

Table 1

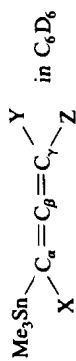
CS $\delta(^{13}\text{C}, ^{119}\text{Sn})$, ppm of stannylallenes

X	Y	Z	$\delta(^{119}\text{Sn})$	$\delta(^{13}\text{C})$					
				C_α	C_β	C_γ	SnCH_3	XCH_3	$\text{C}_{\text{Y,Z}}$
SnMe ₃	H	H	-9.55	75.23	205.98	53.01	-8.53	-8.53	-
	H	SiMe ₃	-3.56	65.06	202.91	55.36	-8.35	-8.35	-0.06
	H	GeMe ₃	-4.94	65.96	201.76	56.70	-8.38	-8.38	-0.82
	H	SnMe ₃	-3.12	61.98	201.32	50.49	-8.38	-8.38	-9.03
	H	SC ₂ H ₅	-5.07	79.59	204.08	65.14	-8.06	-8.06	29.86(CH ₂) 15.09(CH ₃)
SiMe ₃	SnMe ₃	SiMe ₃	3.40	50.78	196.08	52.69	-8.29	-8.29	-8.23(SnMe ₃) 0.67(SiMe ₃)
	SnMe ₃	GeMe ₃	1.87	52.06	196.13	54.20	-8.27	-8.27	-8.21(SnMe ₃) 0.01(GeMe ₃)
	SnMe ₃	SnMe ₃	3.73	47.36	195.58	47.36	-8.32	-8.32	-8.32
	SnMe ₃	SC ₂ H ₅	-1.82	70.04	200.00	64.03	-8.06	-8.06	29.04(CH ₂) 15.41(CH ₃)
	H	SiMe ₃	-5.95	71.44	204.93	59.14	-8.15	0.32	-8.79(SnMe ₃)
SnMe ₃	H	SiMe ₃	-7.73	71.92	203.32	60.05	-8.21	0.32	-0.09
	H	GeMe ₃	-6.08	77.92	206.13	68.63	-7.88	0.53	-0.85
	H	SC ₂ H ₅	0.34	56.79	197.48	56.79	-8.06	0.76	29.74(CH ₂) 15.21(CH ₃)
	SnMe ₃	SiMe ₃	0.34	56.79	197.48	56.79	-8.06	0.76	0.23(SnMe ₃) 0.18(SiMe ₃)

	SnMe ₃	GeMe ₃	-1.48	57.64	196.97	57.73	-8.14	0.74	-8.17(SnMe ₃) 0.04(GeMe ₃)
	SnMe ₃	SnMe ₃	0.02	52.69	196.08	50.78	-8.23	0.67	-8.29
	SnMe ₃	SC ₂ H ₅	-3.68	76.40	200.59	67.52	-7.88	0.38	-8.76(SnMe ₃) 28.81(CH ₂) 15.35(CH ₃)
GeMe ₃	H	SiMe ₃	-7.42	71.59	203.58	59.69	-8.26	-0.29	-0.12
	H	GeMe ₃	-9.01	72.20	202.10	60.71	-8.32	-0.34	-0.89
	H	SC ₂ H ₅	-8.49	78.71	204.36	69.30	-8.00	-0.35	29.30(CH ₂) 15.21(CH ₃)
	SnMe ₃	SiMe ₃	-0.95	57.73	197.48	57.64	-8.17	0.04	-8.14(SnMe ₃) 0.74(SiMe ₃)
	SnMe ₃	GeMe ₃	-2.61	58.60	196.45	58.60	-8.21	-0.04	-
	SnMe ₃	SnMe ₃	-1.03	54.20	196.13	52.06	-8.21	0.01	-8.27(SnMe ₃)
	SnMe ₃	SC ₂ H ₅	-3.96	77.33	199.54	68.66	-7.97	-0.15	-8.76(SnMe ₃) 28.78(CH ₂) 15.41(CH ₃)
H	SnMe ₃	SnMe ₃	-8.66	50.49	201.32	61.98	-9.03	-	-8.38
SC ₂ H ₅	SnMe ₃	SiMe ₃	-1.88	67.52	200.59	76.40	-8.76	28.81(CH ₂) 15.36(CH ₃)	-7.88(SiMe ₃) 0.38(SiMe ₃)
	SnMe ₃	GeMe ₃	-3.48	68.66	199.54	77.33	-8.76	28.78(CH ₂) 15.41(CH ₃)	-7.97(SnMe ₃) -0.15(GeMe ₃)
	SnMe ₃	SnMe ₃	-2.94	64.03	200.00	70.04	-8.79	29.04(CH ₂) 15.41(CH ₃)	-8.06(SnMe ₃)
Br	H	H	2.98	78.51	206.98	74.96	-8.56	-	-

