—C225—H225	120.0
C125—C126—C121	121.3 (2)	C225—C226—C221	121.1 (2)
C125—C126—H126	119.3	C225—C226—H226	119.5
C121—C126—H126	119.3	C221—C226—H226	119.5
C14—C13—C12	116.75 (18)	C24—C23—C22	117.13 (18)
C14—C13—H13A	108.1	C24—C23—H23A	108.0

C12—C13—H13A	108.1	C22—C23—H23A	108.0
C14—C13—H13B	108.1	C24—C23—H23B	108.0
C12—C13—H13B	108.1	C22—C23—H23B	108.0
H13A—C13—H13B	107.3	H23A—C23—H23B	107.3
N15—C14—C141	113.22 (17)	N25—C24—C241	113.98 (18)
N15—C14—C13	111.74 (17)	N25—C24—C23	111.82 (17)
C141—C14—C13	110.08 (17)	C241—C24—C23	109.96 (18)
N15—C14—H14	107.2	N25—C24—H24	106.9
C141—C14—H14	107.2	C241—C24—H24	106.9
C13—C14—H14	107.2	C23—C24—H24	106.9
C146—C141—C142	118.4 (2)	C246—C241—C242	118.4 (2)
C146—C141—C14	118.9 (2)	C246—C241—C24	119.56 (19)
C142—C141—C14	122.66 (19)	C242—C241—C24	121.88 (19)
C143—C142—C141	120.5 (2)	C243—C242—C241	120.4 (2)
C143—C142—H142	119.8	C243—C242—H242	119.8
C141—C142—H142	119.8	C241—C242—H242	119.8
C142—C143—C144	120.6 (2)	C244—C243—C242	120.7 (2)
C142—C143—H143	119.7	C244—C243—H243	119.7
C144—C143—H143	119.7	C242—C243—H243	119.7
C143—C144—C145	119.6 (2)	C243—C244—C245	119.6 (2)
C143—C144—H144	120.2	C243—C244—H244	120.2
C145—C144—H144	120.2	C245—C244—H244	120.2
C144—C145—C146	119.8 (2)	C244—C245—C246	119.6 (2)
C144—C145—H145	120.1	C244—C245—H245	120.2
C146—C145—H145	120.1	C246—C245—H245	120.2
C145—C146—C141	121.2 (2)	C241—C246—C245	121.2 (2)
C145—C146—H146	119.4	C241—C246—H246	119.4
C141—C146—H146	119.4	C245—C246—H246	119.4
C151—N15—C111	121.14 (17)	C251—N25—C211	121.01 (18)
C151—N15—C14	118.90 (17)	C251—N25—C24	118.86 (18)
C111—N15—C14	119.87 (16)	C211—N25—C24	120.07 (16)
O15—C151—N15	120.8 (2)	O25—C251—N25	120.9 (2)
O15—C151—C152	122.3 (2)	O25—C251—C252	121.72 (19)
N15—C151—C152	116.93 (19)	N25—C251—C252	117.41 (19)
C151—C152—H15A	109.5	C251—C252—H25A	109.5
C151—C152—H15B	109.5	C251—C252—H25B	109.5
H15A—C152—H15B	109.5	H25A—C252—H25B	109.5
C151—C152—H15C	109.5	C251—C252—H25C	109.5
H15A—C152—H15C	109.5	H25A—C252—H25C	109.5
H15B—C152—H15C	109.5	H25B—C252—H25C	109.5
C111—C16—C17	120.2 (2)	C211—C26—C27	119.8 (2)
C111—C16—H16	119.9	C211—C26—H26	120.1
C17—C16—H16	119.9	C27—C26—H26	120.1
C18—C17—C16	120.0 (2)	C28—C27—C26	120.2 (2)
C18—C17—H17	120.0	C28—C27—H27	119.9
C16—C17—H17	120.0	C26—C27—H27	119.9
C17—C18—C19	120.3 (2)	C27—C28—C29	120.4 (2)
C17—C18—H18	119.8	C27—C28—H28	119.8

C19—C18—H18	119.8	C29—C28—H28	119.8
C18—C19—C110	120.3 (2)	C28—C29—C210	120.0 (2)
C18—C19—H19	119.8	C28—C29—H29	120.0
C110—C19—H19	119.8	C210—C29—H29	120.0
C19—C110—C111	118.9 (2)	C29—C210—C211	119.6 (2)
C19—C110—S11	119.55 (18)	C29—C210—S21	119.66 (18)
C111—C110—S11	121.26 (16)	C211—C210—S21	120.49 (17)
C16—C111—C110	120.13 (19)	C26—C211—C210	119.9 (2)
C16—C111—N15	120.5 (2)	C26—C211—N25	120.0 (2)
C110—C111—N15	119.40 (19)	C210—C211—N25	120.0 (2)

