

5-[(4-Methylphenyl)sulfonyl]-1-phenylthiopyrano-[4,3-*b*]indole-3(5*H*)-thione dichloromethane monosolvate

Benjamin Dassonneville, Dieter Schollmeyer and Heiner Detert*

University of Mainz, Department of Chemistry, Duesbergweg 10-14, 55099 Mainz, Germany. *Correspondence e-mail: detert@uni-mainz.de

Received 12 April 2023

Accepted 18 April 2023

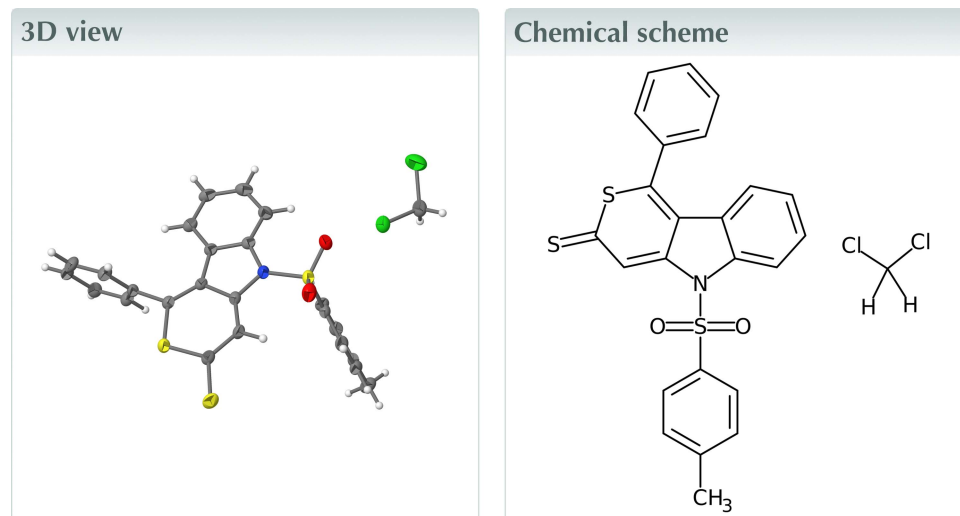
Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

Keywords: crystal structure; sulfur; annulated heterocycles.

CCDC reference: 2077250

Structural data: full structural data are available from iucrdata.iucr.org

Rhodium-catalyzed [2+2+2] cycloaddition of carbon disulfide to *o,N*-dialkynyltosylanilines gives two isomeric indolothiopyranthiones, a violet and a red isomer. This is the first crystal structure of a red isomer, which crystallizes with one solvent molecule of dichloromethane in the asymmetric unit, $C_{24}H_{17}NO_2S_3 \cdot CH_2Cl_2$. In the extended structure, centrosymmetric pairs of the planar annulated system are arranged in strands and solvent molecules fill the space between the strands.



Structure description

Transition-metal-catalyzed [2+2+2] cycloadditions are an atom-economic route to aromatic rings (Reppe *et al.*, 1948; Bönemann, 1978; Vollhardt, 1984). With tethered diynes, annulated systems are accessible, *e.g.* carbazoles and carbolines (Heller & Hapke; 2007; Dassonneville *et al.*, 2011). The first thiopyranthione was reported in 1973 (Wakatsuki & Yamazaki, 1973), followed by rare examples of this heterocycle. The $[RhCl(C_8H_{14})_2]_2$ -BINAP [BINAP is 2,2'-bis(diphenylphosphanyl)-1,1'-binaphthyl] (Tanaka *et al.*, 2006) catalyzed [2+2+2] cycloaddition of carbon disulfide to *o,N*-dialkynyltosylamides gives mainly the violet indolothiopyranthiones with a [3,4-*b*] annulation, in some cases accompanied by their red isomers differing in the annulation pattern (Dassonneville *et al.*, 2023). While the structure of the violet indolothiopyranthiones has been proven exemplarily in a single-crystal XRD study (Dassonneville *et al.*, 2010), the structures of the red isomers were hitherto only based on spectroscopic data. This report gives the first crystal structure of a red isomer. The moderate stability of the red thiopyranthione allowed crystals to be grown by slow evaporation of a solution in dichloromethane/petroleum ether. The title compound (Fig. 1) crystallizes with one

