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DISTINCTION OF *cis* AND *trans* ARRANGEMENTS IN DOUBLE BONDS BY $^{13}C-^{1}H$ COUPLING

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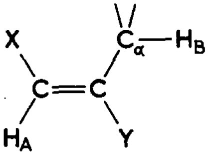
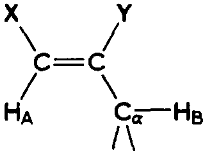
In vicinally-disubstituted olefins, the magnitude of the hydrogen-hydrogen coupling constant usually allows a distinction of *cis* from *trans* configurations. In more highly substituted cases such as 1 or 2 ($X,Y \neq H$), the hydrogen-hydrogen coupling constant which may be available viz. J_{A-B}, is not normally useful in diagnosing configuration. This coupling constant varies between 0 and 2 Hz, so is not easily measured accurately, and the *cis*-coupling in 2 may be greater OR smaller than the *trans*-coupling in 1 depending on the nature of X and Y[2].



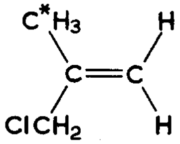
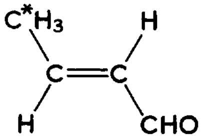
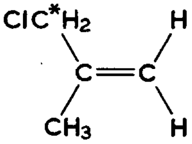
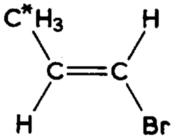
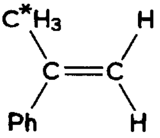
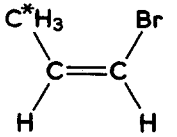
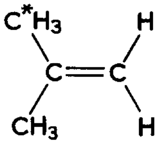
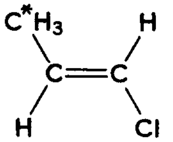
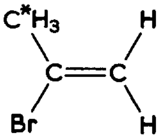
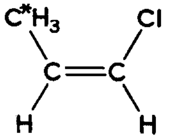
1 *trans*



2 *cis*

I report that the vicinal $^{13}C-^{1}H$ coupling constant $J_{A-\alpha}$ varies markedly with configuration and can be used to distinguish isomers.

Table 1 shows values of *cis* and *trans* $^{13}C-C{=}C-^{1}H$ coupling constants[3] for several simple molecules. The values for $J_{\underline{cis}}$ and $J_{\underline{trans}}$ are normally widely different, the ranges just overlapping. Each range is large indicating that the effect of substituents and their orientation with respect to the coupling pathway may be determined from these couplings and be diagnostic of structure.

J_{cis} Hz		J_{trans} Hz	J_{cis} Hz		J_{trans} Hz
6·0		10·4	5·9		—
7·5		13·9	4·7		—
6·9		11·3	—		7·0
5·2		12·4	4·4		—
4·5		8·9	—		7·2

• REFERENCES

1. 'High Resolution Nuclear Magnetic Resonance Spectroscopy', J.W. Emsley, J. Feeney, and L.H. Sutcliffe, Pergamon Press, London, 1966, Section 10.4.

2. See for example Table 5.8 in reference 1.

3. Determined usually by first-order analysis of natural abundance ^{13}C-spectra without decoupling of hydrogens. Spectra are not always first-order. By analogy with similar ^{1}H-^{1}H values, coupling constants should be positive.