0·253 (7) Å]. The torsion angles of the two ethylenic bridges are —45·6 (6)° for N1—C8—C9—N2 and 49·4 (6)° for N2—C10—C11—N3 and the corresponding C—C bond lengths are 1·502 (10) and 1·510 (10) Å, respectively, in good agreement with the corresponding values found in the Cu(saltrien) complex [both 1·498 (9) Å]. It seems likely that such values are the real ones for the C—C distances while the apparently shorter values found in various salen complexes can be attributed to thermal motion of the ethylene bridges in the crystals (Rotondo *et al.*, 1984; Bresciani-Pahor *et al.*, 1976).

This structure confirms that the presence of a hydrogen bond from the phenoxy oxygen to the terminal nitrogen is usual in these kinds of complexes. The final difference Fourier map, as in the analogous copper compound, shows some electron-density residues of the order 0·9 e Å^{-3} near to the non-coordinated nitrogen (N4) in a position characteristic for three hydrogen atoms bound to sp^3-hybridized nitrogen atoms. One of these hydrogens (H43) forms a short contact of 1·983 (3) Å with the oxygen of the saltren ligand; the separation N4···O1 is 2·705 (6) Å, characteristic of a hydrogen bond. The molecular packing (Fig. 2) is mainly determined by normal van der Waals interactions and by some hydrogen bonds involving the oxygen atoms of the perchlorate anions; one of them makes a long-range interaction with the metal atom [Ni···O8 3·044 (7) Å] in the apical position.

The molar conductivity of the complex in methanol at 298 K is 188 Ω cm^2 mol^{-1}; this value is in the range for a 2:1 electrolyte type and suggests that the complex, analogously to the copper derivative, acts in methanol as a dipositively charged species.

Magnetic susceptibilities measured by the Evans (1959) method revealed that the complex is dia-magnetic when dissolved in methanol. The electronic spectrum in the same solvent shows a very intense band at 380 nm which is typical for all deprotonated salicylaldehydo derivatives; in the tail of this intense band, a shoulder can be seen at 445 nm, attributable to a $d \rightarrow d$ transition of a d^8 Ni atom in an approximately square-planar arrangement. The diffuse reflectance spectrum of the solid powdered compound recorded in the same region shows a well resolved maximum at 448 nm.

References

BETT, G., FENTON, D. E. & TATE, J. R. (1981). *Inorg. Chim. Acta,* 54, 101–102.
BRESCIANI-PAHOR, N., CALLIGARIS, M., DELISE, P., NARDIN, G., RANDACCIO, L., ZOTTI, E., FACCHINETTI, G. & FLORIANI, C. (1976). *J. Chem. Soc. Dalton Trans.* pp. 2310–2316.
CASELLATO, V., VIGATO, P. A., FENTON, D. E. & VIDALI, M. (1979). *Chem. Soc. Rev.* 8, 199–220.
COSTA, G., MESTRONI, G., PUXEDDU, A. & REISENHOFER, E. (1970). *J. Chem. Soc. A,* pp. 2870–2874.
COSTES, J. P., CROSS, G., DARBIEN, M. H. & LAURENT, J. P. (1982). *Inorg. Chim. Acta,* 60, 111–114.
CUSMANO PRIOLO, F., ROTONDO, E., RIZZARDI, G., BRUNO, G. & BOMBIERI, G. (1983). *Acta Cryst.* C39, 550–552.
EVANS, D. F. (1959). *J. Chem. Soc.* pp. 2003–2005.
HOLM, R. H. & O'CONNOR, M. J. (1971). *Prog. Inorg. Chem.* 14, 241–401.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO.* Program for plotting molecular and crystal structures. Univ. of Cambridge, England.
NARDELLI, M. (1983). *Comput. Chem.* 7, 95–98.
ROTONDO, E., CUSMANO PRIOLO, F., BOMBIERI, G. & BRUNO, G. (1984). *Acta Cryst.* C40, 960–962.
ROTONDO, E., CUSMANO PRIOLO, F., ROMEO, M., BRUNO, G. & BOMBIERI, G. (1983). *Acta Cryst.* C39, 1525–1527.
SHELDRICK, G. M. (1976). *SHELX76.* Program for crystal structure determination. Univ. of Cambridge, England.
WILKINS, R. G. (1971). *Adv. Chem. Ser.* No. 100, pp. 111–126.

