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# Structures of the Two New Compounds Distrontium Copper(II) Triselenite(IV) and Distrontium Copper(II) Bis[hydrogenselenite(IV)] Bisselenite(IV)

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**Abstract.** $Sr_2Cu(SeO_3)_3$, $M_r = 619.68$, triclinic, $P\bar{1}$, $a = 7.229$ (3), $b = 7.710$ (3), $c = 8.656$ (3) Å, $\alpha = 102.68$ (3), $\beta = 105.31$ (3), $\gamma = 96.12$ (3)°, $V = 447.0$ Å$^3$, $Z = 2$, $D_x = 4.60$ Mg m$^{-3}$, $\lambda$(Mo $K\alpha$) = 0.71073 Å, $\mu = 26.0$ mm$^{-1}$, $F(000) = 558$, room temperature, $R = 0.033$ for 3330 reflections up to $2\theta = 70°$. $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$, $M_r = 748.65$, triclinic, $P\bar{1}$, $a = 5.260$ (1), $b = 6.961$ (1), $c = 9.052$ (2) Å, $\alpha = 67.86$ (1), $\beta = 75.40$ (1), $\gamma = 80.41$ (1)°, $V = 296.6$ Å$^3$, $Z = 1$, $D_x = 4.19$ Mg m$^{-3}$, $\lambda$(Mo $K\alpha$) = 0.71073 Å, $\mu = 22.6$ mm$^{-1}$, $F(000) = 339$, room temperature, $R = 0.036$ for 2362 reflections up to $2\theta = 70°$. In the two compounds the Sr atoms are [8] and [9] coordinated (Sr—O = 2.52 to 2.93 Å), the Cu atoms have a tetragonal-pyramidal [4 + 1] and a square-planar [4] coordination, respectively. The distance Se—$O_h$ (1.80 Å) is significantly longer than the other Se—O bonds (1.66 to 1.73 Å). In $Sr_2Cu(SeO_3)_3$, the $SrO_8$ polyhedra form a three-dimensional network; in $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$, the $SrO_9$ polyhedra are edge-linked to form sheets which are connected by $CuO_4$ squares, $SeO_3$ groups and the hydrogen bond (O—H···O = 2.88 Å).

**Introduction.** The crystal chemistry of compounds containing selenite(IV) groups $[SeO_3]^{2-}$ or various protonated selenite(IV) groups are characterized by the space requirement of the lone-pair electrons. Many previous studies have been performed by several authors. Examinations of alkaline-earth copper(II) selenites which were grown under hydrothermal conditions yielded the new compounds $SrCu(SeO_3)_2$, three modifications of $BaCu(SeO_3)_2$ (Effenberger, 1987), $Sr_2Cu(SeO_3)_3$ and $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$. For comparison, the crystal structures of the following alkaline-earth selenites have been determined up to now: $MgSeO_3.6H_2O$ (Weiss, Wendling & Grandjean, 1966), $CaSeO_3.H_2O$ (Valkonen, Losoi & Pajunen, 1985), $CaSe_2O_5$ (Delage, Carpy & Goursolle, 1982), $Ca(SeO_2OH)_2.H_2O$ and $Ca_2(SeO_2OH)_2(Se_2O_5)$ (Valkonen, 1986).

**Experimental.** Single crystals suitable for X-ray work were grown under hydrothermal conditions as described by Effenberger (1987). Experimental details are compiled in Table 1. Four-circle diffractometer AED2 (Stoe & Cie, Darmstadt, Federal Republic of Germany), graphite-monochromatized Mo $K\alpha$ radiation; lattice parameters from 75 reflections up to $2\theta = 45°$ each. $2\theta/\omega$ scan mode; min. of 48 steps per reflection increased for $\alpha_1$–$\alpha_2$ dispersion; step time 0.5 and 1.5 s per step; step width 0.03°; 8 steps for background correction at each side; 3 standard reflections monitored every 2 h, intensity variation ≤

