Contribution ID: **266** Contribution code: **P-THU-20** Type: **Poster**

Structure of muoniated trimethylsilylvinyl radicals

Thursday, 1 September 2022 18:40 (20 minutes)

Muoniated vinyl radicals can be produced by Mu addition to triple bonds. Rhodes et al. observed a muoniated radical formed by Mu addition to trimethylsilylacetylene but were unable to determine the structure.¹ We have performed additional transverse field muon spin rotation measurements on trimethylsilylacetylene at 298 K and observed that two muoniated radicals were formed; a major product with muon hyperfine coupling constant (A_{μ}) of 587.3(1) MHz and a minor product with A_{μ} of 570.9(5) MHz. DFT calculations show that Mu addition is preferred to the unsaturated carbon bonded to H and that the resulting radical has a non-linear radical centre. Calculated muon hyperfine coupling constants were used to assign the observed radicals, which are the cis and trans isotopomers with respect to the trimethylsilyl substituent, respectively.

1.C.J. Rhodes et al. *J. Chem. Soc., Chem. Commun.* **1987**, 447

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Session Classification: Posters

Track Classification: Molecular chemistry and chemical physics