Structure of a *nido*-Metalla-Monocarbon Carbaborane, [5-(PPh3)-9,9,9-(H)(PPh3)2-9,6-IrCB8H10]

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Abstract. 5,9,9-Tris(triphenylphosphine)-6,9-carbirida-decaborane(14), $C_{55}H_{56}B_8IrP_3$ (excluding solvent), $M_r = 1088·71$, orthorhombic, $Pna2_1$, $a = 32·796$ (10), $b = 17·945$ (7), $c = 10·656$ (4) Å, $U = 6271$ (3) Å^3, $Z = 4$, $D_x = 1·15$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, μ(Mo $K\alpha$) = 22·2 cm^{-1}, $F(000) = 2192$, $T = 290$ K, $R = 0·069$ for 2206 unique observed $[I/\sigma(I) \geq 3·0]$ reflections. A minor product from

the reaction of $[CB_8H_{13}]^-$ and $[IrCl(PPh_3)_3]$ has been identified as the title compound. It contains 24 skeletal electrons, as expected for *nido* geometry, but the precision of the B—B bond distances is too low for distortions caused by the substitution of C for B to be firmly identified. The geometry differs from the *iso–nido* structure established for one other $[IrCB_8]$ open cage.

Introduction. Polyhedral cage compounds containing both metal and boron atoms are well established, and the structures of many such compounds have been determined by X-ray crystallographic studies (Kennedy, 1986). In contrast, relatively few structures are known for compounds which contain one heteroatom in the cage as well as the metal and boron atoms. In particular, for ten-atom cages, which are commonly *closo* (based on the $B_{10}H_{10}^{2-}$ ion) or *nido* (based on the $B_{10}H_{14}$ framework), structural parameters for MCB_8 cages are known for only a few compounds (Alcock, Jasztal & Wallbridge, 1987). We have previously published the structure of a *closo*-iridium derivative $[1-(PPh_3)-2,2,2-(H)(PPh_3)_2-2,10-IrCB_8H_8]$ which was formed surprisingly from the *arachno*-$[CB_8H_{13}]^-$ ion by reaction with $[IrCl(PPh_3)_3]$ (Alcock, Taylor & Wallbridge, 1983). We also isolated from the same reaction, albeit in lower yield than the *closo* compound, the compound we expected originally, namely the *nido*-$[5-(PPh_3)-9,9,9-(H)(PPh_3)_2-9,6-IrCB_8H_{10}]$. An X-ray structure investigation was undertaken to establish the framework structure of this intermediate unequivocally, since this allows a pathway for the formation of the *closo* compound to be suggested with more confidence than has hitherto been possible.

Experimental. The *arachno*-carbaborane $[CB_8H_{14}]$ (0·11 g, 0·98 mmol) was dissolved in degassed diethyl ether (25 cm³) and LiBu (0·98 mmol) was added to the stirred solution. After evolution of butane, and the formation of Li$[CB_8H_{13}]$, the $[IrCl(PPh_3)_3]$ (1·0 g, 0·98 mmol) was added and the mixture stirred for 6 d. The solvent was evaporated, and the mustard yellow residue dissolved in CH_2Cl_2 (15 cm³). The resulting dark red solution was filtered in air, and the *nido* compound separated by preparative thin-layer chromatography (silica gel, CH_2Cl_2 50%: 60°–80° petroleum ether 50% as eluent, R_f value 0·2, yield 23 mg, 2·1%). The compound was recrystallized from CH_2Cl_2/acetone to give red-orange irregular blocks. The positions of the bridging H atoms could not be established crystallographically (see below), and attempts to locate them from ¹H NMR spectroscopy were only partially successful. The resonance due to the Ir—H proton occurs at −13·5 p.p.m. as a multiplet. Since this appears to be a triplet of doublets we tentatively assign the principal coupling to the two equivalent P nuclei on the Ir (J, H—Ir—P, ~20 Hz), with a further coupling (~6 Hz) due to a bridging hydrogen (J, H—Ir—H—B).

