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Intramolecular interactions in *ortho*-methoxyalkylphenylboronic acids and their catechol esters

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Keywords: boronic acids; boronic esters; ¹⁷O NMR; hydrogen bond

Highlights:

- Synthesis of *ortho*-methoxyalkylphenylboronic acids catechol esters.
- ¹⁷O NMR characterization of the esters and parent acids.
- Influence of hydrogen bond on the properties of the acids.
- No O→B interactions in the investigated compounds.
- Diminished acidity compared with the unsubstituted phenylboronic acid.

Abstract

Catechol esters of *ortho*-methoxyalkylphenylboronic acids have been synthesized and characterized by ¹⁷O NMR spectroscopy. The results were compared with the data for the parent acids. The influence of intramolecular and intermolecular hydrogen bonds on the properties of the boronic acids has been discussed. The ¹⁷O NMR data for the boronic esters proved that there are no O→B interactions in the investigated compounds. This fact is connected with weak Lewis acidity of the parent acids and their low sugars' receptors activity. Crystal structure of *ortho*-methoxyphenylboronic acid catechol ester was determined.

Introduction

Arylboronic acids are systems that attract an increasing scientific interest due to their new applications in organic synthesis, catalysis, supramolecular chemistry, biology, medicine

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