SPIN-IN-A-BOTTLE: ENCAPSULATION STRATEGIES FOR CONTROLLING DECOHERENCE IN CHROMIUM COMPLEXES

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In recent years, many EPR spectroscopists have become interested in quantum information processing. Electron spins indeed can technically serve as elementary units of quantum computation, and when these spins are localized in molecules, the resulting systems are often referred to as *molecular qubits*. Despite the considerable hype in this field, where almost any paramagnetic compound with transverse spin relaxation times long enough to allow pulsed EPR detection is sometimes labeled a molecular qubit, and despite the relatively low probability that such molecules will ultimately be used in practical quantum computing architectures, it must be acknowledged that the interface between chemistry and physics in this area has revealed several phenomena that are unique to molecular systems. In particular, although their use as computational qubits may remain speculative, molecular spins have already demonstrated promising performance as quantum sensors at the laboratory level.

As in other qubit platforms, however, the fragile nature of quantum states presents a major challenge. For molecular qubits, maintaining spin coherence remains difficult because spin superpositions are highly sensitive to magnetic noise and lattice vibrations. Traditional approaches to suppress decoherence rely on strong magnetic dilution in diamagnetic solvents, which minimizes dipolar interactions and nuclear spin noise. While this strategy can produce long coherence times, it lacks orientational control and complicates integration into solid-state devices.

Embedding qubits in diamagnetically diluted crystalline matrices offers orientational control and improved prospects for device integration, but introduces decoherence driven by lattice vibrations. Although primarily associated with spin-lattice relaxation (T_1), these processes can also accelerate phase decoherence (T_m) through spectral diffusion.

Here we demonstrate several approaches in which supramolecular encapsulation [1] of a paramagnetic chromium ion can either effectively shield the qubit from host lattice dynamics [2] or generate a clock transition through delocalization of the unpaired electron onto the ligand framework, leading to a significant increase in the spin coherence times. Our results highlight the potential of supramolecular encapsulation as a general strategy for protecting molecular spin qubits and for advancing their implementation in hybrid quantum devices [3].

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[1] Swain *et al.*, Multifunctional Guest-Hosting Triple-Stranded Helicates: From Anion Recognition to Quantum Information Applications, *Acc. Chem. Res.*, **2026**, 10.1021/acs.accounts.6c00020

[2] Swain *et al.*, *Angew. Chem. Int. Ed*., **2025**, 64, e202510603

[3] Palacios *et al.*, Self-Cooling Molecular Spin Qudits, *Adv. Materials*, **2025**, e11061