

Doing Chemistry with Muons

Stephen Cottrell

ISIS Facility, STFC Rutherford Appleton Lab



Science & Technology Facilities Council

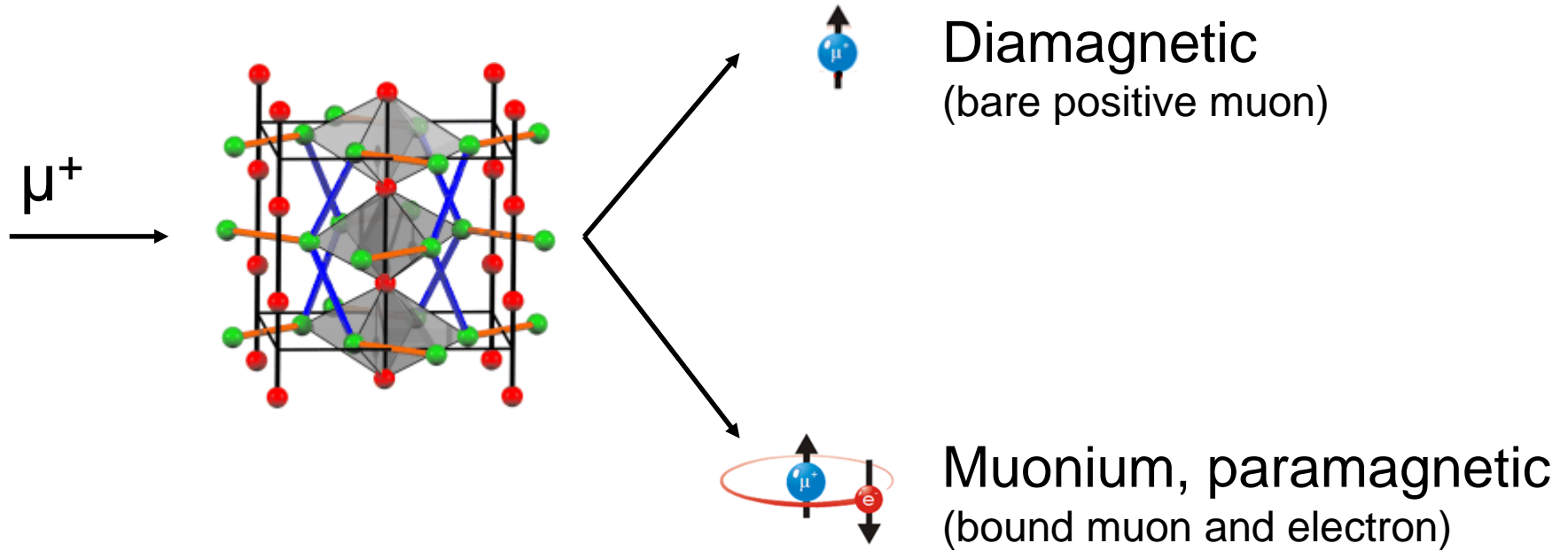
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Outline

- Muons in materials
- Why do chemistry with muons?
- What we might learn?
- Examples



Muons in materials



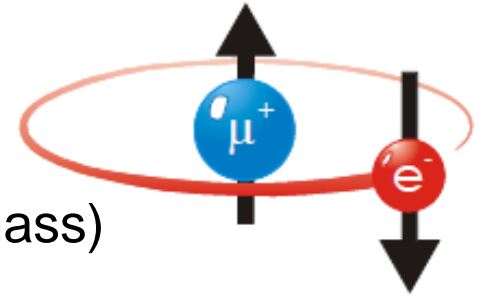
States formed by fraction of muons on implantation

States often coexist



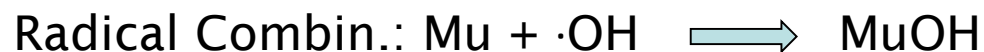
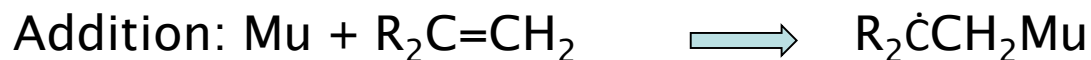
Why do chemistry with Muonium?

