

# Supplementary materials

## Strong antiferromagnetic interactions in the binuclear cobalt(II) complex with a bridged nitroxide diradical

Vitaly A. Morozov<sup>1</sup>, Eugenia V. Peresypkina<sup>2</sup>, Wolfgang Wernsdorfer<sup>3</sup> and Kira E. Vostrikova<sup>4,\*</sup>

<sup>1</sup> International Tomography Center SB RAS, Institutskaya Str. 3a, 630090 Novosibirsk, Russia;

<sup>2</sup> Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße 7, 60438 Frankfurt am Main, Germany;

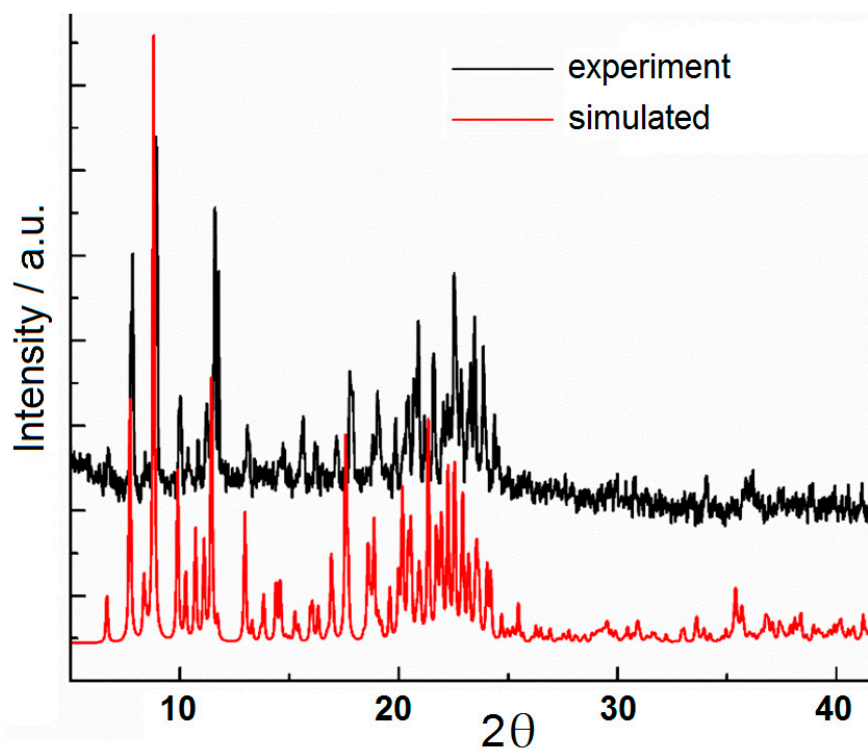
<sup>3</sup> Physikalisches Institut, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany;

<sup>4</sup> Nikolaev Institute of Inorganic Chemistry SB RAS, 3 Lavrentiev Avenue, 630090 Novosibirsk, Russia;

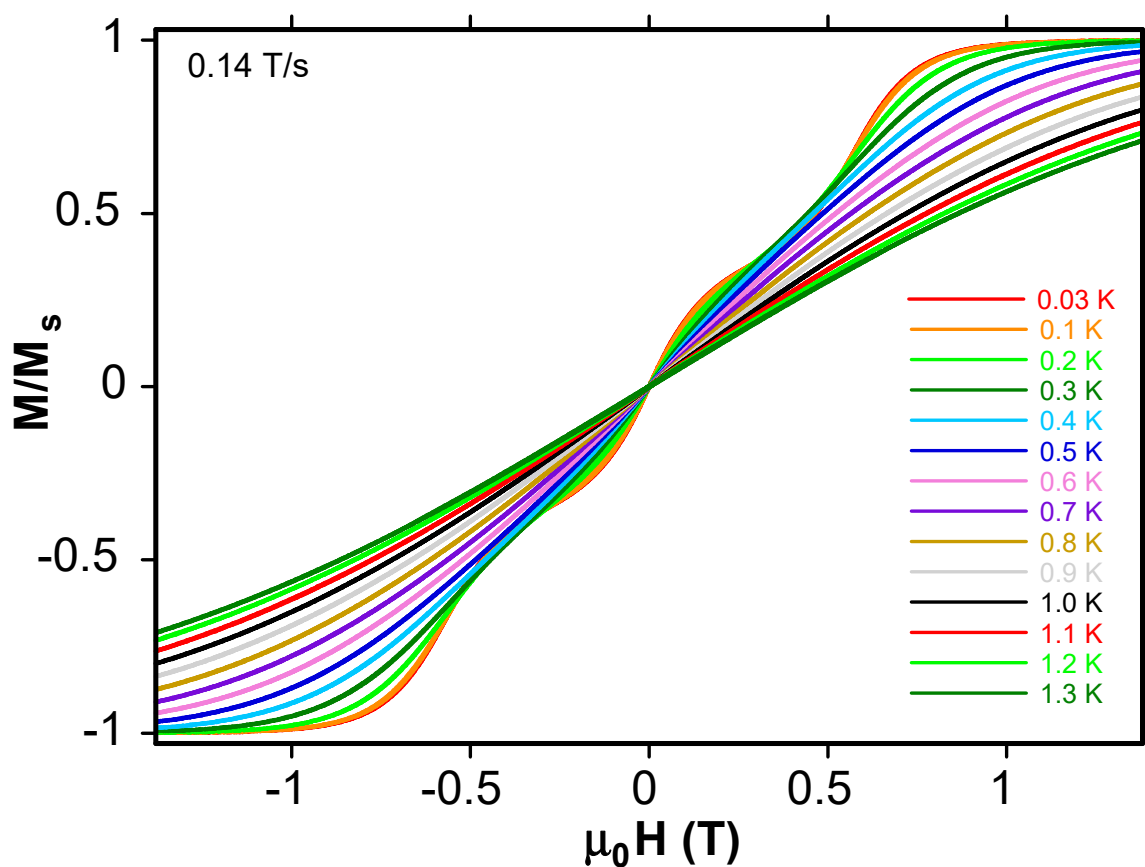
**Table S1.** Crystal data and single-crystal XRD experimental details.

