



Figure 1. Identification of an oxidation product by a combination of high-field EPR spectroscopy and DFT property calculations. Left: one-electron oxidation of the parent compounds leads either to proton migration (NH-forms) or the corresponding OH-forms. On the right side, the deviation between calculated and experimental g -values is shown under assumption of the NH-forms (in red) or the OH-forms (in green). Reproduced with permission from [125]. Copyright © 2005, Wiley–VCH.