- Chemically equivalent to H-atom
(similar Bohr radius, ionisation energy and reduced mass)
- Greatly extends isotopic mass comparison
($m_{\text{Mu}} / m_{\text{H}} \sim 1/9$; $m_{\text{Mu}} / m_{\text{D}} \sim 1/18$)
- High sensitivity ... measurements in extreme dilution
(we're detecting the muon decay positron)



Chemically equivalent to H-atom ...

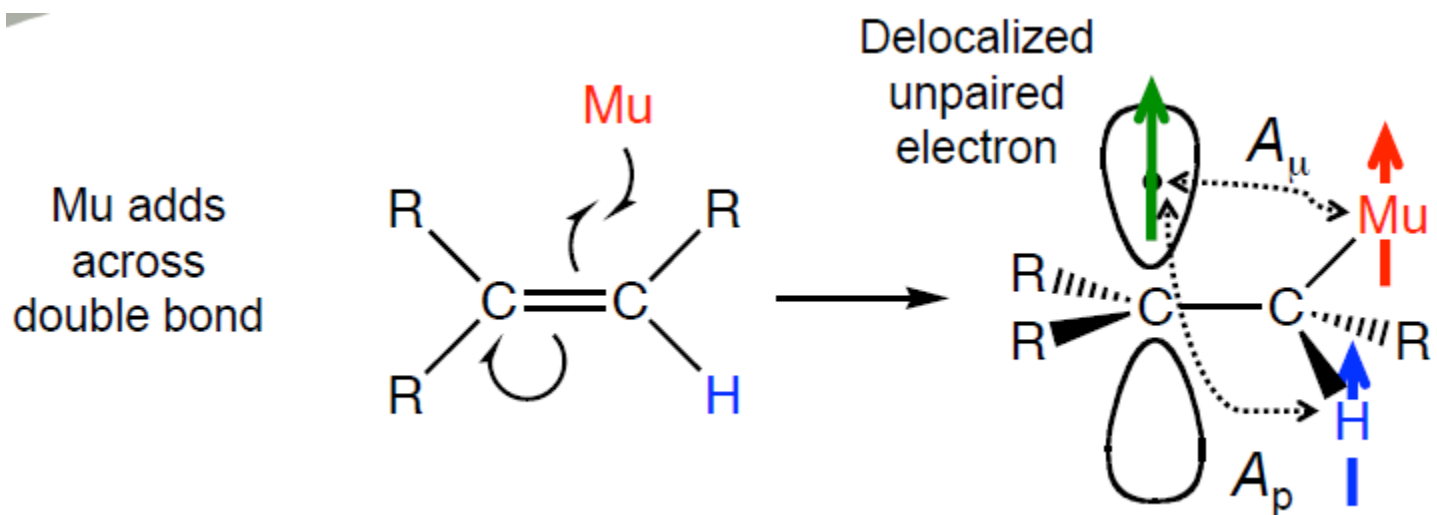
Mu will undergo the same reactions as an H-atom ...



...



Addition Reactions ...

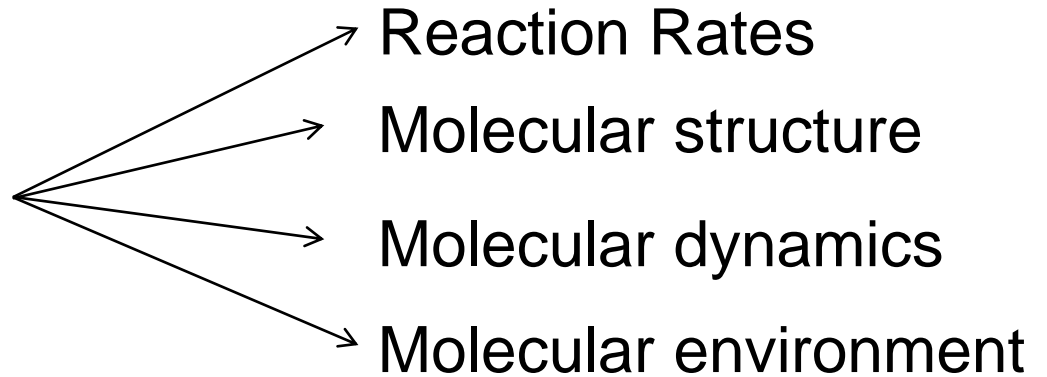


Hyperfine coupling (hfc), A_μ and A_p , makes for an **extremely sensitive probe** species