Table 2

Coupling constants and isotope shifts of stannylallenes



X	Y	Z	Coupling constants (Hz)				Isotope shifts (ppb)		
			SnC _α	SnC _β	SnC _γ	¹¹⁹ Sn- ¹¹⁷ Sn	SnC _{CH₃}	¹¹⁹ Sn(C _α)	¹¹⁹ Sn(C _{CH₃})
SnMe ₃	H	H	261.7	30.5	60.6	158.5	348.2	31.8	9.0
	H	SiMe ₃	264.4	26.3	50.1	169.1	349.4	34.3	7.1
	H	GeMe ₃	269.9	26.8	57.1	190.9	347.6	33.8	7.7
	H	SnMe ₃	274.1	26.1	58.9	199.4(² J)	347.0	34.2	7.7
	H	SC ₂ H ₅	239.8	31.2	65.1	166.5	348.1	37.5	6.6
	SnMe ₃	SiMe ₃	281.7	21.4	48.6	202.6(² J)	348.0	32.2	7.5
	SnMe ₃	GeMe ₃	285.1	22.7	54.5	248.6(⁴ J)	345.9	31.9	9.2
	SnMe ₃	SnMe ₃	292.9	22.1	54.8	226.2(² J)	345.6	31.1	9.3
	SnMe ₃	SC ₂ H ₅	263.2	30.5	66.4	250.5(⁴ J)	343.0	33.2	7.5

SiMe ₃	H	SiMe ₃	254.4	31.6	49.6	-	348.3	35.5	8.0
	H	GeMe ₃	261.6	^a	56.4	-	346.7	35.0	8.0
	H	SC ₂ H ₅	233.5	36.6	64.5	-	346.5	36.5	7.4
	SnMe ₃	SiMe ₃	270.4	27.7	47.8	241.1(^d J)	346.0	33.3	8.3
	SnMe ₃	GeMe ₃	276.8	28.8	53.9	244.6(^d J)	344.6	32.7	8.5
	SnMe ₃	SnMe ₃	284.0	28.2	54.8	248.7(^d J)	347.2	32.2	8.6
	SnMe ₃	SC ₂ H ₅	257.7	28.4	65.7	199.3(^d J)	340.2	34.6	8.2
GeMe ₃	H	SiMe ₃	280.3	23.6	48.5	-	349.1	33.4	8.2
	H	GeMe ₃	286.9	23.0	54.6	-	347.4	30.5	8.5
	H	SC ₂ H ₅	258.9	26.7	62.6	-	347.6	35.6	7.1
	SnMe ₃	SiMe ₃	298.1	19.2	46.3	244.6(^d J)	347.0	31.7	9.2
	SnMe ₃	GeMe ₃	304.6	20.1	52.1	247.3(^d J)	345.7	30.7	9.3
	SnMe ₃	SnMe ₃	310.0	19.3	53.3	250.5(^d J)	344.9	30.0	9.7
	SnMe ₃	SC ₂ H ₅	283.7	26.2	61.6	198.6(^d J)	341.3	33.0	7.9
H	SnMe ₃	SnMe ₃	423.5	6.1	44.8	248.3(^d J)	353.5	22.4	12.1
SC ₂ H ₅	SnMe ₃	SiMe ₃	410.6	35.2	32.2	199.3(^d J)	353.2	38.4	6.3
	SnMe ₃	GeMe ₃	417.0	26.2	35.1	198.6(^d J)	352.6	37.6	6.6
	SnMe ₃	SnMe ₃	433.7	32.1	36.4	202.3(^d J)	350.9	36.6	7.2
Br	H	H	360.8	32.5	27.4	-	371.5	26.4	1.1

^a Not measured.

^{29}Si and tetramethylstannane as an external standard for ^{119}Sn NMR measurements. The sample temperature was 303 K. ^{13}C , ^{29}Si , ^{119}Sn CS were measured with -0.03 ppm accuracy; SSCC -0.07 Hz. ^{13}C , ^{29}Si , ^{119}Sn NMR spectra were obtained using complete proton decoupling. Isotope shifts were measured as follows: ${}^n\Delta^{119}\text{Sn}(^{13/12}\text{C}) = \delta\text{Sn}(\text{Sn}-^{12}\text{C}) - \delta\text{Sn}(\text{Sn}-^{13}\text{C})$

The compounds were prepared according to [5].

