Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methyl-2,4,6-triphenyl-4*H*-thiopyran

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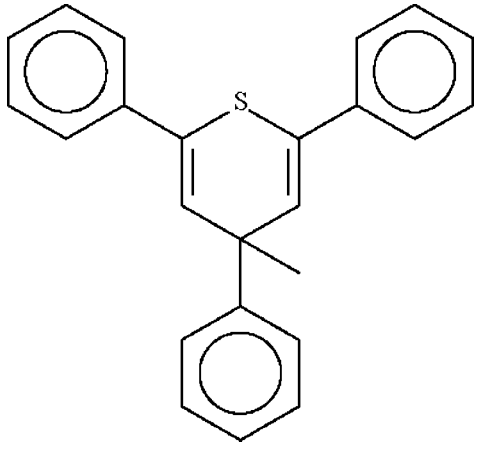
Received 18 February 2009; accepted 19 February 2009

Key indicators: single-crystal X-ray study; T = 115 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.072; data-to-parameter ratio = 17.1.

The six-membered thiopyran ring in the title compound, $C_{24}H_{20}S$, adopts a flattened boat conformation, with the S atom displaced by 0.273 (2) Å and the 3-methylene C atom by 0.294 (3) Å from the plane of the other four sp^2-hydridized C atoms. The methyl group on the methylene carbon lies in a axial position with the phenyl equatorial.

Related literature

2,4,4,6-Tetraaryl- or 4-alkyl-2,4,6-triaryl-4*H*-thiopyrans undergo UV-induced isomerization to form aryl-migrated 2*H*-thiopyrans; for a discussion of the photoisomerization mechanism, see: Pirelahi *et al.* (2004); Pirelahi & Rahmani (1997). 4-Methyl-2,4,6-triphenyl-4*H*-thiopyran does not react in the solid state, but in solution is converted to 4-methyl-2,3,6-triphenyl-2*H*-thiopyran; see: Mori & Maeda (1991). For the synthesis, see: Suld & Price (1962).



Experimental

Crystal data

$C_{24}H_{20}S$
M_r = 340.46
Monoclinic, *Cc*
a = 9.8737 (2) Å
b = 22.5282 (4) Å
c = 9.2288 (2) Å
β = 118.987 (1)°
V = 1795.67 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 115 K
0.35 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.917, T_{max} = 0.982
8464 measured reflections
3883 independent reflections
3698 reflections with $I > \sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.072
S = 1.03
3883 reflections
227 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack (1983), 1825 Friedel pairs
Flack parameter: 0.00 (5)

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).

We thank the Iranian Research Organization for Science and Technology and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2578).

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supplementary materials

Acta Cryst. (2009). E**65**, o603 [**doi:10.1107/S1600536809005911**]

4-Methyl-2,4,6-triphenyl-4*H*-thiopyran

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Comment

(type here to add)

Experimental

The compound was synthesized by the reaction of methyl magnesium bromide and 2,4,6-triphenylthiopyrylium perchlorate in dry ether under an argon atmosphere according to a reported method (Suld & Price, 1962). 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

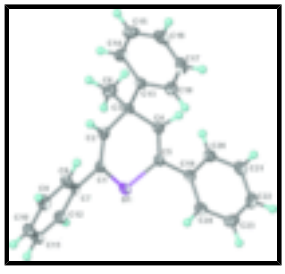


Fig. 1. Thermal ellisoid plot (Barbour, 2001) of $C_{24}H_{20}S$; probability levels are set at 70% and H-atoms are drawn as spheres of arbitrary radius.

4-Methyl-2,4,6-triphenyl-4*H*-thiopyran

Crystal data

$C_{24}H_{20}S$	F_{000} = 720
M_r = 340.46	D_x = 1.259 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 4067 reflections
a = 9.8737 (2) Å	θ = 2.5–28.0º
b = 22.5282 (4) Å	μ = 0.18 mm^{-1}
c = 9.2288 (2) Å	*T* = 115 K
β = 118.987 (1)º	Prism, colorless
V = 1795.67 (6) Å^3	0.35 × 0.20 × 0.10 mm

