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Editors
Jelena **MILOVANOVIĆ**
Vuk **FILIPOVIĆ**
Života **SELAKOVIĆ**
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Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

Page Layout and Design
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

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Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

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Theoretical study of the relationship between molecular geometry and strength of hydrogen bonds in acetylsalicylic acid

Danijela S. Kretić[1], Marija Maslarević[1], Dušan Ž. Veljković[1]
[1] *University of Belgrade - Faculty of Chemistry, Belgrade, Serbia*

Acetylsalicylic acid is a pharmaceutical drug well-known for its anti-inflammatory and antipyretic effects, and it is commonly used for the treatment of pain and fever caused by different diseases.[1] However, it is well known that pharmaceutical properties highly depend on the geometry of chemical compounds. [2] Herein, we present a theoretical study of the relationship between molecular geometry and chemical properties for various acetylsalicylic acid structures obtained from the Cambridge Structural Database (CSD). It is significant to emphasize that studied structures were synthesized and studied under different experimental conditions, and some of them were classified as different polymorphic structures.

In this work, we used quantum chemical calculations to study the influence of differences in geometries on values of calculated electrostatic potentials in critical points of selected acetylsalicylic acid molecules. The results showed that different crystal structures have significant deviations in electrostatic potential values in critical points above the ortho-Ar hydrogen atom. In addition, we studied the influence of geometry differences on the strength of C-H/O interaction between acetylsalicylic acid and water molecules. The results suggest that minor differences in the molecular geometry of acetylsalicylic acid could significantly influence the strength of C-H/O interaction. In conclusion, the geometry differences could have a crucial effect on the strength of non-covalent interactions and pharmaceutical properties of acetylsalicylic acid.

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