Results

The ^{13}C , ^{29}Si , ^{119}Sn NMR chemical shifts (CS) measured for stannylallenes and silylstannylallenes are presented in Tables 1 and 3; the spin-spin coupling constants (SSCC) ${}^nJ(^{119}\text{Sn}-^{13}\text{C})$, ${}^nJ(^{119}\text{Sn}-^{117}\text{Sn})$, ${}^nJ(^{29}\text{Si}-^{13}\text{C})$ and isotope shifts (IS) are given in Tables 2 and 3.

Analysis of CS of ^{13}C and ^{119}Sn for stannylallenes **1** (Table 1) shows that these values are additive and can be described by the equations;

$$\delta(^{13}\text{C}_{\alpha,\gamma}) = 81.2 + \Sigma X_{\alpha} + \Sigma X_{\gamma} \quad (1)$$

$$\delta(^{13}\text{C}_{\beta}) = 219.0 + \Sigma X_{\beta} \quad (2)$$

$$\delta(^{119}\text{Sn}) = -21.6 + X_{\alpha} + \Sigma X_{\gamma} \quad (3)$$

where $X_{\alpha,\beta,\gamma}$ are increments of the corresponding substituents in the α,β,γ -positions with regard to the nuclei under study. The calculated increments of substituents are presented in Table 4. The difference between the calculated ^{13}C , ^{119}Sn CS and their

Table 3

No.	X	Y	Z	$\delta(^{29}\text{Si})$ (ppm)	Coupling constants (Hz)			${}^1\Delta^{29}\text{Si}(\text{C}_{\alpha})$ (ppb)
					$^{29}\text{Si}-\text{C}_{\text{CH}_3}$	$^{29}\text{Si}-\text{C}_{\alpha}$	$^{29}\text{Si}-^{119}\text{Sn}$	
1	SnMe ₃	SiMe ₃	H	-5.06	52.86	66.19	27.74	-9.1
2	GeMe ₃	SiMe ₃	H	-5.12	52.91	65.21	26.94	-9.5
3	SiMe ₃	SiMe ₃	H	-4.94	53.20	64.61	26.68	-9.6
4	SiMe ₃	SnMe ₃	SnMe ₃	-3.59	52.75	58.69	27.56(4J) 23.81(2J)	-9.8
5	SiMe ₃	SnMe ₃	GeMe ₃	-3.66	52.87	57.96	27.16(4J) 23.28(2J)	-10.0
6	SiMe ₃	SnMe ₃	SiMe ₃	-3.98	53.31	57.56	27.06(4J) 20.80(2J)	-10.5
7	SiMe ₃	H	SiMe ₃	-3.89	52.95	55.40	18.03	-10.4
8	SiMe ₃	H	GeMe ₃	-4.01	53.06	55.58	20.14	-10.4
9	SiMe ₃	H	SC ₂ H ₅	-3.41	53.31	52.91	18.49	-11.1
10	SiMe ₃	SnMe ₃	SC ₂ H ₅	-3.34	52.98	55.61	26.26(4J) 21.64(2J)	-10.3
11	Me ₃ Si Br		H H	-0.31				

Table 4

Values of the calculated increments of substituents in stannylallenes **1**

Measured value	Increment of group				
	SnMe ₃	GeMe ₃	SiMe ₃	SC ₂ H ₅	CMe ₃ [6]
$\delta(^{13}\text{C}_\alpha)$	-2.5	+3.6	+2.6	+13.3	+28.6
$\delta(^{13}\text{C}_\beta)$	-6.1	-5.0	-4.4	-1.6	-5.6
$\delta(^{13}\text{C}_\gamma)$	-14.1	-10.0	-10.8	+8.0	-3.5
$\delta(^{119}\text{Sn})$	+12.4(α) +6.6(γ)	+7.6(α) +4.6(γ)	+8.7(α) +6.3(γ)	+6.0(α) +3.0(γ)	
$^1J(^{119}\text{Sn}-^{13}\text{C}_\alpha)$	+130.6(α) +15.9(γ)	-113.4(α) +9.6(γ)	+139.4(α) +5.2(γ)		
$^2J(^{119}\text{Sn}-^{13}\text{C}_\beta)$	+16.0(α) -4.4(γ)	+13.0(α) -3.6(γ)	+22.1(α) -4.6(γ)		
$^3J(^{119}\text{Sn}-^{13}\text{C}_\gamma)$	+10.0(α) -2.1(γ)	+8.0(α) -4.0(γ)	+9.5(α) -10.7(γ)		