$Z = 4$

Data collection

Bruker SMART APEX diffractometer	3883 independent reflections
Radiation source: fine-focus sealed tube	3698 reflections with $I > \sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 115$ K	$\theta_{max} = 27.5^{o}$
ω scans	$\theta_{min} = 1.8^{o}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.917$, $T_{max} = 0.982$	$k = -29 \rightarrow 29$
8464 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.2571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
3883 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
227 parameters	Extinction correction: none
2 restraints	Absolute structure: Flack (1983), 1825 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.00 (5)
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.49977 (4)	0.892322 (17)	0.49963 (4)	0.01993 (9)
C1	0.48277 (17)	0.87133 (6)	0.67575 (18)	0.0169 (3)
C2	0.37550 (18)	0.83350 (7)	0.66660 (19)	0.0197 (3)
H2	0.3740	0.8259	0.7671	0.024*
C3	0.25547 (17)	0.80107 (7)	0.51476 (19)	0.0187 (3)
C4	0.22225 (18)	0.83423 (7)	0.35828 (18)	0.0180 (3)
H4	0.1228	0.8283	0.2651	0.022*
C5	0.31709 (16)	0.87086 (6)	0.33675 (17)	0.0156 (3)
C6	0.3178 (2)	0.73921 (7)	0.5054 (2)	0.0252 (4)
H6A	0.3487	0.7178	0.6092	0.038*
H6B	0.4075	0.7437	0.4879	0.038*
H6C	0.2366	0.7168	0.4131	0.038*
C7	0.59735 (17)	0.90088 (7)	0.83149 (19)	0.0174 (3)
C8	0.55816 (18)	0.91435 (7)	0.95401 (19)	0.0210 (3)

H8	0.4585	0.9041	0.9379	0.025*
C9	0.66275 (19)	0.94253 (7)	1.0990 (2)	0.0241 (3)
H9	0.6341	0.9517	1.1810	0.029*
C10	0.8091 (2)	0.95738 (7)	1.1249 (2)	0.0236 (4)
H10	0.8809	0.9766	1.2245	0.028*
C11	0.84996 (18)	0.94407 (7)	1.0045 (2)	0.0237 (3)
H11	0.9503	0.9540	1.0221	0.028*
C12	0.74509 (18)	0.91643 (7)	0.85877 (19)	0.0207 (3)
H12	0.7738	0.9079	0.7765	0.025*
C13	0.10640 (17)	0.79667 (7)	0.52855 (18)	0.0183 (3)
C14	0.0894 (2)	0.75238 (8)	0.6233 (2)	0.0255 (3)
H14	0.1679	0.7231	0.6742	0.031*
C15	−0.0402 (2)	0.75009 (8)	0.6451 (2)	0.0294 (4)
H15	−0.0487	0.7198	0.7118	0.035*
C16	−0.1572 (2)	0.79169 (8)	0.5702 (2)	0.0284 (4)
H16	−0.2465	0.7899	0.5836	0.034*
C17	−0.14174 (19)	0.83609 (8)	0.47516 (19)	0.0257 (4)
H17	−0.2212	0.8649	0.4232	0.031*
C18	−0.01103 (19)	0.83879 (7)	0.45533 (18)	0.0222 (3)
H18	−0.0016	0.8698	0.3910	0.027*
C19	0.27339 (17)	0.89872 (7)	0.17441 (18)	0.0165 (3)
C20	0.18705 (18)	0.86626 (7)	0.02926 (18)	0.0191 (3)
H20	0.1658	0.8255	0.0359	0.023*
C21	0.13179 (19)	0.89302 (7)	−0.1250 (2)	0.0222 (3)
H21	0.0729	0.8706	−0.2230	0.027*
C22	0.16242 (19)	0.95233 (8)	−0.1358 (2)	0.0238 (4)
H22	0.1232	0.9708	−0.2412	0.029*
C23	0.25068 (19)	0.98482 (7)	0.0078 (2)	0.0242 (3)
H23	0.2722	1.0255	0.0005	0.029*
C24	0.30752 (18)	0.95805 (7)	0.16187 (18)	0.0192 (3)
H24	0.3700	0.9802	0.2594	0.023*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01477 (16)	0.02749 (19)	0.01650 (17)	−0.00309 (16)	0.00676 (13)	−0.00013 (15)
C1	0.0159 (7)	0.0177 (7)	0.0151 (7)	0.0022 (6)	0.0060 (6)	0.0015 (6)
C2	0.0202 (7)	0.0213 (8)	0.0151 (7)	0.0008 (6)	0.0067 (6)	0.0030 (6)
C3	0.0183 (7)	0.0174 (7)	0.0179 (7)	−0.0021 (6)	0.0069 (6)	0.0014 (5)
C4	0.0177 (7)	0.0189 (7)	0.0146 (7)	−0.0021 (6)	0.0056 (6)	−0.0022 (6)
C5	0.0144 (7)	0.0154 (7)	0.0151 (7)	0.0006 (5)	0.0056 (6)	−0.0027 (5)
C6	0.0260 (9)	0.0207 (8)	0.0305 (9)	0.0010 (7)	0.0150 (7)	0.0016 (7)
C7	0.0144 (7)	0.0168 (7)	0.0159 (7)	0.0014 (6)	0.0032 (6)	0.0022 (5)
C8	0.0149 (7)	0.0237 (8)	0.0219 (8)	−0.0006 (6)	0.0070 (6)	−0.0016 (6)
C9	0.0233 (8)	0.0294 (8)	0.0197 (8)	0.0019 (7)	0.0105 (6)	−0.0021 (6)
C10	0.0203 (8)	0.0216 (8)	0.0206 (8)	−0.0008 (7)	0.0034 (6)	−0.0044 (6)
C11	0.0167 (7)	0.0261 (8)	0.0250 (8)	−0.0027 (6)	0.0075 (6)	−0.0014 (6)
C12	0.0201 (8)	0.0237 (8)	0.0190 (8)	−0.0008 (6)	0.0100 (6)	0.0002 (6)

