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Belgrade, 25.02.2019

Dear Editor,

Please find enclosed a manuscript entitled "Hydrogen transfer reaction: Bond formation and bond cleavage through the eyes of Interacting Quantum Atoms" by Branislav Milovanović, Mihajlo Etinski and Milena Petković, which we are submitting for consideration for publication as an article in the special issue of the *Journal of Serbian Chemical Society* dedicated to the 70th birthday of prof. Miljenko Perić.

In this manuscript, we used Density Functional Theory to study the reaction between hydroquinone and methoxy radical with the emphasis on the changes that take place in the vicinity of the transition state. Particularly, we focused on a detailed analysis of the changes of the bond that gets broken (O-H bond in hydroquinone) and the bond that gets formed (O-H bond in methanol). For this purpose, we employed the Interacting Quantum Atoms methodology, which emerged from Bader's Quantum Theory of Atoms in Molecules approach. By dividing the whole system into two fragments, it is possible to monitor the changes of the bond of interest along the minimum energy path starting from the saddle point and going in the direction of the reactants and the products. By defining the fragments as reactants, hydroquinone and methoxy radical, we extract information about the O-H bond in methanol that gets formed. On the other hand, if the products are chosen as fragments, semiquinone and methanol, it is possible to monitor O-H bond cleavage in hydroquinone. Further, we divided the system into three fragments (semiquinone, methoxy radical and hydrogen atom), which enabled simultaneous analysis of both processes, bond formation and bond cleavage, but also interaction between semiquinone and methoxy radical. To the best of our knowledge, the results presented in this manuscript represent the first application of Interacting Quantum Atoms methodology on a system with more than two fragments.

We hope that you share our enthusiasm for the presented results and that you will consider our work for publication in the *Journal of Serbian Chemical Society*.

Sincerely,

Milena Petković

Manuscript title:

Hydrogen transfer reaction: Bond formation and bond cleavage through the eyes of Interacting Quantum Atoms

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