Conformational Analysis of 2-(Diphenylphosphanyl)-N,N-dimethyl-1- benzamide and 2-(Diphenylphosphanyl)-phenyl-pyrrolidin-1-yl-methanone by NMR Spectroscopy

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We have synthesized 2-(Diphenylphosphanyl)-N,N-dimethyl-1- benzamide (1) and 2-(Diphenylphosphanyl)-phenyl-pyrrolidin-1-yl-methanone (2), and examined their conformations on the basis of NMR spectral data. Conformational analysis of the compounds is useful in deducing the structure in which they are active as a catalyst. In the present NMR measurements, ^{1}H- X fg -JHMBC (field gradient J -Resolved Hetero -nuclear Multiple -Bond Correlation) spectroscopy was implemented as a tool for the determination of hetero -nuclear three bond, phosphorus and protons and carbon -protons coupling constants. The experiment utilized proton detection with good sensitivity and benefited considerably from the use of pulsed field gradients. By fitting a sine curve to the experimental data by the method of 3D J -resolved HMBC NMR measurements, accurate ^{n}JHX coupling constants were obtained. From the coupling constants, the corresponding dihedral angles, H3 -C2-C3-P, H12-C12-C11-P, H16-C16-C11-P, H18-C18-C17-P, and H22 -C22-C17-P, of compounds (1) and (2) were determined. The optimized structures of the compounds were obtained by molecular orbital calculations in which the dihedral angles experimentally determined were used.