Table 2. *Bond distances* (Å) *and selected angles* (°)

S1—C2	1.762 (3)	S1—C6	1.771 (3)
S1—O1	1.423 (3)	S1—O2	1.436 (2)
C2—C3	1.315 (3)	C2—C21	1.488 (4)
C3—C4	1.518 (4)	C4—C5	1.505 (4)
C4—C411	1.546 (3)	C4—C421	1.546 (4)
C5—C6	1.329 (3)	C6—C61	1.485 (5)
C21—C22	1.367 (5)	C21—C26	1.391 (5)
C22—C23	1.400 (4)	C23—C24	1.341 (6)
C24—C25	1.352 (6)	C25—C26	1.396 (5)
C61—C62	1.389 (5)	C61—C66	1.388 (4)
C62—C63	1.369 (5)	C63—C64	1.382 (4)
C64—C65	1.383 (4)	C65—C66	1.370 (4)
C411—C412	1.375 (4)	C411—C416	1.400 (4)
C412—C413	1.404 (5)	C413—C414	1.369 (6)
C414—C415	1.369 (6)	C415—C416	1.367 (4)
C421—C422	1.384 (4)	C421—C426	1.392 (4)
C422—C423	1.398 (4)	C423—C424	1.344 (6)
C424—C425	1.403 (6)	C425—C426	1.367 (5)

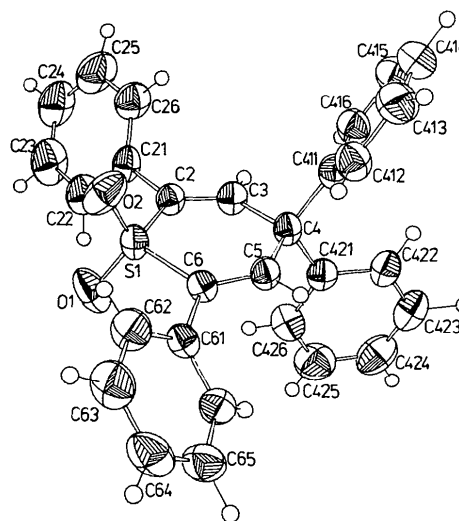| O1—S1—O2	116.6 (2)	C6—S1—O2	109.6 (2)
C6—S1—O1	108.0 (2)	C2—S1—O2	107.9 (2)
C2—S1—O1	109.0 (2)	C2—S1—C6	105.2 (2)
S1—C2—C21	115.4 (2)	S1—C2—C3	121.5 (2)
C2—C3—C4	129.3 (2)	C3—C4—C421	108.1 (2)
C3—C4—C411	106.6 (2)	C3—C4—C5	113.3 (2)
C411—C4—C421	112.6 (2)	C5—C4—C421	105.4 (2)
C5—C4—C411	110.9 (2)	C4—C5—C6	129.5 (3)
S1—C6—C5	120.8 (2)	S1—C6—C61	115.6 (2)
C22—C21—C26	118.7 (3)	C21—C22—C23	120.2 (4)
C21—C26—C25	119.4 (4)	C62—C61—C66	117.8 (3)
C61—C62—C63	121.4 (4)	C61—C66—C65	121.1 (3)
C412—C411—C416	118.5 (2)	C411—C412—C413	120.1 (3)
C411—C416—C415	120.8 (3)	C422—C421—C426	118.1 (3)
C421—C422—C423	120.2 (3)	C421—C426—C425	121.6 (3)

Fig. 1. The atomic numbering scheme with thermal ellipsoids at the 50% probability level.

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To exclude a strong dependence of the photochromic behaviour on substituents at sites 2, 4 and 6, we have studied the series of equally substituted structures $A_1 = A_2 = A_3 = A_4$ = phenyl: X = NH (Iwasaki, Watanabe & Maeda, 1987), X = O (Vojtěchovský & Hašek, 1990), X = S (Vojtěchovský, Hašek, Nešpůrek & Adamec, 1991), X = N—Ph (Vojtěchovský, Hašek, Huml & Ječný, 1990), X = NCH₂C₅H₆ (Hašek & Ondráček, 1990). The title compound (X = SO₂) is not photochromic.

