donor atom O(12) of the hydrogen bond and 1·84 v.u. for its acceptor atom O(23). All the other O atoms have 1·78 to 1·99 v.u. in the two compounds.

The SrO_8 polyhedra in $Sr_2Cu(SeO_3)_3$ are edge- and corner-linked forming a three-dimensional network. Common O–O edges are O(12)–O(12) = 2·825 (7), O(21)–O(31) = 2·898 (5), O(11)–O(32) = 3·257 (5), O(11)–O(11) = 3·316 (7) and O(13)–O(13) = 3·469 (6) Å. The coordination polyhedra of the Cu atoms are not connected with each other. In contrast, the SrO_9 polyhedra in $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ are edge-linked to form a sheet-like arrangement parallel to (001) [common O—O edges O(13)—O(13) = 2·966 (6), O(21)–O(21) = 3·210 (5) and 3·657 (5) Å]. A three-dimensional network is formed by the interconnection with the CuO_4 'square' and the selenite groups. It should be mentioned that the connection of the CuO_4 'squares' with the $Se(2)O_3$ groups might be described as chains of composition $Cu(SeO_3)_2$ parallel to [100], which have already been found in $SrCu(SeO_3)_2$ and $BaCu(SeO_3)_2$-III (Effenberger, 1987).

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Structure of *cis*-$Pt(asb)_2Cl_2$, a Platinum(II) Complex with a Styrylbenzothiazole Ligand

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Abstract. *cis*-Bis[2-(2-acetoxystyryl)benzothiazole]dichloroplatinum(II), $[PtCl_2(C_{17}H_{13}NO_2S)_2]$, M_r = 856·7, triclinic, $P\bar{1}$, a = 12·145 (6), b = 12·859 (4), c = 11·021 (5) Å, α = 105·88 (3), β = 90·64 (4), γ = 87·64 (4)°, V = 1654 (2) Å^3, Z = 2, D_x = 1·72 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 46·1 cm^{-1}, $F(000)$ = 840, T = 296 K, final R = 0·029 for 6121 unique observed reflections. The $[PtCl_2(asb)_2]$ complex has square-planar geometry about the Pt, with the asb coordinated to the Pt through the N of the thiazole ring. The average Pt—N and Pt—Cl bond distances are 2·035 (1) and 2·287 (5) Å. The ligand is non-planar with an average dihedral angle of 36 (3)° between the benzothiazole and the benzene rings. The dihedral angles between the platinum coordination plane and the benzothiazole and benzene rings are 78 (4) and 69 (7)° respectively. The acetoxybenzene rings in the two ligands have different orientations with respect to the olefin C atoms.

Introduction. Since the discovery of the antitumor activity of complexes of platinum, such as *cis*-$Pt(NH_3)_2Cl_2$, there has been considerable interest in preparing new complexes of improved activity (Hacker, Douple & Krakoff, 1984). Among the ligands which have been used for the synthesis of new complexes are heterocyclic ligands such as imidazole and thiazole (van

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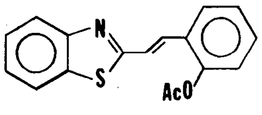
Kralingen, De Ridder & Reedijk, 1979; Dehand & Jordanov, 1976). Since several derivatives of styrylbenzothiazole showed significant biological activity (Cox, Jackson, Vargas, Baez, Colon, Gonzalez & de Leon, 1982), complexes of the type $Pt(L)_2Cl_2$, where L = the styrylbenzothiazole derivative, were prepared and characterized by ^{13}C NMR, UV–visible and IR spectrometry (Cadiz, 1985). It proved to be very difficult to assign the geometry of the complexes and the mode of coordination of the ligand as N or S on the basis of spectroscopic data alone. Thus, the structural study of the title compound was undertaken. The structural formula of the asb ligand is shown below.



