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3,4,5-Trimethyl-2,4,6-triphenyl-4*H*-thiopyran

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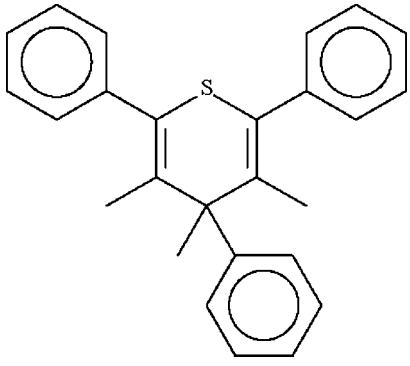
Key indicators: single-crystal X-ray study; T = 115 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.123; data-to-parameter ratio = 18.0.

The six-membered thiopyran ring in the title compound, $C_{26}H_{24}S$, adopts a boat conformation, with the S atom displaced by 0.478 (2) Å and the 3-methylene C atom by 0.644 (2) Å from the plane of the other four sp^2-hydridized C atoms. The methyl group on the methylene carbon lies in a pseudo-equatorial position and the phenyl ring in a pseudo-axial position.

Related literature

For a similar compound, see: Rahmani *et al.* (2009). For the synthesis, see: Rahmani & Pirelahi (1997).



Experimental

Crystal data

$C_{26}H_{24}S$
M_r = 368.51
Monoclinic, $P2_1/n$
a = 8.4525 (1) Å
b = 14.4732 (2) Å
c = 16.2971 (3) Å
β = 103.156 (1)°
V = 1941.37 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 115 K
0.35 × 0.35 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.840, T_{max} = 0.966
17659 measured reflections
4445 independent reflections
3576 reflections with $I > \sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.123
S = 1.05
4445 reflections
247 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2579).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Rahmani, H. & Pirelahi, H. (1997). *Sulfur Lett.* **20**, 159–163.
Rahmani, H., Pirelahi, H. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o603..
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2009). E**65**, o604 [**doi:10.1107/S1600536809005923**]

3,4,5-Trimethyl-2,4,6-triphenyl-4*H*-thiopyran

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Comment

(type here to add)

Experimental

4-Methyl-2,4,6-triphenyl-4*H*-thiopyran was was synthesized by the reaction of methyl magnesium bromide and 3,5-dimethyl-2,4,6triphenyl thiopyrylium perchlorate in dry ether under an argon atmosphere according to a reported method (Rahmani & Pirelahi, 1997). The product was isolated by TLC on neutral alumina (petroleum ether 40–60 °C) and purified by recrystalization from ethanol.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C).

Figures

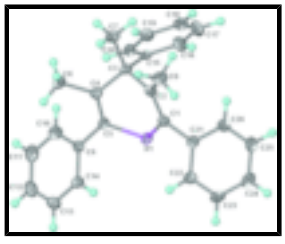


Fig. 1. Thermal ellisoid plot (Barbour, 2001) of $C_{26}H_{24}S$; probability levels are set at 70% and H-atoms are drawn as spheres of arbitrary radius.

3,4,5-Trimethyl-2,4,6-triphenyl-4*H*-thiopyran

Crystal data

$C_{26}H_{24}S$	F_{000} = 784
M_r = 368.51	D_x = 1.261 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5510 reflections
a = 8.4525 (1) Å	θ = 2.5–28.2º
b = 14.4732 (2) Å	μ = 0.17 mm^{-1}
c = 16.2971 (3) Å	T = 115 K
β = 103.156 (1)º	Block, colorless

V = 1941.37 (5) Å^3	0.35 × 0.35 × 0.20 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	4445 independent reflections
Radiation source: fine-focus sealed tube	3576 reflections with $I > \sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 115 K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.9º
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	h = −10→10
T_{min} = 0.840, T_{max} = 0.966	k = −18→18
17659 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.123	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 1.0605P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
4445 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
247 parameters	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.66266 (5)	0.60193 (3)	0.30451 (3)	0.01781 (12)
C1	0.56658 (19)	0.69496 (11)	0.34341 (10)	0.0168 (3)
C2	0.4182 (2)	0.68372 (11)	0.35910 (10)	0.0170 (3)
C3	0.32243 (19)	0.59530 (11)	0.32806 (11)	0.0165 (3)
C4	0.4297 (2)	0.51230 (12)	0.36251 (10)	0.0174 (3)
C5	0.5796 (2)	0.50682 (11)	0.34781 (10)	0.0166 (3)
C6	0.3438 (2)	0.75486 (13)	0.40643 (12)	0.0231 (4)
H6A	0.4224	0.8045	0.4257	0.035*
H6B	0.3145	0.7257	0.4552	0.035*
H6C	0.2462	0.7806	0.3692	0.035*
C7	0.1580 (2)	0.59255 (13)	0.35402 (12)	0.0223 (4)
H7A	0.1768	0.5943	0.4156	0.033*
H7B	0.1002	0.5356	0.3329	0.033*
H7C	0.0924	0.6460	0.3300	0.033*
C8	0.3661 (2)	0.43945 (13)	0.41291 (11)	0.0224 (4)