experimental values for the C _{α,β,γ} -carbon atoms does not exceed -0.6 ppm, for ¹¹⁹Sn CS -0.3 ppm. The relatively small values of these deviations demonstrate that the increments can be used for analytical purposes. The study of increments for ¹³C (Table 4) provides evidence for a considerably larger influence of the MMe₃ group in the γ -position of the allene system than in the α - and β -positions. The negative sign of the γ -increment results from exponential correlation between the group-specific electronegativity of the substituent and the γ -increment value [6]. A significant increase in the shielding of the γ -carbon nucleus (owing to the introduction of a MMe₃ group into the α -position of the allene system) is observed in the sequence CMe₃ < GeMe₃ < SiMe₃ < SnMe₃. This is correlated with the increasing σ -donating capacity of substituents in this sequence, suggesting that the negative values of the γ -increment result from the σ -donating capacity of the MMe₃ group.

Generally, antibate relationships are observed between the ¹¹⁹Sn and ¹³C CS of the β -carbon atom in **1** (Table 1). This speaks in favour of conjugation between the tin atom and the allene system as a downfield shift of the ¹³C _{β} signal corresponds to an upfield shift of the ¹¹⁹Sn resonance. In a series of structurally similar compounds, the relative changes in the shielding of nuclei under the influence of substituents are related to corresponding changes in the electron density of these nuclei. Therefore, one can assume that an increase in the negative charge on the tin atom results from a decrease in the charge of C _{β} : Me₂Sn⁻-C _{α} =C _{β} =C _{γ} ⁻. This conclusion is in agreement with the correlation found earlier between the shielding of the central ¹³C _{β} atom in the allene system and substituent resonance effects [6]. Judging from the β -increments (see Table 4), the π -acceptor capacity of the MMe₃ group increases in the sequence Sn < Ge < Si.

The symbatic changes of $\delta(^{13}\text{C}_\alpha)$ and $\delta(^{13}\text{C}_\beta)$ (Fig. 1) suggest a dramatic shift of electrons in the C _{α} =C _{β} bond under the influence of substituents Y, Z in **1**. Thereby, an increase in the downfield shift of the C _{β} atom resonance is accompanied by a downfield shift of the C _{α} -carbon atom resonance, too. Compounds possessing a SR substituent in the X, Y or Z positions deviate from these relationships. Apparently, this is either due to the conjugation between the unpaired electron pair on the sulphur atom and the MMe₃ group or to differences in the volumes of SR and

MMe₃ groups and hence to the smaller deformation of valency angles at the C_α atom. The deviation of the C_αH derivative from the correlation speaks in favour of the latter assumption.

The ${}^nJ(^{119}\text{Sn}-^{13}\text{C})$ SSCC are summarized in Table 2. We failed to find a correlation between the ^{119}Sn and ^{13}C CS and the corresponding SSCC in **1**. Perhaps this can be explained by the fact that CS are mainly determined by the densities of both *s*- and *p*-electrons while SSCC mainly depends on the state of *s*-electrons in the bond.

The ${}^1J(^{119}\text{Sn}-^{13}\text{C}_\alpha)$ SSCC is smaller than ${}^1J(^{119}\text{Sn}-^{13}\text{CH}_3)$ in its absolute value, despite the fact that in the case of the first SSCC the carbon atom shows *sp*²-hybridization. Apparently, the assumption as to the direct correlation between *s*-character of the bond and the SSCC value is fulfilled only for the $^{13}\text{C}-^{13}\text{C}$ SSCC and does not work in the case of the $^{119}\text{Sn}-^{13}\text{C}$ SSCC.

The SSCC through two bonds (${}^2J(^{119}\text{Sn}-^{117}\text{Sn})$ and ${}^2J(^{119}\text{Sn}-^{13}\text{C}_\beta)$ in **1** (Table 2) (except those containing SR substituents)) have a smaller absolute value than those for ${}^4J(^{119}\text{Sn}-^{117}\text{Sn})$ and ${}^3J(^{119}\text{Sn}-^{13}\text{C}_\gamma)$. This feature was also observed for the ${}^2J(^{119}\text{Sn}-^{29}\text{Si})$ and ${}^4J(^{119}\text{Sn}-^{29}\text{Si})$ SSCC in silyl-substituted stannylallenes (Table 3), being likely due to the different sign of the ${}^2J(^{119}\text{Sn}-\text{X})$ and ${}^4J(^{119}\text{Sn}-\text{X})$ SSCC, as it is known that ${}^2J(^{119}\text{Sn}-^{117}\text{Sn}) > 0$, ${}^4J(^{119}\text{Sn}-^{117}\text{Sn}) < 0$ [1].

