SUPPORTING INFORMATION

Interactions between H-bonded [$Cu^{II}_3(\mu_3\text{-}OH)$]triangles; A combined magnetic susceptibilty and EPR study.

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Details for the simulation of the solide powder EPR spectra

In order to account for broadening effects we assume one nuclear spin per trimer with $I_a = I_b = 3/2$ with a hyperfine interaction $A_{||,i}$ = 280 MHz. It was found that better agreement between theory and experiment can be achieved by allowing for a slight rotation of the $\mathbf{g_a}$ and $\mathbf{g_b}$ along the $\mathbf{r_{ab}}$ vector to an angle ξ = 0.5° and introducing an ordering of the molecules according to the orientation distribution [see reference 26] P(θ) = exp(-U(θ)) with U(θ) = -λ(3 cos2θ - 1)/2), where θ is the angle between the molecular z axis and the static magnetic field. The ordering parameter was fixed to λ = -10 (http://www.easyspin.org/). The simulation of the parallel mode X-band spectrum does not account for several resonances in the 250 - 500 mT range which are remnants from the allowed $\Delta M_S = \pm 1$ transitions. The little difference of the obtained parameters at the two frequencies are attributed to instrumental conditions

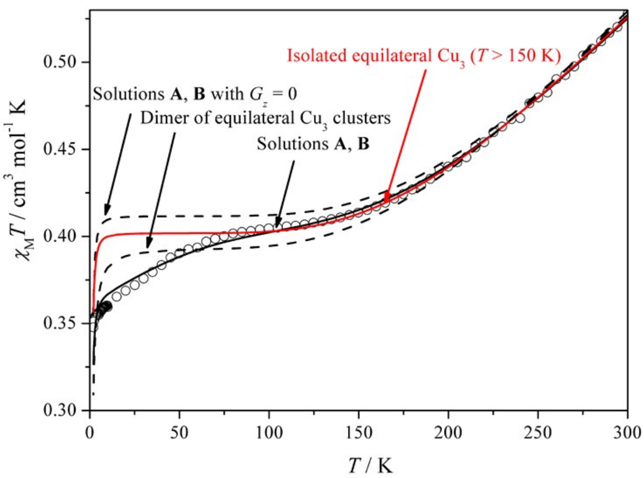

Figure S1. $\chi_M T$ *vs* T experimental data and calculated curves for **1** according to the models described in the text. The solid black line represents fit according to solution **B**. In the dimer of equilateral Cu_3 cluster model $\chi_M T$ is considered per trimeric unit.

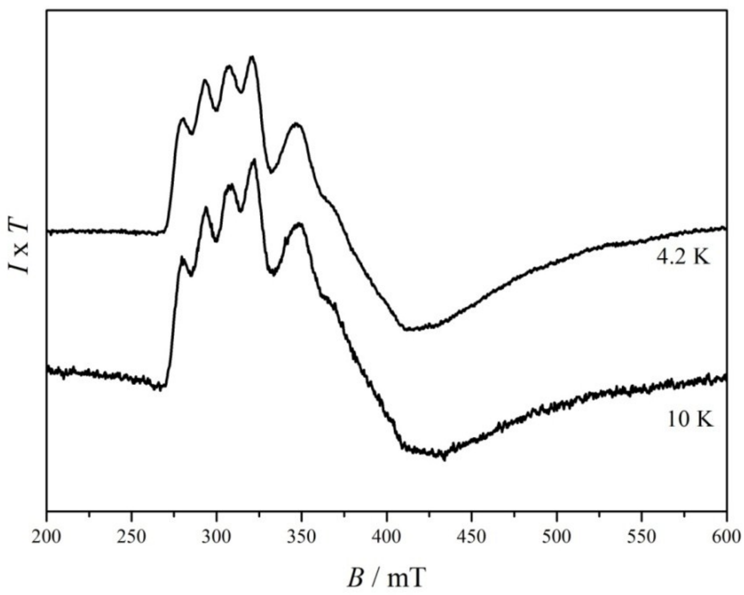

Figure S2. X-band EPR spectra of a frozen solution in THF of **1** at 4.2 and 10 K. The signals, scaled as *I* x *T*, are super-imposable indicating that they arise from a ground state. EPR conditions: microwave frequency, 9.41 GHz; microwave power, 0.7 μW; modulation amplitude,10 G_{pp}.