Table 1. *Atom coordinates* ($\times 10^4$) *and temperature factors* ($\text{Å}^2 \times 10^3$)

	x	y	z	U
Ir	1113 (1)	6498 (1)	5000	30 (1)*
P(1)	485 (3)	6567 (8)	5958 (8)	36 (4)*
P(2)	1402 (3)	5458 (6)	5925 (9)	28 (4)*
P(3)	2374 (3)	7167 (7)	2130 (9)	38 (4)*
B(1)	1443 (14)	7787 (27)	2738 (41)	34 (13)
B(2)	1818 (11)	8380 (25)	3518 (34)	23 (11)
B(3)	1318 (17)	8296 (33)	4104 (51)	59 (18)
B(4)	1000 (15)	7518 (33)	3627 (48)	57 (17)
B(5)	1919 (14)	7454 (29)	3241 (42)	37 (13)
C(6)	2030 (12)	7755 (22)	4519 (31)	43 (12)
B(7)	1680 (13)	8215 (24)	5363 (30)	23 (13)
B(8)	1154 (21)	7706 (37)	5171 (89)	105 (26)
B(10)	1449 (13)	6869 (26)	3049 (38)	31 (12)
C(01)	1299	1191	5055	80
C(02)	1125	570	6196	80
C(03)	1164	697	4378	80
C(112)	−114 (7)	5623 (13)	7034 (20)	43 (12)
C(113)	−322 (7)	4951 (13)	7177 (20)	60 (14)
C(114)	−208 (7)	4330 (13)	6472 (20)	55 (14)
C(115)	115 (7)	4382 (13)	5624 (20)	35 (11)
C(116)	323 (7)	5055 (13)	5481 (20)	24 (10)
C(111)	209 (7)	5675 (13)	6186 (20)	30 (10)
C(122)	87 (7)	7863 (14)	5066 (25)	56 (11)
C(123)	−152 (7)	8240 (14)	4190 (25)	82 (18)
C(124)	−359 (7)	7842 (14)	3264 (25)	83 (17)
C(125)	−327 (7)	7068 (14)	3213 (25)	81 (17)
C(126)	−87 (7)	6691 (14)	4088 (25)	61 (14)
C(121)	120 (7)	7089 (14)	5015 (25)	37 (8)
C(132)	765 (6)	6943 (14)	8348 (22)	35 (10)
C(133)	734 (6)	7222 (14)	9566 (22)	68 (16)
C(134)	375 (6)	7565 (14)	9961 (22)	80 (13)
C(135)	46 (6)	7628 (14)	9139 (22)	57 (14)
C(136)	76 (6)	7349 (14)	7921 (22)	49 (13)
C(131)	436 (6)	7006 (14)	7525 (22)	52 (13)
C(212)	1585 (6)	5599 (14)	8531 (25)	69 (15)
C(213)	1511 (6)	5514 (14)	9813 (25)	56 (11)
C(214)	1157 (6)	5159 (14)	10221 (25)	59 (13)
C(215)	876 (6)	4889 (14)	9348 (25)	33 (10)
C(216)	950 (6)	4974 (14)	8067 (25)	51 (13)
C(211)	1305 (6)	5329 (14)	7658 (25)	29 (10)
C(222)	1275 (7)	4522 (11)	3842 (22)	29 (10)
C(223)	1206 (7)	3847 (11)	3227 (22)	51 (13)
C(224)	1139 (7)	3199 (11)	3921 (22)	75 (16)
C(225)	1141 (7)	3226 (11)	5229 (22)	36 (11)
C(226)	1210 (7)	3901 (11)	5844 (22)	29 (10)
C(221)	1278 (7)	4548 (11)	5151 (22)	86 (16)
C(232)	2200 (7)	4816 (11)	5840 (20)	19 (9)
C(233)	2624 (7)	4863 (11)	5840 (20)	52 (13)
C(234)	2814 (7)	5557 (11)	5917 (20)	63 (14)
C(235)	2580 (7)	6204 (11)	5994 (20)	67 (15)
C(236)	2155 (7)	6157 (11)	5993 (20)	28 (10)
C(231)	1965 (7)	5463 (11)	5916 (20)	25 (10)
C(312)	2724 (6)	7804 (13)	−48 (23)	41 (9)
C(313)	2715 (6)	7998 (13)	−1315 (23)	35 (11)
C(314)	2351 (6)	7946 (13)	−1988 (23)	52 (13)
C(315)	1997 (6)	7700 (13)	−1393 (23)	50 (13)
C(316)	2006 (6)	7506 (13)	−125 (23)	56 (11)
C(311)	2370 (6)	7558 (13)	547 (23)	44 (12)
C(322)	2884 (7)	8200 (14)	3161 (22)	49 (12)
C(323)	3230 (7)	8444 (14)	3800 (22)	56 (12)
C(324)	3533 (7)	7936 (14)	4138 (22)	94 (18)
C(325)	3489 (7)	7184 (14)	3837 (22)	82 (17)
C(326)	3143 (7)	6940 (14)	3198 (22)	69 (16)
C(321)	2840 (7)	7448 (14)	2860 (22)	21 (9)
C(332)	2283 (7)	5636 (15)	2625 (19)	36 (11)
C(333)	2315 (7)	4882 (15)	2320 (19)	121 (24)
C(334)	2488 (7)	4667 (15)	1181 (19)	53 (13)
C(335)	2631 (7)	5207 (15)	347 (19)	85 (19)
C(336)	2600 (7)	5961 (15)	652 (19)	62 (14)
C(331)	2426 (7)	6175 (15)	1791 (19)	27 (10)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Similar small couplings, between terminal metal H and adjacent bridging M—H—B protons, have been observed previously in structurally related metallaboranes, such as $[6-H-6,6-(PPh_3)_2-nido-6-IrB_9H_{13}]$ (Boocock, Bould, Greenwood, Kennedy & McDonald, 1982) and $[2-(PMe_2Ph)-6,6,6,6-(PMe_2Ph)_2ClH-nido-6-$

