Crystal Structure of an Iron–Antimony Molecular Complex Bis-μ-[dicarbonyl(π-cyclopentadienyl)ferriochloro]-bis{[dicarbonyl(π-cyclopentadienyl)ferriochloro]trichloroantimony}

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Crystals of the title complex (I) are triclinic, space group $P\bar{1}$, with a unit cell of dimensions a = 12·513(3), b = 18·618(5), c = 10·899(3) Å, α = 104·20(2), β = 115·50(2), γ = 92·15(2)°, Z = 2. The structure was solved from diffractometer data by Patterson and Fourier methods and refined by least-squares methods to R 7·4% (2001 observed reflections).

Two crystallographically different ' molecules ' of the title compound are found within the triclinic unit cell, each being independent and having a different crystallographic centre of symmetry.

Each ' molecule ' consists of two $SbCl_3$ and two $Fe(C_5H_5)(CO)_2Cl$ units, linked about a centre of symmetry by weak Sb · · · Cl bridges. In the $SbCl_3$ segment a distorted octahedron about antimony is completed by interactions from chlorine atoms from three surrounding $Fe(C_5H_5)(CO)_2Cl$ groups (one terminal and two bridging). The Sb–Cl bonds vary from 2·351(10) to 2·404(9) Å, while the three bridging Sb · · · Cl interactions are 3·025(9)—3·307(9) Å. Fe–Cl bonds are 2·279(9) to 2·312(9) Å.

Numerous complexes with transition metals co-ordinated to Group VA elements have been prepared, and those containing Fe–As or Fe–P bonds have been the subject of extensive X-ray structural investigations.[1] However, compounds with direct iron–antimony bonds have only recently been reported,[2] these being a partial series $[Fe(\pi\text{-}C_5H_5)(CO)_2Cl_x]_m[SbCl_y]_n$, with ratios of $m : n$ of 3 : 1 and 1 : 1. To complete this series, an examin-

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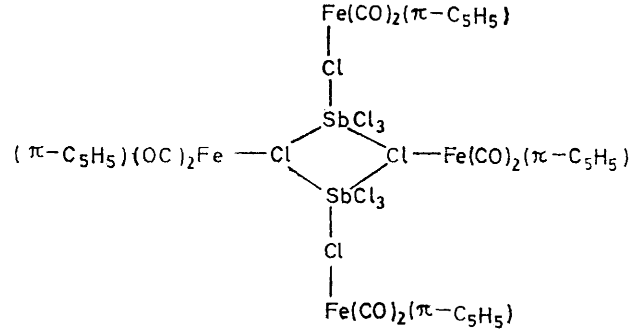
[1] (*a*) D. J. Dahm and R. A. Jacobson, *J. Amer. Chem. Soc.*, 1968, **90**, 5106; (*b*) F. W. B. Einstein and Anne-Marie Svensson, *ibid.*, 1969, **91**, 3663; (*c*) F. W. B. Einstein and R. D. G. Jones, *Inorg. Chem.*, 1972, **12**, 255; (*d*) F. W. B. Einstein and J. Trotter, *J. Chem. Soc.* (*A*), 1967, 824.

[2] Trinh-Toan and L. F. Dahl, *J. Amer. Chem. Soc.*, 1971, **93**, 2654.

ation was undertaken on compound (I) with a corresponding ratio of 2 : 1 whose preparation had been previously reported.[3] Two different structures were found for the reported compounds, and a third different structure was expected for the complex studied.



(I)

EXPERIMENTAL

A 1 : 1 reaction of $SbCl_3$ with $[Fe(C_5H_5)(CO)_2]_2$ in CH_2Cl_2 yielded deep-red triclinic crystals of (I); these crystals were blade-shaped, with the longest direction parallel to *a*. Preliminary Weissenberg and precession photographs (both Cu-K_α) were used to select the axes of the triclinic unit cell.