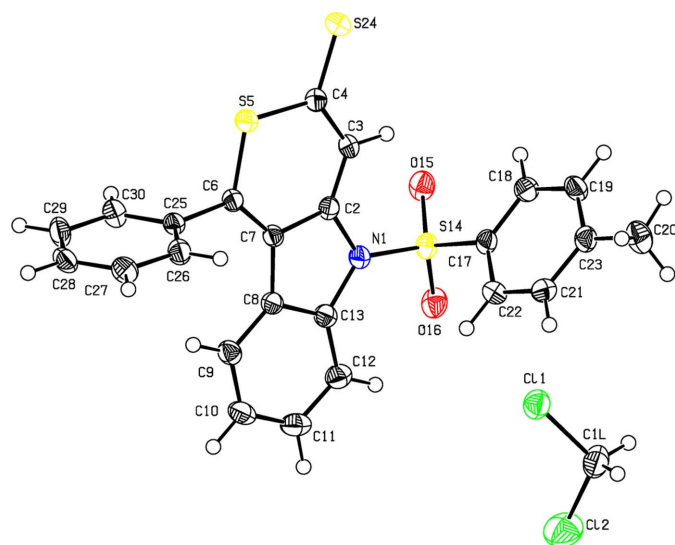


Figure 1
View of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

molecule of the solvent. Centrosymmetric pairs with a distance of 3.5556 (13) Å between the centroids of the N1/C2/C7/C8/C13 and C8–C13 π -systems are arranged in strands along the *a* axis (Fig. 2). The solvent molecules fill the volume between the strands. The heterocyclic framework is essentially planar, the maximum deviation from the mean plane of the π -system is 0.043 (2) Å at the thiocarbonyl C4 atom. With a dihedral angle of 82.44 (8)°, the phenyl ring is close to being orthogonal to the fused-ring system. The tolyl ring is also almost perpendicular [dihedral angle = 83.08 (8)°] to the plane of the three-membered ring system. The N–S–C angle of the sulfonyl group is 103.79 (9)°. The C–N bonds in the pyrrole ring are significantly different, with the N–phenyl bond [1.436 (3) Å] significantly longer than the N–thiopyrane bond

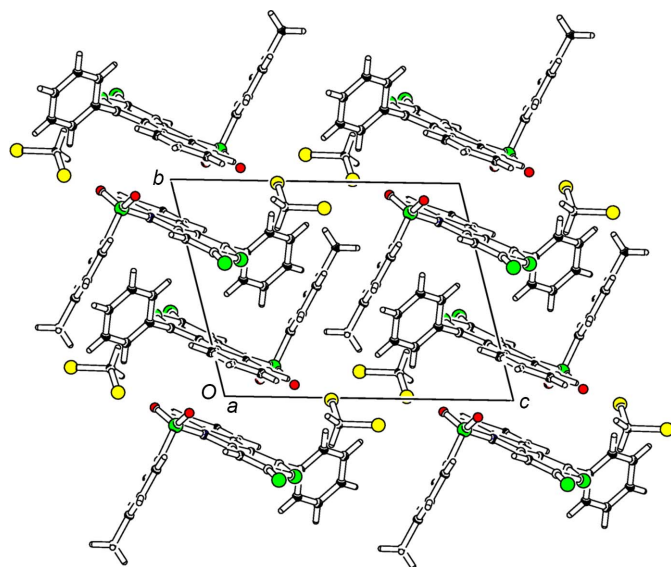


Figure 2
Part of the packing diagram, viewed along the *a* axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	C ₂₄ H ₁₇ NO ₂ S ₃ ·CH ₂ Cl ₂
<i>M</i> _r	532.49
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	193
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.8368 (14), 10.2783 (15), 13.2857 (18)
α , β , γ (°)	97.689 (9), 108.305 (8), 108.103 (8)
<i>V</i> (Å ³)	1171.6 (3)
<i>Z</i>	2
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	5.20
Crystal size (mm)	0.40 × 0.20 × 0.08
Data collection	
Diffractometer	Enraf–Nonius CAD-4
Absorption correction	Numerical (<i>CORINC</i> ; Dräger & Gattow, 1971)
<i>T</i> _{min} , <i>T</i> _{max}	0.24, 0.68
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	4706, 4431, 4039
<i>R</i> _{int}	0.029
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.609
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.038, 0.107, 1.02
No. of reflections	4431
No. of parameters	299
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.49, −0.42

Computer programs: *CAD-4 Software* (Enraf–Nonius, 1989), *CORINC* (Dräger & Gattow, 1971), *SHELXT* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b) and *PLATON* (Spek, 2020).