H8A	0.4540	0.3966	0.4374	0.034*
H8B	0.2777	0.4053	0.3759	0.034*
H8C	0.3253	0.4691	0.4581	0.034*
C9	0.6879 (2)	0.42489 (11)	0.36408 (10)	0.0173 (3)
C10	0.6295 (2)	0.33811 (12)	0.33442 (11)	0.0228 (4)
H10	0.5200	0.3320	0.3038	0.027*
C11	0.7283 (2)	0.26059 (13)	0.34882 (12)	0.0281 (4)
H11	0.6859	0.2019	0.3289	0.034*
C12	0.8894 (2)	0.26882 (13)	0.39231 (13)	0.0287 (4)
H12	0.9577	0.2159	0.4021	0.034*
C13	0.9494 (2)	0.35449 (14)	0.42122 (12)	0.0261 (4)
H13	1.0595	0.3602	0.4510	0.031*
C14	0.8508 (2)	0.43231 (13)	0.40722 (11)	0.0202 (4)
H14	0.8941	0.4909	0.4270	0.024*
C15	0.27841 (19)	0.59420 (11)	0.23067 (11)	0.0165 (3)
C16	0.2352 (2)	0.67542 (12)	0.18567 (12)	0.0240 (4)
H16	0.2420	0.7325	0.2151	0.029*
C17	0.1825 (2)	0.67490 (13)	0.09868 (12)	0.0270 (4)
H17	0.1534	0.7312	0.0692	0.032*
C18	0.1722 (2)	0.59257 (12)	0.05465 (11)	0.0219 (4)
H18	0.1364	0.5921	−0.0050	0.026*
C19	0.2142 (2)	0.51143 (12)	0.09817 (11)	0.0219 (4)
H19	0.2074	0.4546	0.0684	0.026*
C20	0.2667 (2)	0.51212 (12)	0.18537 (11)	0.0201 (4)
H20	0.2951	0.4555	0.2145	0.024*
C21	0.6639 (2)	0.78164 (11)	0.35383 (10)	0.0178 (3)
C22	0.8276 (2)	0.78257 (12)	0.39556 (11)	0.0201 (4)
H22	0.8794	0.7268	0.4178	0.024*
C23	0.9153 (2)	0.86471 (13)	0.40479 (12)	0.0237 (4)
H23	1.0261	0.8647	0.4342	0.028*
C24	0.8427 (2)	0.94655 (13)	0.37156 (12)	0.0251 (4)
H24	0.9032	1.0025	0.3779	0.030*
C25	0.6807 (2)	0.94582 (13)	0.32899 (11)	0.0240 (4)
H25	0.6298	1.0016	0.3061	0.029*
C26	0.5927 (2)	0.86423 (12)	0.31960 (11)	0.0207 (4)
H26	0.4824	0.8645	0.2895	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0159 (2)	0.0162 (2)	0.0235 (2)	0.00008 (15)	0.00897 (16)	0.00014 (16)
C1	0.0155 (8)	0.0169 (8)	0.0175 (8)	0.0015 (6)	0.0030 (6)	−0.0009 (6)
C2	0.0155 (8)	0.0177 (8)	0.0174 (8)	0.0014 (6)	0.0034 (6)	−0.0006 (6)
C3	0.0118 (7)	0.0179 (8)	0.0207 (8)	−0.0009 (6)	0.0054 (6)	−0.0014 (6)
C4	0.0168 (8)	0.0188 (8)	0.0163 (8)	−0.0016 (6)	0.0030 (6)	−0.0007 (6)
C5	0.0166 (8)	0.0163 (8)	0.0170 (8)	−0.0015 (6)	0.0037 (6)	0.0009 (6)
C6	0.0193 (9)	0.0250 (9)	0.0262 (9)	−0.0004 (7)	0.0077 (7)	−0.0062 (7)
C7	0.0153 (8)	0.0278 (9)	0.0254 (9)	−0.0012 (7)	0.0082 (7)	−0.0013 (7)