Experimental. An aqueous solution (4 mL) of K_2PtCl_4 (0·10 g, 0·24 mmol) was mixed with 4 mL of a 1:1 THF/ethanol solution of the ligand asb (0·14 g, 0·48 mmol). The mixture was stirred and heated for 20 min. The sticky, brown solid which formed was recrystallized first from acetone and then from nitromethane in an ethanol-saturated atmosphere.

Orange prismatic crystal, D_m not determined, 0·40 × 0·20 × 0·20 mm, Enraf–Nonius CAD-4 diffractometer, monochromated Mo $K\alpha$, ω–θ scan, scan width $(0·9 + 0·34\tan\theta)°$, $2\theta_{\max} = 53°$, lattice parameters from least squares of 24 reflections in the range of $11 < \theta < 14°$. No systematic absences; $+h\pm k\pm l$ with $h \le 15$, $|k| \le 16$, $|l| \le 13$; three standard reflections, intensities constant within experimental error; total unique reflections measured 7164, 6121 with $F^2 > 2\sigma(F_o)^2$, $\sigma(F_o) = [\sigma(I_{\rm raw})^2 + (0·04F_o^2)^2]^{1/2}/2F$. Absorption corrections from ψ scans, relative transmission factors 0·871 to 0·997. Structure was solved with the Enraf–Nonius *SDP* (Frenz, 1986), heavy-atom and difference-Fourier methods; isotropic then anisotropic refinement on F of all non-H atoms, H atoms at calculated positions [C—H 0·95 Å, U(H) = 1·3U(C)]; 406 parameters refined, R = 0·029, wR = 0·036, $w = 1/[\sigma(F_o)]^2$, S = 1·0; difference syntheses showed no densities above 0·68 e Å^{-3} (min. −0·40 e Å^{-3}); max. Δ/σ = 0·04. Neutral-atom scattering factors were used, except for Pt^{II} [all from *International Tables for X-ray Crystallography* (1974)], and were corrected for anomalous dispersion (Cromer & Liberman, 1970). No correction for secondary extinction.*

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2) *for cis*-$Pt(asb)_2Cl_2$