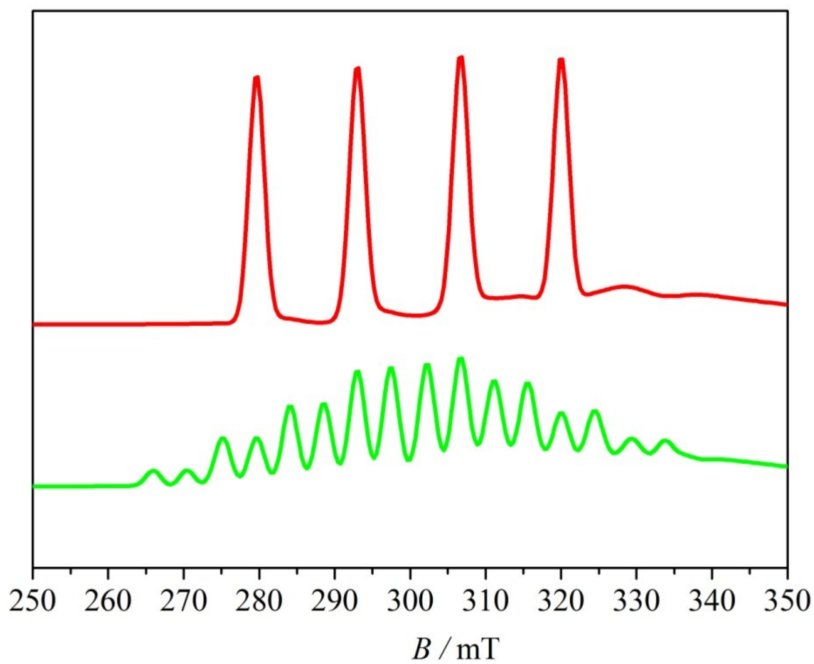

Figure S3. Hyperfine patterns from an axial S=1/2 system in the $g_{||}$ (>$g_{\perp}$) region with three I=3/2 nuclei according to model I (**A_1** = -**a**/3, **A_2** = **A_3** = +2**a**/3 ; green line) and model II (**A_1**= **a**, **A_2** = **A_3** =0; red line). $g_{||}$ = 2.25; $a_{||}$ = 425 MHz. For the simulations an intrinsic line-width of σ_L = 0.8 mT was assumed.