Crystal Data.—$C_{28}H_{20}Cl_{10}Fe_4O_8Sb_2$, $M = 1305{\cdot}8$, Triclinic, $a = 12{\cdot}513(3)$, $b = 18{\cdot}618(5)$, $c = 10{\cdot}899(3)$ Å, $\alpha = 104{\cdot}20(2)$, $\beta = 115{\cdot}50(2)$, $\gamma = 92{\cdot}15(2)°$, $U = 2179$ Å^3, $D_c = 1{\cdot}99$, $Z = 2$, $D_m = 1{\cdot}92$, $F(000) = 1256$. Mo-radiation, $\lambda(\text{Mo-}K_{\alpha_1}) = 0{\cdot}70926$ Å, $\lambda(\text{Mo-}K_\alpha) = 0{\cdot}71069$ Å; $\mu(\text{Mo-}K_\alpha) = 32{\cdot}0$ cm^{-1}. Space group $P1$ or $P\bar{1}$, shown to be the latter from the results.

As this compound was sensitive to both light and air, all crystals were sealed in Lindemann glass capillaries. The crystal used for data collection was ground to a sphere [diameter = 0·16(1) mm], and was mounted with *c* approximately parallel to the ϕ axis. Accurate cell dimensions were obtained from a least-squares analysis of 2θ values for 30 reflections which were centred on a computer controlled, Picker four-circle diffractometer. Errors were determined by a least-squares procedure.

For data collection niobium-filtered Mo-K_α radiation was used, with a scintillation counter equipped with pulse-height analysis; take off angle 2·4°. Intensity data for $2\theta < 40°$ were measured by the θ—2θ scan technique. Each reflection was scanned over a basewidth of 2·0° in 2θ (increased to allow for dispersion effects) at 2° min^{-1}. Background counts were measured at both scan limits for 10 s. Intensities were corrected for background count, variation in the standard count, and the Lorentz-polarization factor. Of 4079 reflections measured, 2001 were considered observed, having a net count $>2{\cdot}3\sigma$; the initial structure determination was based on 1106 reflections $\geqslant 7\sigma$. The net intensity of 2 standard reflections monitored every 100 measurements both decreased during data collection to 75% of their initial values, probably owing to decomposition of the crystal into a powder. The rate of decomposition was reduced by collecting data in the dark. No corrections were made for absorption, which may have resulted in a maximum error of 3% in I_{obs}.

Structure Determination.—The initial model was obtained by Patterson methods. Both Sb and two Fe atoms were located and refined by full-matrix least-squares procedures, to give *R* 35·7%. All reflections were assigned unit weight. Two more Fe and four Cl atoms which had been located in the Patterson map with less confidence were then added and also refined. Two electron-density difference syntheses were required to locate all non-hydrogen atoms. As refinement proceeded additional electron-density difference syntheses were used to determine which parameters were used for our model. All antimony and chlorine atoms in the final cycles were refined anisotropically. Hydrogen atoms for the cyclopentadienyl ring were placed in calculated positions (assuming C–H 0·98 Å).

The final difference map showed that two of the eight different carbonyl groups had anisotropic motion, and that all four cyclopentadienyl rings had anisotropic motion or alternatively some degree of rotational disorder. Since all features were of approximately the same size [maximum *ca.* $\pm 0{\cdot}8(4)$ eÅ^{-3}] a large number of additional variables would be required to correct the deficiencies in the model. While better agreement may be able to be achieved it is very doubtful that chemically useful information could be obtained.

Reflections during final refinement were assigned weights $w = 1/(\sigma F)^2$ where $\sigma F = \sigma I/(Lp)2F_o$. Refinement was completed at *R* 0·074, and *R′* 0·064 for all observed data. Since not all parameters could be varied in each least-squares cycle, two cyclopentadienyl rings were alternately fixed while all other non-hydrogen atoms were varied; errors in all parameters, distances, and angles may therefore be slightly underestimated. The function minimized was $\Sigma w(|F_o| - |F_c|)^2$.

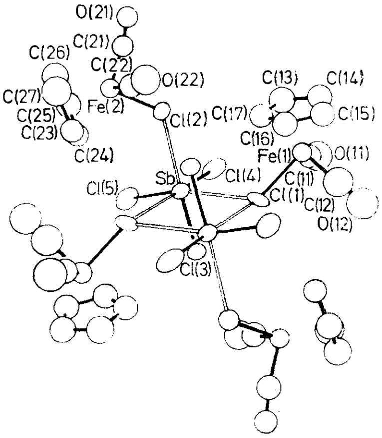


FIGURE 1 Diagram of the molecule, showing the atom numbering system

Table 1 lists final atomic parameters, Table 2 interatomic distances and angles, and Table 3 mean planes calculated through selected groups of atoms. Observed and calculated structure factors are listed in Supplementary Publication No. SUP 20876 (5 pp).* Figure 1 shows a drawng of the molecule and the atom numbering system used in the analysis.