	x	y	z	B_{eq}*(Å^2)
Pt	0·18340 (1)	0·43233 (1)	0·14387 (1)	2·450 (3)
Cl(1)	0·0318 (1)	0·3317 (1)	0·1426 (1)	3·91 (3)
Cl(2)	0·2289 (1)	0·3356 (1)	−0·0569 (1)	4·56 (3)
S1	0·5204 (1)	0·5786 (1)	0·1719 (1)	4·14 (3)
S1′	0·0900 (1)	0·64893 (9)	0·5353 (1)	3·49 (2)
O1	0·4109 (3)	0·1932 (3)	0·2698 (3)	4·34 (8)
O1′	0·1128 (3)	1·0090 (3)	0·4664 (3)	4·19 (8)
O2′	0·2787 (4)	1·0247 (4)	0·3903 (4)	6·7 (1)
O2	0·4979 (4)	0·0378 (4)	0·1694 (4)	7·1 (1)
N1	0·3206 (3)	0·5176 (3)	0·1425 (3)	3·14 (8)
N1′	0·1481 (3)	0·5104 (3)	0·3269 (3)	2·64 (7)
C1	0·3257 (4)	0·6046 (4)	0·0879 (4)	3·32 (9)
C1′	0·1678 (4)	0·4593 (3)	0·4227 (4)	2·70 (8)
C2′	0·2103 (4)	0·3539 (4)	0·4056 (4)	3·4 (1)
C2	0·2394 (5)	0·6427 (4)	0·0246 (5)	4·2 (1)
C3	0·2600 (6)	0·7283 (4)	−0·0222 (5)	5·4 (1)
C3′	0·2309 (5)	0·3176 (4)	0·5110 (5)	4·2 (1)
C4	0·3624 (6)	0·7748 (4)	−0·0103 (6)	5·5 (1)
C4′	0·2059 (5)	0·3841 (5)	0·6316 (5)	4·5 (1)
C5	0·4492 (5)	0·7365 (4)	0·0510 (5)	5·1 (1)
C5′	0·1616 (4)	0·4870 (4)	0·6506 (4)	3·9 (1)
C6	0·4280 (4)	0·6494 (4)	0·0989 (5)	3·9 (1)
C6′	0·1427 (4)	0·5239 (4)	0·5433 (4)	3·22 (9)
C7	0·4171 (4)	0·4949 (4)	0·1882 (4)	3·09 (9)
C7′	0·1082 (4)	0·6101 (3)	0·3736 (4)	2·86 (9)
C8	0·4349 (4)	0·4076 (4)	0·2444 (4)	3·4 (1)
C8′	0·0784 (4)	0·6853 (4)	0·2996 (4)	3·12 (9)
C9	0·5171 (4)	0·4002 (4)	0·3214 (5)	3·8 (1)
C9′	0·0776 (4)	0·7916 (3)	0·3495 (4)	3·19 (9)
C10′	0·0462 (4)	0·8754 (3)	0·2877 (4)	3·3 (1)
C10	0·5388 (4)	0·3182 (4)	0·3892 (4)	3·28 (9)
C11	0·6126 (4)	0·3425 (4)	0·4913 (5)	4·0 (1)
C11′	−0·0094 (5)	0·8526 (4)	0·1726 (5)	4·2 (1)
C12′	−0·0426 (6)	0·9348 (5)	0·1192 (5)	5·2 (1)
C12	0·6316 (4)	0·2734 (5)	0·5685 (5)	4·3 (1)
C13	0·5776 (5)	0·1787 (5)	0·5443 (5)	5·0 (1)
C13′	−0·0202 (6)	1·0411 (4)	0·1805 (5)	5·4 (1)
C14′	0·0363 (5)	1·0656 (4)	0·2930 (6)	5·1 (1)
C14	0·5069 (5)	0·1494 (4)	0·4423 (6)	4·8 (1)
C15′	0·0670 (4)	0·9834 (4)	0·3450 (4)	3·6 (1)
C15	0·4886 (4)	0·2188 (4)	0·3668 (5)	3·6 (1)
C16	0·4217 (5)	0·0973 (4)	0·1768 (5)	4·7 (1)
C16′	0·2213 (5)	1·0296 (4)	0·4789 (5)	4·4 (1)
C17	0·3233 (6)	0·0854 (5)	0·0950 (6)	6·0 (2)
C17′	0·2563 (6)	1·0568 (6)	0·6144 (6)	6·2 (2)

* Anisotropically refined atoms are given in the form of the equivalent isotropic displacement parameter defined as:

$$\tfrac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

Discussion. The atomic coordinates and equivalent isotropic temperature factors are listed in Table 1, and bond lengths and angles in Table 2. An *ORTEP* plot (Johnson, 1976) of the title compound with the atom numbering is shown in Fig. 1, and the packing of the molecules (Motherwell & Clegg, 1976) in Fig. 2.

The complex has approximately square-planar geometry about the Pt. The average Pt—Cl and Pt—N bond distances are 2·287 (5) and 2·035 (1) Å, respectively, which are typical for complexes of Pt^{II}. The Pt and the four coordinated atoms are very nearly planar, with no atom farther than 0·0377 (2) Å from the least-squares plane. The two coordinated asb molecules are non-planar, with an average dihedral angle of 36 (3)° between the benzothiazole and the benzene rings. This is considerably smaller than the dihedral angle of 60·1 (4)° which was found between the benzothiazole and nitrobenzene rings in the related $[NEt_4][Pt(nsb)Br_3]$ complex, where nsb = 2-(2-chloro-

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* Lists of structure factors, anisotropic thermal factors, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44632 (93 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å) *and angles* (°) *for cis-*Pt(asb)$_2$Cl$_2$

