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

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Ultrahigh resolution ^{15}N NMR spectra were measured for two nitroalkanes ($MeNO_2$ **1a**, ^{t}BuNO$_2$ **1c**), two isocyanates (^{t}BuNCO **2c**, Me_3SiNCO **2d**), four isothiocyanates (MeNCS **3a**, EtNCS **3b**, ^{t}BuNCS **3c**, Me_3SiNCS **3d**), one carbodiimide ($Me_3SiNCNSiMe_3$ **4d**), one keteneimine [$Me_3SiNCC(SiMe_3)_2$ **5d**], two sulphinyl imides (^{t}BuNSO **6c**, Me_3SiNSO **6d**), and N-*tert*-butyl-pyrrole **7c**, in order to determine coupling constants $J(^{15}N,^{13}C)$ and isotope induced chemical shifts $^1\Delta^{12/13}C(^{15}N)$ at the natural abundance of the isotopes. The values $^1\Delta^{12/13}C(^{15}N)$ 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 $^1\Delta^{12/13}C(^{15}N)$ become more negative with a decrease in the absolute magnitude of $|^1J(^{15}N,^{13}C)|$. The corresponding values $^1\Delta^{14/15}N(^{13}C)$ show a similar behaviour. However, N-substituted pyrroles appear to be exceptional in this respect.

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