Atomic scattering factors for all non-hydrogen atoms were from ref. 4, those for hydrogen from ref. 5, with

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* See Notice to Authors No. 7 in *J.C.S. Dalton*, 1972, Index issue. Items less than 10 pp. are sent as full size copies.

[3] W. R. Cullen, D. J. Patmore, J. R. Sams, M. J. Newlands, and L. K. Thompson, *Chem. Comm.*, 1971, 952.

[4] D. T. Cromer and D. T. Waber, *Acta Cryst.*, 1965, **18**, 104.

[5] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, 1965, **42**, 3175.

corrections for anomalous scattering of antimony from ref. 6. Computer programs used are listed in ref. 7.

DISCUSSION

Two crystallographically different 'molecules' of composition $[Fe(\pi\text{-}C_5H_5)(CO)_2Cl]_4[SbCl_3]_2$ are found within the triclinic unit cell (Figure 2). The asymmetric unit comprises two independent half-molecules, (A) and (B), each molecule having a different crystallographic centre of symmetry.

TABLE 1

Final atomic parameters [a]

	Molecule (A)				Molecule (B)			
Atom	*x*	*y*	*z*	$U^{b,c}$	*x*	*y*	*z*	$U^{b,c}$
Sb	−2066(2)	−31(2)	−1904(3)		6890(2)	5052(2)	729(3)	
Cl(1)	362(8)	1034(5)	−55(10)		4727(8)	4046(5)	−2019(5)	
Cl(2)	−3040(8)	903(5)	−49(9)		7627(9)	4033(5)	2727(9)	
Cl(3)	−1305(9)	−574(6)	−3535(10)		6450(8)	5822(5)	−760(9)	
Cl(4)	−2817(10)	860(6)	−3126(10)		8143(9)	4425(6)	−57(10)	
Cl(5)	−3915(9)	−900(6)	−3199(12)		8504(8)	6008(6)	2643(9)	
Fe(1)	655(4)	2197(3)	−302(5)	44(1)	4466(5)	2741(3)	−2916(5)	51(1)
Fe(2)	−2614(4)	811(3)	2156(5)	42(1)	7496(5)	4265(3)	4819(5)	49(1)
O(11)	26(3)	161(2)	−321(3)	106(9)	636(3)	274(2)	−374(3)	119(10)
O(12)	322(3)	220(2)	95(3)	100(9)	264(3)	269(2)	−569(4)	128(11)
O(21)	−405(3)	194(2)	256(3)	117(10)	856(2)	297(2)	542(3)	74(7)
O(22)	−45(3)	191(2)	351(3)	95(8)	505(3)	349(2)	357(3)	107(9)
C(11)	39(4)	181(2)	−202(4)	87(13)	563(4)	281(2)	−338(4)	88(12)
C(12)	217(4)	223(2)	46(4)	75(11)	335(5)	271(3)	−457(6)	129(18)
C(21)	−347(4)	151(3)	241(4)	101(14)	815(3)	347(2)	511(4)	66(10)
C(22)	−136(4)	143(3)	287(4)	92(13)	609(4)	381(2)	399(4)	90(12)
C(13)	−87(4)	272(2)	−101(4)	86(12)	543(4)	219(3)	−146(5)	93(12)
C(14)	19(4)	321(2)	−51(4)	90(13)	447(4)	166(2)	−280(4)	75(11)
C(15)	100(4)	327(3)	99(5)	103(13)	341(4)	183(2)	−303(4)	72(11)
C(16)	37(4)	279(2)	136(4)	93(12)	357(4)	244(2)	−183(4)	88(12)
C(17)	−81(4)	245(2)	3(4)	76(12)	472(4)	271(2)	−89(4)	80(12)
C(23)	−193(4)	−20(3)	219(5)	99(14)	800(4)	544(2)	527(4)	66(10)
C(24)	−310(4)	−35(2)	128(4)	78(11)	895(4)	517(2)	615(4)	79(12)
C(25)	−376(4)	−9(2)	196(4)	69(11)	837(4)	480(3)	692(4)	90(13)
C(26)	−297(4)	27(2)	340(4)	75(11)	723(4)	490(3)	647(5)	90(13)
C(27)	−180(4)	20(3)	353(4)	83(13)	702(4)	534(2)	536(4)	79(12)
H(13)	−152	259	−194		468	219	−143	
H(14)	64	369	−29		523	157	−276	
H(15)	128	372	87		267	160	−384	
H(16)	−12	299	177		292	264	−171	
H(17)	−81	275	87		557	283	−51	
H(23)	−129	−33	197		806	569	463	
H(24)	−342	−61	30		934	478	647	
H(25)	−461	−14	153		904	518	724	
H(26)	−317	50	412		672	527	630	
H(27)	−107	40	437		653	494	536	

