A Computational Approach to the Study of Free Radical Chemistry

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Radicals are ubiquitous in chemistry and biology. Because they are reactive species, they are often difficult to study experimentally and therefore theory has a potentially useful role to play in their characterization. However, there are also challenges for theory, particularly in the form of so-called spin contamination. In recent years, we have been involved in formulating theoretical procedures that provide an improved description for radicals. We have also been using such procedures to investigate the structures, stabilities and reactivities of radicals. Highlights from this research will be presented.