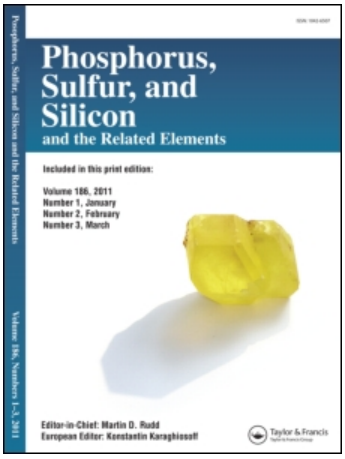

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Synthesis and NMR Spectroscopic Properties of C-Fluorinated Bisphosphonic Acids

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SYNTHESIS AND NMR SPECTROSCOPIC PROPERTIES OF C-FLUORINATED BISPHOSPHONIC ACIDS

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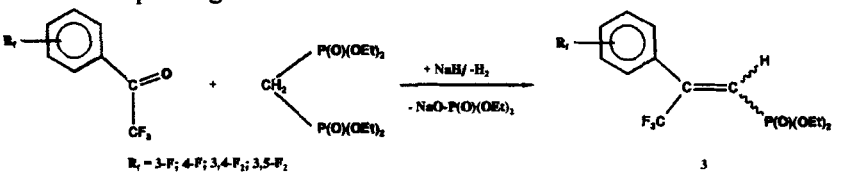
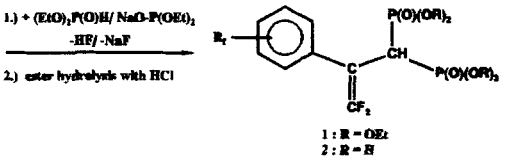
INTRODUCTION

Fluorinated and halogenated bisphosphonates have gained widespread interests in chemistry, pharmacy and medicine. The concept of biochemical activity with metal-chelating agents has encouraged our research team to study synthesis, NMR and analytic chemistry of fluorinated aromatic and olefinic geminal bisphosphonates.

RESULTS AND DISCUSSION

We have developed a reaction pathway for a novel type of fluorinated bisphosphonic acid esters **1** and corresponding acids **2**:





Fluorinated acetophenones and methylenediphosphonic acid ester react under the conditions of the Wittig-Horner-Emmons-Reaction to yield the vinylphosphonates **3**, which add diethyl phosphite. After the nucleophilic addition of the phosphonate group a fluoride ion elimination takes place leading to the bisphosphonic acid esters **1**, which are cleaved by hydrochloric acid to the parent acids **2**. The bisphosphonates **1** and **2** are characterised by 1D-, 2D-, DR- and NOE spectroscopic methods using nuclei ^{1}H, ^{13}C, ^{19}F and ^{31}P. Variable temperature $^{31}P\{^{1}H\}$- and ^{19}F-NMR deduced the dynamic behaviour of the model compounds.