	Molecule (A)						Molecule (B)					
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sb	481(18)	484(17)	545(17)	136(13)	280(14)	182(13)	487(18)	509(17)	492(17)	161(14)	256(14)	198(13)
Cl(1)	64(8)	54(7)	90(8)	12(6)	23(6)	37(6)	74(8)	34(6)	75(7)	18(6)	20(6)	19(5)
Cl(2)	74(8)	82(8)	62(7)	30(6)	45(6)	41(6)	121(9)	65(7)	50(7)	34(7)	50(7)	21(6)
Cl(3)	72(8)	82(8)	72(8)	29(6)	39(6)	6(6)	82(8)	56(7)	55(7)	15(6)	27(6)	28(6)
Cl(4)	117(9)	102(9)	78(8)	61(8)	57(7)	45(7)	89(9)	135(10)	62(7)	73(8)	44(7)	49(7)
Cl(5)	81(9)	104(10)	129(11)	−21(7)	58(7)	−17(8)	51(7)	92(8)	62(7)	−9(6)	13(6)	27(6)

[a] Estimated standard deviations are in parentheses. Antimony, chlorine, and iron × 10^4; oxygen, carbon, and hydrogen × 10^3; isotropic temperature factors Å^2 × 10^3. [b] Anisotropic thermal parameters for Sb (Å^2 × 10^4) and Cl (Å^2 × 10^3) atoms in the form: $\exp -2\pi(U_{11}a^{*2}h^2 + U_{22}b^{*2}k^2 + U_{33}c^{*2}l^2 + 2U_{12}a^*b^*hk + 2U_{13}a^*c^*hl + 2U_{23}b^*c^*kl)$, with parameters. [c] Hydrogen atoms assigned *B* 0·089 Å^2.

Each molecule has two $SbCl_3$ units bridged by the chlorine atoms from two of the four surrounding $Fe(C_5H_5)(CO)_2Cl$ groups. The other two $Fe(C_5H_5)(CO)_2Cl$ groups are linked through similar chlorine bridges, one to each antimony, completing a distorted octahedral environment about the antimony atom. (The term 'molecule' is used somewhat loosely to describe an arrangement of groups held together by weak Sb $\cdots$ Cl interactions.)

Antimony Environment.—The antimony trichloride segments of this complex consist of three chlorine atoms bonded to antimony in the expected *fac*-configuration with interbond angles in the range of 90·7(4)—94·0(4)°, and bond lengths 2·351(10)—2·404(9) Å (Table 2). Studies of $SbCl_3$ by electron diffraction,[8] microwave,[9] and *X*-ray diffraction [10] all show similar geometry. The

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[6] 'International Tables for *X*-Ray Crystallography,' vol. III, 1962, Kynoch Press, Birmingham, p. 213.

[7] F. W. B. Einstein and R. D. G. Jones, *Inorg. Chem.*, 1972, **11**, 395.

[8] P. W. Allen and L. E. Sutton, *Acta Cryst.*, 1950, **3**, 46.

[9] P. Kisliuk, *J. Chem. Phys.*, 1954, **22**, 86.

[10] I. Lindqvist and A. Niggli, *J. Inorg. Nuclear Chem.*, 1956, **2**, 345.

three other chlorine atoms which complete the distorted octahedron are at distances between **3·025(9)** and 3·307(9) Å. This type of distorted octahedral geometry, with long contacts, has been reported previously, though the long contacts have not always been noted. An additional feature is the chlorine atoms which bridge between one iron and two antimony atoms. Direct interactions are suggested between these chlorine and antimony atoms for the following reasons. Van der Waals' radii suggest an antimony–chlorine contact distance of 4·0 Å, whereas each antimony atom has an octahedral environment comprising six contacts $<3·4$ Å. A graph of Sb · · · Cl distance *vs.* *trans*-Sb–Cl bond length (Figure 3) for four antimony(III) compounds[11-13] shows a uniform curve, indicating an inverse relationship between the *trans*-related Sb–Cl distances. The shortest bond distance of *ca.* 2·3 Å is observed where there is a *trans*-chlorine distance of