C110—S11—C12—C121	−146.32 (15)	C210—S21—C22—C221	−146.81 (15)
C110—S11—C12—C13	−18.1 (2)	C210—S21—C22—C23	−18.37 (19)
C13—C12—C121—C126	95.0 (2)	C23—C22—C221—C226	99.2 (2)
S11—C12—C121—C126	−136.62 (19)	S21—C22—C221—C226	−132.44 (19)
C13—C12—C121—C122	−83.6 (3)	C23—C22—C221—C222	−79.2 (3)
S11—C12—C121—C122	44.7 (3)	S21—C22—C221—C222	49.1 (3)
C126—C121—C122—C123	0.8 (4)	C226—C221—C222—C223	−0.1 (3)
C12—C121—C122—C123	179.5 (2)	C22—C221—C222—C223	178.4 (2)
C121—C122—C123—C124	0.3 (4)	C221—C222—C223—C224	0.9 (4)
C122—C123—C124—C125	−0.9 (4)	C222—C223—C224—C225	−0.9 (4)
C123—C124—C125—C126	0.5 (4)	C223—C224—C225—C226	0.0 (4)
C124—C125—C126—C121	0.6 (4)	C224—C225—C226—C221	0.9 (4)
C122—C121—C126—C125	−1.3 (4)	C222—C221—C226—C225	−0.9 (4)
C12—C121—C126—C125	180.0 (2)	C22—C221—C226—C225	−179.4 (2)
C121—C12—C13—C14	61.4 (3)	C221—C22—C23—C24	61.8 (3)
S11—C12—C13—C14	−64.6 (2)	S21—C22—C23—C24	−64.5 (2)
C12—C13—C14—N15	64.1 (2)	C22—C23—C24—N25	64.2 (2)
C12—C13—C14—C141	−169.21 (18)	C22—C23—C24—C241	−168.13 (18)
N15—C14—C141—C146	−129.7 (2)	N25—C24—C241—C246	−121.1 (2)
C13—C14—C141—C146	104.4 (2)	C23—C24—C241—C246	112.4 (2)
N15—C14—C141—C142	52.5 (3)	N25—C24—C241—C242	63.2 (3)
C13—C14—C141—C142	−73.4 (3)	C23—C24—C241—C242	−63.3 (3)
C146—C141—C142—C143	1.4 (3)	C246—C241—C242—C243	1.4 (3)
C14—C141—C142—C143	179.2 (2)	C24—C241—C242—C243	177.2 (2)
C141—C142—C143—C144	−0.8 (3)	C241—C242—C243—C244	−1.0 (4)
C142—C143—C144—C145	0.0 (3)	C242—C243—C244—C245	0.2 (4)
C143—C144—C145—C146	0.2 (4)	C243—C244—C245—C246	0.0 (4)
C144—C145—C146—C141	0.4 (4)	C242—C241—C246—C245	−1.2 (3)
C142—C141—C146—C145	−1.2 (3)	C24—C241—C246—C245	−177.1 (2)
C14—C141—C146—C145	−179.1 (2)	C244—C245—C246—C241	0.5 (3)
C141—C14—N15—C151	91.6 (2)	C241—C24—N25—C251	90.3 (2)
C13—C14—N15—C151	−143.5 (2)	C23—C24—N25—C251	−144.2 (2)
C141—C14—N15—C111	−91.9 (2)	C241—C24—N25—C211	−92.6 (2)
C13—C14—N15—C111	33.1 (3)	C23—C24—N25—C211	32.9 (3)
C111—N15—C151—O15	177.7 (2)	C211—N25—C251—O25	176.8 (2)
C14—N15—C151—O15	−5.7 (3)	C24—N25—C251—O25	−6.1 (3)
C111—N15—C151—C152	−3.0 (3)	C211—N25—C251—C252	−4.9 (3)

C14—N15—C151—C152	173.53 (19)	C24—N25—C251—C252	172.23 (19)
C111—C16—C17—C18	1.0 (3)	C211—C26—C27—C28	1.8 (3)
C16—C17—C18—C19	−1.0 (3)	C26—C27—C28—C29	−1.6 (3)
C17—C18—C19—C110	−0.1 (3)	C27—C28—C29—C210	−0.7 (3)
C18—C19—C110—C111	1.0 (3)	C28—C29—C210—C211	2.8 (3)
C18—C19—C110—S11	−173.21 (17)	C28—C29—C210—S21	−171.13 (17)
C12—S11—C110—C19	−121.78 (18)	C22—S21—C210—C29	−122.94 (18)
C12—S11—C110—C111	64.11 (19)	C22—S21—C210—C211	63.2 (2)
C17—C16—C111—C110	−0.1 (3)	C27—C26—C211—C210	0.4 (3)
C17—C16—C111—N15	−179.64 (19)	C27—C26—C211—N25	177.87 (19)
C19—C110—C111—C16	−1.0 (3)	C29—C210—C211—C26	−2.7 (3)
S11—C110—C111—C16	173.18 (16)	S21—C210—C211—C26	171.23 (16)
C19—C110—C111—N15	178.62 (18)	C29—C210—C211—N25	179.85 (19)
S11—C110—C111—N15	−7.2 (3)	S21—C210—C211—N25	−6.3 (3)
C151—N15—C111—C16	−75.7 (3)	C251—N25—C211—C26	−72.4 (3)
C14—N15—C111—C16	107.7 (2)	C24—N25—C211—C26	110.6 (2)
C151—N15—C111—C110	104.7 (2)	C251—N25—C211—C210	105.1 (2)
C14—N15—C111—C110	−71.8 (3)	C24—N25—C211—C210	−72.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C145—H145···O25^{i}	0.95	2.47	3.336 (3)	152
C245—H245···O15^{i}	0.95	2.41	3.268 (3)	150

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

(II) (2RS,4RS)-*N*-Chloroacetyl-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine

