

Microsolvation of multifunctional nitroxide spin labels in inert gas matrices.

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Matrix isolation FTIR spectroscopy is used to investigate the microsolvation of EPR active nitroxide spin labels such as Hexamethyl imidazolidine nitroxide radical (HMI) and 2,2,6,6-Tetramethyl-1-piperidinyloxy (TEMPO) in inert gas matrices. These spin labels are stable paramagnetic organic radicals and are popular in biochemistry as highly sensitive probes of local pH and are also used as catalysts. The nitroxide radicals show rich conformational diversity and can form strong 1:1 hydrogen bonded complexes with solvent molecules such as water or methanol. The interaction energy of these hydrogen bonded complexes ranges from 6 to 8 kcal/mol. HMI has two competing sites – the ring nitrogen and the oxygen of the nitroxide radical and it is intriguing to understand the preference of solvent molecule (water) for hydration amongst these competing sites. TEMPO having only one hydrogen bonding site serves as a reference to understand more complicated HMI molecule.