[1.405 (3) Å]. This and alternating bond lengths between the indole-N atom and the thiocarbonyl are an indication of an electronic coupling between the nitrogen thiocarbonyl group. Other structural features of the tricyclic core are similar to those of the isomeric system with a methyl instead of phenyl substituent. The two isomers differ in color and in the relative position of the indole-N atom to the thiocarbonyl group. In the violet isomer, these units are in perfect conjugation whereas the *meta*-conjunction in the red isomer restricts electronic interaction, thus shifting the absorption maximum about 60 nm to higher energies.

Synthesis and crystallization

The synthetic and spectroscopic details for the title compound have been reported previously (Dassonneville *et al.*, 2023).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed at calculated positions and refined in the riding-model approximation, with aromatic C–H = 0.95 Å, methylene C–H = 0.99 Å and methyl C–H = 0.98 Å, and with *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl H atoms and 1.2*U*_{eq}(C) otherwise.

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full crystallographic data

IUCrData (2023). **8**, x230354 [<https://doi.org/10.1107/S2414314623003541>]

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(I)

Crystal data

$C_{24}H_{17}NO_2S_3 \cdot CH_2Cl_2$

$M_r = 532.49$

Triclinic, $P\bar{1}$

$a = 9.8368$ (14) Å

$b = 10.2783$ (15) Å

$c = 13.2857$ (18) Å

$\alpha = 97.689$ (9)°

$\beta = 108.305$ (8)°

$\gamma = 108.103$ (8)°

$V = 1171.6$ (3) Å³

$Z = 2$

$F(000) = 548$

$D_x = 1.509$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 25 reflections

$\theta = 65\text{--}70^\circ$

$\mu = 5.20$ mm⁻¹

$T = 193$ K

Plate, red

$0.40 \times 0.20 \times 0.08$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: rotating anode

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: numerical

(CORINC; Dräger & Gattow, 1971)

$T_{\min} = 0.24$, $T_{\max} = 0.68$

4706 measured reflections

4431 independent reflections

4039 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 70.0^\circ$, $\theta_{\min} = 3.6^\circ$

$h = -11 \rightarrow 0$

$k = -11 \rightarrow 12$

$l = -15 \rightarrow 16$

3 standard reflections every 60 min

intensity decay: 2%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.107$

$S = 1.02$

4431 reflections

299 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2 + 0.8284P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.49$ e Å⁻³