Crystal data

$C_{23}H_{20}ClNOS$
M_r = 393.92
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 12.6348 (4) Å
b = 11.9337 (5) Å
c = 12.7904 (5) Å
β = 92.549 (2)°
V = 1926.63 (13) Å^3
Z = 4
$F(000)$ = 824
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4418 reflections
θ = 3.2–27.5°
μ = 0.32 mm^{-1}
T = 120 K
Plate, colourless
0.28 × 0.24 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.926, T_{max} = 0.987
26344 measured reflections
4418 independent reflections
2950 reflections with $I > 2\sigma(I)$
R_{int} = 0.081
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −16→16
k = −15→15
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.098$
$S = 1.00$
4418 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Cl5	0.91507 (4)	0.23886 (5)	0.38523 (4)	0.03279 (15)
S1	0.62010 (4)	0.10640 (4)	0.09520 (4)	0.02562 (14)
O5	0.68726 (10)	0.23583 (11)	0.41271 (10)	0.0254 (3)
N5	0.62888 (12)	0.29611 (13)	0.25199 (12)	0.0210 (3)
C2	0.48382 (14)	0.11544 (15)	0.14149 (15)	0.0211 (4)
C3	0.45311 (15)	0.23221 (15)	0.18065 (15)	0.0223 (4)
C4	0.51655 (14)	0.27594 (15)	0.27657 (15)	0.0213 (4)
C6	0.68342 (15)	0.43814 (16)	0.12682 (15)	0.0239 (4)
C7	0.71108 (15)	0.46821 (17)	0.02638 (15)	0.0266 (4)
C8	0.70979 (16)	0.38876 (16)	−0.05196 (15)	0.0262 (4)
C9	0.67862 (15)	0.27932 (16)	−0.03213 (15)	0.0245 (4)
C10	0.65120 (15)	0.24793 (15)	0.06785 (15)	0.0219 (4)
C11	0.65492 (15)	0.32806 (15)	0.14771 (14)	0.0207 (4)
C21	0.46712 (14)	0.02588 (15)	0.22280 (15)	0.0216 (4)
C22	0.53824 (15)	0.00511 (15)	0.30613 (15)	0.0235 (4)
C23	0.51420 (16)	−0.07096 (16)	0.38456 (16)	0.0264 (4)
C24	0.41872 (17)	−0.12711 (17)	0.37951 (17)	0.0315 (5)
C25	0.34730 (17)	−0.10777 (17)	0.29671 (18)	0.0324 (5)
C26	0.37133 (15)	−0.03237 (16)	0.21828 (16)	0.0264 (4)
C41	0.46579 (14)	0.37879 (15)	0.32295 (15)	0.0218 (4)
C42	0.42153 (15)	0.36996 (17)	0.42056 (15)	0.0251 (4)
C43	0.37349 (15)	0.46205 (18)	0.46527 (16)	0.0288 (5)
C44	0.36970 (15)	0.56379 (18)	0.41354 (16)	0.0291 (5)
C45	0.41336 (16)	0.57349 (17)	0.31652 (17)	0.0299 (5)
C46	0.45954 (16)	0.48096 (16)	0.27098 (16)	0.0274 (5)
C51	0.70636 (15)	0.26827 (15)	0.32498 (15)	0.0218 (4)
C52	0.81861 (15)	0.27880 (19)	0.28850 (16)	0.0294 (5)
H2	0.4348	0.0978	0.0802	0.025*
H22	0.6043	0.0432	0.3100	0.028*
H23	0.5636	−0.0840	0.4414	0.032*
H24	0.4022	−0.1789	0.4328	0.038*
H25	0.2814	−0.1461	0.2933	0.039*
H26	0.3220	−0.0205	0.1611	0.032*
H3A	0.4607	0.2863	0.1228	0.027*

H3B	0.3773	0.2306	0.1972	0.027*
H4	0.5163	0.2157	0.3309	0.026*
H42	0.4242	0.3005	0.4568	0.030*
H43	0.3432	0.4550	0.5316	0.035*
H44	0.3373	0.6268	0.4444	0.035*
H45	0.4117	0.6435	0.2811	0.036*
H46	0.4872	0.4876	0.2034	0.033*
H52A	0.8314	0.3575	0.2680	0.035*
H52B	0.8261	0.2313	0.2258	0.035*
H6	0.6840	0.4927	0.1809	0.029*
H7	0.7308	0.5433	0.0119	0.032*
H8	0.7303	0.4089	−0.1200	0.031*
H9	0.6761	0.2257	−0.0871	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0297 (3)	0.0194 (2)	0.0285 (3)	0.0014 (2)	0.0100 (2)	0.0002 (2)
C2	0.0211 (9)	0.0201 (9)	0.0222 (10)	−0.0001 (8)	0.0011 (7)	−0.0001 (8)
C21	0.0223 (10)	0.0157 (9)	0.0272 (11)	0.0008 (8)	0.0047 (8)	−0.0049 (8)
C22	0.0246 (10)	0.0196 (9)	0.0266 (11)	−0.0006 (8)	0.0038 (8)	−0.0025 (8)
C23	0.0363 (11)	0.0198 (9)	0.0233 (11)	0.0030 (9)	0.0046 (9)	0.0005 (8)
C24	0.0424 (13)	0.0212 (10)	0.0323 (12)	−0.0009 (9)	0.0176 (10)	−0.0006 (9)
C25	0.0312 (11)	0.0226 (10)	0.0445 (14)	−0.0079 (9)	0.0145 (10)	−0.0070 (9)
C26	0.0236 (10)	0.0229 (10)	0.0329 (12)	−0.0009 (9)	0.0017 (8)	−0.0064 (9)
C3	0.0219 (9)	0.0211 (10)	0.0240 (10)	0.0027 (8)	0.0014 (8)	−0.0008 (8)
C4	0.0234 (9)	0.0201 (9)	0.0206 (10)	0.0005 (8)	0.0030 (8)	0.0008 (8)
C41	0.0211 (9)	0.0226 (10)	0.0216 (10)	0.0002 (8)	−0.0003 (8)	−0.0028 (8)
C42	0.0210 (9)	0.0286 (11)	0.0256 (11)	−0.0023 (8)	0.0014 (8)	−0.0006 (9)
C43	0.0229 (10)	0.0368 (12)	0.0270 (11)	−0.0006 (9)	0.0044 (8)	−0.0085 (9)
C44	0.0233 (10)	0.0285 (11)	0.0353 (12)	0.0031 (9)	−0.0022 (9)	−0.0126 (9)
C45	0.0346 (11)	0.0203 (10)	0.0344 (12)	0.0026 (9)	−0.0015 (9)	−0.0039 (9)
C46	0.0311 (11)	0.0247 (10)	0.0267 (11)	0.0029 (9)	0.0045 (9)	−0.0016 (8)
N5	0.0227 (8)	0.0228 (8)	0.0176 (8)	−0.0002 (7)	0.0033 (6)	0.0027 (6)
C51	0.0277 (10)	0.0183 (9)	0.0196 (10)	0.0000 (8)	0.0015 (8)	−0.0021 (8)
O5	0.0304 (8)	0.0288 (7)	0.0170 (7)	−0.0003 (6)	0.0027 (6)	0.0022 (6)
C52	0.0241 (10)	0.0399 (12)	0.0240 (11)	0.0002 (9)	−0.0011 (8)	0.0062 (9)
Cl5	0.0266 (3)	0.0420 (3)	0.0293 (3)	0.0002 (2)	−0.0039 (2)	0.0037 (2)
C6	0.0270 (10)	0.0224 (10)	0.0222 (10)	−0.0021 (8)	0.0001 (8)	−0.0008 (8)
C7	0.0299 (10)	0.0246 (10)	0.0254 (11)	−0.0031 (9)	0.0010 (8)	0.0057 (9)
C8	0.0284 (10)	0.0307 (11)	0.0197 (10)	−0.0014 (9)	0.0025 (8)	0.0079 (9)
C9	0.0284 (11)	0.0265 (10)	0.0186 (10)	0.0008 (9)	0.0030 (8)	−0.0019 (8)
C10	0.0224 (9)	0.0224 (10)	0.0212 (10)	0.0018 (8)	0.0022 (8)	0.0015 (8)
C11	0.0215 (9)	0.0235 (10)	0.0172 (10)	0.0019 (8)	0.0014 (7)	0.0031 (8)

