# The two-dimensional Heisenberg antiferromagnet $CuF_2(H_2O)_2(pyz)$ studied with muon spin rotation

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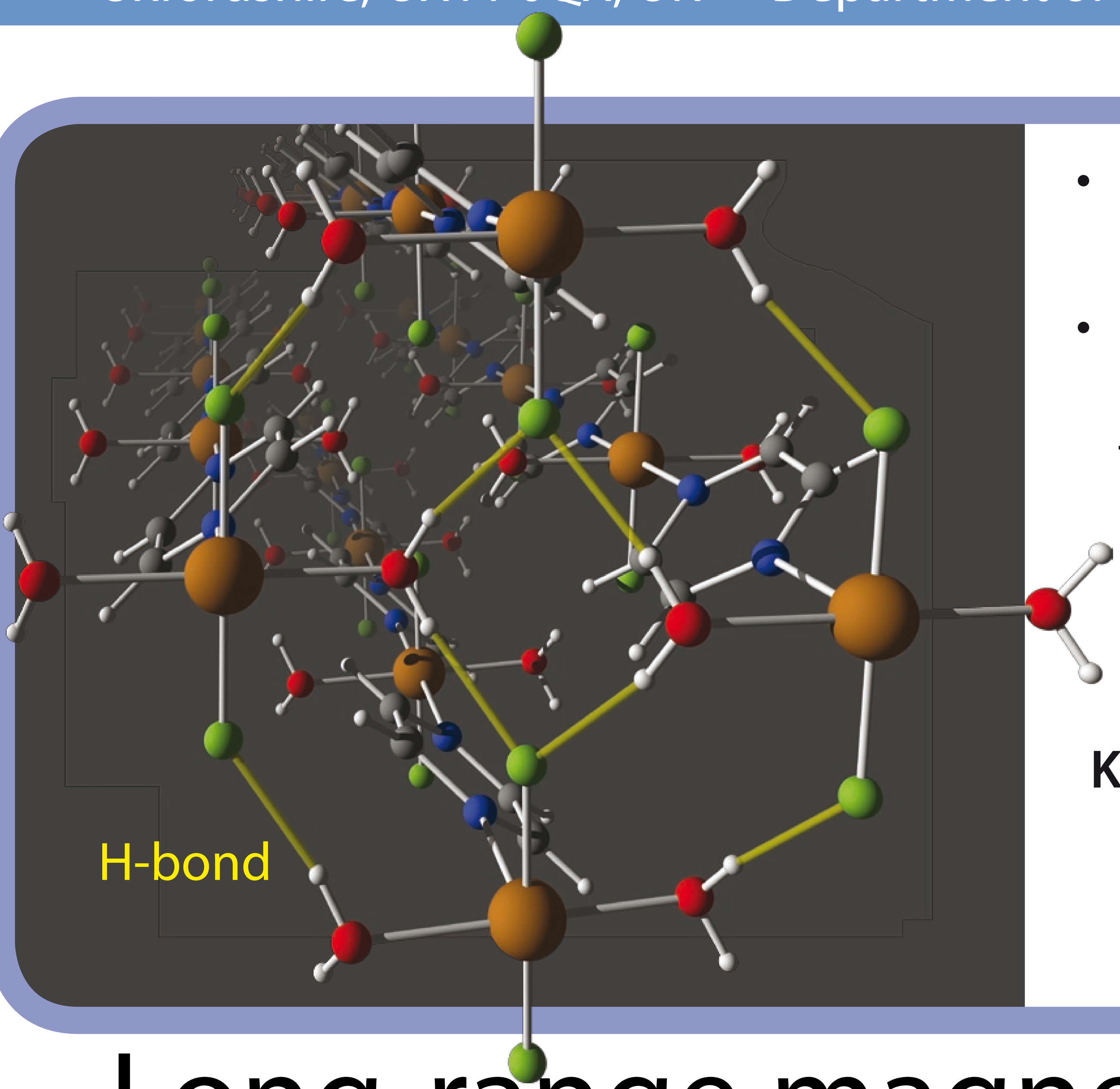
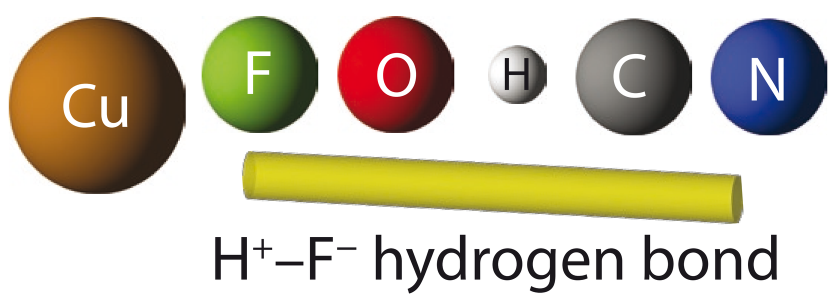
## Structure




