Crystal Structure of and *ab initio* Calculations on $[(C_6H_5)(CH_3)CH\text{-}NH]\text{-}P(O)(p\text{-}OC_6H_4CH_3)_2$, Syntheses and Spectroscopic Characterization of *N*-Benzyl Phosphoramidic Acid (4-Methylphenyl)ester Derivatives

Khodayar Gholivand, Zahra Shariatinia, and Mehrdad Pourayoubi

Department of Chemistry, Faculty of Sciences, Tarbiat Modarres University,
P. O. Box 14115-175, Tehran, Iran

Reprint requests to Prof. K. Gholivand. E-mail: gholi_kh@modares.ac.ir

Z. Naturforsch. **60b,** 67 – 74 (2005); received May 17, 2004

Some new *N*-benzyl phosphoramidic acid (4-methylphenyl)ester derivatives were synthesized and characterized by ^{1}H, ^{13}C, ^{31}P NMR and IR spectroscopy and elemental analysis. The structure of $[(C_6H_5)(CH_3)CH\text{-}NH]P(O)(p\text{-}OC_6H_4CH_3)_2$ (**2**) was investigated. This compound exists in polymeric zigzag chains in the crystalline lattice produced by hydrogen bonding built from two alternating independent molecules. NMR data indicate two diastereotopic *p*-cresol groups as confirmed by X-ray crystallography. *Ab initio* calculations were performed on the geometry of compound **2** at the UHF/6-311G** and B3LYP/6-311G** levels. The optimized structure of each independent molecule contains two different *p*-cresol groups, in agreement with the experimental results.

Key words: *N*-Benzyl Phosphoramidic Acid (4-methylphenyl)esters, X-Ray Crystallography, NMR, *ab initio* Calculations