Geometric parameters (Å, º)

S1—C10	1.7725 (19)	C42—H42	0.95
S1—C2	1.8487 (18)	C43—C44	1.383 (3)
C2—C21	1.513 (3)	C43—H43	0.95
C2—C3	1.536 (2)	C44—C45	1.385 (3)
C2—H2	1.00	C44—H44	0.95
C21—C22	1.386 (3)	C45—C46	1.389 (3)
C21—C26	1.395 (3)	C45—H45	0.95
C22—C23	1.396 (3)	C46—H46	0.95
C22—H22	0.95	N5—C51	1.363 (2)
C23—C24	1.379 (3)	N5—C11	1.439 (2)
C23—H23	0.95	C51—O5	1.221 (2)
C24—C25	1.380 (3)	C51—C52	1.518 (3)
C24—H24	0.95	C52—Cl5	1.763 (2)
C25—C26	1.391 (3)	C52—H52A	0.99
C25—H25	0.95	C52—H52B	0.99
C26—H26	0.95	C6—C11	1.391 (3)
C3—C4	1.527 (3)	C6—C7	1.393 (3)
C3—H3A	0.99	C6—H6	0.95
C3—H3B	0.99	C7—C8	1.379 (3)
C4—N5	1.487 (2)	C7—H7	0.95
C4—C41	1.518 (3)	C8—C9	1.391 (3)
C4—H4	1.00	C8—H8	0.95
C41—C46	1.389 (3)	C9—C10	1.391 (3)
C41—C42	1.394 (3)	C9—H9	0.95
C42—C43	1.391 (3)	C10—C11	1.399 (3)
C10—S1—C2	103.03 (8)	C44—C43—C42	120.24 (18)
C21—C2—C3	111.82 (15)	C44—C43—H43	119.9
C21—C2—S1	109.84 (12)	C42—C43—H43	119.9
C3—C2—S1	114.18 (13)	C43—C44—C45	119.70 (18)
C21—C2—H2	106.9	C43—C44—H44	120.1
C3—C2—H2	106.9	C45—C44—H44	120.1
S1—C2—H2	106.9	C44—C45—C46	120.06 (19)
C22—C21—C26	118.33 (18)	C44—C45—H45	120.0
C22—C21—C2	123.36 (16)	C46—C45—H45	120.0
C26—C21—C2	118.10 (17)	C45—C46—C41	120.86 (18)
C21—C22—C23	120.97 (18)	C45—C46—H46	119.6
C21—C22—H22	119.5	C41—C46—H46	119.6
C23—C22—H22	119.5	C51—N5—C11	120.82 (15)
C24—C23—C22	120.0 (2)	C51—N5—C4	118.61 (14)
C24—C23—H23	120.0	C11—N5—C4	119.90 (15)
C22—C23—H23	120.0	O5—C51—N5	122.77 (17)
C23—C24—C25	119.71 (19)	O5—C51—C52	122.29 (17)
C23—C24—H24	120.1	N5—C51—C52	114.93 (16)
C25—C24—H24	120.1	C51—C52—Cl5	112.83 (14)
C24—C25—C26	120.35 (19)	C51—C52—H52A	109.0