The additivity rule for SSCC in stannylallenes works worse than for CS (see Table 2, 3). Nevertheless, ${}^nJ(^{119}\text{Sn}-^{13}\text{C})$ in **1** can be predicted satisfactorily using the equations:

$${}^1J(^{119}\text{Sn}-^{13}\text{C}_\alpha) = 390.6 + X_\alpha + \Sigma X_\gamma \quad (4)$$

$${}^2J(^{119}\text{Sn}-^{13}\text{C}_\beta) = 14.7 + X_\alpha + \Sigma X_\gamma \quad (5)$$

$${}^3J(^{119}\text{Sn}-^{13}\text{C}_\gamma) = 50.6 + X_\alpha + \Sigma X_\gamma \quad (6)$$

$X_{\alpha,\gamma}$ are the increments of substituents (Table 4). The accuracy of prediction is equal to -2.0 Hz for ${}^1J(^{119}\text{Sn}-^{13}\text{C}_\alpha)$, -1.0 Hz for ${}^2J(^{119}\text{Sn}-^{13}\text{C}_\beta)$ and -2.0 Hz for ${}^3J(^{119}\text{Sn}-^{13}\text{C}_\gamma)$. It is known [6] that the so-called pairwise interactions can be used for the improvement of the results. However, due to the large mutual spacing of the groups this approach seems applicable to allenes only if one assumes the interaction between the nuclei through space. Apparently, the latter assumption can be used to explain the increase in the ${}^2J(^{119}\text{Sn}-^{117}\text{Sn})$ value in **1** with $\text{X} = \text{SnMe}_3$ in the sequence of substituents Y, Z: $\text{H} < \text{SiMe}_3 \approx \text{SC}_2\text{H}_5 < \text{GeMe}_3 < \text{SnMe}_3$.

In contrast with the ^{119}Sn resonance, the ^{29}Si CS of the stannylsilylallenes that have been studied are much less sensitive to the electronic effects of substituents and fall within the range -4 ± 1 ppm (Table 3). The SSCC involving the ^{29}Si nucleus also change within a considerably smaller range than those corresponding to ${}^nJ(^{119}\text{Sn}-^{13}\text{C})$. The ${}^1J(^{29}\text{Si}-^{13}\text{C}_\alpha)$ SSCC being an exception to the rule, becomes smaller by 7–7.5 Hz under the influence of the α -SnMe₃ group (Table 3).

The isotope shifts resulting from the substitution of ^{12}C by ^{13}C , in different parts of the molecule can easily be measured during the study of SSCC in ^{119}Sn and ^{29}Si NMR spectra. The results of these measurements are summarized in Table 2 (for ^{119}Sn) and in Table 3 (for ^{29}Si). According to [7], the isotope shift is a function of changes in the dynamic properties of a molecule as well as of deviations from the

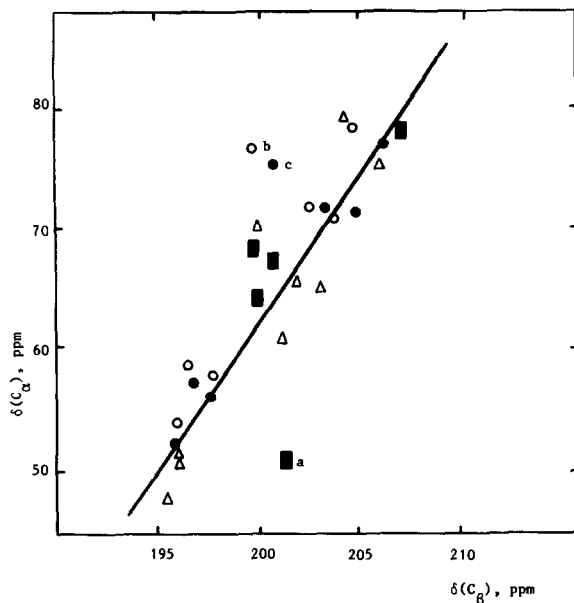


Fig. 1. Relationship between $\delta(C_\alpha)$ and $\delta(C_\beta)$ CS in stannylallenes **1** (X = Δ ; SnMe₃; \bullet : SiMe₃; \circ : GeMe₃; \blacksquare : H, SC₂H₅, Br).
 $\delta(C_\alpha) = -406.6 + 2.35\delta(C_\beta)$ ($r = 0.82$; $n = 28$); a: X = H; b, c: Z = SC₂H₅.

