²⁹Si-H Spin Coupling Constants

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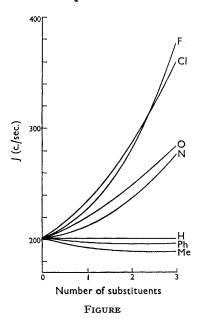
WE are at present engaged in a study of spin couplings in Si-H fragments. Data have been collected on 62 compounds, of which 31 have already appeared in the literature. We have noticed that an empirical equation of the type used by Malinowski¹ to correlate ¹³C-H couplings is applicable to ²⁵Si-H couplings. The coupling constant for the compound SiHXYZ can be written

$$J_{\mathbf{X},\mathbf{Y},\mathbf{Z}} = J_{\mathbf{X}\mathbf{Y}}' + J_{\mathbf{Y}\mathbf{Z}}' + J_{\mathbf{Z}\mathbf{X}}'$$

where the J' are constants for each pair of substituents. The equation has been tested over a range of compounds in which X, Y, and Z are all possible combinations of hydrogen, methyl, phenyl, and chlorine. The following parameters were obtained (in c./sec.)

$$J'_{
m HH} = 67.6$$
 $J'_{
m HCl} = 84.7 \ J'_{
m HMe} = 63.5 \ J'_{
m HPh} = 66.0$ $J'_{
m ClCl} = 120.5 \ J'_{
m ClMe} = 79.9 \ J'_{
m ClPh} = 84.6$ $J'_{
m MeMe} = 63.1 \ J'_{
m MePh} = 63.4$ $J'_{
m PhPh} = 66.1$

We have also extended previously recorded data to enable us to draw a Figure which shows the variation in $J(^{29}\text{Si-H})$ as 1, 2, or 3 substitutents are introduced into SiH₄.



Variation in $J(^{29}Si-H)$ as substituents are introduced into SiH_4 .

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¹ E. R. Malinowski and T. Vladimiroff, J. Amer. Chem. Soc., 1964, 86, 3375.