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

Takeshi Kinoshita, Sadao Sato, Yoji Furukawa, and Chihiro Tamura

Central Research Laboratories, Sankyo Co., Ltd.

Shinagawa-ku, Tokyo, Japan

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 ($\delta CCl_4 - \delta C_6D_6$) 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 ($\delta CCl_4 - \delta C_6D_6$) 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^o parameter.