Pt	Cl(1)	2·291 (1)	C2′	C3′	1·382 (8)
Pt	Cl(2)	2·283 (1)	C2	C3	1·370 (9)
Pt	N1	2·035 (4)	C3	C4	1·391 (9)
Pt	N1′	2·034 (3)	C3′	C4′	1·399 (6)
S1	C6	1·741 (6)	C4	C5	1·390 (9)
S1	C7	1·728 (5)	C4′	C5′	1·370 (8)
S1′	C6′	1·730 (5)	C5	C6	1·397 (8)
S1′	C7′	1·728 (4)	C5′	C6′	1·403 (7)
O1	C15	1·398 (6)	C7	C8	1·430 (7)
O1	C16	1·374 (6)	C7′	C8′	1·458 (7)
O1′	C15′	1·401 (6)	C8	C9	1·320 (7)
O1′	C16′	1·354 (7)	C8′	C9′	1·327 (6)
O2′	C16′	1·192 (7)	C9	C10	1·464 (8)
O2	C16	1·165 (7)	C9′	C10′	1·461 (7)
N1	C1	1·411 (6)	C10′	C11′	1·394 (7)
N1	C7	1·323 (6)	C10′	C15′	1·392 (6)
N1′	C1′	1·402 (6)	C10	C11	1·406 (7)
N1′	C7′	1·318 (5)	C10	C15	1·398 (7)
C1	C2	1·397 (7)	C11	C12	1·399 (9)
C1	C6	1·381 (7)	C11′	C12′	1·387 (9)
C1′	C2′	1·394 (6)	C12′	C13′	1·387 (7)
C1′	C6′	1·390 (5)	C12	C13	1·367 (8)
C13	C14	1·384 (8)	C14	C15	1·387 (9)
C13′	C14′	1·375 (9)	C16	C17	1·476 (9)
C14′	C15′	1·370 (8)	C16′	C17′	1·498 (9)

Cl(1)	Pt	Cl(2)	91·58 (5)	C1′	C2′	C3′	118·5 (4)
Cl(1)	Pt	N1	178·3 (1)	C1	C2	C3	117·0 (5)
Cl(1)	Pt	N1′	87·9 (1)	C2	C3	C4	122·2 (6)
Cl(2)	Pt	N1	87·2 (1)	C2′	C3′	C4′	120·5 (5)
Cl(2)	Pt	N1′	176·1 (1)	C3	C4	C5	121·2 (6)
N1	Pt	N1′	93·2 (1)	C3′	C4′	C5′	122·0 (5)
C6	S1	C7	90·1 (2)	C4	C5	C6	116·5 (5)
C6′	S1′	C7′	90·0 (2)	C4′	C5′	C6′	117·1 (4)
C15	O1	C16	120·0 (4)	S1	C6	C1	110·4 (4)
C15′	O1′	C16′	118·3 (4)	S1	C6	C5	127·7 (4)
Pt	N1	C1	124·2 (3)	C1	C6	C5	121·8 (5)
Pt	N1	C7	123·8 (3)	S1′	C6′	C1′	109·8 (4)
C1	N1	C7	112·0 (4)	S1′	C6′	C5′	128·4 (3)
Pt	N1′	C1′	120·8 (2)	C1′	C6′	C5′	121·7 (4)
Pt	N1′	C7′	128·1 (3)	S1	C7	N1	114·1 (4)
C1′	N1′	C7′	111·0 (3)	S1	C7	C8	122·9 (4)
N1	C1	C2	125·5 (5)	N1	C7	C8	123·0 (4)
N1	C1	C6	113·4 (4)	S1′	C7′	N1′	114·9 (4)
C2	C1	C6	121·1 (5)	S1′	C7′	C8′	120·0 (3)
N1′	C1′	C2′	125·7 (4)	N1′	C7′	C8′	125·1 (4)
N1′	C1′	C6′	114·2 (4)	C7	C8	C9	124·5 (5)
C2′	C1′	C6′	120·1 (4)	C7′	C8′	C9′	121·7 (4)
C8	C9	C10	128·6 (5)	C13′	C14′	C15′	118·8 (5)
C8′	C9′	C10′	127·3 (4)	C13	C14	C15	119·3 (5)
C9′	C10′	C11′	122·3 (4)	O1′	C15′	C10′	117·6 (4)
C9′	C10′	C15′	120·6 (4)	O1′	C15′	C14′	119·1 (4)
C11′	C10′	C15′	117·0 (5)	C10′	C15′	C14′	123·0 (5)
C9	C10	C11	117·9 (4)	O1	C15	C10	117·8 (5)
C9	C10	C15	126·3 (4)	O1	C15	C14	119·4 (4)
C11	C10	C15	115·7 (5)	C10	C15	C14	122·7 (5)
C10	C11	C12	122·2 (5)	O1	C16	O2	122·7 (5)
C10′	C11′	C12′	120·9 (5)	O1	C16	C17	108·9 (5)
C11′	C12′	C13′	119·8 (5)	O2	C16	C17	128·4 (5)
C11	C12	C13	119·5 (5)	O1′	C16′	O2′	122·1 (5)
C12	C13	C14	120·5 (6)	O1′	C16′	C17′	111·4 (5)
C12′	C13′	C14′	120·4 (6)	O2′	C16′	C17′	126·5 (6)