C13	0.0172 (7)	0.0187 (7)	0.0153 (7)	−0.0034 (6)	0.0048 (6)	−0.0022 (5)
C14	0.0258 (8)	0.0221 (8)	0.0262 (8)	−0.0006 (7)	0.0107 (7)	0.0051 (6)
C15	0.0318 (9)	0.0282 (9)	0.0302 (9)	−0.0090 (7)	0.0167 (8)	0.0027 (7)
C16	0.0208 (8)	0.0378 (10)	0.0267 (9)	−0.0079 (7)	0.0115 (7)	−0.0065 (7)
C17	0.0198 (8)	0.0340 (9)	0.0182 (8)	0.0035 (7)	0.0050 (6)	−0.0011 (6)
C18	0.0246 (8)	0.0228 (8)	0.0166 (8)	−0.0005 (6)	0.0079 (7)	0.0008 (5)
C19	0.0140 (7)	0.0203 (7)	0.0165 (8)	0.0010 (6)	0.0084 (6)	−0.0008 (6)
C20	0.0188 (7)	0.0198 (7)	0.0202 (8)	−0.0007 (6)	0.0106 (6)	−0.0012 (6)
C21	0.0184 (8)	0.0318 (9)	0.0166 (8)	−0.0006 (6)	0.0086 (6)	−0.0019 (6)
C22	0.0195 (8)	0.0346 (9)	0.0197 (8)	0.0068 (7)	0.0113 (7)	0.0079 (7)
C23	0.0262 (8)	0.0216 (8)	0.0314 (9)	−0.0006 (7)	0.0191 (7)	0.0027 (6)
C24	0.0182 (7)	0.0222 (8)	0.0192 (8)	−0.0019 (6)	0.0106 (6)	−0.0027 (6)

