

## Supporting information

### “Structural and magnetic characterization of a 1D chain of [Co(II)<sub>2</sub>(μ-aqua)(μ-carboxylate)<sub>2</sub>] strung cores”

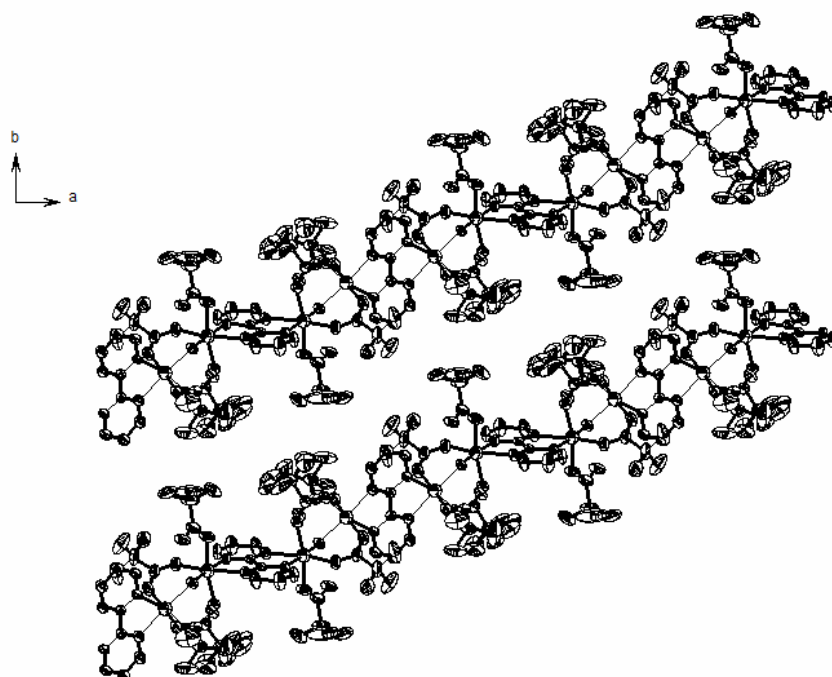
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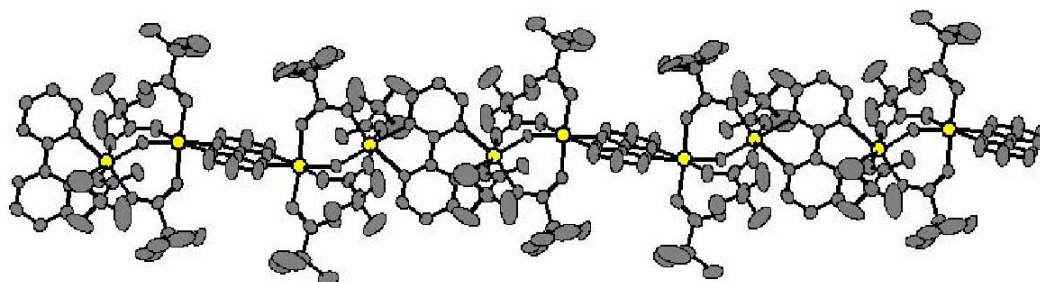
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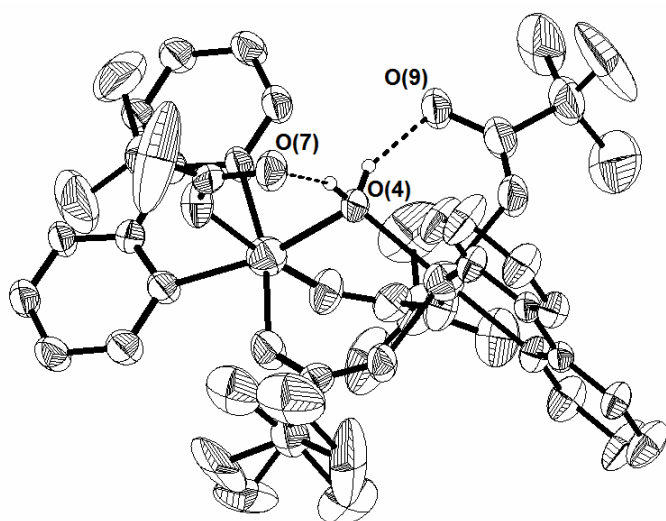
*E-mail: albores@uni-mainz.de; rentschl@uni-mainz.de*



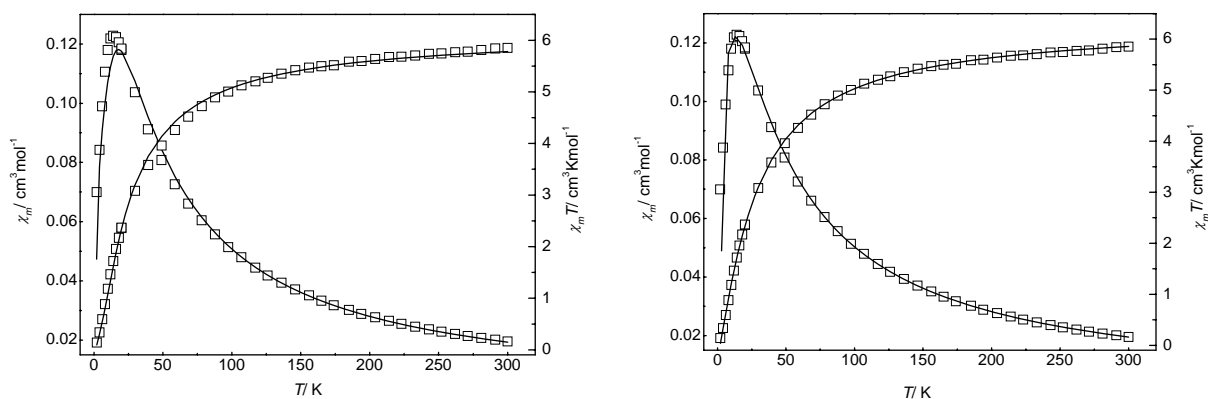
**Figure S1.** Chains packing view along *c* axis direction. Hydrogen atoms omitted for clarity.



