



**Figure 7.** The DPNO radical in coordination with explicit solvent molecules (one, two, and three water or methanol molecules). Two solvent molecules form H-bonds to the nitroxide oxygen atoms, while the third solvent molecule is hydrogen bonded to another solvent molecule. The COSMO model was used in the geometry optimization ( $\epsilon = 80.4$  for water and  $\epsilon = 32.63$  for methanol). Reproduced with permission from [133]. Copyright © 2006, American Chemical Society.