Table 2. *Selected bond lengths* (Å)

Ir—P(1)	2·30 (1)	B(2)—B(5)	1·72 (7)
Ir—P(2)	2·31 (1)	B(2)—C(6)	1·70 (6)
Ir—B(4)	2·38 (6)	B(2)—B(7)	2·04 (8)
Ir—B(8)	2·18 (7)	B(3)—B(4)	1·81 (8)
Ir—B(10)	2·44 (4)	B(3)—B(7)	1·80 (7)
B(5)—P(3)	1·97 (5)	B(3)—B(8)	1·65 (10)
B(1)—B(2)	1·83 (6)	B(4)—B(8)	1·75 (11)
B(1)—B(3)	1·77 (7)	B(4)—B(10)	1·98 (7)
B(1)—B(4)	1·80 (7)	B(5)—C(6)	1·51 (6)
B(1)—B(5)	1·76 (7)	B(5)—B(10)	1·88 (7)
B(1)—B(10)	1·68 (7)	C(6)—B(7)	1·68 (5)
B(2)—B(3)	1·76 (7)	B(7)—B(8)	1·96 (8)

ReB$_9$H$_{12}$] (Beckett, Greenwood, Kennedy & Thornton-Pett, 1985). This, therefore, suggests that the two bridging H atoms are placed between the Ir and the B(8) and B(10) atoms, as found in the parent [*nido*-CB$_9$H$_{12}$]$^-$ anion (Jelinek, Stibr, Plesek & Hermanek, 1986). The single C—H proton occurs as a singlet at 6 p.p.m., with the remaining B—H terminal protons occurring as overlapping broad quartets. Attempts to obtain ^{1}H{^{11}B/^{31}P} NMR spectra were unsuccessful due to thermal degradation of the sample.