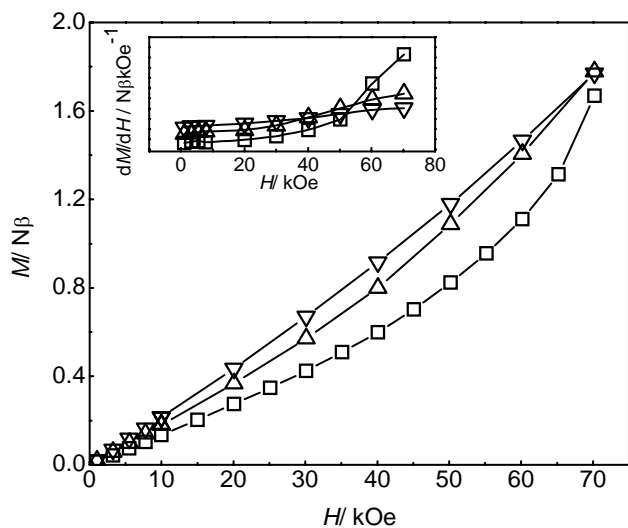
**Figure S2.** Perspective of the zigzag arrangement of Co(II) sites along the chain.



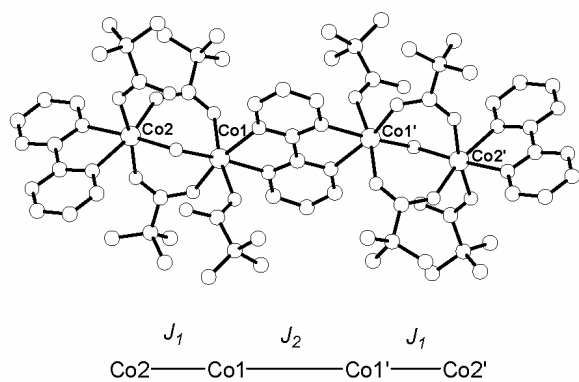
**Figure S3.** ORTEP (50% ellipsoid probability) representation of the dinuclear [Co<sub>2</sub>(μ-OH<sub>2</sub>)(μ-O<sub>2</sub>CC(CH<sub>3</sub>)<sub>3</sub>)<sub>2</sub>] unit of the chain showing the H-bond interaction of the non-bridging carboxylate with the bridging aqua ligand.



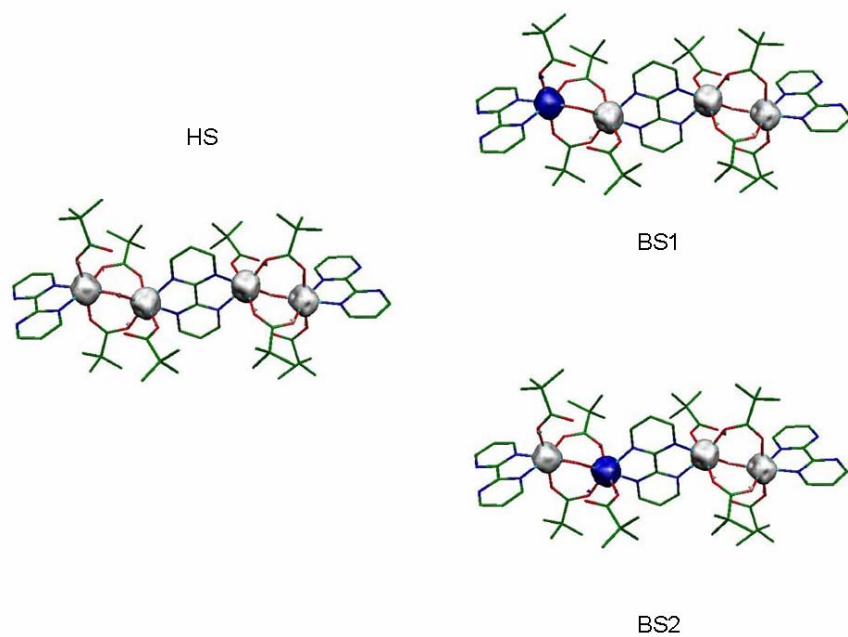
**Figure S4.**  $\chi_m T$  vs  $T$  and  $\chi_m$  vs  $T$  plots in the 2-300K range. Empty squares: experimental data. Full line: best fitting curves with model b); left panel and model d); right panel.



**Figure S5.**  $M$  vs  $H$  plot at three different temperatures: ( $\nabla$ ) 10K, ( $\Delta$ ), 6K and ( $\square$ ) 1.8K. Inset: field derivative of the magnetization. Lines are only for eye guideline.



**Figure S6.** Co<sub>4</sub> tetranuclear model, extracted from the X-ray structure geometry, employed in the DFT calculations. The considered magnetic exchange interactions are additionally shown.



**Figure S7.** Spin density surfaces (0.03 a.u. isogrid values) of the three possible spin topologies calculated. White and blue colours represent positive and negative regions.