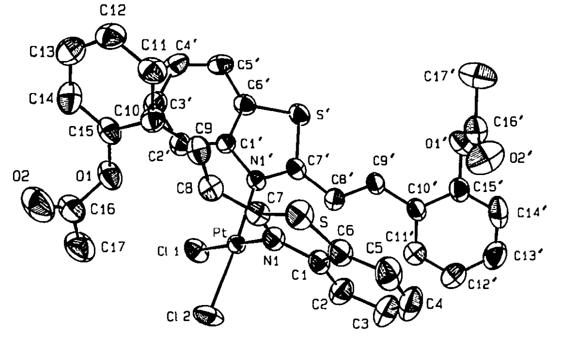

Fig. 1. Labeling of atoms in [Pt(asb)$_2$Cl$_2$] (50% probability ellipsoids). The two ligand molecules are not symmetrically related, but a parallel numbering scheme has been used to indicate similar positions in the molecules.

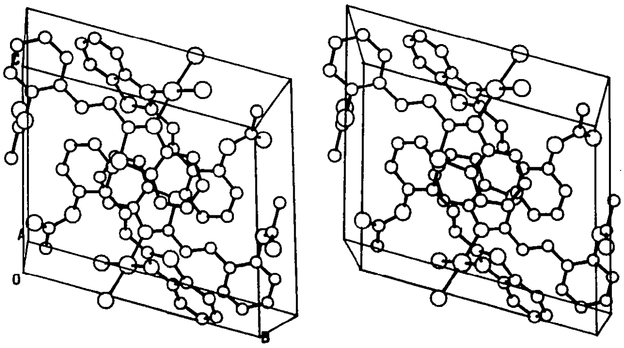

Fig. 2. Packing diagram of [Pt(asb)$_2$Cl$_2$] in the unit cell.

5-nitrostyryl)benzothiazole (Muir, Gomez, Muir, Cox & Cadiz, 1987). In the nsb complex, the large deviation from planarity was postulated to facilitate parallel stacking of the nitrobenzene moieties at a distance which would permit π interactions. In the present complex, with a pair of *cis* asb molecules, such stacking interactions are hindered by the overall geometry. The smaller dihedral angles observed presumably result from avoidance of non-bonded interactions between H atoms on the olefin C atoms, C8, C9, C8′ and C9′, and nearby atoms. With the average dihedral angles obtained, there are no non-bonded distances between those H atoms and other atoms shorter than 1·94 Å. It is interesting to note that the acetoxybenzene rings in the two ligands have different orientations with respect to the olefin C atoms. Thus, C8 is closest to O1, while C8′ is closest to C11′.

The benzothiazole and acetoxybenzene rings in both ligands show only very small deviations from planarity. The largest deviations from the least-squares planes are for C6, 0·026 (5) Å; C2′, 0·031 (5) Å; and C7′, 0·030 (4) Å. The distances and angles in the ligands are normal.