C24—C25—H25	119.8	Cl5—C52—H52A	109.0
C26—C25—H25	119.8	C51—C52—H52B	109.0
C25—C26—C21	120.6 (2)	Cl5—C52—H52B	109.0
C25—C26—H26	119.7	H52A—C52—H52B	107.8
C21—C26—H26	119.7	C11—C6—C7	119.87 (18)
C4—C3—C2	116.15 (16)	C11—C6—H6	120.1
C4—C3—H3A	108.2	C7—C6—H6	120.1
C2—C3—H3A	108.2	C8—C7—C6	119.84 (18)
C4—C3—H3B	108.2	C8—C7—H7	120.1
C2—C3—H3B	108.2	C6—C7—H7	120.1
H3A—C3—H3B	107.4	C7—C8—C9	120.49 (18)
N5—C4—C41	112.07 (15)	C7—C8—H8	119.8
N5—C4—C3	110.93 (14)	C9—C8—H8	119.8
C41—C4—C3	112.00 (15)	C8—C9—C10	120.31 (18)
N5—C4—H4	107.2	C8—C9—H9	119.8
C41—C4—H4	107.2	C10—C9—H9	119.8
C3—C4—H4	107.2	C9—C10—C11	119.05 (17)
C46—C41—C42	118.57 (17)	C9—C10—S1	120.30 (15)
C46—C41—C4	122.60 (16)	C11—C10—S1	120.53 (14)
C42—C41—C4	118.82 (17)	C6—C11—C10	120.39 (17)
C43—C42—C41	120.54 (19)	C6—C11—N5	120.00 (17)
C43—C42—H42	119.7	C10—C11—N5	119.61 (16)
C41—C42—H42	119.7		

C10—S1—C2—C21	−147.32 (13)	C4—C41—C46—C45	−179.36 (18)
C10—S1—C2—C3	−20.80 (16)	C41—C4—N5—C51	93.70 (19)
C3—C2—C21—C22	−80.5 (2)	C3—C4—N5—C51	−140.30 (17)
S1—C2—C21—C22	47.4 (2)	C41—C4—N5—C11	−95.62 (19)
C3—C2—C21—C26	94.2 (2)	C3—C4—N5—C11	30.4 (2)
S1—C2—C21—C26	−138.00 (15)	C11—N5—C51—O5	−176.57 (17)
C26—C21—C22—C23	−0.9 (3)	C4—N5—C51—O5	−6.0 (3)
C2—C21—C22—C23	173.68 (17)	C11—N5—C51—C52	2.5 (3)
C21—C22—C23—C24	0.3 (3)	C4—N5—C51—C52	173.09 (16)
C22—C23—C24—C25	0.0 (3)	O5—C51—C52—Cl5	0.3 (3)
C23—C24—C25—C26	0.3 (3)	N5—C51—C52—Cl5	−178.73 (14)
C24—C25—C26—C21	−0.9 (3)	C11—C6—C7—C8	0.2 (3)
C22—C21—C26—C25	1.2 (3)	C6—C7—C8—C9	1.5 (3)
C2—C21—C26—C25	−173.69 (17)	C7—C8—C9—C10	−1.8 (3)
C21—C2—C3—C4	62.1 (2)	C8—C9—C10—C11	0.3 (3)
S1—C2—C3—C4	−63.4 (2)	C8—C9—C10—S1	−175.75 (15)
C2—C3—C4—N5	66.3 (2)	C2—S1—C10—C9	−121.43 (16)
C2—C3—C4—C41	−167.65 (15)	C2—S1—C10—C11	62.6 (2)
N5—C4—C41—C46	58.2 (2)	C7—C6—C11—C10	−1.7 (3)
C3—C4—C41—C46	−67.2 (2)	C7—C6—C11—N5	178.44 (17)
N5—C4—C41—C42	−123.23 (18)	C9—C10—C11—C6	1.4 (3)
C3—C4—C41—C42	111.4 (2)	S1—C10—C11—C6	177.46 (14)
C46—C41—C42—C43	−0.8 (3)	C9—C10—C11—N5	−178.70 (17)
C4—C41—C42—C43	−179.44 (17)	S1—C10—C11—N5	−2.6 (2)

C41—C42—C43—C44	−0.4 (3)	C51—N5—C11—C6	−83.9 (2)
C42—C43—C44—C45	0.4 (3)	C4—N5—C11—C6	105.6 (2)
C43—C44—C45—C46	0.8 (3)	C51—N5—C11—C10	96.2 (2)
C44—C45—C46—C41	−2.1 (3)	C4—N5—C11—C10	−74.3 (2)
C42—C41—C46—C45	2.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24—H24···O5^{i}	0.95	2.42	3.295 (3)	153
C44—H44···O5^{ii}	0.95	2.48	3.364 (2)	154

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

(III) (2RS,4RS)-*N*-Benzoyl-2,3,4,5-tetrahydro-2,4-diphenyl-1,5-benzothiazepine

Crystal data

$C_{28}H_{23}NOS$
M_r = 421.53
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 30.1891 (8) Å
b = 14.8005 (3) Å
c = 9.7965 (3) Å
β = 102.2570 (16)°
V = 4277.43 (19) Å^3
Z = 8
F(000) = 1776
D_x = 1.309 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4894 reflections
θ = 3.0–27.5°
µ = 0.17 mm^{-1}
T = 120 K
Block, colourless
0.36 × 0.26 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and *ω* scans with *κ* offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.937, T_{max} = 0.973
21732 measured reflections
4894 independent reflections
3535 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −39→35
k = −19→18
l = −11→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.109
S = 1.03
4894 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 1.1026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.094107 (14)	0.42954 (3)	0.77386 (4)	0.02642 (13)