C8	0.0193 (9)	0.0247 (9)	0.0244 (9)	−0.0028 (7)	0.0075 (7)	0.0031 (7)
C9	0.0164 (8)	0.0189 (8)	0.0177 (8)	0.0008 (6)	0.0062 (6)	0.0019 (6)
C10	0.0217 (9)	0.0229 (9)	0.0237 (9)	−0.0003 (7)	0.0050 (7)	−0.0012 (7)
C11	0.0338 (11)	0.0217 (9)	0.0317 (10)	0.0018 (8)	0.0133 (9)	0.0009 (8)
C12	0.0294 (10)	0.0257 (10)	0.0351 (10)	0.0113 (8)	0.0160 (8)	0.0091 (8)
C13	0.0177 (9)	0.0349 (11)	0.0267 (9)	0.0053 (8)	0.0069 (7)	0.0094 (8)
C14	0.0161 (8)	0.0244 (9)	0.0210 (8)	−0.0016 (7)	0.0058 (7)	0.0023 (7)
C15	0.0092 (7)	0.0202 (8)	0.0207 (8)	−0.0001 (6)	0.0044 (6)	0.0002 (6)
C16	0.0274 (9)	0.0162 (8)	0.0263 (9)	0.0046 (7)	0.0016 (7)	−0.0038 (7)
C17	0.0314 (10)	0.0194 (9)	0.0271 (10)	0.0042 (7)	0.0000 (8)	0.0032 (7)
C18	0.0181 (8)	0.0265 (9)	0.0200 (8)	0.0004 (7)	0.0019 (7)	−0.0008 (7)
C19	0.0207 (8)	0.0186 (8)	0.0251 (9)	−0.0001 (7)	0.0027 (7)	−0.0044 (7)
C20	0.0188 (8)	0.0167 (8)	0.0239 (9)	−0.0007 (6)	0.0030 (7)	0.0014 (7)
C21	0.0177 (8)	0.0193 (8)	0.0177 (8)	−0.0010 (6)	0.0067 (6)	−0.0012 (6)
C22	0.0172 (8)	0.0211 (9)	0.0221 (8)	0.0012 (6)	0.0050 (7)	0.0000 (7)
C23	0.0160 (8)	0.0286 (10)	0.0267 (9)	−0.0041 (7)	0.0050 (7)	−0.0019 (7)
C24	0.0271 (10)	0.0227 (9)	0.0277 (10)	−0.0061 (7)	0.0106 (8)	−0.0022 (7)
C25	0.0274 (10)	0.0195 (9)	0.0256 (9)	−0.0002 (7)	0.0070 (8)	0.0038 (7)
C26	0.0188 (8)	0.0223 (9)	0.0207 (8)	0.0004 (7)	0.0039 (7)	−0.0005 (7)

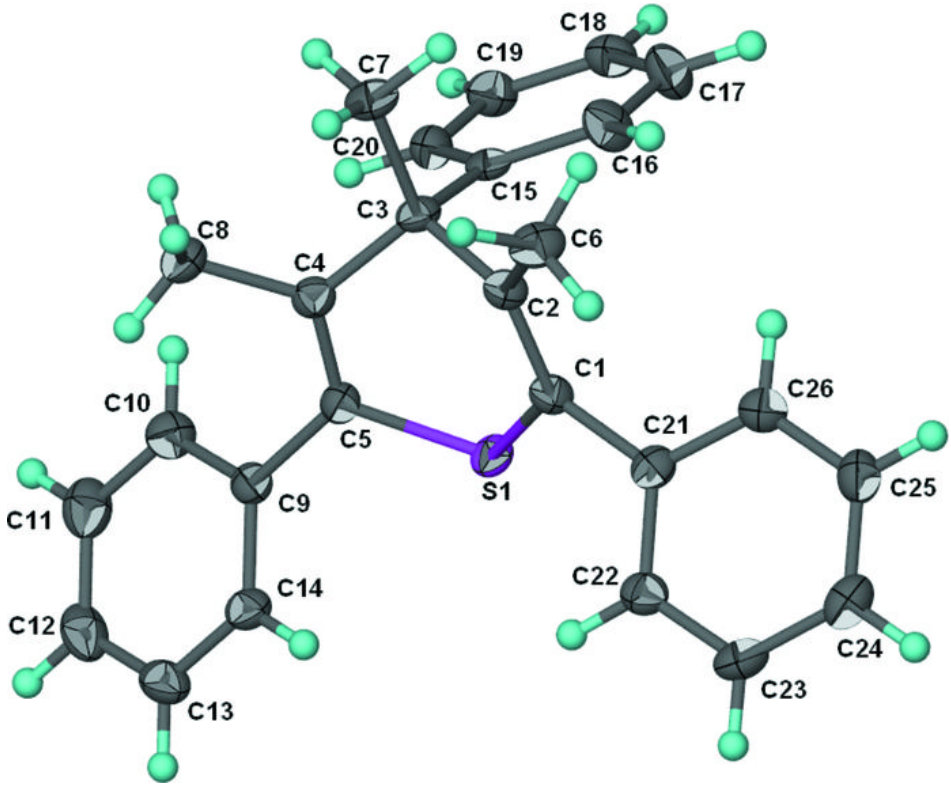
Geometric parameters (Å, °)

