SOME PARTICULARITIES OF THE REACTION BETWEEN ANTIOXIDANT PHENOLIC ACIDS AND THE FREE RADICAL ABTS$^{\bullet+}$: DFT STUDY

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Abstract. The detailed mechanism of the interaction of the radical cation ABTS$^{\bullet+}$ with a number of food (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 sulfonic 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…H and the experimental values of the antioxidant activity of the food acids under study was found.

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