

# Preface

Electron Paramagnetic Resonance, EPR, has been widely used for nearly 60 years in studies of intermediate products like free radicals, triplet state molecules and other paramagnetic species, formed by irradiation. The applications of EPR (ESR) in radiation research have since then been reviewed in several monographs and edited works. The progress made during the last two decades has so far not been treated in a single volume, however, in spite of the significant progress reached by applying modern continuous wave (CW) and pulsed EPR, development of detection methods with high resolution and sensitivity, application of sophisticated matrix isolation techniques and by the advancement in quantitative EPR to mention a few recent experimental trends. On the theoretical side methods based on first principles have been developed and applied for the calculation of hyperfine couplings, zero-field splittings and g-factors as well as in spectral simulations. In the present work an effort was made to present developments of particular interest for radiation research in 19 chapters written by invited specialists.

Elementary radiation processes is treated in the first four chapters. The subject is introduced in Chap. 1 and is illustrated by recent applications in radiation chemistry employing steady-state and pulse radiolysis. Experimental EPR studies of the radicals and radical ions formed by radiolysis of crystalline organophosphorus compounds, metal complexes, and halocarbons are reviewed in the following two chapters, with assignments supported by state-of-the-art quantum chemistry calculations. Recent progress in studies of hydrogen molecular ions is reviewed in Chap. 4. EPR studies in solid para-hydrogen matrices at cryogenic temperatures were reported. Several applications of EPR in solid state radiation chemistry are considered in the three following chapters. A combination of EPR and IR methods was used in Chap. 5 to obtain information on the structure and dynamics of radicals and radical ions produced by *in situ* irradiation with fast electrons. A rigorous matrix isolation approach using solid noble gases was applied. Research towards identification of radiation-induced radicals in solid state sugars and sugar phosphates is treated in Chap. 6. EPR and ENDOR single crystal measurements combined with DFT calculations were utilized to obtain information of initial radiation damages and thermally induced transformation mechanisms. Structures of radiation-induced defects in silica ( $\text{SiO}_2$ ) were investigated by pulsed ENDOR and ESEEM as well

as EPR in Chap. 7. Recent progress made on selected radiation-induced defects in crystalline  $\text{SiO}_2$  and amorphous  $\text{SiO}_2$  doped (and undoped) with diamagnetic impurities is reviewed. Direct and indirect radiation effects are considered in two chapters devoted to biochemistry, biophysics, and biology applications. In Chap. 8 EPR studies of radical formation by direct ionization of DNA are reviewed. Mechanisms that lead to production of stable damage, such as strand breaks were considered. A method presented in Chap. 9 combining EPR, spin trapping and chromatographic separation made it possible to identify free radicals in nucleic-acid and protein-related compounds. Applications in material science are treated in three chapters. As explained in Chap. 10 EPR studies of polymers have been closely related to the research and development of polymer modification by radiation processing. EPR in combination with theoretical modeling and optical and electrical characterizations were used in Chap. 11 for studies of radiation-induced defects in SiC and III-nitrides. The use of intrinsic defects in controlling properties of materials for power electronics was discussed. The radiation induced reactions and fragmentation in room temperature ionic liquids using EPR spectroscopy are reviewed in Chap. 12 with particular emphasis on applications in nuclear fuel cycle separations. Radiation metrology is treated in two chapters concerned with EPR dosimetry. In Chap. 13 the alanine-EPR metrology system for high-dose radiation dosimetry at NIST is presented. The use of EPR dosimetry in medicine, predominantly within radiotherapy, is reviewed in Chap. 14. Most applications have employed polycrystalline alanine, but the use of other materials is also discussed. The utilization of CW and pulsed EPR measurements as a tool for astrobiology in search of primitive organic matter is considered in Chap. 15. Materials originating from meteorites and terrestrial substances could for example be distinguished. Studies involving pulsed EPR and optical detection are treated in two chapters presenting advanced methods. EPR methods to determine the distribution of radiation damage products in solids are reviewed in Chap. 16. The emphasis is on pulsed EPR methods that measure weak dipolar interactions between paramagnetic centers. Radical ion pairs in irradiated solutions were investigated by optically detected EPR and related techniques in Chap. 17. A brief history, a theoretical background, methodological details, as well as the unique experimental results obtained with these sensitive techniques are discussed. Quantum chemistry calculations and spectrum simulation tools applied to irradiated systems are presented in the last two chapters. Periodic density-functional calculations were employed for confrontation with experimental results in Chap. 18. Software for EPR and ENDOR simulations by exact and perturbation methods are presented in Chap. 19.

Applications of EPR in Radiation Research

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