S1—C1	1.7631 (17)	C12—C13	1.381 (3)
S1—C5	1.7638 (16)	C12—H12	0.9500
C1—C2	1.346 (2)	C13—C14	1.389 (3)
C1—C21	1.488 (2)	C13—H13	0.9500
C2—C6	1.507 (2)	C14—H14	0.9500
C2—C3	1.537 (2)	C15—C16	1.390 (2)
C3—C4	1.532 (2)	C15—C20	1.390 (2)
C3—C7	1.543 (2)	C16—C17	1.386 (3)
C3—C15	1.546 (2)	C16—H16	0.9500
C4—C5	1.345 (2)	C17—C18	1.383 (2)
C4—C8	1.509 (2)	C17—H17	0.9500
C5—C9	1.485 (2)	C18—C19	1.376 (2)
C6—H6A	0.9800	C18—H18	0.9500
C6—H6B	0.9800	C19—C20	1.389 (2)
C6—H6C	0.9800	C19—H19	0.9500
C7—H7A	0.9800	C20—H20	0.9500
C7—H7B	0.9800	C21—C26	1.396 (2)
C7—H7C	0.9800	C21—C22	1.397 (2)
C8—H8A	0.9800	C22—C23	1.391 (2)
C8—H8B	0.9800	C22—H22	0.9500
C8—H8C	0.9800	C23—C24	1.386 (3)
C9—C10	1.395 (2)	C23—H23	0.9500
C9—C14	1.400 (2)	C24—C25	1.387 (3)
C10—C11	1.387 (3)	C24—H24	0.9500
C10—H10	0.9500	C25—C26	1.386 (2)
C11—C12	1.389 (3)	C25—H25	0.9500
C11—H11	0.9500	C26—H26	0.9500

C1—S1—C5	101.20 (8)	C13—C12—C11	119.49 (17)
C2—C1—C21	126.50 (15)	C13—C12—H12	120.3
C2—C1—S1	120.10 (13)	C11—C12—H12	120.3
C21—C1—S1	113.39 (12)	C12—C13—C14	120.77 (17)
C1—C2—C6	122.02 (15)	C12—C13—H13	119.6
C1—C2—C3	118.81 (14)	C14—C13—H13	119.6
C6—C2—C3	119.17 (14)	C13—C14—C9	120.34 (17)
C4—C3—C2	107.98 (13)	C13—C14—H14	119.8
C4—C3—C7	111.96 (14)	C9—C14—H14	119.8
C2—C3—C7	111.78 (13)	C16—C15—C20	117.66 (16)
C4—C3—C15	110.63 (13)	C16—C15—C3	120.41 (15)
C2—C3—C15	109.40 (13)	C20—C15—C3	121.70 (15)
C7—C3—C15	105.07 (13)	C17—C16—C15	121.32 (16)
C5—C4—C8	121.52 (15)	C17—C16—H16	119.3
C5—C4—C3	118.93 (14)	C15—C16—H16	119.3
C8—C4—C3	119.54 (14)	C18—C17—C16	120.20 (17)
C4—C5—C9	125.67 (15)	C18—C17—H17	119.9
C4—C5—S1	120.16 (13)	C16—C17—H17	119.9
C9—C5—S1	114.17 (12)	C19—C18—C17	119.29 (17)
C2—C6—H6A	109.5	C19—C18—H18	120.4
C2—C6—H6B	109.5	C17—C18—H18	120.4
H6A—C6—H6B	109.5	C18—C19—C20	120.40 (16)
C2—C6—H6C	109.5	C18—C19—H19	119.8
H6A—C6—H6C	109.5	C20—C19—H19	119.8
H6B—C6—H6C	109.5	C19—C20—C15	121.13 (16)
C3—C7—H7A	109.5	C19—C20—H20	119.4
C3—C7—H7B	109.5	C15—C20—H20	119.4
H7A—C7—H7B	109.5	C26—C21—C22	118.38 (16)
C3—C7—H7C	109.5	C26—C21—C1	119.97 (15)
H7A—C7—H7C	109.5	C22—C21—C1	121.63 (15)
H7B—C7—H7C	109.5	C23—C22—C21	120.38 (16)
C4—C8—H8A	109.5	C23—C22—H22	119.8
C4—C8—H8B	109.5	C21—C22—H22	119.8
H8A—C8—H8B	109.5	C24—C23—C22	120.70 (17)
C4—C8—H8C	109.5	C24—C23—H23	119.6
H8A—C8—H8C	109.5	C22—C23—H23	119.6
H8B—C8—H8C	109.5	C23—C24—C25	119.19 (17)
C10—C9—C14	118.23 (16)	C23—C24—H24	120.4
C10—C9—C5	120.13 (15)	C25—C24—H24	120.4
C14—C9—C5	121.62 (15)	C26—C25—C24	120.39 (17)
C11—C10—C9	121.18 (17)	C26—C25—H25	119.8
C11—C10—H10	119.4	C24—C25—H25	119.8
C9—C10—H10	119.4	C25—C26—C21	120.93 (16)
C10—C11—C12	119.97 (18)	C25—C26—H26	119.5
C10—C11—H11	120.0	C21—C26—H26	119.5
C12—C11—H11	120.0		
C5—S1—C1—C2	−29.19 (15)	C10—C11—C12—C13	0.3 (3)
C5—S1—C1—C21	151.99 (12)	C11—C12—C13—C14	−0.1 (3)
C21—C1—C2—C6	−12.4 (3)	C12—C13—C14—C9	0.6 (3)

