**EPR Investigation of the ErSc$_2$N@C$_{80}$ Fullerene**


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**Introduction**

Atoms, ions and even small clusters encapsulated inside a carbon cage can exhibit a highly isolated behaviour within a solid state environment which could be exploited for quantum information processing. Fullerenes doped with luminescent ions, such as Er$^{3+}$, have potential for optical readout if they are also electron-spin active. In this study, we present electron paramagnetic resonance (EPR) results of the ErSc$_2$N@C$_{80}$ molecule, composed of a triangular ErSc$_2$N unit held within a C$_{80}$ cage and known to emit at around 1.5 microns.

**Experimental**

The high frequency homodyne EPR spectrometer (multifrequency up to 600 GHz) and superconducting 15 T magnet was used to run experiments at a number of different frequencies (105 GHz, 209 GHz, 302 GHz and 419 GHz). Optical illumination was provided to the sample in the cryostat prior to EPR measurements by shining a torch down the microwave waveguide.

**Results and Discussion**

In X-band, at low temperature, the EPR spectrum of ErSc$_2$N@C$_{80}$ in toluene is composed of the superposition of the powder spectrum of two different types of Er$^{3+}$, corresponding to two different orientations of the ErSc$_2$N cluster inside the C$_{80}$ cage. Each configuration can be simulated with the EasySpin software [1] assuming a pseudo-spin $S = 1/2$. Each EPR spectrum is characterized by a strong anisotropy of the g matrix (Er$^{3+}$(1): $g_{\text{par}} = 13.1$, $g_{\text{perp}} = 3.0$ and Er$^{3+}$(2): $g_{\text{par}} = 11.3$, $g_{\text{perp}} = 5.6$) and of the hyperfine tensor (Er$^{3+}$(1): $A_{\text{par}} = 1400$ MHz, $A_{\text{perp}} = 280$ MHz and Er$^{3+}$(2): $A_{\text{par}} = 1600$ MHz, $A_{\text{perp}} = 150$ MHz). At 5 K, the two configurations are present in similar proportions (57:43). Illuminating the fullerene with a visible light beam (532 nm) induces a switch of the molecular cluster inside the cage from one configuration to the other. The final proportion is: 30:70. The change in configuration can persist for a very long time (over 20 hours at 5 K) [2].

**Conclusions**

By using high frequency EPR (105 GHz, 209 GHz, 302 GHz and 419 GHz), it was possible to verify the X-band g-factor analysis for one configuration, revealing an extremely small g-strain of the gpar component, thus proving its unique and well defined structure. The possibility to interconvert between both configurations with visible light was also confirmed.

**References**