

RELATIONSHIP BETWEEN THE MOLECULAR STRUCTURES OF 1,2,4-THIA-
DIAZOLIDINE DERIVATIVES AND THEIR NMR SOLVENT EFFECTS

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The n.m.r. spectra of 2,4-dimethyl(or diethyl)-3,5-diarylimino-1,2,4-thiadiazolidines, 2-aryl-3-methyl(or ethyl)imino-4-methyl(or ethyl)-5-arylimino-1,2,4-thiadiazolidines, 2-methyl(or ethyl)-3-arylimino-4-aryl-5-methyl(or ethyl)imino-1,2,4-thiadiazolidines and 2,4-dimethyl(or diethyl)-3,5-diarylimino-1,2,4-thiadiazolidine-1-oxides have been obtained. The n.m.r. solvent shifts (δCCl_4 - $\delta\text{C}_6\text{D}_6$) for these 1,2,4-thiadiazolidine derivatives are shown in the tables.

On the para-substituted compounds, a reasonably good correlation has been found between the relative solvent shifts (δCCl_4 - $\delta\text{C}_6\text{D}_6$) for the sp^2 -like N-methyl or methylene protons and the corresponding Hammett σ parameter. On the other hand, the solvent shifts for the sp^3 -like N-methyl or methylene protons have been shown to be correlated with Taft σ° parameter.