Table 1. *Details on data collection and structure refinement*

| | $Sr_2Cu(SeO_3)_3$ | $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ |
|---|---|---|
| Crystal dimensions (mm) | 0.06 × 0.11 × 0.15 | 0.04 × 0.09 × 0.11 |
| Colour | Light blue | Bright blue |
| Crystallographic forms | {010}, {001}, {110}, {01$\bar{1}$}, {$\bar{2}$01} | {010}, {001}, {111} |
| $2\theta_{max}$(°) | 70 | 70 |
| Measured reflections | 4202 | 5225 |
| $h, k, l$ | −11→11, −12→0, −13→13 | −8→8, −11→11, −14→14 |
| Unique reflections | 3931 | 2612 |
| $R_{int}$ | 0.048 | 0.055 |
| Reflections with $\|F_o\| > 3\sigma(F_o)$ | 3330 | 2362 |
| Absorption correction | Gaussian integration | 3 $\psi$ scans |
| Transmission factors | 0.024 to 0.142 | 0.014 to 0.075 |
| $R$, $wR$, $w = [\sigma(F_o)]^{-2}$ | 0.033, 0.030 | 0.036, 0.030 |
| Variable parameters | 137 | 93 |
| Final difference Fourier map excursions (e Å$^{-3}$) | −1.5 to 1.9 | −1.8 to 1.6 |
| Extinction (Zachariasen, 1967): $g$ | 6.2 (4) × 10$^{-6}$ | 1.67 (7) × 10$^{-5}$ |
| Max. $\Delta/\sigma$ | <0.001 | <0.001 |

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Table 2. *Atomic fractional coordinates and equivalent isotropic temperature parameters* (Å$^2$) *with e.s.d.'s in parentheses*

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

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| $Sr_2Cu(SeO_3)_3$ | | | | |
| Sr(1) | 0·24224 (6) | 0·08944 (5) | 0·39070 (5) | 0·0119 |
| Sr(2) | 0·37523 (6) | 0·51505 (5) | 0·19242 (5) | 0·0137 |
| Cu | 0·91278 (7) | 0·65866 (7) | 0·25028 (6) | 0·0116 |
| Se(1) | 0·63532 (6) | 0·91769 (5) | 0·20247 (5) | 0·0115 |
| Se(2) | 0·89877 (6) | 0·20267 (5) | 0·03236 (5) | 0·0110 |
| Se(3) | 0·77115 (6) | 0·36721 (5) | 0·41231 (5) | 0·0111 |
| O(11) | 0·4853 (5) | 0·8722 (4) | 0·3147 (4) | 0·015 |
| O(12) | 0·8476 (4) | 0·9844 (5) | 0·3540 (4) | 0·017 |
| O(13) | 0·6567 (4) | 0·7006 (4) | 0·1131 (4) | 0·019 |
| O(21) | 1·1226 (5) | 0·2468 (4) | 0·1661 (4) | 0·016 |
| O(22) | 0·8160 (5) | 0·3993 (5) | 0·0634 (5) | 0·023 |
| O(23) | 0·9387 (5) | 0·1872 (4) | −0·1547 (4) | 0·017 |
| O(31) | 0·5294 (5) | 0·2980 (5) | 0·3544 (5) | 0·022 |
| O(32) | 0·7760 (5) | 0·5919 (4) | 0·4103 (4) | 0·017 |
| O(33) | 0·8302 (5) | 0·3752 (5) | 0·6169 (4) | 0·017 |
| $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ | | | | |
| Sr | 0·83119 (6) | 0·80657 (5) | 0·44133 (3) | 0·0143 |
| Cu | 0 | 0 | 0 | 0·0133 |
| Se(1) | 0·80535 (7) | 0·44989 (5) | 0·21859 (3) | 0·0150 |
| Se(2) | 0·40121 (6) | 0·02819 (5) | 0·18651 (3) | 0·0122 |
| O(11) | 0·8701 (6) | 0·2015 (5) | 0·2382 (3) | 0·024 |
| O(12) | 0·4534 (6) | 0·4481 (5) | 0·2776 (3) | 0·024 |
| O(13) | 0·8772 (6) | 0·4666 (4) | 0·3820 (3) | 0·019 |
| O(21) | 0·3345 (5) | −0·0409 (4) | 0·3897 (3) | 0·017 |
| O(22) | 0·6951 (4) | −0·1179 (4) | 0·1620 (2) | 0·014 |
| O(23) | 0·2063 (4) | −0·1360 (4) | 0·1690 (2) | 0·015 |
| H | 0·401 (10) | 0·545 (8) | 0·270 (5) | 0·015† |

† Fixed during refinement.

