
Structure and Reactivity of Baicalein Radical Cation

ZORAN S. MARKOVIĆ,¹ SVETLANA MARKOVIĆ,²
JASMINA M. DIMITRIĆ MARKOVIĆ,³ DEJAN MILENKOVIĆ⁴

¹Department of Bio-chemical and Medical Sciences, State University of Novi Pazar, Vuka Karadžića bb, 36300 Novi Pazar, Republic of Serbia

²Department of Chemistry, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Republic of Serbia

³Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Republic of Serbia

⁴Bioengineering Research and Development Center, Prooslava Stojanovića 6, 34000 Kragujevac, Republic of Serbia

Received 28 February 2011; accepted 13 May 2011

Published online 18 July 2011 in Wiley Online Library (wileyonlinelibrary.com).

DOI 10.1002/qua.23175

ABSTRACT: Neutral baicalein, corresponding radical cation, and three possible radicals obtained by proton removal from the radical cation were investigated using density functional theory. The structure and UV spectrum of baicalein were very well reproduced by the B3LYP/6-311+G(2df,p) level of theory. The results showed that the loss of an electron from baicalein molecule induced the transfer of H4 to O5. The reasons for this rearrangement were pointed out. It was found that delocalization of spin density is most pronounced in the thermodynamically most stable C6—OH radical. It was supposed that this radical plays a significant role in the antioxidant activity of baicalein within the single-electron transfer-proton transfer mechanism. © 2011 Wiley Periodicals, Inc. *Int J Quantum Chem* 112: 2009–2017, 2012

Key words: baicalein; radical cation; SET-PT mechanism; DFT

Correspondence to: J. M. Dimitrić Marković; e-mail: arkovich@ffh.bg.ac.rs (or) Z. S. Marković; e-mail: zmarkovic@np.ac.rs

Contract grant sponsor: Ministry of Science of the Republic of Serbia.

Contract grant numbers: 172015 and 172016.

Additional Supporting Information may be found in the online version of this article.