$\Delta\rho_{\min} = -0.42$ e Å⁻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>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.30399 (19)	0.17913 (18)	0.10488 (13)	0.0247 (4)
C2	0.3290 (2)	0.2383 (2)	0.01978 (15)	0.0225 (4)
C3	0.4616 (2)	0.2740 (2)	−0.00101 (16)	0.0257 (4)
H3	0.546346	0.256542	0.044845	0.031*
C4	0.4787 (2)	0.3357 (2)	−0.08731 (16)	0.0260 (4)
S5	0.32556 (6)	0.36665 (6)	−0.17392 (4)	0.02863 (14)
C6	0.1753 (2)	0.3113 (2)	−0.12982 (16)	0.0233 (4)
C7	0.1890 (2)	0.2571 (2)	−0.04071 (15)	0.0217 (4)
C8	0.0808 (2)	0.2101 (2)	0.01257 (16)	0.0232 (4)
C9	−0.0709 (2)	0.2027 (2)	−0.01054 (17)	0.0274 (4)
H9	−0.121736	0.232427	−0.071261	0.033*
C10	−0.1450 (3)	0.1512 (2)	0.05678 (19)	0.0325 (5)
H10	−0.248258	0.144580	0.041628	0.039*
C11	−0.0704 (3)	0.1089 (2)	0.1464 (2)	0.0343 (5)
H11	−0.123337	0.075406	0.192183	0.041*
C12	0.0799 (3)	0.1145 (2)	0.17078 (18)	0.0306 (5)
H12	0.130386	0.085282	0.231982	0.037*
C13	0.1528 (2)	0.1643 (2)	0.10218 (16)	0.0242 (4)
S14	0.43707 (6)	0.13882 (5)	0.19537 (4)	0.02610 (14)
O15	0.51358 (18)	0.08036 (17)	0.13778 (13)	0.0340 (4)
O16	0.35700 (18)	0.05745 (16)	0.25269 (13)	0.0348 (4)
C17	0.5680 (2)	0.3040 (2)	0.28468 (16)	0.0255 (4)
C18	0.7232 (2)	0.3448 (2)	0.30206 (17)	0.0292 (4)
H18	0.758342	0.286801	0.262936	0.035*
C19	0.8268 (2)	0.4717 (2)	0.37757 (18)	0.0300 (5)
H19	0.933551	0.500361	0.389998	0.036*
C20	0.7767 (2)	0.5579 (2)	0.43548 (17)	0.0283 (4)
C21	0.6195 (3)	0.5153 (2)	0.41441 (17)	0.0296 (4)
H21	0.583515	0.574240	0.451815	0.036*
C22	0.5146 (2)	0.3889 (2)	0.34013 (17)	0.0293 (4)
H22	0.407732	0.360408	0.327132	0.035*
C23	0.8899 (3)	0.6957 (3)	0.5167 (2)	0.0407 (6)
H23A	0.864225	0.774195	0.492812	0.061*
H23B	0.994618	0.707837	0.521106	0.061*
H23C	0.884507	0.694728	0.589017	0.061*
S24	0.63754 (6)	0.38421 (7)	−0.11578 (5)	0.03617 (16)
C25	0.0371 (2)	0.3359 (2)	−0.19783 (16)	0.0241 (4)
C26	0.0170 (2)	0.4602 (2)	−0.16453 (17)	0.0296 (4)
H26	0.086969	0.525949	−0.096614	0.035*