1·5%. Corrections for Lorentz and polarization effects; complex neutral atomic scattering functions (*International Tables for X-ray Crystallography*, 1974). All calculations were performed with the program system *STRUCSY* (Stoe & Cie, 1984).

Some of the Sr, Se and Cu atoms were found by direct methods, the remainder and the O atoms in Fourier and difference Fourier summations. Convergencies were reached after several cycles of least-squares refinements on $F$ with anisotropic temperature parameters for all atoms. The difference Fourier summation of $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ showed its highest peak at that position which was expected from crystal chemical considerations for the H atom. The H atom was included in refinement, its atomic coordinates were allowed to vary, $U_{iso}$ was fixed to 0·015 Å$^2$. Atomic coordinates and equivalent isotropic temperature parameters are compiled in Table 2,* some important interatomic distances and bond angles are listed in Table 3.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44640 (32 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Selected interatomic bond lengths* (Å) *and angles* (°)

E.s.d.'s are ~0·003 Å for Sr—O, Cu—O and Se—O, ~0·005 Å for O—O, ~0·05 Å for O—H, ~0·2° for O—Cu—O and O—Se—O and 5° for O—H—O.

$Sr_2Cu(SeO_3)_3$

| | | | |
|---|---|---|---|
| Sr(1)—O(21) | 2·524 | Sr(2)—O(21) | 2·536 |
| Sr(1)—O(23) | 2·552 | Sr(2)—O(22) | 2·544 |
| Sr(1)—O(31) | 2·617 | Sr(2)—O(33) | 2·568 |
| Sr(1)—O(12) | 2·620 | Sr(2)—O(31) | 2·571 |
| Sr(1)—O(11) | 2·661 | Sr(2)—O(11) | 2·673 |
| Sr(1)—O(32) | 2·712 | Sr(2)—O(13) | 2·684 |
| Sr(1)—O(11) | 2·714 | Sr(2)—O(13) | 2·734 |
| Sr(1)—O(12) | 2·795 | Sr(2)—O(32) | 2·926 |

$Sr_2Cu(SeO_2OH)_2(SeO_3)_2$

| | | | |
|---|---|---|---|
| Sr—O(21) | 2·548 | Sr—O(23) | 2·685 |
| Sr—O(13) | 2·552 | Sr—O(12) | 2·725 |
| Sr—O(13) | 2·579 | Sr—O(21) | 2·742 |
| Sr—O(22) | 2·640 | Sr—O(21) | 2·884 |
| Sr—O(11) | 2·677 | | |

$Sr_2Cu(SeO_3)_3$

| Cu | O(23) | O(33) | O(13) | O(32) | O(22) |
|---|---|---|---|---|---|
| O(23) | 1·969 | 2·703 | 2·864 | 3·919 | 3·299 |
| O(33) | 86·2 | 1·987 | 4·006 | 2·907 | 3·228 |
| O(13) | 91·8 | 177·9 | 2·019 | 2·827† | 2·702† |
| O(32) | 158·2 | 93·0 | 88·8 | 2·022 | 3·146 |
| O(22) | 104·9 | 101·2 | 79·8 | 96·6 | 2·188 |

$Sr_2Cu(SeO_2OH)_2(SeO_3)_2$

| Cu | O(22) | O(22) | O(23) | O(23) |
|---|---|---|---|---|
| O(22) | 1·936 | 3·873 | 2·691 | 2·811 |
| O(22) | 180 | 1·936 | 2·811 | 2·691 |
| O(23) | 87·5 | 92·5 | 1·955 | 3·910 |
| O(23) | 92·5 | 87·5 | 180 | 1·955 |

$Sr_2Cu(SeO_3)_3$

| Se(1) | O(11) | O(12) | O(13) |
|---|---|---|---|
| O(11) | 1·694 | 2·578* | 2·609† |
| O(12) | 99·8 | 1·677 | 2·622 |
| O(13) | 99·5 | 100·9 | 1·725 |
| Se(2) | O(21) | O(22) | O(23) |
| O(21) | 1·672 | 2·657 | 2·655 |
| O(22) | 104·8 | 1·681 | 2·620 |
| O(23) | 103·9 | 101·6 | 1·700 |
| Se(3) | O(31) | O(32) | O(33) |
| O(31) | 1·677 | 2·598† | 2·602 |
| O(32) | 99·2 | 1·733 | 2·689 |
| O(33) | 101·0 | 103·3 | 1·694 |