TABLE 2

Selected interatomic distances and angles within the molecule, with estimated standard deviations in parentheses

(*a*) Interatomic distances (Å)

	Molecule (A)	Molecule (B)
Sb–Cl(1)	3·089(9)	3·196(9)
Sb–Cl(1′)	3·307(9)	3·257(9)
Sb–Cl(2)	3·025(9)	3·052(9)
Sb–Cl(3)	2·395(9)	2·380(8)
	2·412(9) *	2·391(9) *
Sb–Cl(4)	2·351(10)	2·367(10)
	2·375(10) *	2·391(10) *
Sb–Cl(5)	2·398(10)	2·404(9)
	2·437(10) *	2·420(9) *
Sb–Sb′	5·022(5)	4·258(5)
Cl(1)–Cl(1′)	3·966(16)	4·848(17)
Fe(1)–Cl(1)	2·280(10)	2·312(9)
Fe(1)–C(1)	1·71(4)	1·74(4)
Fe(1)–C(2)	1·70(4)	1·73(5)
Fe(1)–C(3)	2·10(4)	2·07(4)
Fe(1)–C(4)	2·04(4)	2·06(4)
Fe(1)–C(5)	2·05(4)	2·06(4)
Fe(1)–C(6)	2·05(4)	2·10(4)
Fe(1)–C(7)	2·06(4)	2·11(4)
C(1)–O(1)	1·19(4)	1·15(4)
C(2)–O(2)	1·20(4)	1·14(5)
C(3)–C(4)	1·39(5)	1·50(5)
C(4)–C(5)	1·48(5)	1·31(5)
C(5)–C(6)	1·41(5)	1·44(5)
C(6)–C(7)	1·52(5)	1·34(5)
C(7)–C(3)	1·33(4)	1·53(5)
Fe(1)–O(1)	2·90(3)	2·88(3)
Fe(1)–O(2)	2·89(3)	2·87(3)
Fe(2)–Cl(2)	2·279(9)	2·292(10)
Fe(2)–C(1)	1·76(5)	1·75(4)
Fe(2)–C(2)	1·67(4)	1·67(4)
Fe(2)–C(3)	2·09(4)	2·13(4)
Fe(2)–C(4)	2·09(4)	2·14(4)
Fe(2)–C(5)	2·08(4)	2·02(4)
Fe(2)–C(6)	2·05(4)	2·06(4)
Fe(2)–C(7)	2·04(4)	2·12(4)
C(1)–O(1)	1·13(5)	1·13(4)
C(2)–O(2)	1·23(4)	1·24(4)
C(3)–C(4)	1·34(5)	1·37(5)
C(4)–C(5)	1·36(4)	1·58(5)
C(5)–C(6)	1·41(4)	1·33(5)
C(6)–C(7)	1·42(5)	1·56(5)
C(7)–C(3)	1·40(5)	1·28(5)
Fe(2)–O(1)	1·89(3)	2·87(3)
Fe(2)–O(2)	1·89(3)	2·90(3)

* Value corrected for thermal motion. The second atom assumed to ride on the first.

TABLE 2 (*Continued*)

(*b*] Interatomic angles (°)