- 1D chains of copper linked with pyrazine bridges repeat along **a** (into the poster).
- Hydrogen bonds create a 2D square lattice of copper ions whose plane is skewed 21° from normal to the **a** direction.

$$Cu^{2+}, S = ½, \mu_{Cu} \approx \mu_B$$

Key:

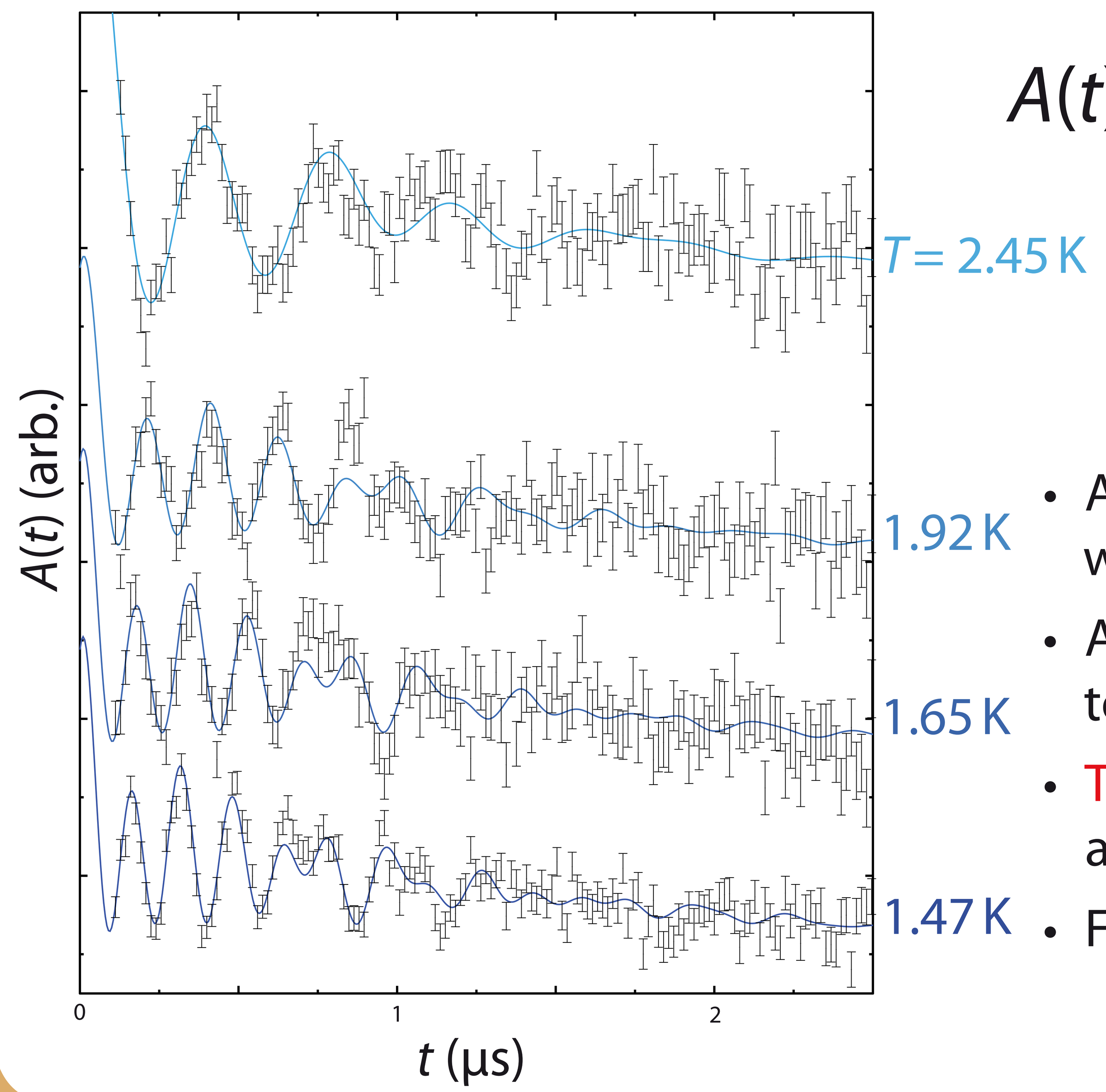



- The Cu *d*-orbitals align towards O and F, reducing coupling along the chains.
- The ratio of exchange along the chains, $J_\perp$, to that via the hydrogen bonds, $J$, derived from μSR $T_N$ measurement (see below) and high-field magnetisation.

$$|J_\perp / J| \approx 3 \times 10^{-4}$$

- Orientation of moments in the ordered state is uncertain. Coupling via hydrogen bonds is known to be antiferromagnetic, coupling along isolated pyrazine chains is also known to be antiferromagnetic.