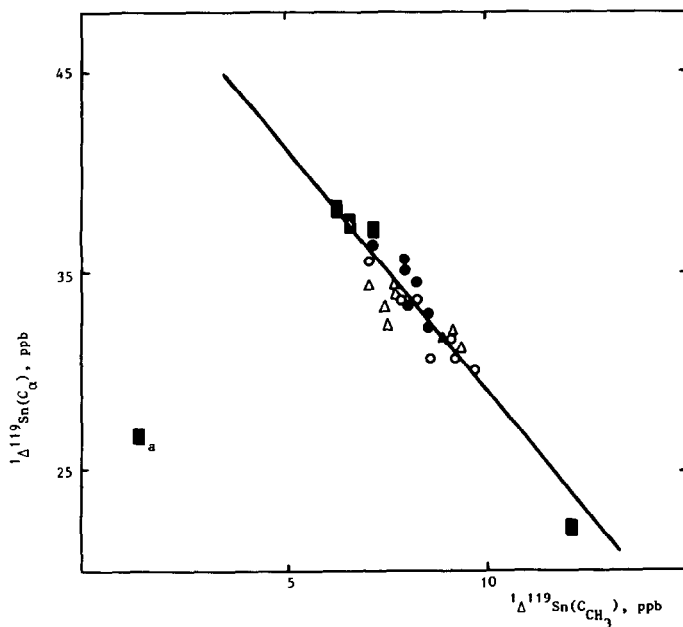


Fig. 2. Dependence of IS ${}^1\Delta^{119}\text{Sn}(C_\alpha)$ on ${}^1\Delta^{119}\text{Sn}(C_{\text{CH}_3})$ in stannylallenes **1** (X = Δ : SnMe₃; \bullet : SiMe₃; \circ : GeMe₃; \blacksquare : H, SC₂H₅, Br).
 ${}^1\Delta^{119}\text{Sn}(C_\alpha) = 53.42 - 2.46 {}^1\Delta^{119}\text{Sn}(C_{\text{CH}_3})$ ($r = 0.934$; $n = 27$); a: X = Br.

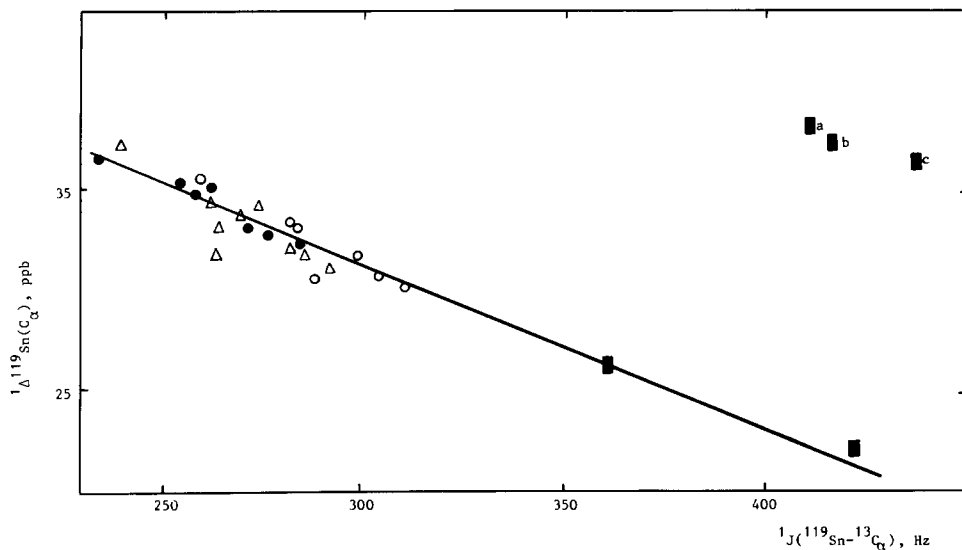


Fig. 3. Dependence between ${}^1\Delta^{119}\text{Sn}(\text{C}_\alpha)$ IS and ${}^1J(^{119}\text{Sn}-^{13}\text{C}_\alpha)$ SSCC in stannylallenes **1** ($\text{X} = \Delta$: SnMe_3 ; \bullet : SiMe_3 ; \circ : GeMe_3 ; \blacksquare : H , SC_2H_5 , Br); a, b, c: $\text{X} = \text{SC}_2\text{H}_5$.

