Muoniated Radical States in the Group 16 Elements: Computational Studies

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Longitudinal field repolarization and avoided level-crossing studies on positive muon implantation into sulfur led to the observation of two separate paramagnetic species in addition to a diamagnetic muon state [1,2]; while one of these can clearly be attributed to interstitial muonium, computational studies suggest that the muoniated sulfanyl radical, SMu, is a likely candidate for the other [3]. Subsequent experimental studies on positive muon implantation into selenium and tellurium have been interpreted on the basis that the primary paramagnetic species observed is likely to be XMu (X = Se or Te), the analogous muonium-substituted diatomic hydride radical for that element [4,5,6]. However, a full account of the temperature-dependent effects on spin relaxation rate, signal intensity, and hyperfine parameters remains a fascinating problem still not yet fully solved.

From a theoretical perspective these diatomic hydride species are computationally challenging despite their small size as a result of the interplay of electronic degeneracy, spin-orbit coupling, environmental effects, and vibrational and reorientational averaging. In this work computational studies are carried out on all hydrogen isotopomers of the series OH, SH, SeH and TeH. Several different methodological approaches are compared, and the effects of spin-orbit coupling and of zero-point and temperature-dependent vibrational corrections on the isotropic and anisotropic components of the hyperfine interaction examined. Additionally, other candidate species for the muoniated radical state in sulfur are considered.

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