$Sr_2Cu(SeO_2OH)_2(SeO_3)_2$

| Se(1) | O(11) | O(12) | O(13) |
|---|---|---|---|
| O(11) | 1·656 | 2·590 | 2·638 |
| O(12) | 97·1 | 1·797 | 2·674 |
| O(13) | 105·2 | 101·1 | 1·665 |
| Se(2) | O(21) | O(22) | O(23) |
| O(21) | 1·673 | 2·582‡ | 2·590‡ |
| O(22) | 99·1 | 1·718 | 2·583 |
| O(23) | 99·1 | 97·0 | 1·731 |

O(12)—H = 0·67
H···O(23) = 2·24
O(12)···O(23) = 2·878
O(12)—H···O(23) = 161

* Common O—O edge with $Sr(1)O_8$.
† Common O—O edge with $Sr(2)O_8$.
‡ Common O—O edge with $SrO_9$.

**Discussion.** The two title compounds are chemically related to each other as the ratio Sr:Cu is in both cases 2:1 and the anion groups are selenites. In one of the two compounds half of the selenite groups are protonated. This results in two principally different structures with distinct coordination numbers of the Sr and Cu atoms. Both the structures consist of networks with dissimilar interconnections of the coordination polyhedra (Figs. 1 and 2).

The coordination polyhedra around the three crystallographically different Sr atoms within the two title compounds are clear-cut. The individual Sr—O bond lengths range from 2·524 (3) to 2·926 (4) Å. The two

Sr atoms in $Sr_2Cu(SeO_3)_3$ are surrounded by eight ligands with average Sr—O bond lengths of 2·649 and 2·655 Å. In $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ the Sr atom is nine coordinated; in accordance with the larger coordination number the average Sr—O bond length is 2·670 Å. The $SrO_8$ and $SrO_9$ coordination polyhedra are irregular. Next Sr—O distances exceed 3·40 Å. These types of Sr coordination frequently occur in oxygen-bearing compounds (*cf.* Fischer, 1972).

The Cu atoms are coordinated to four nearest O-atom neighbours in an approximately square-planar arrangement with Cu—O bond lengths from 1·936 (2) to 2·022 (3) Å – a well known coordination for formally divalent Cu atoms (*cf.* Zemann, 1961, 1972; Eysel, Breuer & Lambert, 1984; Hathaway, 1984; Wells, 1984). In $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ the $CuO_4$ 'square' is exactly planar due to the site symmetry $\bar{1}$ and the average Cu—O bond length is 1·946 Å; two further O atoms have a Cu—O distance of 2·881 (3) Å

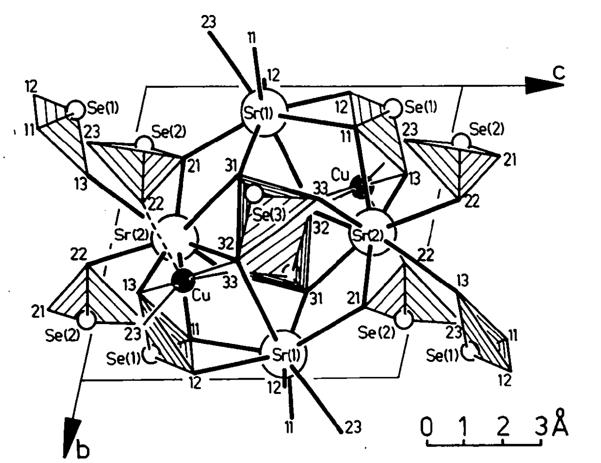


Fig. 1. The crystal structure of $Sr_2Cu(SeO_3)_3$ in a projection onto (100).