C27	-0.1056 (3)	0.4880 (2)	-0.23081 (19)	0.0314 (5)
H27	-0.119603	0.572988	-0.208273	0.038*
C28	-0.2076 (2)	0.3919 (2)	-0.32976 (18)	0.0314 (5)
H28	-0.291812	0.410854	-0.374891	0.038*
C29	-0.1870 (3)	0.2687 (2)	-0.36283 (19)	0.0347 (5)
H29	-0.257127	0.203008	-0.430764	0.042*
C30	-0.0641 (2)	0.2401 (2)	-0.29718 (18)	0.0307 (5)
H30	-0.049704	0.155542	-0.320298	0.037*
C1L	0.4146 (3)	0.1202 (3)	0.6269 (2)	0.0428 (6)
H1L1	0.497653	0.085655	0.659362	0.051*
H1L2	0.444766	0.217600	0.670815	0.051*
Cl1	0.39459 (7)	0.12334 (6)	0.49086 (4)	0.03707 (15)
Cl2	0.24155 (10)	0.01018 (8)	0.63246 (7)	0.0643 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0217 (8)	0.0301 (9)	0.0224 (8)	0.0102 (7)	0.0071 (7)	0.0091 (7)
C2	0.0227 (9)	0.0237 (9)	0.0193 (9)	0.0093 (8)	0.0057 (7)	0.0043 (7)
C3	0.0196 (9)	0.0334 (11)	0.0231 (10)	0.0117 (8)	0.0053 (8)	0.0071 (8)
C4	0.0223 (10)	0.0309 (10)	0.0223 (9)	0.0099 (8)	0.0068 (8)	0.0031 (8)
S5	0.0234 (3)	0.0407 (3)	0.0251 (3)	0.0134 (2)	0.0100 (2)	0.0135 (2)
C6	0.0208 (9)	0.0260 (9)	0.0217 (9)	0.0094 (8)	0.0066 (8)	0.0039 (7)
C7	0.0186 (9)	0.0221 (9)	0.0214 (9)	0.0068 (7)	0.0061 (7)	0.0025 (7)
C8	0.0215 (9)	0.0231 (9)	0.0227 (9)	0.0069 (8)	0.0083 (8)	0.0025 (7)
C9	0.0235 (10)	0.0272 (10)	0.0293 (10)	0.0101 (8)	0.0087 (8)	0.0016 (8)
C10	0.0233 (10)	0.0323 (11)	0.0392 (12)	0.0074 (9)	0.0148 (9)	0.0009 (9)
C11	0.0353 (12)	0.0315 (11)	0.0389 (12)	0.0082 (9)	0.0228 (10)	0.0065 (9)
C12	0.0332 (11)	0.0310 (11)	0.0290 (10)	0.0106 (9)	0.0146 (9)	0.0088 (8)
C13	0.0230 (10)	0.0222 (9)	0.0251 (9)	0.0070 (7)	0.0088 (8)	0.0026 (7)
S14	0.0270 (3)	0.0274 (3)	0.0231 (2)	0.0119 (2)	0.0059 (2)	0.00851 (19)
O15	0.0368 (9)	0.0359 (8)	0.0311 (8)	0.0212 (7)	0.0083 (7)	0.0065 (6)
O16	0.0364 (9)	0.0340 (8)	0.0311 (8)	0.0104 (7)	0.0087 (7)	0.0158 (6)
C17	0.0249 (10)	0.0295 (10)	0.0205 (9)	0.0101 (8)	0.0059 (8)	0.0086 (8)
C18	0.0282 (11)	0.0358 (11)	0.0283 (10)	0.0171 (9)	0.0108 (9)	0.0105 (9)
C19	0.0209 (10)	0.0388 (12)	0.0316 (11)	0.0132 (9)	0.0079 (8)	0.0131 (9)
C20	0.0268 (10)	0.0320 (11)	0.0246 (10)	0.0107 (9)	0.0063 (8)	0.0114 (8)
C21	0.0299 (11)	0.0347 (11)	0.0272 (10)	0.0136 (9)	0.0130 (9)	0.0080 (9)
C22	0.0228 (10)	0.0359 (11)	0.0294 (11)	0.0109 (9)	0.0107 (8)	0.0074 (9)
C23	0.0306 (12)	0.0359 (12)	0.0424 (13)	0.0075 (10)	0.0049 (10)	0.0022 (10)
S24	0.0232 (3)	0.0523 (3)	0.0324 (3)	0.0119 (2)	0.0123 (2)	0.0099 (2)
C25	0.0207 (9)	0.0302 (10)	0.0236 (9)	0.0107 (8)	0.0085 (8)	0.0105 (8)
C26	0.0259 (10)	0.0337 (11)	0.0267 (10)	0.0128 (9)	0.0067 (8)	0.0040 (8)
C27	0.0295 (11)	0.0330 (11)	0.0360 (12)	0.0171 (9)	0.0121 (9)	0.0101 (9)
C28	0.0203 (10)	0.0405 (12)	0.0357 (11)	0.0133 (9)	0.0093 (9)	0.0157 (9)
C29	0.0235 (10)	0.0380 (12)	0.0294 (11)	0.0072 (9)	0.0000 (9)	0.0023 (9)
C30	0.0262 (11)	0.0293 (10)	0.0321 (11)	0.0108 (9)	0.0059 (9)	0.0051 (9)
C1L	0.0435 (14)	0.0464 (14)	0.0294 (12)	0.0120 (11)	0.0072 (10)	0.0091 (10)

C11	0.0385 (3)	0.0410 (3)	0.0320 (3)	0.0176 (2)	0.0107 (2)	0.0099 (2)
C12	0.0688 (5)	0.0593 (4)	0.0611 (5)	0.0072 (4)	0.0338 (4)	0.0209 (4)

Geometric parameters (Å, °)