Structure of 1-Oxo-2,4,4,6-tetraphenyl-4*H*-thiopyran Benzene Solvate

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Abstract. $C_{29}H_{22}OS.\frac{1}{4}C_6H_6$, M_r = 439.57, triclinic, $P\bar{1}$, a = 10.622 (3), b = 11.448 (2), c = 12.343 (3) Å, α = 96.08 (2), β = 69.42 (2), γ = 67.69 (2)°, V = 1249.3 (6) Å³, Z = 2, D_x = 1.161 g cm⁻³, λ(Cu $K\alpha$) = 1.54184 Å, μ = 12.49 cm⁻¹, $F(000)$ = 461, T = 294 K, R = 0.064 for 3032 unique observed reflections. The central ring has a boat conformation with S1 and C4 displaced by 0.237 (11) and 0.116 (6) Å out of the least-squares plane defined by the remaining atoms. Within this ring the C2—C3 and

$C_{29}H_{22}OS.\frac{1}{4}C_6H_6$

Table 1. Final coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\times 10^3$ Å^2) with e.s.d.'s in parentheses for the non-H atoms

$$U_{eq} = \frac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C2	1229 (4)	3488 (3)	−2390 (3)	65 (2)
C3	2696 (4)	3112 (3)	−2826 (3)	70 (2)
C4	3610 (4)	3658 (3)	−3650 (3)	65 (2)
C5	2615 (4)	4928 (3)	−3797 (3)	65 (2)
C6	1149 (4)	5489 (3)	−3450 (3)	63 (2)
C21	468 (4)	2876 (3)	−1562 (3)	71 (2)
C22	661 (6)	2802 (4)	−509 (4)	93 (2)
C23	−5 (7)	2192 (5)	245 (4)	119 (3)
C24	−838 (7)	1667 (6)	−11 (6)	130 (3)
C25	−1077 (5)	1746 (4)	−1061 (6)	117 (3)
C26	−406 (4)	2363 (4)	−1828 (4)	87 (2)
C61	319 (4)	6756 (3)	−3649 (3)	64 (2)
C62	700 (4)	7774 (4)	−3500 (3)	71 (2)
C63	−15 (5)	8939 (4)	−3739 (4)	87 (2)
C64	−1147 (5)	9104 (4)	−4111 (4)	95 (2)
C65	−1550 (5)	8107 (4)	−4244 (4)	93 (2)
C66	−827 (4)	6947 (4)	−4011 (3)	78 (2)
C411	4638 (4)	2627 (3)	−4870 (3)	65 (2)
C412	4683 (4)	2898 (4)	−5944 (3)	82 (2)
C413	5641 (5)	1953 (4)	−7032 (4)	102 (3)
C414	6583 (5)	702 (4)	−7079 (4)	92 (2)
C415	6548 (4)	416 (4)	−6027 (4)	84 (2)
C416	5593 (4)	1360 (4)	−4934 (4)	77 (2)
C421	4527 (4)	4022 (3)	−3046 (3)	68 (2)
C422	3781 (5)	4809 (4)	−1878 (4)	93 (2)
C423	4549 (6)	5207 (5)	−1334 (5)	109 (2)
C424	6052 (5)	4818 (4)	−1941 (5)	96 (3)
C425	6805 (5)	4023 (4)	−3094 (4)	88 (3)
C426	6051 (4)	3617 (4)	−3648 (3)	72 (2)
S1	−37 (1)	4747 (1)	−2757 (1)	74 (1)
O1	−1251 (3)	5698 (3)	−1619 (2)	98 (2)
C7	3511 (14)	1187 (21)	1114 (17)	1668 (31)
C8	4164 (14)	1584 (21)	122 (16)	731 (44)
C9	5396 (14)	653 (21)	−906 (17)	780 (32)
C10	5975 (14)	−674 (21)	−943 (16)	502 (21)
C11	5321 (14)	−1071 (21)	49 (17)	269 (18)
C12	4089 (14)	−140 (21)	1078 (17)	566 (35)

Table 2. Bond distances (Å) and selected angles (°)

