Some Applications of Ultrahigh Resolution $^{15}$N NMR Spectroscopy

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NMR Data, Ultrahigh Resolution

Ultrahigh resolution $^{15}$N NMR spectra were measured for two nitroalkanes (MeNO$_2$ 1a, t-BuNO$_2$ 1c), two isocyanates (t-BuNCO 2c, Me$_3$SiNCO 2d), four isothiocyanates (MeNCS 3a, EtNCS 3b, t-BuNCS 3c, Me$_3$SiNCS 3d), one carbodiimide (Me$_3$SiNCNSiMe$_3$ 4d), one keteneimine [Me$_3$SiNCC(SiMe$_3$)$_2$ 5d], two sulphinyl imides (t-BuNSO 6c, Me$_3$SiNSO 6d), and N-tert-butyl-pyrrole 7c, in order to determine coupling constants $J^{(\text{N}^{15}, \text{C}^{13})}$ and isotope induced chemical shifts $\Delta^{12,13}\text{C}(^{15}\text{N})$ at the natural abundance of the isotopes. The values $\Delta^{12,13}\text{C}(^{15}\text{N})$ can be separated into two groups, one dealing with NC single and another one with NC double bonds. In each group (with few exceptions), the values $\Delta^{12,13}\text{C}(^{15}\text{N})$ become more negative with a decrease in the absolute magnitude of $|J^{(\text{N}^{15}, \text{C}^{13})}|$. The corresponding values $\Delta^{14,15}\text{N}(^{13}\text{C})$ show a similar behaviour. However, N-substituted pyrroles appear to be exceptional in this respect.

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