N1—C2	1.405 (3)	C18—C19	1.389 (3)
N1—C13	1.436 (3)	C18—H18	0.9500
N1—S14	1.6771 (17)	C19—C20	1.395 (3)
C2—C3	1.367 (3)	C19—H19	0.9500
C2—C7	1.446 (3)	C20—C21	1.391 (3)
C3—C4	1.412 (3)	C20—C23	1.506 (3)
C3—H3	0.9500	C21—C22	1.382 (3)
C4—S24	1.665 (2)	C21—H21	0.9500
C4—S5	1.732 (2)	C22—H22	0.9500
S5—C6	1.721 (2)	C23—H23A	0.9800
C6—C7	1.361 (3)	C23—H23B	0.9800
C6—C25	1.494 (3)	C23—H23C	0.9800
C7—C8	1.453 (3)	C25—C30	1.386 (3)
C8—C9	1.401 (3)	C25—C26	1.388 (3)
C8—C13	1.402 (3)	C26—C27	1.388 (3)
C9—C10	1.381 (3)	C26—H26	0.9500
C9—H9	0.9500	C27—C28	1.385 (3)
C10—C11	1.391 (3)	C27—H27	0.9500
C10—H10	0.9500	C28—C29	1.380 (3)
C11—C12	1.391 (3)	C28—H28	0.9500
C11—H11	0.9500	C29—C30	1.391 (3)
C12—C13	1.383 (3)	C29—H29	0.9500
C12—H12	0.9500	C30—H30	0.9500
S14—O15	1.4257 (16)	C1L—C12	1.757 (3)
S14—O16	1.4274 (16)	C1L—C11	1.761 (2)
S14—C17	1.758 (2)	C1L—H1L1	0.9900
C17—C18	1.384 (3)	C1L—H1L2	0.9900
C17—C22	1.391 (3)		
C2—N1—C13	109.41 (16)	C17—C18—C19	119.0 (2)
C2—N1—S14	123.30 (14)	C17—C18—H18	120.5
C13—N1—S14	127.27 (14)	C19—C18—H18	120.5
C3—C2—N1	126.56 (18)	C18—C19—C20	121.1 (2)
C3—C2—C7	126.24 (18)	C18—C19—H19	119.5
N1—C2—C7	107.19 (17)	C20—C19—H19	119.5
C2—C3—C4	123.21 (18)	C21—C20—C19	118.5 (2)
C2—C3—H3	118.4	C21—C20—C23	120.8 (2)
C4—C3—H3	118.4	C19—C20—C23	120.6 (2)
C3—C4—S24	125.67 (16)	C22—C21—C20	121.3 (2)
C3—C4—S5	119.70 (15)	C22—C21—H21	119.4
S24—C4—S5	114.63 (12)	C20—C21—H21	119.4
C6—S5—C4	107.18 (10)	C21—C22—C17	119.0 (2)
C7—C6—C25	126.27 (18)	C21—C22—H22	120.5