O5	0.17444 (4)	0.15956 (8)	0.69736 (13)	0.0315 (3)
N5	0.12068 (4)	0.26493 (8)	0.62342 (14)	0.0208 (3)
C2	0.14420 (5)	0.46165 (11)	0.70379 (17)	0.0232 (4)
C3	0.14544 (6)	0.41805 (10)	0.56286 (17)	0.0228 (3)
C4	0.15486 (5)	0.31680 (10)	0.56536 (16)	0.0213 (3)
C6	0.04472 (6)	0.24342 (11)	0.47728 (17)	0.0252 (4)
C7	0.00021 (6)	0.27212 (12)	0.43145 (18)	0.0289 (4)
C8	−0.01450 (6)	0.35052 (12)	0.48598 (18)	0.0297 (4)
C9	0.01483 (6)	0.39916 (11)	0.58627 (18)	0.0256 (4)
C10	0.05930 (5)	0.37055 (11)	0.63496 (17)	0.0222 (3)
C11	0.07424 (5)	0.29148 (10)	0.57957 (16)	0.0212 (3)
C21	0.18738 (5)	0.44868 (10)	0.81379 (16)	0.0211 (3)
C22	0.22147 (6)	0.51296 (11)	0.82174 (18)	0.0258 (4)
C23	0.26166 (6)	0.50527 (12)	0.92018 (19)	0.0300 (4)
C24	0.26810 (6)	0.43394 (12)	1.01364 (19)	0.0290 (4)
C25	0.23471 (6)	0.36931 (11)	1.00595 (17)	0.0274 (4)
C26	0.19454 (6)	0.37592 (11)	0.90624 (17)	0.0234 (4)
C41	0.15783 (5)	0.27965 (10)	0.42232 (16)	0.0205 (3)
C42	0.12596 (6)	0.30039 (11)	0.30132 (17)	0.0237 (4)
C43	0.12925 (6)	0.26244 (12)	0.17391 (18)	0.0270 (4)
C44	0.16410 (6)	0.20381 (11)	0.16507 (18)	0.0285 (4)
C45	0.19614 (6)	0.18313 (12)	0.28431 (18)	0.0291 (4)
C46	0.19296 (6)	0.22055 (11)	0.41200 (18)	0.0251 (4)
C51	0.10328 (6)	0.12645 (10)	0.74628 (17)	0.0239 (4)
C52	0.07184 (6)	0.15941 (11)	0.81872 (18)	0.0290 (4)
C53	0.04732 (7)	0.10049 (13)	0.8830 (2)	0.0378 (5)
C54	0.05359 (7)	0.00808 (13)	0.8753 (2)	0.0428 (5)
C55	0.08459 (7)	−0.02543 (12)	0.8026 (2)	0.0427 (5)
C56	0.10975 (6)	0.03312 (11)	0.7399 (2)	0.0332 (4)
C57	0.13505 (6)	0.18430 (11)	0.68621 (17)	0.0243 (4)
H2	0.1415	0.5282	0.6860	0.028*
H22	0.2171	0.5627	0.7589	0.031*
H23	0.2849	0.5491	0.9236	0.036*
H24	0.2954	0.4295	1.0827	0.035*
H25	0.2392	0.3199	1.0693	0.033*
H26	0.1719	0.3307	0.9011	0.028*
H3A	0.1159	0.4292	0.4985	0.027*
H3B	0.1690	0.4489	0.5235	0.027*
H4	0.1850	0.3068	0.6292	0.026*
H42	0.1018	0.3407	0.3058	0.028*
H43	0.1073	0.2770	0.0921	0.032*
H44	0.1661	0.1779	0.0778	0.034*
H45	0.2204	0.1433	0.2789	0.035*
H46	0.2150	0.2057	0.4934	0.030*
H52	0.0672	0.2227	0.8240	0.035*
H53	0.0260	0.1235	0.9329	0.045*
H54	0.0366	−0.0322	0.9198	0.051*
H55	0.0886	−0.0888	0.7958	0.051*

H56	0.1316	0.0099	0.6922	0.040*
H6	0.0550	0.1906	0.4384	0.030*
H7	−0.0201	0.2382	0.3630	0.035*
H8	−0.0448	0.3706	0.4541	0.036*
H9	0.0046	0.4529	0.6226	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0271 (2)	0.0301 (2)	0.0232 (2)	−0.00194 (18)	0.00794 (17)	−0.00742 (18)
C2	0.0304 (9)	0.0193 (8)	0.0210 (8)	−0.0017 (7)	0.0079 (7)	−0.0007 (7)
C21	0.0266 (8)	0.0202 (8)	0.0184 (8)	−0.0001 (6)	0.0092 (6)	−0.0043 (6)
C22	0.0338 (9)	0.0232 (8)	0.0244 (9)	−0.0018 (7)	0.0155 (7)	−0.0006 (7)
C23	0.0274 (9)	0.0324 (9)	0.0329 (10)	−0.0069 (7)	0.0124 (8)	−0.0079 (8)
C24	0.0249 (9)	0.0380 (10)	0.0245 (9)	0.0021 (8)	0.0060 (7)	−0.0084 (8)
C25	0.0365 (10)	0.0260 (8)	0.0209 (9)	0.0034 (7)	0.0090 (7)	−0.0009 (7)
C26	0.0292 (9)	0.0200 (8)	0.0220 (9)	−0.0040 (7)	0.0073 (7)	−0.0034 (7)
C3	0.0277 (8)	0.0223 (8)	0.0190 (8)	−0.0016 (7)	0.0063 (7)	0.0003 (7)
C4	0.0245 (8)	0.0221 (8)	0.0178 (8)	−0.0003 (6)	0.0057 (6)	0.0003 (6)
C41	0.0239 (8)	0.0192 (7)	0.0199 (8)	−0.0034 (6)	0.0080 (6)	−0.0005 (6)
C42	0.0254 (8)	0.0245 (8)	0.0228 (9)	0.0024 (7)	0.0083 (7)	−0.0009 (7)
C43	0.0294 (9)	0.0326 (9)	0.0192 (9)	0.0020 (7)	0.0053 (7)	0.0003 (7)
C44	0.0352 (10)	0.0305 (9)	0.0223 (9)	0.0009 (8)	0.0121 (7)	−0.0039 (7)
C45	0.0305 (9)	0.0306 (9)	0.0286 (9)	0.0062 (7)	0.0120 (7)	−0.0023 (8)
C46	0.0254 (8)	0.0255 (8)	0.0250 (9)	0.0013 (7)	0.0064 (7)	0.0019 (7)
N5	0.0260 (7)	0.0185 (6)	0.0192 (7)	0.0020 (5)	0.0074 (6)	0.0032 (5)
C57	0.0322 (9)	0.0218 (8)	0.0199 (8)	0.0037 (7)	0.0080 (7)	−0.0002 (7)
O5	0.0314 (7)	0.0292 (6)	0.0357 (7)	0.0084 (5)	0.0110 (5)	0.0087 (5)
C51	0.0329 (9)	0.0210 (8)	0.0179 (8)	0.0030 (7)	0.0057 (7)	0.0028 (7)
C52	0.0419 (10)	0.0220 (8)	0.0257 (9)	0.0052 (7)	0.0128 (8)	0.0036 (7)
C53	0.0498 (12)	0.0326 (10)	0.0382 (11)	0.0089 (9)	0.0253 (9)	0.0064 (8)
C54	0.0541 (12)	0.0297 (10)	0.0526 (13)	0.0012 (9)	0.0289 (10)	0.0127 (9)
C55	0.0593 (13)	0.0206 (9)	0.0556 (14)	0.0039 (9)	0.0292 (11)	0.0067 (9)
C56	0.0426 (11)	0.0248 (9)	0.0376 (11)	0.0068 (8)	0.0206 (9)	0.0021 (8)
C6	0.0319 (9)	0.0222 (8)	0.0228 (9)	−0.0043 (7)	0.0089 (7)	−0.0019 (7)
C7	0.0283 (9)	0.0357 (10)	0.0217 (9)	−0.0090 (7)	0.0031 (7)	−0.0001 (8)
C8	0.0247 (9)	0.0351 (10)	0.0286 (9)	0.0000 (7)	0.0042 (7)	0.0054 (8)
C9	0.0282 (9)	0.0235 (8)	0.0259 (9)	0.0022 (7)	0.0072 (7)	0.0040 (7)
C10	0.0262 (8)	0.0217 (8)	0.0191 (8)	−0.0012 (6)	0.0060 (6)	0.0019 (7)
C11	0.0257 (8)	0.0203 (8)	0.0185 (8)	−0.0001 (6)	0.0064 (6)	0.0036 (6)