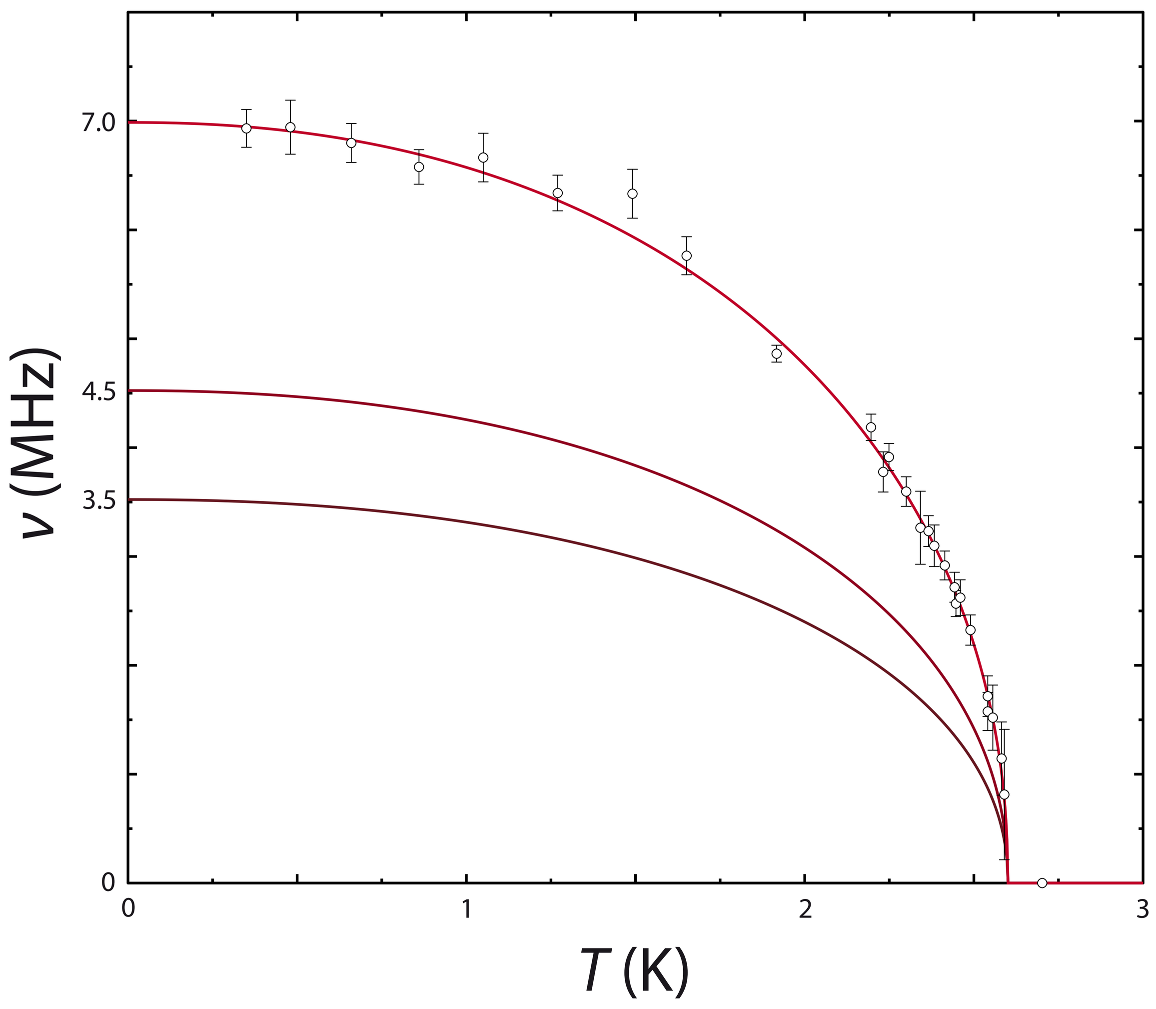
## Long-range magnetic order




$$A(t) = A_0[p_1\cos(2\pi\nu_1 t+\varphi_1)e^{-\lambda_1 t} + p_2\cos(2\pi P_2\nu_1 t+\varphi_2)e^{-\lambda_2 t} + p_3\cos(2\pi P_3\nu_1 t+\varphi_3)e^{-\lambda_3 t} + p_4 e^{-\lambda_4 t}] + A_{bg}e^{-\lambda_{bg} t}$$

