

Application of the electron localization function of radical systems

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An application of the topological electron localization function (ELF) analysis of free radical systems is presented. A separation of the ELF function into its α -spin and β -spin contributions has been performed. Methyl and phenyl radicals, ortho-, meta-, and para-benzyne biradicals, and their corresponding radical anions have been chosen with the aim to validate the new ELF α and ELF β proposed functions. The results show that the ELF separation yields complementary information about the localization of the unpaired electron.