Data were collected with a Syntex $P2_1$ four-circle diffractometer in ω–2θ mode. Maximum 2θ was 50°, with scan range $\pm 1\cdot 1°$ (2θ) around the $K\alpha_1$–$K\alpha_2$ angles, scan speed 2–29° min^{-1}, depending on the intensity of a 2 s prescan; backgrounds were measured at each end of the scan for 0·25 of the scan time. Because the crystals were weakly diffracting, reflections with $40 < 2\theta < 50°$ were only collected if their count rate exceeded a preset minimum [approximately corresponding to $I \geq 2\sigma(I)$]. *hkl* ranges were 0/32; 0/18; −12/10. Three standard reflections were monitored every 200 reflections, and showed no changes during data collection. Unit-cell dimensions and standard deviations were obtained by least-squares fit to 15 reflections ($18 < 2\theta < 20°$). Reflections were processed using profile analysis to give 4521 unique reflections; 2206 were considered observed [$I/\sigma(I) \geq 3\cdot 0$] and used in refinement; they were corrected for Lorentz, polarization and absorption effects, the last by the analytical method (Alcock, 1970); maximum and minimum transmission factors were 0·74 and 0·60. Crystal dimensions were 0·23 × 0·14 × 0·46 mm. Systematic absences: $0kl$, $k+l \neq 2n$; $h0l$, $h \neq 2n$ indicate either $Pna2_1$ or $Pnam$ (non-standard setting of $Pnma$). The first was assumed from consideration of the likely Z value. The Ir atom was located by the Patterson interpretation section of *SHELXTL* (Sheldrick, 1983) and the light atoms then found on successive Fourier syntheses. The C atom was placed by consideration of its temperature factor on refinement (when all atoms treated as B), and the distances to neighbouring atoms.

The crystals were found to contain a partially occupied disordered molecule of solvent which was approximated by three carbon atoms (positions and temperature factors fixed; occupations refined to

0·34–0·46 (6)]. Anisotropic temperature factors were used for Ir and P only; attempts to refine more atoms in this way led to numerous non-positive definite values. Phenyl rings were treated as rigid hexagons with C—C 1·39 and C—H 0·96 Å. Cage and metal H atoms could not be located. The chirality of the individual crystal chosen was tested by refinement of an f'' multiplier to 0·74 (6). The z coordinate for Ir was held at 0·5 to fix the origin. Final refinement was on F by cascaded least squares refining 183 parameters. Largest positive and negative peaks on a final difference Fourier synthesis were of height +3·0 and −1·5 e Å^{-3} (both near Ir).

A weighting scheme of the form $w = 1/[\sigma^2(F) + gF^2]$ with $g = 0\cdot 0024$ was used and shown to be satisfactory by a weight analysis. Final $R = 0\cdot 069$, $wR = 0\cdot 070$. Maximum shift/e.s.d. in final cycle 0·4. Computing with *SHELXTL* (Sheldrick, 1983) on a Data General Nova 3, apart from absorption correction on a Burroughs B6700. Scattering factors in the analytical form and anomalous-dispersion factors taken from *International Tables for X-ray Crystallography* (1974). Final atomic coordinates are given in Table 1, and selected bond lengths and angles in Table 2.*

Discussion. Fig. 1 shows the structure of the *nido* product from the reaction of [CB$_8$H$_{13}$]$^-$ with [IrCl-(PPh$_3$)$_3$], with the crystallographic numbering (identical to the IUPAC system for the cage). It is established as *nido*-[5(PPh$_3$)-9,9,9-(H)(PPh$_3$)$_2$-9,6-IrCB$_8$H$_{10}$]. The H attached to Ir is probably located in the direction completing an approximate octahedron around Ir with the two Ir—P and three Ir—B bonds. The C atom in the cage is in the position originally surmised. Thus, the reaction route proposed for the formation of the

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* Lists of structure factors, anisotropic thermal parameters and full bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51270 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
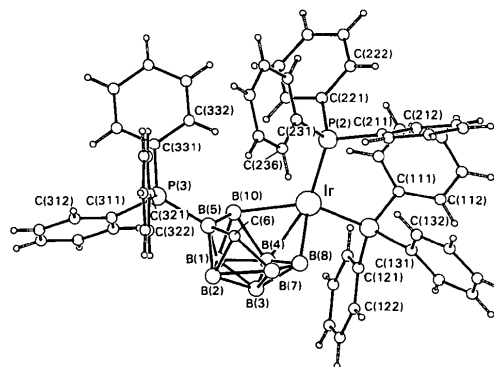

Fig. 1. Molecular structure of the title compound, showing the atomic numbering.

closo-[IrCB$_8$] cluster (Alcock *et al.*, 1983) is supported by the present determination.

The cluster geometry is of standard *nido* form, corresponding to that of the parent borane, $B_{10}H_{14}$. However, the relatively low precision of the determination means that detailed comparisons of the cage dimensions cannot be made. One point should however be noted: the unusually long B(2)—B(7) distance of 2·04 (8) Å which is significantly different from the shorter cage bonds. This probably arises as a consequence of the distortions introduced by the C atom.