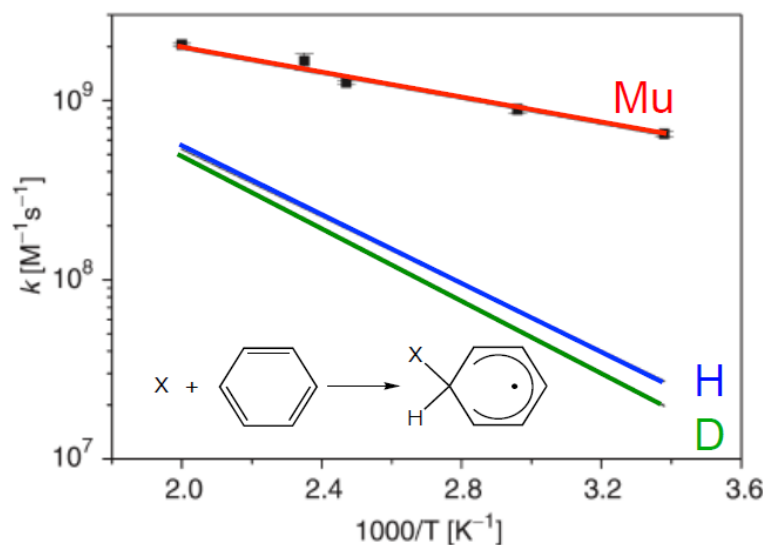
What we might learn?

Study
atoms and molecules
containing muons



Reaction Kinetics ...

Reaction rate constants, k_{Mu} , Activation energy, E_a , can be investigated ...



Example: formation of cyclohexadienyl radical

Isotope effects seen both in k_{Mu} and in E_a

(Roduner *et al.* Ber. Bunsenges.
Phys. Chem. 1990, 94, 1224)



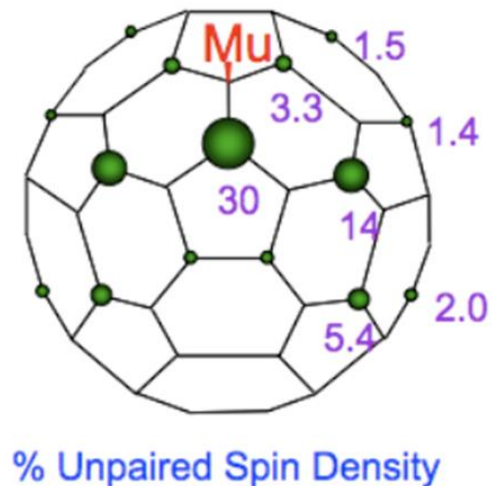
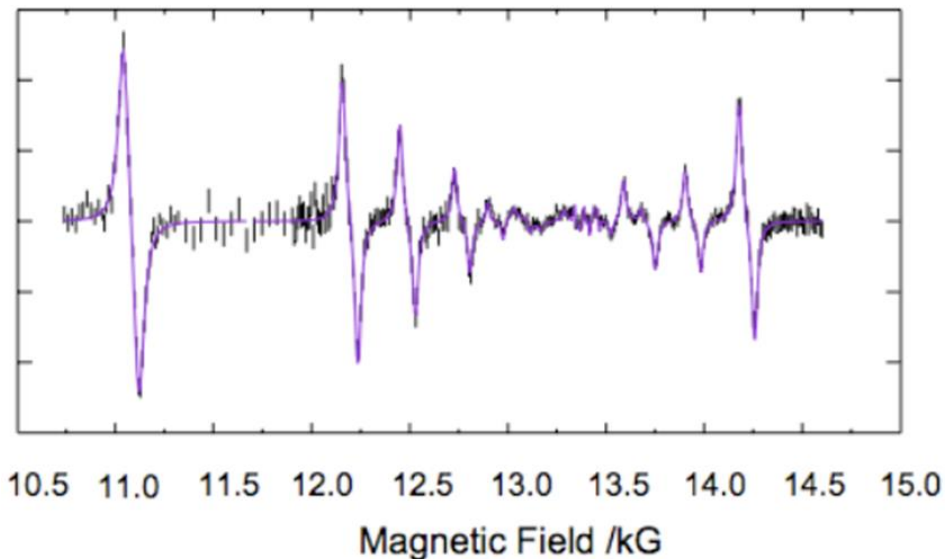
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Molecular Structure ...

Muon Avoided Level Crossing allows investigation of unpaired spin density across the C_{60} molecule ...