Complex	{(hfac)Co <sup>II</sup> (BN)Co <sup>II</sup> (hfac)}	{(hfac)Mn <sup>II</sup> (BN)Mn <sup>II</sup> (hfac)} <sup>1</sup>
Crystal data		
Chemical formula	<i>C</i> <sub>34</sub> <i>H</i> <sub>28</sub> <i>Co</i> <sub>2</sub> <i>F</i> <sub>24</sub> <i>N</i> <sub>4</sub> <i>O</i> <sub>12</sub>	<i>C</i> <sub>34</sub> <i>H</i> <sub>28</sub> <i>Mn</i> <sub>2</sub> <i>F</i> <sub>24</sub> <i>N</i> <sub>4</sub> <i>O</i> <sub>12</sub>
<i>M</i> <sub>r</sub>	1258.46	1250.44
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	150	295
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.1513(5), 12.8362(7), 18.2903(8)	11.0825(6), 13.305(1), 18.617(1)
$\alpha$ , $\beta$ , $\gamma$ (°)	103.061(1), 100.898(2), 102.250(1)	103.359(6), 100.968(5), 101.885(5)
<i>V</i> (Å <sup>3</sup> )	2413.8 (2)	2530.72
<i>Z</i>	2	2
Radiation type	Mo <i>K</i> $\alpha$	Cu <i>K</i> $\alpha$
$\mu$ (mm <sup>−1</sup> )	0.84	
Crystal size (mm)	0.19 × 0.16 × 0.08	
Data collection for {(hfac)Co <sup>II</sup> (BN)Co <sup>II</sup> (hfac)}		
Diffractometer	Bruker X8Apex CCD detector diffractometer	
Absorption correction	Empirical (using intensity measurements) based on intensities ( <i>SADABS</i> , Bruker, 2005)	
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.857, 0.937	
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	13224, 9057, 6509	
<i>R</i> <sub>int</sub>	0.019	
(sin θ/λ) <sub>max</sub> (Å <sup>−1</sup> )	0.611	
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.045, 0.105, 1.02	
No. of reflections	9057	
No. of parameters	828	
No. of restraints	6	
H-atom treatment	H-atom parameters constrained	
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>−3</sup> )	0.53, −0.56	
Computer programs: Apex2 V.1.27 (Bruker, 2005), <i>SHELXS</i> 97 (Sheldrick, 1990), <i>SHELXL</i> 97 (Sheldrick, 1997), <i>SHELXTL</i> V6.22 (Bruker, 2000–2005), local programs.		

<sup>1</sup>Tanaka, M.; Matsuda, K.; Itoh, T.; Iwamura, H. *Angew. Chemie Int. Ed.* **1998**, *37*, 810–812