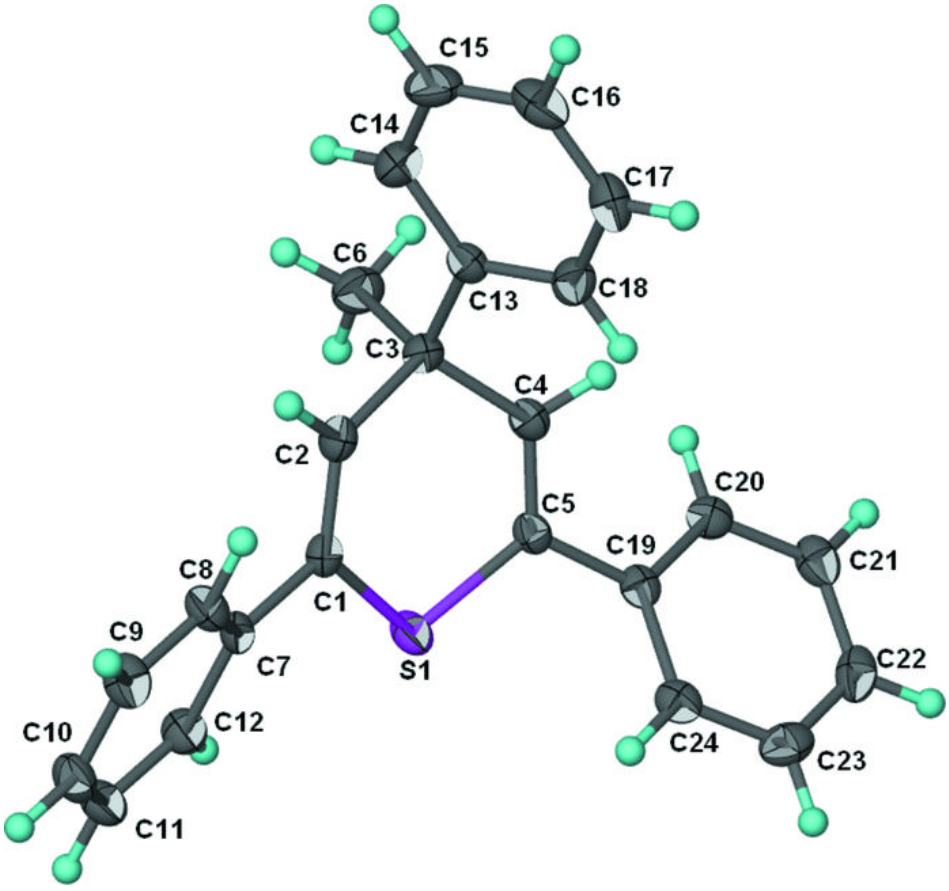
Geometric parameters (Å, °)

S1—C5	1.7661 (14)	C11—H11	0.9500
S1—C1	1.7772 (15)	C12—H12	0.9500
C1—C2	1.330 (2)	C13—C14	1.390 (2)
C1—C7	1.488 (2)	C13—C18	1.393 (2)
C2—C3	1.514 (2)	C14—C15	1.390 (2)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.514 (2)	C15—C16	1.384 (3)
C3—C13	1.541 (2)	C15—H15	0.9500
C3—C6	1.543 (2)	C16—C17	1.386 (3)
C4—C5	1.333 (2)	C16—H16	0.9500
C4—H4	0.9500	C17—C18	1.390 (2)
C5—C19	1.483 (2)	C17—H17	0.9500
C6—H6A	0.9800	C18—H18	0.9500
C6—H6B	0.9800	C19—C20	1.396 (2)
C6—H6C	0.9800	C19—C24	1.397 (2)
C7—C8	1.394 (2)	C20—C21	1.391 (2)
C7—C12	1.399 (2)	C20—H20	0.9500
C8—C9	1.386 (2)	C21—C22	1.384 (2)
C8—H8	0.9500	C21—H21	0.9500
C9—C10	1.387 (3)	C22—C23	1.390 (2)
C9—H9	0.9500	C22—H22	0.9500
C10—C11	1.386 (2)	C23—C24	1.388 (2)
C10—H10	0.9500	C23—H23	0.9500
C11—C12	1.386 (2)	C24—H24	0.9500
C5—S1—C1	101.27 (7)	C11—C12—C7	120.71 (15)
C2—C1—C7	123.89 (14)	C11—C12—H12	119.6
C2—C1—S1	122.53 (12)	C7—C12—H12	119.6
C7—C1—S1	113.57 (11)	C14—C13—C18	117.92 (14)
C1—C2—C3	127.59 (14)	C14—C13—C3	120.65 (14)
C1—C2—H2	116.2	C18—C13—C3	121.32 (14)
C3—C2—H2	116.2	C15—C14—C13	121.22 (16)
C4—C3—C2	110.82 (12)	C15—C14—H14	119.4
C4—C3—C13	109.66 (12)	C13—C14—H14	119.4
C2—C3—C13	107.77 (13)	C16—C15—C14	120.43 (16)