With the normal assumption of a +3 oxidation state for Ir, the title compound has 24 skeletal electrons, as expected for a *nido* cage. Three other [IrCB$_8$] cages have been characterized, none of which share this geometry. Two have 22 skeletal electrons and show the expected *closo* geometry (Alcock *et al.*, 1983; Crook, Greenwood, Kennedy & McDonald, 1983). However, the third, [μ-1,2-(MeCOO)-2-H-2,10(PPh$_3$)$_2$-*closo*-1,2-ClIrB$_8$H$_7$] (Crook, Greenwood, Kennedy & McDonald, 1981), apparently also with 22 electrons, has *iso–nido* geometry, which is explained by postulating Ir^V rather than Ir^{III}. The importance compared with the present compound lies in the demonstration of alternative cage geometries. The difference can be correlated with the two bridging H atoms in the present structure and in $B_{10}H_{14}$. These provide 'support' for the open face of the cluster; in their absence the Ir moves inward, to span

five rather than *three* boron atoms, in the *iso–nido* geometry.

References

ALCOCK, N. W. (1970). *Crystallographic Computing,* edited by F. R. AHMED, pp. 271–278. Copenhagen: Munksgaard.
ALCOCK, N. W., JASZTAL, M. J. & WALLBRIDGE, M. G. H. (1987). *J. Chem. Soc. Dalton Trans.* pp. 2793–2802.
ALCOCK, N. W., TAYLOR, J. G., & WALLBRIDGE, M. G. H. (1983). *J. Chem. Soc. Chem. Commun.* pp. 1168–1169.
BECKETT, M. A., GREENWOOD, N. N., KENNEDY, J. D. & THORNTON-PETT, M. (1985). *J. Chem. Soc. Dalton Trans.* pp. 1119–1129.
BOOCOCK, S. K., BOULD, J., GREENWOOD, N. N., KENNEDY, J. D. & MCDONALD, W. S. (1982). *J. Chem. Soc. Dalton Trans.* pp. 713–719.
CROOK, J. E., GREENWOOD, N. N., KENNEDY, J. D. & MCDONALD, W. S. (1981). *J. Chem. Soc. Chem. Commun.* pp. 933–934.
CROOK, J. E., GREENWOOD, N. N., KENNEDY, J. D. & MCDONALD, W. S. (1983). *J. Chem. Soc. Chem. Commun.* pp. 1983, 83–84.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
JELINEK, T., STIBR, B., PLESEK, J. & HERMANEK, S. (1986). *Organomet. Chem.* 307, C13–15.
KENNEDY, J. D. (1986). *Prog. Inorg. Chem.* 34, 211–434.
SHELDRICK, G. M. (1983). *SHELXTL User Manual.* Nicolet XRD Corporation, Madison, Wisconsin, USA.

[*N,N*-Bis(2-hydroxyethyl)dithiocarbamato-*S,S'*]dichlorogold(III)

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Abstract. [Au(C$_5$H$_{10}$NO$_2$S$_2$)Cl$_2$], $M_r = 448 \cdot 1$, space group $P2_12_12_1$ (No. 19), $a = 7 \cdot 446$ (2), $b = 11 \cdot 434$ (4), $c = 13 \cdot 110$ (3) Å, $V = 1116 \cdot 2$ (5) Å^3, $Z = 4$, $D_m = 2 \cdot 74$ (5), $D_x = 2 \cdot 67$ g cm^{-3}, graphite-monochromatized Mo $K\alpha$ radiation, $\lambda = 0 \cdot 71069$ Å, $\mu = 144 \cdot 0$ cm^{-1}, $F(000) = 832 \cdot 2$, $T = 298$ K, $R = 0 \cdot 0432$, $wR = 0 \cdot 0397$ for 1974 unique reflections and 118 parameters. The gold atom is in a roughly square-planar environment, distorted as a result of the small bite distance of the chelating dithiocarbamate ligand. Molecules pack in the crystal lattice such that there are linear $\cdots$S$\cdots$Au$\cdots$S$\cdots$ chains parallel to the a axis.

Introduction. We have been investigating the mutagenic activity and DNA binding of a series of Au^{III} square-planar compounds. Without exception the compounds were cytotoxic rather than mutagenic when tested in Ames assays of TA102 Salmonella bacteria