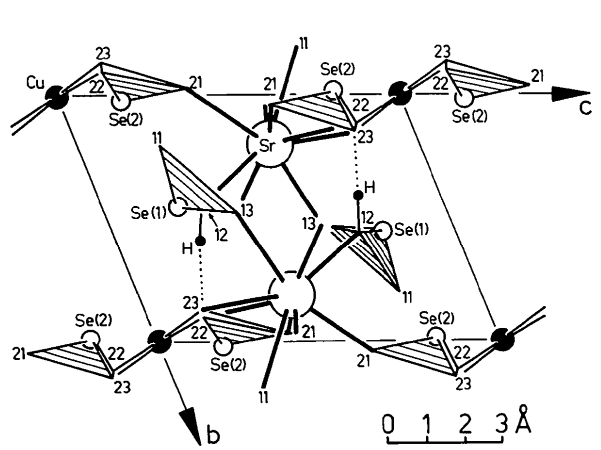


Fig. 2. The crystal structure of $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ in a projection onto (100). The hydrogen bond is dotted.

giving a formal bond valence calculated according to Trömel (1984) of 0·03 v.u. only (v.u. = valence unit). In $Sr_2Cu(SeO_3)_3$, the average Cu—O bond length to the four nearest neighbours is 1·999 Å. A fifth O atom is at 2·188 (4) Å. The coordination polyhedron can be described as a distorted tetragonal pyramid with the Cu atom near to the centre of the basal plane and the fifth ligand at the apex. As common for [4 + 1] coordinated Cu atoms with all the Cu—O bond lengths <2·30 Å, the $CuO_4$ 'square' is bent; one of the two O—Cu—O angles between opposite O atoms is near to the ideal value of 180°, but the other one deviates by 21·8 (2)°. Therefore, this coordination polyhedron is considered a representative for a transition from a tetragonally pyramidal [4 + 1] coordination towards a trigonally bipyramidal [5] coordination (*cf.* Effenberger, 1988). It should be mentioned that a sixth O atom follows at 2·612 (4) Å and at least a weak chemical interaction is assumed (formal bond valence 0·06 v.u.; Trömel, 1984). Coordination polyhedra of $Cu^{II}$ atoms with five Cu—O bonds <2·20 Å and a sixth Cu—O distance at ~2·60 Å have seldom been described in inorganic crystal structures; usually there are larger gaps between the five Cu—O bond lengths below 2·20 Å and the sixth Cu—O distance.

The selenite groups form trigonal pyramids with the Se atoms at the apexes. In agreement with values from the literature (Fischer & Zemann, 1974), the Se—O bond lengths in the $SeO_3$ groups of the two title compounds vary from 1·672 (3) to 1·733 (3) Å. Protonation causes an elongation of the Se—$O_h$ bond length [1·797 (3) Å] in the $SeO_2OH$ group while the two other Se—O bond lengths are the shortest in the two compounds [1·656 (3) and 1·665 (2) Å]. Ferraris & Ivaldi (1984) gave 1·759 ± 0·02 Å as the mean Se—$O_h$ bond length derived from 18 distances in $SeO_2OH$ groups. Longer Se—$O_h$ bond lengths in $SeO_2OH$ groups were compiled by Valkonen & Leskelä (1978); additional examples are $Cu(SeO_2OH)_2$ [1·773 (2) Å; Effenberger, 1985], $NH_4Mn(SeO_2OH)_3$ [1·738 (7) to 1·776 (7) Å; Valkonen & Jalkanen, 1985], $Cd(SeO_2OH)NO_3$ [1·778 (8) Å; Leskelä, Valkonen & Leskelä, 1984], $Ca(SeO_2OH)_2.H_2O$ [Se(1): 1·784 (1) Å; Valkonen, 1986], $Ca_2(SeO_2OH)_2(Se_2O_5)$ [1·773 (10) Å; Valkonen, 1986]. The average Se—O bond lengths vary from 1·684 to 1·701 Å for the selenite groups in $Sr_2Cu(SeO_3)_3$ and they are 1·706 and 1·707 Å in $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$. The bond valences calculated according to Brown & Wu (1976) range from 3·67 to 3·88 v.u. for the two compounds. Next Se—O bond lengths exceed 2·80 Å.

The coordination numbers of the O atoms are three and four with the exception of atom O(11) in $Sr_2Cu(SeO_2OH)_2(SeO_3)_2$ which is coordinated only to one Se and one Cu atom. If the H atom is neglected, the sums of the bond valences at the O atoms are 1·62 v.u. for the [2] coordinated O(11) atom, 1·17 v.u. for the 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, $\alpha$ = 105·88 (3), $\beta$ = 90·64 (4), $\gamma$ = 87·64 (4)°, $V$ = 1654 (2) Å$^3$, $Z$ = 2, $D_x$ = 1·72 g cm$^{-3}$, $\lambda$(Mo $K\alpha$) = 0·71073 Å, $\mu$ = 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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