Geometric parameters (Å, º)

S1—C10	1.7637 (16)	C44—H44	0.95
S1—C2	1.8507 (16)	C45—C46	1.390 (2)
C2—C21	1.517 (2)	C45—H45	0.95
C2—C3	1.532 (2)	C46—H46	0.95
C2—H2	1.00	N5—C57	1.370 (2)

C21—C22	1.391 (2)	N5—C11	1.431 (2)
C21—C26	1.394 (2)	C57—O5	1.227 (2)
C22—C23	1.385 (3)	C57—C51	1.496 (2)
C22—H22	0.95	C51—C52	1.389 (2)
C23—C24	1.384 (3)	C51—C56	1.398 (2)
C23—H23	0.95	C52—C53	1.380 (3)
C24—C25	1.380 (2)	C52—H52	0.95
C24—H24	0.95	C53—C54	1.385 (3)
C25—C26	1.390 (2)	C53—H53	0.95
C25—H25	0.95	C54—C55	1.383 (3)
C26—H26	0.95	C54—H54	0.95
C3—C4	1.525 (2)	C55—C56	1.379 (3)
C3—H3A	0.99	C55—H55	0.95
C3—H3B	0.99	C56—H56	0.95
C4—N5	1.492 (2)	C6—C11	1.388 (2)
C4—C41	1.526 (2)	C6—C7	1.390 (2)
C4—H4	1.00	C6—H6	0.95
C41—C42	1.393 (2)	C7—C8	1.389 (3)
C41—C46	1.395 (2)	C7—H7	0.95
C42—C43	1.391 (2)	C8—C9	1.378 (2)
C42—H42	0.95	C8—H8	0.95
C43—C44	1.381 (2)	C9—C10	1.392 (2)
C43—H43	0.95	C9—H9	0.95
C44—C45	1.384 (2)	C10—C11	1.404 (2)

C10—S1—C2	103.94 (7)	C44—C45—C46	120.14 (16)
C21—C2—C3	113.92 (13)	C44—C45—H45	119.9
C21—C2—S1	110.53 (11)	C46—C45—H45	119.9
C3—C2—S1	113.85 (11)	C45—C46—C41	120.93 (16)
C21—C2—H2	105.9	C45—C46—H46	119.5
C3—C2—H2	105.9	C41—C46—H46	119.5
S1—C2—H2	105.9	C57—N5—C11	124.79 (13)
C22—C21—C26	118.75 (15)	C57—N5—C4	116.13 (13)
C22—C21—C2	117.84 (14)	C11—N5—C4	117.18 (12)
C26—C21—C2	123.41 (14)	O5—C57—N5	120.57 (15)
C23—C22—C21	120.73 (16)	O5—C57—C51	118.97 (14)
C23—C22—H22	119.6	N5—C57—C51	120.43 (14)
C21—C22—H22	119.6	C52—C51—C56	119.12 (15)
C24—C23—C22	120.18 (16)	C52—C51—C57	124.39 (14)
C24—C23—H23	119.9	C56—C51—C57	116.14 (15)
C22—C23—H23	119.9	C53—C52—C51	120.17 (15)
C25—C24—C23	119.61 (16)	C53—C52—H52	119.9
C25—C24—H24	120.2	C51—C52—H52	119.9
C23—C24—H24	120.2	C52—C53—C54	120.42 (17)
C24—C25—C26	120.52 (16)	C52—C53—H53	119.8
C24—C25—H25	119.7	C54—C53—H53	119.8
C26—C25—H25	119.7	C55—C54—C53	119.84 (17)
C25—C26—C21	120.18 (15)	C55—C54—H54	120.1