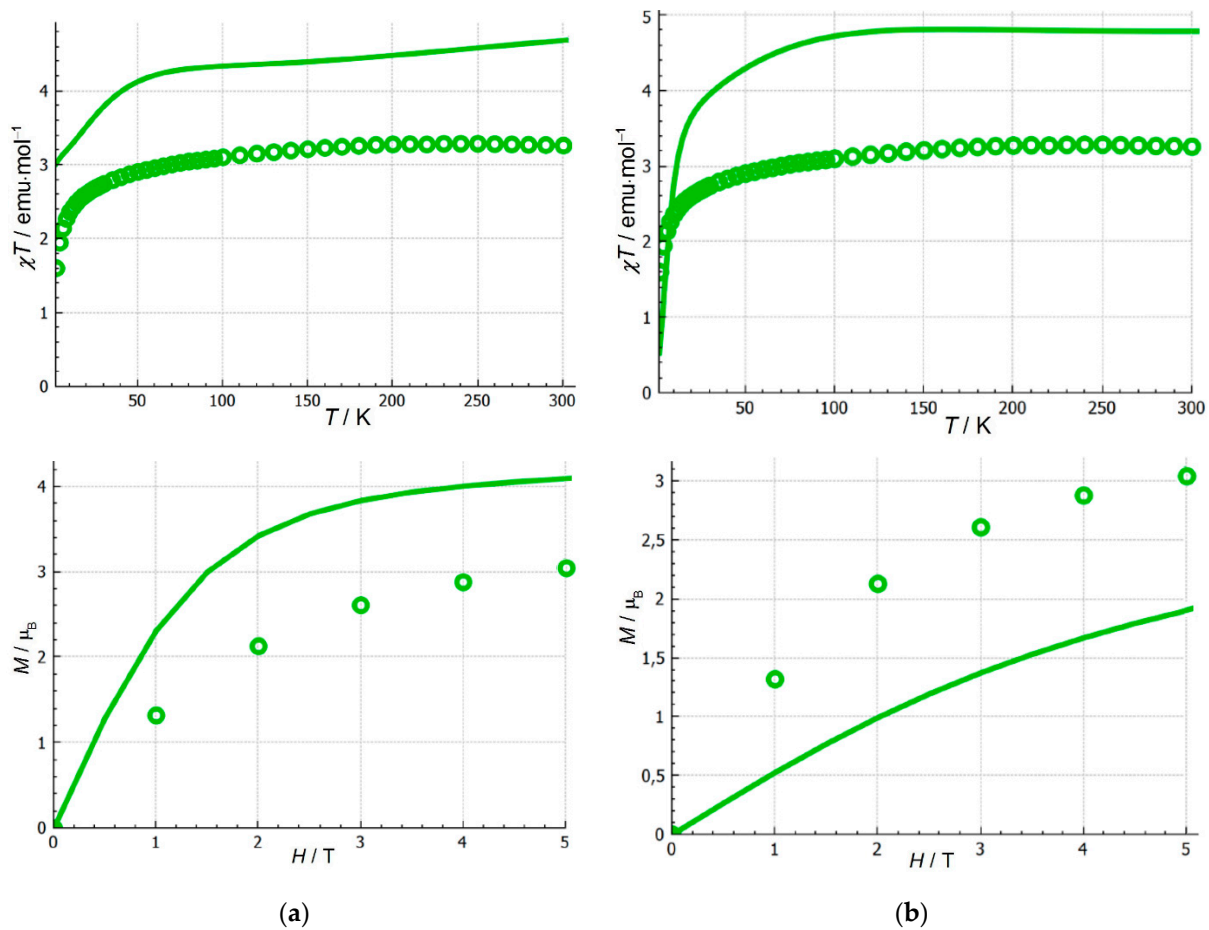
**Figure S1.** Powder X-Ray Diffraction pattern of  $\{(\text{hfac})_2\text{Co}^{\text{II}}(\text{BN})\text{Co}^{\text{II}}(\text{hfac})_2\}$  measured at room temperature compared to the pattern simulated from the single crystal structure measured at 150 K.



**Figure S2.** Field dependences of the normalized magnetizations measured at a sweep rate of  $0.14 \text{ T s}^{-1}$  at low temperatures from single crystals of  $\{(\text{hfac})_2\text{Co}^{\text{II}}(\text{BN})\text{Co}^{\text{II}}(\text{hfac})_2\}$ .

**Table S2.** The first 40 levels and their energy values for  $\{(\text{hfac})_2\text{Co}^{\text{II}}(\text{BN})\text{Co}^{\text{II}}(\text{hfac})_2\}$  obtained by *ab initio* calculations.

Level №	Energy, cm <sup>-1</sup>
1	0
2	0.69
3	13.01
4	113.55
5	119.64
6	125.02
7	192.32
8	194.33
9	221.21
10	668.8
11	672.17
12	674.56
13	693.6
14	693.79
15	725.11
16	733.43
17	739.35
18	765.97
19	772.97
20	773.37
21	788.67
22	794.84
23	811.62
24	815.86
25	816.65
26	831.36
27	833.51
28	835.93
29	842.71
30	843.14
31	854.13
32	860.7
33	870.72
34	879.06
35	908.5
36	915.26
37	928.79
38	949.55
39	952.72
40	1018.93



**Figure S3.** The simulations at  $\lambda = -180 \text{ cm}^{-1}$  for the  $\chi T(T)$  and  $M(H)$  using two different sets of spin-Hamiltonian parameters: (a) Set1 and (b) Set 2. Open circles are the experimental values.