equilibrium geometry (both caused by isotopic replacement). Substituents change the electronic properties of a molecule and affect the isoshielding derivative in the vicinity of nuclei and, in turn, change the values of isotope shifts in NMR spectra. Therefore, the latter are linearly correlated with the physical or electronic properties

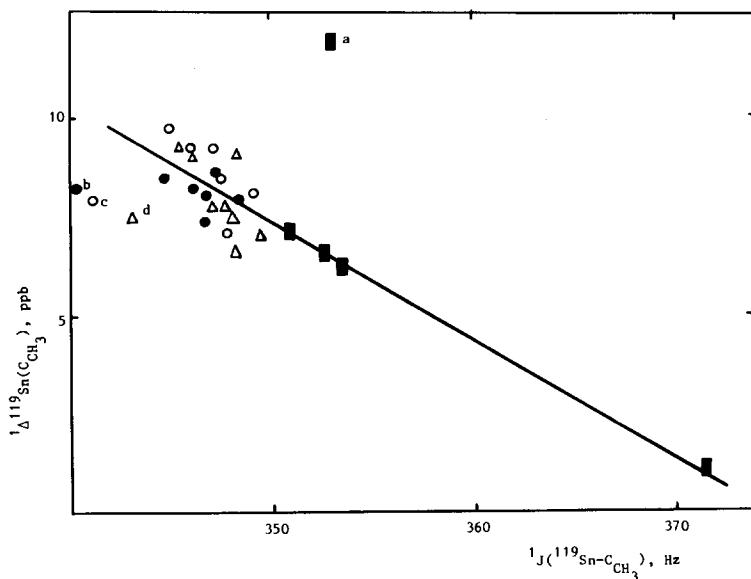


Fig. 4. Relationship between ${}^1\Delta^{119}\text{Sn}(\text{C}_{\text{CH}_3})$ IS and ${}^1J(^{119}\text{Sn}-^{13}\text{C}_{\text{CH}_3})$ SSCC in stannylallenes **1** ($\text{X} = \Delta$: SnMe_3 ; \bullet : SiMe_3 ; \circ : GeMe_3 ; \blacksquare : H , SC_2H_5 , Br); a: $\text{X} = \text{H}$; b, c, d: $\text{Z} = \text{SC}_2\text{H}_5$.

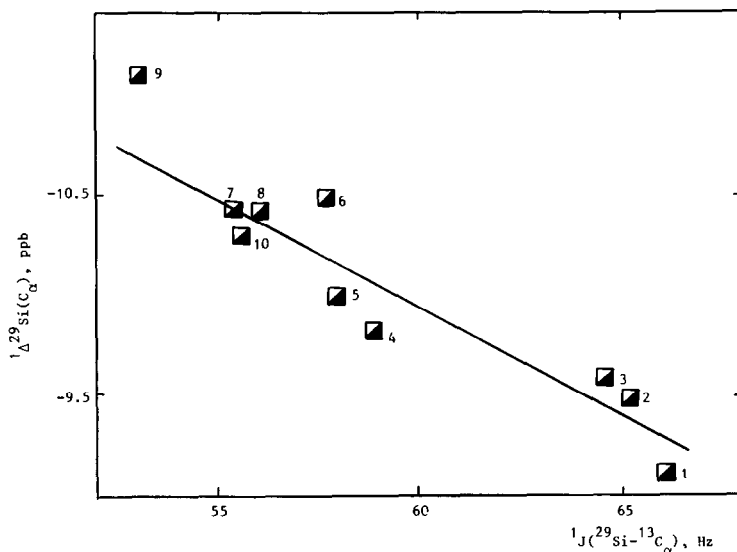


Fig. 5. Dependence of ${}^1\Delta^{29}\text{Si}(\text{C}_\alpha)$ IS on ${}^1J(^{29}\text{Si}-\text{C}_\alpha)$ SSCC in silyllallenes. Numeration of compounds as in Table 3.