$Mu^{13}C_{60}$ Avoided Level Crossing Resonance

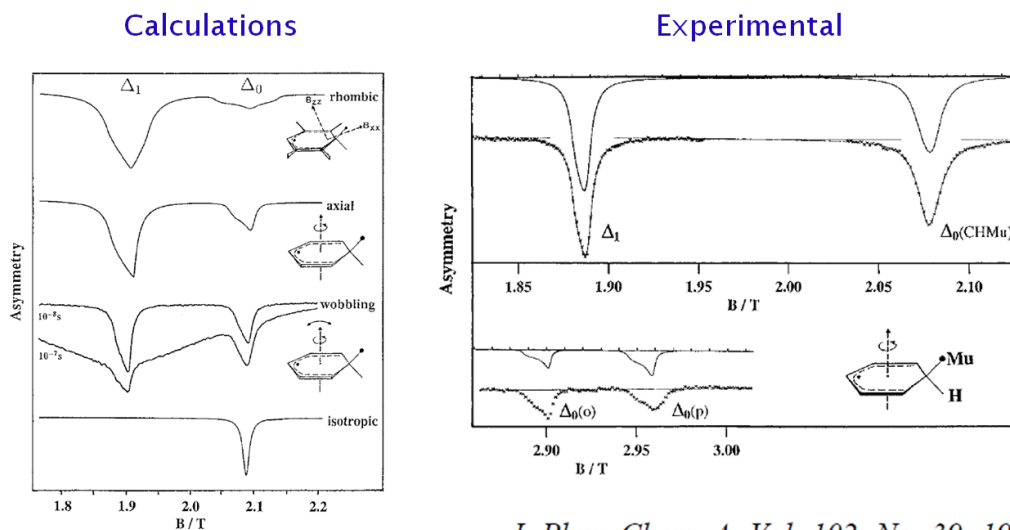


(Percival *et al.* Chem. Phys. Lett. 1995, 245, 90)



Molecular Dynamics ...

The dynamics of molecules tagged with a muon (in this case Benzene in a zeolite cage) can be investigated ...

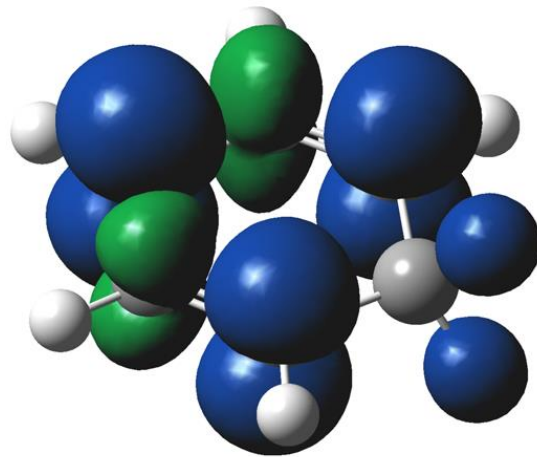


Line shape reflects mode of reorientation

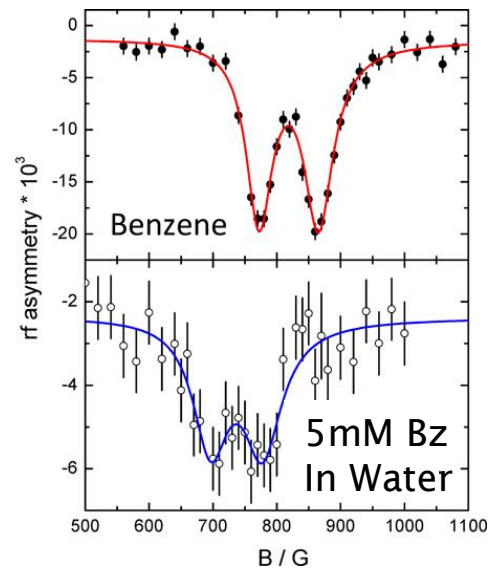


Molecular Environment ...

Solvent effects can be investigated. In this case Benzene in dilute aqueous solutions has been studied ...



Muoniated cyclohexadienyl radical



Signal shift defines shift in hyperfine parameters

(McKenziel *et al.* J. Phys. Chem. B 2013, 117, 13614)



Iain McKenzie will be talking about all this
(and a great deal more)
during his lectures on *Saturday morning*

