

Accepted Manuscript

New hybrid cluster-continuum model for pKa values calculations: Case study of neurotransmitters' amino group acidity

Miroslav M. Ristić, Milena Petković, Branislav Milovanović, Jelena Belić, Mihajlo Etinski

PII: S0301-0104(18)30548-2

DOI: <https://doi.org/10.1016/j.chemphys.2018.08.022>

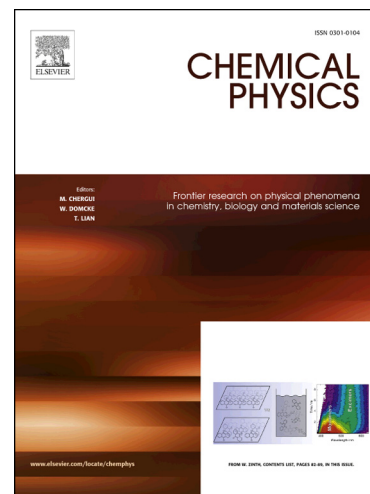
Reference: CHEMPH 10138

To appear in: *Chemical Physics*

Received Date: 21 May 2018

Revised Date: 13 August 2018

Accepted Date: 14 August 2018



Please cite this article as: M.M. Ristić, M. Petković, B. Milovanović, J. Belić, M. Etinski, New hybrid cluster-continuum model for pKa values calculations: Case study of neurotransmitters' amino group acidity, *Chemical Physics* (2018), doi: <https://doi.org/10.1016/j.chemphys.2018.08.022>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

New hybrid cluster-continuum model for pK_a values calculations: Case study of neurotransmitters' amino group acidity

Miroslav M. Ristić*, Milena Petković, Branislav Milovanović, Jelena Belić, Mihajlo Etinski

Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, P. O. Box 47, 11158

Belgrade, Serbia

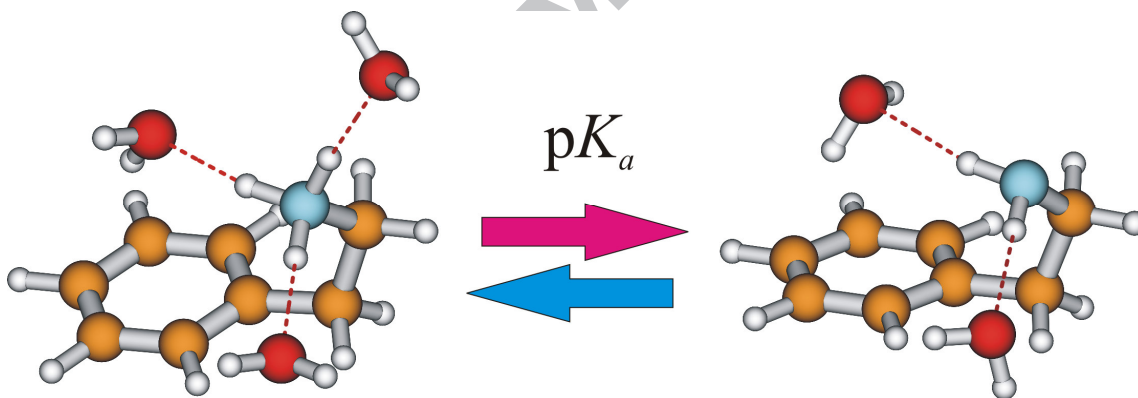
e-mail: ristic@ffh.bg.ac.rs

Hybrid cluster-continuum model.

pK_a values calculations.

Primary amines.

Molecular dynamics simulations.



Abstract: Acid dissociation constant is a quantitative measure of chemical species ability to donate a proton to water molecule and plays important role in aqueous chemistry. Many computational strategies were conceived in order to properly address an acid dissociation equilibrium. In this work, we present new economical cluster-continuum method based on the density functional theory for the accurate calculation of pK_a values. By analysing hydration properties of neutral and protonated 2-phenylethylamine sampled in the first principle molecular dynamics simulations, we were able to find key interactions between water

Download English Version:

<https://daneshyari.com/en/article/8948397>

Download Persian Version:

<https://daneshyari.com/article/8948397>

[Daneshyari.com](https://daneshyari.com)