Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information:

Electron paramagnetic resonance study of ferroelectric phase transition and dynamic effects in Mn^{2+} doped $[NH_4][Zn(HCOO)_3]$ hybrid formate framework

Marius Navickas, Laisvydas Giriūnas, Vidmantas Kalendra, Timur Biktagirov, Uwe Gerstmann, Wolf Gero Schmidt, Mirosław Mączka, Andreas Pöppl, Jūras Banys and Mantas Šimėnas*

*e-mail: mantas.simenas@ff.vu.lt

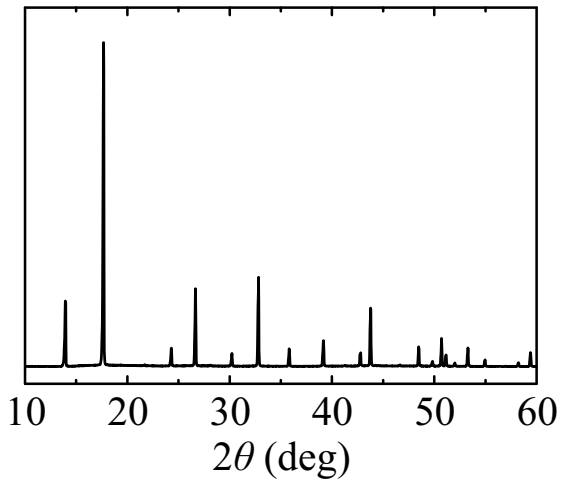

Figure S1: Room temperature powder XRD pattern of the investigated compound. Measurement performed using CuKα1 radiation.

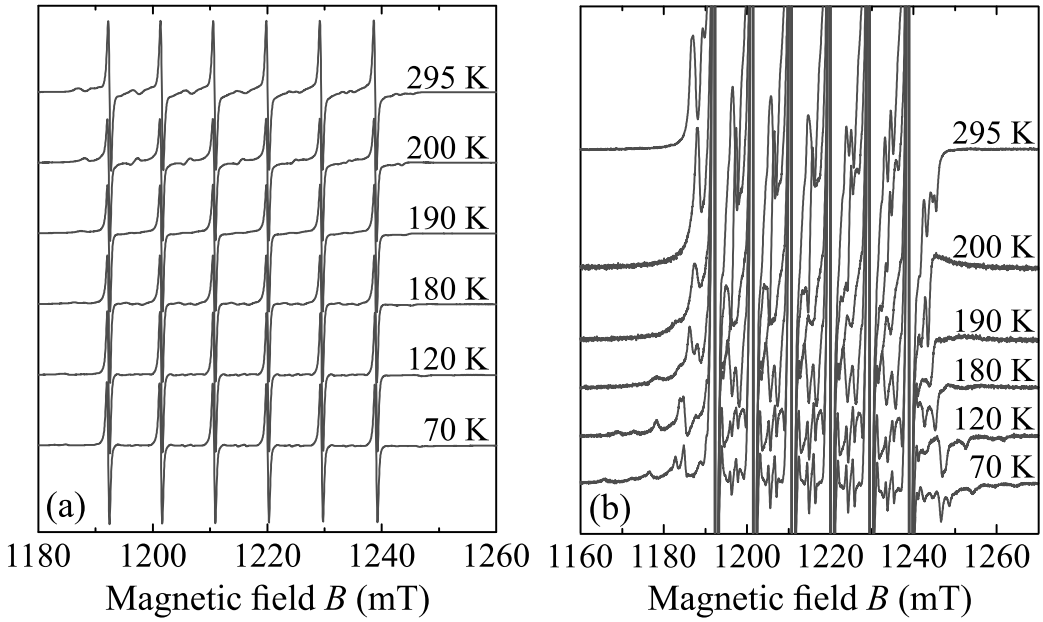

Figure S2: (a) Central and (b) outer fine structure transitions of the temperature dependent Q-band CW EPR spectra of AmZn:Mn^{2+}.

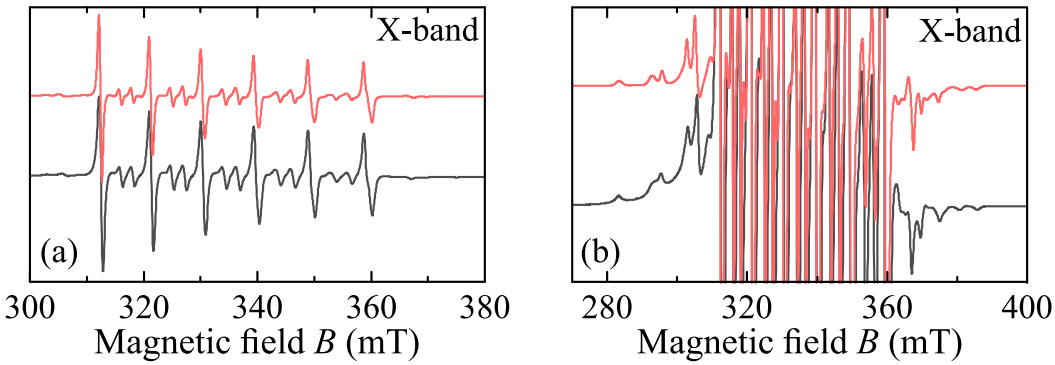

Figure S3: Simulation of the X-band CW EPR spectra of AmZn:Mn^{2+} recorded at 26 K. Experimental and simulated spectra are shown in black and red, respectively. The emphasis is on the (a) central and (b) outer fine structure transitions. Fine structure parameters used for simulation: $D = -193(2)$, $E = 25(1)$, $a = 32(1)$, $F = -30(1)$, $B_4^{-1} = 2.5(1)$, $B_4^{-2} = 1.0(5)$ and $B_4^{-3} = 0.5(5)$ MHz.