which are related to the different electronic configurations of a molecule (bond length, bond order, etc). Comparison of IS for ${}^1\Delta^{119}\text{Sn}(\text{C}_\alpha)$ and ${}^1\Delta^{119}\text{Sn}(\text{C}_{\text{CH}_3})$ bonds (Fig. 2) shows that these values are interrelated. An increase in the ${}^1\Delta^{119}\text{Sn}(\text{C}_{\text{CH}_3})$ value is accompanied by a decrease in ${}^1\Delta^{119}\text{Sn}(\text{C}_\alpha)$. In other words, an increase in the strength of the Sn- C_α bond (increased ${}^1\Delta^{119}\text{Sn}(\text{C}_\alpha)$) is connected with a decrease in the strength of the Sn- CH_3 bond (decreased ${}^1\Delta^{119}\text{Sn}(\text{C}_{\text{CH}_3})$).

Linear correlations are observed between the ${}^1J(^{119}\text{Sn}-^{13}\text{C}_i)$ SSCC and the corresponding isotope shift ${}^1\Delta^{119}\text{Sn}(\text{C}_i)$ (Figs. 3 and 4). Thus, an increase in SSCC is accompanied by a decrease in IS values:

$${}^1\Delta^{119}\text{Sn}(\text{C}_\alpha) = 54.64 - 0.08 {}^1J(^{119}\text{Sn}-^{13}\text{C}_\alpha) \quad (7)$$

$(r = 0.96; n = 25)$

$${}^1\Delta^{119}\text{Sn}(\text{C}_{\text{CH}_3}) = 111.64 - 0.298 {}^1J(^{119}\text{Sn}-^{13}\text{C}_{\text{CH}_3}) \quad (8)$$

$(r = 0.925; n = 24)$

An analogous correlation has been found between ${}^1J(^{29}\text{Si}-^{13}\text{C}_\alpha)$ and ${}^1\Delta^{29}\text{Si}(\text{C}_\alpha)$ (Fig. 5):

$${}^1\Delta^{29}\text{Si}(\text{C}_\alpha) = -16.91 + 0.12 {}^1J(^{29}\text{Si}-^{13}\text{C}_\alpha) \quad (9)$$

$(r = 0.93; n = 10)$

Similarity has been observed between the IS values in ^{119}Sn and ^{29}Si NMR spectra caused by the $^{12/13}\text{C}$ isotope substitution. The correlation between ${}^1\Delta^{119}\text{Sn}(\text{C}_\alpha)$ and ${}^1\Delta^{29}\text{Si}(\text{C}_\alpha)$ found in isostructural stannyl- and silyllallenes supports this interpretation to (Fig. 6):

$${}^1\Delta^{29}\text{Si}(\text{C}_\alpha) = -6.14 - 0.13 {}^1\Delta^{119}\text{Sn}(\text{C}_\alpha) \quad (10)$$

$(r = 0.94; n = 8)$

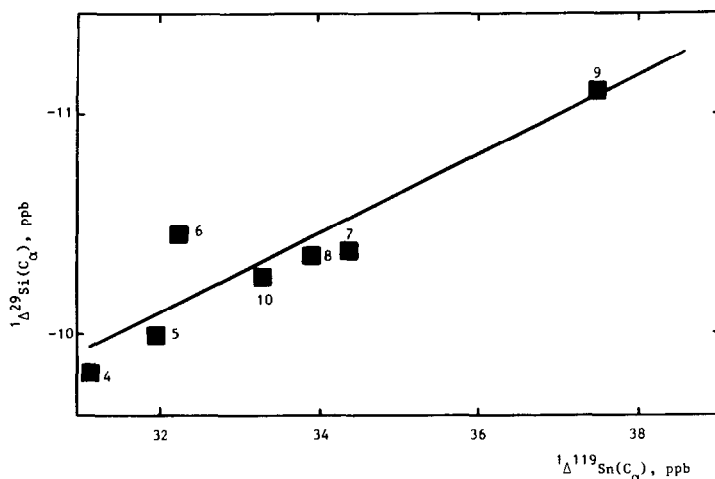


Fig. 6. Relationship between $\Delta^{29}\text{Si}(\text{C}_\alpha)$ and $\Delta^{119}\text{Sn}(\text{C}_\alpha)$ IS in isostructural stannyl- and silylallenes. Numeration of compounds as in Table 3.

Judging by this equation the sensitivity of ^{119}Sn resonance considerably exceeds that of ^{29}Si resonance; this is in agreement with the total range of CS changes observed for these nuclei.

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