S1—C2	1.785 (4)	S1—C6	1.802 (4)
S1—O1	1.469 (2)	C2—C21	1.480 (6)
C2—C3	1.325 (6)	C4—C5	1.512 (5)
C3—C4	1.506 (6)	C4—C421	1.559 (7)
C4—C411	1.530 (4)	C6—C61	1.483 (5)
C5—C6	1.317 (5)	C21—C26	1.379 (7)
C21—C22	1.391 (7)	C23—C24	1.343 (12)
C22—C23	1.380 (8)	C25—C26	1.397 (8)
C24—C25	1.411 (11)	C61—C66	1.389 (7)
C61—C62	1.386 (7)	C63—C64	1.388 (8)
C62—C63	1.384 (6)	C65—C66	1.378 (6)
C64—C65	1.376 (8)	C411—C416	1.393 (5)
C411—C412	1.382 (6)	C413—C414	1.382 (6)
C412—C413	1.380 (5)	C415—C416	1.383 (5)
C414—C415	1.364 (7)	C421—C426	1.378 (5)
C421—C422	1.378 (5)	C423—C424	1.363 (7)
C422—C423	1.388 (9)	C425—C426	1.388 (8)
C424—C425	1.366 (6)		

|			
C6—S1—O1	107.9 (2)	C2—S1—C6	99.8 (2)
C2—S1—O1	107.4 (2)	S1—C2—C3	124.3 (3)
S1—C2—C21	112.6 (3)	C3—C4—C421	108.2 (3)
C2—C3—C4	128.8 (4)	C3—C4—C5	111.5 (3)
C3—C4—C411	108.9 (3)	C5—C4—C421	105.6 (3)
C411—C4—C421	111.8 (3)	C4—C5—C6	129.7 (4)
C5—C4—C411	110.8 (3)	S1—C6—C61	113.2 (3)
S1—C6—C5	123.2 (3)	C21—C22—C23	119.3 (5)
C22—C21—C26	119.8 (4)	C62—C61—C66	118.4 (4)
C21—C26—C25	120.6 (5)	C61—C66—C65	121.1 (4)
C61—C62—C63	120.8 (4)	C411—C412—C413	121.2 (4)
C412—C411—C416	117.2 (4)	C422—C421—C426	118.6 (4)
C411—C416—C415	121.4 (4)	C421—C426—C425	120.4 (4)
C421—C422—C423	120.4 (5)		
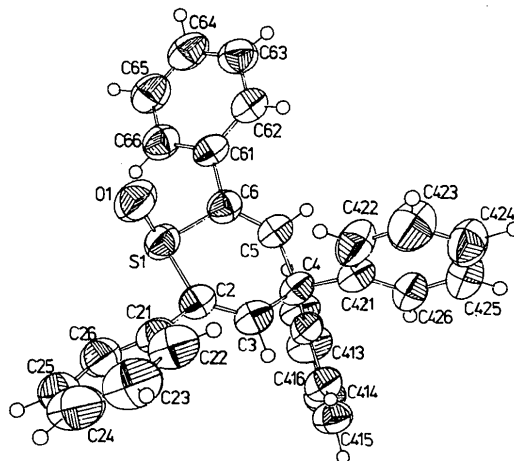
Fig. 1. The atomic numbering scheme of the title compound with thermal ellipsoids at the 50% probability level.

C5—C6 distances, 1.325 (6) and 1.317 (5) Å, respectively, indicate localized double bonds and the phenyl rings at C2 and C6 make dihedral angles of − 58.7 (4) and 43.8 (3)° with the least-squares plane. The orientations of the phenyl substituents at C4 are given by the torsion angles C411—C4—C421—C426 = 10.1 (5) and C421—C4—C411—C416 = 65.9 (5)°. The disordered solvent molecule had to be fixed during the refinement.

Experimental. The crystallization and diffraction experiments were made in a similar manner to that used for 1,1-dioxo-2,4,4,6-tetraphenyl-4H-thiopyran (Vojtěchovský & Hašek, 1992). The crystal size was 0.5 × 0.4 × 0.3 mm; 15 reflections used for refinement of the cell constants in the range 9.7 < 2θ < 27.0°. The data collection with $2\theta_{max} = 120°$ and indices h −11/11, k −12/0, l −13/13 resulted in 3425 unique reflections, of which 3032 were taken as observed [$I > 1.96\sigma(I)$]. Three standard reflections (00$\bar{3}$, 0$\bar{1}$0, 100) did not vary significantly during the measurement. The program MULTAN87 (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987)