C25—C26—H26	119.9	C53—C54—H54	120.1
C21—C26—H26	119.9	C56—C55—C54	120.05 (17)
C4—C3—C2	116.10 (13)	C56—C55—H55	120.0
C4—C3—H3A	108.3	C54—C55—H55	120.0
C2—C3—H3A	108.3	C55—C56—C51	120.37 (16)
C4—C3—H3B	108.3	C55—C56—H56	119.8
C2—C3—H3B	108.3	C51—C56—H56	119.8
H3A—C3—H3B	107.4	C11—C6—C7	120.36 (15)
N5—C4—C3	111.71 (13)	C11—C6—H6	119.8
N5—C4—C41	110.18 (12)	C7—C6—H6	119.8
C3—C4—C41	112.75 (13)	C8—C7—C6	119.82 (16)
N5—C4—H4	107.3	C8—C7—H7	120.1
C3—C4—H4	107.3	C6—C7—H7	120.1
C41—C4—H4	107.3	C9—C8—C7	120.07 (16)
C42—C41—C46	118.36 (15)	C9—C8—H8	120.0
C42—C41—C4	122.51 (14)	C7—C8—H8	120.0
C46—C41—C4	119.11 (15)	C8—C9—C10	120.83 (16)
C43—C42—C41	120.42 (15)	C8—C9—H9	119.6
C43—C42—H42	119.8	C10—C9—H9	119.6
C41—C42—H42	119.8	C9—C10—C11	119.13 (15)
C44—C43—C42	120.70 (16)	C9—C10—S1	119.14 (13)
C44—C43—H43	119.7	C11—C10—S1	121.54 (12)
C42—C43—H43	119.7	C6—C11—C10	119.77 (15)
C43—C44—C45	119.45 (16)	C6—C11—N5	120.93 (14)
C43—C44—H44	120.3	C10—C11—N5	119.17 (14)
C45—C44—H44	120.3		

C10—S1—C2—C21	−138.65 (11)	C11—N5—C57—O5	166.53 (15)
C10—S1—C2—C3	−9.0 (2)	C4—N5—C57—O5	2.7 (2)
C3—C2—C21—C22	89.28 (17)	C11—N5—C57—C51	−15.4 (2)
S1—C2—C21—C22	−141.05 (12)	C4—N5—C57—C51	−179.24 (13)
C3—C2—C21—C26	−90.52 (18)	O5—C57—C51—C52	138.48 (18)
S1—C2—C21—C26	39.15 (19)	N5—C57—C51—C52	−39.6 (2)
C26—C21—C22—C23	−0.4 (2)	O5—C57—C51—C56	−34.6 (2)
C2—C21—C22—C23	179.76 (14)	N5—C57—C51—C56	147.28 (16)
C21—C22—C23—C24	−1.0 (3)	C56—C51—C52—C53	−0.2 (3)
C22—C23—C24—C25	1.6 (3)	C57—C51—C52—C53	−173.12 (17)
C23—C24—C25—C26	−0.7 (2)	C51—C52—C53—C54	−0.4 (3)
C24—C25—C26—C21	−0.7 (2)	C52—C53—C54—C55	−0.1 (3)
C22—C21—C26—C25	1.3 (2)	C53—C54—C55—C56	1.1 (3)
C2—C21—C26—C25	−178.91 (15)	C54—C55—C56—C51	−1.7 (3)
C21—C2—C3—C4	57.31 (18)	C52—C51—C56—C55	1.2 (3)
S1—C2—C3—C4	−70.67 (16)	C57—C51—C56—C55	174.73 (18)
C2—C3—C4—N5	58.11 (18)	C11—C6—C7—C8	1.5 (3)
C2—C3—C4—C41	−177.16 (13)	C6—C7—C8—C9	−0.7 (3)
N5—C4—C41—C42	78.61 (18)	C7—C8—C9—C10	−0.4 (3)
C3—C4—C41—C42	−47.0 (2)	C8—C9—C10—C11	0.6 (2)
N5—C4—C41—C46	−99.49 (16)	C8—C9—C10—S1	−174.59 (13)

C3—C4—C41—C46	134.95 (15)	C2—S1—C10—C9	−124.66 (14)
C46—C41—C42—C43	0.3 (2)	C2—S1—C10—C11	60.3 (2)
C4—C41—C42—C43	−177.82 (14)	C7—C6—C11—C10	−1.3 (2)
C41—C42—C43—C44	−0.1 (2)	C7—C6—C11—N5	−177.27 (15)
C42—C43—C44—C45	−0.3 (3)	C9—C10—C11—C6	0.2 (2)
C43—C44—C45—C46	0.6 (3)	S1—C10—C11—C6	175.31 (12)
C44—C45—C46—C41	−0.4 (3)	C9—C10—C11—N5	176.30 (14)
C42—C41—C46—C45	−0.1 (2)	S1—C10—C11—N5	−8.6 (2)
C4—C41—C46—C45	178.12 (15)	C57—N5—C11—C6	−62.8 (2)
C3—C4—N5—C57	−152.61 (14)	C4—N5—C11—C6	100.87 (17)
C41—C4—N5—C57	81.25 (17)	C57—N5—C11—C10	121.19 (17)
C3—C4—N5—C11	42.3 (2)	C4—N5—C11—C10	−75.1 (2)
C41—C4—N5—C11	−83.85 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···O5^{i}	0.95	2.49	3.347 (2)	150
C24—H24···O5^{ii}	0.95	2.53	3.295 (2)	138

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