C7—C6—S5	121.92 (15)	C17—C22—H22	120.5
C25—C6—S5	111.76 (14)	C20—C23—H23A	109.5
C6—C7—C2	121.71 (18)	C20—C23—H23B	109.5
C6—C7—C8	130.91 (18)	H23A—C23—H23B	109.5
C2—C7—C8	107.38 (17)	C20—C23—H23C	109.5
C9—C8—C13	119.53 (19)	H23A—C23—H23C	109.5
C9—C8—C7	132.47 (19)	H23B—C23—H23C	109.5
C13—C8—C7	108.00 (17)	C30—C25—C26	120.25 (19)
C10—C9—C8	118.6 (2)	C30—C25—C6	120.14 (18)
C10—C9—H9	120.7	C26—C25—C6	119.45 (18)
C8—C9—H9	120.7	C27—C26—C25	119.8 (2)
C9—C10—C11	120.9 (2)	C27—C26—H26	120.1
C9—C10—H10	119.6	C25—C26—H26	120.1
C11—C10—H10	119.6	C28—C27—C26	120.1 (2)
C10—C11—C12	121.6 (2)	C28—C27—H27	120.0
C10—C11—H11	119.2	C26—C27—H27	120.0
C12—C11—H11	119.2	C29—C28—C27	120.0 (2)
C13—C12—C11	117.3 (2)	C29—C28—H28	120.0
C13—C12—H12	121.4	C27—C28—H28	120.0
C11—C12—H12	121.4	C28—C29—C30	120.3 (2)
C12—C13—C8	122.10 (19)	C28—C29—H29	119.8
C12—C13—N1	129.92 (19)	C30—C29—H29	119.8
C8—C13—N1	107.98 (17)	C25—C30—C29	119.5 (2)
O15—S14—O16	120.02 (10)	C25—C30—H30	120.2
O15—S14—N1	108.03 (9)	C29—C30—H30	120.2
O16—S14—N1	105.28 (9)	C12—C1L—C1I	111.26 (14)
O15—S14—C17	109.01 (10)	C12—C1L—H1L1	109.4
O16—S14—C17	109.45 (10)	C1I—C1L—H1L1	109.4
N1—S14—C17	103.79 (9)	C12—C1L—H1L2	109.4
C18—C17—C22	121.13 (19)	C1I—C1L—H1L2	109.4
C18—C17—S14	119.48 (16)	H1L1—C1L—H1L2	108.0
C22—C17—S14	119.34 (16)		
C13—N1—C2—C3	176.94 (19)	C2—N1—C13—C8	2.0 (2)
S14—N1—C2—C3	-1.4 (3)	S14—N1—C13—C8	-179.75 (14)
C13—N1—C2—C7	-2.0 (2)	C2—N1—S14—O15	-39.63 (18)
S14—N1—C2—C7	179.68 (13)	C13—N1—S14—O15	142.36 (17)
N1—C2—C3—C4	-178.83 (18)	C2—N1—S14—O16	-169.00 (16)
C7—C2—C3—C4	-0.1 (3)	C13—N1—S14—O16	12.99 (19)
C2—C3—C4—S24	178.86 (16)	C2—N1—S14—C17	76.01 (17)
C2—C3—C4—S5	-1.0 (3)	C13—N1—S14—C17	-102.00 (18)
C3—C4—S5—C6	0.5 (2)	O15—S14—C17—C18	-10.2 (2)
S24—C4—S5—C6	-179.37 (11)	O16—S14—C17—C18	122.83 (17)
C4—S5—C6—C7	1.1 (2)	N1—S14—C17—C18	-125.19 (17)
C4—S5—C6—C25	178.86 (14)	O15—S14—C17—C22	172.41 (16)
C25—C6—C7—C2	-179.66 (18)	O16—S14—C17—C22	-54.52 (19)
S5—C6—C7—C2	-2.2 (3)	N1—S14—C17—C22	57.47 (18)
C25—C6—C7—C8	-0.2 (3)	C22—C17—C18—C19	1.0 (3)

S5—C6—C7—C8	177.20 (16)	S14—C17—C18—C19	-176.29 (16)
C3—C2—C7—C6	1.9 (3)	C17—C18—C19—C20	-0.1 (3)
N1—C2—C7—C6	-179.21 (17)	C18—C19—C20—C21	-1.3 (3)
C3—C2—C7—C8	-177.69 (19)	C18—C19—C20—C23	-179.6 (2)
N1—C2—C7—C8	1.2 (2)	C19—C20—C21—C22	1.7 (3)
C6—C7—C8—C9	1.2 (4)	C23—C20—C21—C22	-179.9 (2)
C2—C7—C8—C9	-179.3 (2)	C20—C21—C22—C17	-0.8 (3)
C6—C7—C8—C13	-179.5 (2)	C18—C17—C22—C21	-0.6 (3)
C2—C7—C8—C13	0.0 (2)	S14—C17—C22—C21	176.71 (16)
C13—C8—C9—C10	0.5 (3)	C7—C6—C25—C30	-100.3 (3)
C7—C8—C9—C10	179.7 (2)	S5—C6—C25—C30	82.0 (2)
C8—C9—C10—C11	0.7 (3)	C7—C6—C25—C26	84.2 (3)
C9—C10—C11—C12	-1.1 (3)	S5—C6—C25—C26	-93.4 (2)
C10—C11—C12—C13	0.2 (3)	C30—C25—C26—C27	0.4 (3)
C11—C12—C13—C8	1.1 (3)	C6—C25—C26—C27	175.86 (19)
C11—C12—C13—N1	-178.4 (2)	C25—C26—C27—C28	0.1 (3)
C9—C8—C13—C12	-1.4 (3)	C26—C27—C28—C29	-0.3 (3)
C7—C8—C13—C12	179.21 (18)	C27—C28—C29—C30	0.0 (3)
C9—C8—C13—N1	178.17 (17)	C26—C25—C30—C29	-0.7 (3)
C7—C8—C13—N1	-1.2 (2)	C6—C25—C30—C29	-176.1 (2)
C2—N1—C13—C12	-178.4 (2)	C28—C29—C30—C25	0.4 (3)
S14—N1—C13—C12	-0.2 (3)		