C4—C3—C6	107.47 (13)	C16—C15—H15	119.8
C2—C3—C6	109.47 (13)	C14—C15—H15	119.8
C13—C3—C6	111.67 (12)	C15—C16—C17	118.94 (16)
C5—C4—C3	127.18 (13)	C15—C16—H16	120.5
C5—C4—H4	116.4	C17—C16—H16	120.5
C3—C4—H4	116.4	C16—C17—C18	120.56 (16)
C4—C5—C19	122.09 (13)	C16—C17—H17	119.7
C4—C5—S1	122.96 (11)	C18—C17—H17	119.7
C19—C5—S1	114.91 (11)	C17—C18—C13	120.92 (15)
C3—C6—H6A	109.5	C17—C18—H18	119.5
C3—C6—H6B	109.5	C13—C18—H18	119.5
H6A—C6—H6B	109.5	C20—C19—C24	118.78 (14)
C3—C6—H6C	109.5	C20—C19—C5	119.41 (13)
H6A—C6—H6C	109.5	C24—C19—C5	121.68 (13)
H6B—C6—H6C	109.5	C21—C20—C19	120.60 (15)
C8—C7—C12	118.32 (14)	C21—C20—H20	119.7
C8—C7—C1	120.06 (14)	C19—C20—H20	119.7
C12—C7—C1	121.62 (14)	C22—C21—C20	120.09 (15)
C9—C8—C7	120.86 (15)	C22—C21—H21	120.0
C9—C8—H8	119.6	C20—C21—H21	120.0
C7—C8—H8	119.6	C21—C22—C23	119.82 (15)
C8—C9—C10	120.22 (15)	C21—C22—H22	120.1
C8—C9—H9	119.9	C23—C22—H22	120.1
C10—C9—H9	119.9	C24—C23—C22	120.22 (15)
C11—C10—C9	119.59 (15)	C24—C23—H23	119.9
C11—C10—H10	120.2	C22—C23—H23	119.9
C9—C10—H10	120.2	C23—C24—C19	120.44 (14)
C12—C11—C10	120.30 (15)	C23—C24—H24	119.8
C12—C11—H11	119.9	C19—C24—H24	119.8
C10—C11—H11	119.9		
C5—S1—C1—C2	17.61 (15)	C4—C3—C13—C14	157.18 (14)
C5—S1—C1—C7	−161.33 (11)	C2—C3—C13—C14	−82.11 (17)
C7—C1—C2—C3	−179.48 (15)	C6—C3—C13—C14	38.2 (2)
S1—C1—C2—C3	1.7 (2)	C4—C3—C13—C18	−26.78 (19)
C1—C2—C3—C4	−24.4 (2)	C2—C3—C13—C18	93.93 (16)
C1—C2—C3—C13	−144.35 (16)	C6—C3—C13—C18	−145.80 (14)
C1—C2—C3—C6	94.01 (19)	C18—C13—C14—C15	−0.2 (2)
C2—C3—C4—C5	26.5 (2)	C3—C13—C14—C15	175.99 (16)
C13—C3—C4—C5	145.30 (15)	C13—C14—C15—C16	1.0 (3)
C6—C3—C4—C5	−93.12 (19)	C14—C15—C16—C17	−0.9 (3)
C3—C4—C5—C19	177.18 (14)	C15—C16—C17—C18	0.0 (3)
C3—C4—C5—S1	−5.5 (2)	C16—C17—C18—C13	0.8 (2)
C1—S1—C5—C4	−15.81 (15)	C14—C13—C18—C17	−0.7 (2)
C1—S1—C5—C19	161.67 (11)	C3—C13—C18—C17	−176.85 (14)
C2—C1—C7—C8	−31.3 (2)	C4—C5—C19—C20	−37.1 (2)
S1—C1—C7—C8	147.59 (12)	S1—C5—C19—C20	145.37 (12)
C2—C1—C7—C12	149.37 (16)	C4—C5—C19—C24	138.58 (16)
S1—C1—C7—C12	−31.71 (19)	S1—C5—C19—C24	−38.92 (19)
C12—C7—C8—C9	0.1 (2)	C24—C19—C20—C21	−2.1 (2)

C1—C7—C8—C9	−179.21 (15)	C5—C19—C20—C21	173.78 (14)
C7—C8—C9—C10	−0.5 (3)	C19—C20—C21—C22	0.1 (2)
C8—C9—C10—C11	0.2 (3)	C20—C21—C22—C23	1.0 (2)
C9—C10—C11—C12	0.4 (3)	C21—C22—C23—C24	−0.3 (2)
C10—C11—C12—C7	−0.8 (3)	C22—C23—C24—C19	−1.7 (2)
C8—C7—C12—C11	0.5 (2)	C20—C19—C24—C23	2.8 (2)
C1—C7—C12—C11	179.82 (15)	C5—C19—C24—C23	−172.93 (14)

Fig. 1


C15
C16
C14
C17
C6
C13
C18
C3
C4
C2
C20
C5
C19
C21
C8
C1
C9
C7
S1
C22
C10
C12
C24
C23
C11