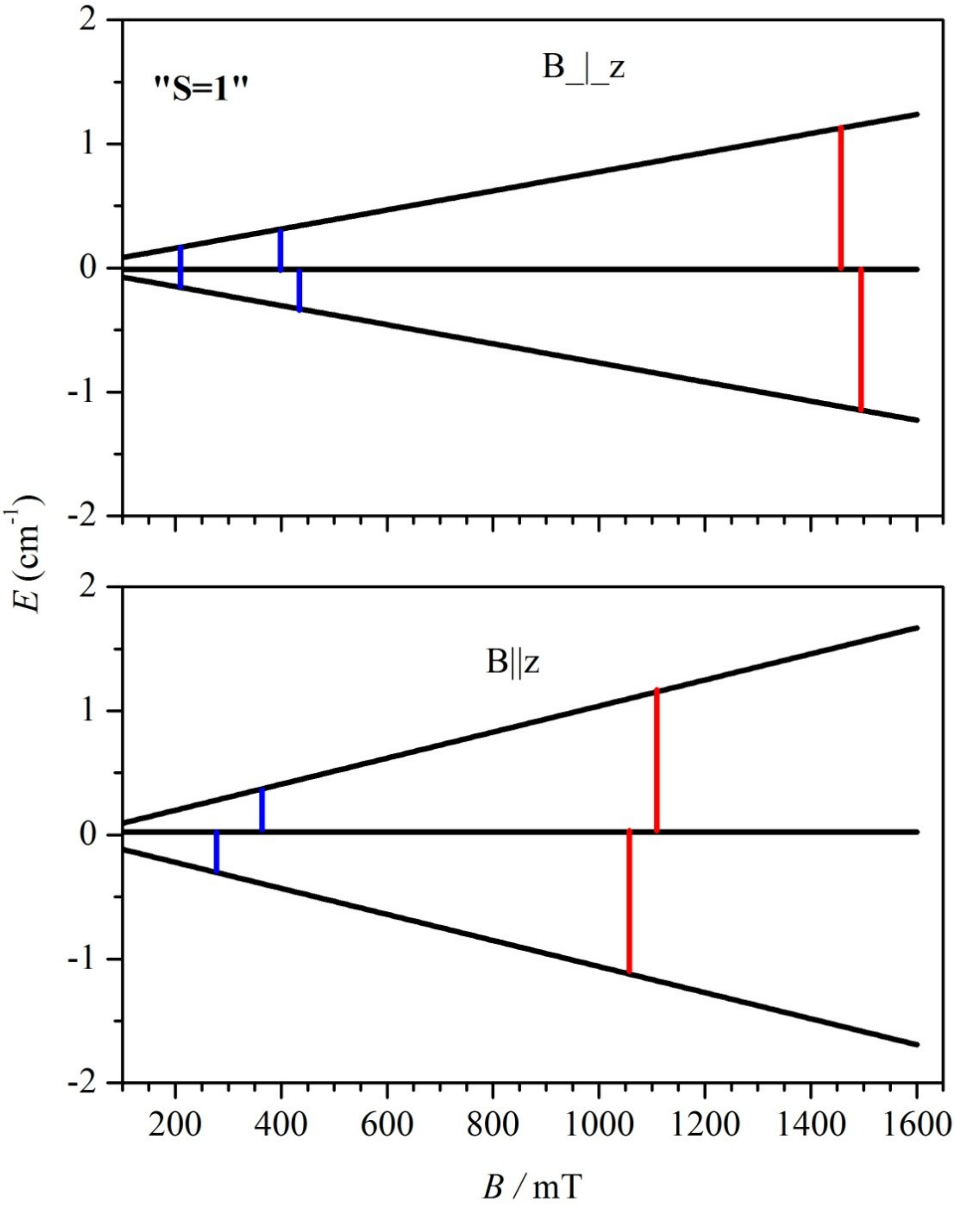

Figure S4. Dependence of the energy levels on the magnetic field for an effective S = 1 system characterized by the spin Hamiltonian H_{zfs} = DS_z^2 +β**BgS** for two orientations of the magnetic field relative to the z-axis of the ***D***-tensor. D=-0.033 cm^{-1}, ***g*** = [1.65, 1.65, 2.25]. The blue and red vertical bars indicate the EPR transitions at X- and Q-band respectively.

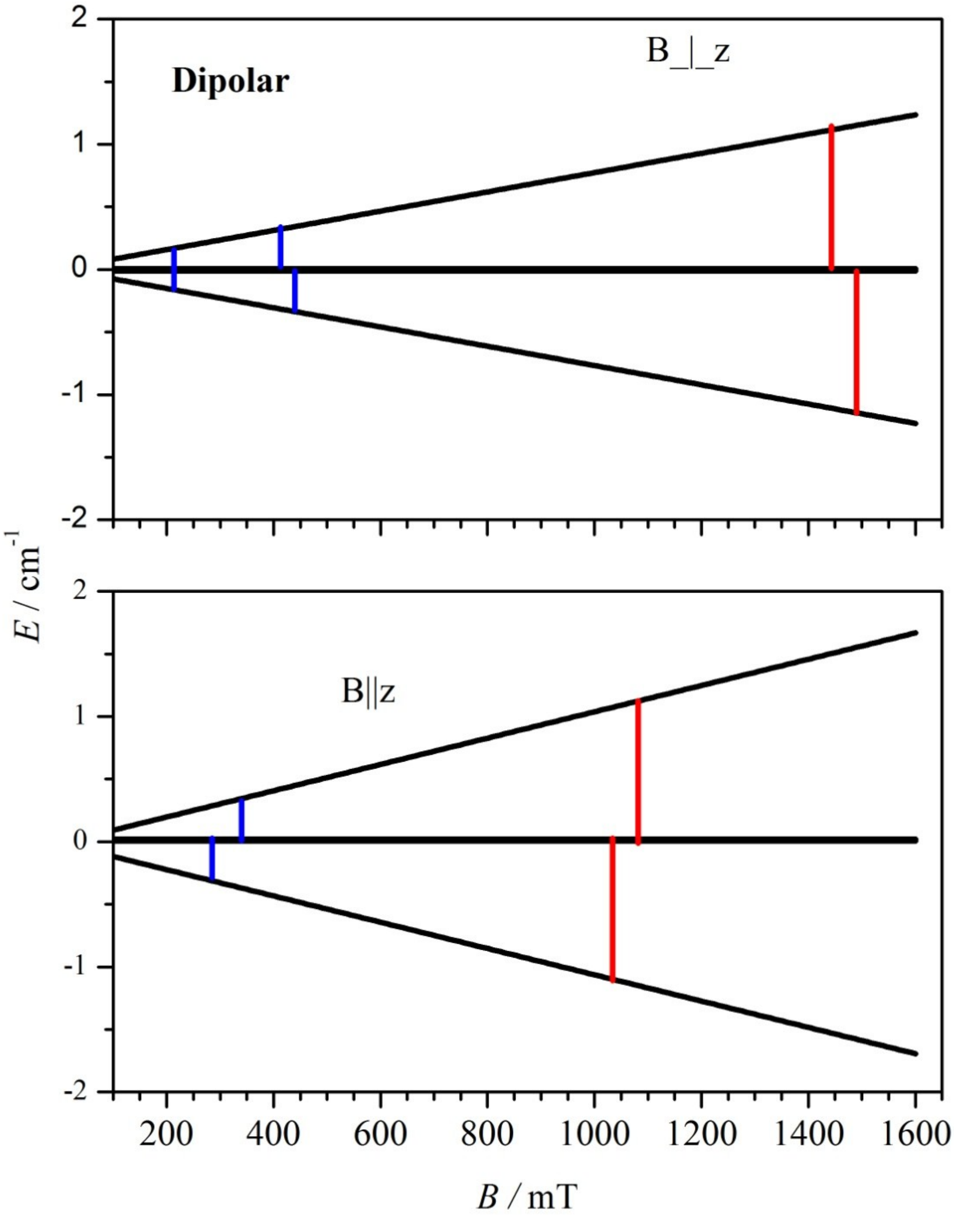

Figure S5. Dependence of the energy levels on the magnetic field for two spins with S_a = S_b = 1/2 in the point dipolar approximation. $\boldsymbol{g_{a,b}}$ = [1.65, 1.65, 2.25], r_{ab} = 4.4 Å. The two **g**-tensors are assumed co-linear. The blue and red vertical bars indicate the EPR transitions at X- and Q-band respectively.