	Molecule (A)	Molecule (B)
Cl(1)–Sb–Cl(1′)	76·6(3)	97·4(3)
Cl(1)–Sb–Cl(2)	88·3(3)	104·7(3)
Cl(1)–Sb–Cl(3)	88·3(3)	76·0(3)
Cl(1)–Sb–Cl(4)	89·9(4)	85·6(3)
Cl(1)–Sb–Cl(5)	175·7(4)	166·9(3)
Cl(1′)–Sb–Cl(2)	104·3(3)	97·0(3)
Cl(1′)–Sb–Cl(3)	84·6(3)	87·6(3)
Cl(1′)–Sb–Cl(4)	165·8(3)	177·0(4)
Cl(1′)–Sb–Cl(5)	99·7(4)	83·6(3)
Cl(2)–Sb–Cl(3)	169·4(3)	175·3(3)
Cl(2)–Sb–Cl(4)	79·2(3)	82·2(3)
Cl(2)–Sb–Cl(5)	90·7(3)	88·4(3)
Cl(3)–Sb–Cl(4)	90·9(4)	93·2(4)
Cl(3)–Sb–Cl(5)	93·3(4)	90·7(4)
Cl(4)–Sb–Cl(5)	94·0(4)	93·5(4)
Sb–Cl(1)–Sb′	103·4(3)	82·6(3)
Sb–Cl′–Fe(1)	135·0(4)	124·0(4)
Sb–Cl–Fe(1)	121·5(3)	124·8(4)
Cl–Fe(1)–C(1)	91·2(12)	90·1(12)
Cl–Fe(1)–C(2)	91·6(12)	92·5(15)
C(1)–Fe(1)–C(2)	97·3(16)	94·4(19)
C(7)–C(3)–C(4)	108(4)	103(4)
C(3)–C(4)–C(5)	112(4)	111(4)
C(4)–C(5)–C(6)	104(4)	107(4)
C(5)–C(6)–C(7)	106(4)	114(4)
C(6)–C(7)–C(3)	110(4)	105(4)
Fe(1)–C(1)–O(1)	173(4)	170(4)
Fe(1)–C(2)–O(2)	175(4)	178(5)
Sb–Cl–Fe(2)	122·7(4)	123·8(4)
Cl–Fe(2)–C(1)	91·9(13)	89·3(11)
Cl–Fe(2)–C(2)	90·5(13)	91·6(12)
C(1)–Fe(2)–C(2)	93·0(17)	94·8(16)
C(7)–C(3)–C(4)	108(4)	116(4)
C(3)–C(4)–C(5)	110(4)	102(4)
C(4)–C(5)–C(6)	108(4)	109(4)
C(5)–C(6)–C(7)	106(4)	105(4)
C(6)–C(7)–C(3)	107(4)	108(4)
Fe(2)–C(1)–O(1)	178(4)	173(3)
Fe(2)–C(2)–O(2)	174(4)	170(4)

Primed atoms are centrosymmetrically related to unprimed atoms

(*c*) Important non-bonded distances (Å), non-hydrogen contacts ($\leqslant 3·3$Å)

Contact	Type	Distance
O(12) · · · O(22)	(A) · · · (B)	3·13
O(12) · · · O(21$^{\mathrm{I}}$)	(A) · · · (A)	3·22
O(21) · · · O(22$^{\mathrm{II}}$)	(A) · · · (B)	3·26
O(22) · · · O(21$^{\mathrm{II}}$)	(A) · · · (B)	3·19
O(11) · · · O(21$^{\mathrm{III}}$)	(B) · · · (B)	3·29

Roman numeral superscripts denote the following equivalent positions relative to the reference molecule at x, y, z:

I $1 + x, y, z$
II $x - 1, y, z$
III $x, y, z - 1$

TABLE 3

Equations of selected mean planes (in the form $Ax' + By' + Cz' + D = 0$) and χ^2 [$\Sigma p^2/\sigma^2(p)$, where p is the distance (Å) of the atom normal to the plane]. Coordinates (Å) are orthogonalized such that: x' parallel to a, y' in ab plane, 90° from a, and z' is perpendicular to $a'b'$ plane

Atoms in Plane	Molecule	*A*	*B*	*C*	*D*	χ^2
C(13)—(17)	(A)	0·653	−0·696	−0·299	−3·954	0·04
C(23)—(27)	(A)	0·133	0·968	−0·212	1·842	0·15
C(13)—(17)	(B)	0·310	0·807	−0·502	6·574	1·24
C(23)—(27)	(B)	0·084	−0·687	−0·722	8·111	0·13

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[11] F. W. Einstein and R. D. G. Jones, *Inorg. Chem.*, 1972, **12,** 1690.

[12] M. Webster and S. Keats, *J. Chem. Soc.* (*A*), 1971, 298.

[13] S. K. Porter and R. A. Jacobson, *J. Chem. Soc.* (*A*), 1970, 1356.