provided the coordinates of all non-H atoms of the title compound. Benzene atoms were set to the peaks around $0,0,\frac{1}{2}$ and then refined as a regular hexagon. Their site occupation factors converged close to 0.25 and were fixed at this value. The refinement of 386 parameters in the program SHELX76 (Sheldrick, 1976) {function minimized $\Sigma[w(|F_o| - |F_c|)^2]$, where $w = [\sigma^2(F_o) + 0.0009|F_o|^2]^{-1}$} converged at R = 0.064, wR = 0.089 and S = 2.14. Nine H atoms were kept at fixed distances to the corresponding C atoms during the refinement. The maxima on the final

difference electron density map were 0.30 and $-0.25 \, e \, \text{Å}^{-3}$. The refinement was terminated when the parameter shifts fell below 0.09 of the corresponding e.s.d.'s and those for the solvent molecule below 0.4 e.s.d.'s. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Molecular geometry and interatomic distances were calculated by *PARST* (Nardelli, 1978). The fractional coordinates and the equivalent isotropic thermal parameters of all non-H atoms are listed in Table 1. The atomic numbering scheme with thermal ellipsoids for non-H atoms is drawn using *ORTEP* (Johnson, 1976) in Fig. 1. Interatomic distances and selected angles are listed in Table 2.*

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* List of structure factors, H-atom positions and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54896 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI9092]

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Structure of a Cyclopenta[*hi*]indolizine

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Abstract. Ethyl 3,4-dihydrocyclopenta[*hi*]indolizine-1-carboxylate, $C_{13}H_{13}NO_2$, $M_r = 215.25$, triclinic, $P\bar{1}$, $a = 8.239 \, (1)$, $b = 9.750 \, (1)$, $c = 7.856 \, (1) \, \text{Å}$, $\alpha = 105.67 \, (1)°$, $\beta = 118.14 \, (1)°$, $\gamma = 79.85 \, (1)°$, $V = 534.8 \, (1) \, \text{Å}^3$, $Z = 2$, $D_x = 1.336 \, \text{g cm}^{-3}$, $\lambda(\text{Mo} \, K\alpha) = 0.71069 \, \text{Å}$, $\mu = 0.85 \, \text{cm}^{-1}$, $F(000) = 228$, $T = 297 \, \text{K}$, final $R = 0.037$ for 1732 observed $[I > 3.00\sigma(I)]$ reflections. The pyrrole and pyridine rings in the indolizine skeleton are planar with mean deviations 0.001 (1) and 0.004 (2) Å, respectively, and inclined to one another at 0.98°. The planar five-membered ring attached to the indolizine ring is slightly corrugated with larger mean deviation of 0.012 (2) Å, but this ring is also almost coplanar with the pyrrole ring with a dihedral angle of 1.49°. The delocalized ring system extends to the ester carbonyl group as indicated by the shortened Cl_{ring}—$Cl1_{ester}$ bond of 1.442 (2) Å. The ester group at the 1-position is also coplanar with the indolizine ring with a dihedral angle of 1.61°.
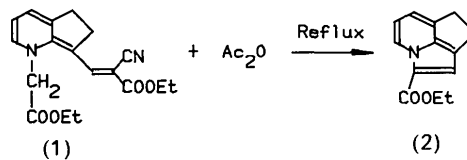
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Experimental. The reaction of ethyl 3-[2-cyano-2-(ethoxycarbonyl)vinyl]-1,2-dihydro-4*H*-cyclopenta-[*b*]pyridine-4-acetate (1) (328 mg) with acetic anhydride (3 μm³) under reflux for 12 h smoothly afforded the title compound, ethyl 3,4-dihydro-cyclopenta[*hi*]indolizine-1-carboxylate (2), in a 41% yield (Kakehi, Ito & Yotsuya, 1986).

Recrystallization from ethanol gave white prisms. D_m not determined. Crystal $0.24 \times 0.40 \times 0.48$ mm. Rigaku AFC-5S diffractometer, graphite-monochromated Mo $K\alpha$ radiation. Cell constants from setting angles of 25 reflections ($39.31 < 2\theta < 39.90°$). ω–2θ scans. Correction for Lorentz–polarization effects. $2\theta_{max} = 55.0°$ with $0 \leq h \leq 10$, $-12 \leq k \leq 12$,