S1—C1—C2—C6	168.91 (13)	C10—C9—C14—C13	−1.3 (2)
C21—C1—C2—C3	167.85 (15)	C5—C9—C14—C13	−179.74 (16)
S1—C1—C2—C3	−10.8 (2)	C4—C3—C15—C16	−156.56 (15)
C1—C2—C3—C4	54.54 (19)	C2—C3—C15—C16	−37.7 (2)
C6—C2—C3—C4	−125.18 (16)	C7—C3—C15—C16	82.42 (18)
C1—C2—C3—C7	178.12 (15)	C4—C3—C15—C20	29.1 (2)
C6—C2—C3—C7	−1.6 (2)	C2—C3—C15—C20	147.93 (15)
C1—C2—C3—C15	−65.93 (19)	C7—C3—C15—C20	−91.92 (18)
C6—C2—C3—C15	114.35 (16)	C20—C15—C16—C17	−0.1 (3)
C2—C3—C4—C5	−54.04 (19)	C3—C15—C16—C17	−174.63 (16)
C7—C3—C4—C5	−177.52 (15)	C15—C16—C17—C18	−0.1 (3)
C15—C3—C4—C5	65.65 (19)	C16—C17—C18—C19	0.2 (3)
C2—C3—C4—C8	125.17 (16)	C17—C18—C19—C20	−0.1 (3)
C7—C3—C4—C8	1.7 (2)	C18—C19—C20—C15	−0.1 (3)
C15—C3—C4—C8	−115.13 (16)	C16—C15—C20—C19	0.2 (3)
C8—C4—C5—C9	11.4 (3)	C3—C15—C20—C19	174.69 (15)
C3—C4—C5—C9	−169.35 (15)	C2—C1—C21—C26	−49.4 (2)
C8—C4—C5—S1	−169.24 (13)	S1—C1—C21—C26	129.31 (14)
C3—C4—C5—S1	10.0 (2)	C2—C1—C21—C22	132.24 (18)
C1—S1—C5—C4	29.71 (15)	S1—C1—C21—C22	−49.03 (19)
C1—S1—C5—C9	−150.90 (12)	C26—C21—C22—C23	2.0 (2)
C4—C5—C9—C10	50.0 (2)	C1—C21—C22—C23	−179.63 (16)
S1—C5—C9—C10	−129.34 (15)	C21—C22—C23—C24	−1.1 (3)
C4—C5—C9—C14	−131.58 (18)	C22—C23—C24—C25	0.2 (3)
S1—C5—C9—C14	49.07 (19)	C23—C24—C25—C26	−0.2 (3)
C14—C9—C10—C11	1.5 (3)	C24—C25—C26—C21	1.1 (3)
C5—C9—C10—C11	179.99 (16)	C22—C21—C26—C25	−2.0 (3)
C9—C10—C11—C12	−1.0 (3)	C1—C21—C26—C25	179.61 (16)

Fig. 1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