TITLE: ^{13}C NMR Spectroscopy: Transmission Effects in 3,5-Diaryl-4-Bromoisoxazoles

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Introduction:
Transmission effects have been studied in 3,5-diarylisoxazoles.The present study seeks to investigate if transmission is altered in isoxazoles when a bulky group has been added to the central position of the ring to force the 3,5-diaryl groups to twist. ^{13}C NMR spectral data will be plotted against that of the parent system to determine the effect.
Methods:
3,5-Diarylisoxazoles were prepared by published procedures. The 4-bromoisoxazole derivatives will be prepared from the isoxazoles by a reaction with NBS in acetic acid. Compounds were purified and characterized by standard methods. ^{13}C NMR spectra will be collected using standard NMR parameters in DMSO-d6. Collected data for known compounds were in agreement with those previously published. Molecular modeling studies were conducted using the Spartan'14 program. X-ray analysis will be obtained commercially to verify the three-dimensional geometry (dihedral angles between the aromatic rings) of the heterocyclic system.
Results:
Molecular modeling results for 3,5-diarylisoxazoles and the corresponding 4-bromoisoxazoles showed the former to be flat and the latter to be twisted with dihedral angles between the two aryl groups and the central isoxazole ring of about 15^{o} and 35^{o} respectively. ^{13}C spectra data of both series of compounds were obtained and assigned. In agreement with published work, transmission of substituent effects were observed on the chemical shift of C_4 for 3,5-diarylisoxazoles. Electron donating groups on the 5-aryl group resulted in amplified shifts of the signal for C_4 of the isoxazoles while electron withdrawing groups showed the opposite. Substituents on the 3-aryl groups had little to no effect of the C_4 shift signal. Plots of the C_4 chemical shifts for the series of 5-aryl substituted isoxazoles vs. those of the 4-bromoisoxazoles should be linear, and the slope of which should allow determination of any changes in transmission efficiency.
Discussion:
Molecular modeling is valuable in predicting three-dimensional structures of molecules including the distortions created as a result of adding bulky groups. Comprehending transmission of substituent effects in heterocyclic compounds will lead to a better understanding of the properties of these molecules and their reactivity in chemical reactions.