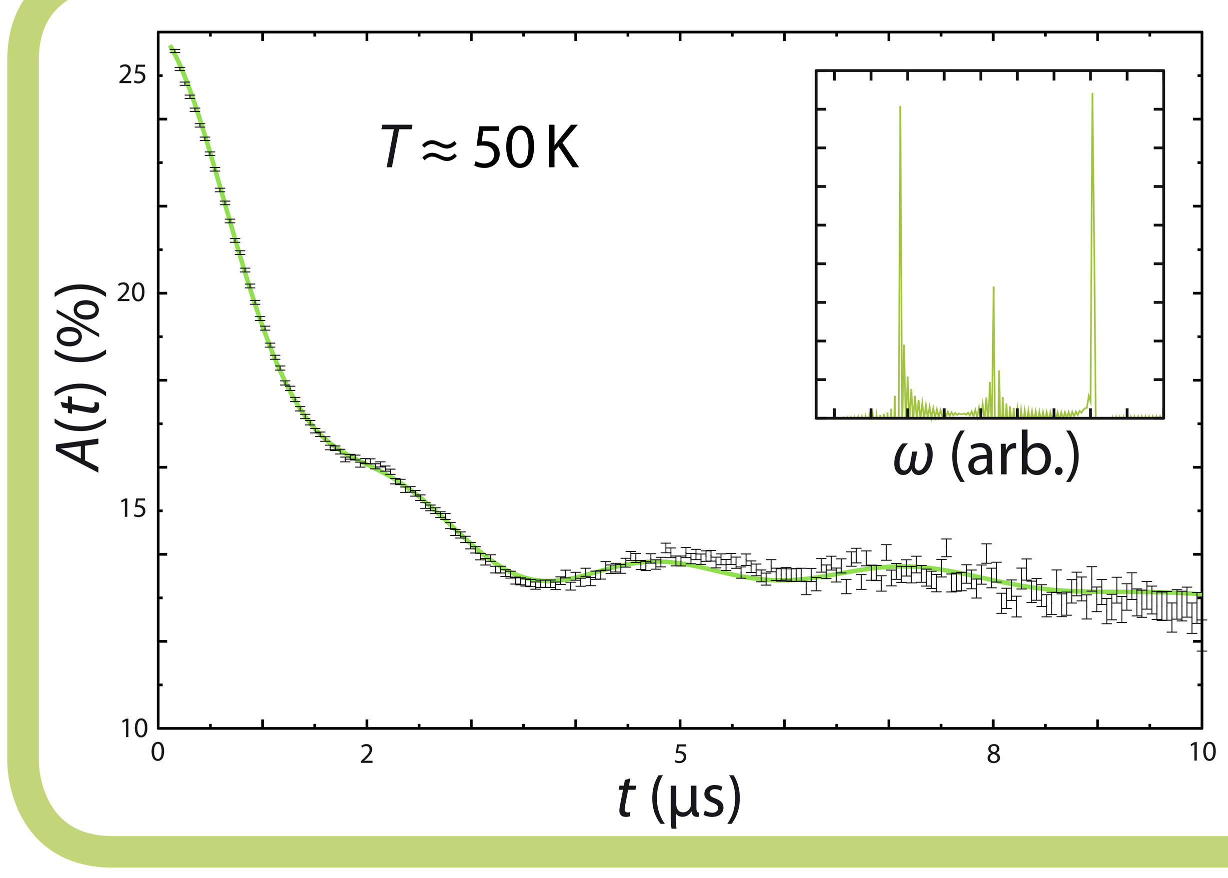
- A true 2D Heisenberg antiferromagnet would not order for $T > 0$.
- An ordered phase is observed for $T < T_N$ due to nonzero coupling along the chains.
- Three distinct frequencies are observed, along with a fast-relaxing component.
- Fit precession frequencies:

$$\nu(T) = \nu(0)\ [1 - (T/T_N)^{\alpha}]^{\beta}$$




$T_N = 2.61(3)$ K
$\alpha = 2.2(1)$; $\beta = 0.36(5)$

## μ–F dipole–dipole interactions

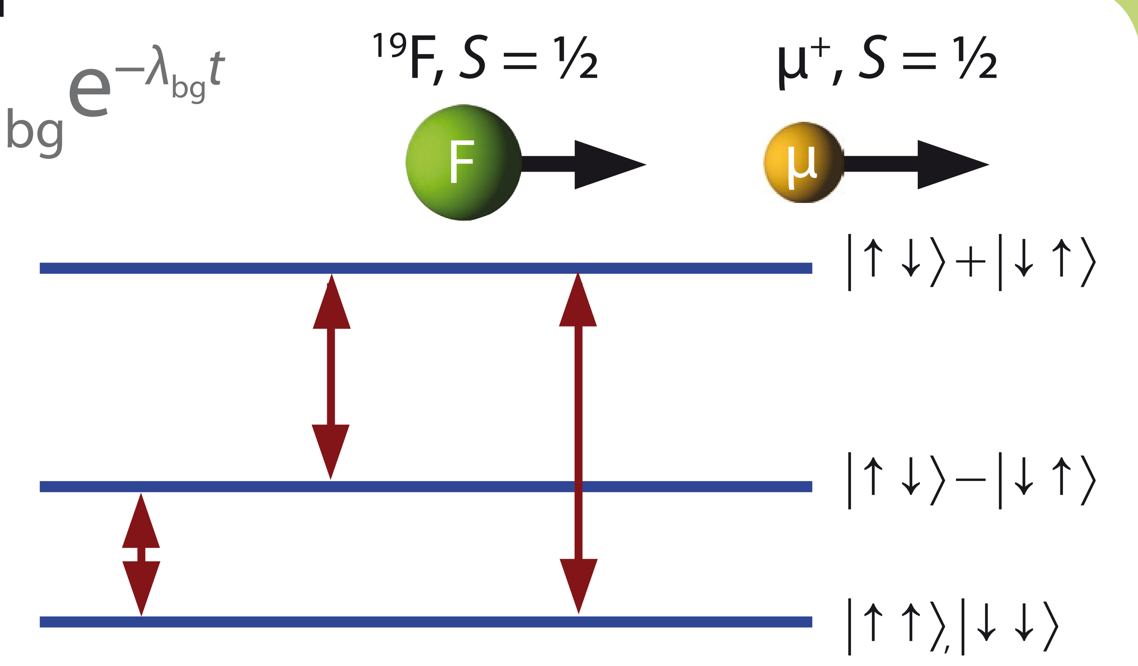



$$A(t) = A_0(p_1 D_z(t)e^{-\lambda_1 t} + p_2 e^{-\lambda_2 t}) + A_{bg}e^{-\lambda_{bg} t}$$

