CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2022, 17(1), 24-30
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.asm.md
http://dx.doi.org/10.19261/cjm.2021.919

SOME PARTICULARITIES OF THE REACTION BETWEEN ANTIOXIDANT PHENOLIC ACIDS AND THE FREE RADICAL ABTS$^{\bullet+}$: A COMPARATIVE DFT STUDY FOR THE GAS PHASE AND ETHANOL

Mikhail Gorbachev, Natalia Gorinchoy *, Iolanta Balan

Institute of Chemistry, 3, Academiei str., Chisinau MD-2028, Republic of Moldova
**email: ngorinchoy@yahoo.com; natalia.gorincioi@ichem.md*

Abstract. The detailed mechanism of the interaction of the radical cation ABTS$^{\bullet+}$ with a number of food acids (gallic, ferulic, caffeic, vanillic, cinnamic, syringic, *p*-coumaric) is revealed by means of the DFT calculations. It is shown that the interaction between the neutral molecules of the studied food acids and ABTS$^{\bullet+}$ does not lead to any charge transfer from these molecules onto ABTS$^{\bullet+}$. The almost complete conversion of the ABTS radical cation into its diamagnetic derivative occurs due to the interaction of one of the sulphonic groups of ABTS$^{\bullet+}$ with the acid anions through the formation of the corresponding intermolecular hydrogen bond. The clear-cut correlation between the bond lengths SO$^{\cdots}$H and the experimental values of the antioxidant activity of the food acids under study was found. DFT calculations taking into account the solvent (ethanol), allow one to reveal the second clear-cut correlation between the studied activity and the values of the charge transfer from the anions of the studied food acids to ABTS$^{\bullet+}$.

Keywords: antioxidant activity, radical cation ABTS$^{\bullet+}$, food acid, charge transfer complex, DFT calculation.

Received: 24 December 2021/ Revised final: 17 January 2022/ Accepted: 20 January 2022