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Structure of a Bis(η^4-exocyclic-1,3-diene)Fe(CO)$_3$ Complex

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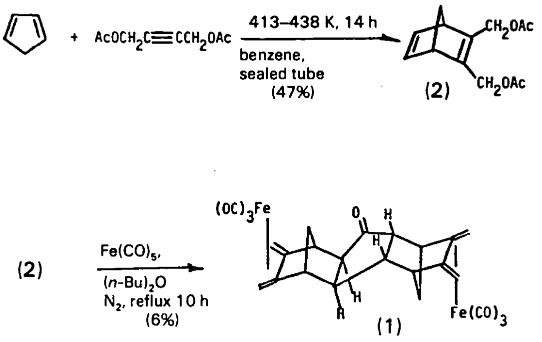
Abstract. *trans*-μ-(12–13-η:14–15-η-1,2,3,4,4a,4b,5,6,7,8,8a,9a-Dodecahydro-2,3,6,7-tetramethylene-1,4:5,8-dimethanofluoren-9-one)-bis(tricarbonyliron), [$Fe_2(CO)_6(C_{19}H_{20}O)$], $M_r = 544{\cdot}12$, triclinic, $P\bar{1}$, $a = 6{\cdot}940\,(1)$, $b = 12{\cdot}418\,(2)$, $c = 13{\cdot}894\,(2)$ Å, $\alpha = 93{\cdot}65\,(1)$, $\beta = 94{\cdot}50\,(1)$, $\gamma = 95{\cdot}31\,(1)°$, $V = 1185{\cdot}4\,(3)$ Å^3, $Z = 2$, $D_x = 1{\cdot}524$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 12{\cdot}64$ cm^{-1}, $F(000) = 556$, $T = 294$ K, $R = 0{\cdot}0412$ for 2432 reflections. The Fe^0 atoms exhibit distorted tetragonal pyramidal geometries with the bases defined by two C—O groups and the midpoints of the C=C bonds of the (*S-cis*)-butadiene moieties. The norbornene rings are fused to a planar cyclopentanone ring in an *exo–trans–exo* fashion.

Introduction. As part of a continuing program that is involved with the study of the stereochemistry and mechanism of thermal reactions of iron pentacarbonyl with substituted norbornadienes (Speert, Gelan, Anteunis, Marchand & Laszlo, 1973; Marchand & Hayes, 1977; Marchand, Goodin, Hossain & van der Helm, 1984; Marchand, Earlywine & Heeg, 1986), we have examined the corresponding reaction of 2,3-bis(acetoxy)norbornadiene with Fe(CO)$_5$. Reactions of this kind have been found typically to afford a variety of norbornadiene dimers and also to afford products that are derived *via* Fe(CO)$_5$-promoted coupling of the strained alkene substrate to carbon monoxide (Weissberger & Laszlo, 1976).

In the past, no effort has been made in our laboratory to isolate iron-containing intermediates and/or products that might result from these reactions. Instead, such Fe^0 complexes are routinely destroyed oxidatively by stirring the crude reaction product with a solution of ferric chloride in acetone (Marchand & Hayes, 1977; Marchand, Goodin, Hossain & van der Helm, 1984; Marchand, Earlywine & Heeg, 1986). However, when this procedure was applied to the product of the thermal reaction of 2,3-bis(acetoxy)norbornadiene with Fe(CO)$_5$, a pale yellow crystalline solid was obtained in low yield; this material proved to be the unusually stable bis(η^4-1,3-diene)Fe(CO)$_3$ complex (1).



Experimental. A pale yellow crystal of dimensions 0·35 × 0·10 × 0·175 mm; Nicolet $R3m/\mu$ update of a $P2_1$ diffractometer; data collected in the Wyckoff mode ($4 \leq 2\theta \leq 45°$, 2θ fixed, ω varied), variable scan rate (4 to 29·3° min^{-1}), graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from a least-squares

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