- For $T_N < T < 100$ K, small-amplitude, low-frequency oscillations are observed.
- Fit $D_z(t)$ to find the muon–fluorine separation and number of entangled spins.

$$r_{\mu\text{–}F} = 0.110(2)\ \text{nm}$$

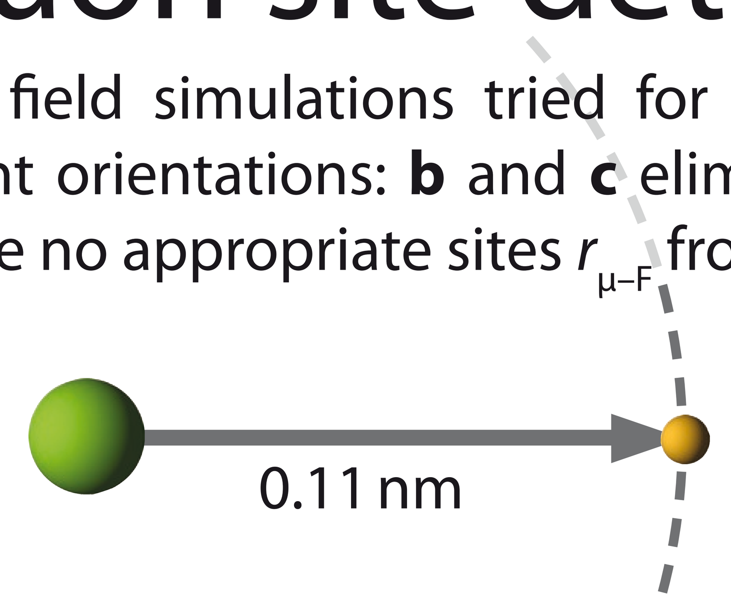
[See T. Lancaster *et al*, PRL **99**, 267601 (2007)]



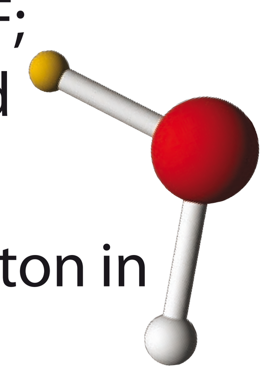

- Caused by transitions between energy levels of entangled μ–F system.

## Muon site determination

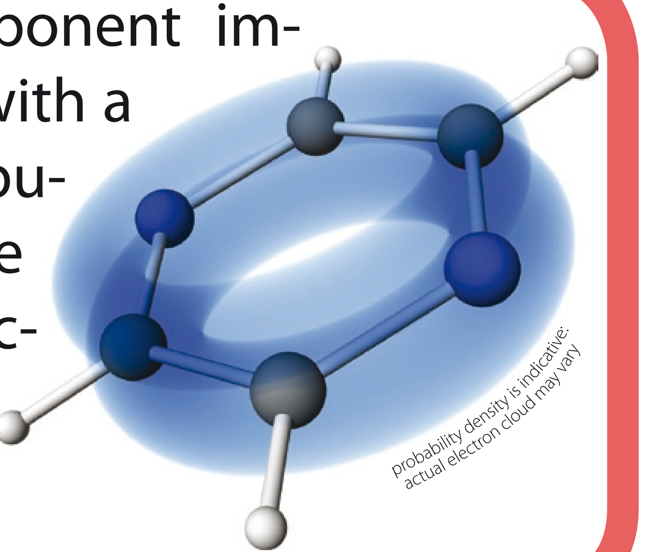
- Dipole field simulations tried for several moment orientations: **b** and **c** eliminated because no appropriate sites $r_{\mu\text{-F}}$ from an F.




- For moments pointing along **a**, both ferro- and antiferromagnetic coupling along chains give several sites near F; plausible fields are also found near O and pyrazine.
- Muons often substitute for a proton in water, turning $H_2O$ into HμO.



- Fast-relaxing component implies a muon site with a large field distribution: possibly in the delocalised electrons near the pyrazine.



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