ON MODELING THE ELECTRONIC STRUCTURE OF HIGHLY REACTIVE RADICALS IN WATER

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Frequent serious discrepancies between the structural models of short-lived radicals in water derived from their vibrational spectra , chemical properties and theoretical structure calculations will be discussed using the example of phenoxyl radicals. It will be shown that the apparent agreement between some of the calculated frequencies of the radicals with a few experimentally observed frequencies is not sufficient to proceed with the vibrational mode assignments. The protonation/deprotonation site in the radical structure and acid-base properties provide a simple chemical test for the adequacy of the structural models in interpreting the molecular spectra and the chemistry in solution.