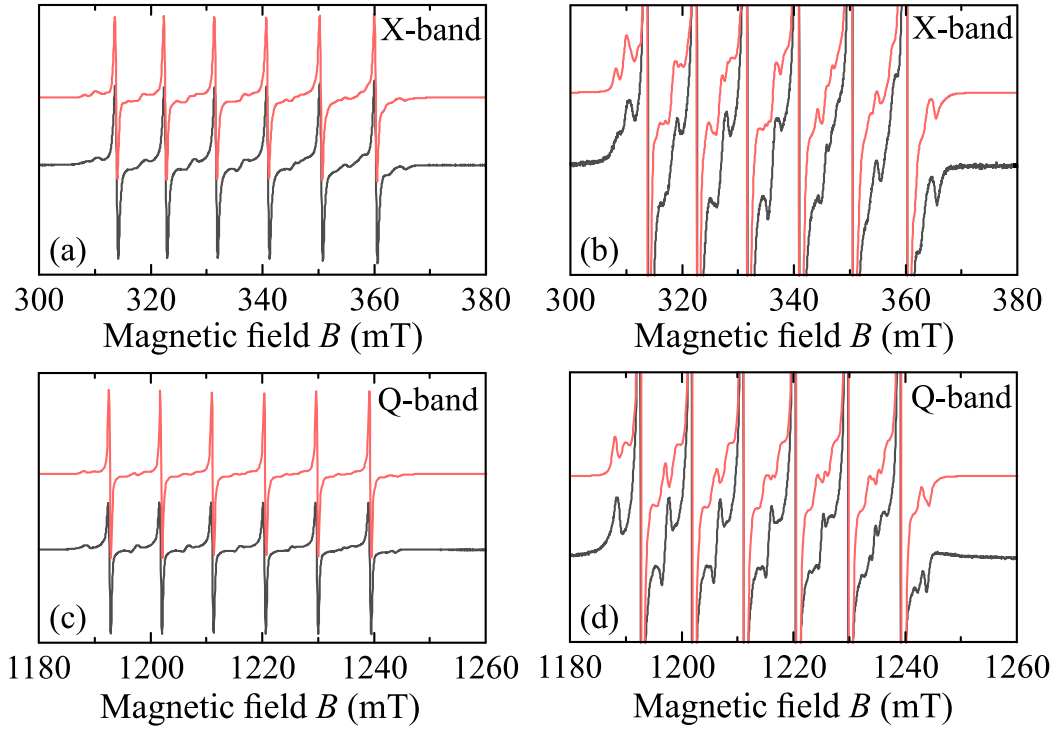

Figure S4: Simulation of the X- and Q-band CW EPR spectra of AmZn:Mn^{2+} recorded at 199 K. Experimental and simulated spectra are shown in black and red, respectively. The emphasis is on the (a, c) central and (b, d) outer transitions. Fine structure parameters used for simulation: $D = -20(5)$, $E = 2(1)$, $a = 45(1)$, $F = -40(1)$, $B_2^1 = 5(2)$, $B_2^{-1} = 2(1)$ and $B_2^{-2} = 19(2)$ MHz.

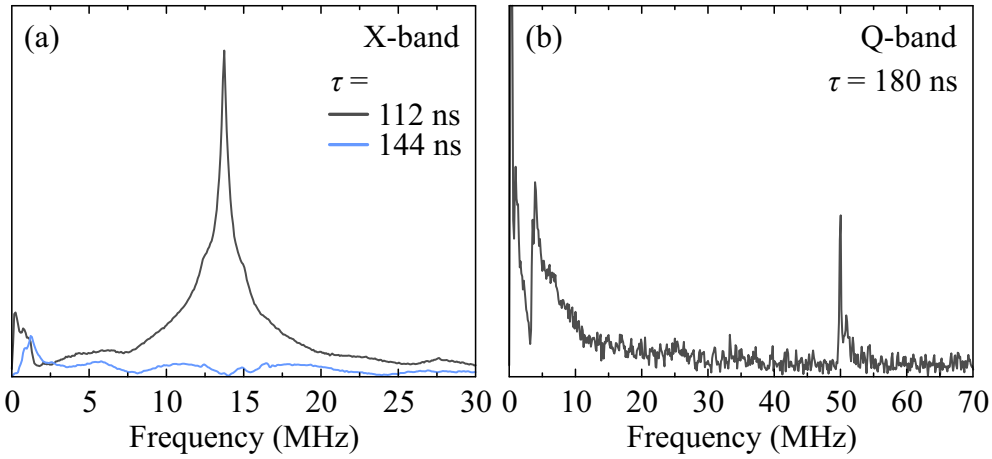

Figure S5: (a) X- and (b) Q-band 3p ESEEM of AmZn:Mn^{2+} recorded at 325.6 (τ = 112 and 144 ns) and 1193.3 mT (τ = 180), respectively. Measurements performed at 15 K.