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PROBING METHYL GROUP TUNNELING IN $[(CH_3)_2NH_2][Zn(HCOO)_3]$ HYBRID PEROVSKITE USING Co^{2+} EPR

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At high temperature, methyl group exhibits classical reorientation dynamics around its symmetry axis, while at lower temperatures, it acts as a quantum rotor exhibiting rotational quantum tunneling, which is highly sensitive to a local methyl group environment (Fig. 1a). Recently, we observed this effect using pulsed electron paramagnetic resonance (EPR) in two dimethylammonium containing hybrid perovskites doped with paramagnetic Mn^{2+} ions [1].

In this work, we investigate the feasibility of using a fast-relaxing Co^{2+} paramagnetic center to study the methyl group tunneling in dimethylammonium zinc formate $[(CH_3)_2NH_2][Zn(HCOO)_3]$ (Fig. 1b) hybrid perovskite using a multifrequency EPR experiments. Our pulsed EPR experiments reveal magnetic field independent electron spin echo envelope modulation (ESEEM) signals, which are assigned to the methyl group tunneling. The extracted tunnel frequency of 1.84 MHz from the experimental data is used in density operator simulations, which allows us to calculate the rotational barrier of the methyl groups. The comparison of these results [2] with the previously reported Mn^{2+} [1] case shows that our approach can detect very small changes in the local methyl group environment opening pathway for a new spectroscopic tool.

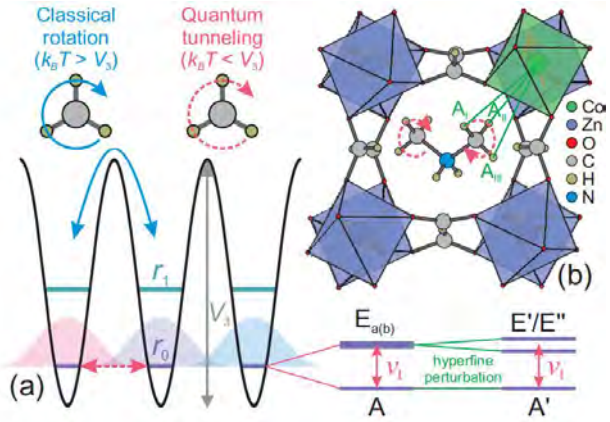

Fig. 1. (a) Schematic energy level diagram of a methyl group rotor with rotational barrier V_3. At lower temperatures, the group acts as a hindered quantum rotor enabled by the wave-function overlap, which also splits the ro-librational levels by the tunnel splitting ν_t. (b) Low-temperature structure of DMAZn:Co. The hyperfine interactions between the paramagnetic Co^{2+} ion and protons of the nearest methyl group are indicated by green lines.

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[1] M. Šimėnas, et al., Magnetic excitation and readout of methyl group tunnel coherence. *Sci. Adv.* 2020, **6**, eaba1517.
[2] G. Usevičius, et al. Probing Methyl Group Tunneling in $[(CH_3)_2NH_2][Zn(HCOO)_3]$ Hybrid Perovskite Using Co^{2+} EPR. *Molecules* 2023 **28**, 979.