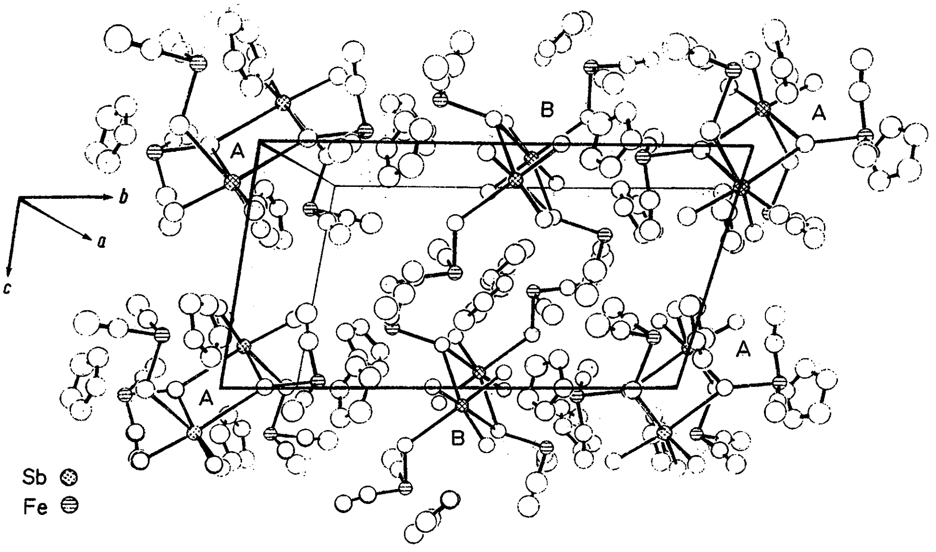

FIGURE 2 Unit-cell packing diagram

3·4 Å. Both bonds are of equal distance at *ca.* 2·6 Å. This may presumably be simply described as a four-electron three-centre bond involving the antimony and two chlorine atoms. This distance of *ca.* 2·6 Å would therefore correspond to a formal bond order of $\frac{1}{2}$.

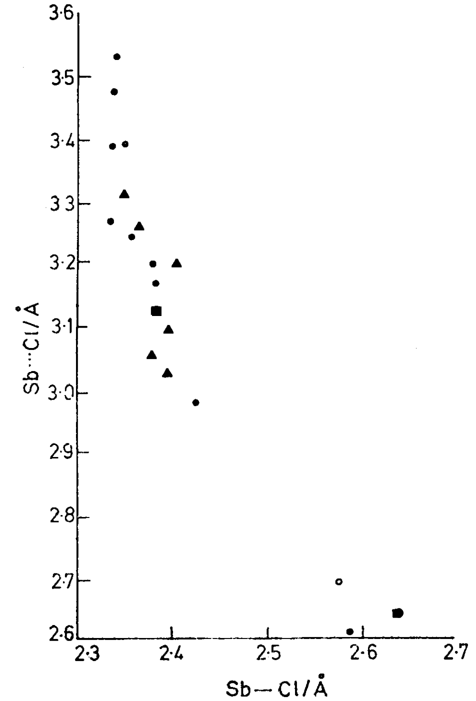

FIGURE 3 Graph of Sb–Cl bond distance *vs.* *trans*-Sb · · · Cl distance, for octahedral antimony(III) compounds. Circle, from ref. 11; triangle, present work; open circle, from ref 12; square, from ref. 13

Differences in the dimensions of the four-membered Sb_2Cl_2 ring between molecules (A) and (B) are significant. For molecule (A) Sb · · · Cl distances are 3·089(9) and 3·307(9) Å, with Cl · · · Sb · · · Cl 76·6(3)°, while for molecule (B) these values are 3·196(9) and 3·257(9) Å, and 97·4(3)°. Such differences should not be unexpected, however, owing to the weak and presumably flexible nature of the interactions which hold the ring together.

Iron Environment.—Each iron is approximately octahedrally co-ordinated to two carbonyl groups, one chlorine atom, and a terdentate cyclopentadienyl group. Bond distances and angles (Table 2) are similar to those found in other iron complexes.[1c,2] All the cyclopentadienyl rings are planar (Table 3). The four Fe–Cl distances are nearly equal and therefore independent of Cl · · · Sb contacts.

Each iron atom can be assumed to receive five electrons from the π-cyclopentadienyl group, two electrons from each of two carbonyl groups, and one electron from chlorine, in agreement with the e.a.n. rule formalism.

We thank Dr. W. R. Cullen for providing the samples of crystals, and the National Research Council of Canada for financial support of this work.

[3/1492 *Received*, 16*th July*, 1973]